



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 03:47 am BST

PDB ID : 2VYX  
Title : Crystal structure of the T. thermophilus dodecin W38F mutant  
Authors : Essen, L.-O.; Meissner, B.  
Deposited on : 2008-07-29  
Resolution : 1.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

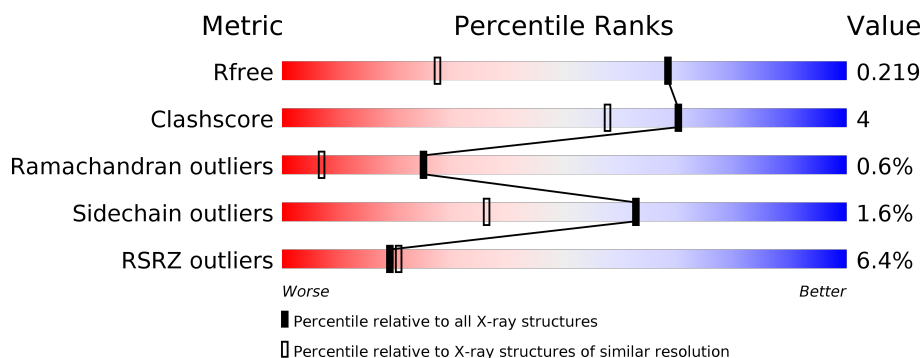
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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

Mol	Chain	Length	Quality of chain
1	A	69	<div> <div>7%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	B	69	<div> <div>6%</div> <div>84%</div> <div>10%</div> <div>..</div> </div>
1	C	69	<div> <div>4%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	D	69	<div> <div>6%</div> <div>94%</div> <div>..</div> </div>
1	E	69	<div> <div>7%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	F	69	<div> <div>4%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	69	
1	H	69	
1	I	69	
1	J	69	
1	K	69	
1	L	69	

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
3	COA	A	1071	X	-	-	-
3	COA	K	1070	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7888 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 TTHA1431.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	68	Total	C	N	O	0	0	1
			528	336	93	99			
1	B	66	Total	C	N	O	0	0	0
			518	331	91	96			
1	C	68	Total	C	N	O	0	0	0
			535	340	93	102			
1	D	68	Total	C	N	O	0	2	1
			540	344	93	103			
1	E	68	Total	C	N	O	0	2	1
			543	346	95	102			
1	F	68	Total	C	N	O	0	2	1
			534	339	95	100			
1	G	68	Total	C	N	O	0	3	1
			550	351	96	103			
1	H	68	Total	C	N	O	0	0	1
			528	336	93	99			
1	I	68	Total	C	N	O	0	1	1
			534	340	93	101			
1	J	68	Total	C	N	O	0	0	1
			528	336	93	99			
1	K	68	Total	C	N	O	0	2	0
			547	349	94	104			
1	L	66	Total	C	N	O	0	0	0
			518	331	91	96			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	PHE	TRP	engineered mutation	UNP Q5SIE3
B	38	PHE	TRP	engineered mutation	UNP Q5SIE3
C	38	PHE	TRP	engineered mutation	UNP Q5SIE3
D	38	PHE	TRP	engineered mutation	UNP Q5SIE3
E	38	PHE	TRP	engineered mutation	UNP Q5SIE3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	38	PHE	TRP	engineered mutation	UNP Q5SIE3
G	38	PHE	TRP	engineered mutation	UNP Q5SIE3
H	38	PHE	TRP	engineered mutation	UNP Q5SIE3
I	38	PHE	TRP	engineered mutation	UNP Q5SIE3
J	38	PHE	TRP	engineered mutation	UNP Q5SIE3
K	38	PHE	TRP	engineered mutation	UNP Q5SIE3
L	38	PHE	TRP	engineered mutation	UNP Q5SIE3

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- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system (rings 1, 2, and 4) with atoms N1, N3, N5, N9, and N10. The ring is substituted with a ribitol chain at position 10 (C10) and a phosphate group at position 2 (C2). The ribitol chain consists of a ribose ring (C3', C4', C5') and a terminal phosphate group (O1P, O2P, O3P). The ribose ring is substituted with a hydroxyl group (OH) at C3' and a phosphate group (O4P, O5P) at C4'. The ribitol chain is further substituted with a phosphate group (O1P, O2P, O3P) at the terminal position (C5'). The ribitol chain is further substituted with a phosphate group (O1P, O2P, O3P) at the terminal position (C5').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	B	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	B	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	C	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	C	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	D	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	D	1	Total 31	C 17	N 4	O 9	P 1	0	0

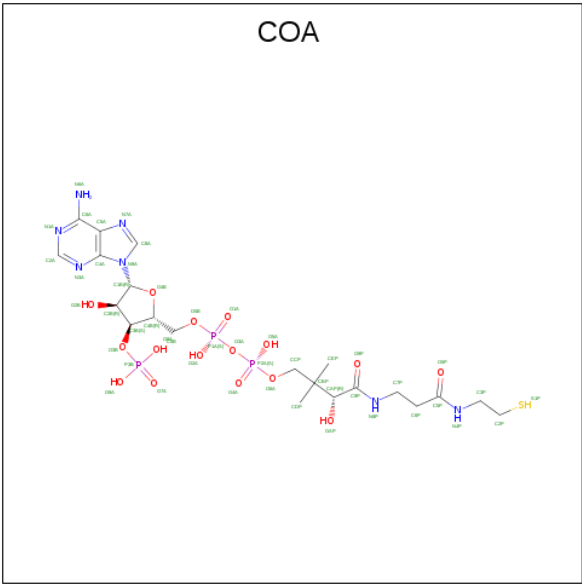


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**PDB**  
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	16	3		
3	A	1	Total	C	N	O	P	0	0
			48	21	7	16	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	16	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	16	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	16	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	16	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	16	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	I	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	J	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	K	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	42	Total	O	0	0
			42	42		
6	B	52	Total	O	0	0
			52	52		
6	C	52	Total	O	0	0
			52	52		
6	D	56	Total	O	0	0
			56	56		
6	E	43	Total	O	0	0
			43	43		

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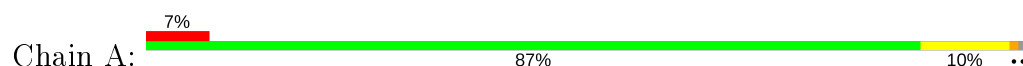
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	52	Total 52	O 52	0	0
6	G	50	Total 50	O 50	0	0
6	H	37	Total 37	O 37	0	0
6	I	43	Total 43	O 43	0	0
6	J	43	Total 43	O 43	0	0
6	K	34	Total 34	O 34	0	0
6	L	28	Total 28	O 28	0	0



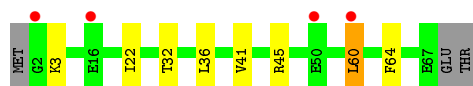
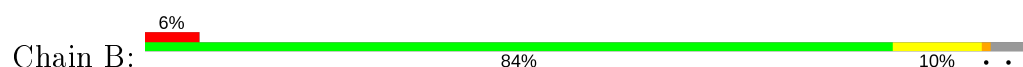
### 3 Residue-property plots [i](#)

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: TTHA1431



- Molecule 1: TTHA1431



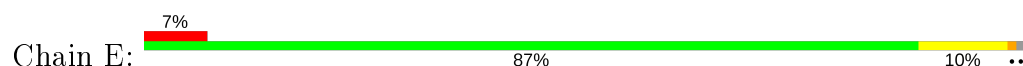
- Molecule 1: TTHA1431



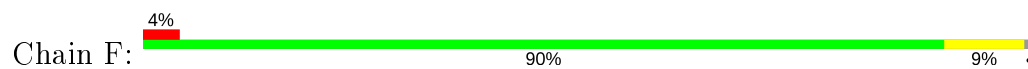
- Molecule 1: TTHA1431



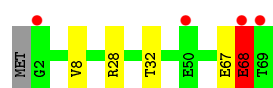
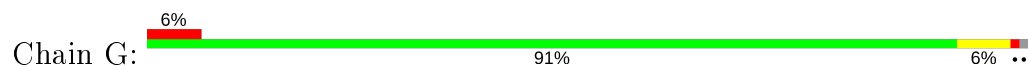
- Molecule 1: TTHA1431



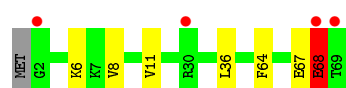
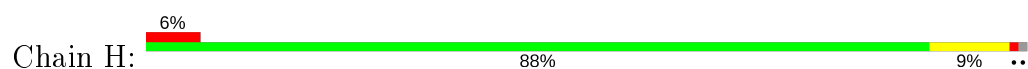
- Molecule 1: TTHA1431



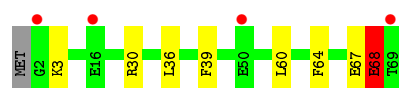
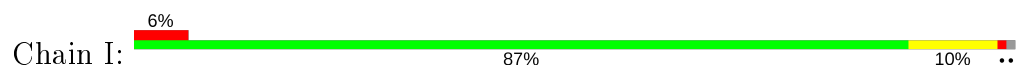
• Molecule 1: TTHA1431



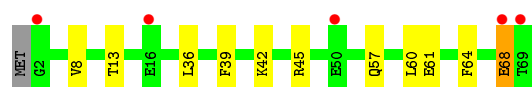
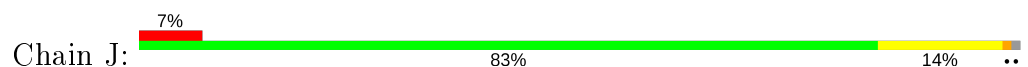
• Molecule 1: TTHA1431



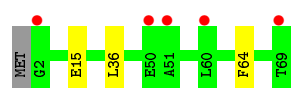
• Molecule 1: TTHA1431



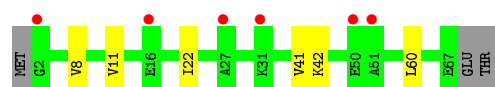
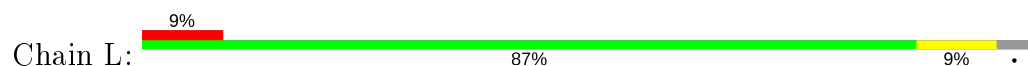
• Molecule 1: TTHA1431



• Molecule 1: TTHA1431



• Molecule 1: TTHA1431



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.63Å 98.55Å 139.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.99 – 1.50 9.97 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (9.99-1.50) 97.6 (9.97-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.05 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.218 , 0.250 0.226 , 0.219	Depositor DCC
$R_{free}$ test set	7305 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.49 , 68.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, FMN, CL, NA

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	0.45	0/533	0.65	0/713
1	B	0.52	0/523	0.75	1/699 (0.1%)
1	C	0.48	0/540	0.69	0/721
1	D	0.52	0/551	0.70	0/737
1	E	0.50	0/551	0.65	0/736
1	F	0.64	0/538	0.76	0/719
1	G	0.56	0/558	0.74	1/746 (0.1%)
1	H	0.50	0/533	0.65	0/713
1	I	0.51	0/542	0.72	0/725
1	J	0.50	0/533	0.69	0/713
1	K	0.45	0/558	0.62	0/744
1	L	0.43	0/523	0.59	0/699
All	All	0.51	0/6483	0.69	2/8665 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	LEU	CA-CB-CG	5.86	128.77	115.30
1	G	28	ARG	NE-CZ-NH1	5.56	123.08	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	528	0	544	7	0
1	B	518	0	538	6	0
1	C	535	0	551	3	0
1	D	540	0	556	3	0
1	E	543	0	562	4	0
1	F	534	0	546	5	0
1	G	550	0	570	3	0
1	H	528	0	544	5	0
1	I	534	0	550	4	0
1	J	528	0	544	6	0
1	K	547	0	570	2	0
1	L	518	0	538	4	0
2	A	62	0	38	1	0
2	B	62	0	38	2	0
2	C	62	0	38	1	0
2	D	62	0	38	2	0
2	F	62	0	38	1	0
2	H	62	0	38	1	0
3	A	96	0	64	2	0
3	B	48	0	32	4	0
3	C	48	0	32	0	0
3	D	48	0	32	0	0
3	E	48	0	32	1	0
3	F	48	0	32	0	0
3	G	48	0	32	3	0
3	I	48	0	32	0	0
3	J	48	0	32	1	0
3	K	48	0	32	1	0
3	L	48	0	32	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	42	0	0	0	0
6	B	52	0	0	1	0
6	C	52	0	0	0	0
6	D	56	0	0	0	0
6	E	43	0	0	0	0
6	F	52	0	0	0	0
6	G	50	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	37	0	0	0	0
6	I	43	0	0	0	0
6	J	43	0	0	0	0
6	K	34	0	0	1	0
6	L	28	0	0	0	0
All	All	7888	0	7225	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 53 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)
3:A:1071:COA:O9P	3:A:1071:COA:H141	1.90	0.69
1:K:15:GLU:OE1	6:K:2003:HOH:O	2.13	0.66
1:F:6:LYS:HE3	1:G:8[A]:VAL:HG13	1.80	0.64
1:C:36:LEU:HD23	1:C:64:PHE:HB3	1.81	0.62
1:J:42:LYS:HE3	1:J:61:GLU:HG3	1.85	0.58

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	66/69 (96%)	65 (98%)	1 (2%)	0	100	100
1	B	64/69 (93%)	64 (100%)	0	0	100	100
1	C	66/69 (96%)	66 (100%)	0	0	100	100
1	D	68/69 (99%)	67 (98%)	1 (2%)	0	100	100
1	E	68/69 (99%)	67 (98%)	0	1 (2%)	10	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	67/69 (97%)	67 (100%)	0	0	100	100
1	G	69/69 (100%)	68 (99%)	0	1 (1%)	11	1
1	H	66/69 (96%)	65 (98%)	0	1 (2%)	10	1
1	I	67/69 (97%)	65 (97%)	1 (2%)	1 (2%)	10	1
1	J	66/69 (96%)	62 (94%)	3 (4%)	1 (2%)	10	1
1	K	68/69 (99%)	67 (98%)	1 (2%)	0	100	100
1	L	64/69 (93%)	62 (97%)	2 (3%)	0	100	100
All	All	799/828 (96%)	785 (98%)	9 (1%)	5 (1%)	25	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	68	GLU
1	H	68	GLU
1	I	68	GLU
1	J	68	GLU
1	G	68	GLU

### 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	53/55 (96%)	52 (98%)	1 (2%)	57	27
1	B	52/55 (94%)	51 (98%)	1 (2%)	57	27
1	C	54/55 (98%)	54 (100%)	0	100	100
1	D	55/55 (100%)	55 (100%)	0	100	100
1	E	55/55 (100%)	53 (96%)	2 (4%)	35	8
1	F	53/55 (96%)	53 (100%)	0	100	100
1	G	56/55 (102%)	55 (98%)	1 (2%)	59	30
1	H	53/55 (96%)	52 (98%)	1 (2%)	57	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	54/55 (98%)	52 (96%)	2 (4%)	34	8
1	J	53/55 (96%)	52 (98%)	1 (2%)	57	27
1	K	56/55 (102%)	56 (100%)	0	100	100
1	L	52/55 (94%)	51 (98%)	1 (2%)	57	27
All	All	646/660 (98%)	636 (98%)	10 (2%)	62	39

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	68	GLU
1	H	68	GLU
1	I	68	GLU
1	E	68	GLU
1	I	3	LYS

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 5 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FMN	D	1072	-	31,33,33	1.47	4 (12%)	40,50,50	1.55	6 (15%)
2	FMN	H	1071	-	31,33,33	1.38	4 (12%)	40,50,50	1.78	7 (17%)
3	COA	C	1071	-	41,50,50	1.61	3 (7%)	52,75,75	1.23	2 (3%)
2	FMN	B	1070	-	31,33,33	1.38	4 (12%)	40,50,50	1.73	6 (15%)
3	COA	K	1070	-	41,50,50	1.66	3 (7%)	52,75,75	1.28	3 (5%)
3	COA	A	1073	-	41,50,50	1.68	3 (7%)	52,75,75	1.14	3 (5%)
2	FMN	F	1072	-	31,33,33	1.42	5 (16%)	40,50,50	1.52	5 (12%)
3	COA	B	1069	-	41,50,50	1.58	4 (9%)	52,75,75	1.17	4 (7%)
3	COA	E	1070	-	41,50,50	1.63	3 (7%)	52,75,75	1.11	3 (5%)
2	FMN	F	1070	-	31,33,33	1.35	3 (9%)	40,50,50	1.79	6 (15%)
3	COA	F	1071	-	41,50,50	1.62	3 (7%)	52,75,75	1.31	3 (5%)
2	FMN	H	1070	-	31,33,33	1.35	4 (12%)	40,50,50	1.78	7 (17%)
2	FMN	C	1072	-	31,33,33	1.41	5 (16%)	40,50,50	1.60	6 (15%)
3	COA	A	1071	-	41,50,50	1.72	3 (7%)	52,75,75	1.25	3 (5%)
3	COA	L	1068	-	41,50,50	1.63	3 (7%)	52,75,75	1.19	2 (3%)
3	COA	G	1070	-	41,50,50	1.65	3 (7%)	52,75,75	1.36	6 (11%)
2	FMN	A	1070	-	31,33,33	1.52	5 (16%)	40,50,50	1.61	4 (10%)
2	FMN	C	1070	-	31,33,33	1.44	4 (12%)	40,50,50	1.73	6 (15%)
2	FMN	A	1072	-	31,33,33	1.53	4 (12%)	40,50,50	1.72	8 (20%)
2	FMN	B	1068	-	31,33,33	1.43	4 (12%)	40,50,50	1.48	4 (10%)
2	FMN	D	1070	-	31,33,33	1.46	5 (16%)	40,50,50	1.63	5 (12%)
3	COA	D	1071	-	41,50,50	1.62	3 (7%)	52,75,75	1.24	3 (5%)
3	COA	I	1070	-	41,50,50	1.62	4 (9%)	52,75,75	1.29	3 (5%)
3	COA	J	1070	-	41,50,50	1.61	3 (7%)	52,75,75	1.23	4 (7%)

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	FMN	D	1072	-	-	0/18/18/18	0/3/3/3
2	FMN	H	1071	-	-	0/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	C	1071	-	-	5/44/64/64	0/3/3/3
2	FMN	B	1070	-	-	0/18/18/18	0/3/3/3
3	COA	K	1070	-	1/1/11/13	11/44/64/64	0/3/3/3
3	COA	A	1073	-	-	13/44/64/64	0/3/3/3
2	FMN	F	1072	-	-	0/18/18/18	0/3/3/3
3	COA	B	1069	-	-	9/44/64/64	0/3/3/3
3	COA	E	1070	-	-	6/44/64/64	0/3/3/3
2	FMN	F	1070	-	-	0/18/18/18	0/3/3/3
3	COA	F	1071	-	-	1/44/64/64	0/3/3/3
2	FMN	H	1070	-	-	2/18/18/18	0/3/3/3
2	FMN	C	1072	-	-	3/18/18/18	0/3/3/3
3	COA	A	1071	-	1/1/11/13	18/44/64/64	0/3/3/3
3	COA	L	1068	-	-	12/44/64/64	0/3/3/3
3	COA	G	1070	-	-	7/44/64/64	0/3/3/3
2	FMN	A	1070	-	-	0/18/18/18	0/3/3/3
2	FMN	C	1070	-	-	0/18/18/18	0/3/3/3
2	FMN	A	1072	-	-	0/18/18/18	0/3/3/3
2	FMN	B	1068	-	-	0/18/18/18	0/3/3/3
2	FMN	D	1070	-	-	4/18/18/18	0/3/3/3
3	COA	D	1071	-	-	4/44/64/64	0/3/3/3
3	COA	I	1070	-	-	6/44/64/64	0/3/3/3
3	COA	J	1070	-	-	3/44/64/64	0/3/3/3

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1071	COA	O9P-C9P	9.11	1.41	1.23
3	K	1070	COA	O9P-C9P	8.93	1.41	1.23
3	G	1070	COA	O9P-C9P	8.88	1.41	1.23
3	F	1071	COA	O9P-C9P	8.59	1.40	1.23
3	E	1070	COA	O9P-C9P	8.59	1.40	1.23

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1070	COA	N3A-C2A-N1A	-6.40	118.68	128.68
2	H	1070	FMN	C4-N3-C2	6.29	120.45	115.14
2	F	1070	FMN	C4-N3-C2	6.27	120.43	115.14
3	C	1071	COA	N3A-C2A-N1A	-6.24	118.93	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1071	COA	N3A-C2A-N1A	-6.23	118.94	128.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	K	1070	COA	CAP
3	A	1071	COA	CAP

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1071	COA	C5B-O5B-P1A-O1A
3	C	1071	COA	C5B-O5B-P1A-O2A
3	K	1070	COA	C5B-O5B-P1A-O1A
3	K	1070	COA	C5B-O5B-P1A-O2A
3	K	1070	COA	O9P-C9P-CAP-OAP

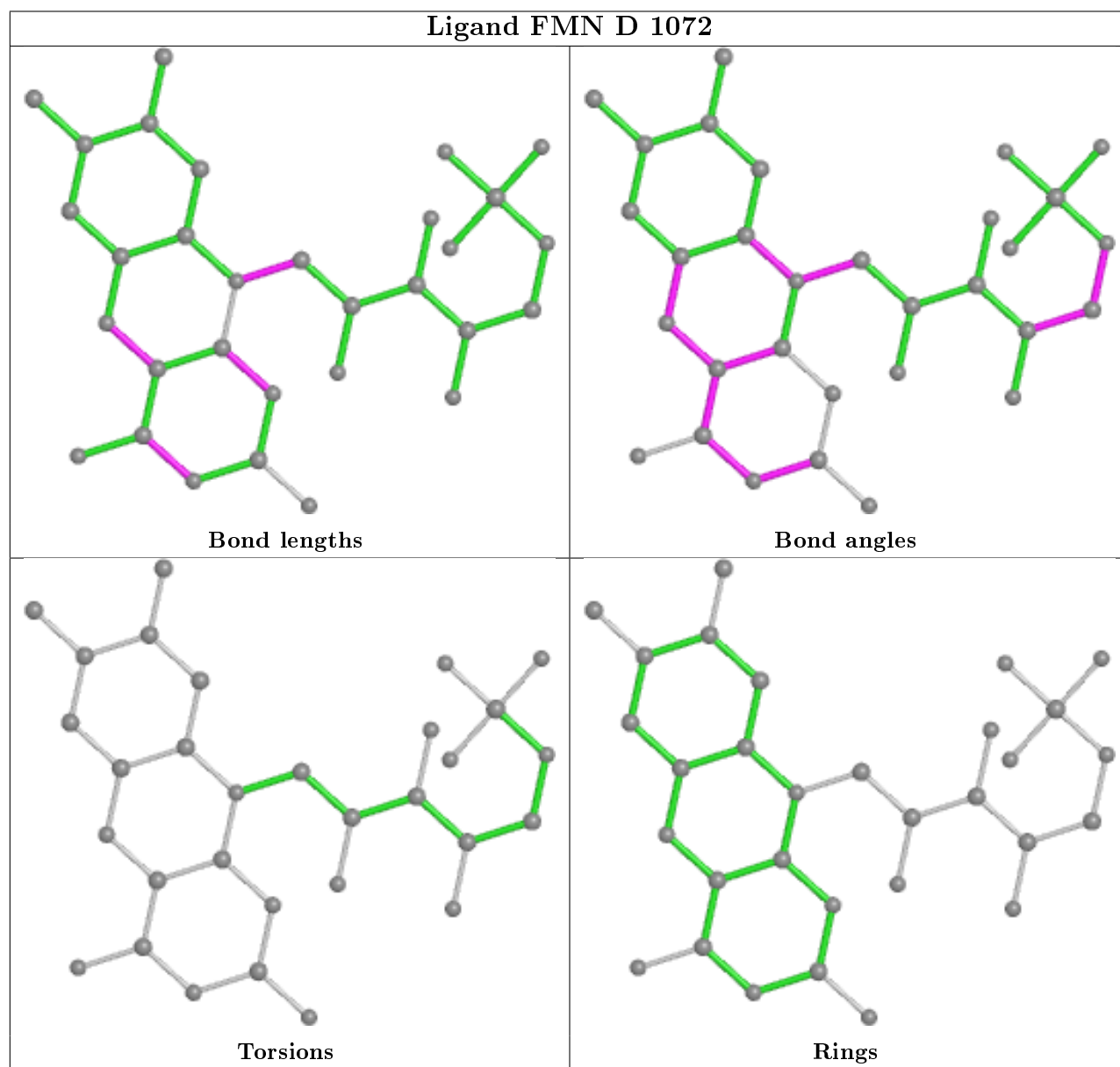
There are no ring outliers.

14 monomers are involved in 18 short contacts:

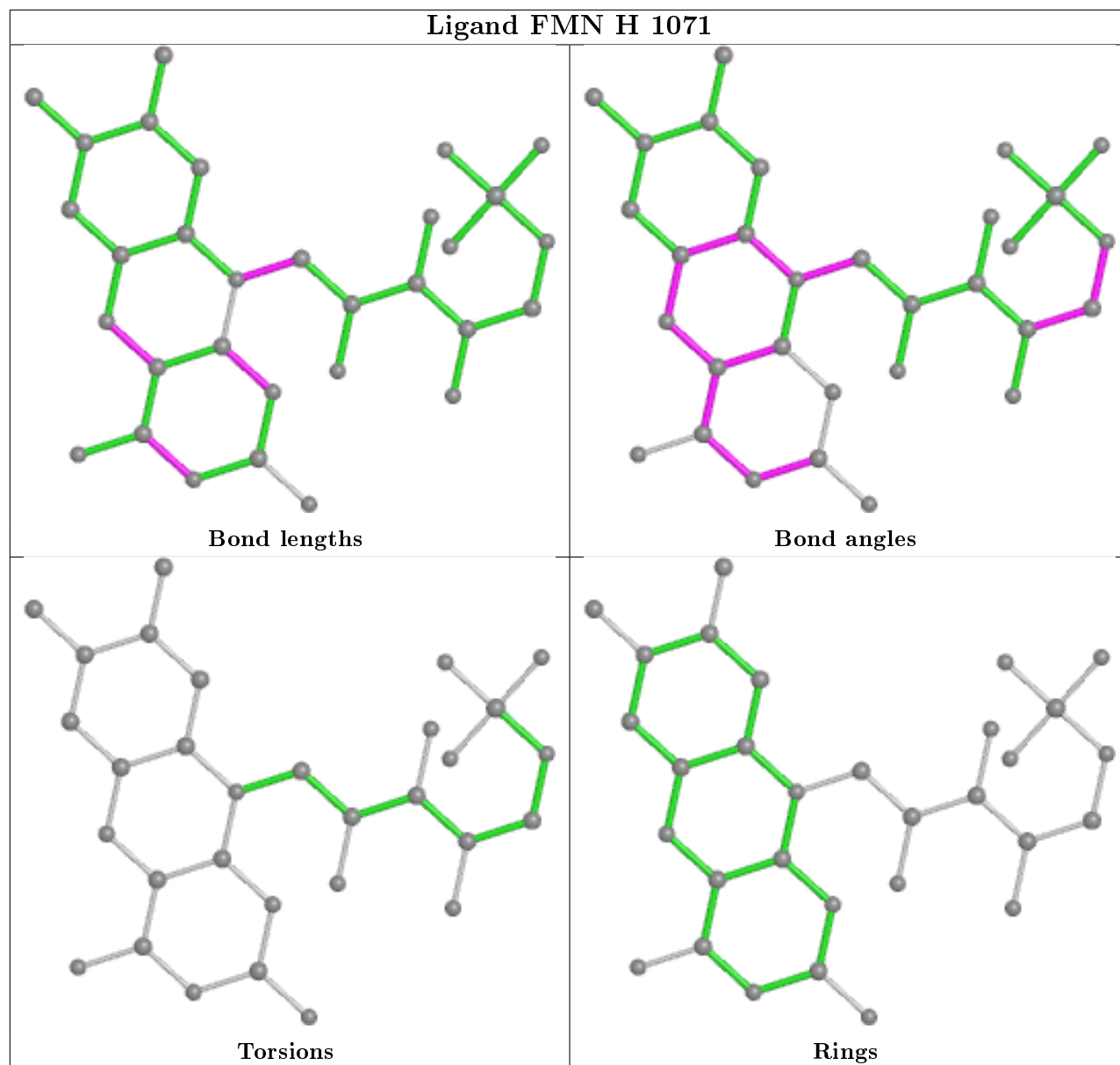
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1072	FMN	1	0
2	B	1070	FMN	1	0
3	K	1070	COA	1	0
2	F	1072	FMN	1	0
3	B	1069	COA	4	0
3	E	1070	COA	1	0
2	H	1070	FMN	1	0
3	A	1071	COA	2	0
3	G	1070	COA	3	0
2	C	1070	FMN	1	0
2	A	1072	FMN	1	0
2	B	1068	FMN	1	0
2	D	1070	FMN	1	0
3	J	1070	COA	1	0

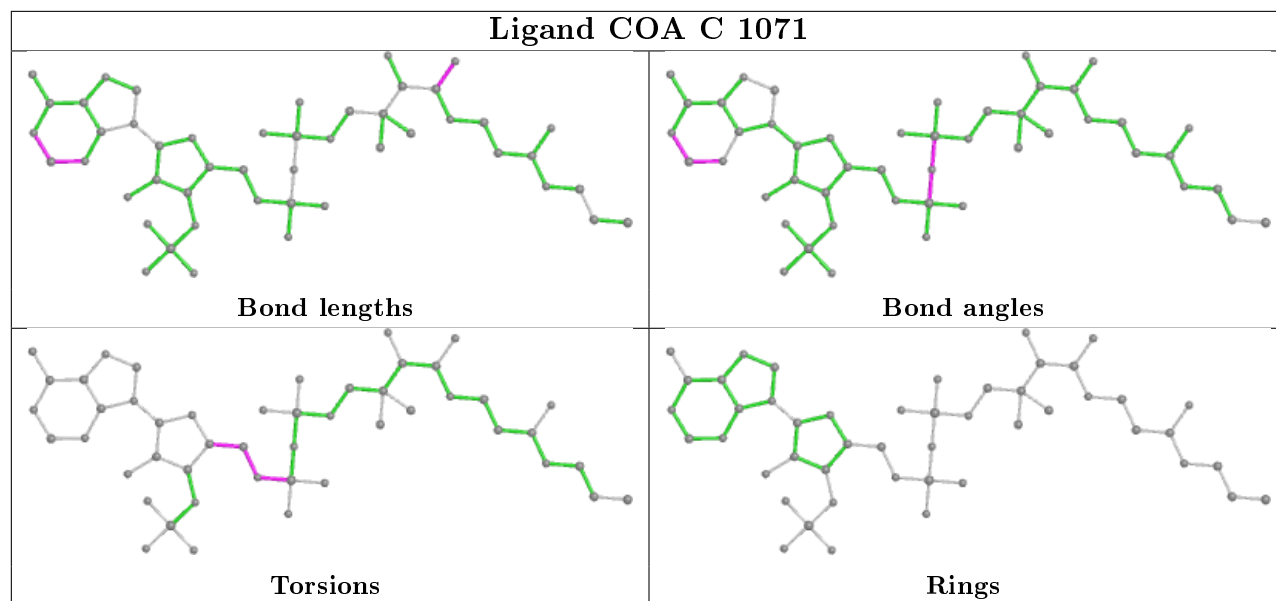
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

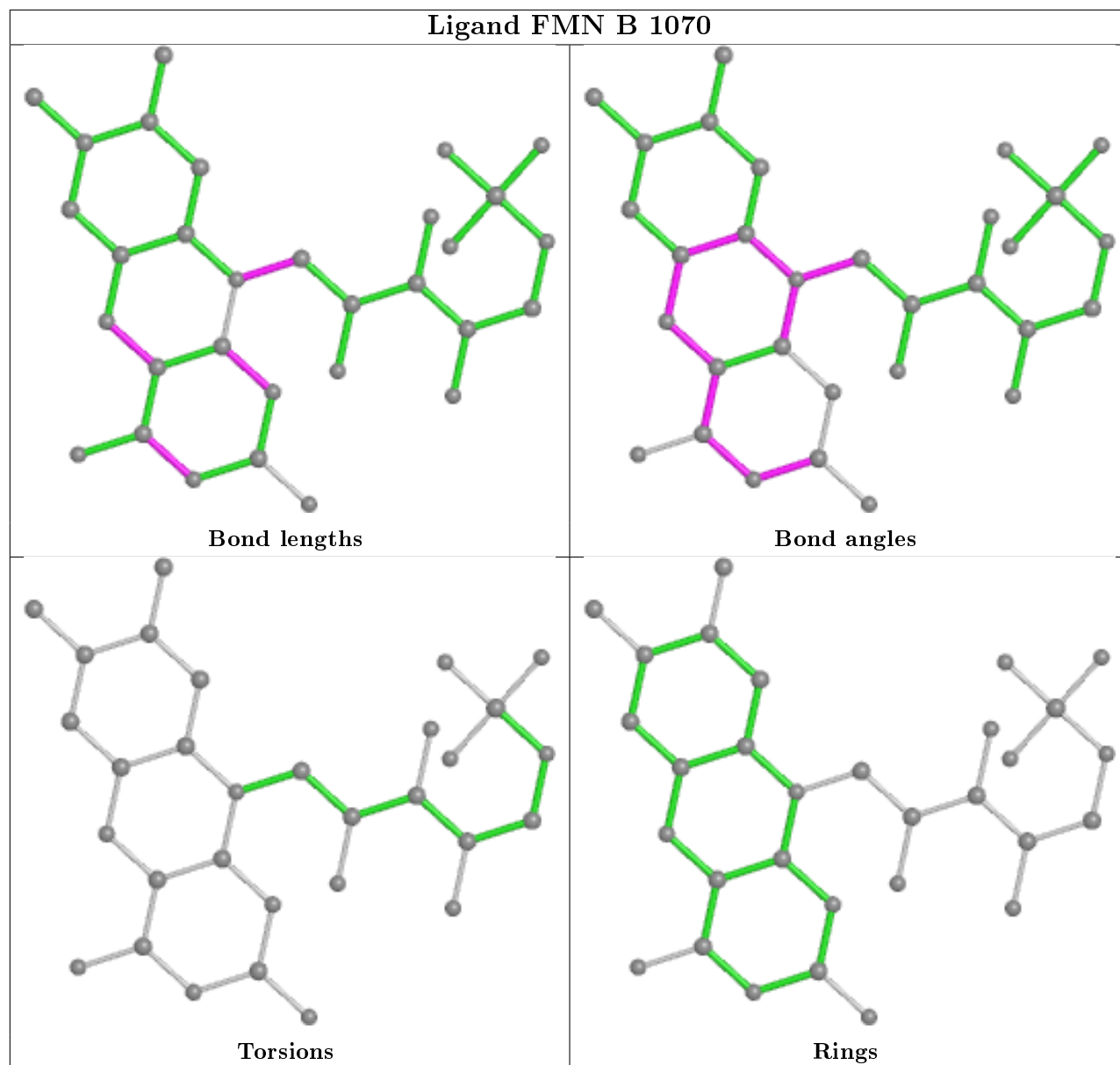


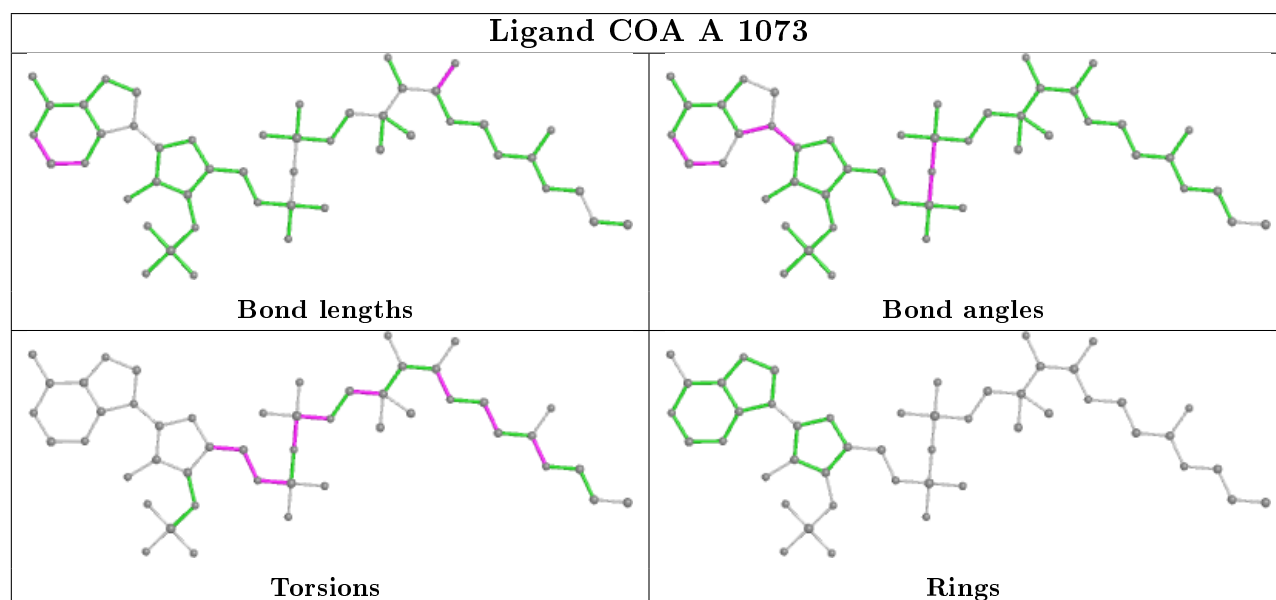
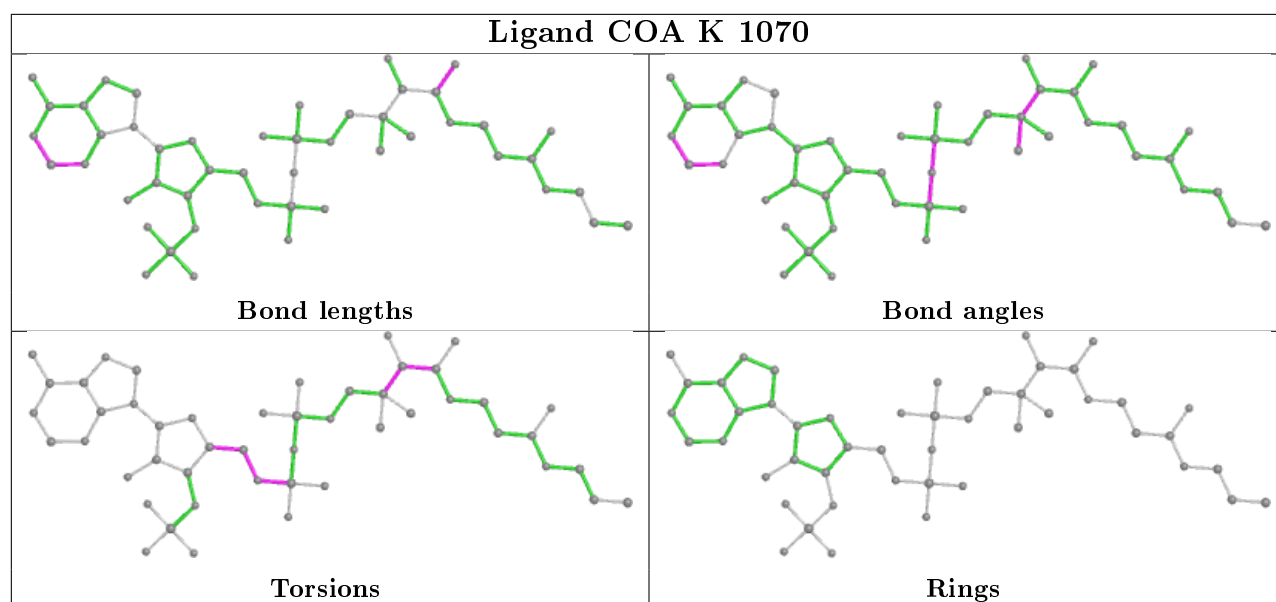
## Ligand FMN H 1071





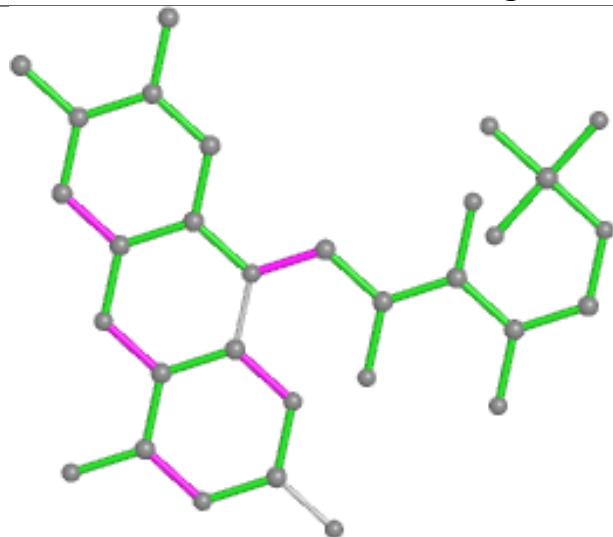
## Ligand FMN B 1070



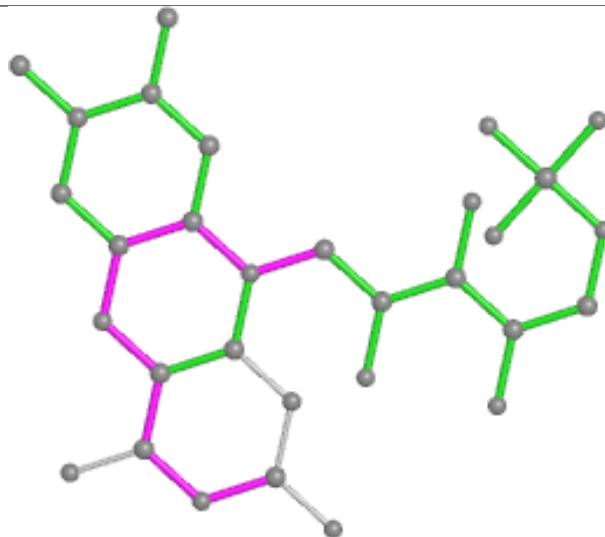




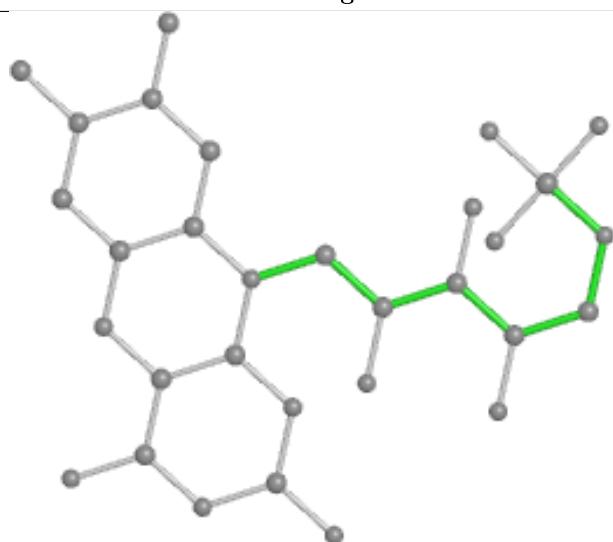
## Ligand FMN F 1072



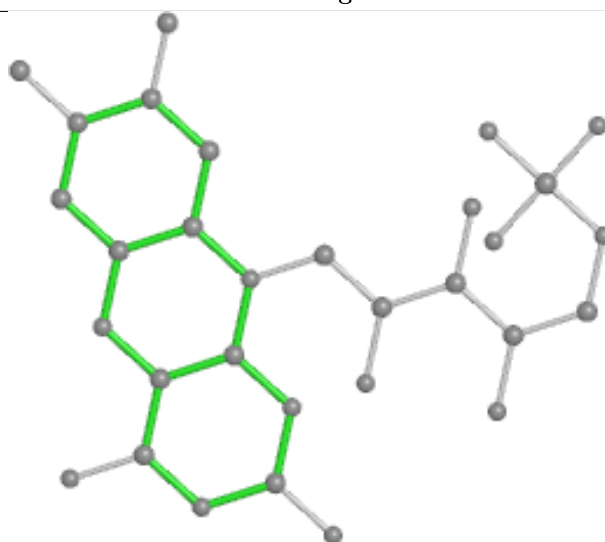
Bond lengths



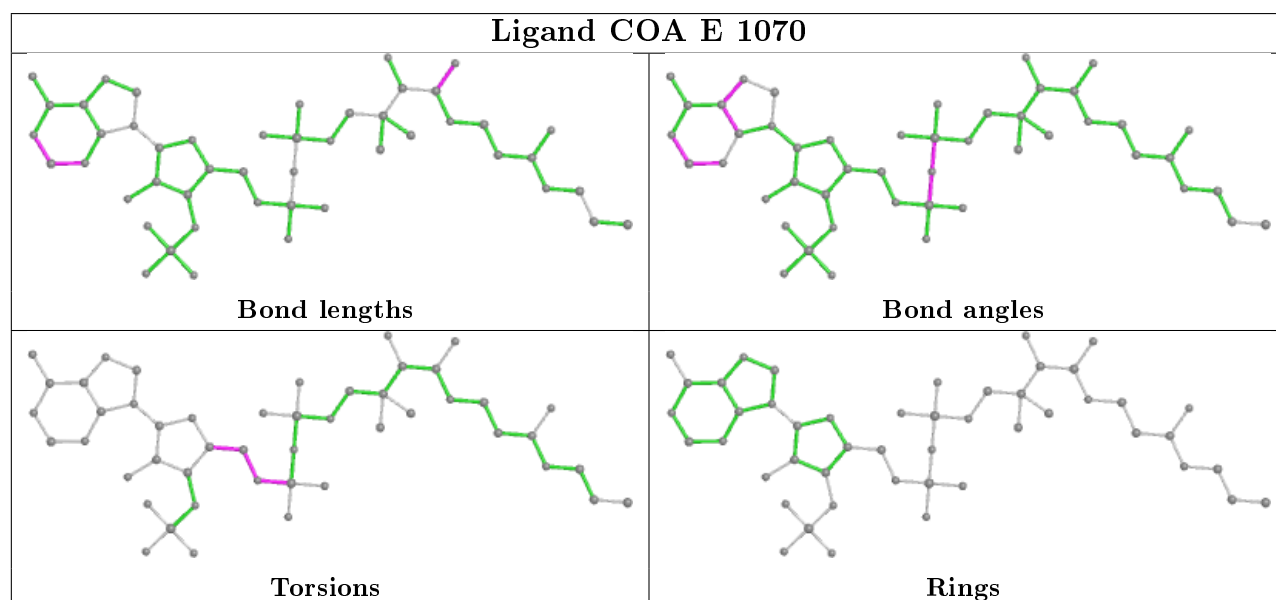
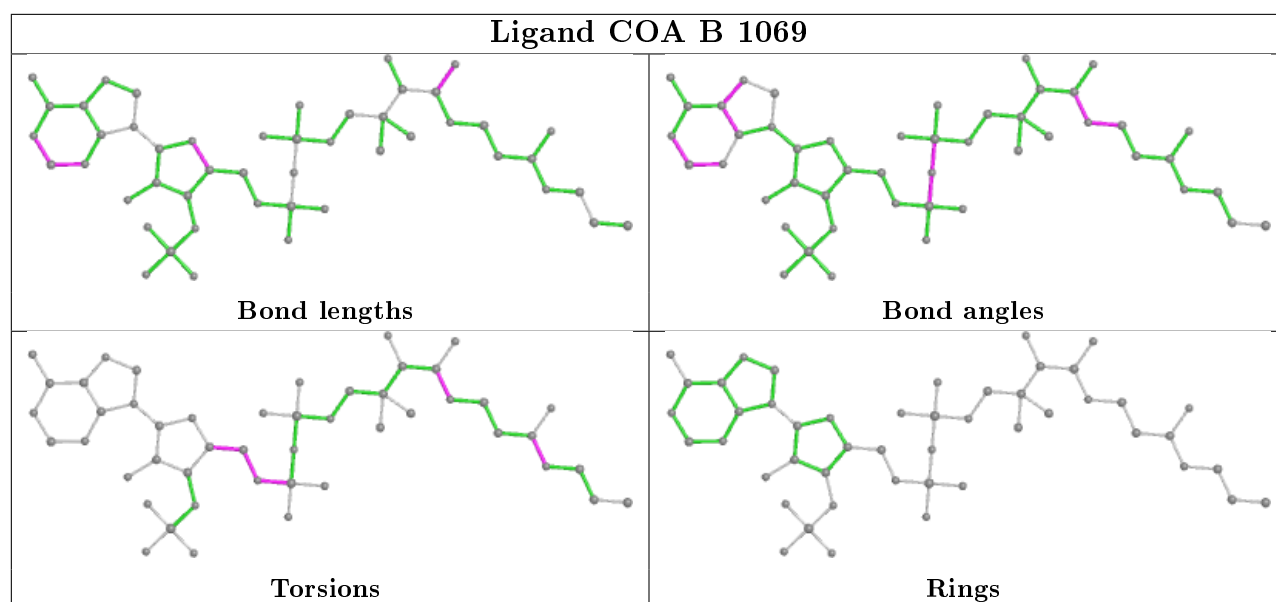
Bond angles



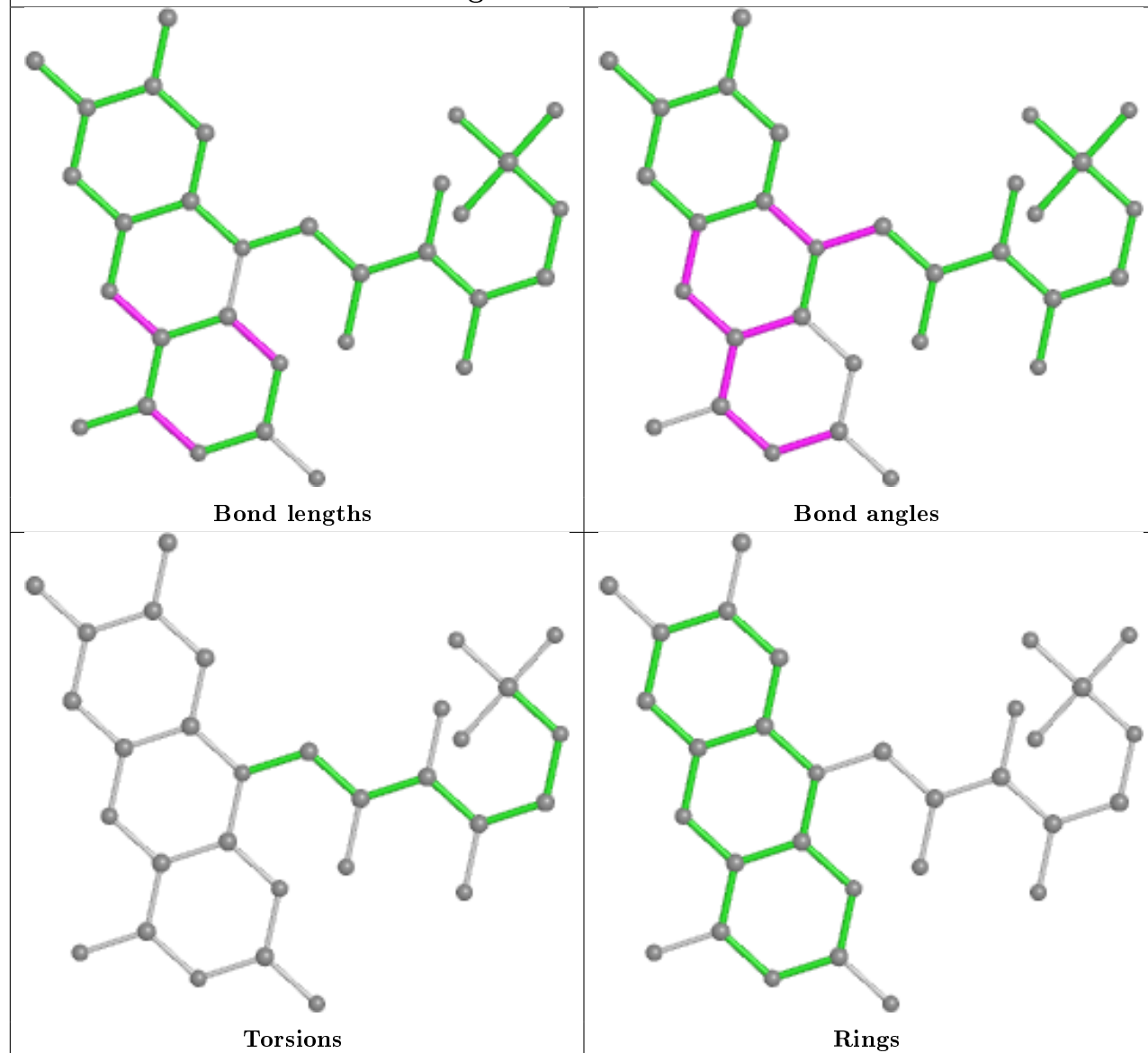
Torsions

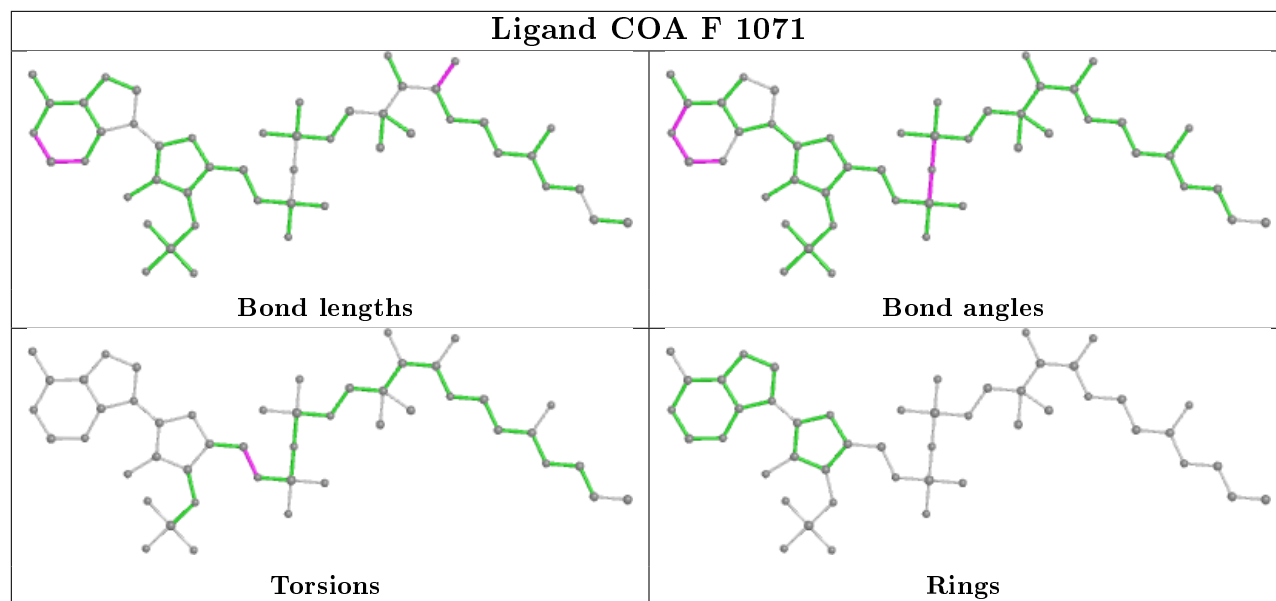


Rings

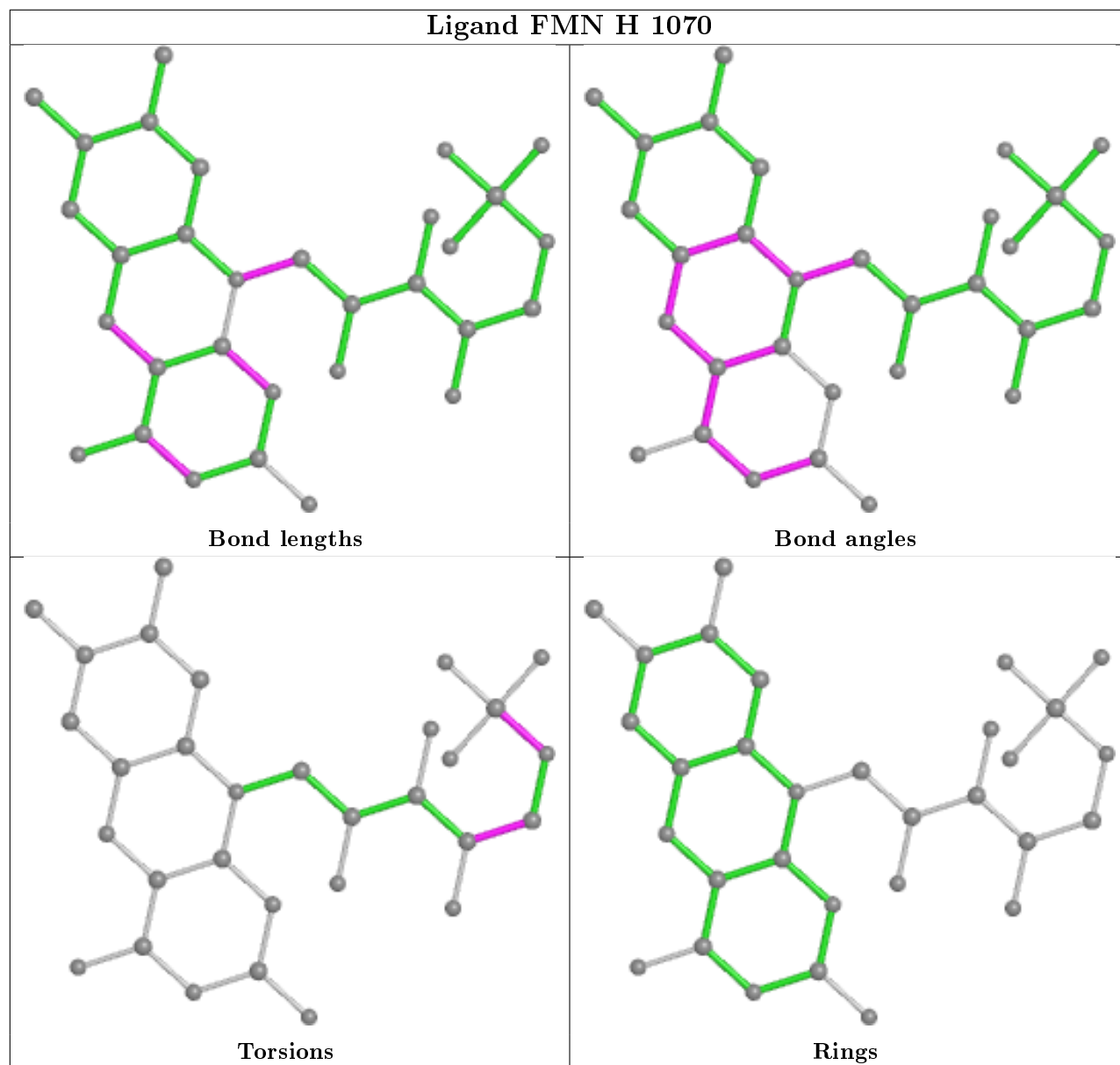


## Ligand FMN F 1070

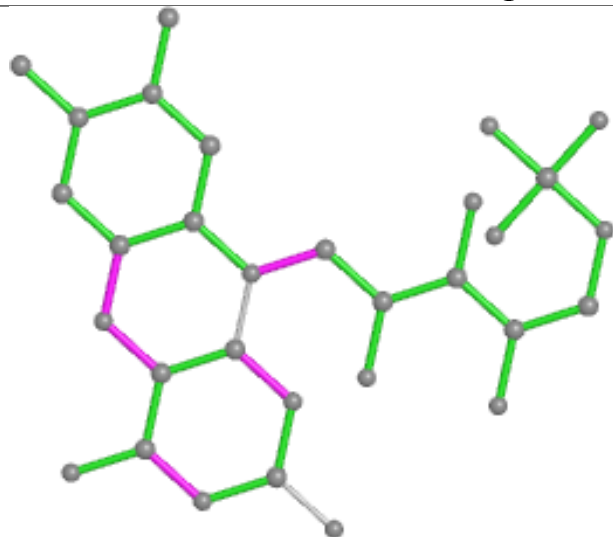




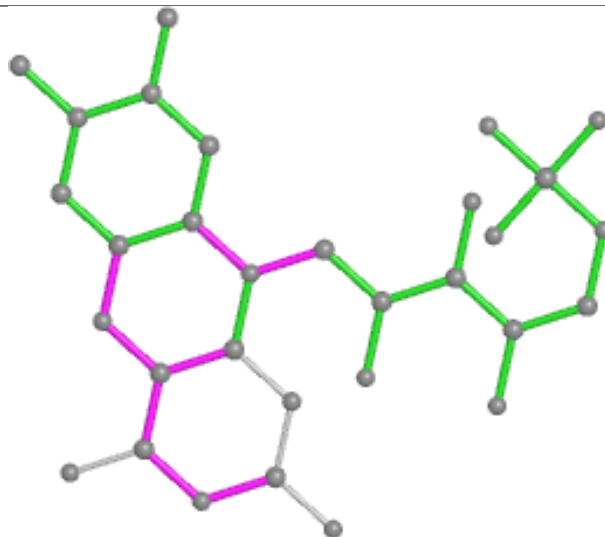
## Ligand FMN H 1070



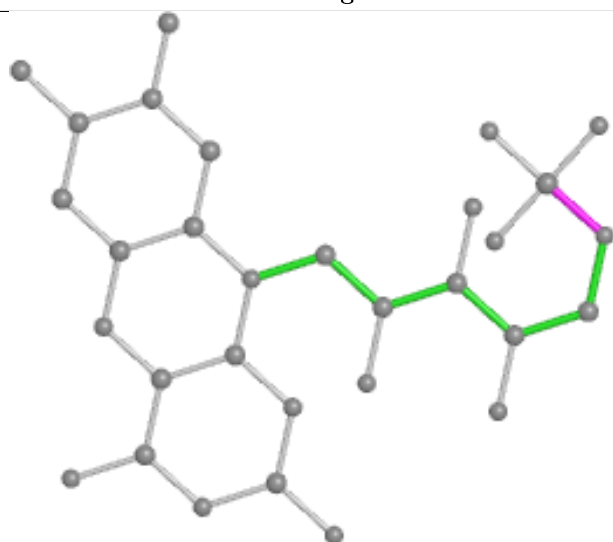
## Ligand FMN C 1072



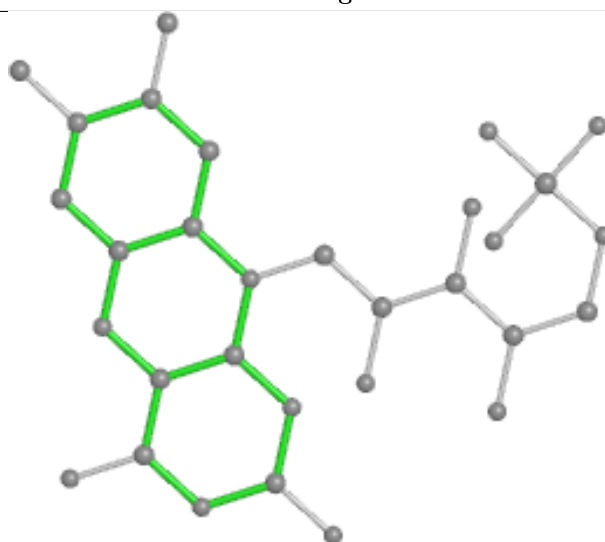
Bond lengths



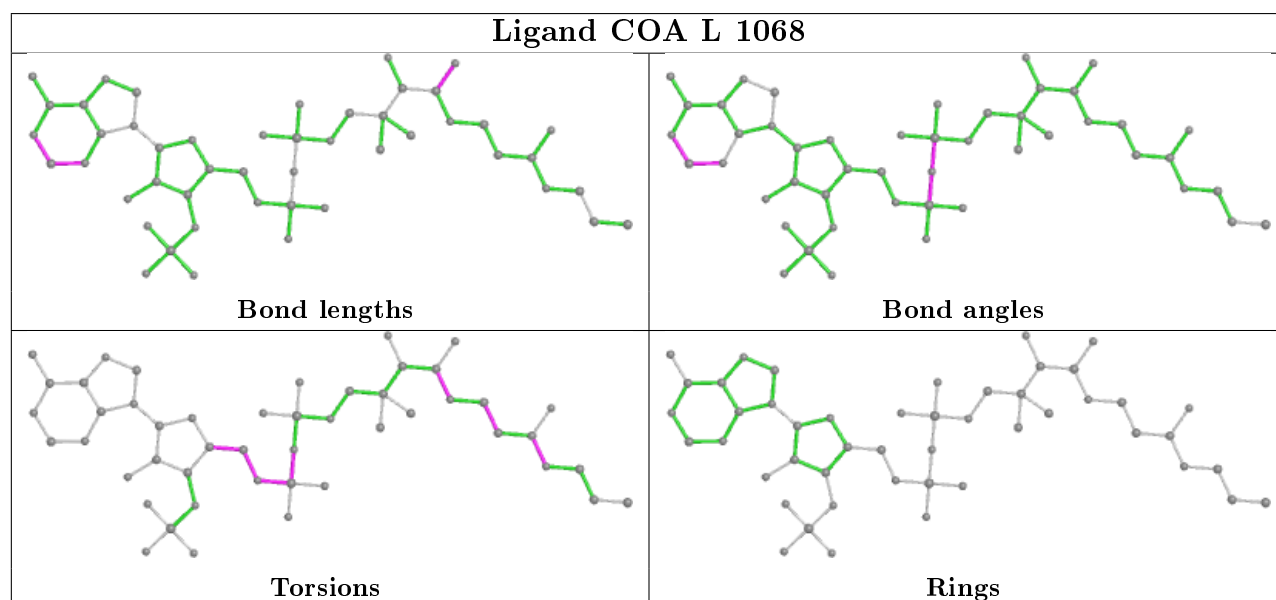
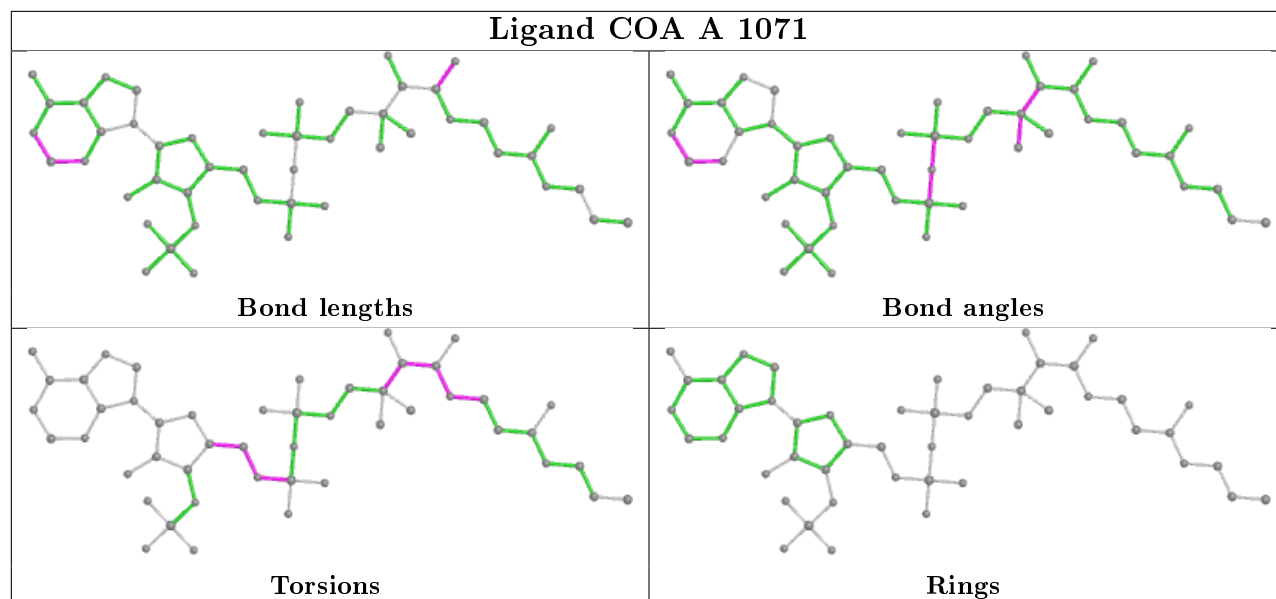
Bond angles

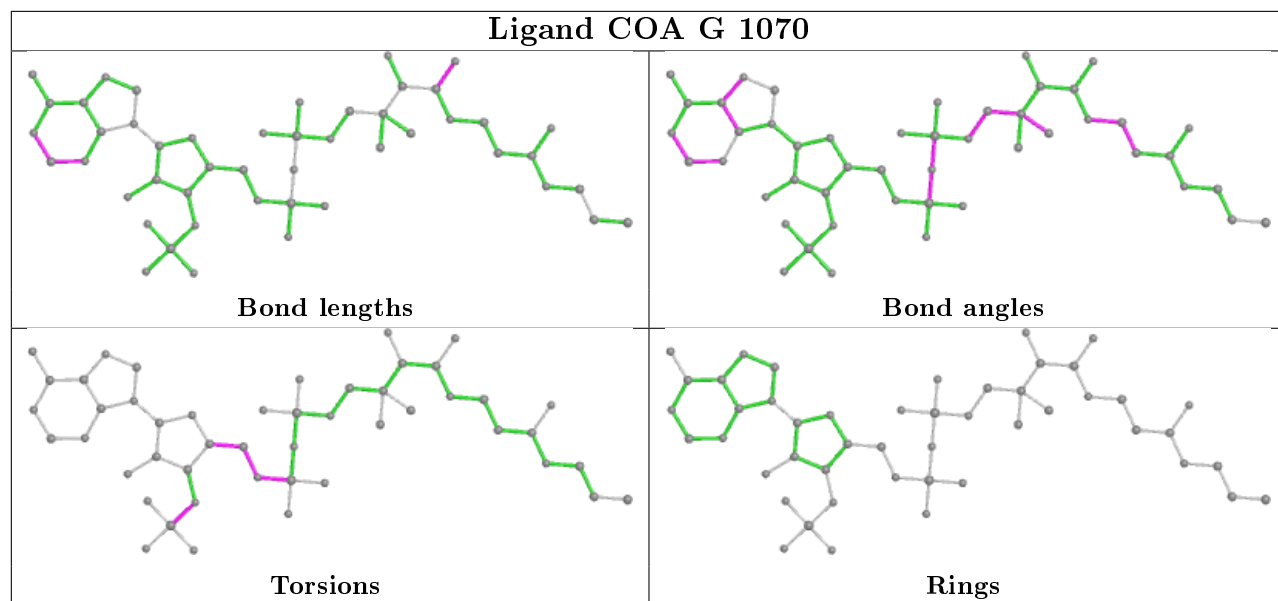


Torsions



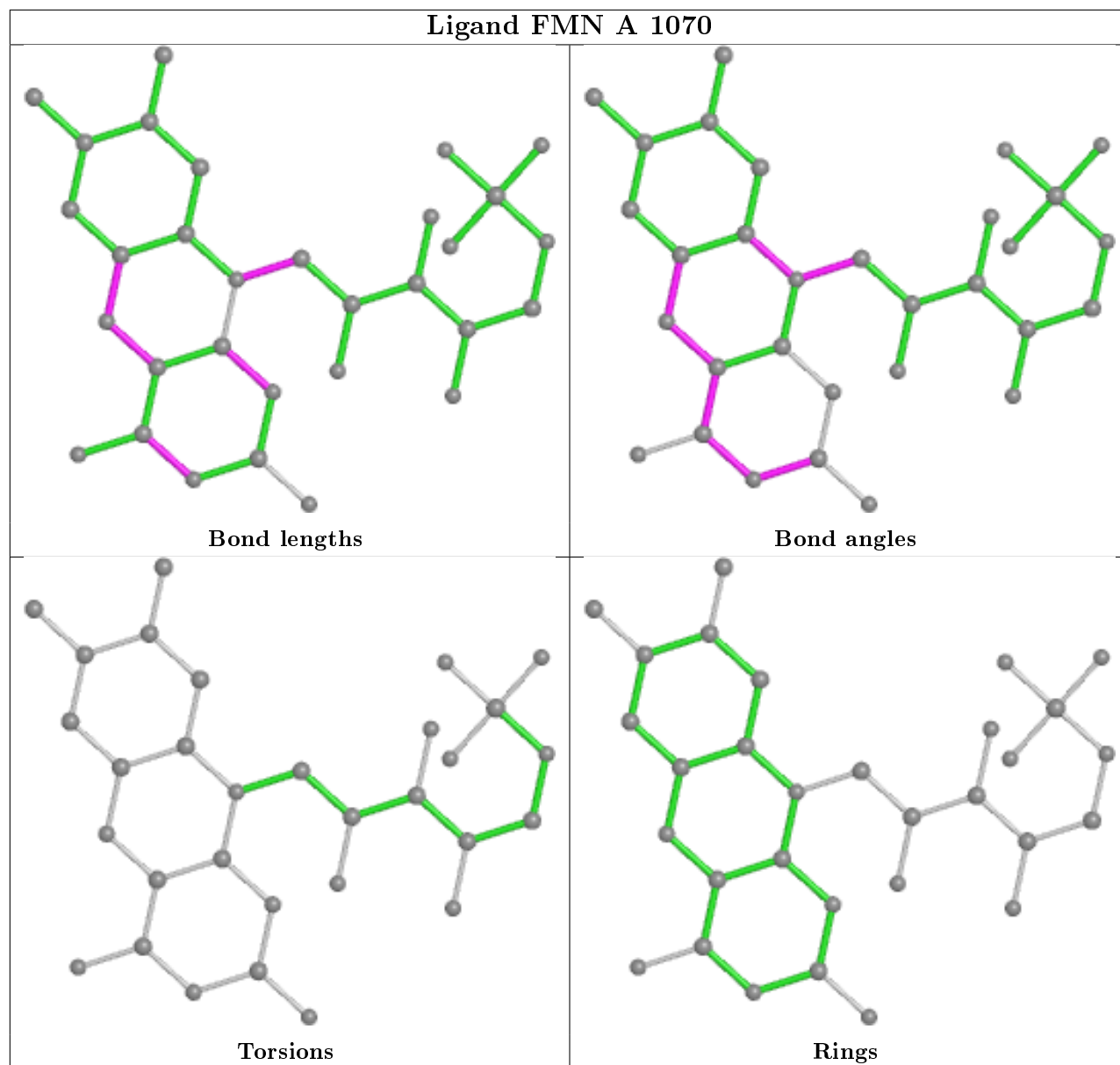
Rings



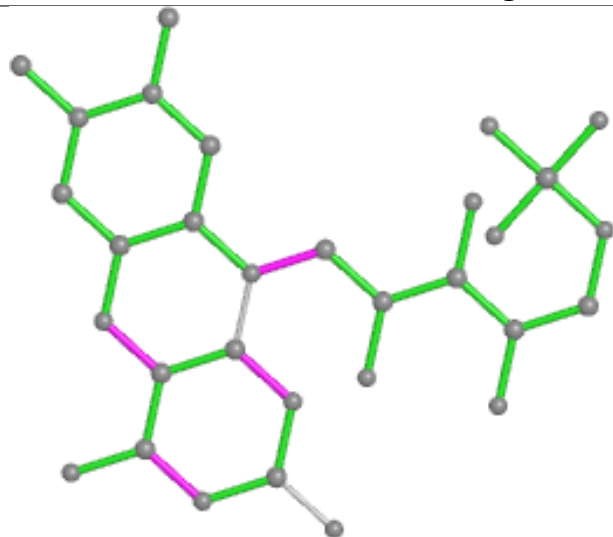




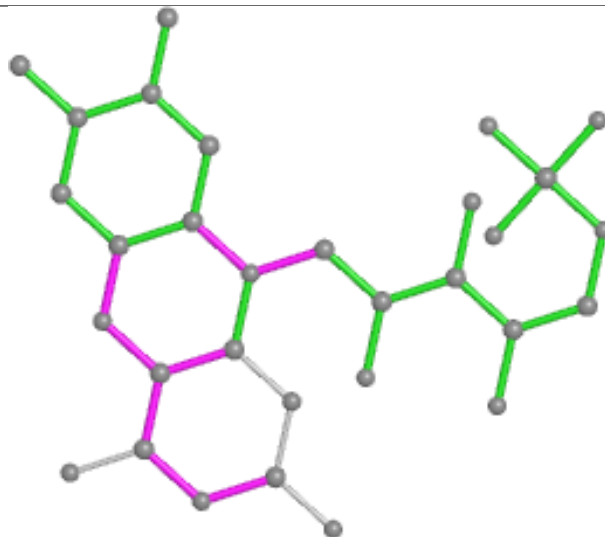
## Ligand FMN A 1070



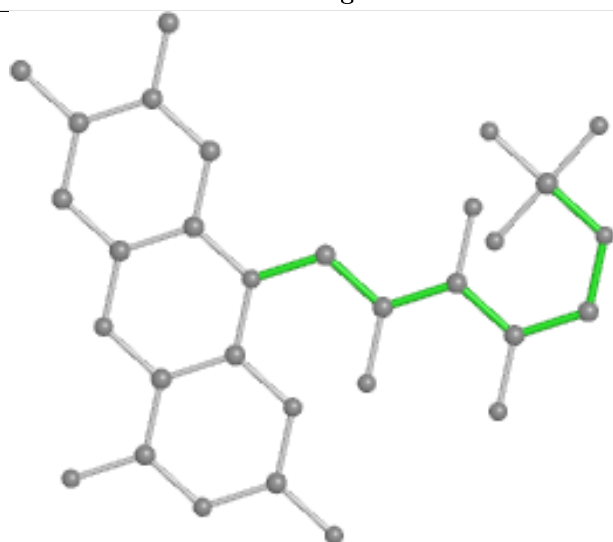
## Ligand FMN C 1070



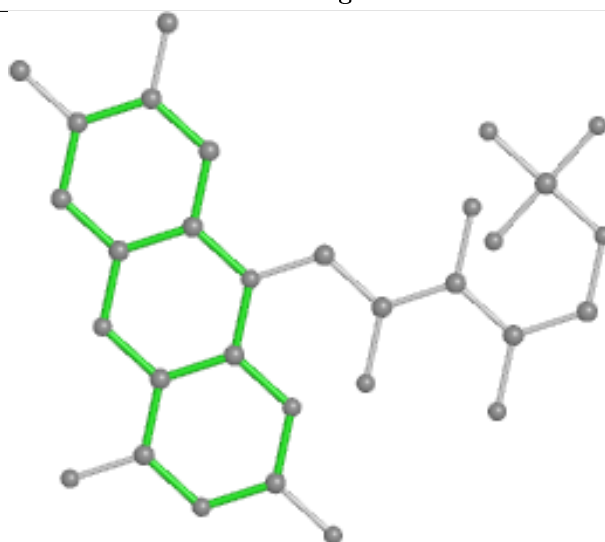
Bond lengths



Bond angles

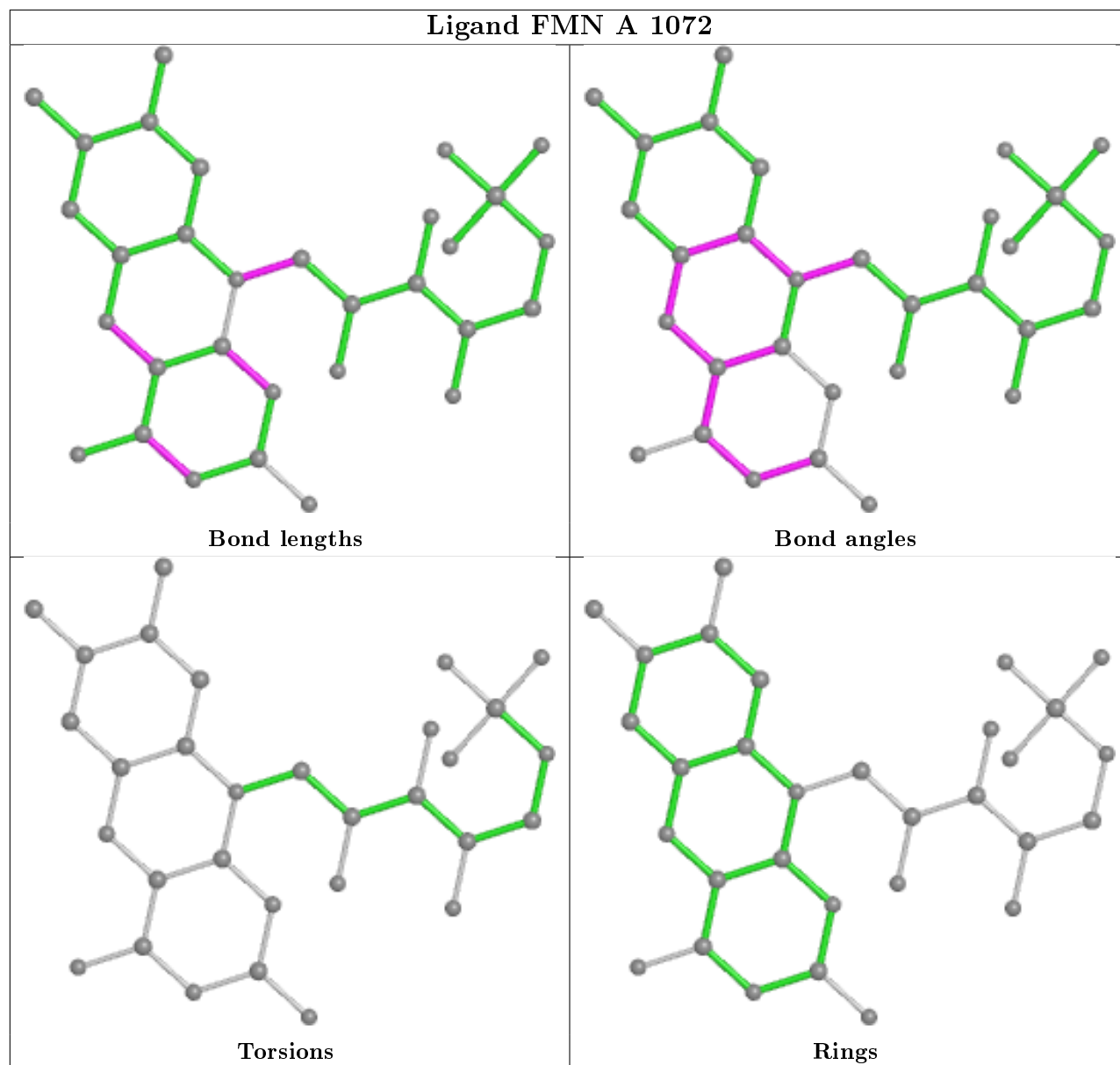


Torsions

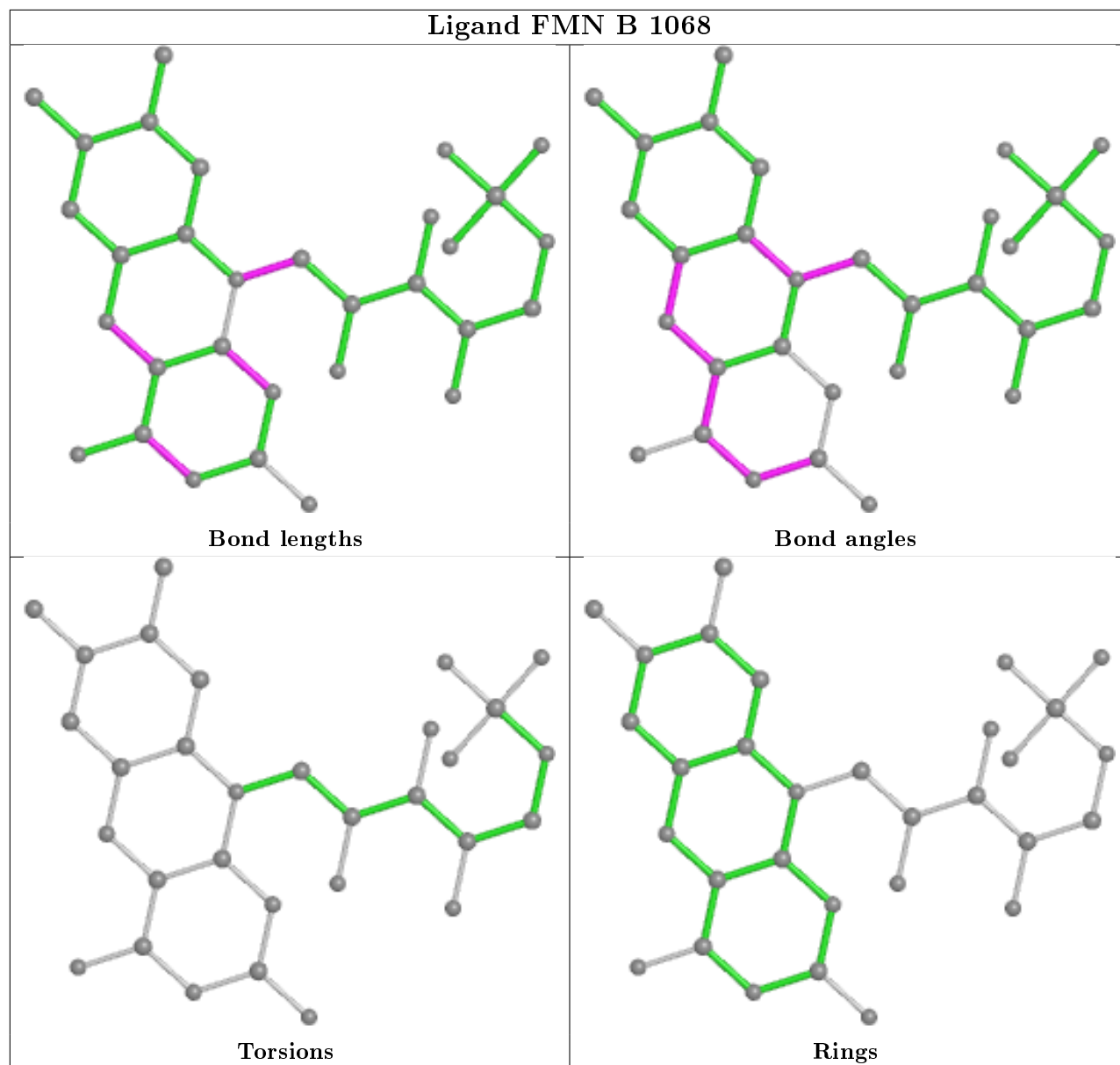


Rings

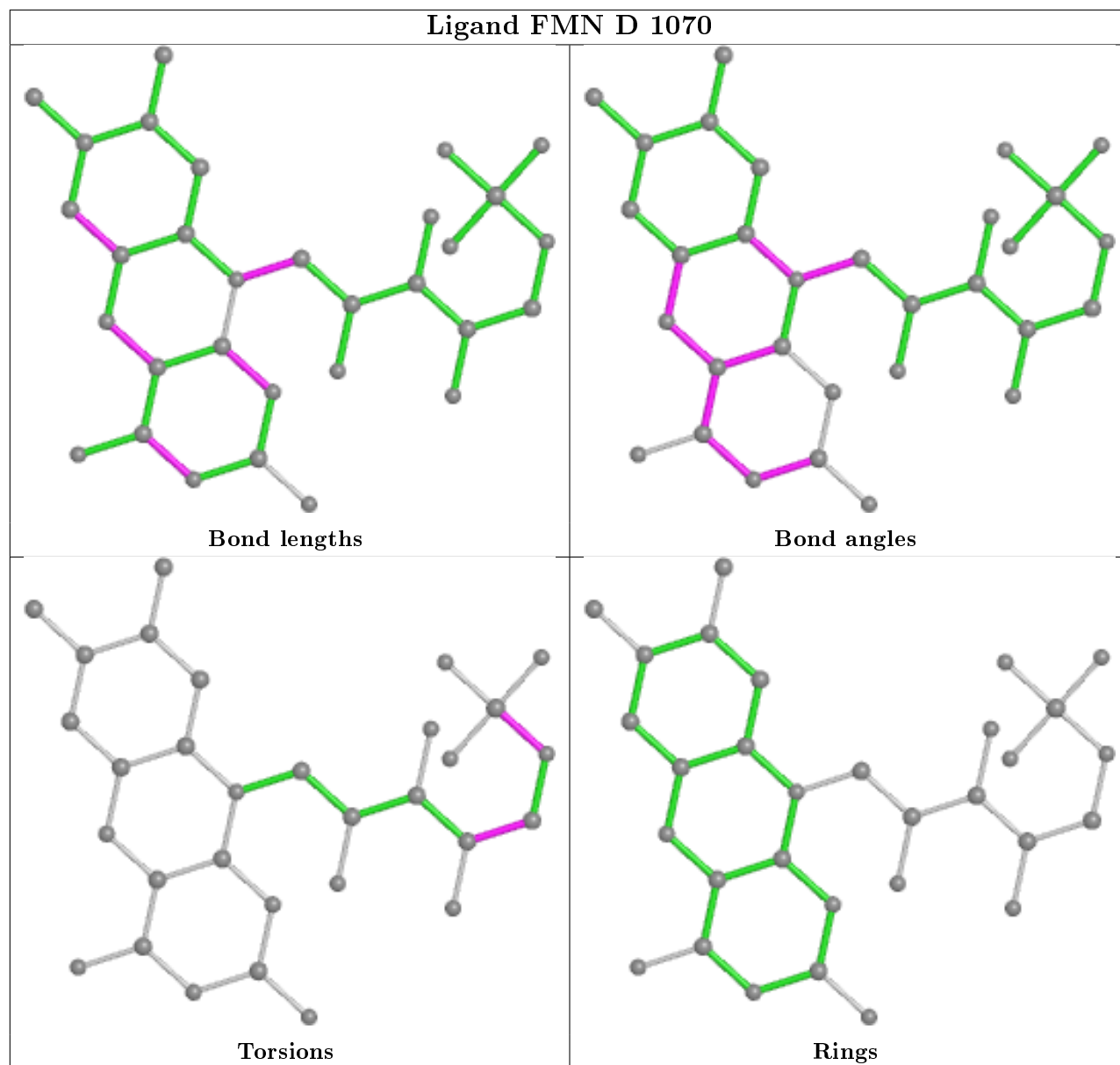
## Ligand FMN A 1072

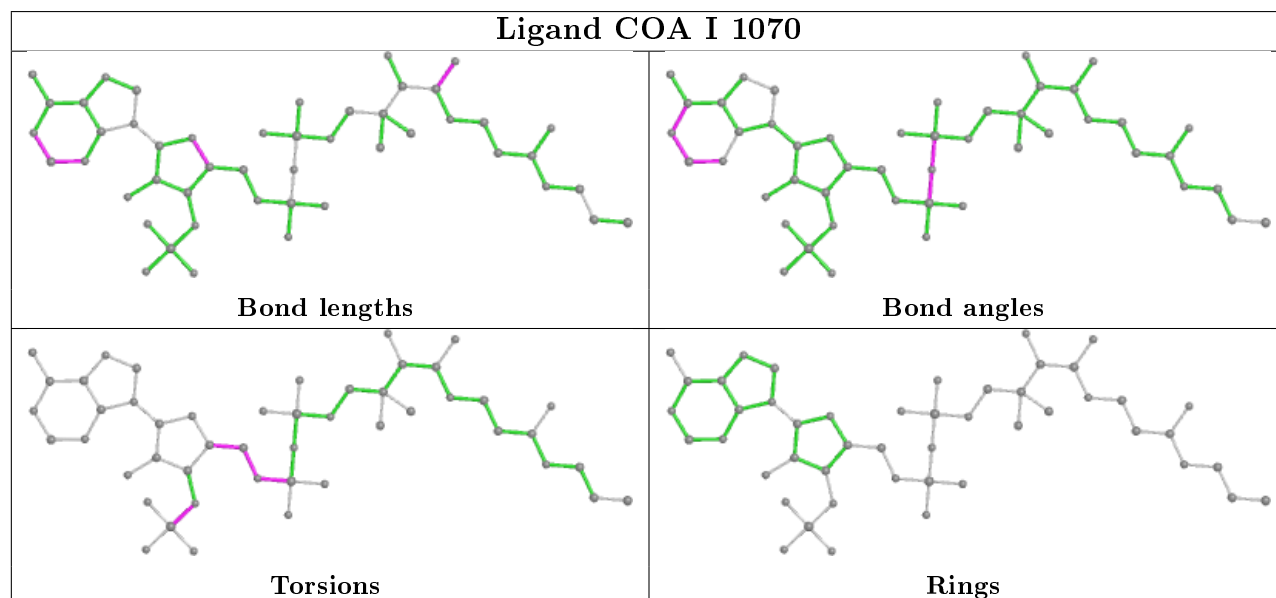
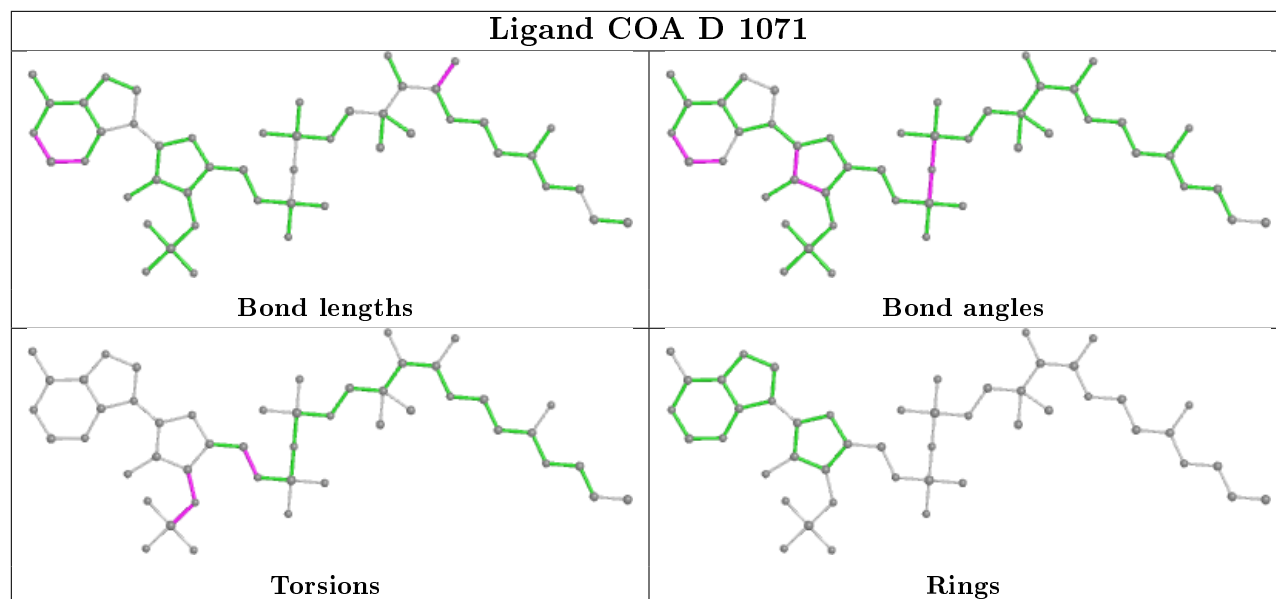


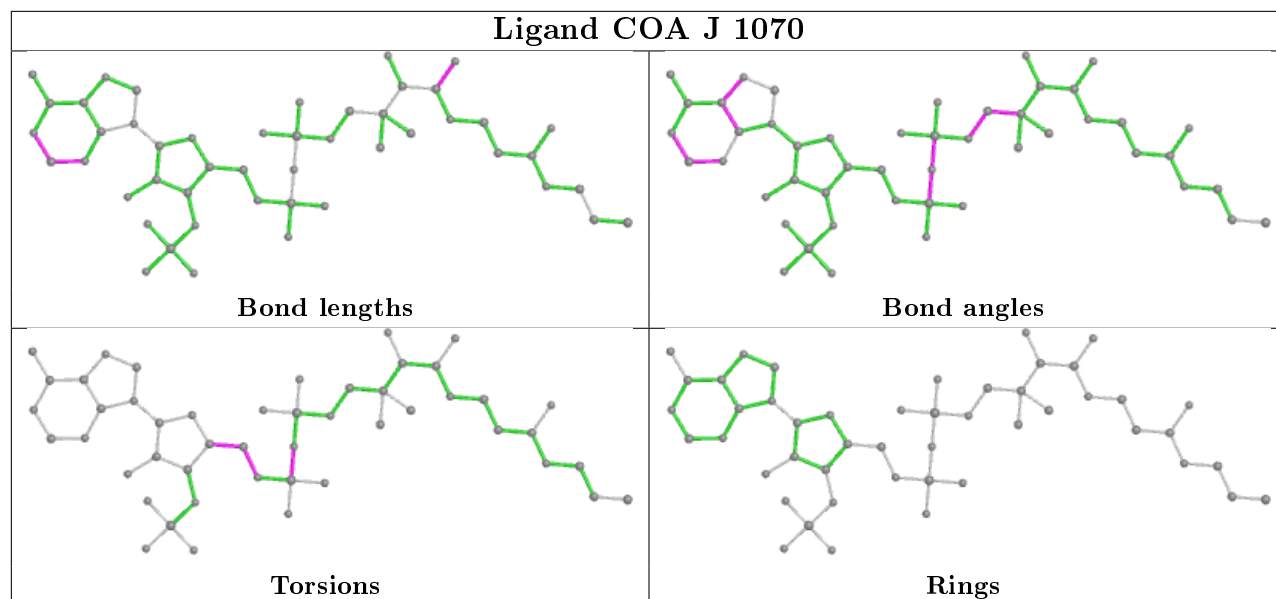
## Ligand FMN B 1068



## Ligand FMN D 1070







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	68/69 (98%)	0.61	5 (7%) 14 15	18, 24, 36, 42	0
1	B	66/69 (95%)	0.17	4 (6%) 21 23	13, 19, 29, 36	0
1	C	68/69 (98%)	0.14	3 (4%) 34 38	14, 21, 29, 31	0
1	D	68/69 (98%)	0.27	4 (5%) 22 24	12, 20, 30, 37	0
1	E	68/69 (98%)	0.36	5 (7%) 14 15	14, 19, 30, 36	0
1	F	68/69 (98%)	0.09	3 (4%) 34 38	10, 17, 26, 33	0
1	G	68/69 (98%)	0.14	4 (5%) 22 24	11, 18, 27, 34	0
1	H	68/69 (98%)	0.65	4 (5%) 22 24	15, 23, 36, 45	0
1	I	68/69 (98%)	0.33	4 (5%) 22 24	11, 18, 28, 33	0
1	J	68/69 (98%)	0.48	5 (7%) 14 15	16, 23, 32, 39	0
1	K	68/69 (98%)	0.53	5 (7%) 14 15	16, 23, 31, 35	0
1	L	66/69 (95%)	0.69	6 (9%) 9 9	19, 25, 35, 37	0
All	All	812/828 (98%)	0.37	52 (6%) 19 20	10, 21, 33, 45	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	69	THR	12.7
1	H	69	THR	10.8
1	E	69	THR	8.0
1	J	69	THR	6.3
1	A	69	THR	5.9

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

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



## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

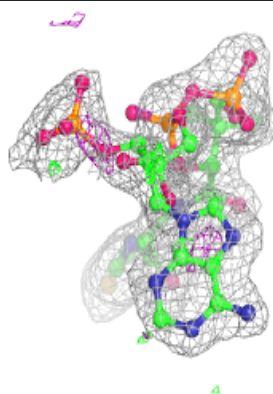
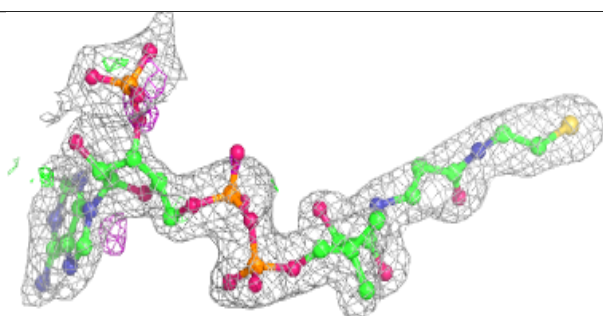
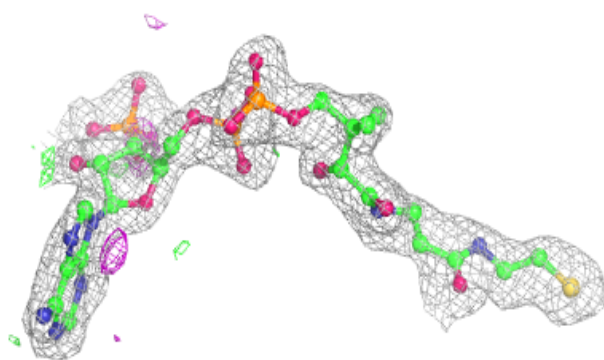
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	COA	A	1073	48/48	0.83	0.13	31,37,47,48	0
3	COA	L	1068	48/48	0.84	0.14	30,38,43,44	0
3	COA	A	1071	48/48	0.85	0.13	27,36,45,46	0
2	FMN	B	1070	31/31	0.85	0.13	25,26,37,38	0
2	FMN	B	1068	31/31	0.85	0.14	25,27,32,34	0
2	FMN	H	1070	31/31	0.88	0.10	20,21,41,42	0
3	COA	K	1070	48/48	0.90	0.11	18,28,36,37	0
3	COA	F	1071	48/48	0.91	0.10	15,23,34,35	0
3	COA	J	1070	48/48	0.91	0.10	19,27,37,39	0
2	FMN	C	1070	31/31	0.92	0.09	19,20,29,32	0
2	FMN	H	1071	31/31	0.92	0.09	20,22,35,36	0
3	COA	D	1071	48/48	0.92	0.11	20,26,44,45	0
2	FMN	C	1072	31/31	0.92	0.09	20,21,32,33	0
3	COA	C	1071	48/48	0.93	0.09	19,25,35,37	0
2	FMN	D	1070	31/31	0.93	0.09	17,19,29,32	0
3	COA	B	1069	48/48	0.93	0.10	16,24,33,34	0
3	COA	I	1070	48/48	0.93	0.09	16,24,32,34	0
3	COA	E	1070	48/48	0.93	0.09	15,24,30,35	0
2	FMN	A	1072	31/31	0.94	0.09	17,18,25,26	0
3	COA	G	1070	48/48	0.94	0.09	15,24,33,34	0
2	FMN	F	1072	31/31	0.95	0.07	12,14,23,25	0
2	FMN	A	1070	31/31	0.95	0.07	19,20,29,30	0
2	FMN	D	1072	31/31	0.95	0.07	18,19,27,28	0
2	FMN	F	1070	31/31	0.96	0.07	11,14,21,24	0
5	NA	F	1073	1/1	0.98	0.10	33,33,33,33	0
4	CL	C	1073	1/1	0.99	0.03	21,21,21,21	0
4	CL	D	1073	1/1	0.99	0.04	20,20,20,20	0
4	CL	B	1071	1/1	0.99	0.03	15,15,15,15	0
4	CL	A	1074	1/1	0.99	0.04	30,30,30,30	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.

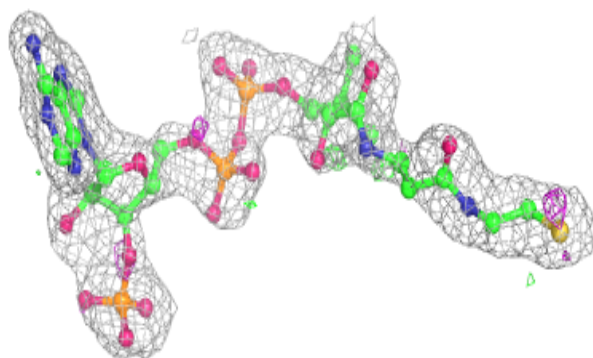
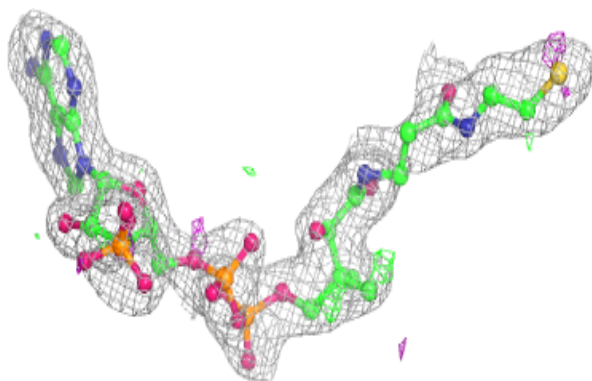
**Electron density around COA A 1073:**

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



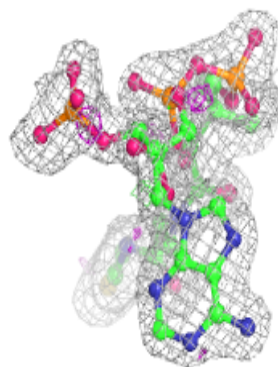
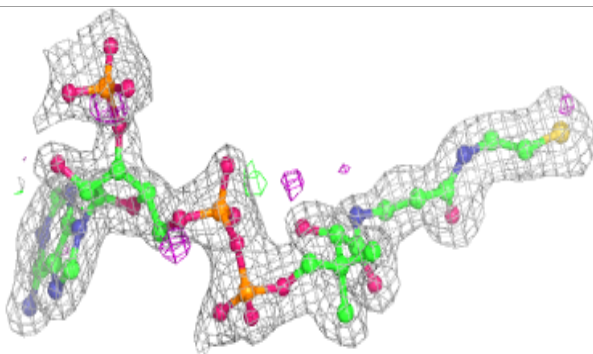
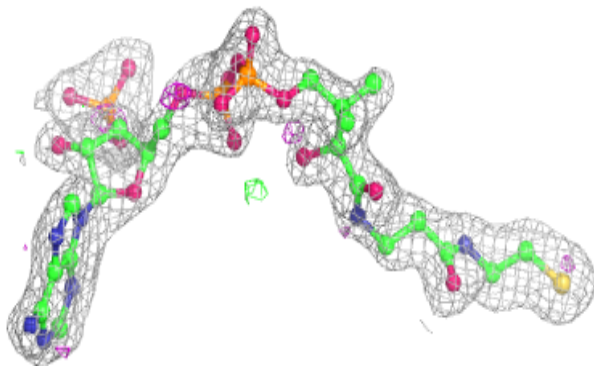
**Electron density around COA L 1068:**

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



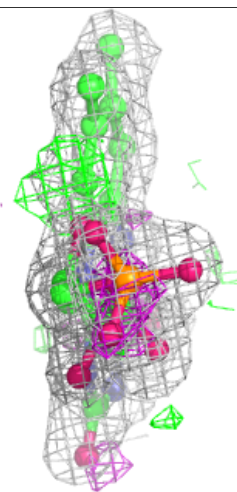
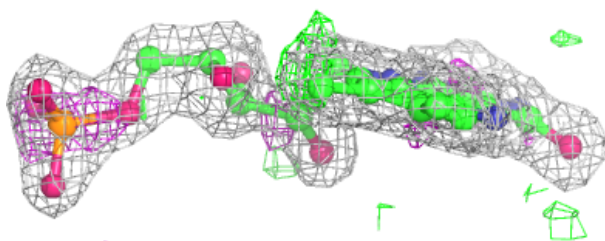
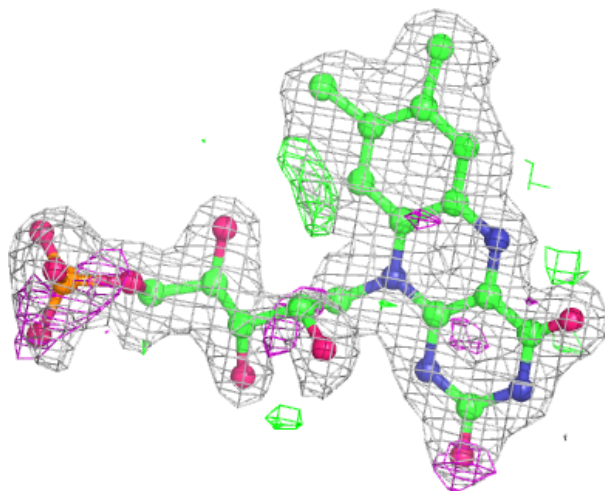
**Electron density around COA A 1071:**

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



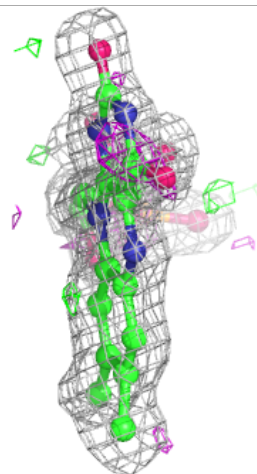
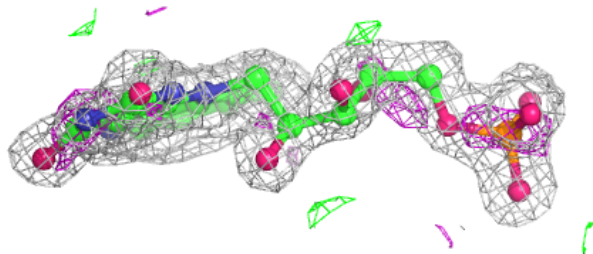
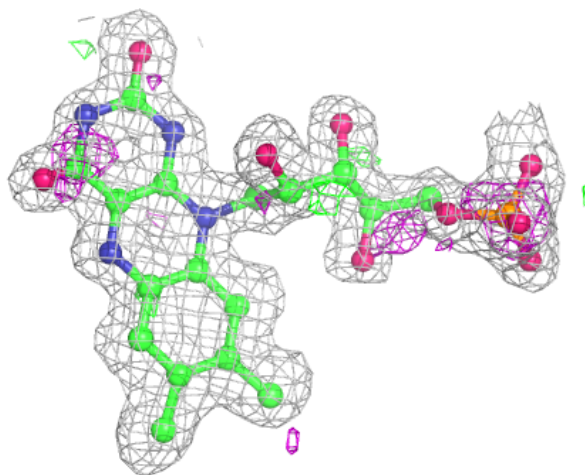
**Electron density around FMN B 1070:**

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



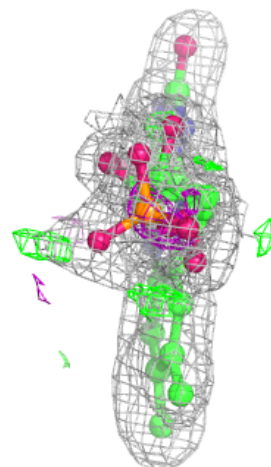
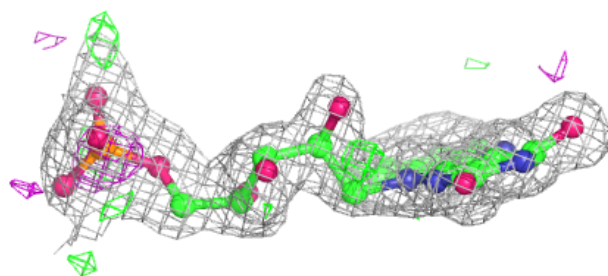
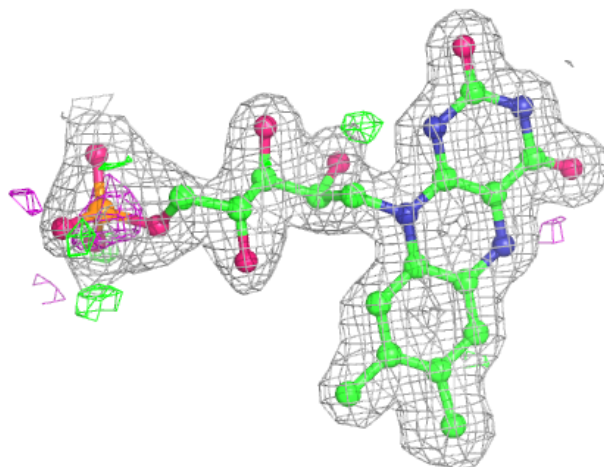
**Electron density around FMN B 1068:**

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



**Electron density around FMN H 1070:**

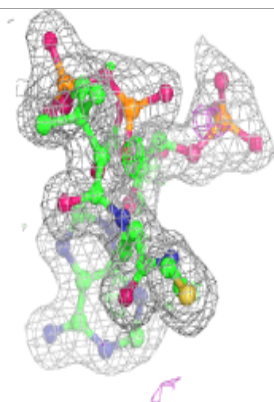
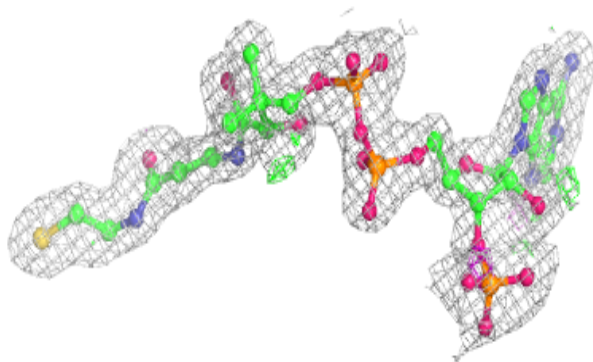
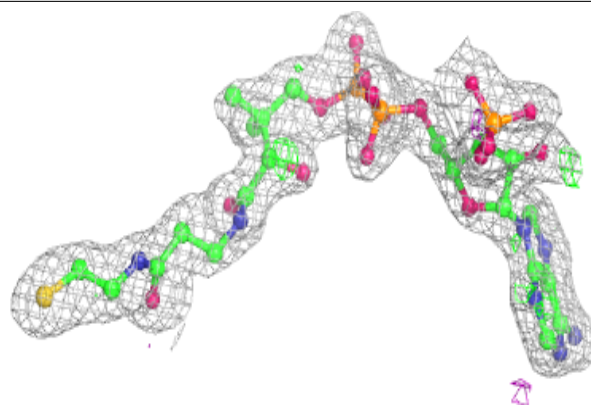
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



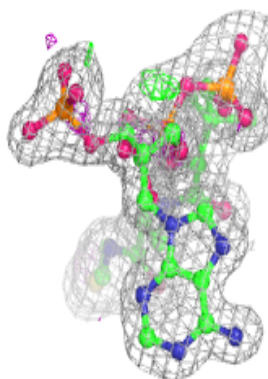
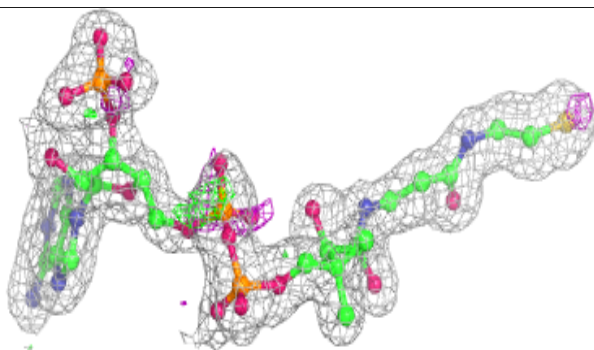
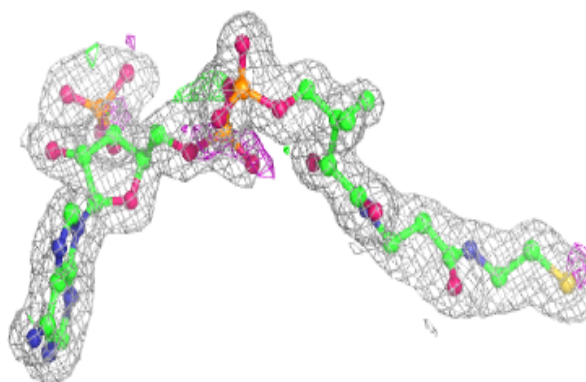


**Electron density around COA K 1070:**

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

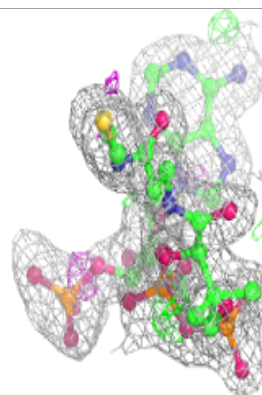
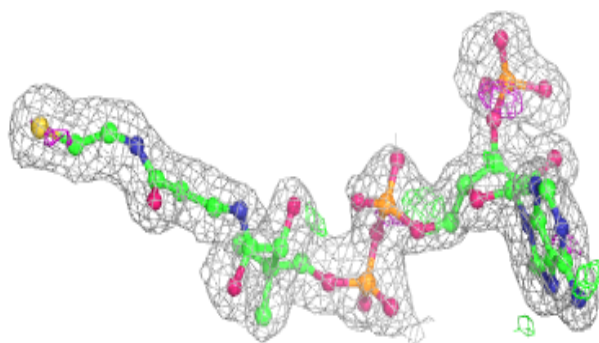
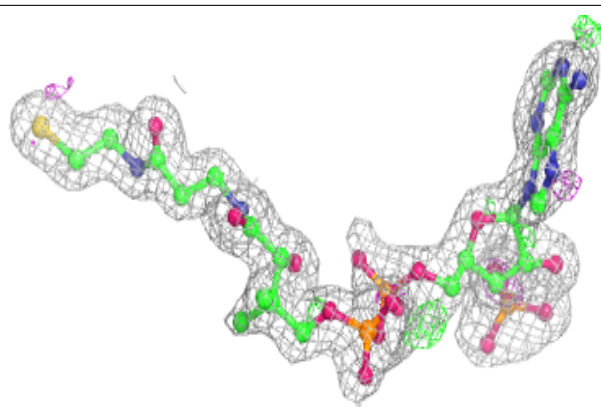
**Electron density around COA F 1071:**

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



**Electron density around COA J 1070:**

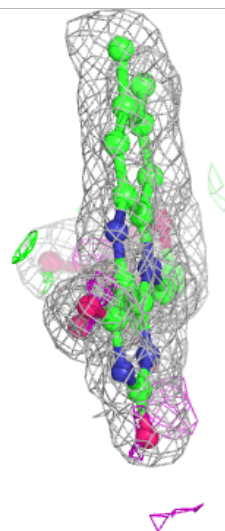
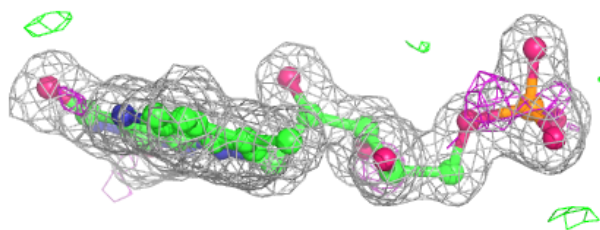
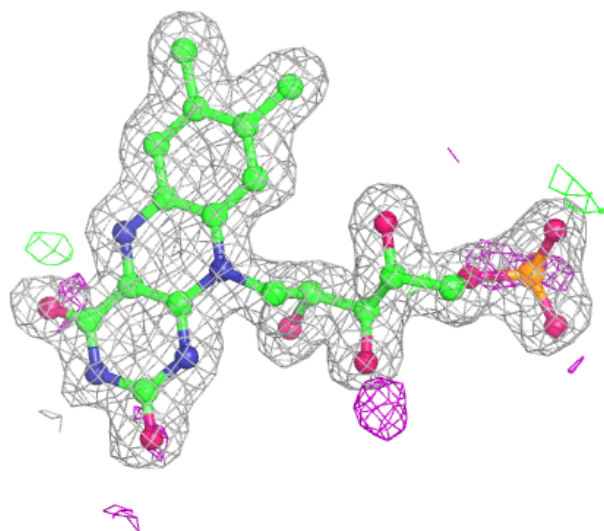
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





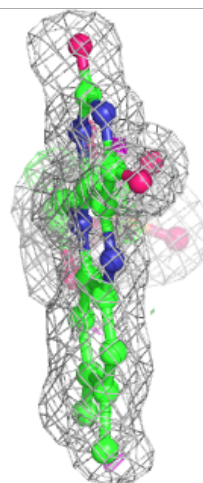
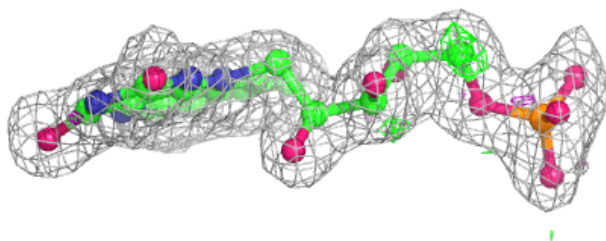
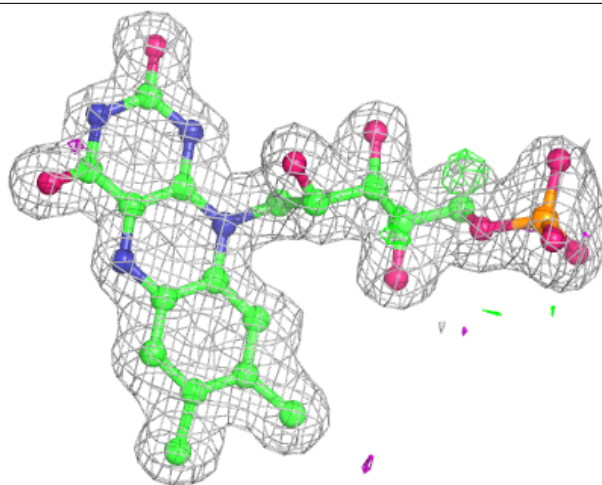
**Electron density around FMN C 1070:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



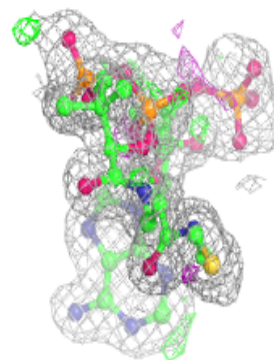
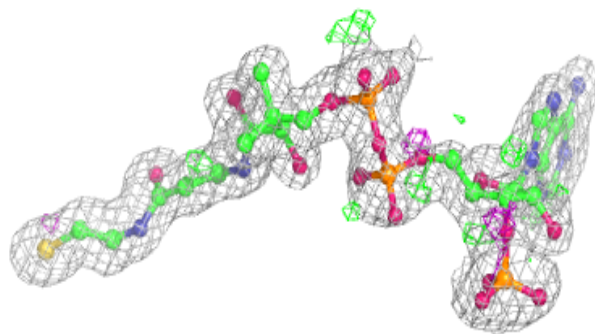
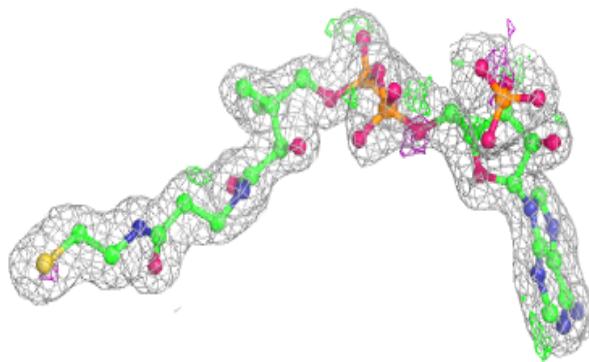
**Electron density around FMN H 1071:**

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



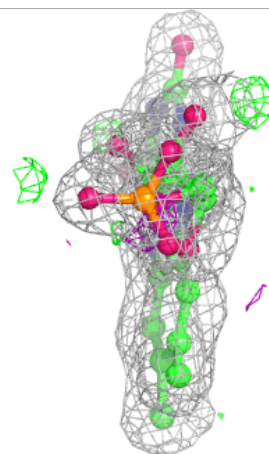
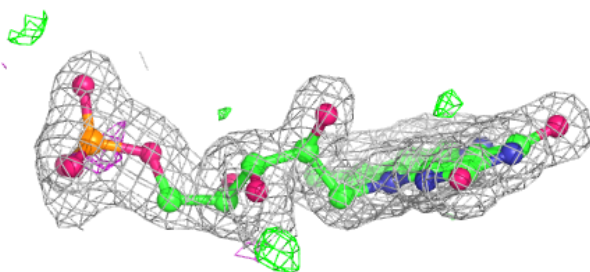
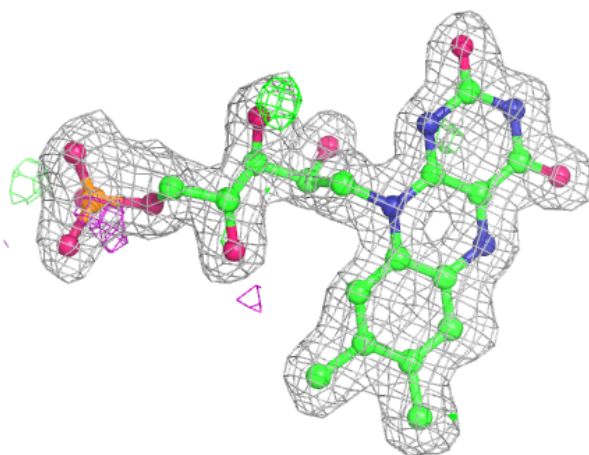
**Electron density around COA D 1071:**

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



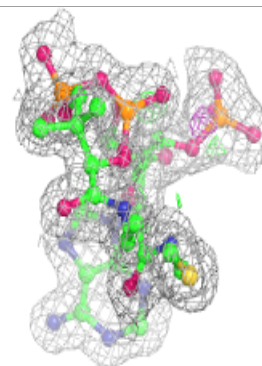
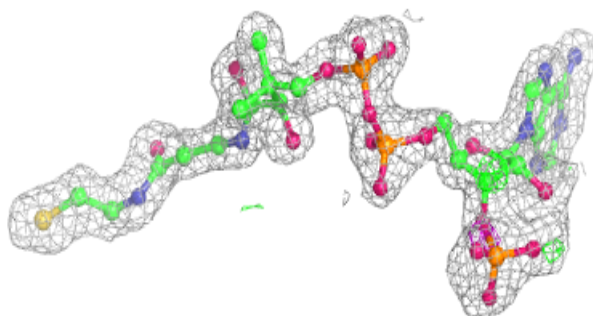
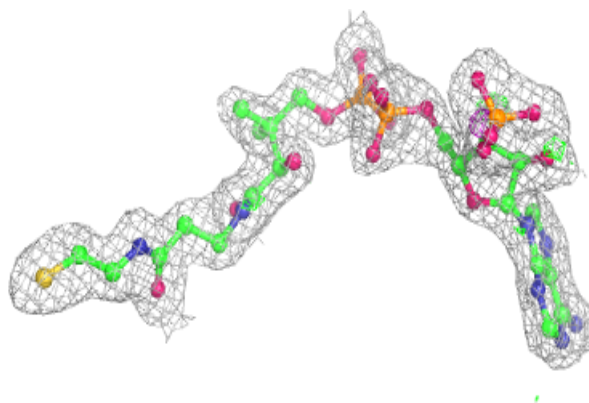
**Electron density around FMN C 1072:**

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



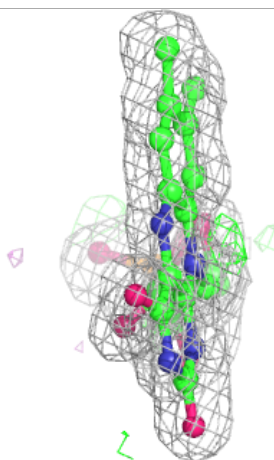
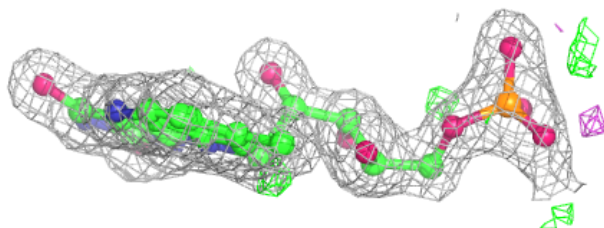
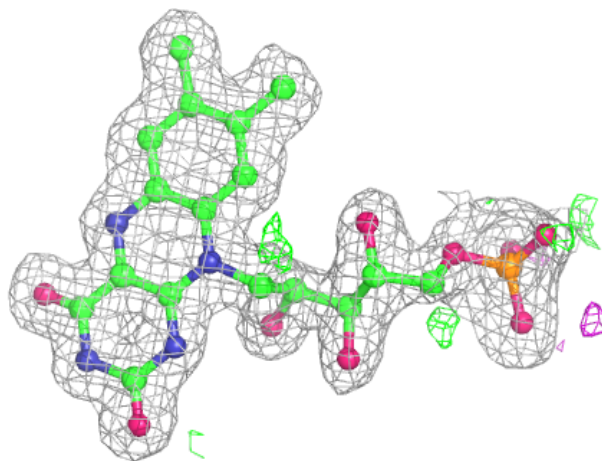
**Electron density around COA C 1071:**

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



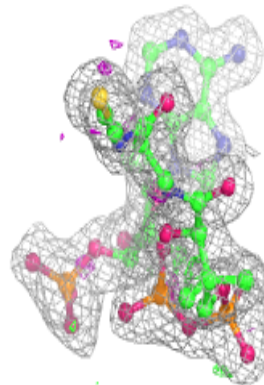
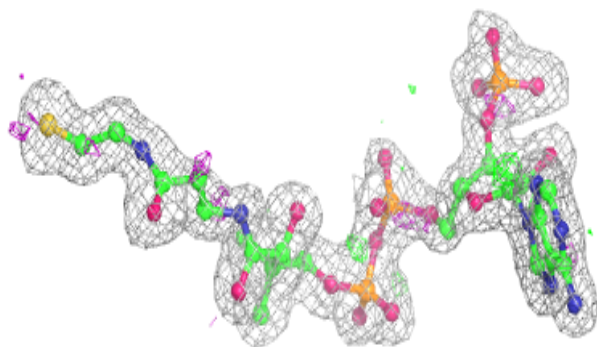
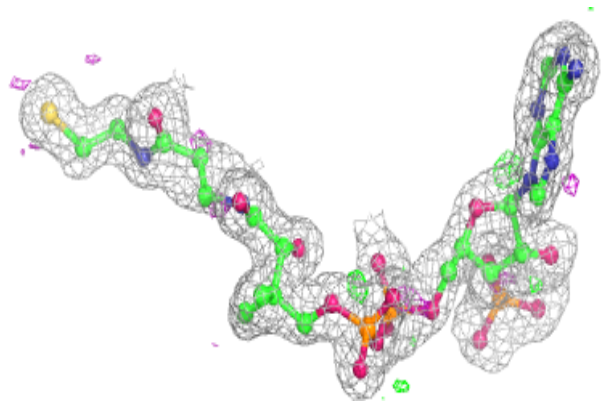
**Electron density around FMN D 1070:**

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

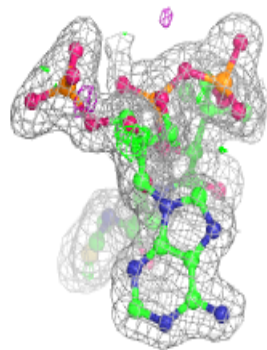
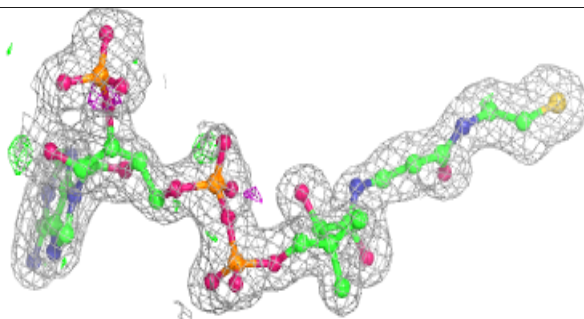
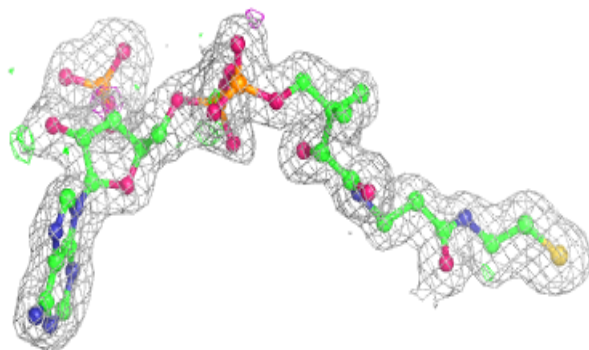


**Electron density around COA B 1069:**

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

**Electron density around COA I 1070:**

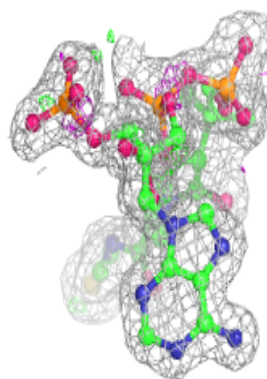
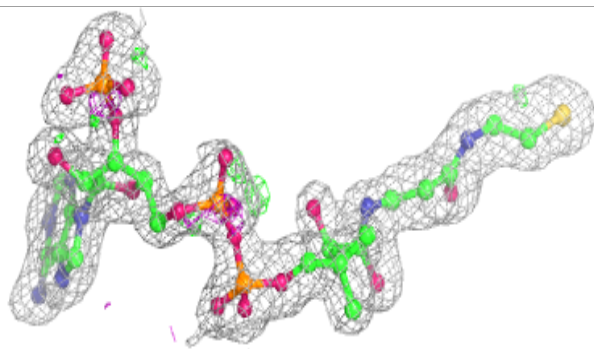
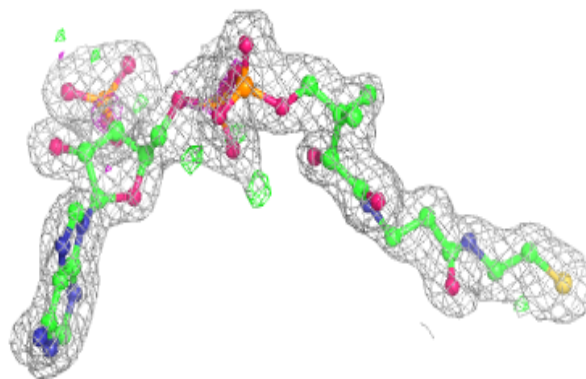
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and green (positive)





**Electron density around COA E 1070:**

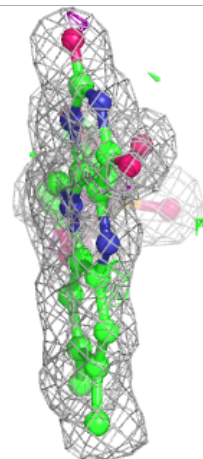
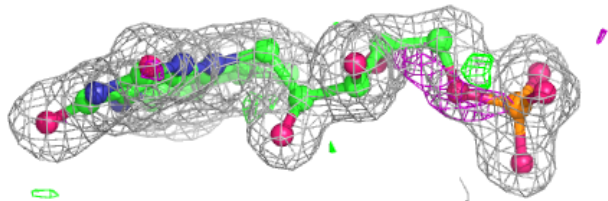
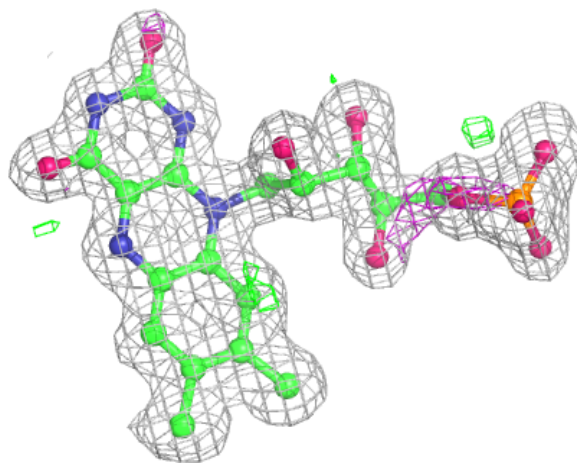
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





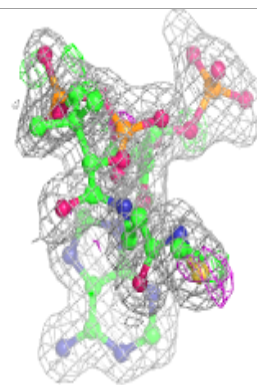
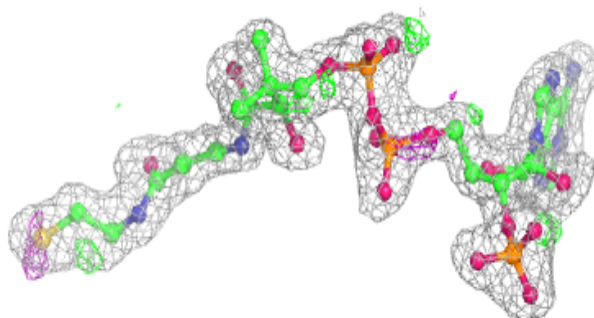
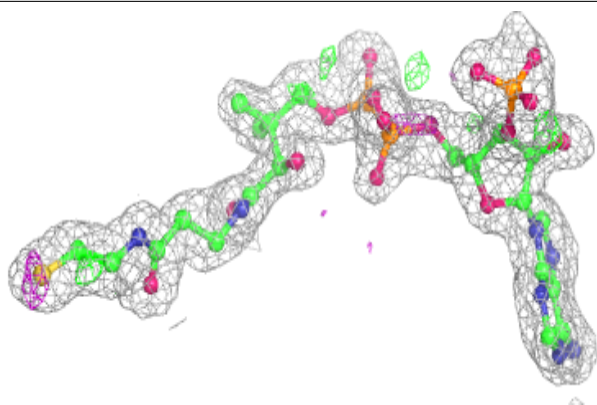
**Electron density around FMN A 1072:**

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



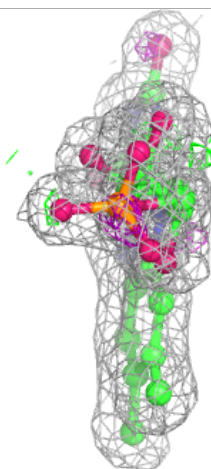
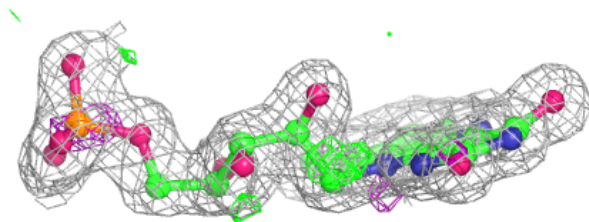
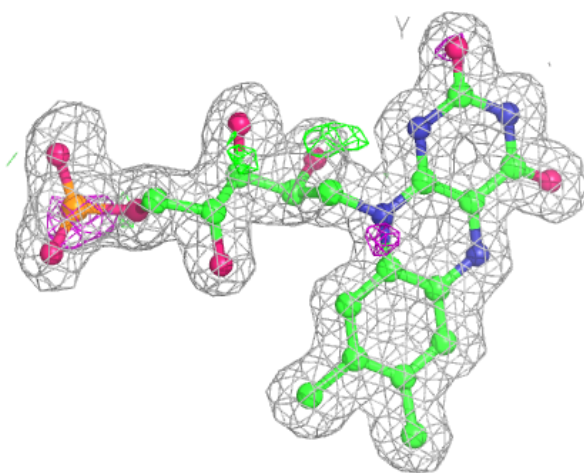
**Electron density around COA G 1070:**

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



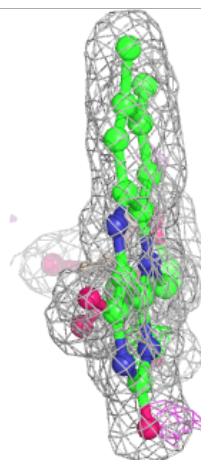
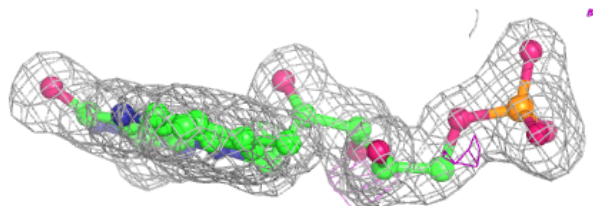
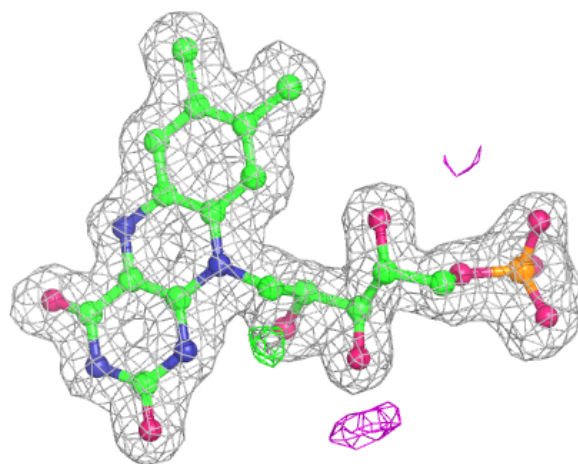
**Electron density around FMN F 1072:**

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



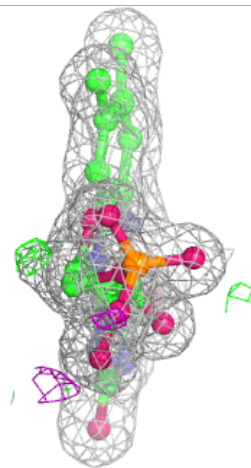
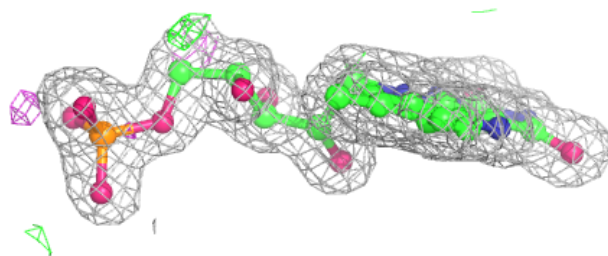
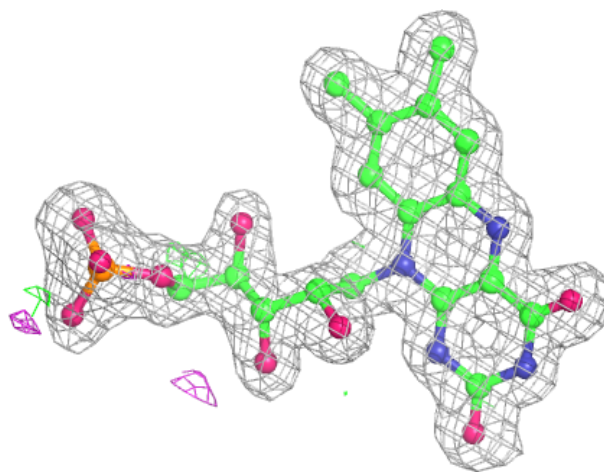
**Electron density around FMN A 1070:**

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



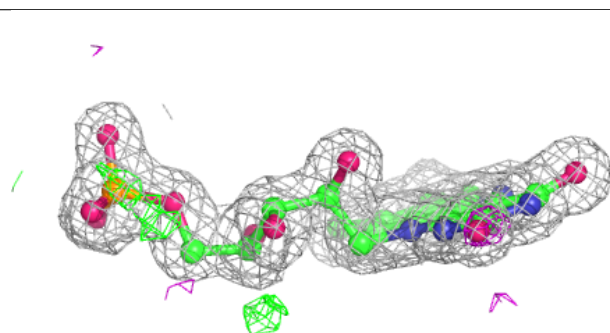
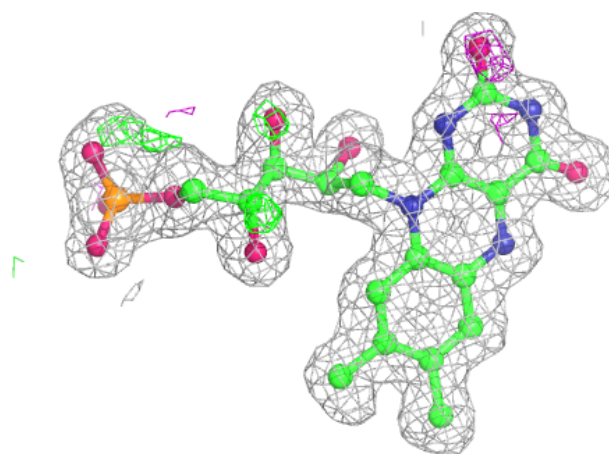
**Electron density around FMN D 1072:**

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



**Electron density around FMN F 1070:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.