wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 07:58 pm BST

PDB ID	:	6H23
Title	:	Crystal structure of the hClpP Y118A mutant with an activating small molecule
Authors	:	Kick, L.M.; Sieber, S.A.; Schneider, S.
Deposited on	:	2018-07-13
Resolution	:	3.09 Å(reported)

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

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

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

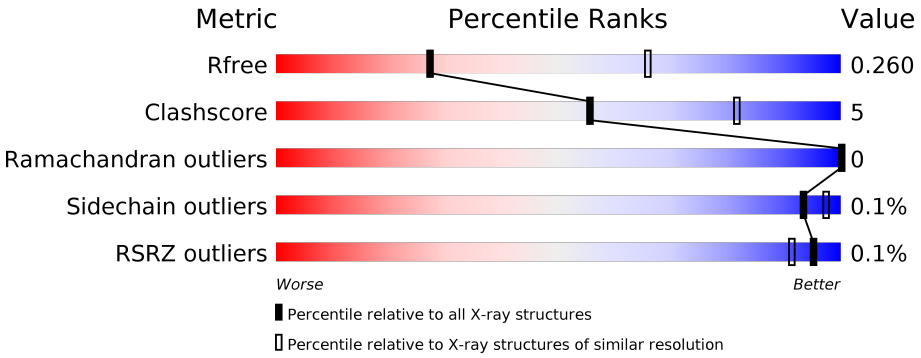
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.09 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	229	61% 11% 28%
1	B	229	62% 10% 28%
1	C	229	62% 10% 28%
1	D	229	59% 13% 28%
1	E	229	62% 11% 28%
1	F	229	64% 9% 28%

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Mol	Chain	Length	Quality of chain
1	G	229	62% 11% 26%
1	H	229	66% 7% 27%
1	I	229	57% 16% 27%
1	J	229	61% 11% 28%
1	K	229	66% 7% 28%
1	L	229	66% 7% 28%
1	M	229	60% 12% 28%
1	N	229	67% 7% 27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FJT	B	301[A]	-	-	-	X
2	FJT	B	301[B]	-	-	-	X
2	FJT	M	301[A]	-	-	-	X
2	FJT	M	301[B]	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18505 atoms, of which 0 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 ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1253	796	212	232	13			
1	B	166	Total	C	N	O	S	0	0	0
			1260	801	213	233	13			
1	C	166	Total	C	N	O	S	0	0	0
			1258	799	213	233	13			
1	D	164	Total	C	N	O	S	0	0	0
			1254	796	214	231	13			
1	E	166	Total	C	N	O	S	0	1	0
			1266	804	216	233	13			
1	F	166	Total	C	N	O	S	0	1	0
			1272	807	217	234	14			
1	G	169	Total	C	N	O	S	0	0	0
			1276	810	216	237	13			
1	H	167	Total	C	N	O	S	0	2	0
			1277	811	217	236	13			
1	I	167	Total	C	N	O	S	0	2	0
			1282	813	218	237	14			
1	J	166	Total	C	N	O	S	0	0	0
			1264	802	216	233	13			
1	K	166	Total	C	N	O	S	0	0	0
			1260	799	215	233	13			
1	L	166	Total	C	N	O	S	0	1	0
			1270	806	216	235	13			
1	M	166	Total	C	N	O	S	0	1	0
			1272	807	219	233	13			
1	N	168	Total	C	N	O	S	0	1	0
			1285	815	219	237	14			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	ALA	TYR	engineered mutation	UNP Q16740
A	278	TRP	-	expression tag	UNP Q16740
A	279	SER	-	expression tag	UNP Q16740
A	280	HIS	-	expression tag	UNP Q16740
A	281	PRO	-	expression tag	UNP Q16740
A	282	GLN	-	expression tag	UNP Q16740
A	283	PHE	-	expression tag	UNP Q16740
A	284	GLU	-	expression tag	UNP Q16740
A	285	LYS	-	expression tag	UNP Q16740
B	118	ALA	TYR	engineered mutation	UNP Q16740
B	278	TRP	-	expression tag	UNP Q16740
B	279	SER	-	expression tag	UNP Q16740
B	280	HIS	-	expression tag	UNP Q16740
B	281	PRO	-	expression tag	UNP Q16740
B	282	GLN	-	expression tag	UNP Q16740
B	283	PHE	-	expression tag	UNP Q16740
B	284	GLU	-	expression tag	UNP Q16740
B	285	LYS	-	expression tag	UNP Q16740
C	118	ALA	TYR	engineered mutation	UNP Q16740
C	278	TRP	-	expression tag	UNP Q16740
C	279	SER	-	expression tag	UNP Q16740
C	280	HIS	-	expression tag	UNP Q16740
C	281	PRO	-	expression tag	UNP Q16740
C	282	GLN	-	expression tag	UNP Q16740
C	283	PHE	-	expression tag	UNP Q16740
C	284	GLU	-	expression tag	UNP Q16740
C	285	LYS	-	expression tag	UNP Q16740
D	118	ALA	TYR	engineered mutation	UNP Q16740
D	278	TRP	-	expression tag	UNP Q16740
D	279	SER	-	expression tag	UNP Q16740
D	280	HIS	-	expression tag	UNP Q16740
D	281	PRO	-	expression tag	UNP Q16740
D	282	GLN	-	expression tag	UNP Q16740
D	283	PHE	-	expression tag	UNP Q16740
D	284	GLU	-	expression tag	UNP Q16740
D	285	LYS	-	expression tag	UNP Q16740
E	118	ALA	TYR	engineered mutation	UNP Q16740
E	278	TRP	-	expression tag	UNP Q16740
E	279	SER	-	expression tag	UNP Q16740
E	280	HIS	-	expression tag	UNP Q16740
E	281	PRO	-	expression tag	UNP Q16740
E	282	GLN	-	expression tag	UNP Q16740
E	283	PHE	-	expression tag	UNP Q16740

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Chain	Residue	Modelled	Actual	Comment	Reference
E	284	GLU	-	expression tag	UNP Q16740
E	285	LYS	-	expression tag	UNP Q16740
F	118	ALA	TYR	engineered mutation	UNP Q16740
F	278	TRP	-	expression tag	UNP Q16740
F	279	SER	-	expression tag	UNP Q16740
F	280	HIS	-	expression tag	UNP Q16740
F	281	PRO	-	expression tag	UNP Q16740
F	282	GLN	-	expression tag	UNP Q16740
F	283	PHE	-	expression tag	UNP Q16740
F	284	GLU	-	expression tag	UNP Q16740
F	285	LYS	-	expression tag	UNP Q16740
G	118	ALA	TYR	engineered mutation	UNP Q16740
G	278	TRP	-	expression tag	UNP Q16740
G	279	SER	-	expression tag	UNP Q16740
G	280	HIS	-	expression tag	UNP Q16740
G	281	PRO	-	expression tag	UNP Q16740
G	282	GLN	-	expression tag	UNP Q16740
G	283	PHE	-	expression tag	UNP Q16740
G	284	GLU	-	expression tag	UNP Q16740
G	285	LYS	-	expression tag	UNP Q16740
H	118	ALA	TYR	engineered mutation	UNP Q16740
H	278	TRP	-	expression tag	UNP Q16740
H	279	SER	-	expression tag	UNP Q16740
H	280	HIS	-	expression tag	UNP Q16740
H	281	PRO	-	expression tag	UNP Q16740
H	282	GLN	-	expression tag	UNP Q16740
H	283	PHE	-	expression tag	UNP Q16740
H	284	GLU	-	expression tag	UNP Q16740
H	285	LYS	-	expression tag	UNP Q16740
I	118	ALA	TYR	engineered mutation	UNP Q16740
I	278	TRP	-	expression tag	UNP Q16740
I	279	SER	-	expression tag	UNP Q16740
I	280	HIS	-	expression tag	UNP Q16740
I	281	PRO	-	expression tag	UNP Q16740
I	282	GLN	-	expression tag	UNP Q16740
I	283	PHE	-	expression tag	UNP Q16740
I	284	GLU	-	expression tag	UNP Q16740
I	285	LYS	-	expression tag	UNP Q16740
J	118	ALA	TYR	engineered mutation	UNP Q16740
J	278	TRP	-	expression tag	UNP Q16740
J	279	SER	-	expression tag	UNP Q16740
J	280	HIS	-	expression tag	UNP Q16740

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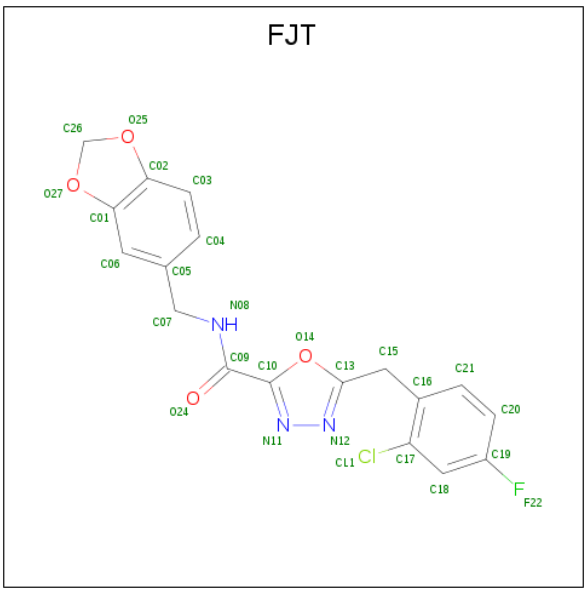
Chain	Residue	Modelled	Actual	Comment	Reference
J	281	PRO	-	expression tag	UNP Q16740
J	282	GLN	-	expression tag	UNP Q16740
J	283	PHE	-	expression tag	UNP Q16740
J	284	GLU	-	expression tag	UNP Q16740
J	285	LYS	-	expression tag	UNP Q16740
K	118	ALA	TYR	engineered mutation	UNP Q16740
K	278	TRP	-	expression tag	UNP Q16740
K	279	SER	-	expression tag	UNP Q16740
K	280	HIS	-	expression tag	UNP Q16740
K	281	PRO	-	expression tag	UNP Q16740
K	282	GLN	-	expression tag	UNP Q16740
K	283	PHE	-	expression tag	UNP Q16740
K	284	GLU	-	expression tag	UNP Q16740
K	285	LYS	-	expression tag	UNP Q16740
L	118	ALA	TYR	engineered mutation	UNP Q16740
L	278	TRP	-	expression tag	UNP Q16740
L	279	SER	-	expression tag	UNP Q16740
L	280	HIS	-	expression tag	UNP Q16740
L	281	PRO	-	expression tag	UNP Q16740
L	282	GLN	-	expression tag	UNP Q16740
L	283	PHE	-	expression tag	UNP Q16740
L	284	GLU	-	expression tag	UNP Q16740
L	285	LYS	-	expression tag	UNP Q16740
M	118	ALA	TYR	engineered mutation	UNP Q16740
M	278	TRP	-	expression tag	UNP Q16740
M	279	SER	-	expression tag	UNP Q16740
M	280	HIS	-	expression tag	UNP Q16740
M	281	PRO	-	expression tag	UNP Q16740
M	282	GLN	-	expression tag	UNP Q16740
M	283	PHE	-	expression tag	UNP Q16740
M	284	GLU	-	expression tag	UNP Q16740
M	285	LYS	-	expression tag	UNP Q16740
N	118	ALA	TYR	engineered mutation	UNP Q16740
N	278	TRP	-	expression tag	UNP Q16740
N	279	SER	-	expression tag	UNP Q16740
N	280	HIS	-	expression tag	UNP Q16740
N	281	PRO	-	expression tag	UNP Q16740
N	282	GLN	-	expression tag	UNP Q16740
N	283	PHE	-	expression tag	UNP Q16740
N	284	GLU	-	expression tag	UNP Q16740
N	285	LYS	-	expression tag	UNP Q16740

- Molecule 2 is {N}-(1,3-benzodioxol-5-ylmethyl)-5-[(2-chloranyl-4-fluoranyl-phenyl)methyl]-

1,3,4-oxadiazole-2-carboxamide (three-letter code: FJT) (formula: $C_{18}H_{13}ClFN_3O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		
2	B	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		
2	D	1	Total	C	Cl	F	N	O	0	0
			27	18	1	1	3	4		
2	D	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		
2	E	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		
2	F	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		
2	G	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		
2	H	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		
2	H	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		
2	J	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		
2	K	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		
2	L	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		
2	M	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		

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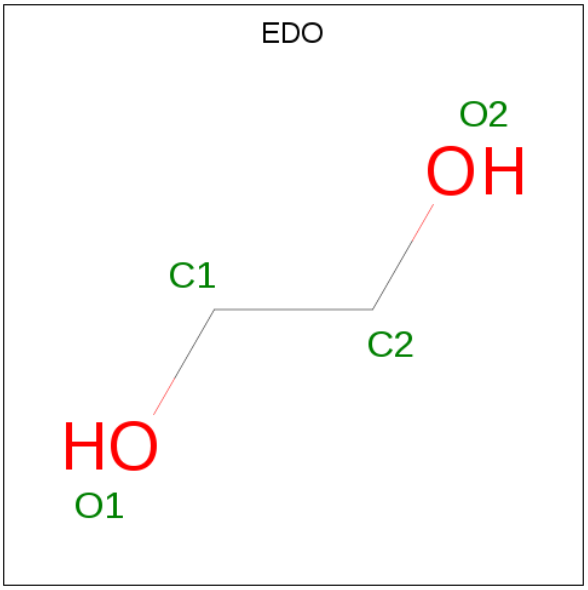
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	M	1	Total	C	Cl	F	N	O	0	1
			54	36	2	2	6	8		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	N	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	O	0	0
			1	1		
4	E	2	Total	O	0	0
			2	2		
4	F	2	Total	O	0	0
			2	2		
4	G	2	Total	O	0	0
			2	2		

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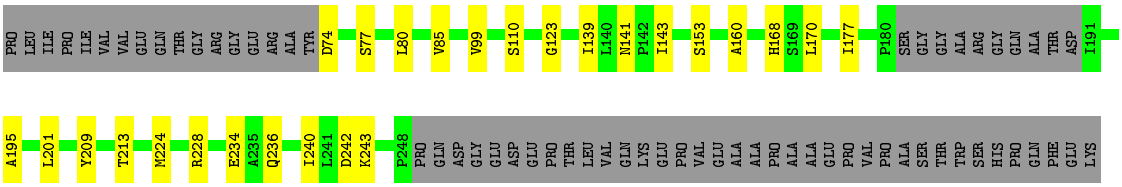
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O 1 1	0	0
4	I	1	Total O 1 1	0	0
4	K	1	Total O 1 1	0	0
4	N	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

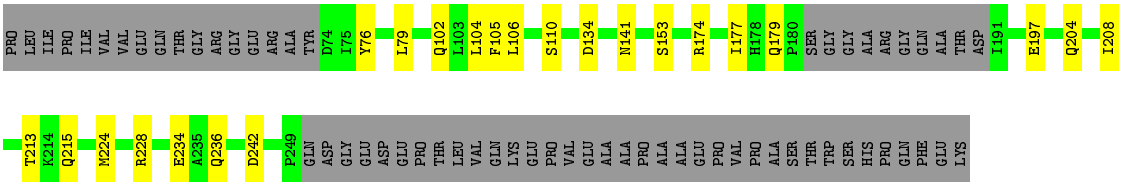
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain A:



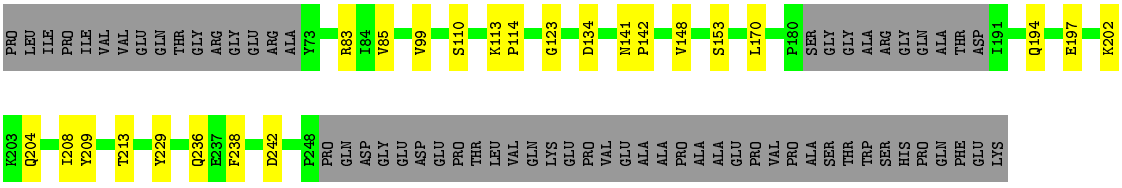
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain B:



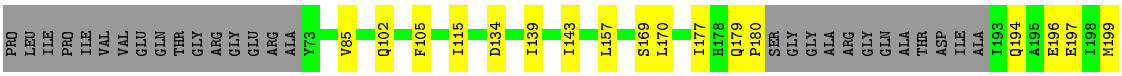
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain C:



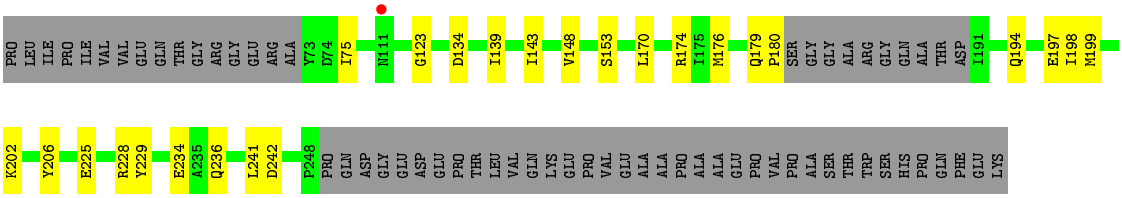
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain D:



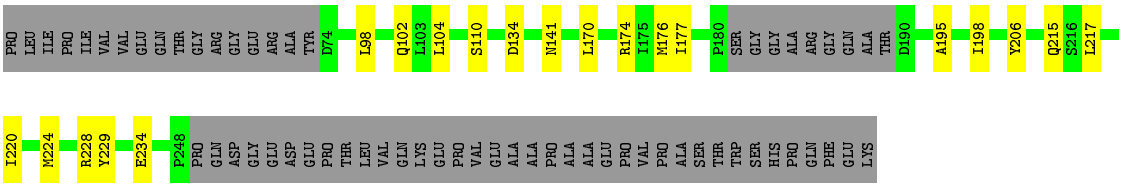
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain E:



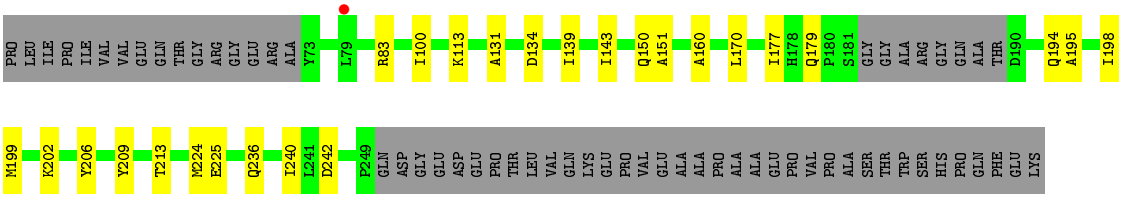
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain F:



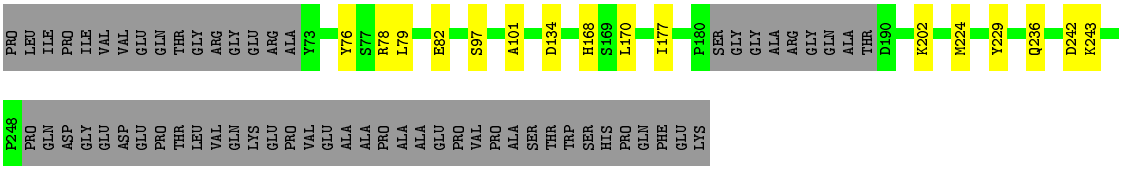
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain G:



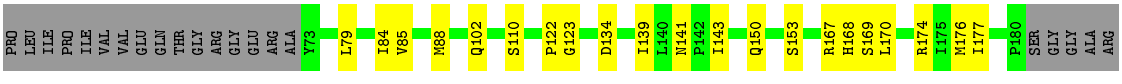
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

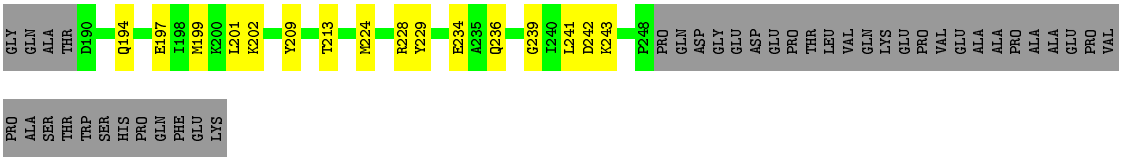
Chain H:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

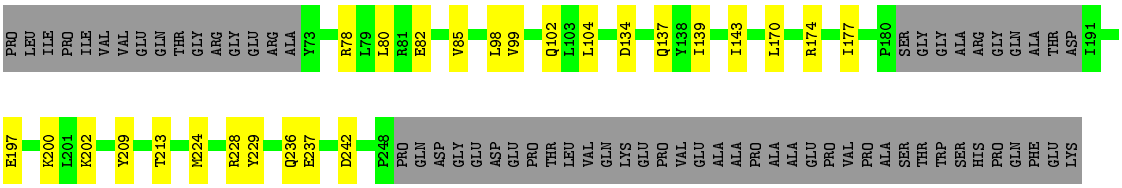
Chain I:





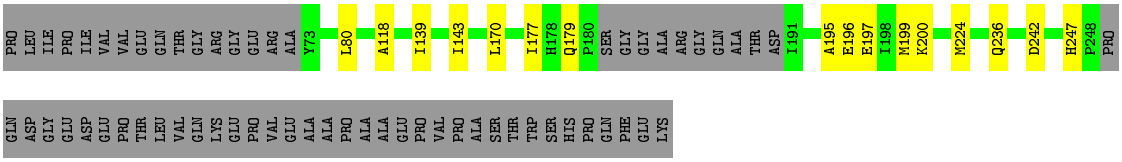
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain J:



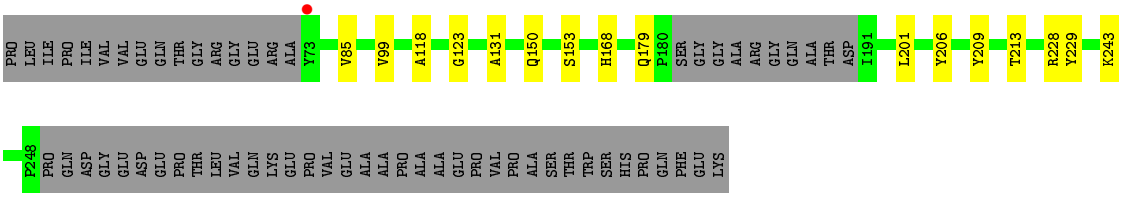
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain K:



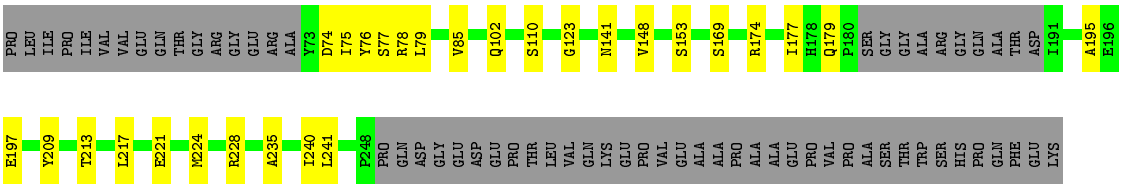
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain L:



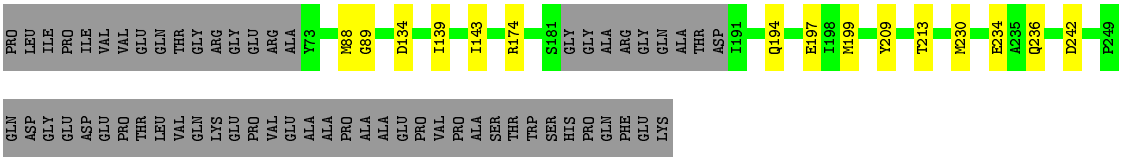
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain M:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain N:


PRO LEU ILE PRO ILE VAL VAL GLU GLN THR GLY ARG GLY GLU ARG ALA Y73 M88 G89 D134 I139 I143 R174 S181 GLY GLY ALA ARG GLY GLN ALA THR ASP I191 Q194 E197 I198 M199 Y209 T213 M230 E234 A235 Q236 D242 P249
GLN ASP GLY GLU ASP GLU PRO THR LEU VAL GLN LYS GLU PRO VAL GLU ALA ALA PRO ALA ALA GLU PRO VAL PRO ALA SER THR TRP SER HIS PRO GLN PHE GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.50Å 97.15Å 127.25Å 90.00° 93.53° 90.00°	Depositor
Resolution (Å)	42.34 – 3.09 49.25 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.34-3.09) 98.8 (49.25-3.09)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.261 0.215 , 0.260	Depositor DCC
R_{free} test set	2569 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18505	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% 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

5.1 Standard geometry

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

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	0/1275	0.41	0/1728
1	B	0.23	0/1283	0.42	0/1740
1	C	0.23	0/1280	0.43	0/1735
1	D	0.23	0/1276	0.40	0/1728
1	E	0.24	0/1291	0.43	0/1749
1	F	0.24	0/1294	0.41	0/1752
1	G	0.24	0/1299	0.42	0/1762
1	H	0.24	0/1305	0.42	0/1768
1	I	0.24	0/1307	0.48	0/1770
1	J	0.24	0/1286	0.42	0/1742
1	K	0.23	0/1282	0.41	0/1738
1	L	0.24	0/1295	0.40	0/1754
1	M	0.24	0/1297	0.42	0/1756
1	N	0.24	0/1308	0.43	0/1772
All	All	0.24	0/18078	0.42	0/24494

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1253	0	1259	15	0
1	B	1260	0	1266	16	0
1	C	1258	0	1261	16	0
1	D	1254	0	1265	20	0
1	E	1266	0	1274	23	0
1	F	1272	0	1280	15	0
1	G	1276	0	1275	16	0
1	H	1277	0	1282	12	0
1	I	1282	0	1284	25	0
1	J	1264	0	1272	18	0
1	K	1260	0	1261	14	0
1	L	1270	0	1278	11	0
1	M	1272	0	1285	17	0
1	N	1285	0	1292	11	0
2	A	54	0	0	0	0
2	B	54	0	0	1	0
2	D	81	0	0	0	0
2	E	54	0	0	0	0
2	F	54	0	0	1	0
2	G	54	0	0	0	0
2	H	108	0	0	0	0
2	J	54	0	0	0	0
2	K	54	0	0	2	0
2	L	54	0	0	2	0
2	M	108	0	0	0	0
3	A	4	0	6	2	0
3	E	4	0	6	1	0
3	F	4	0	6	0	0
3	N	4	0	6	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	N	1	0	0	0	0
All	All	18505	0	17858	184	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 5.

The worst 5 of 184 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:197:GLU:HB3	1:N:174:ARG:HH12	1.48	0.77
1:I:174[A]:ARG:HH21	1:I:174[A]:ARG:HG3	1.52	0.75
1:J:98:LEU:HG	1:J:102:GLN:HE21	1.59	0.66
1:I:236:GLN:NE2	1:I:242:ASP:O	2.29	0.65
1:C:236:GLN:NE2	1:C:242:ASP:O	2.30	0.64

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	161/229 (70%)	157 (98%)	4 (2%)	0	100	100
1	B	162/229 (71%)	158 (98%)	4 (2%)	0	100	100
1	C	162/229 (71%)	158 (98%)	4 (2%)	0	100	100
1	D	160/229 (70%)	156 (98%)	4 (2%)	0	100	100
1	E	163/229 (71%)	159 (98%)	4 (2%)	0	100	100
1	F	163/229 (71%)	159 (98%)	4 (2%)	0	100	100
1	G	165/229 (72%)	160 (97%)	5 (3%)	0	100	100
1	H	165/229 (72%)	161 (98%)	4 (2%)	0	100	100
1	I	165/229 (72%)	160 (97%)	5 (3%)	0	100	100
1	J	162/229 (71%)	158 (98%)	4 (2%)	0	100	100
1	K	162/229 (71%)	157 (97%)	5 (3%)	0	100	100
1	L	163/229 (71%)	159 (98%)	4 (2%)	0	100	100
1	M	163/229 (71%)	157 (96%)	6 (4%)	0	100	100
1	N	165/229 (72%)	160 (97%)	5 (3%)	0	100	100
All	All	2281/3206 (71%)	2219 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	136/192 (71%)	136 (100%)	0	100 100
1	B	137/192 (71%)	137 (100%)	0	100 100
1	C	136/192 (71%)	136 (100%)	0	100 100
1	D	137/192 (71%)	137 (100%)	0	100 100
1	E	137/192 (71%)	137 (100%)	0	100 100
1	F	138/192 (72%)	138 (100%)	0	100 100
1	G	138/192 (72%)	138 (100%)	0	100 100
1	H	138/192 (72%)	138 (100%)	0	100 100
1	I	139/192 (72%)	139 (100%)	0	100 100
1	J	137/192 (71%)	136 (99%)	1 (1%)	84 92
1	K	136/192 (71%)	136 (100%)	0	100 100
1	L	138/192 (72%)	137 (99%)	1 (1%)	84 92
1	M	138/192 (72%)	138 (100%)	0	100 100
1	N	140/192 (73%)	140 (100%)	0	100 100
All	All	1925/2688 (72%)	1923 (100%)	2 (0%)	93 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	237	GLU
1	L	150	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	107	GLN
1	G	150	GLN
1	L	107	GLN
1	E	150	GLN

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Mol	Chain	Res	Type
1	L	150	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

31 ligands are modelled in this entry.

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	FJT	H	302[A]	-	26,30,30	1.73	6 (23%)	33,42,42	1.95	8 (24%)
2	FJT	D	302[A]	-	26,30,30	1.73	7 (26%)	33,42,42	1.97	7 (21%)
2	FJT	H	302[B]	-	26,30,30	1.63	5 (19%)	33,42,42	1.72	8 (24%)
2	FJT	L	301[B]	-	26,30,30	1.67	8 (30%)	33,42,42	1.66	6 (18%)
2	FJT	D	302[B]	-	26,30,30	1.69	7 (26%)	33,42,42	1.67	6 (18%)
2	FJT	H	301[B]	-	26,30,30	1.71	7 (26%)	33,42,42	1.53	6 (18%)
3	EDO	E	302	-	3,3,3	0.46	0	2,2,2	0.34	0
2	FJT	L	301[A]	-	26,30,30	1.70	8 (30%)	33,42,42	1.66	6 (18%)
2	FJT	D	301	-	26,30,30	1.65	6 (23%)	33,42,42	1.49	6 (18%)
2	FJT	H	301[A]	-	26,30,30	1.69	8 (30%)	33,42,42	1.54	6 (18%)
3	EDO	N	301	-	3,3,3	0.46	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FJT	M	301[B]	-	26,30,30	1.69	7 (26%)	33,42,42	1.81	6 (18%)
2	FJT	M	301[A]	-	26,30,30	1.74	6 (23%)	33,42,42	2.16	8 (24%)
2	FJT	G	301[A]	-	26,30,30	1.68	7 (26%)	33,42,42	1.63	6 (18%)
2	FJT	G	301[B]	-	26,30,30	1.67	6 (23%)	33,42,42	1.62	6 (18%)
2	FJT	J	301[A]	-	26,30,30	1.67	6 (23%)	33,42,42	1.58	6 (18%)
2	FJT	J	301[B]	-	26,30,30	1.68	7 (26%)	33,42,42	1.67	6 (18%)
2	FJT	F	301[A]	-	26,30,30	1.76	7 (26%)	33,42,42	2.18	7 (21%)
2	FJT	F	301[B]	-	26,30,30	1.66	7 (26%)	33,42,42	1.61	5 (15%)
2	FJT	B	301[A]	-	26,30,30	1.63	5 (19%)	33,42,42	1.65	7 (21%)
2	FJT	B	301[B]	-	26,30,30	1.69	8 (30%)	33,42,42	1.61	7 (21%)
2	FJT	K	301[A]	-	26,30,30	1.71	7 (26%)	33,42,42	1.76	6 (18%)
2	FJT	E	301[B]	-	26,30,30	1.71	8 (30%)	33,42,42	1.88	6 (18%)
3	EDO	F	302	-	3,3,3	0.46	0	2,2,2	0.34	0
2	FJT	E	301[A]	-	26,30,30	1.69	8 (30%)	33,42,42	1.71	6 (18%)
2	FJT	A	301[B]	-	26,30,30	1.69	7 (26%)	33,42,42	1.71	5 (15%)
2	FJT	K	301[B]	-	26,30,30	1.68	6 (23%)	33,42,42	1.67	5 (15%)
2	FJT	A	301[A]	-	26,30,30	1.67	7 (26%)	33,42,42	1.69	7 (21%)
2	FJT	M	302[A]	-	26,30,30	1.68	6 (23%)	33,42,42	1.55	6 (18%)
2	FJT	M	302[B]	-	26,30,30	1.67	7 (26%)	33,42,42	1.72	5 (15%)
3	EDO	A	302	-	3,3,3	0.46	0	2,2,2	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FJT	H	302[A]	-	-	2/8/19/19	0/4/4/4
2	FJT	D	302[A]	-	-	0/8/19/19	0/4/4/4
2	FJT	H	302[B]	-	-	0/8/19/19	0/4/4/4
2	FJT	L	301[B]	-	-	1/8/19/19	0/4/4/4
2	FJT	D	302[B]	-	-	0/8/19/19	0/4/4/4
2	FJT	H	301[B]	-	-	0/8/19/19	0/4/4/4
3	EDO	E	302	-	-	0/1/1/1	-
2	FJT	L	301[A]	-	-	0/8/19/19	0/4/4/4
2	FJT	D	301	-	-	0/8/19/19	0/4/4/4
2	FJT	H	301[A]	-	-	1/8/19/19	0/4/4/4
3	EDO	N	301	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FJT	M	301[B]	-	-	0/8/19/19	0/4/4/4
2	FJT	M	301[A]	-	-	2/8/19/19	0/4/4/4
2	FJT	G	301[A]	-	-	1/8/19/19	0/4/4/4
2	FJT	G	301[B]	-	-	0/8/19/19	0/4/4/4
2	FJT	J	301[A]	-	-	0/8/19/19	0/4/4/4
2	FJT	J	301[B]	-	-	0/8/19/19	0/4/4/4
2	FJT	F	301[A]	-	-	2/8/19/19	0/4/4/4
2	FJT	F	301[B]	-	-	1/8/19/19	0/4/4/4
2	FJT	B	301[A]	-	-	0/8/19/19	0/4/4/4
2	FJT	B	301[B]	-	-	1/8/19/19	0/4/4/4
2	FJT	K	301[A]	-	-	3/8/19/19	0/4/4/4
2	FJT	E	301[B]	-	-	3/8/19/19	0/4/4/4
3	EDO	F	302	-	-	0/1/1/1	-
2	FJT	E	301[A]	-	-	1/8/19/19	0/4/4/4
2	FJT	A	301[B]	-	-	1/8/19/19	0/4/4/4
2	FJT	K	301[B]	-	-	0/8/19/19	0/4/4/4
2	FJT	A	301[A]	-	-	1/8/19/19	0/4/4/4
2	FJT	M	302[A]	-	-	1/8/19/19	0/4/4/4
2	FJT	M	302[B]	-	-	0/8/19/19	0/4/4/4
3	EDO	A	302	-	-	0/1/1/1	-

The worst 5 of 184 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301[A]	FJT	C09-N08	5.88	1.46	1.33
2	M	301[A]	FJT	C09-N08	5.76	1.46	1.33
2	H	302[A]	FJT	C09-N08	5.75	1.46	1.33
2	D	302[A]	FJT	C09-N08	5.64	1.46	1.33
2	H	301[B]	FJT	C09-N08	5.62	1.46	1.33

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301[A]	FJT	C10-C09-N08	8.94	124.48	115.60
2	M	301[A]	FJT	C10-C09-N08	8.63	124.18	115.60
2	H	302[A]	FJT	C10-C09-N08	7.16	122.71	115.60
2	D	302[A]	FJT	C10-C09-N08	6.74	122.30	115.60
2	E	301[B]	FJT	C10-C09-N08	5.87	121.44	115.60

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	301[B]	FJT	N12-C13-C15-C16
2	G	301[A]	FJT	N12-C13-C15-C16
2	K	301[A]	FJT	N12-C13-C15-C16
2	E	301[B]	FJT	N12-C13-C15-C16
2	E	301[B]	FJT	C13-C15-C16-C17

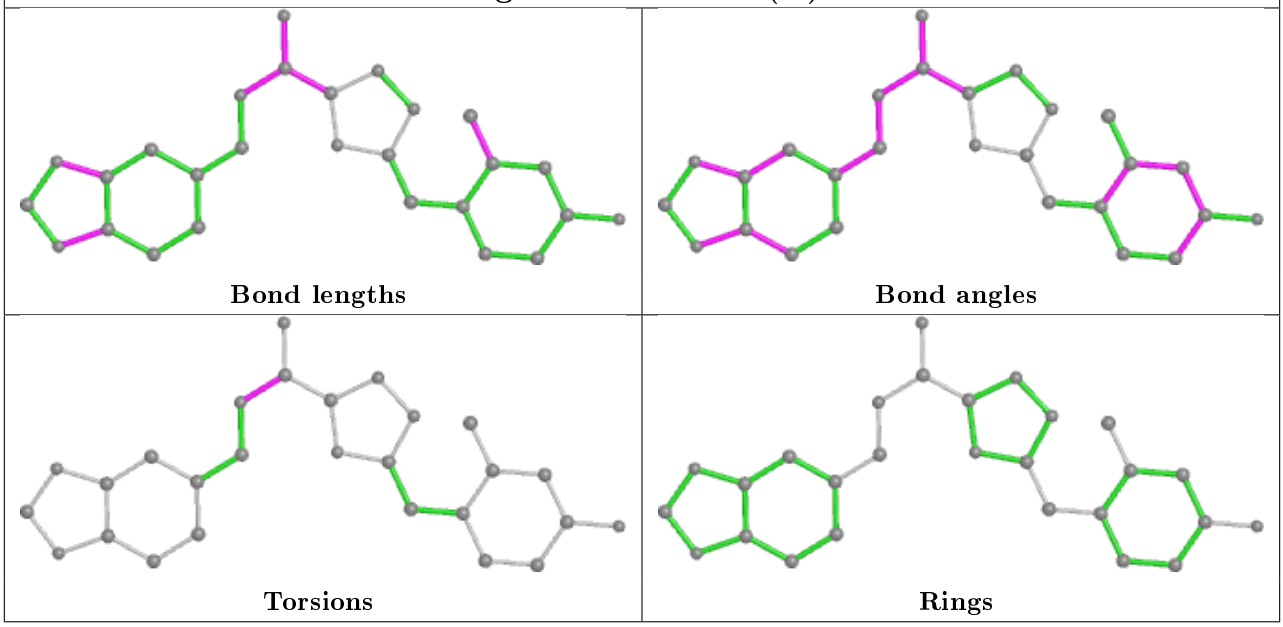
There are no ring outliers.

7 monomers are involved in 9 short contacts:

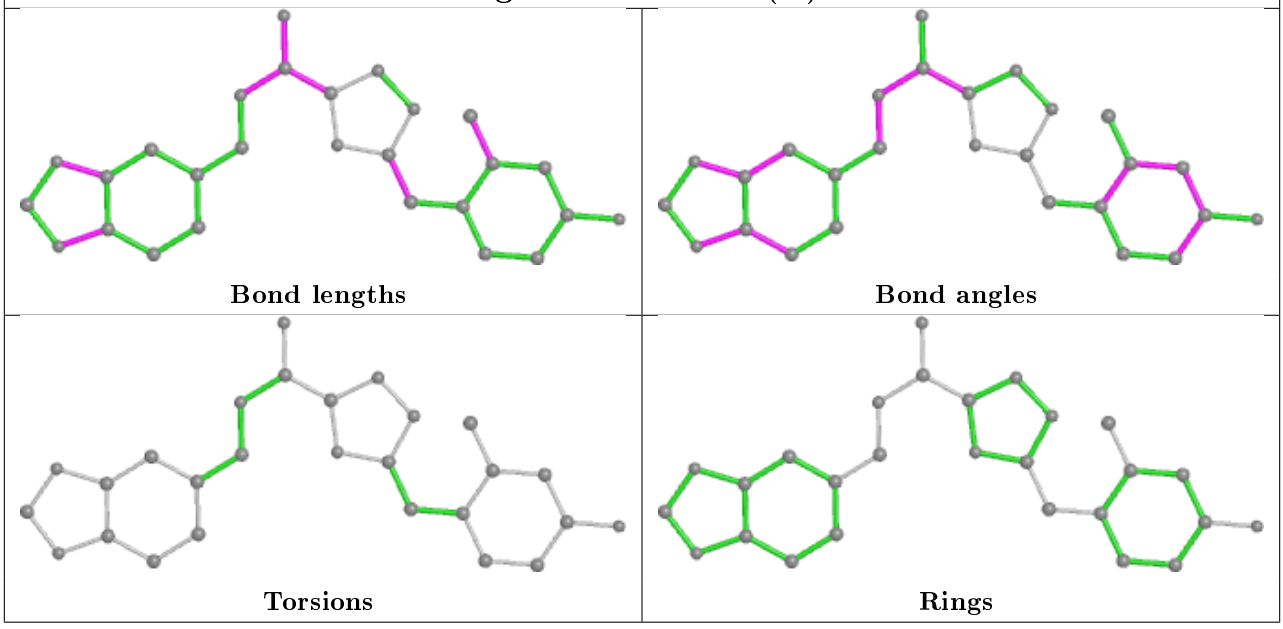
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	301[B]	FJT	1	0
3	E	302	EDO	1	0
2	L	301[A]	FJT	1	0
2	F	301[A]	FJT	1	0
2	B	301[A]	FJT	1	0
2	K	301[B]	FJT	2	0
3	A	302	EDO	2	0

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

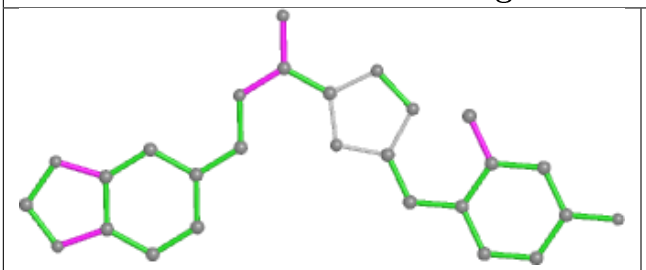
Ligand FJT H 302 (A)



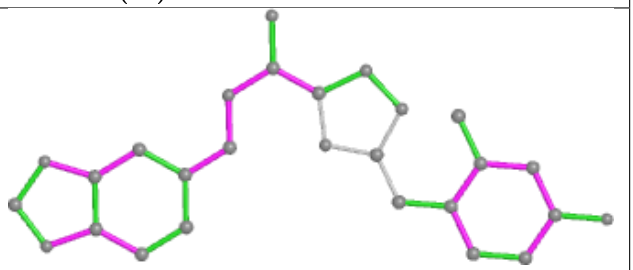
Ligand FJT D 302 (A)



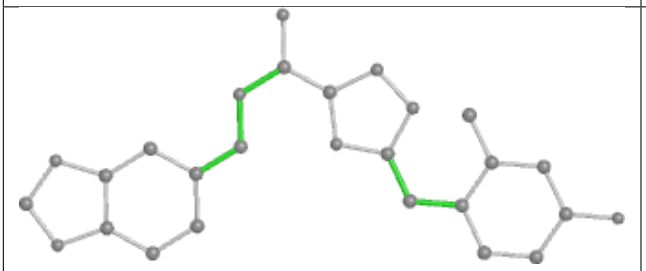
Ligand FJT H 302 (B)



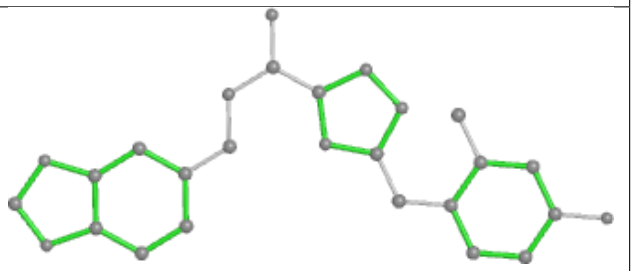
Bond lengths



Bond angles

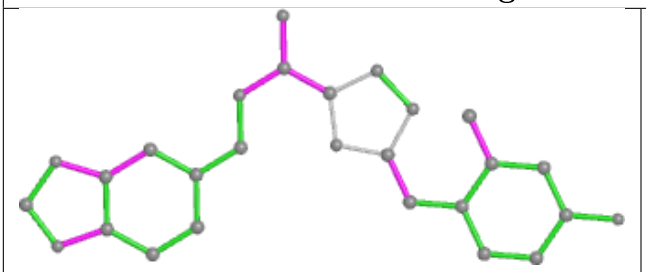


Torsions

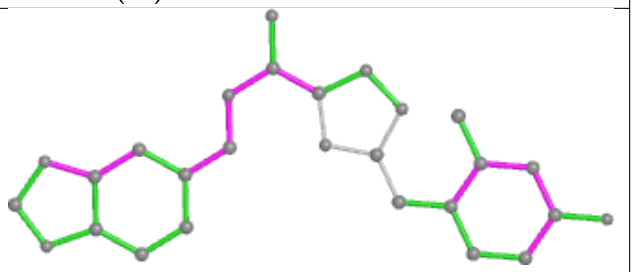


Rings

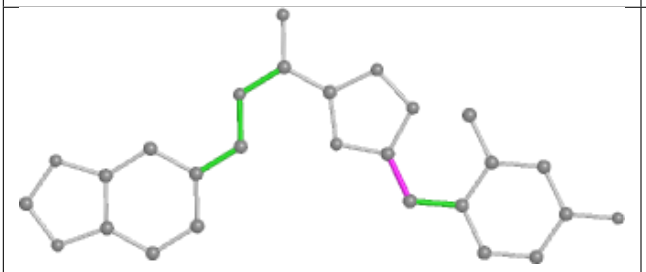
Ligand FJT L 301 (B)



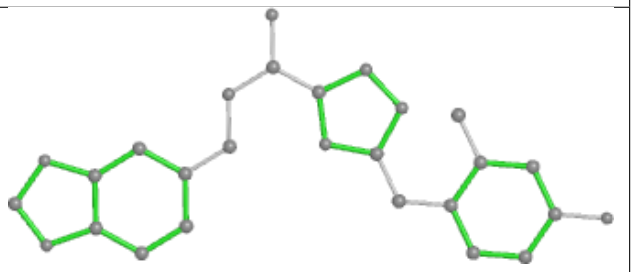
Bond lengths



Bond angles

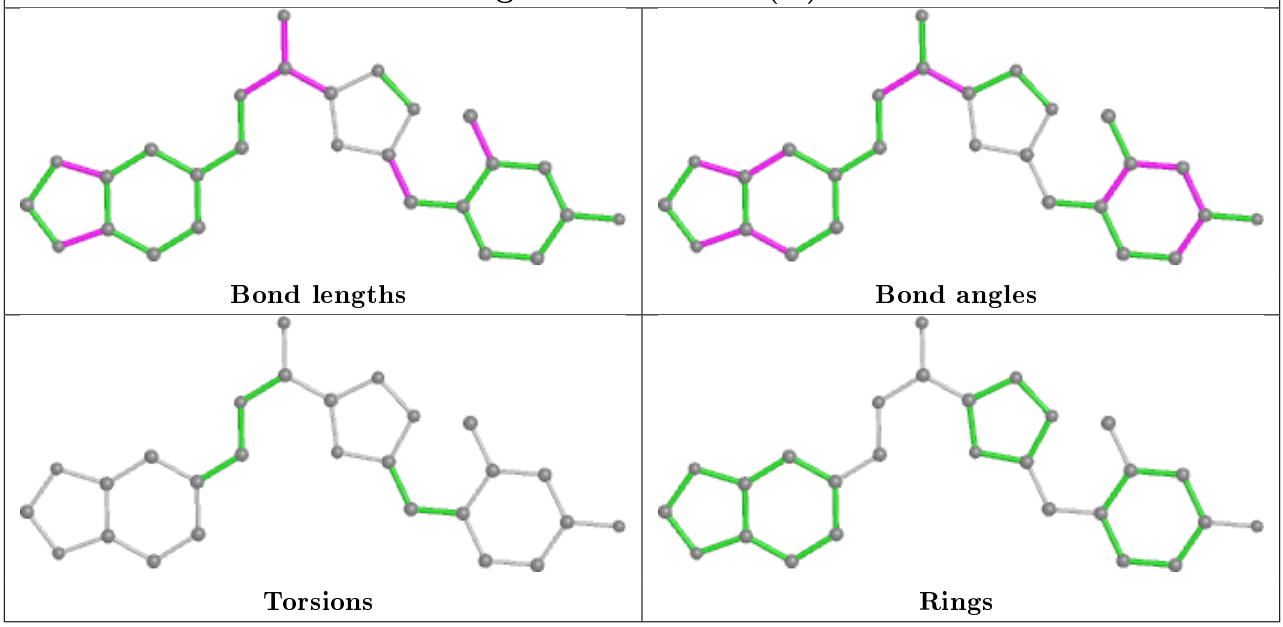


Torsions

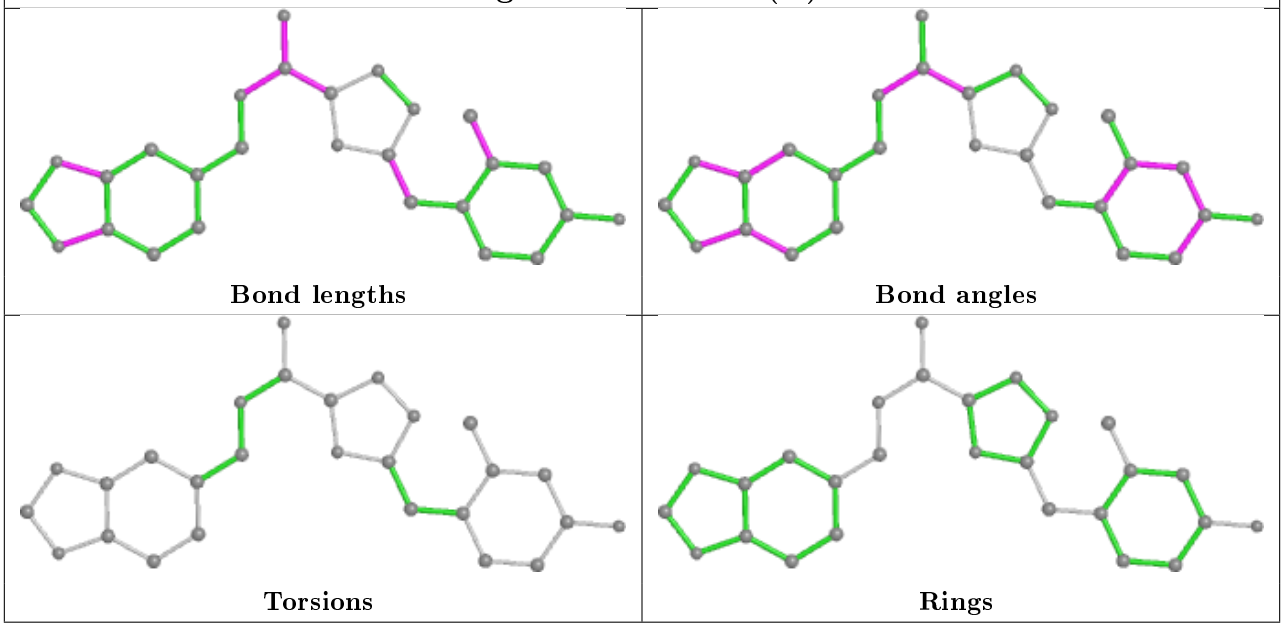


Rings

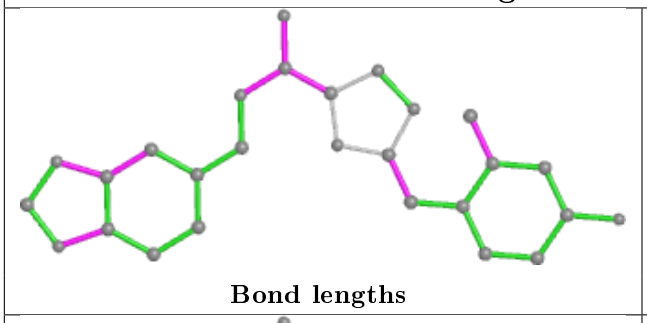
Ligand FJT D 302 (B)



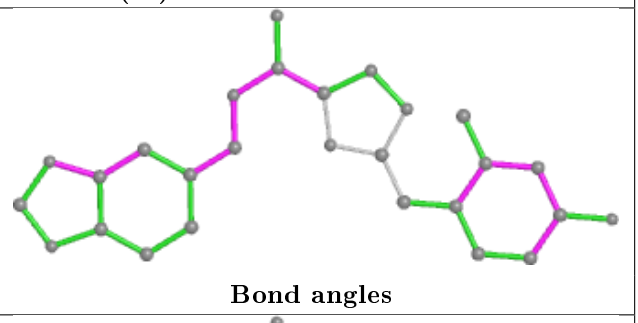
Ligand FJT H 301 (B)



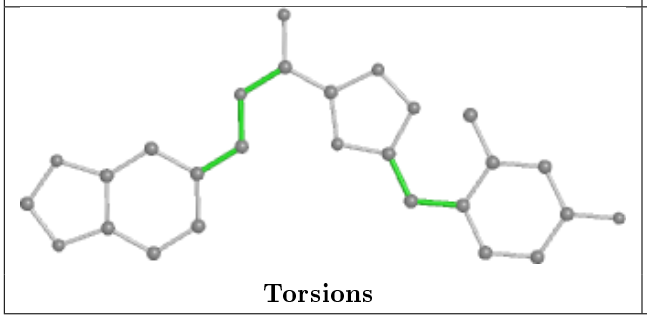
Ligand FJT L 301 (A)



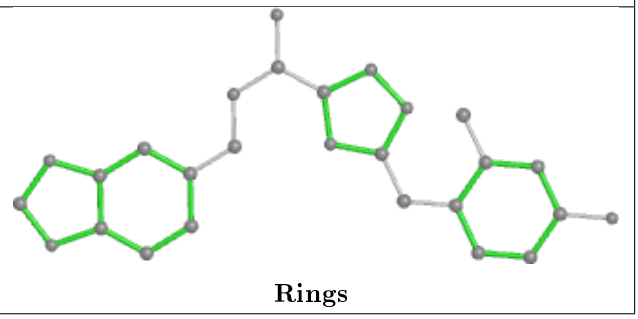
Bond lengths



Bond angles

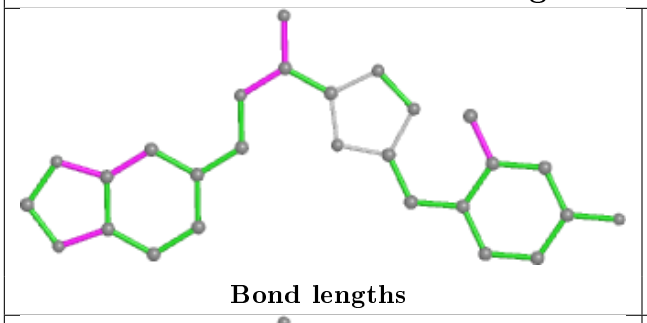


Torsions

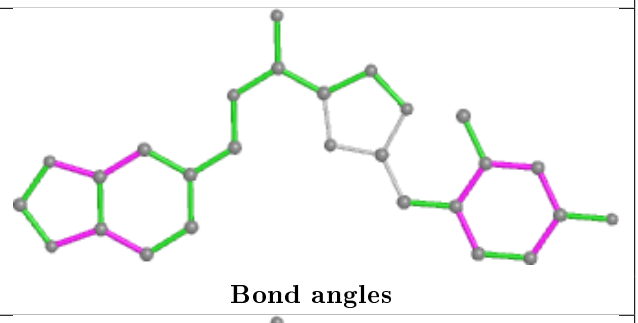


Rings

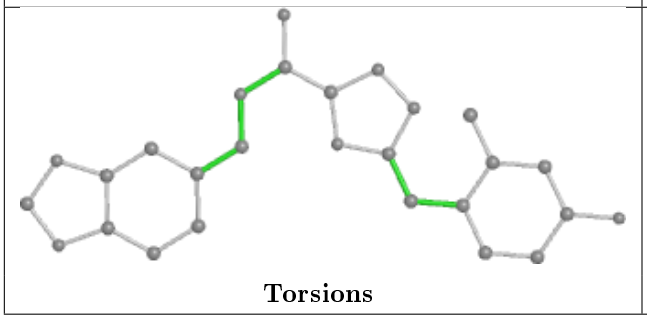
Ligand FJT D 301



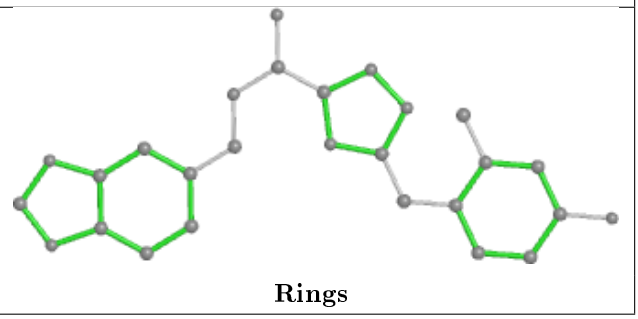
Bond lengths



Bond angles

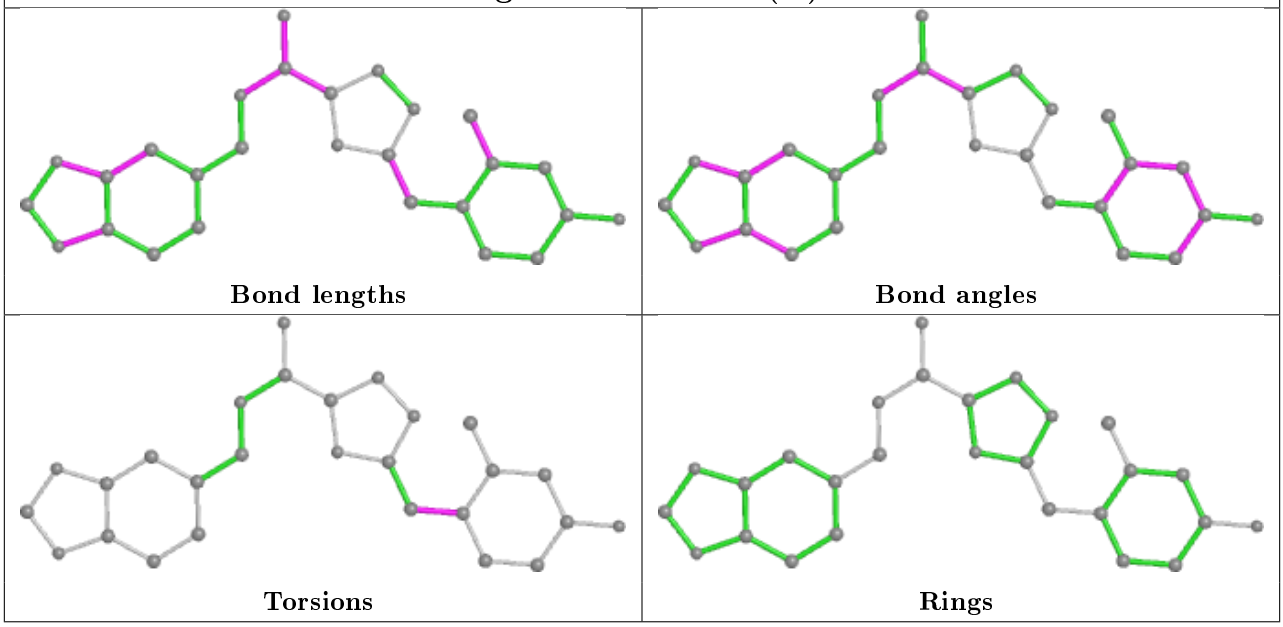


Torsions

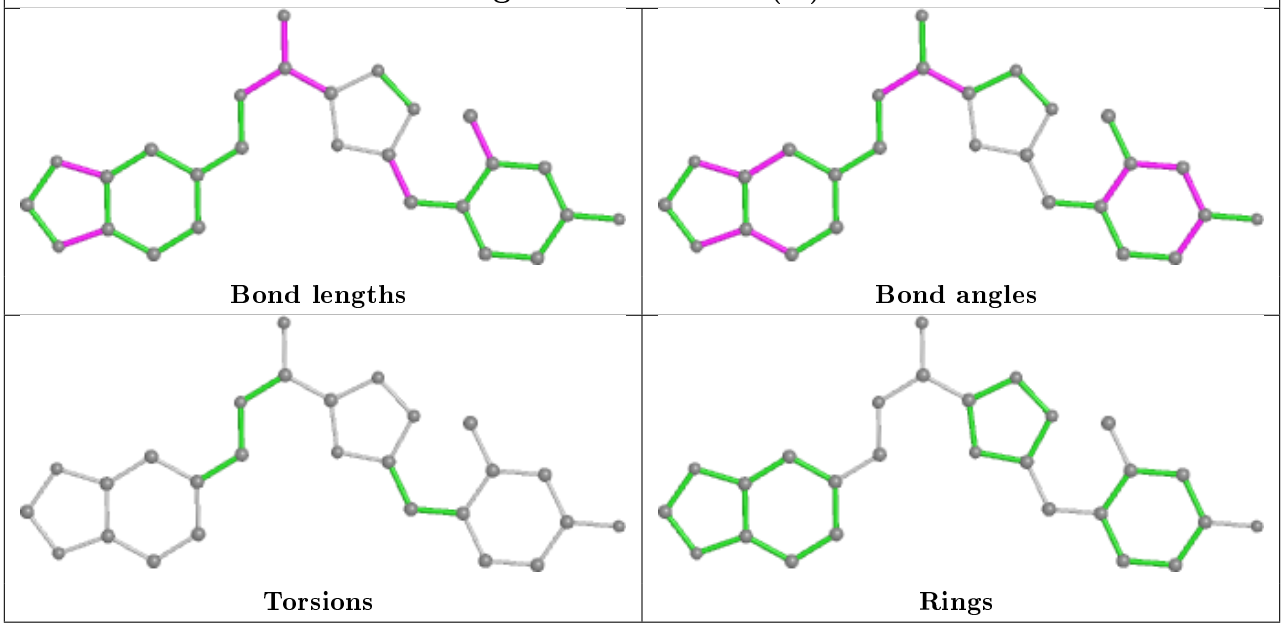


Rings

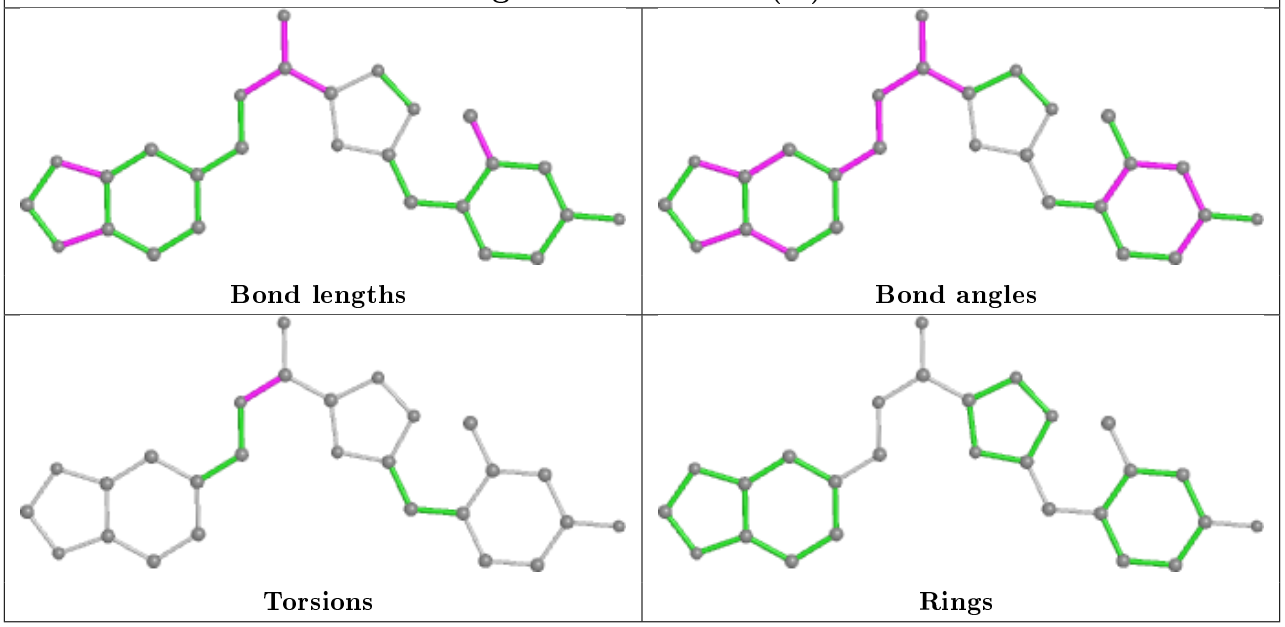
Ligand FJT H 301 (A)



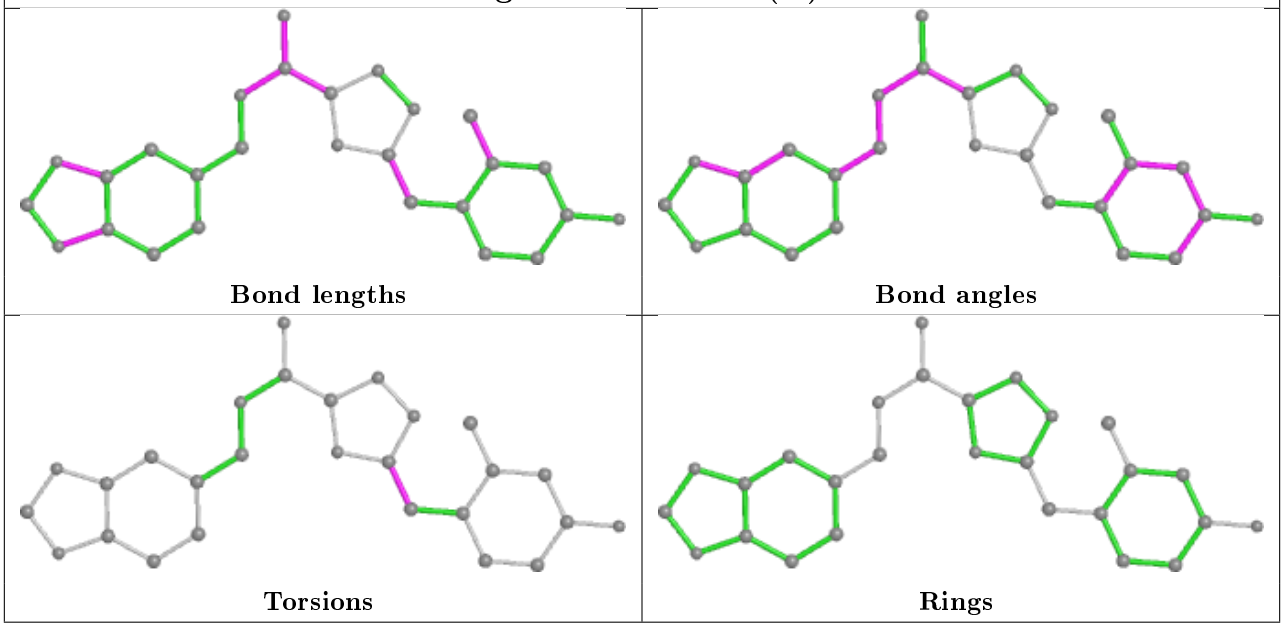
Ligand FJT M 301 (B)



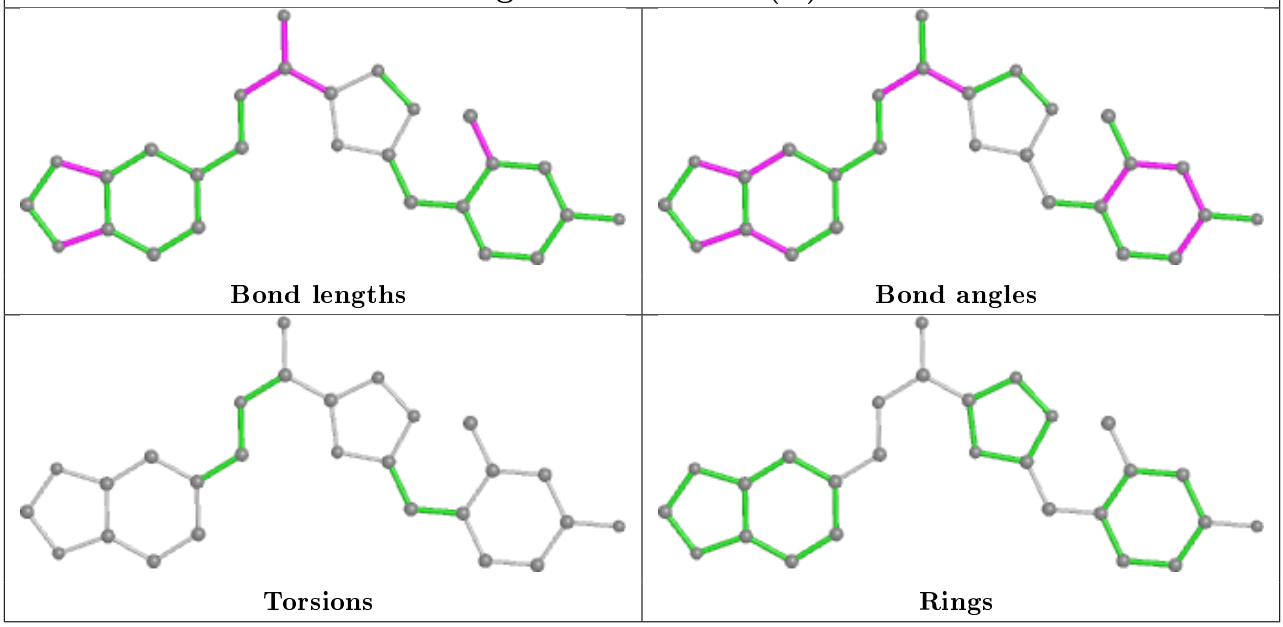
Ligand FJT M 301 (A)



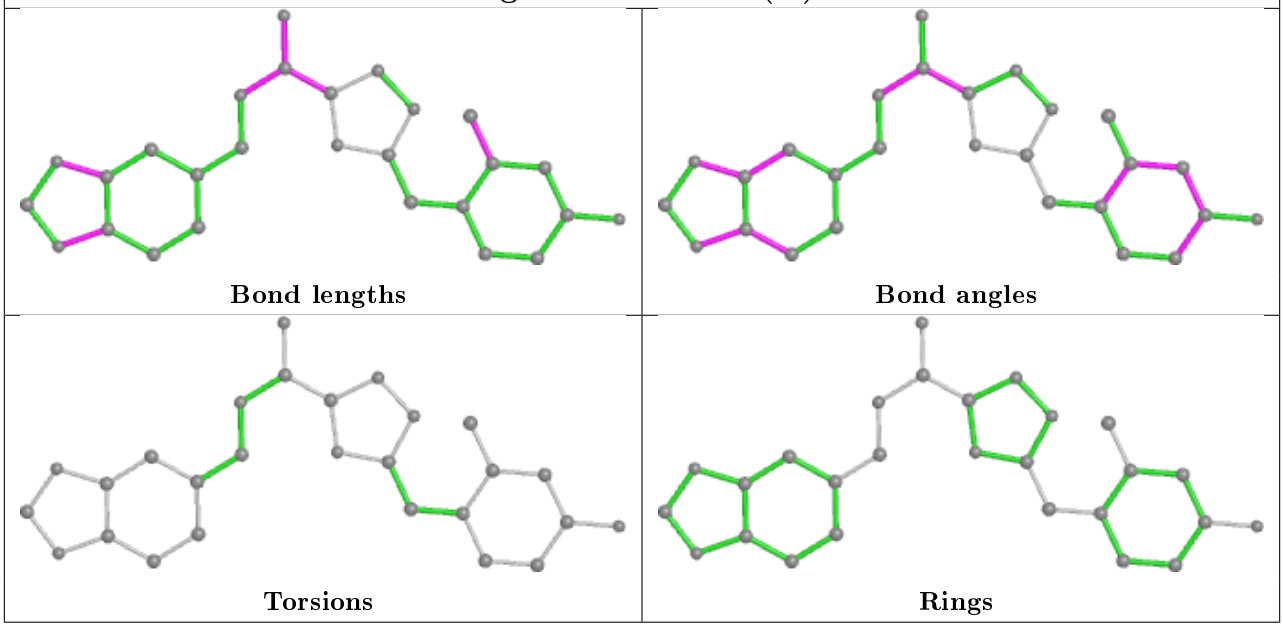
Ligand FJT G 301 (A)



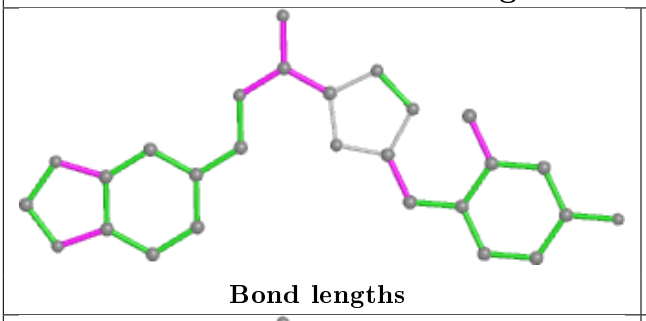
Ligand FJT G 301 (B)



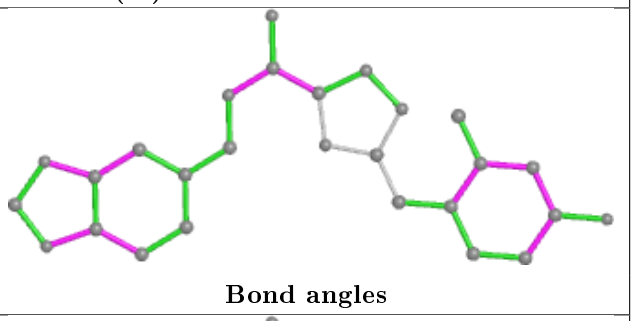
Ligand FJT J 301 (A)



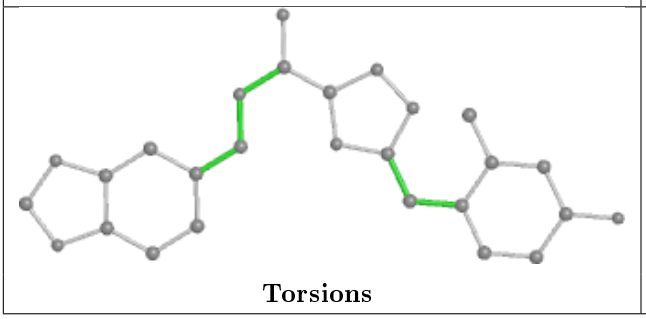
Ligand FJT J 301 (B)



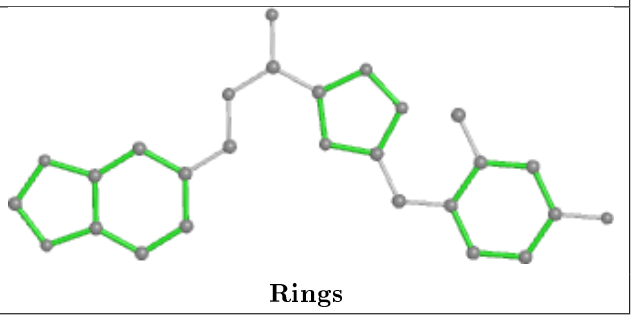
Bond lengths



Bond angles

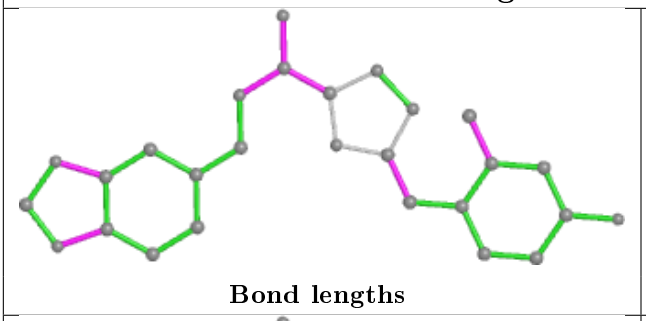


Torsions

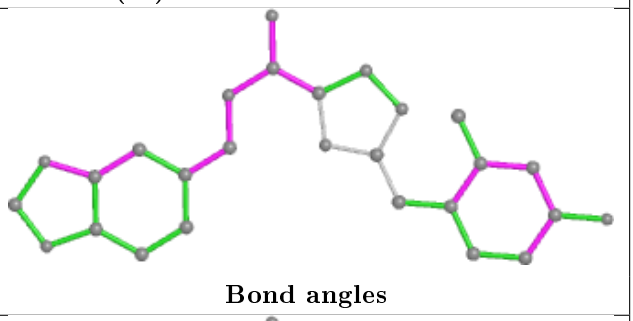


Rings

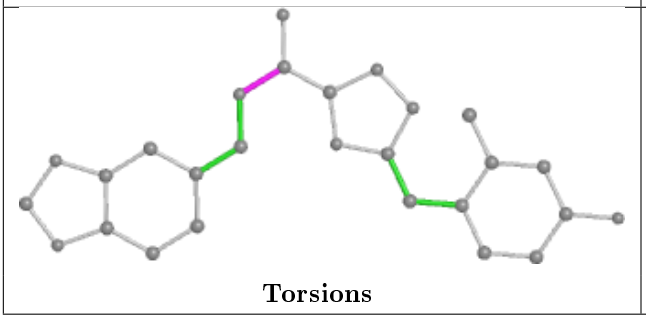
Ligand FJT F 301 (A)



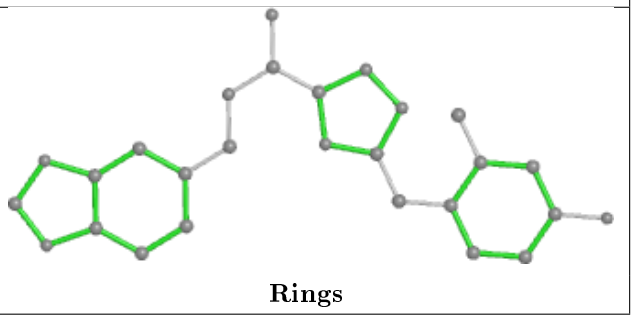
Bond lengths



Bond angles

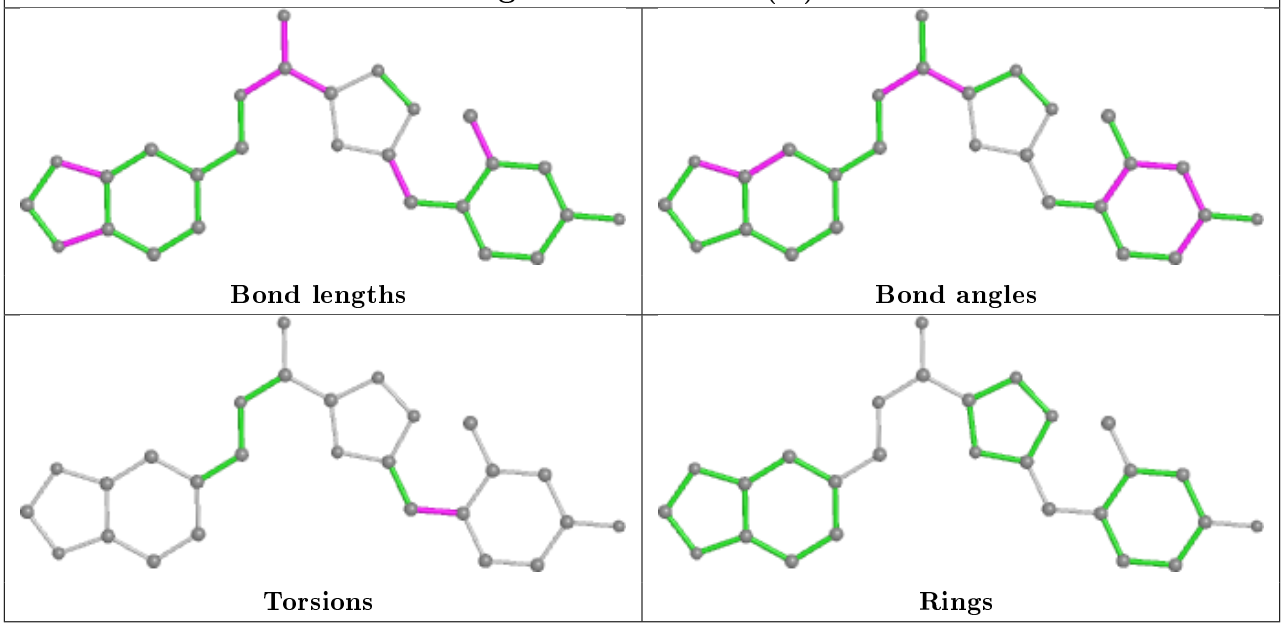


Torsions

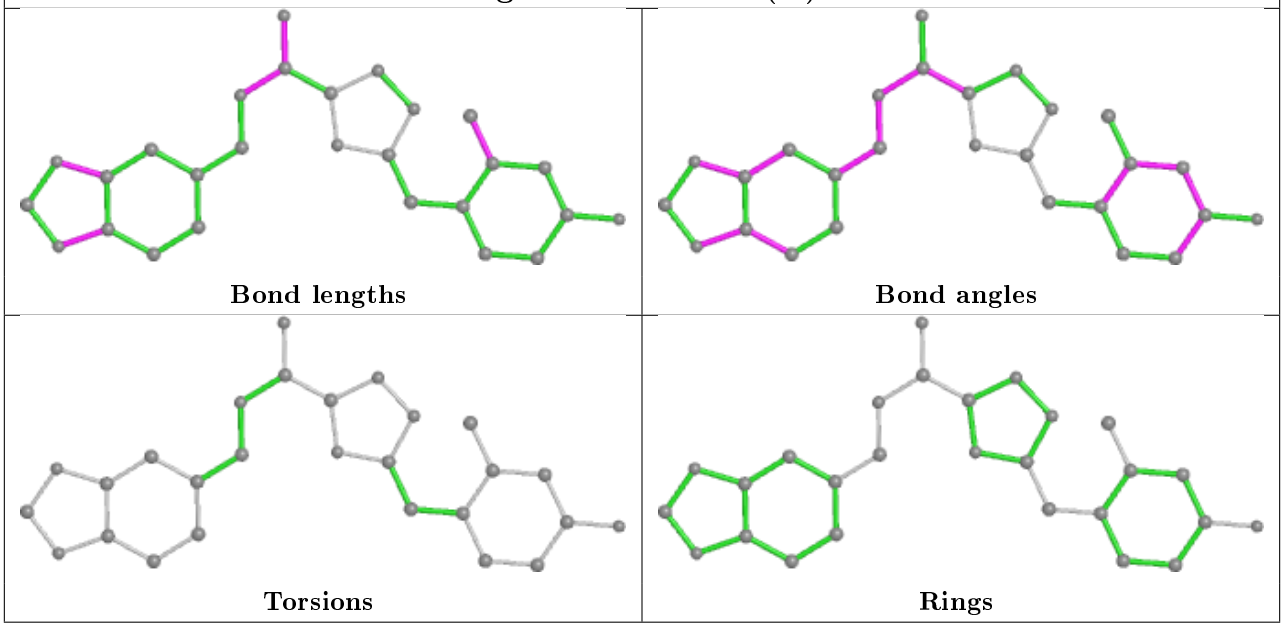


Rings

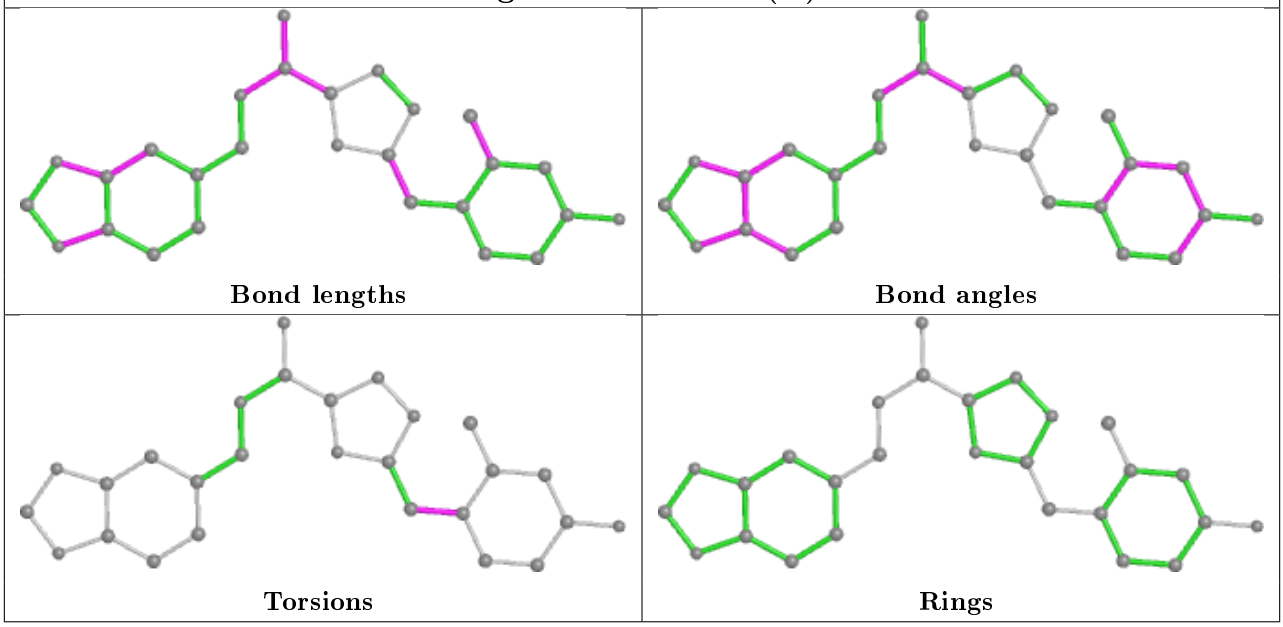
Ligand FJT F 301 (B)



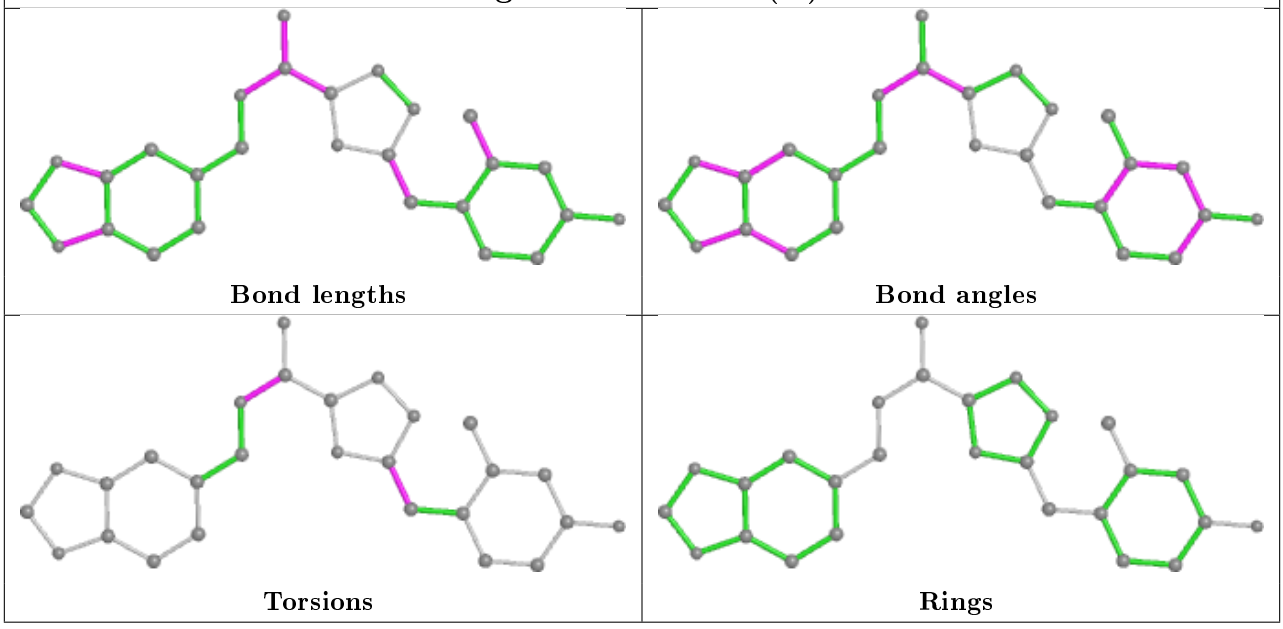
Ligand FJT B 301 (A)



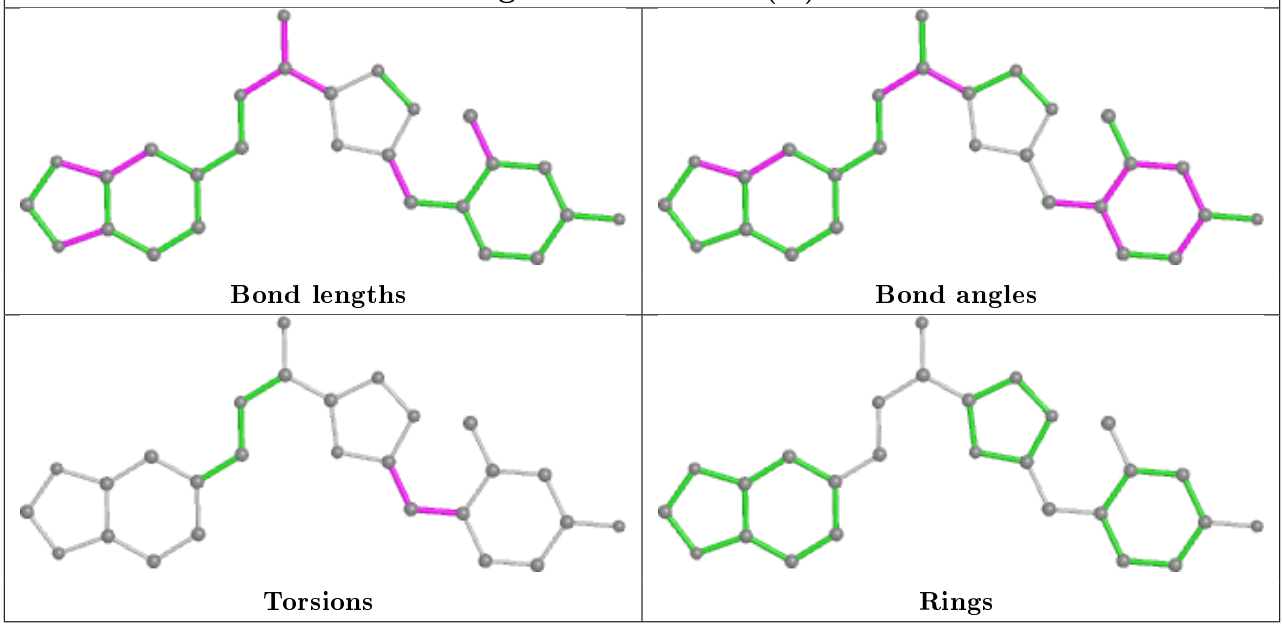
Ligand FJT B 301 (B)



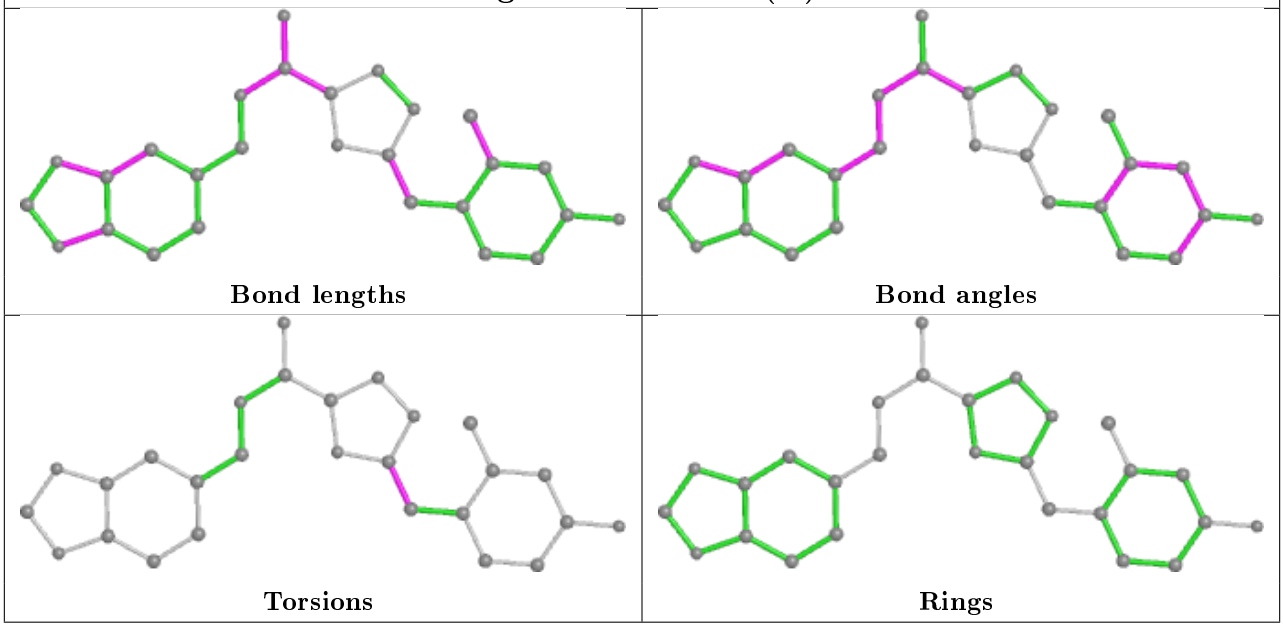
Ligand FJT K 301 (A)



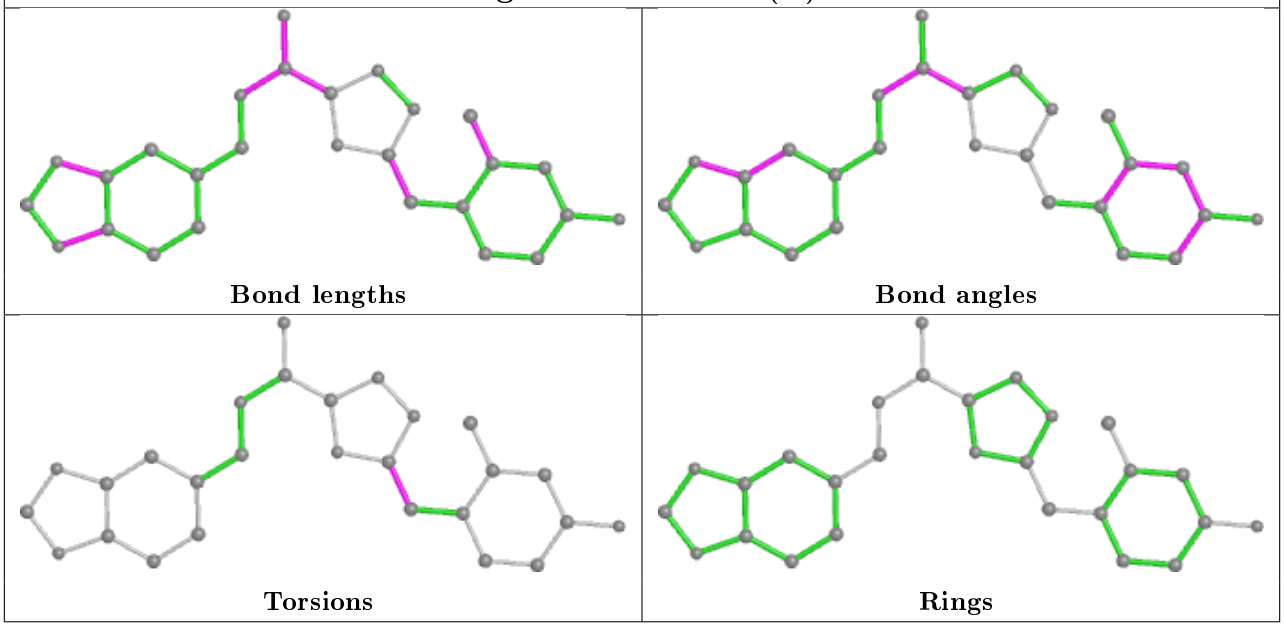
Ligand FJT E 301 (B)



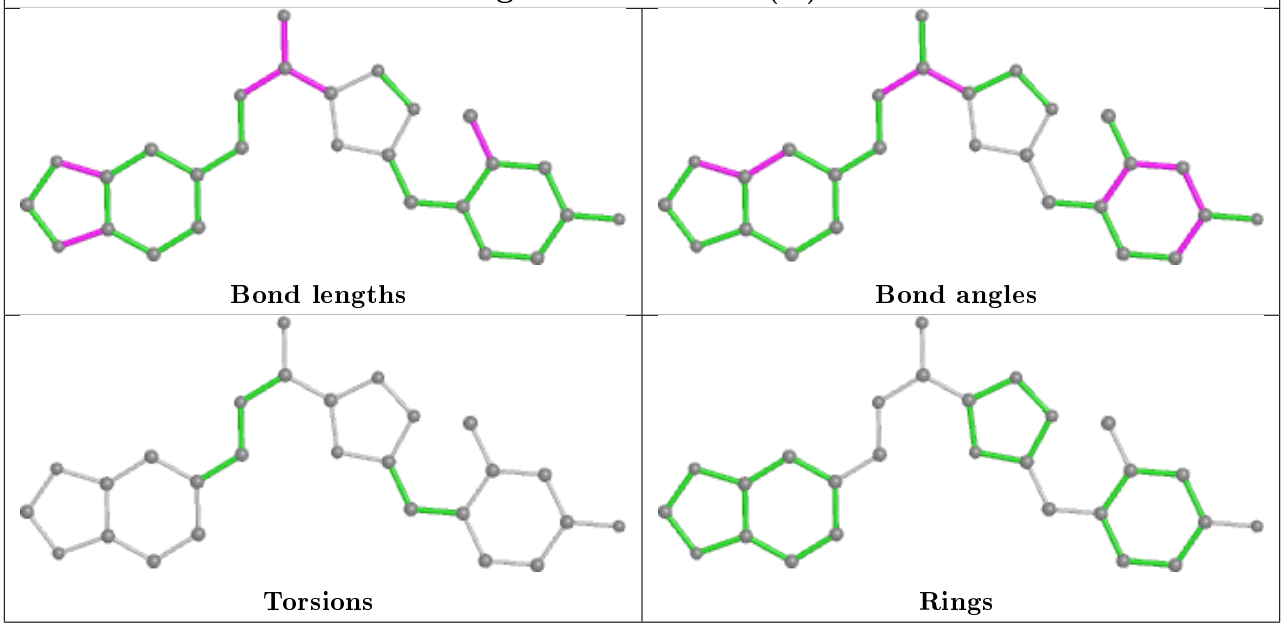
Ligand FJT E 301 (A)



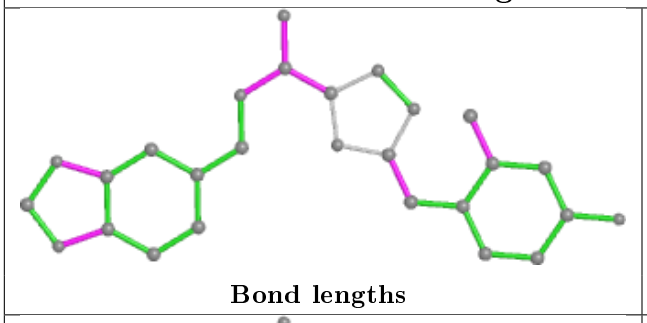
Ligand FJT A 301 (B)



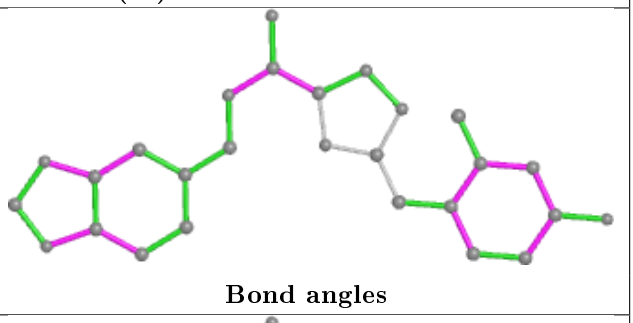
Ligand FJT K 301 (B)



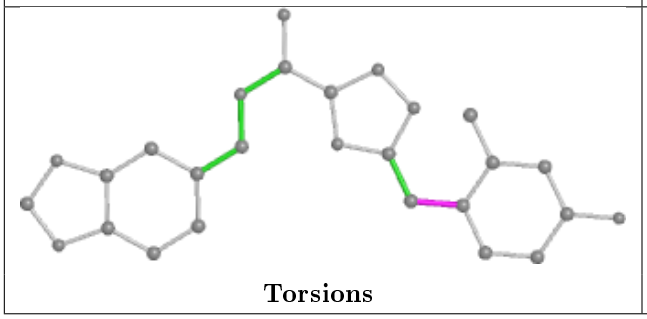
Ligand FJT A 301 (A)



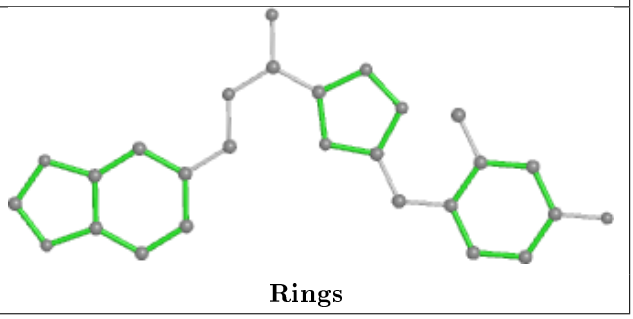
Bond lengths



Bond angles

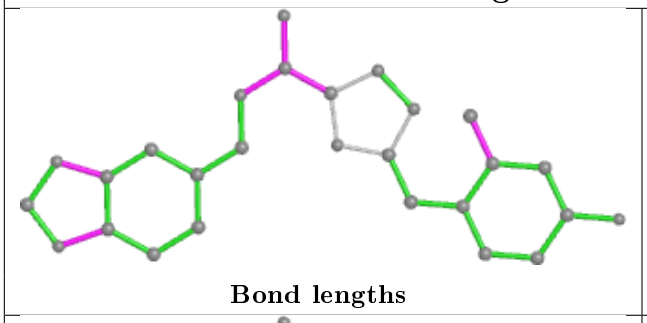


Torsions

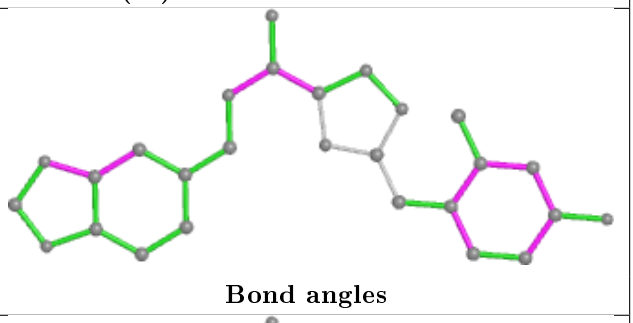


Rings

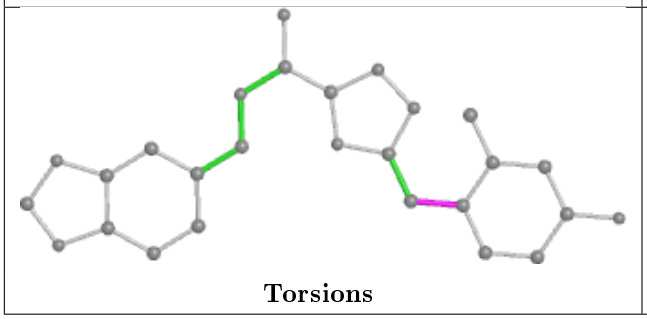
Ligand FJT M 302 (A)



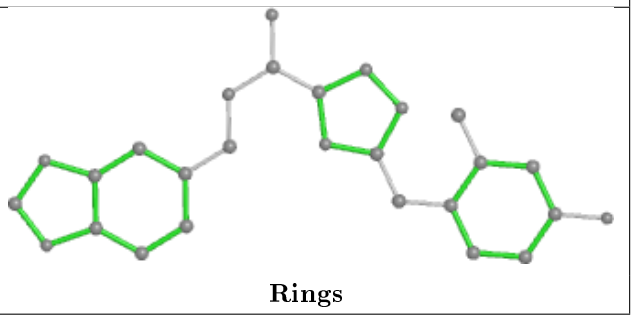
Bond lengths



Bond angles

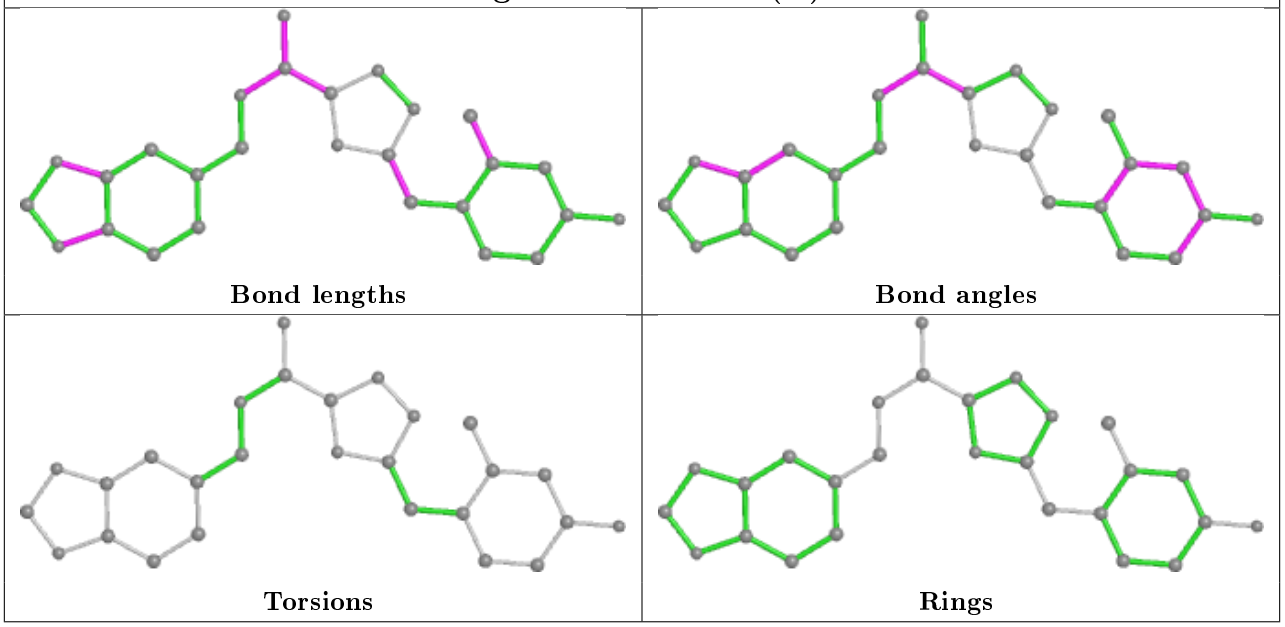


Torsions



Rings

Ligand FJT M 302 (B)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	165/229 (72%)	-0.22	0 100 100	50, 65, 88, 107	0
1	B	166/229 (72%)	-0.16	0 100 100	53, 67, 95, 103	0
1	C	166/229 (72%)	-0.03	0 100 100	49, 69, 103, 117	0
1	D	164/229 (71%)	-0.22	0 100 100	50, 63, 84, 109	0
1	E	166/229 (72%)	-0.22	1 (0%) 89 77	44, 59, 82, 110	0
1	F	166/229 (72%)	-0.15	0 100 100	47, 58, 85, 101	0
1	G	169/229 (73%)	-0.13	1 (0%) 89 77	51, 65, 98, 113	0
1	H	167/229 (72%)	-0.08	0 100 100	51, 63, 88, 110	0
1	I	167/229 (72%)	-0.15	0 100 100	49, 62, 86, 110	0
1	J	166/229 (72%)	-0.23	0 100 100	47, 60, 86, 112	0
1	K	166/229 (72%)	-0.19	0 100 100	47, 61, 88, 118	0
1	L	166/229 (72%)	-0.21	1 (0%) 89 77	44, 55, 81, 117	0
1	M	166/229 (72%)	-0.21	0 100 100	50, 62, 86, 111	0
1	N	168/229 (73%)	-0.24	0 100 100	47, 62, 85, 108	0
All	All	2328/3206 (72%)	-0.18	3 (0%) 95 91	44, 63, 91, 118	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	73	TYR	3.1
1	G	79	LEU	2.2
1	E	111	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

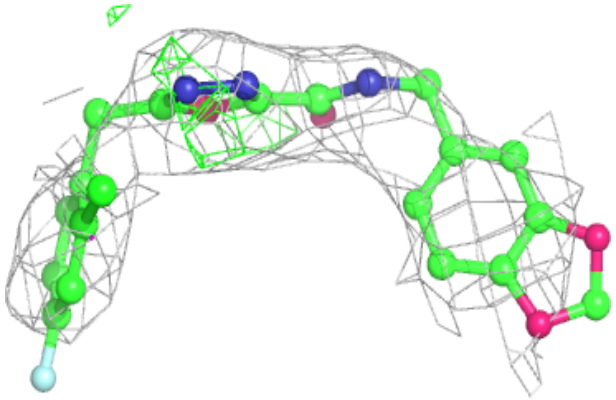
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

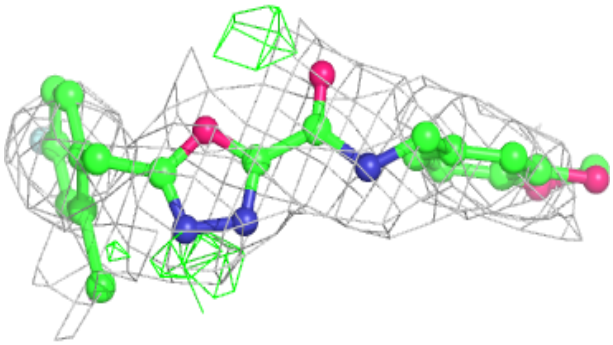
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FJT	B	301[A]	27/27	0.76	0.45	81,92,95,95	27
2	FJT	B	301[B]	27/27	0.76	0.45	82,91,94,96	27
2	FJT	M	301[B]	27/27	0.78	0.46	64,70,74,75	27
2	FJT	M	301[A]	27/27	0.78	0.46	66,70,73,74	27
2	FJT	G	301[A]	27/27	0.80	0.53	79,85,88,90	27
2	FJT	G	301[B]	27/27	0.80	0.53	79,85,88,89	27
2	FJT	F	301[A]	27/27	0.81	0.56	70,78,81,82	27
2	FJT	F	301[B]	27/27	0.81	0.56	71,79,81,82	27
2	FJT	A	301[B]	27/27	0.81	0.56	81,83,86,86	27
2	FJT	A	301[A]	27/27	0.81	0.56	81,83,85,89	27
2	FJT	L	301[B]	27/27	0.82	0.47	68,78,81,84	27
2	FJT	L	301[A]	27/27	0.82	0.47	68,77,80,83	27
2	FJT	M	302[A]	27/27	0.83	0.50	63,74,78,79	27
2	FJT	M	302[B]	27/27	0.83	0.50	64,74,79,79	27
3	EDO	A	302	4/4	0.83	0.25	49,55,60,61	0
3	EDO	F	302	4/4	0.84	0.29	53,58,59,62	0
2	FJT	D	302[A]	27/27	0.84	0.38	68,78,81,82	27
2	FJT	D	301	27/27	0.84	0.33	71,85,89,90	27
2	FJT	H	302[B]	27/27	0.84	0.55	69,81,82,83	27
2	FJT	H	302[A]	27/27	0.84	0.55	70,81,83,84	27
2	FJT	D	302[B]	27/27	0.84	0.38	68,77,81,82	27
2	FJT	K	301[A]	27/27	0.85	0.49	72,77,81,83	27
2	FJT	J	301[A]	27/27	0.85	0.34	70,75,81,83	27
2	FJT	J	301[B]	27/27	0.85	0.34	71,75,81,83	27
2	FJT	K	301[B]	27/27	0.85	0.49	72,77,81,83	27
2	FJT	E	301[B]	27/27	0.88	0.46	62,71,73,76	27
2	FJT	E	301[A]	27/27	0.88	0.46	66,71,74,77	27
2	FJT	H	301[B]	27/27	0.89	0.41	71,80,84,84	27
2	FJT	H	301[A]	27/27	0.89	0.41	73,79,84,84	27
3	EDO	E	302	4/4	0.92	0.20	56,57,61,65	0
3	EDO	N	301	4/4	0.93	0.20	59,62,66,67	0

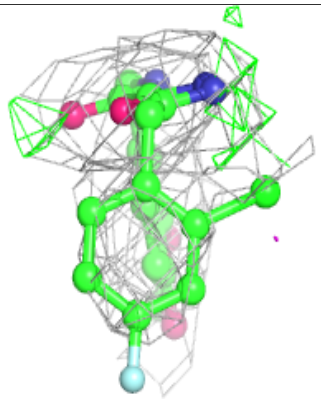
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FJT B 301 (A):

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

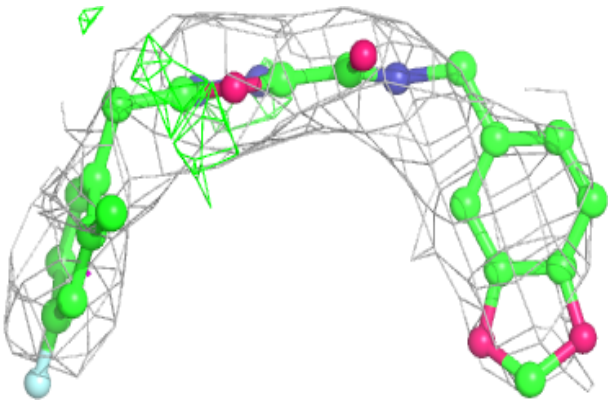


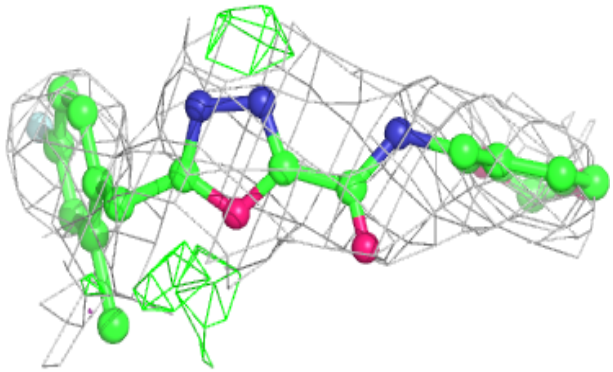


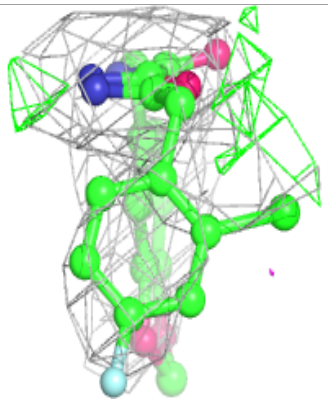


Electron density around FJT B 301 (B):

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

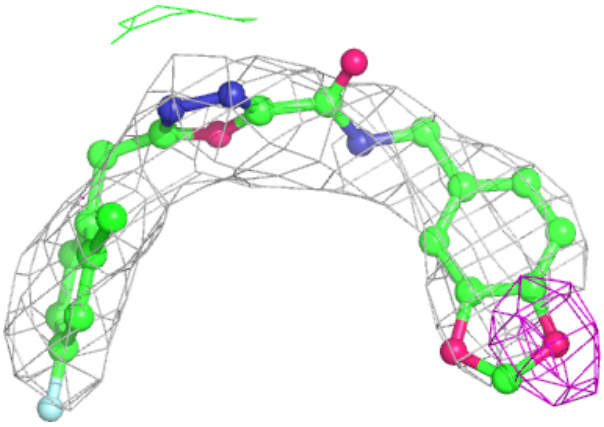


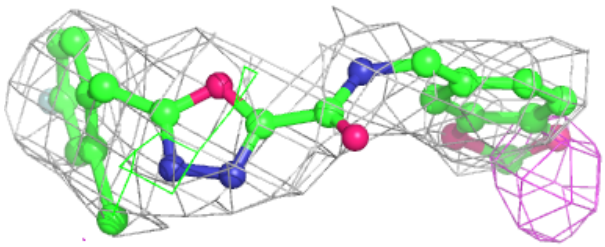


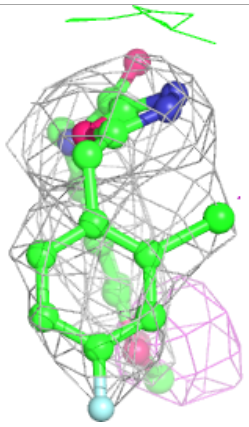


Electron density around FJT M 301 (B):

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

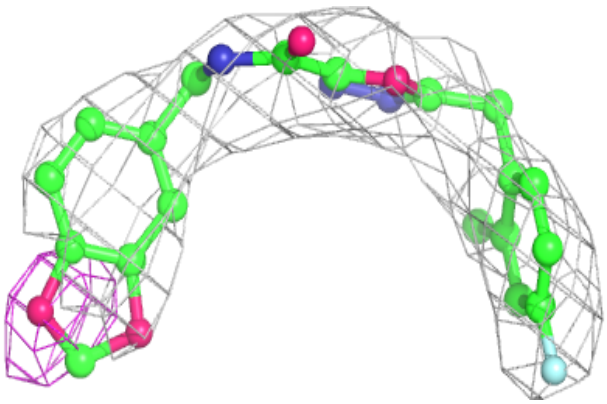


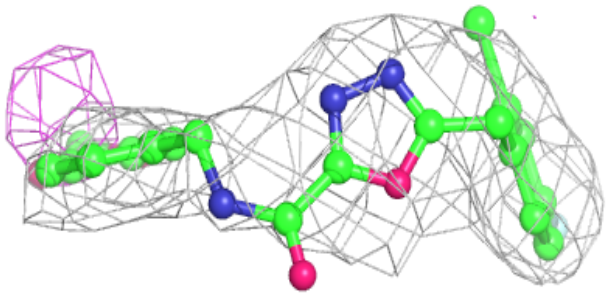


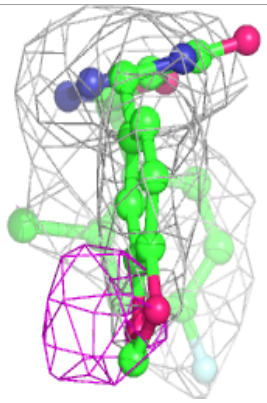


Electron density around FJT M 301 (A):

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

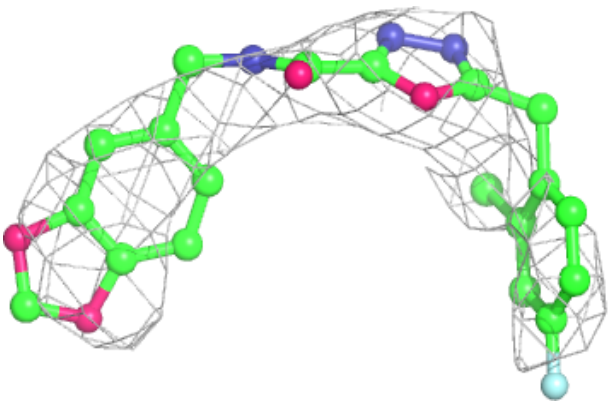


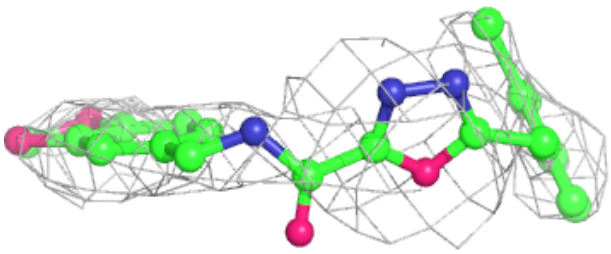


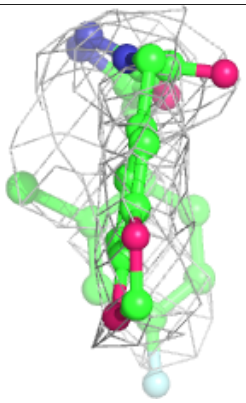


Electron density around FJT G 301 (A):

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

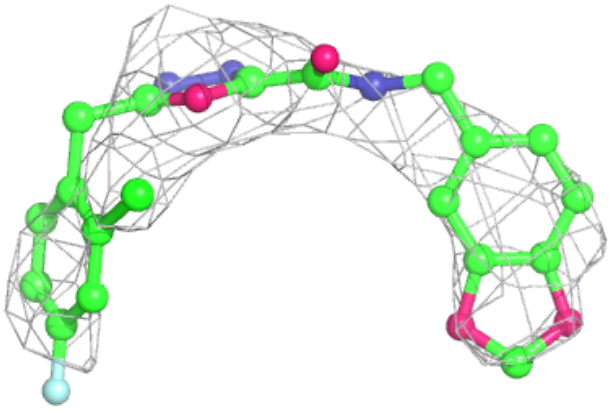


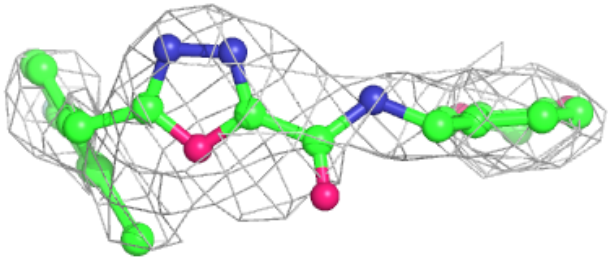


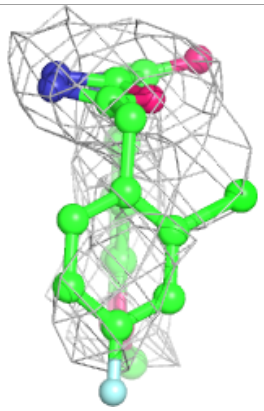


Electron density around FJT G 301 (B):

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

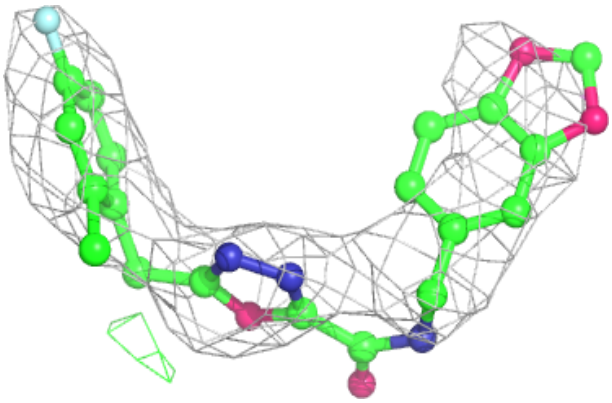


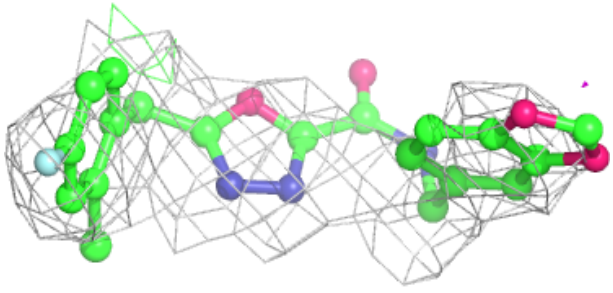


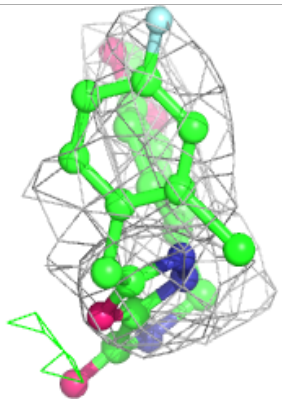


Electron density around FJT F 301 (A):

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

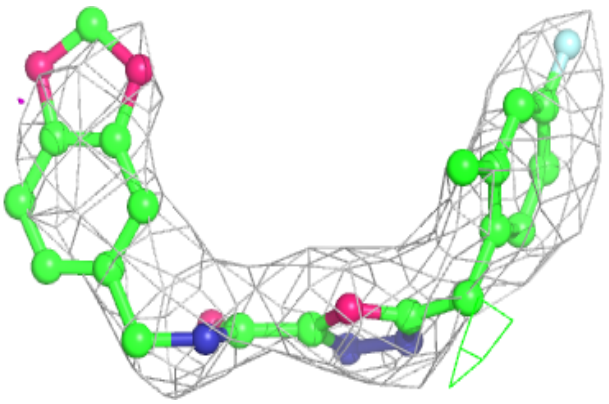


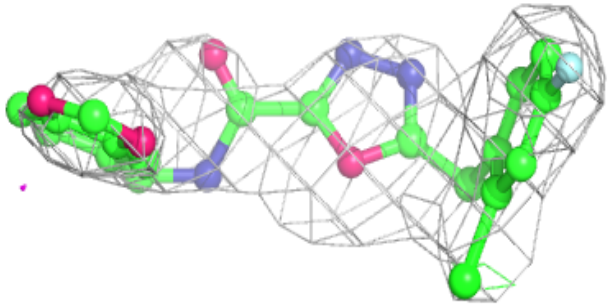


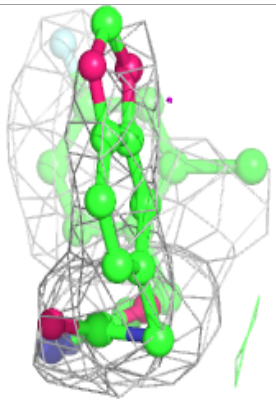


Electron density around FJT F 301 (B):

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

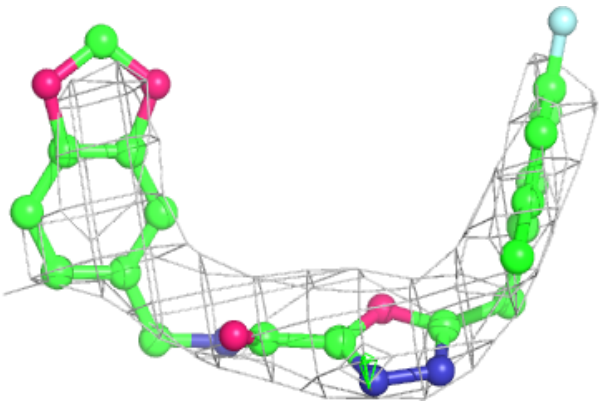


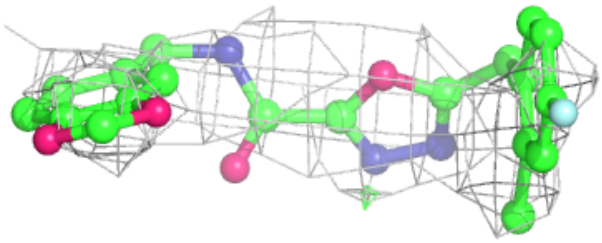


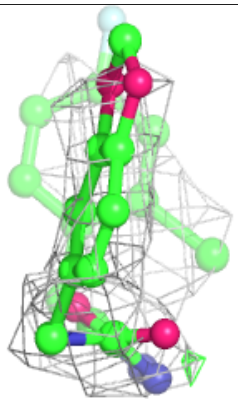


Electron density around FJT A 301 (B):

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

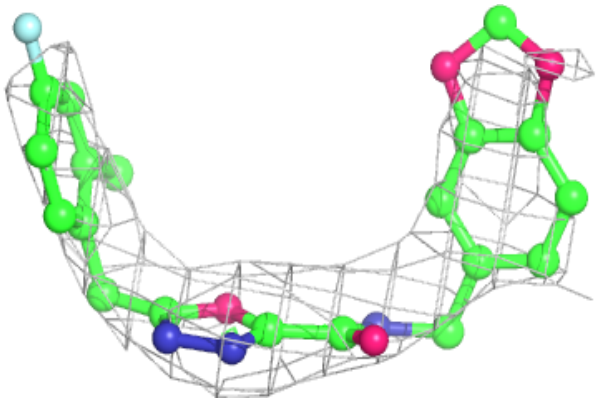


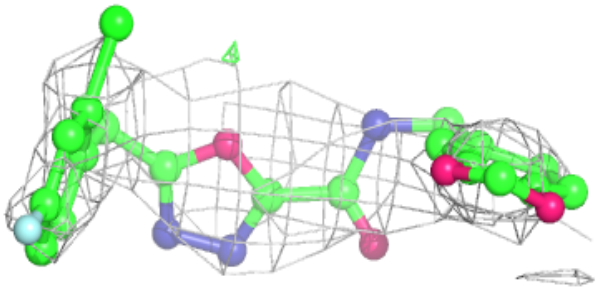


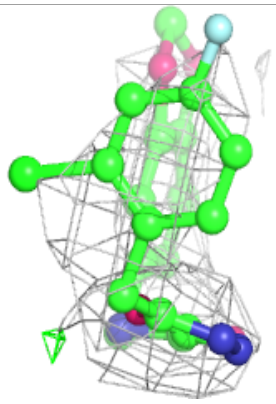


Electron density around FJT A 301 (A):

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

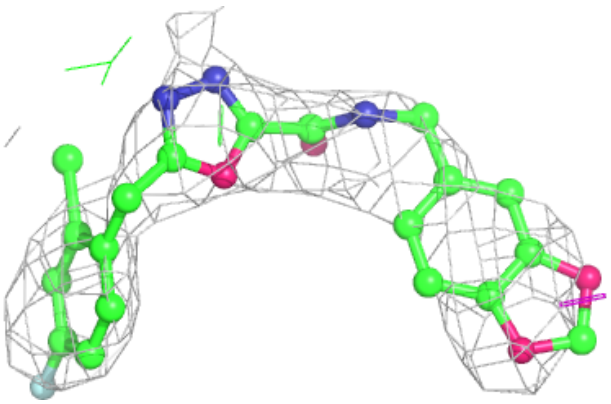


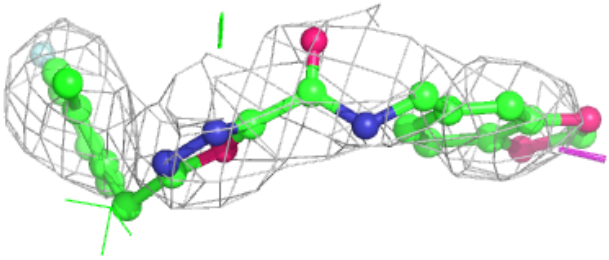


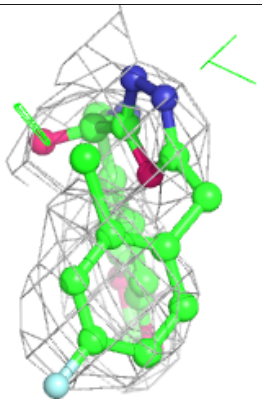


Electron density around FJT L 301 (B):

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

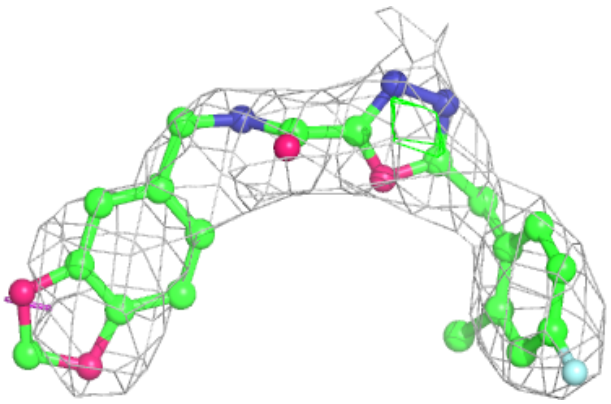


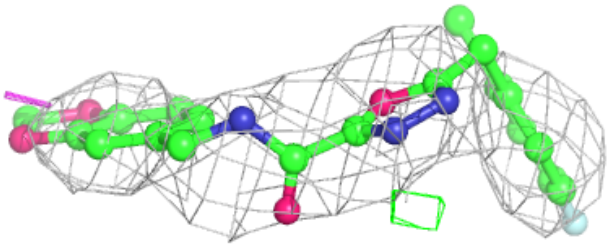




Electron density around FJT L 301 (A):

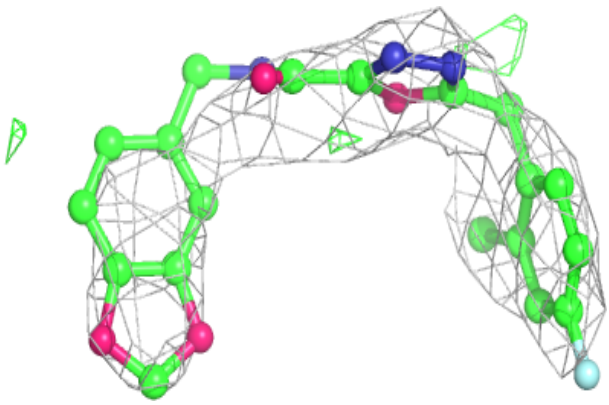
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

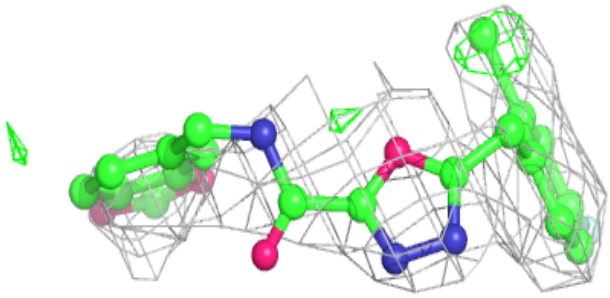


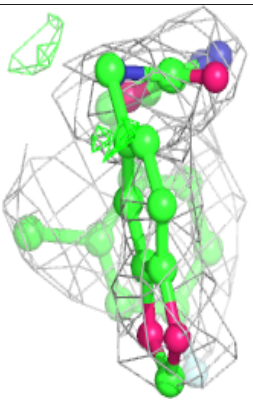


Electron density around FJT M 302 (A):

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

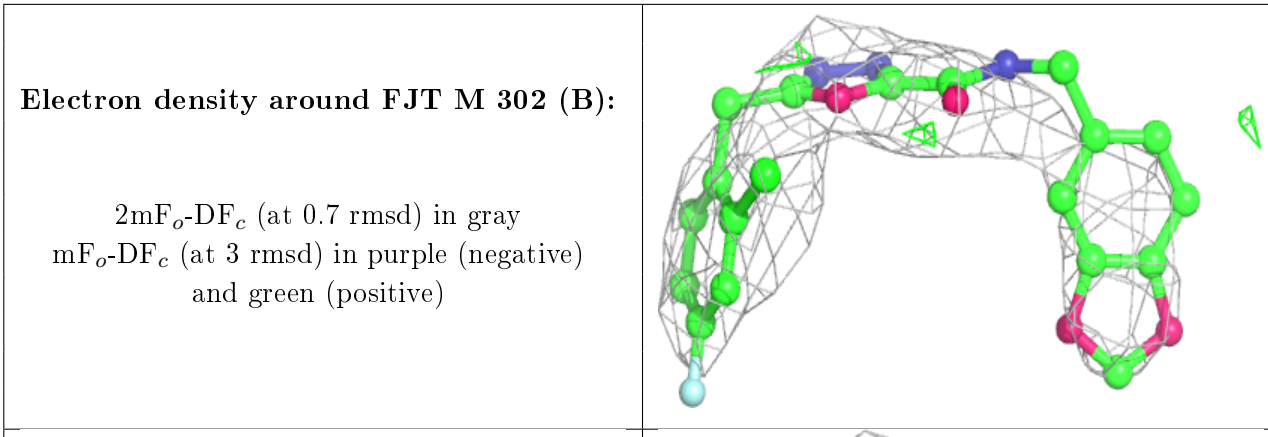






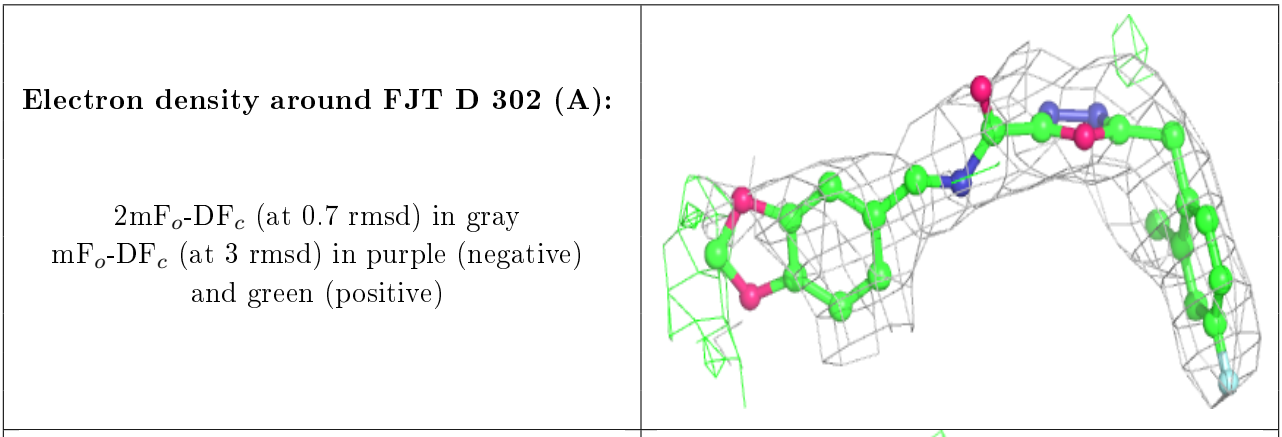
Electron density around FJT M 302 (B):

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



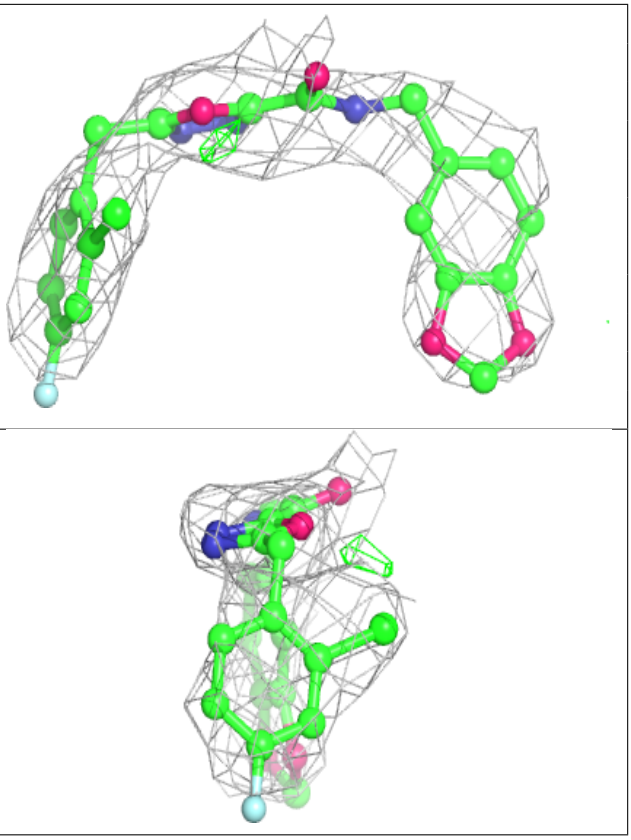
Electron density around FJT D 302 (A):

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



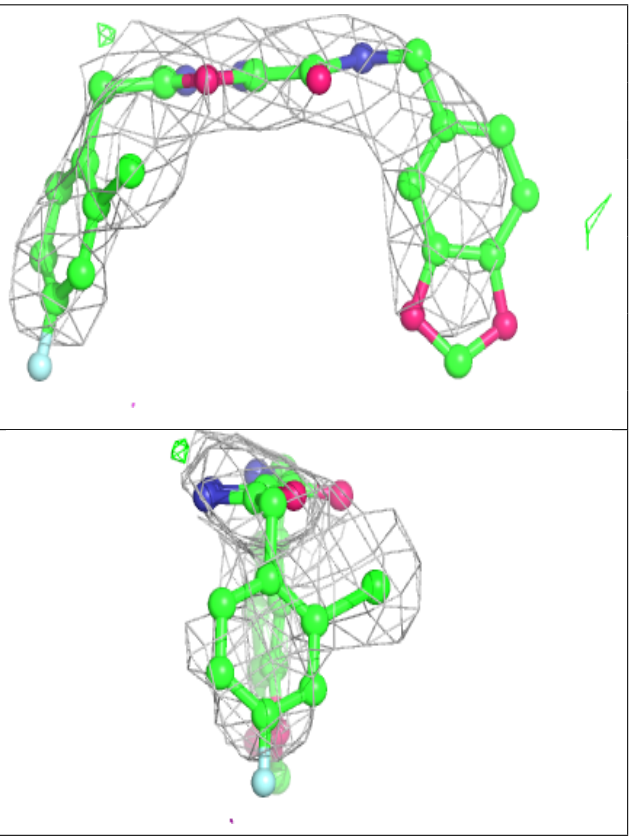
Electron density around FJT D 301:

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



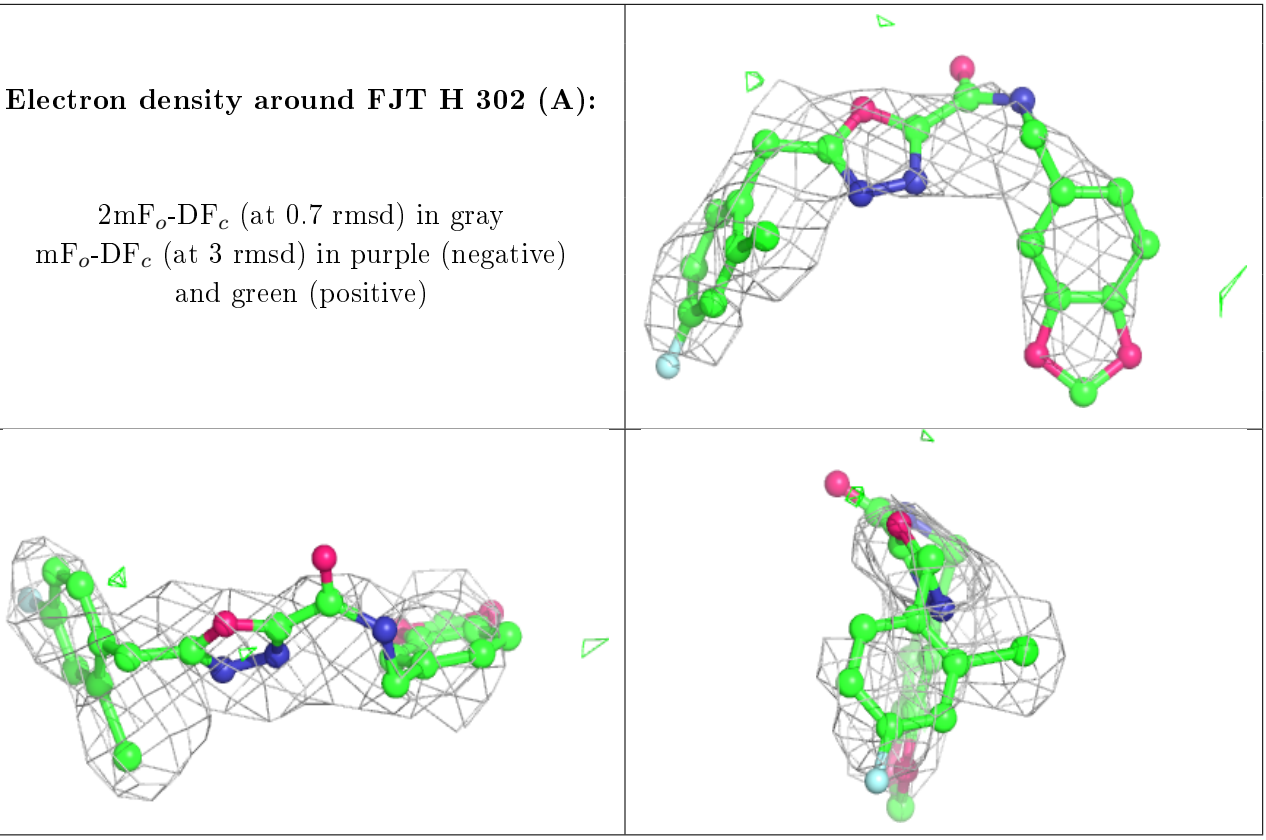
Electron density around FJT H 302 (B):

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



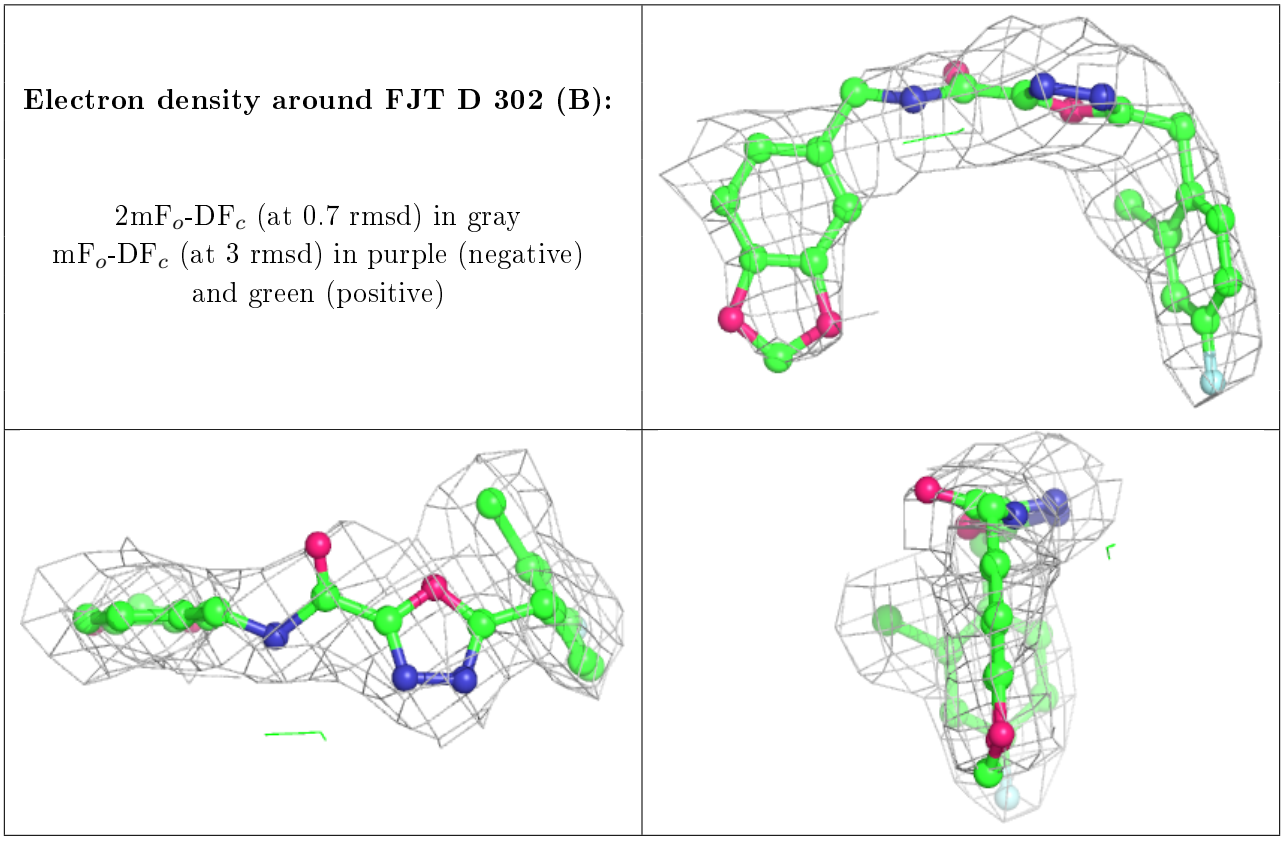
Electron density around FJT H 302 (A):

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



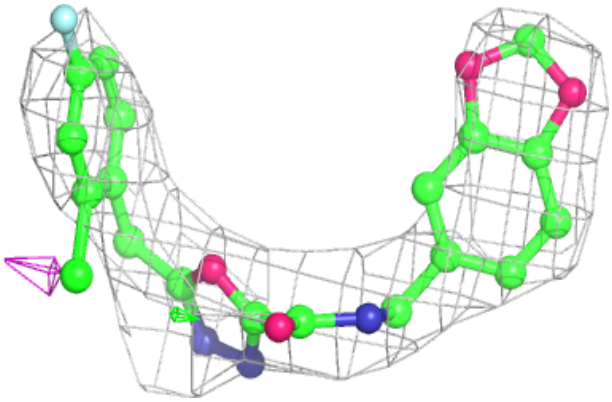
Electron density around FJT D 302 (B):

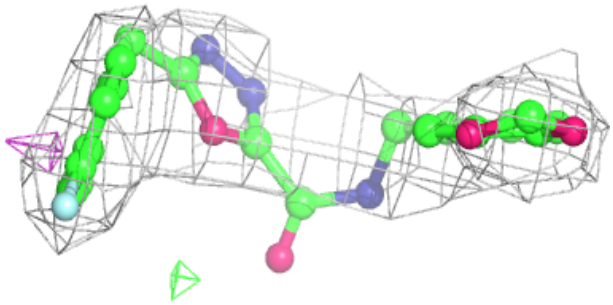
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

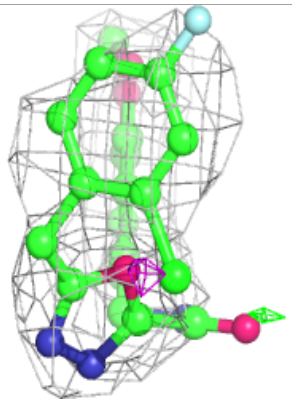


Electron density around FJT K 301 (A):

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

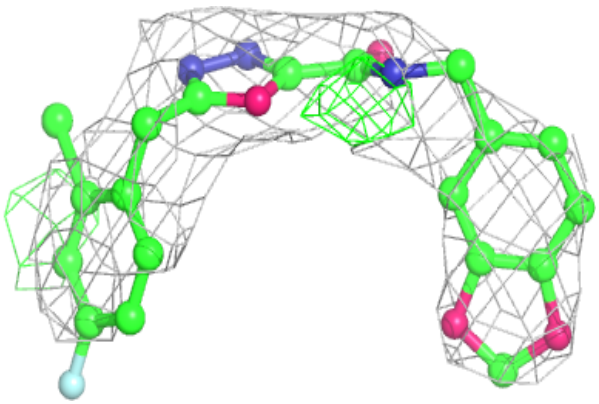


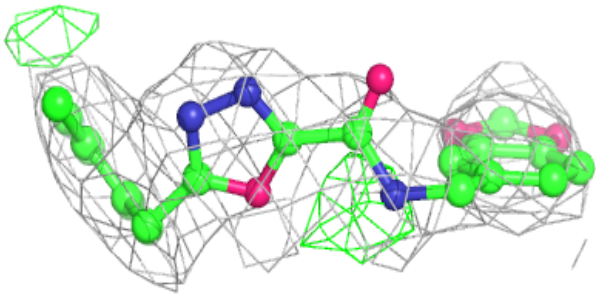


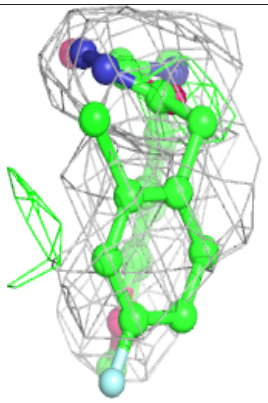


Electron density around FJT J 301 (A):

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

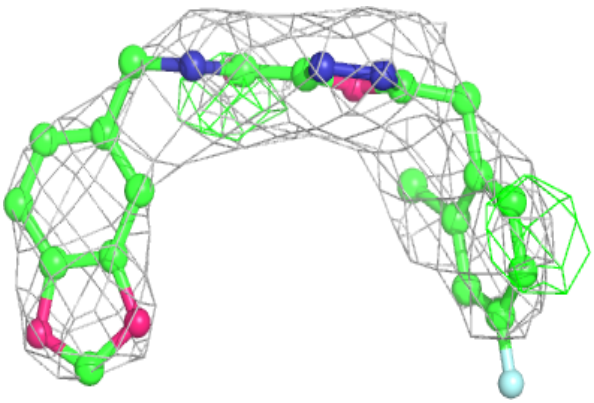


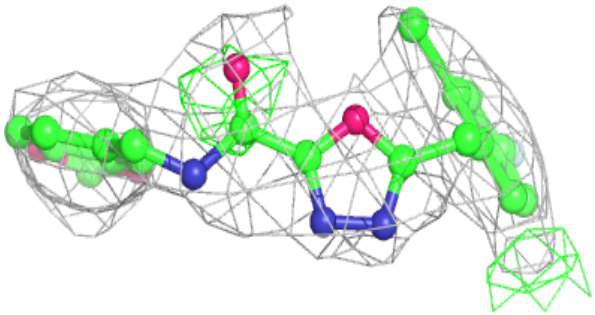


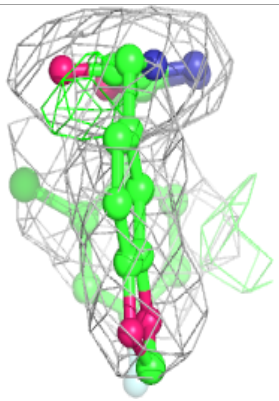


Electron density around FJT J 301 (B):

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

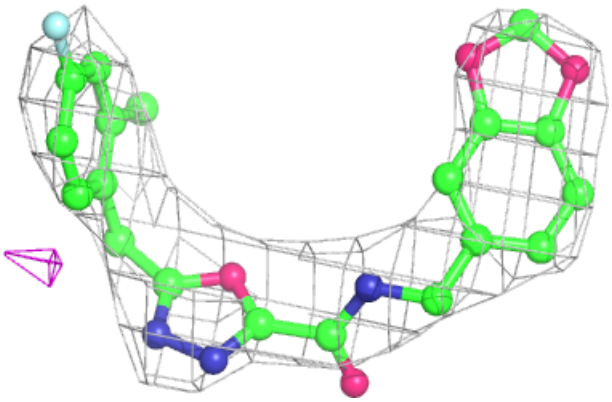


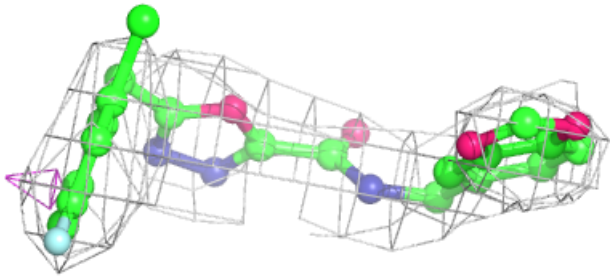


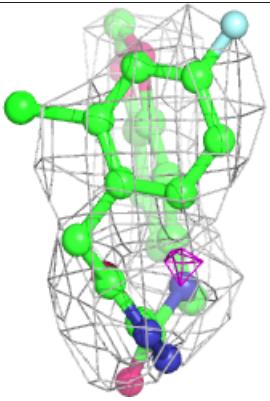


Electron density around FJT K 301 (B):

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

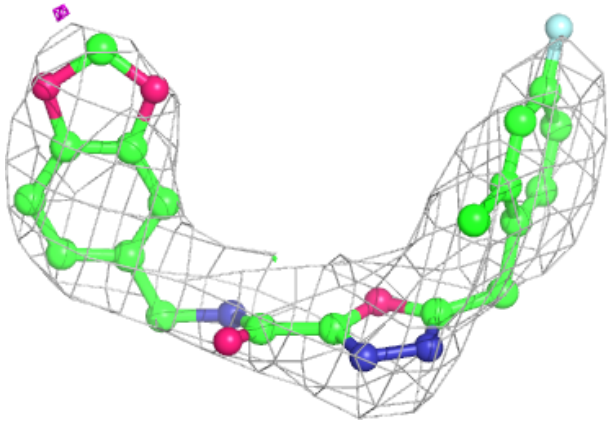


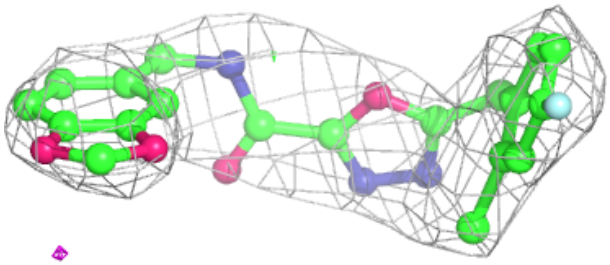


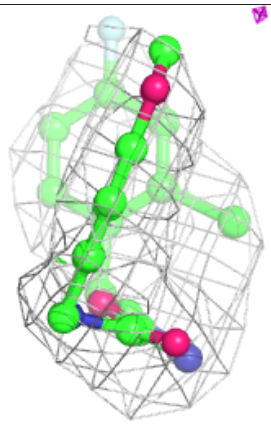


Electron density around FJT E 301 (B):

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

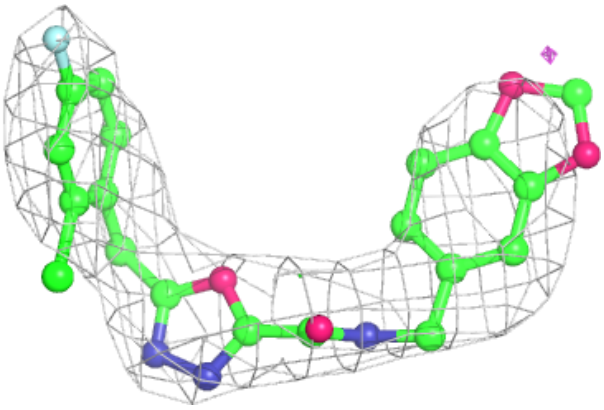


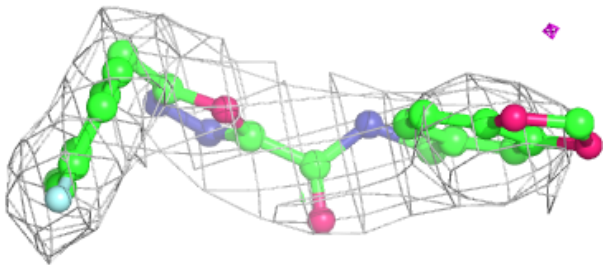


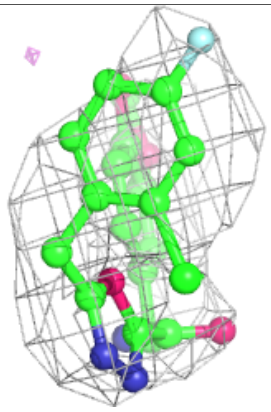


Electron density around FJT E 301 (A):

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

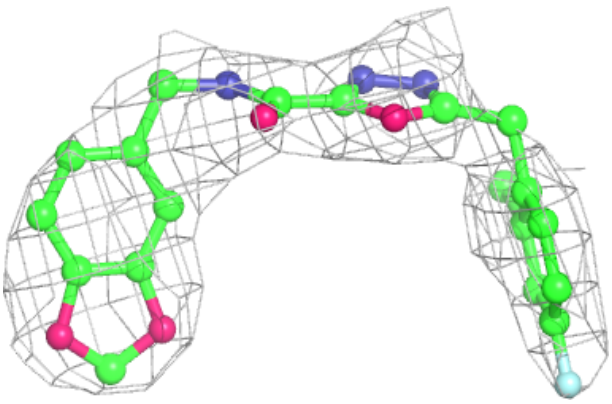


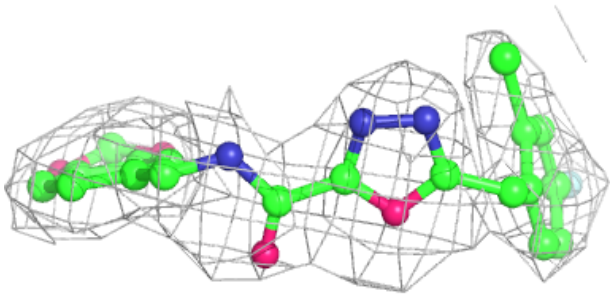


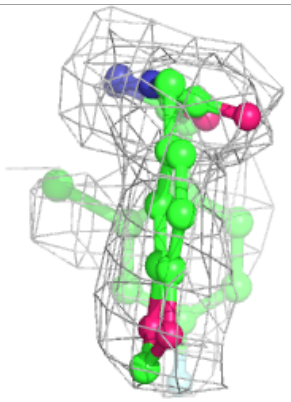


Electron density around FJT H 301 (B):

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

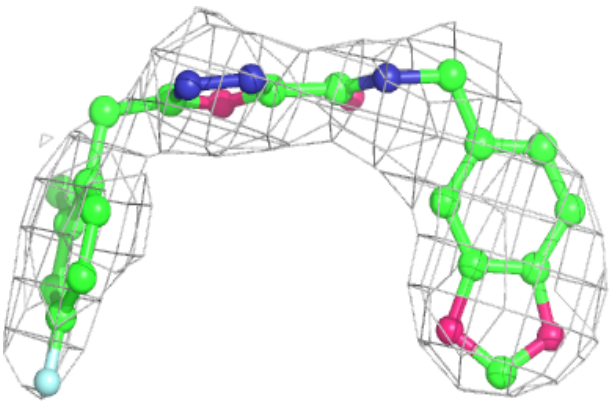


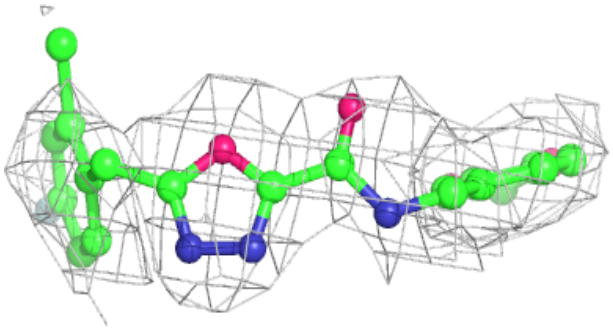


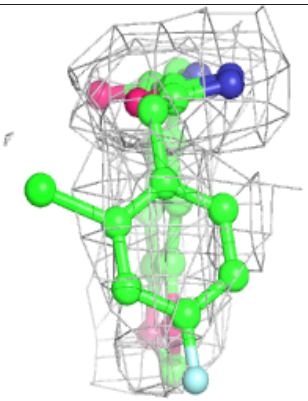


Electron density around FJT H 301 (A):

$2mF_o$-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.