



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 04:04 pm BST

PDB ID : 4A99
Title : STRUCTURE OF THE TETRACYCLINE DEGRADING MONOOXYGENASE TETX IN COMPLEX WITH MINOCYCLINE
Authors : Volkers, G.; Palm, G.J.; Weiss, M.S.; Hinrichs, W.
Deposited on : 2011-11-25
Resolution : 2.18 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 ⓘ symbol.

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

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

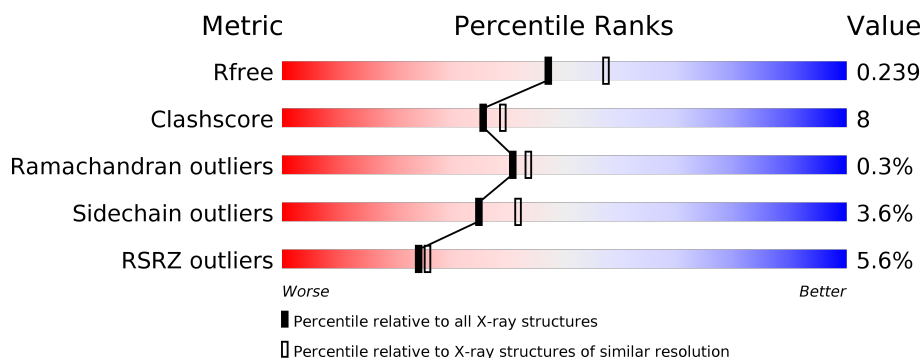
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	398	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	398	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	398	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	398	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>•</div> <div>8%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12662 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 TETX2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2886	1826	489	559	12			
1	B	368	Total	C	N	O	S	0	0	0
			2883	1826	489	556	12			
1	C	367	Total	C	N	O	S	0	0	0
			2868	1817	485	554	12			
1	D	367	Total	C	N	O	S	0	0	0
			2859	1812	485	550	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP Q93L51
A	-8	GLY	-	expression tag	UNP Q93L51
A	-7	SER	-	expression tag	UNP Q93L51
A	-6	SER	-	expression tag	UNP Q93L51
A	-5	HIS	-	expression tag	UNP Q93L51
A	-4	HIS	-	expression tag	UNP Q93L51
A	-3	HIS	-	expression tag	UNP Q93L51
A	-2	HIS	-	expression tag	UNP Q93L51
A	-1	HIS	-	expression tag	UNP Q93L51
A	0	HIS	-	expression tag	UNP Q93L51
A	1	SER	-	expression tag	UNP Q93L51
A	2	SER	-	expression tag	UNP Q93L51
A	3	GLY	-	expression tag	UNP Q93L51
A	4	LEU	-	expression tag	UNP Q93L51
A	5	VAL	-	expression tag	UNP Q93L51
A	6	PRO	-	expression tag	UNP Q93L51
A	7	ARG	-	expression tag	UNP Q93L51
A	8	GLY	-	expression tag	UNP Q93L51
A	9	SER	-	expression tag	UNP Q93L51
A	10	HIS	-	expression tag	UNP Q93L51
B	-9	MET	-	expression tag	UNP Q93L51

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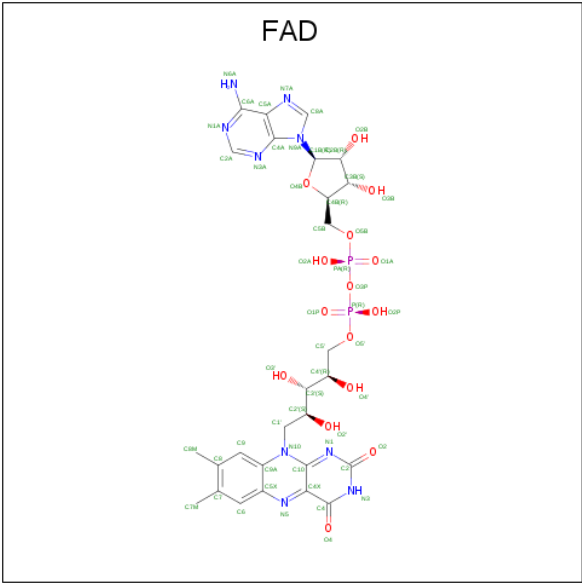
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q93L51
B	-7	SER	-	expression tag	UNP Q93L51
B	-6	SER	-	expression tag	UNP Q93L51
B	-5	HIS	-	expression tag	UNP Q93L51
B	-4	HIS	-	expression tag	UNP Q93L51
B	-3	HIS	-	expression tag	UNP Q93L51
B	-2	HIS	-	expression tag	UNP Q93L51
B	-1	HIS	-	expression tag	UNP Q93L51
B	0	HIS	-	expression tag	UNP Q93L51
B	1	SER	-	expression tag	UNP Q93L51
B	2	SER	-	expression tag	UNP Q93L51
B	3	GLY	-	expression tag	UNP Q93L51
B	4	LEU	-	expression tag	UNP Q93L51
B	5	VAL	-	expression tag	UNP Q93L51
B	6	PRO	-	expression tag	UNP Q93L51
B	7	ARG	-	expression tag	UNP Q93L51
B	8	GLY	-	expression tag	UNP Q93L51
B	9	SER	-	expression tag	UNP Q93L51
B	10	HIS	-	expression tag	UNP Q93L51
C	-9	MET	-	expression tag	UNP Q93L51
C	-8	GLY	-	expression tag	UNP Q93L51
C	-7	SER	-	expression tag	UNP Q93L51
C	-6	SER	-	expression tag	UNP Q93L51
C	-5	HIS	-	expression tag	UNP Q93L51
C	-4	HIS	-	expression tag	UNP Q93L51
C	-3	HIS	-	expression tag	UNP Q93L51
C	-2	HIS	-	expression tag	UNP Q93L51
C	-1	HIS	-	expression tag	UNP Q93L51
C	0	HIS	-	expression tag	UNP Q93L51
C	1	SER	-	expression tag	UNP Q93L51
C	2	SER	-	expression tag	UNP Q93L51
C	3	GLY	-	expression tag	UNP Q93L51
C	4	LEU	-	expression tag	UNP Q93L51
C	5	VAL	-	expression tag	UNP Q93L51
C	6	PRO	-	expression tag	UNP Q93L51
C	7	ARG	-	expression tag	UNP Q93L51
C	8	GLY	-	expression tag	UNP Q93L51
C	9	SER	-	expression tag	UNP Q93L51
C	10	HIS	-	expression tag	UNP Q93L51
D	-9	MET	-	expression tag	UNP Q93L51
D	-8	GLY	-	expression tag	UNP Q93L51
D	-7	SER	-	expression tag	UNP Q93L51

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	expression tag	UNP Q93L51
D	-5	HIS	-	expression tag	UNP Q93L51
D	-4	HIS	-	expression tag	UNP Q93L51
D	-3	HIS	-	expression tag	UNP Q93L51
D	-2	HIS	-	expression tag	UNP Q93L51
D	-1	HIS	-	expression tag	UNP Q93L51
D	0	HIS	-	expression tag	UNP Q93L51
D	1	SER	-	expression tag	UNP Q93L51
D	2	SER	-	expression tag	UNP Q93L51
D	3	GLY	-	expression tag	UNP Q93L51
D	4	LEU	-	expression tag	UNP Q93L51
D	5	VAL	-	expression tag	UNP Q93L51
D	6	PRO	-	expression tag	UNP Q93L51
D	7	ARG	-	expression tag	UNP Q93L51
D	8	GLY	-	expression tag	UNP Q93L51
D	9	SER	-	expression tag	UNP Q93L51
D	10	HIS	-	expression tag	UNP Q93L51

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



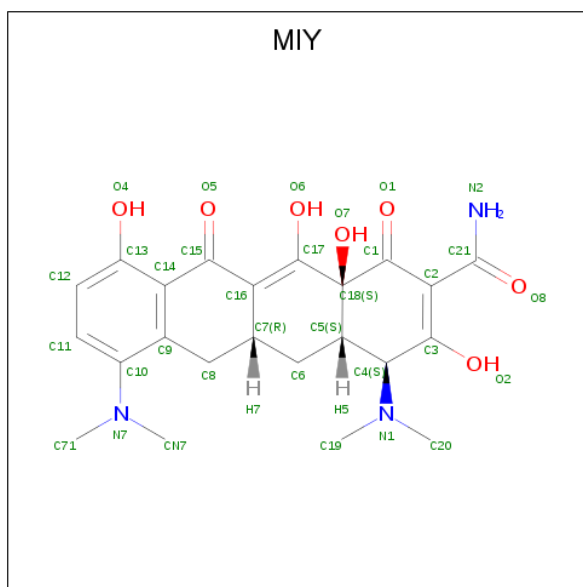
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: $C_{23}H_{27}N_3O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			33	23	3	7			
3	A	1	Total	C	N	O		0	0
			33	23	3	7			
3	B	1	Total	C	N	O		0	0
			33	23	3	7			
3	C	1	Total	C	N	O		0	0
			33	23	3	7			
3	C	1	Total	C	N	O		0	0
			33	23	3	7			
3	D	1	Total	C	N	O		0	0
			33	23	3	7			
3	D	1	Total	C	N	O		0	0
			33	23	3	7			
3	D	1	Total	C	N	O		0	0
			33	23	3	7			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	0
			203	203		

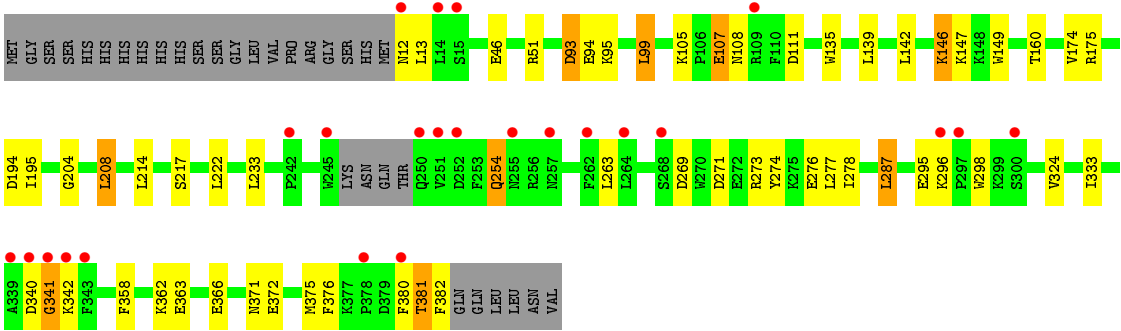
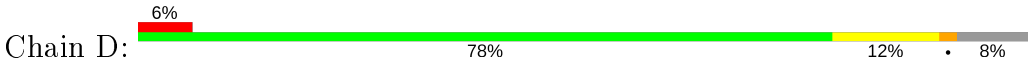
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	189	Total 189	O 189	0	0
5	C	134	Total 134	O 134	0	0
5	D	114	Total 114	O 114	0	0



● Molecule 1: TETX2 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.88Å 80.33Å 86.63Å 110.82° 90.27° 93.39°	Depositor
Resolution (Å)	80.94 – 2.18 47.66 – 2.18	Depositor EDS
% Data completeness (in resolution range)	95.5 (80.94-2.18) 95.5 (47.66-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.185 , 0.235 0.188 , 0.239	Depositor DCC
R_{free} test set	4301 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12662	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MIY, SO4, FAD

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	0.90	5/2944 (0.2%)	0.89	3/3988 (0.1%)
1	B	0.92	3/2941 (0.1%)	0.99	10/3983 (0.3%)
1	C	0.79	1/2926 (0.0%)	0.83	4/3965 (0.1%)
1	D	0.82	3/2917 (0.1%)	0.85	6/3954 (0.2%)
All	All	0.86	12/11728 (0.1%)	0.89	23/15890 (0.1%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	GLU	CD-OE2	-9.28	1.15	1.25
1	B	94	GLU	CD-OE1	-6.89	1.18	1.25
1	A	135	TRP	CD2-CE2	5.91	1.48	1.41
1	A	78	GLN	CD-NE2	-5.83	1.18	1.32
1	A	276	GLU	CD-OE1	5.72	1.31	1.25

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ARG	NE-CZ-NH2	-13.46	113.57	120.30
1	A	175	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	B	94	GLU	OE1-CD-OE2	-10.97	110.13	123.30
1	B	93	ASP	CB-CG-OD2	9.83	127.15	118.30
1	B	175	ARG	NE-CZ-NH1	9.81	125.20	120.30

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	2886	0	2800	39	0
1	B	2883	0	2797	51	0
1	C	2868	0	2771	39	0
1	D	2859	0	2761	42	0
2	A	53	0	31	4	0
2	B	53	0	31	3	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
3	A	66	0	48	3	0
3	B	33	0	24	2	0
3	C	66	0	49	7	0
3	D	99	0	73	7	0
4	A	5	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
5	A	203	0	0	6	0
5	B	189	0	0	10	0
5	C	134	0	0	2	0
5	D	114	0	0	3	0
All	All	12662	0	11447	189	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 8.

The worst 5 of 189 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:A:269:ASP:HB2	5:A:2163:HOH:O	1.28	1.29
1:A:218:HIS:HD2	5:A:2063:HOH:O	1.43	0.99
1:B:381:THR:HA	5:B:2185:HOH:O	1.64	0.96
1:D:12:ASN:HD21	1:D:341:GLY:CA	1.83	0.92
1:D:12:ASN:HD21	1:D:341:GLY:HA2	1.35	0.91

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/398 (92%)	352 (97%)	11 (3%)	1 (0%)	41	43
1	B	364/398 (92%)	350 (96%)	12 (3%)	2 (0%)	29	28
1	C	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	41	43
1	D	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	41	43
All	All	1454/1592 (91%)	1398 (96%)	51 (4%)	5 (0%)	41	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	LEU
1	A	341	GLY
1	B	341	GLY
1	D	341	GLY
1	C	341	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/345 (90%)	299 (96%)	13 (4%)	30	35
1	B	310/345 (90%)	298 (96%)	12 (4%)	32	38
1	C	307/345 (89%)	296 (96%)	11 (4%)	35	42
1	D	305/345 (88%)	296 (97%)	9 (3%)	41	49
All	All	1234/1380 (89%)	1189 (96%)	45 (4%)	35	42

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	269	ASP
1	C	107	GLU
1	D	269	ASP
1	B	353	TYR
1	C	110	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	254	GLN
1	C	12	ASN
1	D	190	ASN
1	B	371	ASN
1	C	68	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 ⓘ

22 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
3	MIY	C	392	-	35,36,36	1.51	7 (20%)	41,58,58	2.37	12 (29%)
3	MIY	A	392	-	35,36,36	1.31	4 (11%)	41,58,58	2.24	12 (29%)
4	SO4	D	1384	-	4,4,4	0.33	0	6,6,6	0.28	0
3	MIY	D	391	-	35,36,36	1.08	2 (5%)	41,58,58	1.79	10 (24%)
2	FAD	A	389	-	51,58,58	1.54	10 (19%)	60,89,89	1.91	11 (18%)
4	SO4	B	1384	-	4,4,4	0.36	0	6,6,6	0.22	0
4	SO4	B	1383	-	4,4,4	0.44	0	6,6,6	0.38	0
4	SO4	C	1384	-	4,4,4	0.38	0	6,6,6	0.36	0
4	SO4	C	1383	-	4,4,4	0.57	0	6,6,6	0.20	0
2	FAD	C	389	-	51,58,58	1.82	8 (15%)	60,89,89	2.62	14 (23%)
4	SO4	D	1385	-	4,4,4	0.43	0	6,6,6	0.28	0
4	SO4	B	1385	-	4,4,4	0.43	0	6,6,6	0.25	0
2	FAD	B	389	-	51,58,58	1.78	11 (21%)	60,89,89	2.47	11 (18%)
3	MIY	A	391	-	35,36,36	1.41	4 (11%)	41,58,58	1.66	10 (24%)
4	SO4	C	1385	-	4,4,4	0.31	0	6,6,6	0.21	0
4	SO4	A	1383	-	4,4,4	0.38	0	6,6,6	0.23	0
4	SO4	D	1383	-	4,4,4	0.58	0	6,6,6	0.33	0
3	MIY	C	391	-	35,36,36	1.08	0	41,58,58	1.80	10 (24%)
3	MIY	D	393	-	35,36,36	1.08	3 (8%)	41,58,58	2.45	15 (36%)
3	MIY	D	392	-	35,36,36	1.40	6 (17%)	41,58,58	2.37	15 (36%)
2	FAD	D	389	-	51,58,58	1.81	10 (19%)	60,89,89	2.57	11 (18%)
3	MIY	B	391	-	35,36,36	1.25	5 (14%)	41,58,58	1.67	10 (24%)

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
3	MIY	C	392	-	-	1/12/70/70	0/4/4/4
3	MIY	A	392	-	-	0/12/70/70	0/4/4/4
3	MIY	D	392	-	-	1/12/70/70	0/4/4/4
3	MIY	B	391	-	-	0/12/70/70	0/4/4/4
3	MIY	D	391	-	-	0/12/70/70	0/4/4/4
2	FAD	D	389	-	-	5/30/50/50	0/6/6/6
2	FAD	A	389	-	-	4/30/50/50	0/6/6/6
2	FAD	C	389	-	-	5/30/50/50	0/6/6/6
2	FAD	B	389	-	-	4/30/50/50	0/6/6/6
3	MIY	A	391	-	-	0/12/70/70	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MIY	C	391	-	-	0/12/70/70	0/4/4/4
3	MIY	D	393	-	-	1/12/70/70	0/4/4/4

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	389	FAD	C10-N1	6.31	1.41	1.33
2	C	389	FAD	C10-N1	6.05	1.41	1.33
2	C	389	FAD	C4X-N5	4.90	1.40	1.33
2	B	389	FAD	C10-N1	4.71	1.39	1.33
2	C	389	FAD	C4X-C10	4.66	1.43	1.38

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	389	FAD	C5'-C4'-C3'	-13.47	86.19	112.20
2	C	389	FAD	C5'-C4'-C3'	-13.07	86.95	112.20
2	B	389	FAD	C5'-C4'-C3'	-12.73	87.62	112.20
3	D	393	MIY	C9-C10-N7	8.73	129.57	118.91
2	D	389	FAD	N3A-C2A-N1A	-7.36	117.18	128.68

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	389	FAD	C2'-C1'-N10-C10
2	A	389	FAD	C5'-O5'-P-O2P
2	A	389	FAD	C5'-O5'-P-O3P
2	C	389	FAD	C2'-C1'-N10-C10
2	C	389	FAD	C5'-O5'-P-O2P

There are no ring outliers.

11 monomers are involved in 29 short contacts:

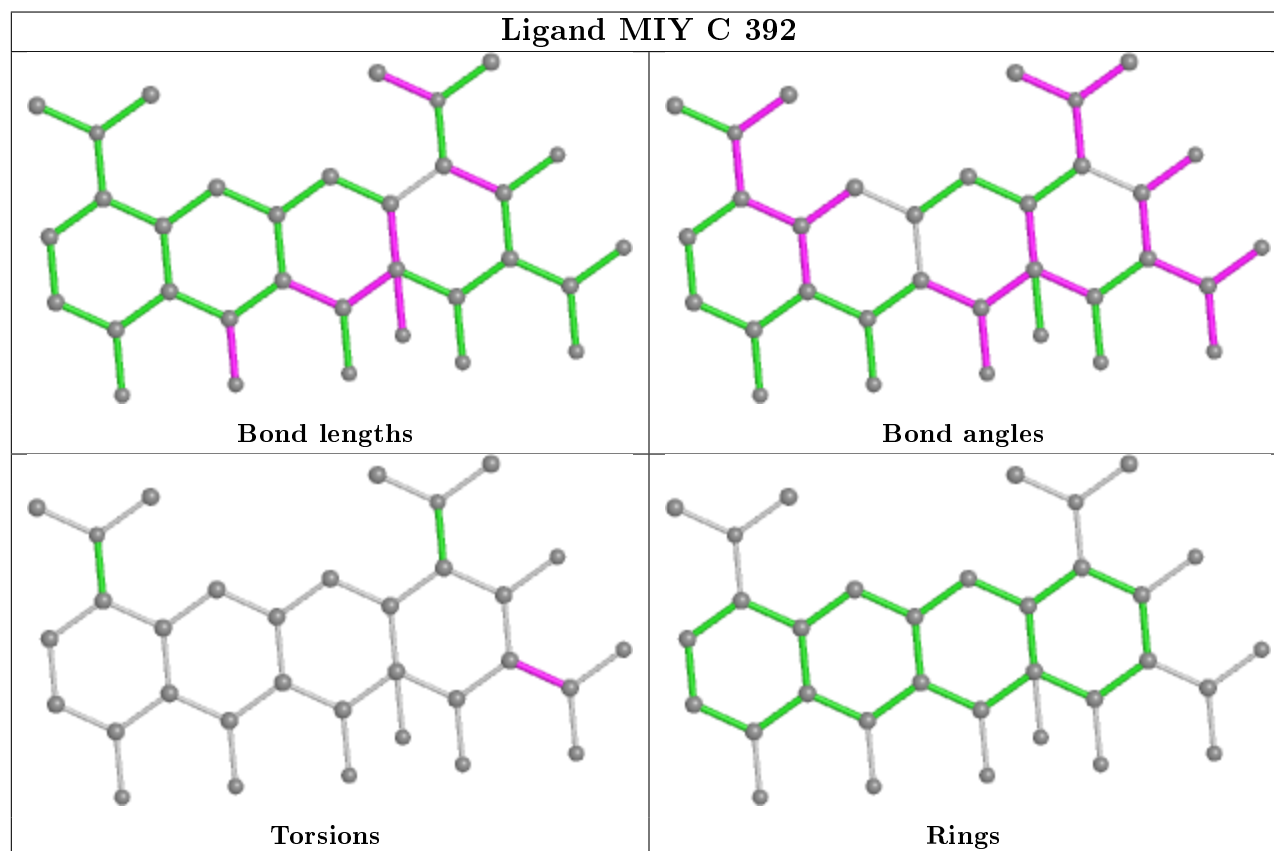
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	392	MIY	6	0
3	A	392	MIY	1	0
2	A	389	FAD	4	0
2	C	389	FAD	2	0
2	B	389	FAD	3	0
3	A	391	MIY	2	0

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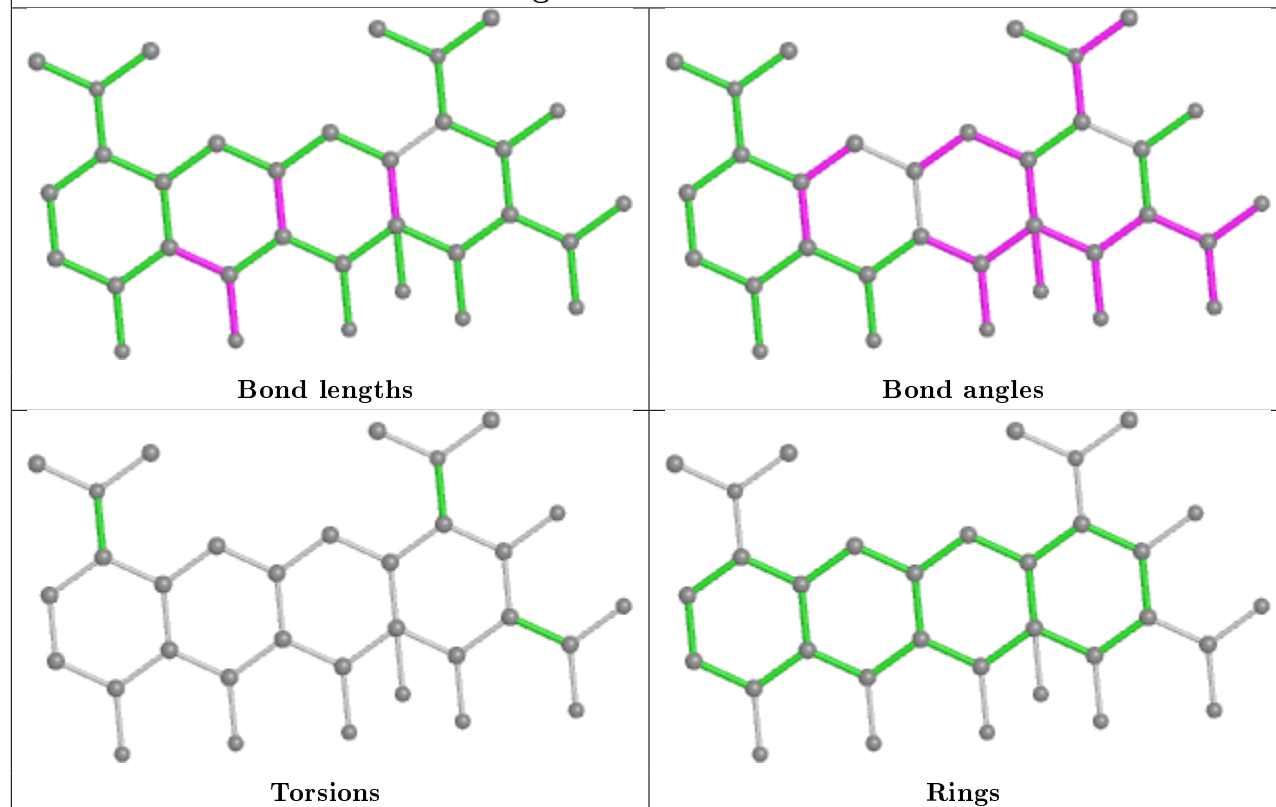
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	391	MIY	1	0
3	D	393	MIY	5	0
3	D	392	MIY	2	0
2	D	389	FAD	3	0
3	B	391	MIY	2	0

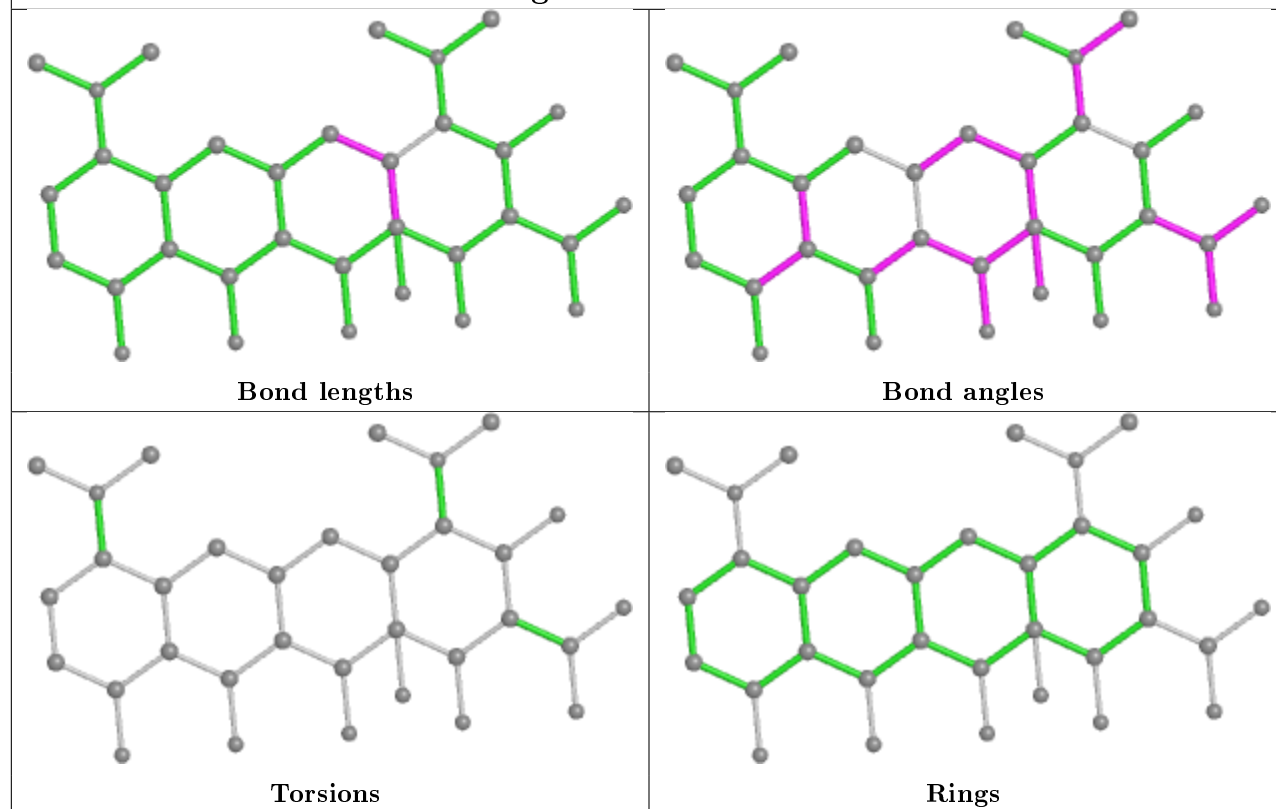
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

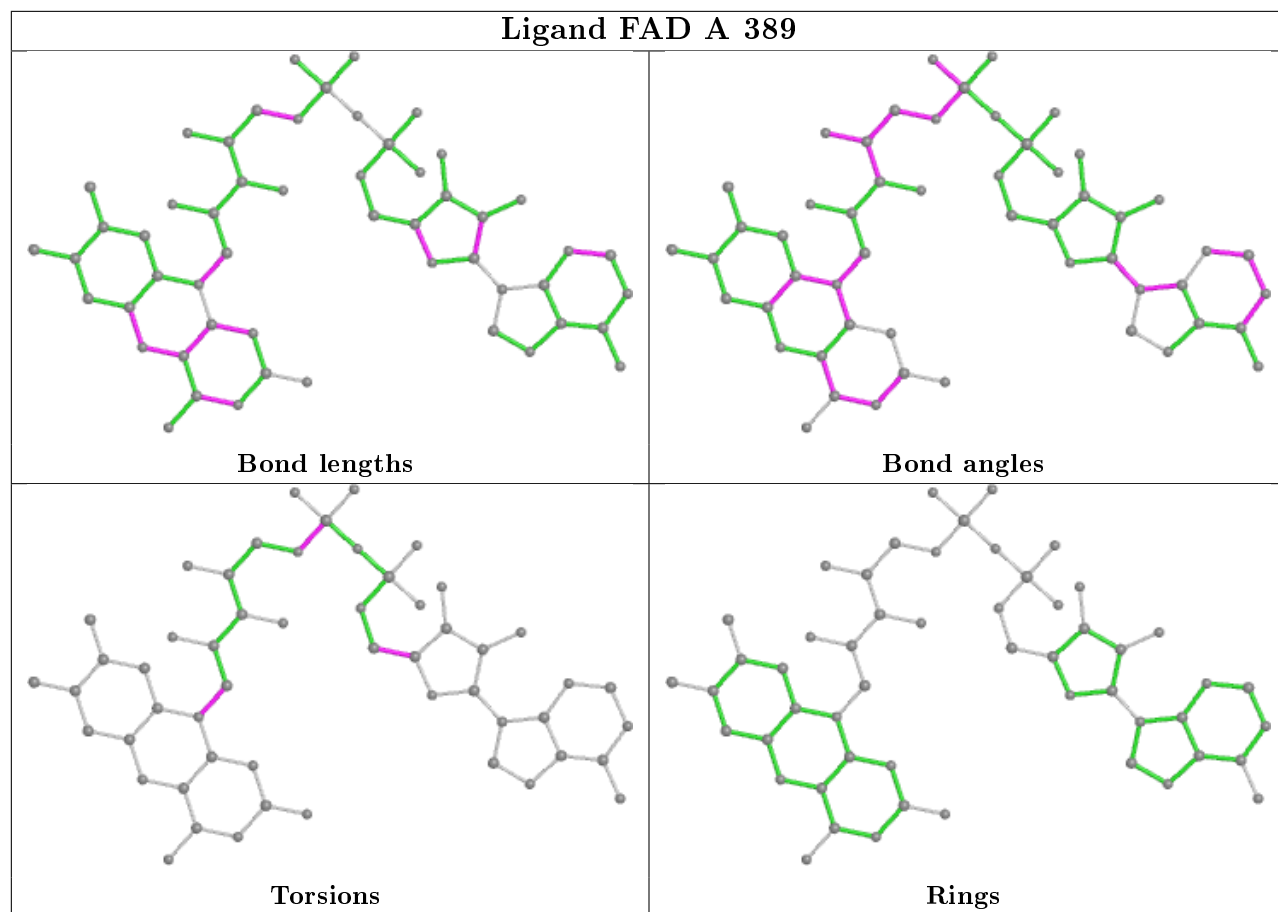


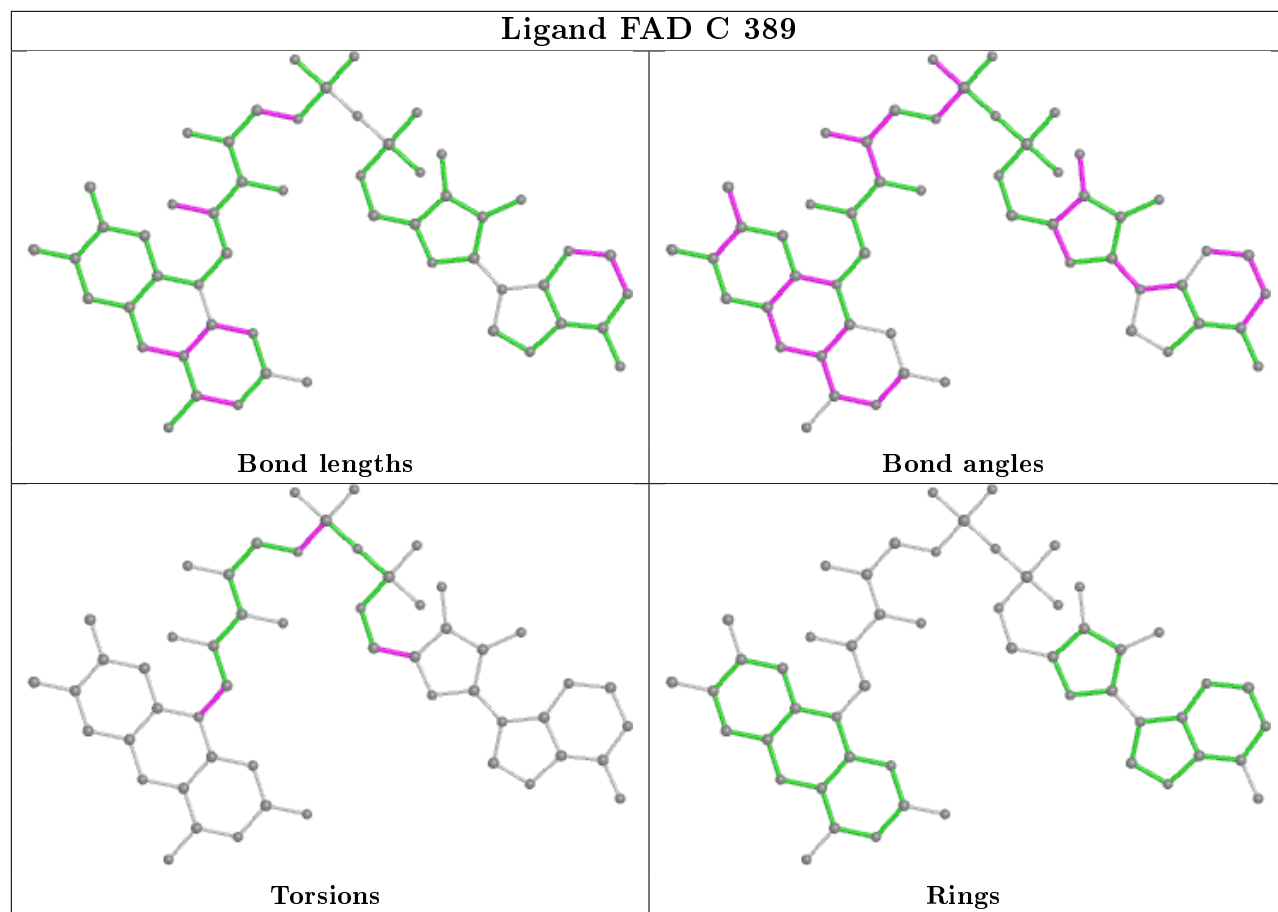
Ligand MIY A 392



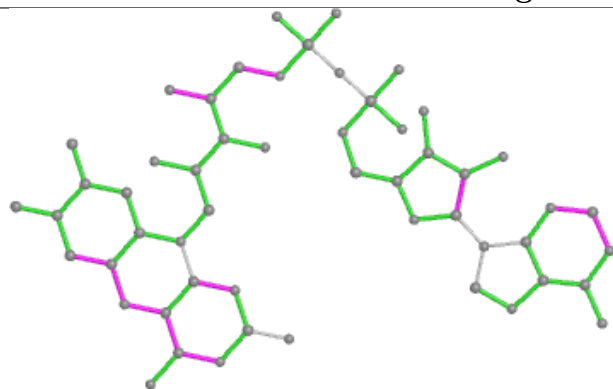
Ligand MIY D 391



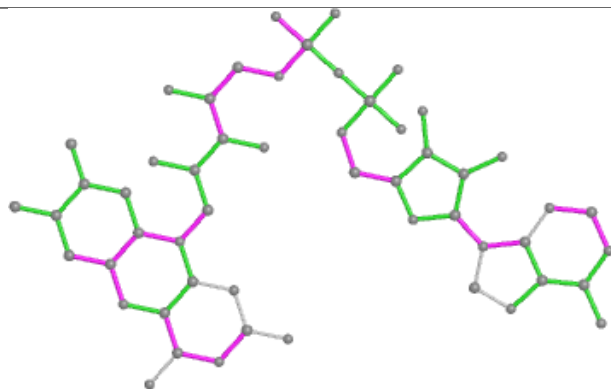




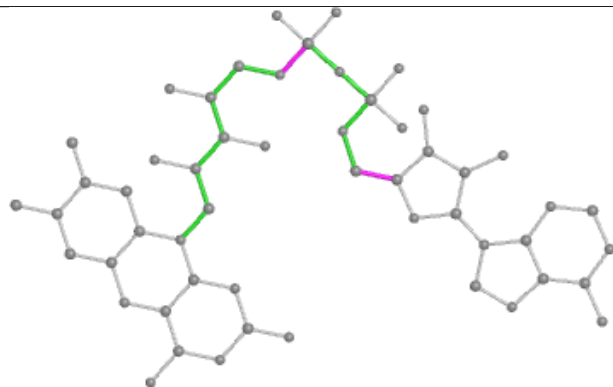
Ligand FAD B 389



Bond lengths



Bond angles

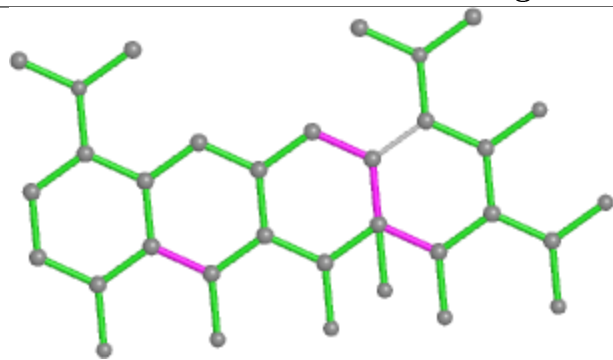


Torsions

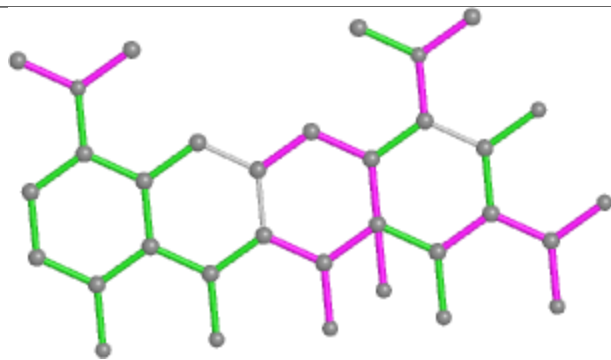


Rings

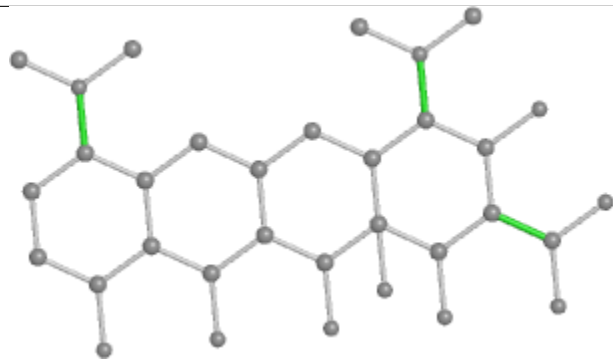
Ligand MIY A 391



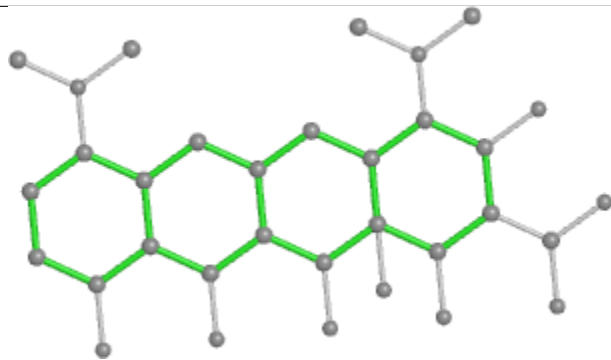
Bond lengths



Bond angles

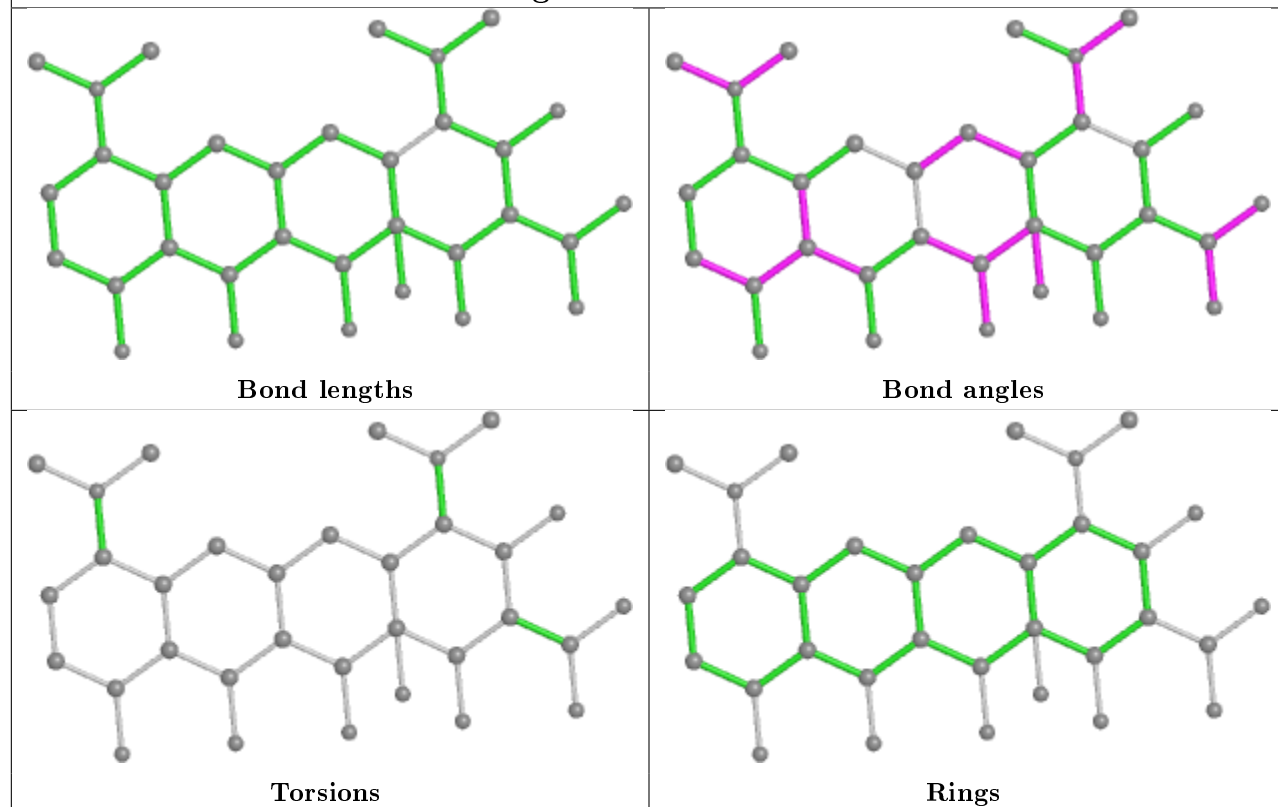


Torsions

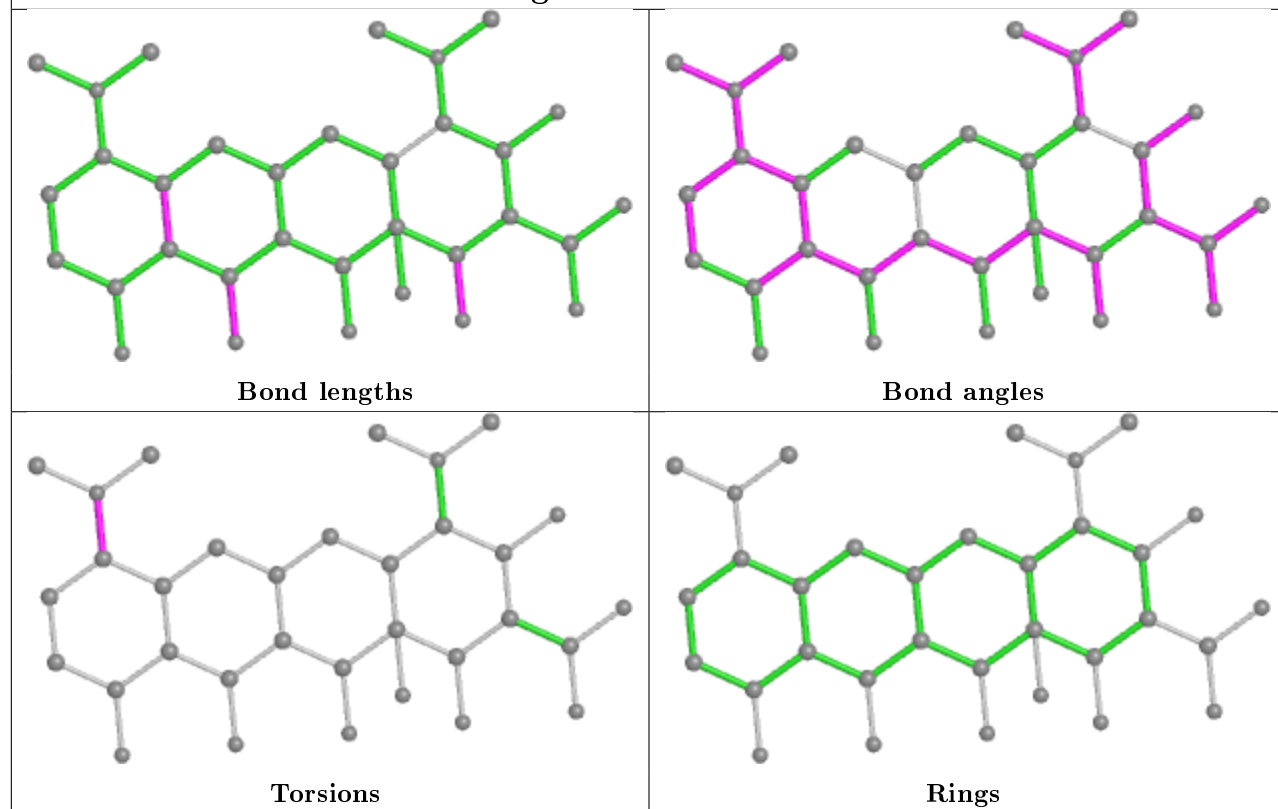


Rings

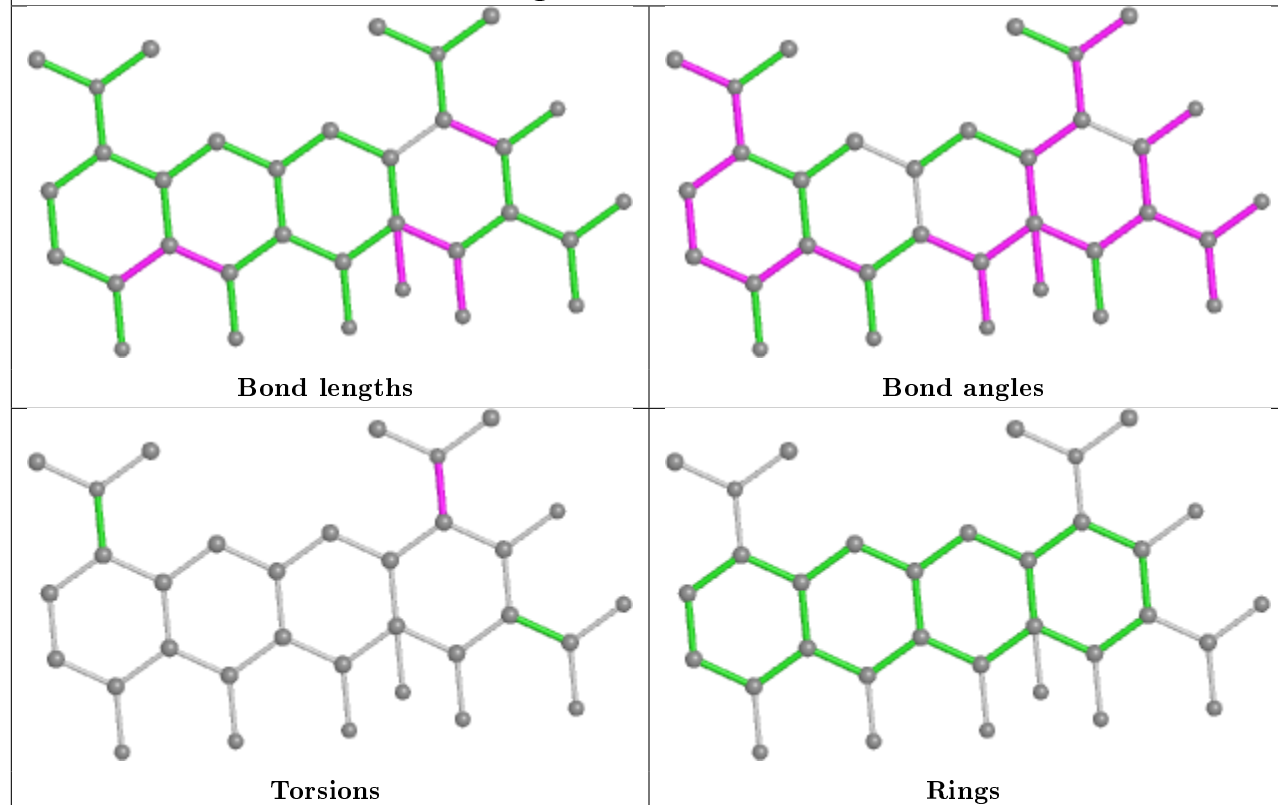
Ligand MIY C 391



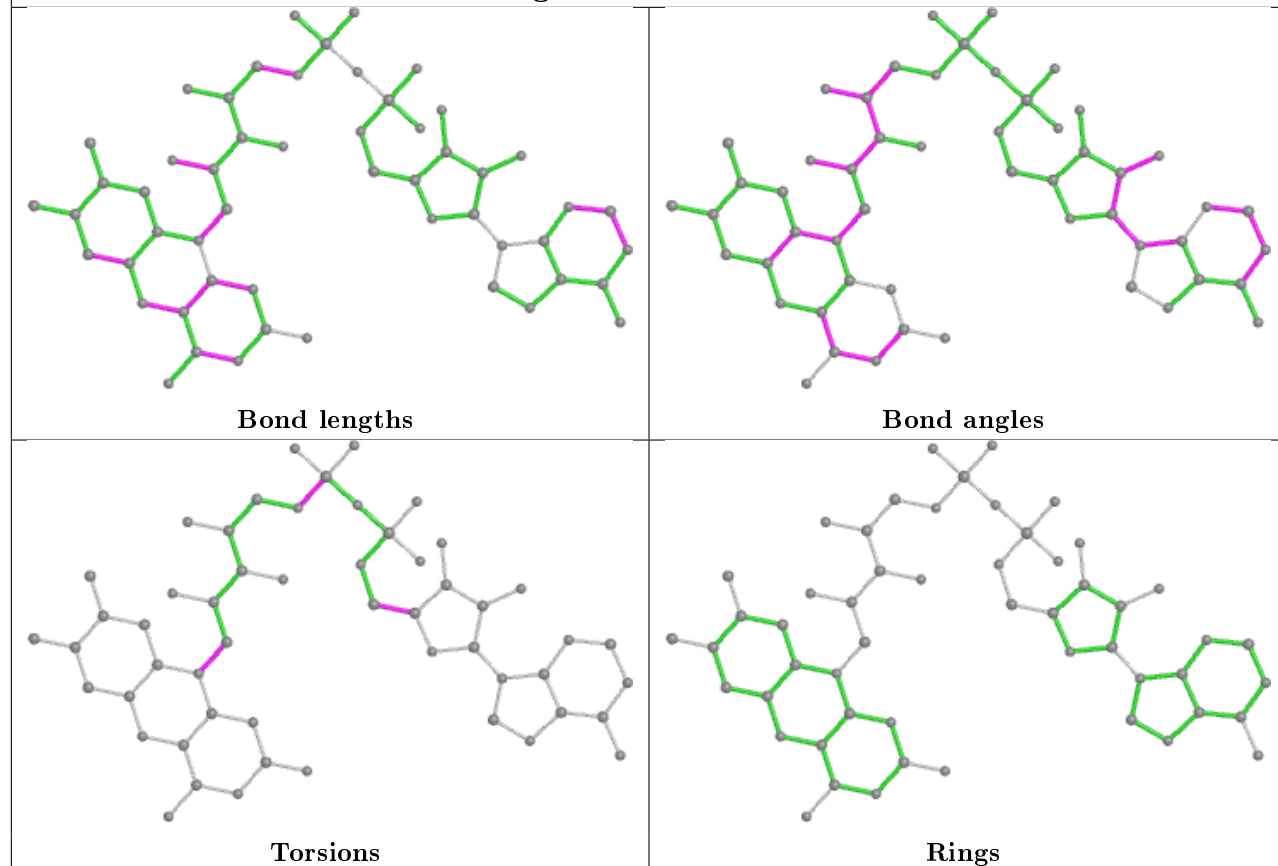
Ligand MIY D 393

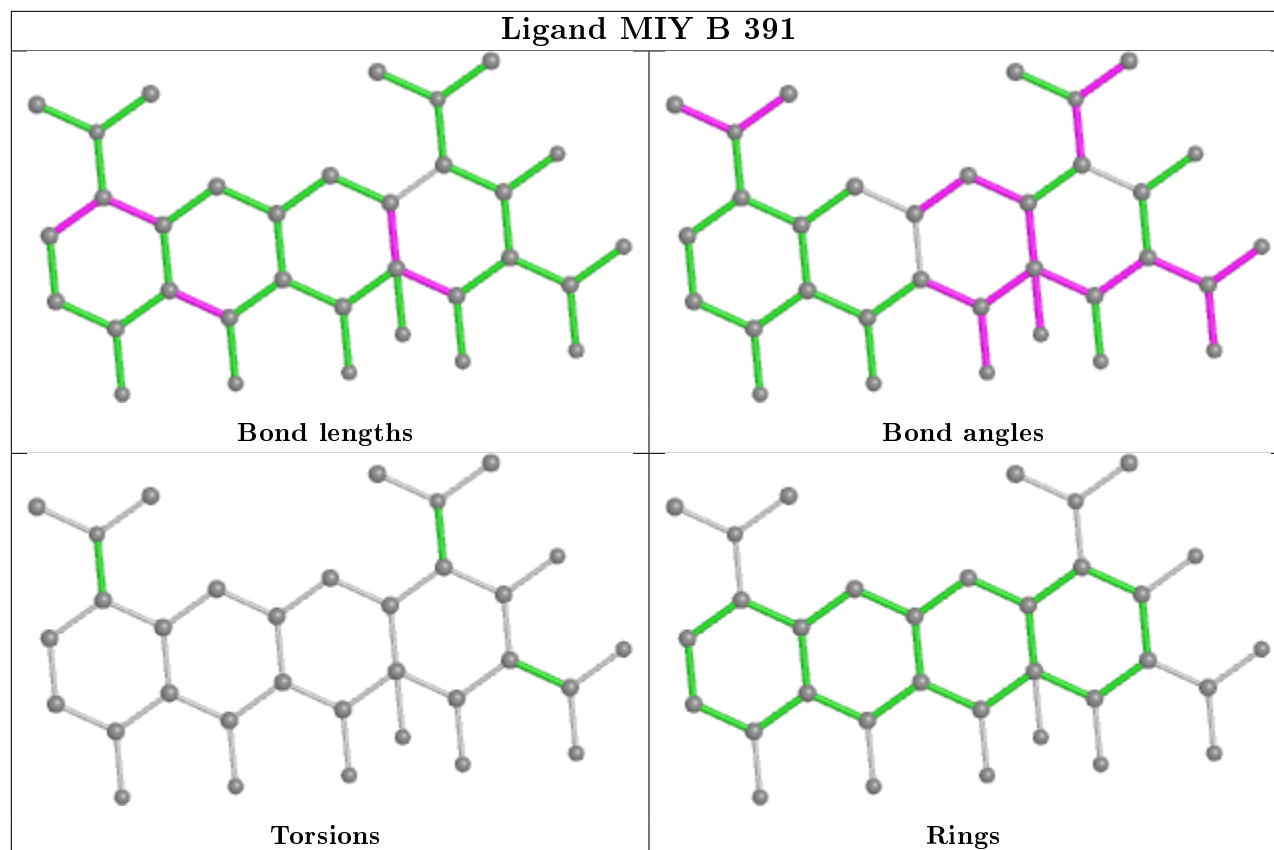


Ligand MIY D 392



Ligand FAD D 389





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	368/398 (92%)	0.22	11 (2%) 50 51	33, 47, 77, 124	0
1	B	368/398 (92%)	0.41	18 (4%) 29 31	32, 48, 80, 124	0
1	C	367/398 (92%)	0.44	29 (7%) 12 13	36, 53, 85, 119	0
1	D	367/398 (92%)	0.40	24 (6%) 18 19	33, 52, 84, 118	0
All	All	1470/1592 (92%)	0.37	82 (5%) 24 26	32, 50, 83, 124	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	THR	6.9
1	D	341	GLY	6.7
1	D	251	VAL	5.9
1	C	251	VAL	5.0
1	B	378	PRO	4.9

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 carbohydrates in this entry.

6.4 Ligands [i](#)

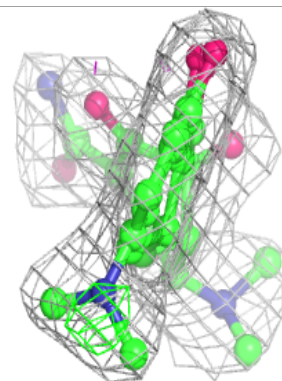
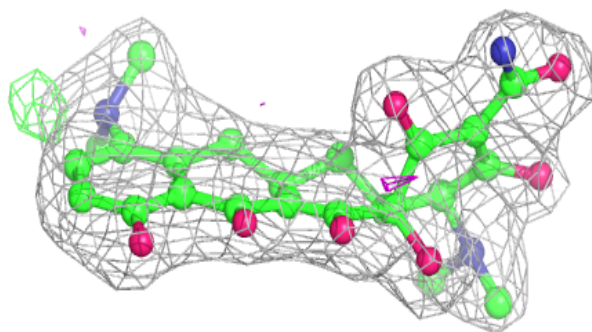
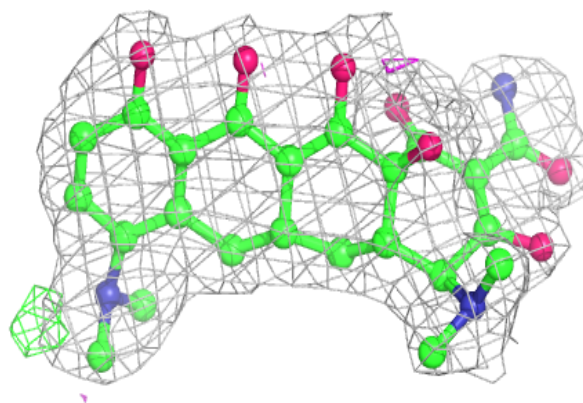
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	B	1385	5/5	0.67	0.33	74,87,92,95	5
4	SO4	D	1385	5/5	0.81	0.21	81,86,93,98	5
4	SO4	C	1383	5/5	0.85	0.18	81,85,105,109	0
4	SO4	C	1385	5/5	0.89	0.11	101,102,111,113	0
4	SO4	D	1383	5/5	0.91	0.18	72,93,95,102	0
3	MIY	D	393	33/33	0.92	0.12	42,50,54,60	0
3	MIY	B	391	33/33	0.92	0.13	32,47,62,71	0
3	MIY	C	392	33/33	0.93	0.11	42,52,55,62	0
3	MIY	C	391	33/33	0.93	0.11	41,50,58,63	0
3	MIY	A	391	33/33	0.94	0.11	32,43,57,59	0
3	MIY	D	391	33/33	0.94	0.11	38,55,64,71	0
3	MIY	D	392	33/33	0.94	0.12	38,45,54,69	0
3	MIY	A	392	33/33	0.94	0.11	42,50,55,56	0
4	SO4	B	1383	5/5	0.95	0.10	92,94,101,104	0
2	FAD	B	389	53/53	0.96	0.14	31,40,55,59	0
2	FAD	C	389	53/53	0.96	0.12	33,42,60,68	0
4	SO4	D	1384	5/5	0.96	0.25	65,70,80,83	0
4	SO4	B	1384	5/5	0.96	0.26	80,81,83,96	0
4	SO4	A	1383	5/5	0.97	0.21	86,88,91,92	0
4	SO4	C	1384	5/5	0.97	0.21	79,80,84,87	0
2	FAD	D	389	53/53	0.97	0.13	33,42,56,62	0
2	FAD	A	389	53/53	0.97	0.12	29,38,52,67	0

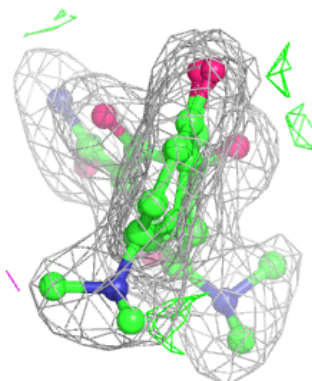
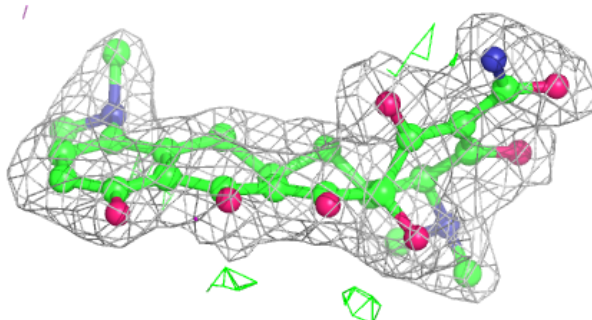
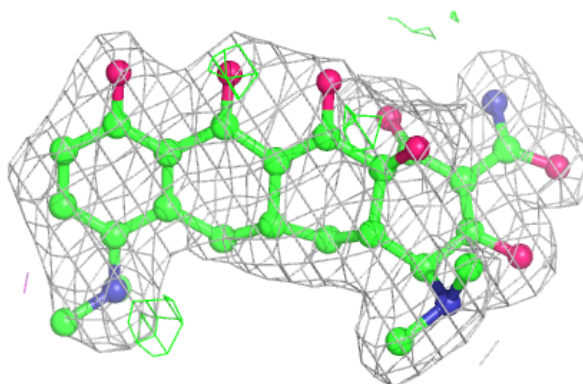
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MIY D 393:

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

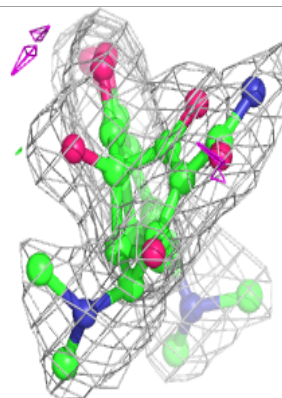
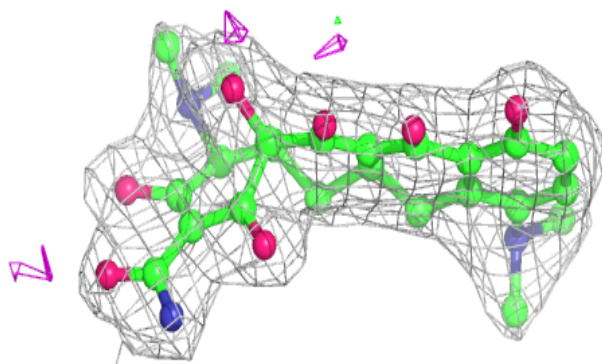
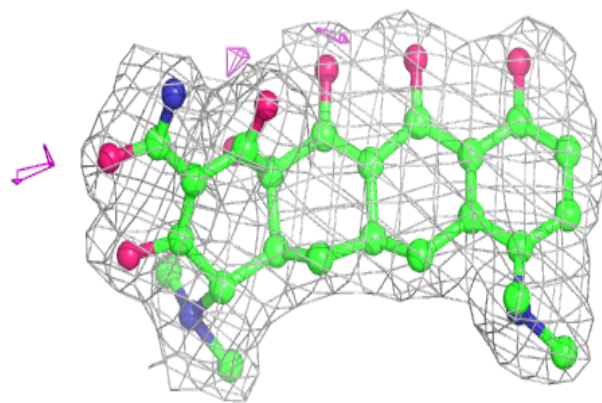
**Electron density around MIY B 391:**

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

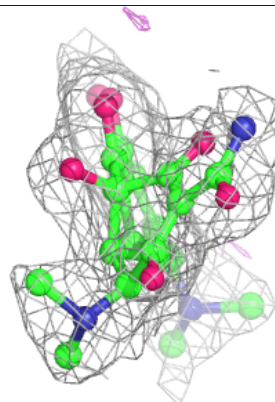
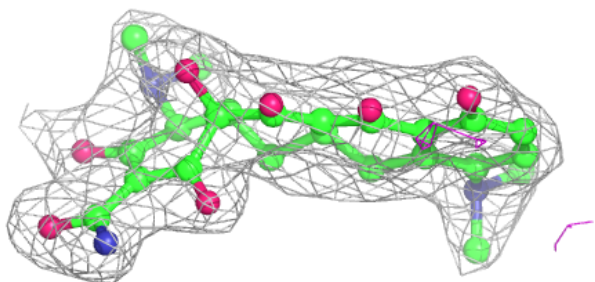
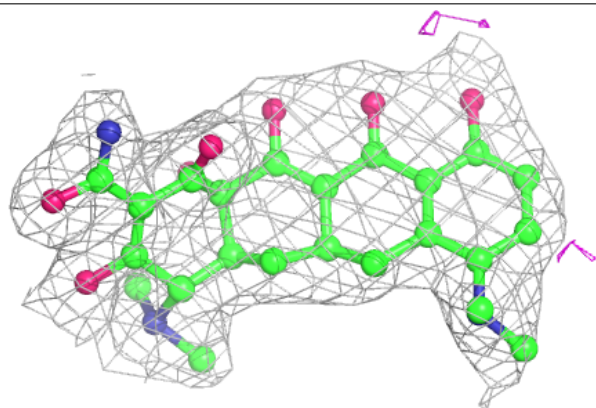


Electron density around MIY C 392:

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

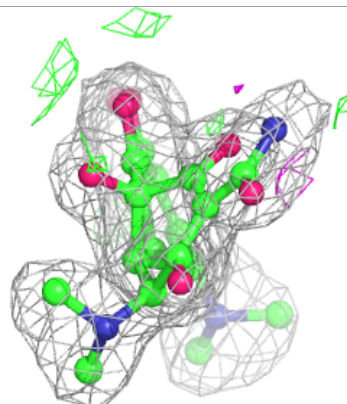
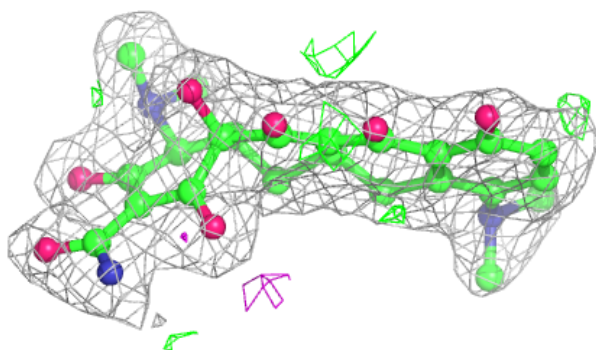
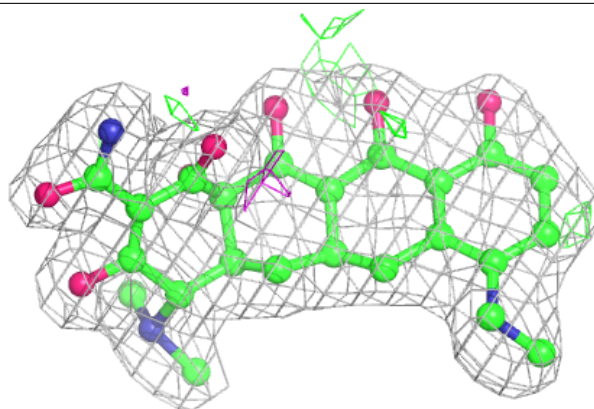
**Electron density around MIY C 391:**

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

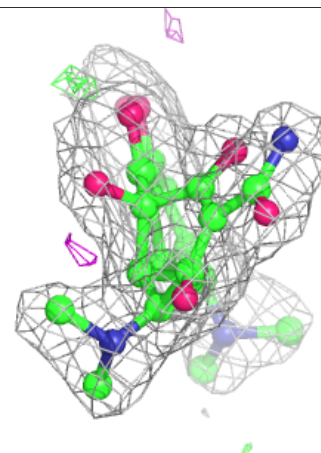
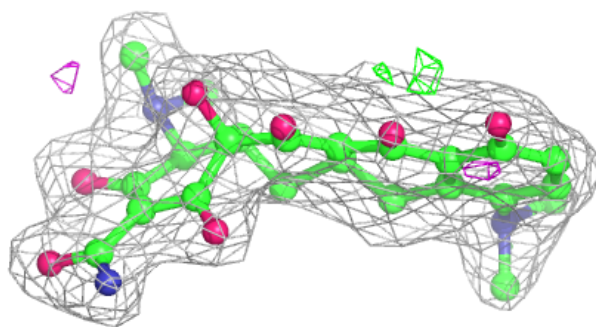
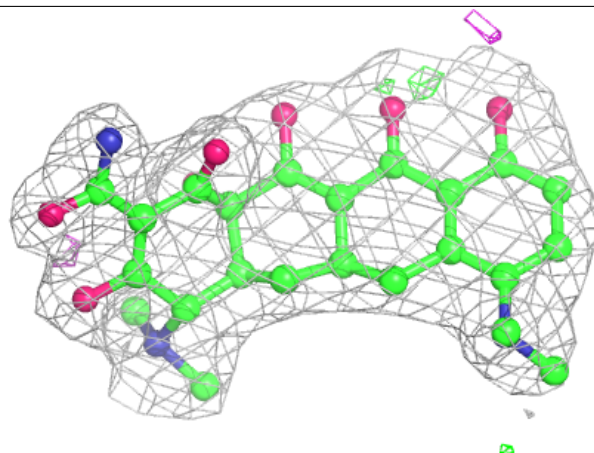


Electron density around MIY A 391:

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and green (positive)

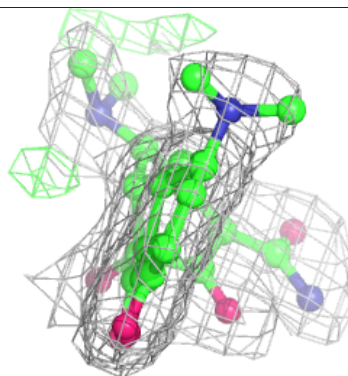
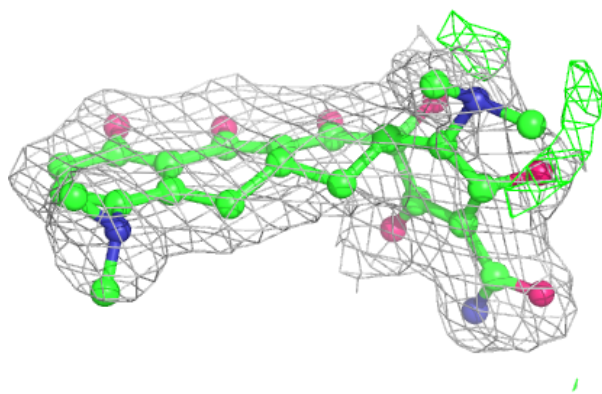
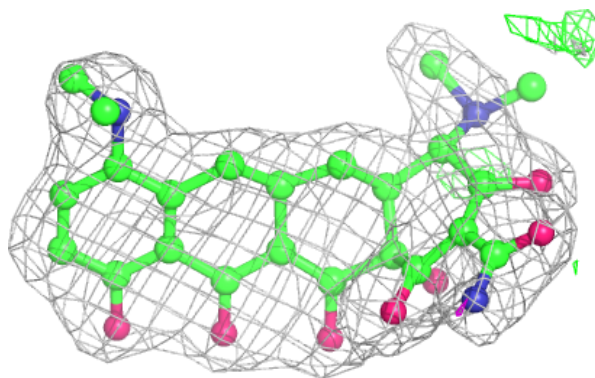
**Electron density around MIY D 391:**

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and green (positive)



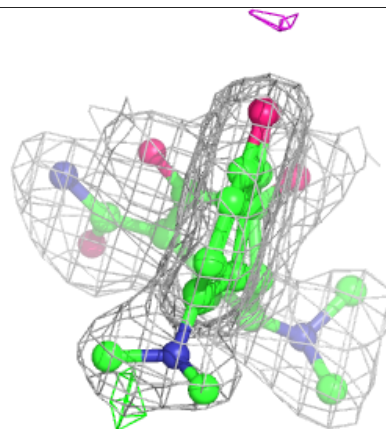
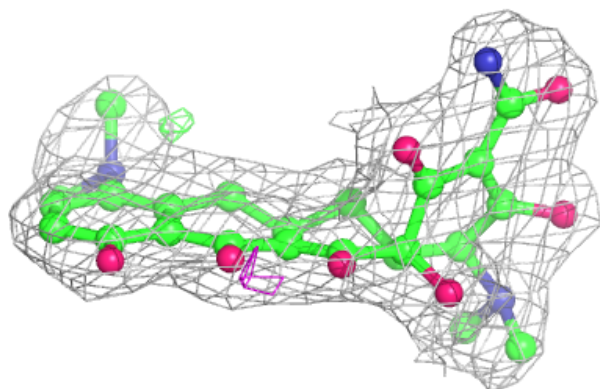
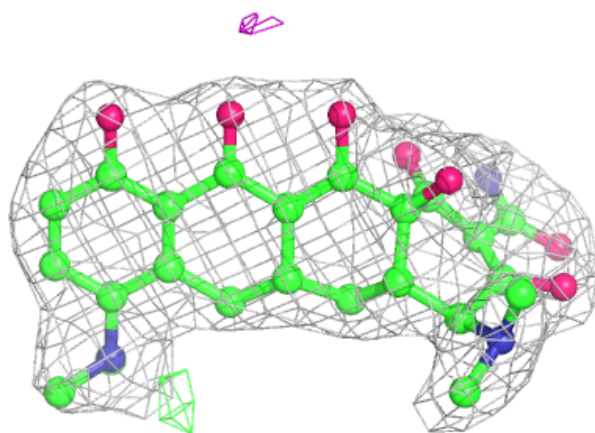
Electron density around MIY D 392:

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and green (positive)

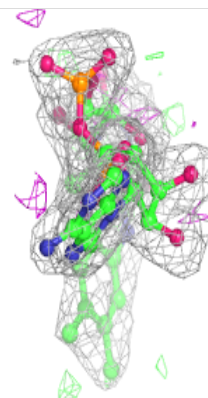
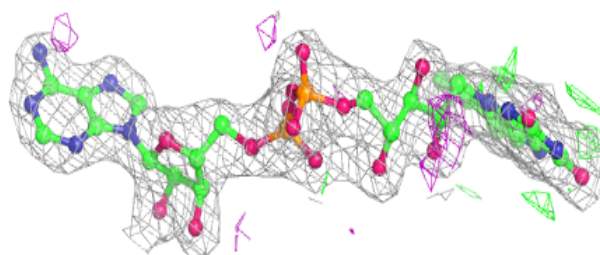
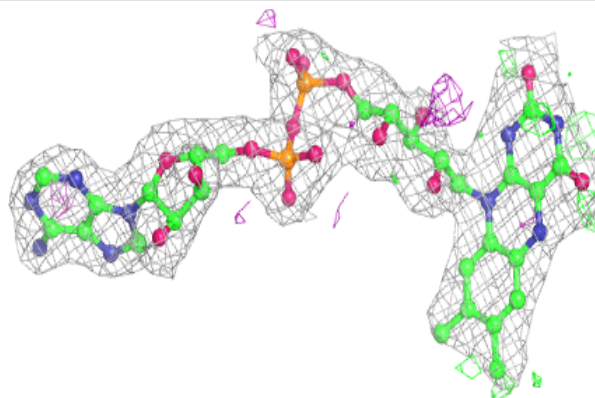


Electron density around MIY A 392:

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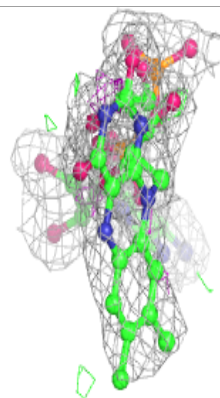
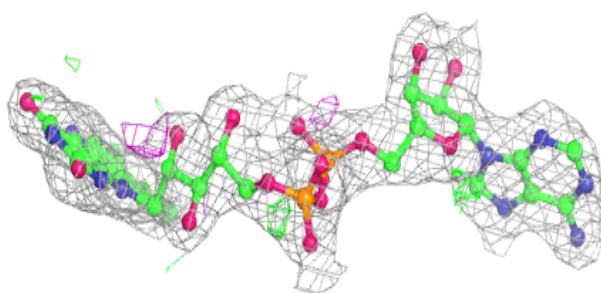
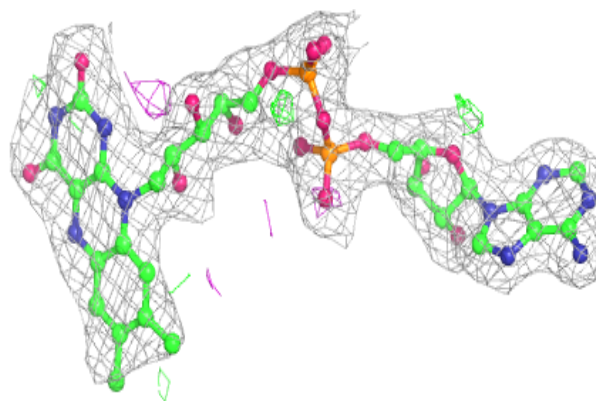
**Electron density around FAD B 389:**

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and green (positive)

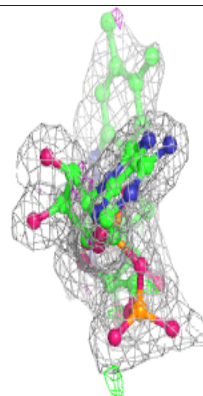
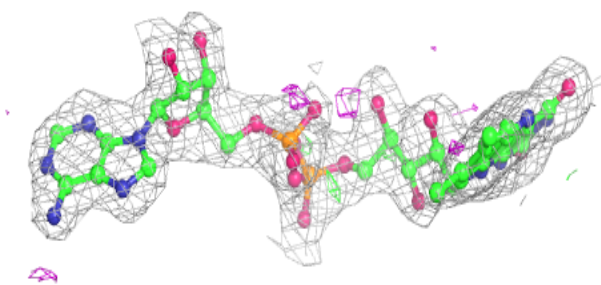
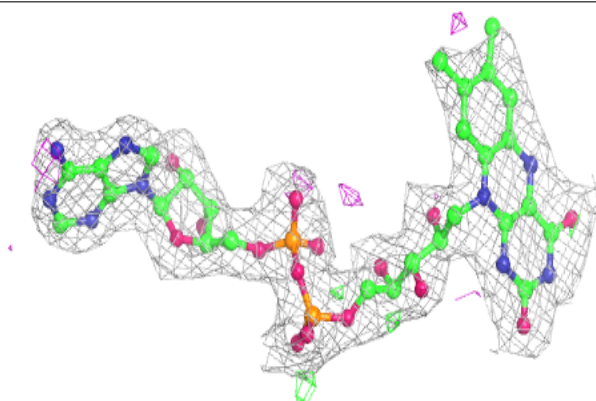


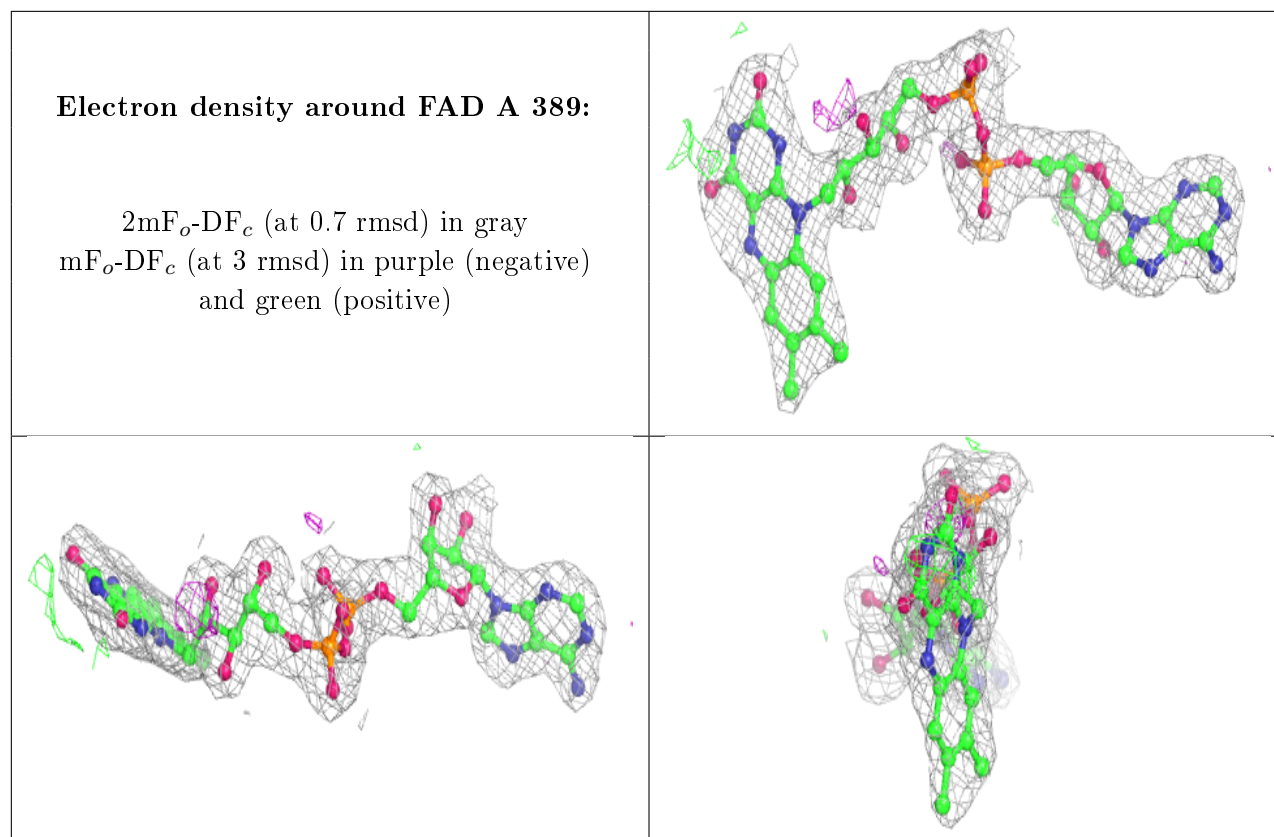
Electron density around FAD C 389:

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

**Electron density around FAD D 389:**

$2mF_o-DF_c$ (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.