



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2021 – 12:21 PM EDT

PDB ID : 7LJT  
Title : Porcine Dihydropyrimidine Dehydrogenase (DPD) soaked with 5-Ethynyluracil (5EU), NADPH - 20 minutes  
Authors : Butrin, A.; Forouzesh, D.; Beaupre, B.; Wawrzak, Z.; Liu, D.; Moran, G.  
Deposited on : 2021-01-30  
Resolution : 1.98 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 : 2.18  
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) : 2.18

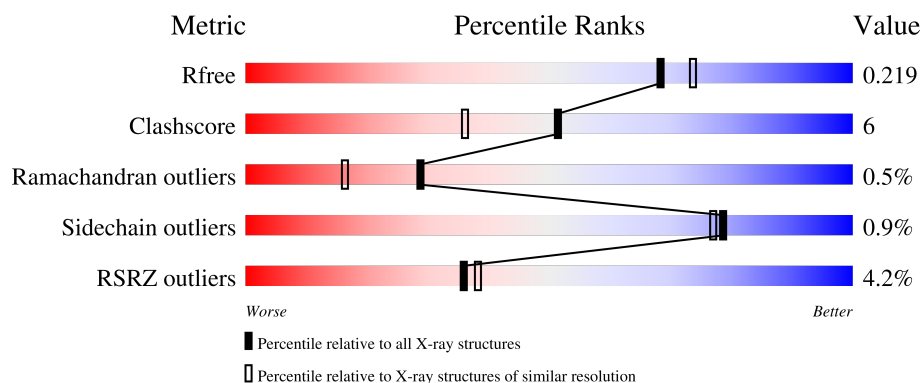
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1025	<div> <div>4%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	B	1025	<div> <div>5%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	C	1025	<div> <div>5%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	D	1025	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35103 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.

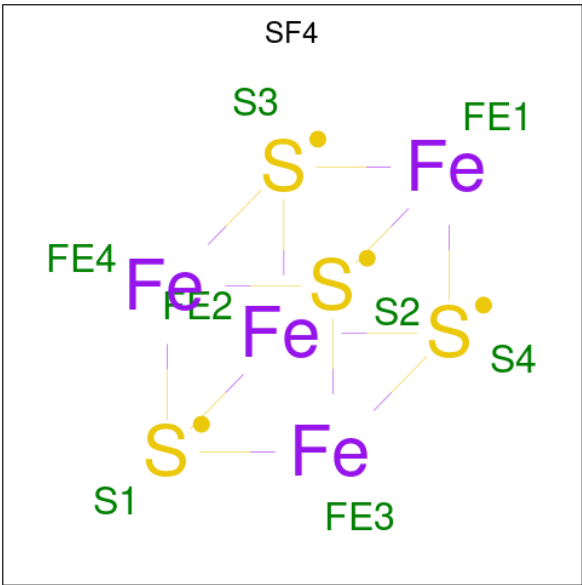
- Molecule 1 is a protein called Dihydropyrimidine dehydrogenase [NADP(+)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	66	0	0
			7694	4880	1302	1459	53			
1	B	1016	Total	C	N	O	S	70	0	0
			7732	4903	1312	1463	54			
1	C	1015	Total	C	N	O	S	0	0	0
			7700	4885	1306	1457	52			
1	D	1017	Total	C	N	O	S	43	0	0
			7721	4898	1311	1458	54			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



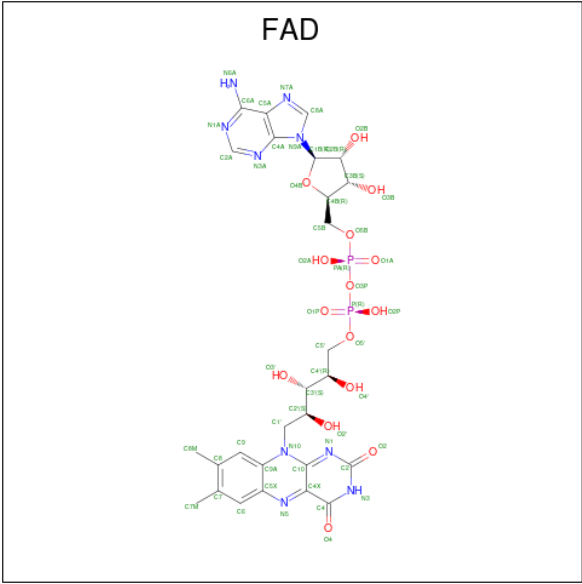
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

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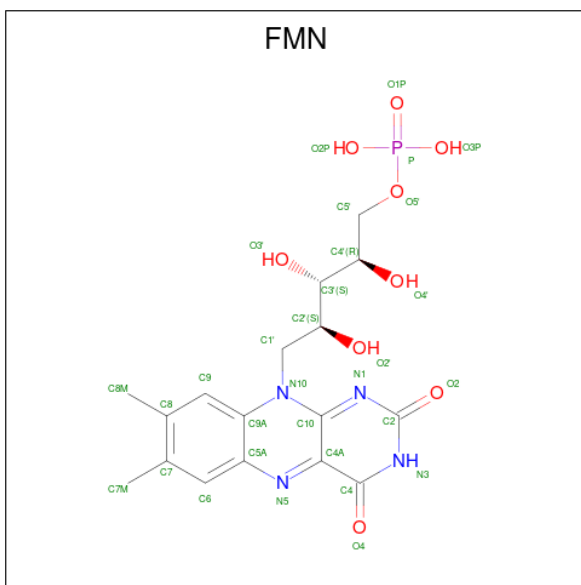
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	D	1	8	4	4	0	0
2	D	1	8	4	4	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



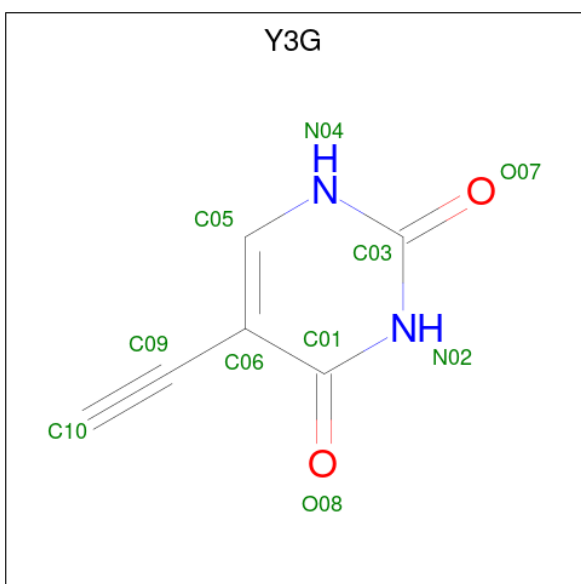
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0
3	C	1	53	27	9	15	2	0	0
3	D	1	53	27	9	15	2	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



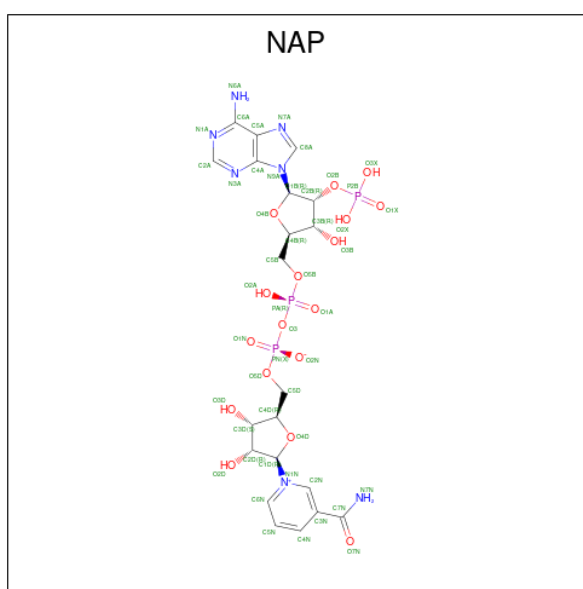
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 5 is 5-ethynylpyrimidine-2,4(1H,3H)-dione (three-letter code: Y3G) (formula:  $C_6H_4N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	6	2	2		
5	B	1	Total	C	N	O	0	0
			10	6	2	2		
5	C	1	Total	C	N	O	0	0
			10	6	2	2		
5	D	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 6 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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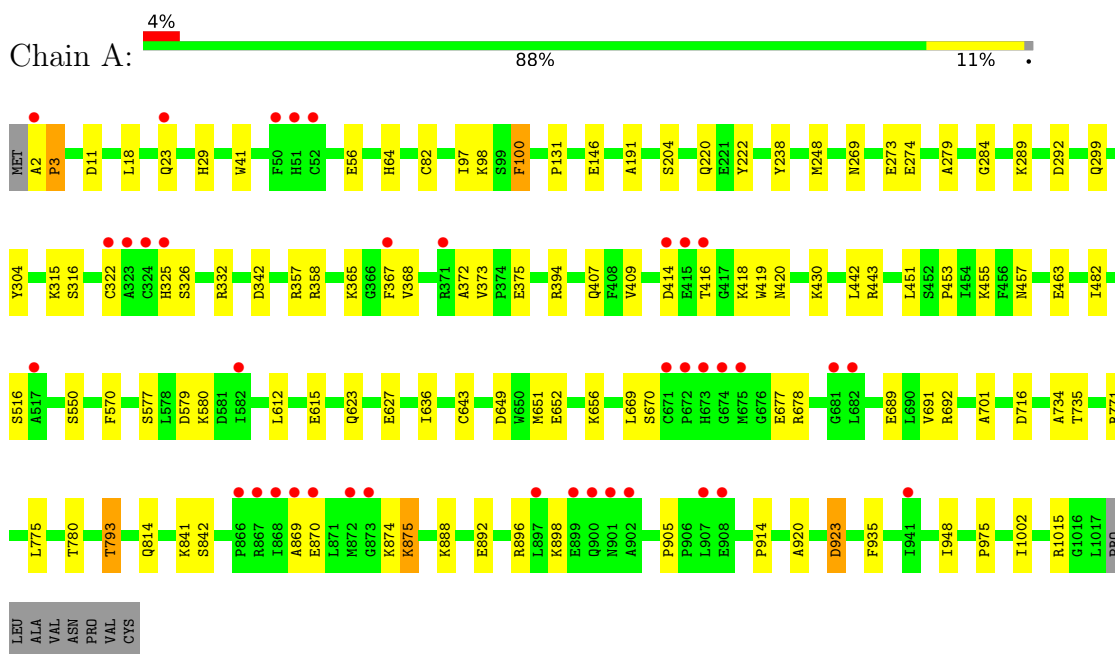
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	818	Total 818	O 818	0	0
7	C	916	Total 916	O 916	0	0
7	D	955	Total 955	O 955	0	0



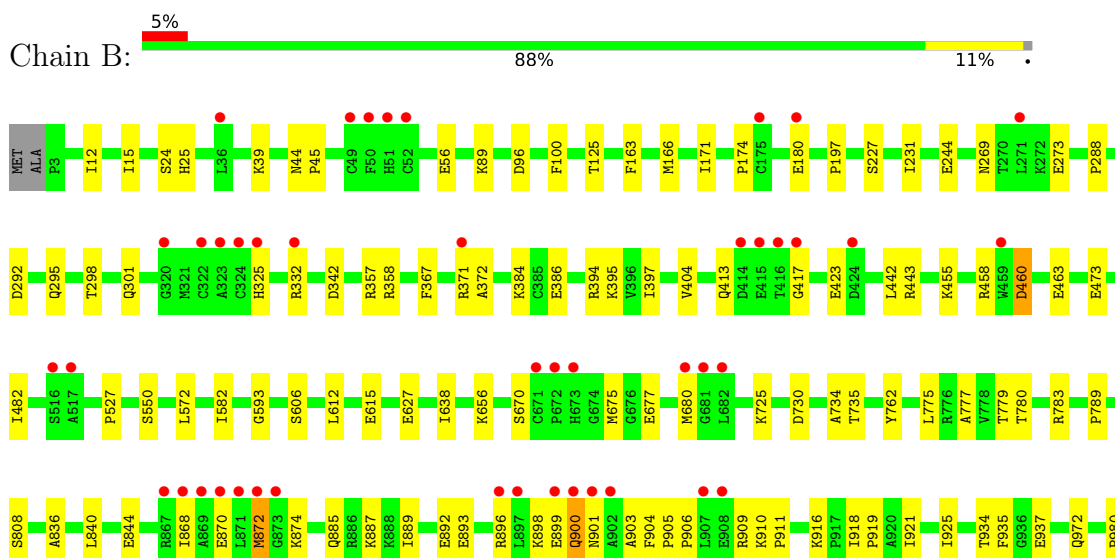
### 3 Residue-property plots

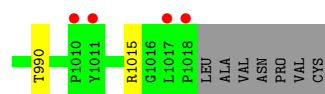
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Dihydropyrimidine dehydrogenase [NAD(+)]

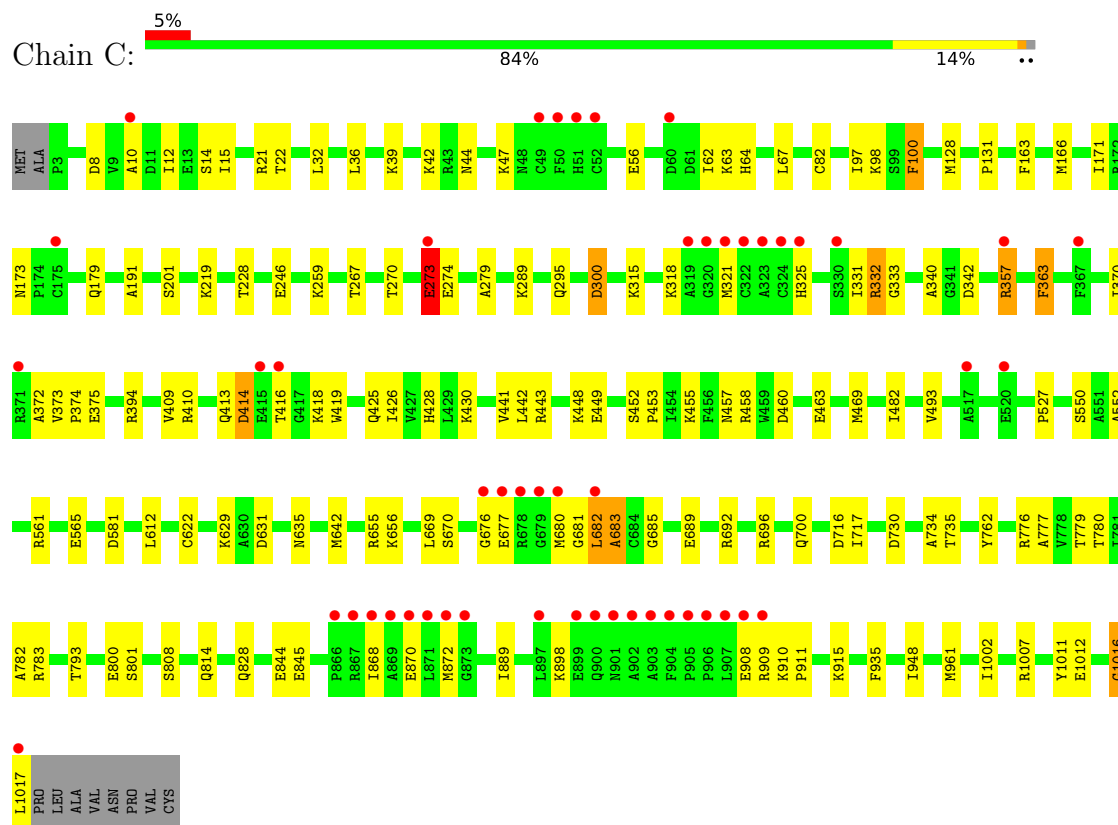


• Molecule 1: Dihydropyrimidine dehydrogenase [NAD(+)]

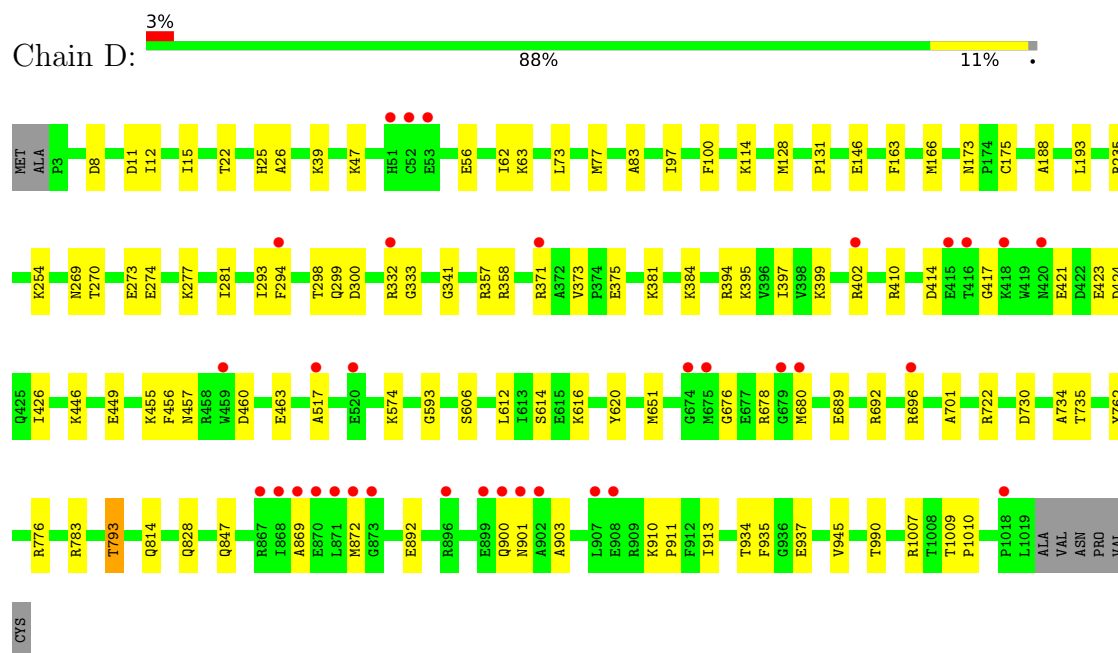




- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.25Å 158.86Å 162.10Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	60.53 – 1.98 71.26 – 1.98	Depositor EDS
% Data completeness (in resolution range)	88.5 (60.53-1.98) 88.5 (71.26-1.98)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.183 , 0.219 0.183 , 0.219	Depositor DCC
$R_{free}$ test set	12778 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.8	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	35103	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: FMN, FAD, Y3G, SF4, NAP

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	0.43	0/7851	0.63	0/10646
1	B	0.43	0/7892	0.63	1/10697 (0.0%)
1	C	0.45	0/7858	0.79	6/10654 (0.1%)
1	D	0.44	0/7881	0.64	0/10686
All	All	0.44	0/31482	0.67	7/42683 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	5

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	GLU	OE1-CD-OE2	-32.47	84.34	123.30
1	C	273	GLU	CG-CD-OE1	21.28	160.86	118.30
1	C	273	GLU	CG-CD-OE2	-16.92	84.47	118.30
1	C	682	LEU	CB-CG-CD2	-6.88	99.30	111.00
1	B	460	ASP	CB-CG-OD2	6.20	123.88	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1016	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	21	ARG	Sidechain
1	C	273	GLU	Sidechain
1	C	458	ARG	Sidechain
1	C	681	GLY	Peptide

## 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	7694	0	7695	84	1
1	B	7732	0	7754	84	1
1	C	7700	0	7708	108	2
1	D	7721	0	7732	86	1
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
3	A	53	0	31	2	0
3	B	53	0	31	1	0
3	C	53	0	31	2	0
3	D	53	0	31	2	0
4	A	31	0	19	1	0
4	B	31	0	19	1	0
4	C	31	0	19	2	0
4	D	31	0	19	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	A	48	0	25	6	0
6	B	48	0	25	3	0
6	C	48	0	24	4	0
6	D	48	0	24	3	0
7	A	871	0	0	21	2
7	B	818	0	0	28	2
7	C	916	0	0	27	2
7	D	955	0	0	32	2
All	All	35103	0	31187	347	7

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 6.

The worst 5 of 347 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:C:844:GLU:HG3	1:C:915:LYS:HG3	1.32	1.10
1:D:696:ARG:NH1	7:D:1202:HOH:O	1.93	1.01
1:D:381:LYS:NZ	7:D:1203:HOH:O	1.96	0.99
1:D:455:LYS:NZ	1:D:463:GLU:OE2	1.98	0.97
1:B:371:ARG:HG2	7:B:1240:HOH:O	1.68	0.93

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1828:HOH:O	7:C:1965:HOH:O[2_645]	1.98	0.22
7:A:1997:HOH:O	7:B:1929:HOH:O[1_455]	1.99	0.21
1:B:460:ASP:OD2	1:D:395:LYS:NZ[1_656]	2.00	0.20
7:C:2108:HOH:O	7:D:2143:HOH:O[1_655]	2.05	0.15
1:A:443:ARG:NH1	1:C:295:GLN:OE1[1_556]	2.06	0.14

## 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	1014/1025 (99%)	965 (95%)	43 (4%)	6 (1%)	25	14
1	B	1014/1025 (99%)	968 (96%)	38 (4%)	8 (1%)	19	9
1	C	1013/1025 (99%)	967 (96%)	41 (4%)	5 (0%)	29	16
1	D	1015/1025 (99%)	971 (96%)	41 (4%)	3 (0%)	41	29
All	All	4056/4100 (99%)	3871 (95%)	163 (4%)	22 (0%)	29	16

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	905	PRO
1	B	180	GLU
1	B	905	PRO
1	C	414	ASP
1	C	677	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	832/854 (97%)	824 (99%)	8 (1%)	76	73
1	B	841/854 (98%)	836 (99%)	5 (1%)	86	85
1	C	833/854 (98%)	824 (99%)	9 (1%)	73	70
1	D	837/854 (98%)	830 (99%)	7 (1%)	81	80
All	All	3343/3416 (98%)	3314 (99%)	29 (1%)	78	77

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	64	HIS
1	D	680	MET
1	C	332	ARG
1	D	173	ASN
1	C	300	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	106	ASN
1	D	173	ASN
1	A	269	ASN
1	A	804	GLN
1	B	301	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

32 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	$\# Z  > 2$
5	Y3G	D	1107	-	9,10,10	2.25	4 (44%)	6,13,13	6.06	5 (83%)
4	FMN	B	1106	-	31,33,33	1.43	3 (9%)	40,50,50	1.55	5 (12%)
2	SF4	B	1104	1	0,12,12	0.00	-	-		
5	Y3G	A	1107	-	9,10,10	2.14	5 (55%)	6,13,13	5.72	5 (83%)
2	SF4	A	1102	1	0,12,12	0.00	-	-		
3	FAD	A	1105	-	51,58,58	1.29	5 (9%)	60,89,89	2.17	7 (11%)
2	SF4	D	1103	1	0,12,12	0.00	-	-		
6	NAP	B	1108	-	45,52,52	2.69	16 (35%)	56,80,80	1.88	11 (19%)
3	FAD	B	1105	-	51,58,58	1.29	6 (11%)	60,89,89	2.25	7 (11%)
2	SF4	B	1101	1	0,12,12	0.00	-	-		
2	SF4	D	1104	1	0,12,12	0.00	-	-		
2	SF4	B	1103	1	0,12,12	0.00	-	-		
2	SF4	B	1102	1	0,12,12	0.00	-	-		
2	SF4	C	1103	1	0,12,12	0.00	-	-		
6	NAP	A	1108	-	45,52,52	2.83	11 (24%)	56,80,80	1.93	14 (25%)
3	FAD	D	1105	-	51,58,58	1.19	5 (9%)	60,89,89	2.20	7 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SF4	A	1104	1	0,12,12	0.00	-	-		
4	FMN	C	1106	-	31,33,33	1.62	6 (19%)	40,50,50	1.55	6 (15%)
2	SF4	D	1102	1	0,12,12	0.00	-	-		
4	FMN	D	1106	-	31,33,33	1.34	5 (16%)	40,50,50	1.62	6 (15%)
2	SF4	D	1101	1	0,12,12	0.00	-	-		
2	SF4	A	1101	1	0,12,12	0.00	-	-		
2	SF4	A	1103	1	0,12,12	0.00	-	-		
3	FAD	C	1105	-	51,58,58	1.25	5 (9%)	60,89,89	2.21	7 (11%)
5	Y3G	B	1107	-	9,10,10	2.13	3 (33%)	6,13,13	5.61	5 (83%)
2	SF4	C	1104	1	0,12,12	0.00	-	-		
6	NAP	D	1108	-	45,52,52	2.74	14 (31%)	56,80,80	2.07	16 (28%)
4	FMN	A	1106	-	31,33,33	1.38	5 (16%)	40,50,50	1.53	8 (20%)
2	SF4	C	1101	1	0,12,12	0.00	-	-		
6	NAP	C	1108	-	45,52,52	2.69	10 (22%)	56,80,80	1.92	13 (23%)
2	SF4	C	1102	1	0,12,12	0.00	-	-		
5	Y3G	C	1107	-	9,10,10	2.10	3 (33%)	6,13,13	5.99	5 (83%)

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
5	Y3G	D	1107	-	-	0/0/2/2	0/1/1/1
4	FMN	B	1106	-	-	4/18/18/18	0/3/3/3
5	Y3G	A	1107	-	-	0/0/2/2	0/1/1/1
2	SF4	B	1104	1	-	-	0/6/5/5
2	SF4	A	1102	1	-	-	0/6/5/5
3	FAD	A	1105	-	-	2/30/50/50	0/6/6/6
6	NAP	B	1108	-	-	6/31/67/67	0/5/5/5
2	SF4	D	1103	1	-	-	0/6/5/5
3	FAD	B	1105	-	-	2/30/50/50	0/6/6/6
2	SF4	B	1101	1	-	-	0/6/5/5
2	SF4	D	1104	1	-	-	0/6/5/5
2	SF4	B	1103	1	-	-	0/6/5/5
2	SF4	B	1102	1	-	-	0/6/5/5
6	NAP	A	1108	-	-	4/31/67/67	0/5/5/5
2	SF4	C	1103	1	-	-	0/6/5/5
3	FAD	D	1105	-	-	1/30/50/50	0/6/6/6
2	SF4	A	1104	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	C	1106	-	-	1/18/18/18	0/3/3/3
2	SF4	D	1102	1	-	-	0/6/5/5
4	FMN	D	1106	-	-	3/18/18/18	0/3/3/3
2	SF4	D	1101	1	-	-	0/6/5/5
2	SF4	A	1101	1	-	-	0/6/5/5
3	FAD	C	1105	-	-	1/30/50/50	0/6/6/6
5	Y3G	B	1107	-	-	0/0/2/2	0/1/1/1
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	C	1104	1	-	-	0/6/5/5
6	NAP	D	1108	-	-	5/31/67/67	0/5/5/5
4	FMN	A	1106	-	-	1/18/18/18	0/3/3/3
2	SF4	C	1101	1	-	-	0/6/5/5
6	NAP	C	1108	-	-	1/31/67/67	0/5/5/5
2	SF4	C	1102	1	-	-	0/6/5/5
5	Y3G	C	1107	-	-	0/0/2/2	0/1/1/1

The worst 5 of 106 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1108	NAP	P2B-O2B	12.91	1.83	1.59
6	D	1108	NAP	P2B-O2B	12.83	1.83	1.59
6	A	1108	NAP	P2B-O2B	12.42	1.82	1.59
6	B	1108	NAP	P2B-O2B	11.59	1.81	1.59
6	A	1108	NAP	C4N-C3N	7.01	1.51	1.39

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1105	FAD	C4-N3-C2	13.33	126.40	115.14
3	C	1105	FAD	C4-N3-C2	12.92	126.05	115.14
3	D	1105	FAD	C4-N3-C2	12.82	125.97	115.14
3	A	1105	FAD	C4-N3-C2	12.71	125.87	115.14
5	D	1107	Y3G	N04-C03-N02	-10.94	119.73	128.43

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1105	FAD	PA-O3P-P-O5'
6	B	1108	NAP	C5D-O5D-PN-O1N
6	D	1108	NAP	C2B-O2B-P2B-O2X

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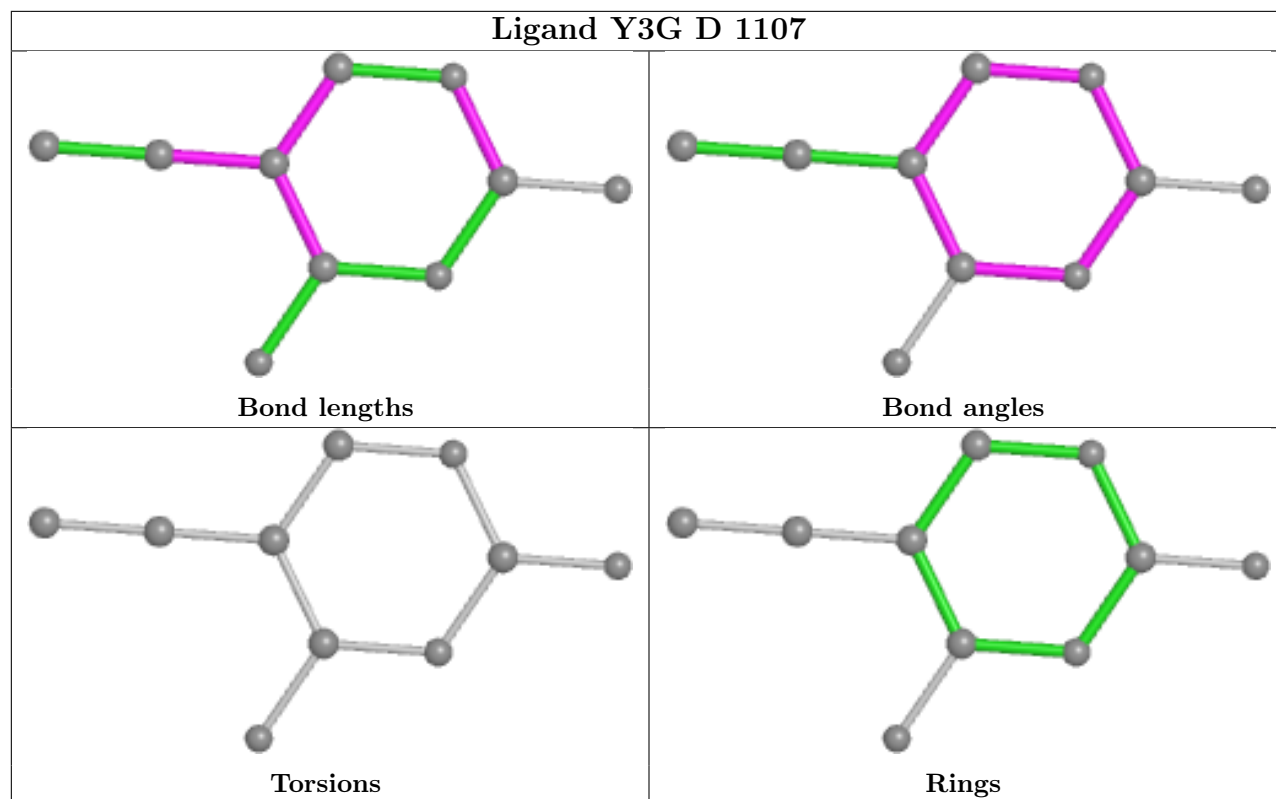
Mol	Chain	Res	Type	Atoms
6	D	1108	NAP	O4D-C1D-N1N-C2N
6	A	1108	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

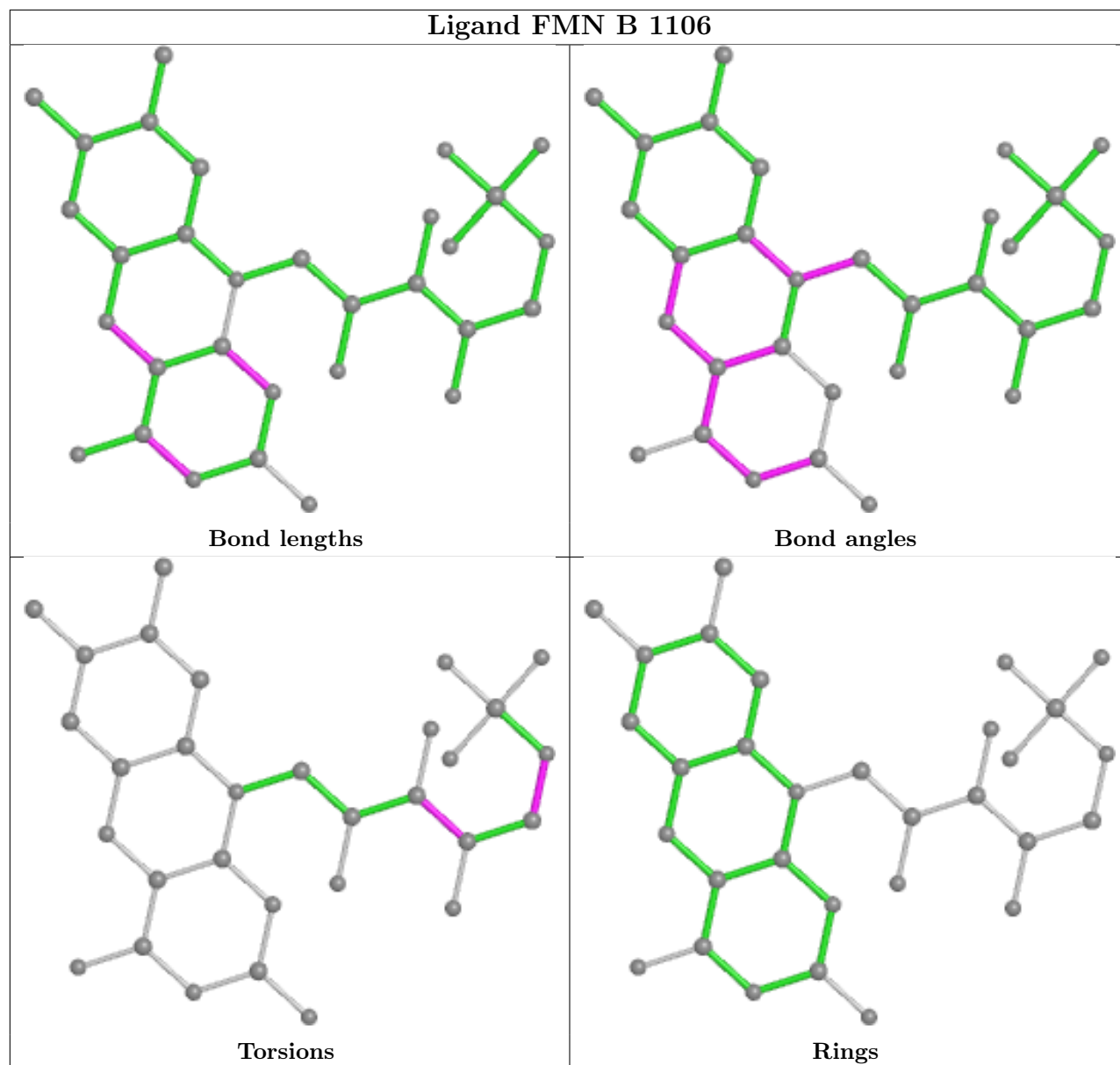
11 monomers are involved in 20 short contacts:

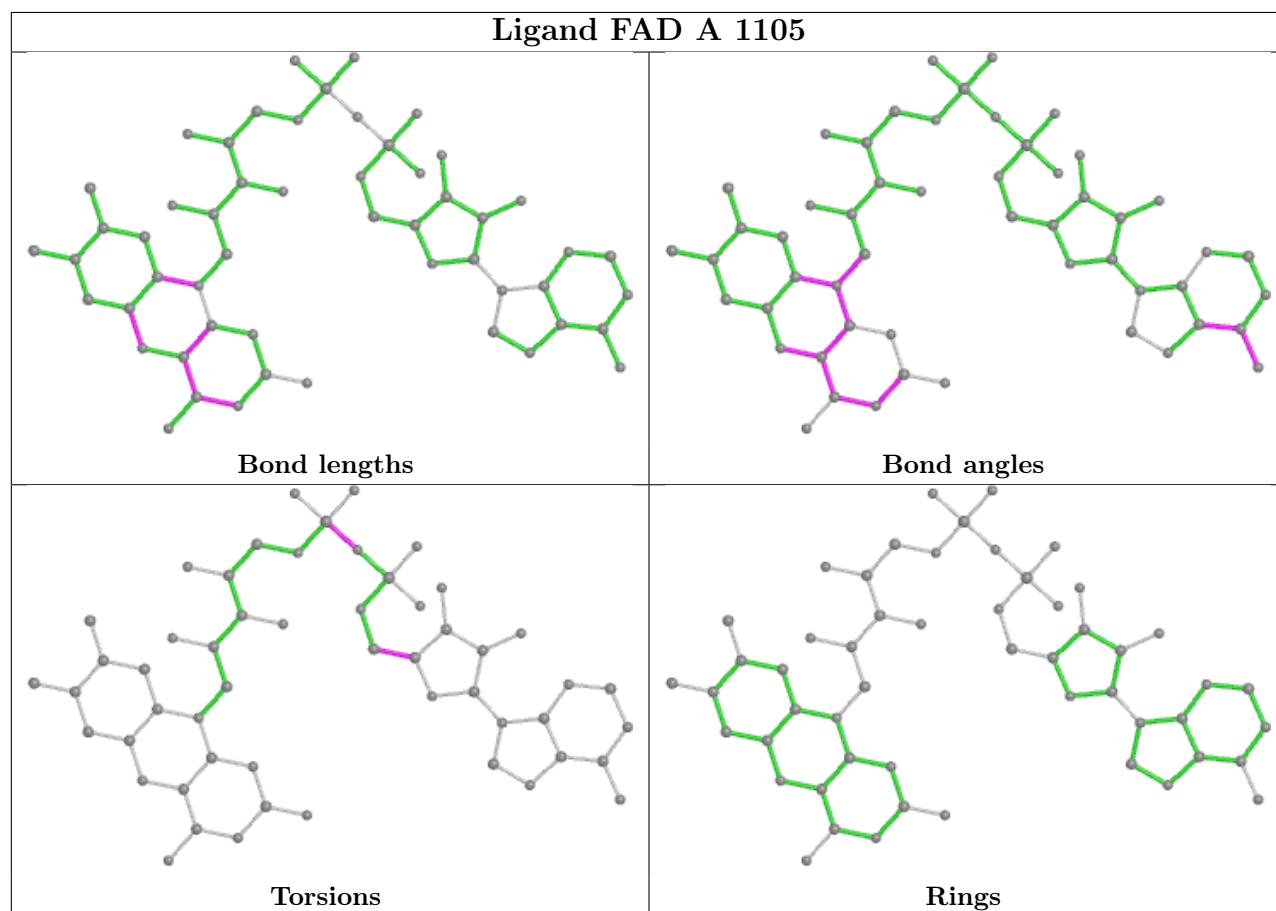
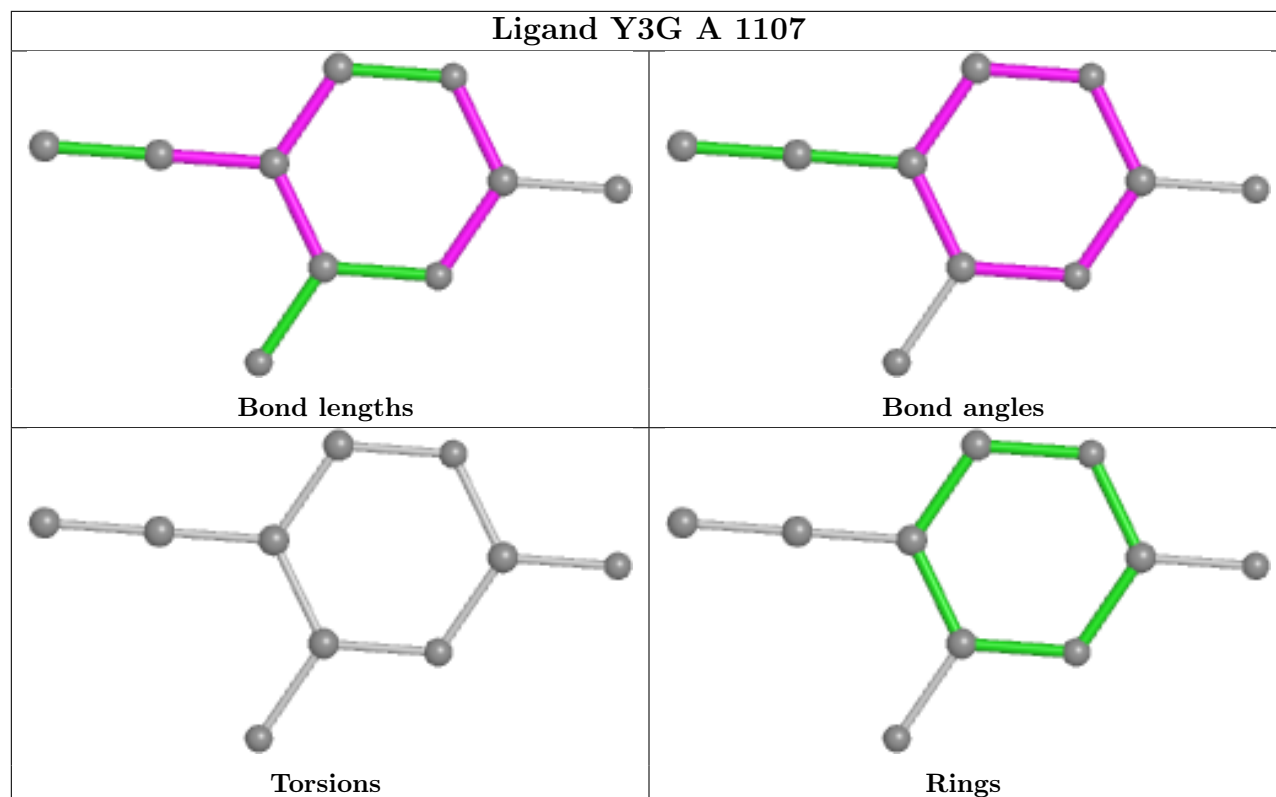
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1106	FMN	1	0
3	A	1105	FAD	2	0
6	B	1108	NAP	3	0
3	B	1105	FAD	1	0
6	A	1108	NAP	6	0
3	D	1105	FAD	2	0
4	C	1106	FMN	2	0
3	C	1105	FAD	2	0
6	D	1108	NAP	3	0
4	A	1106	FMN	1	0
6	C	1108	NAP	4	0

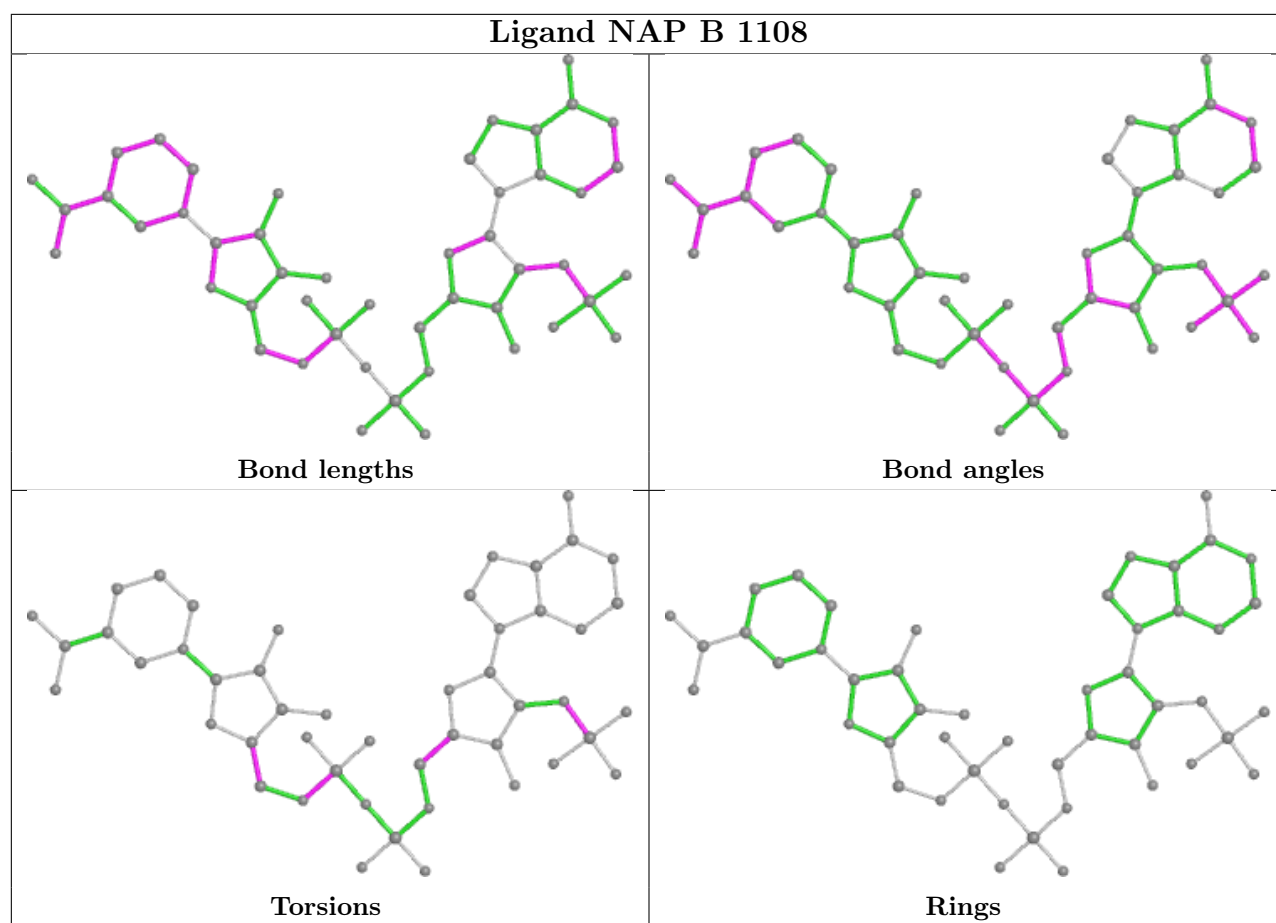
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

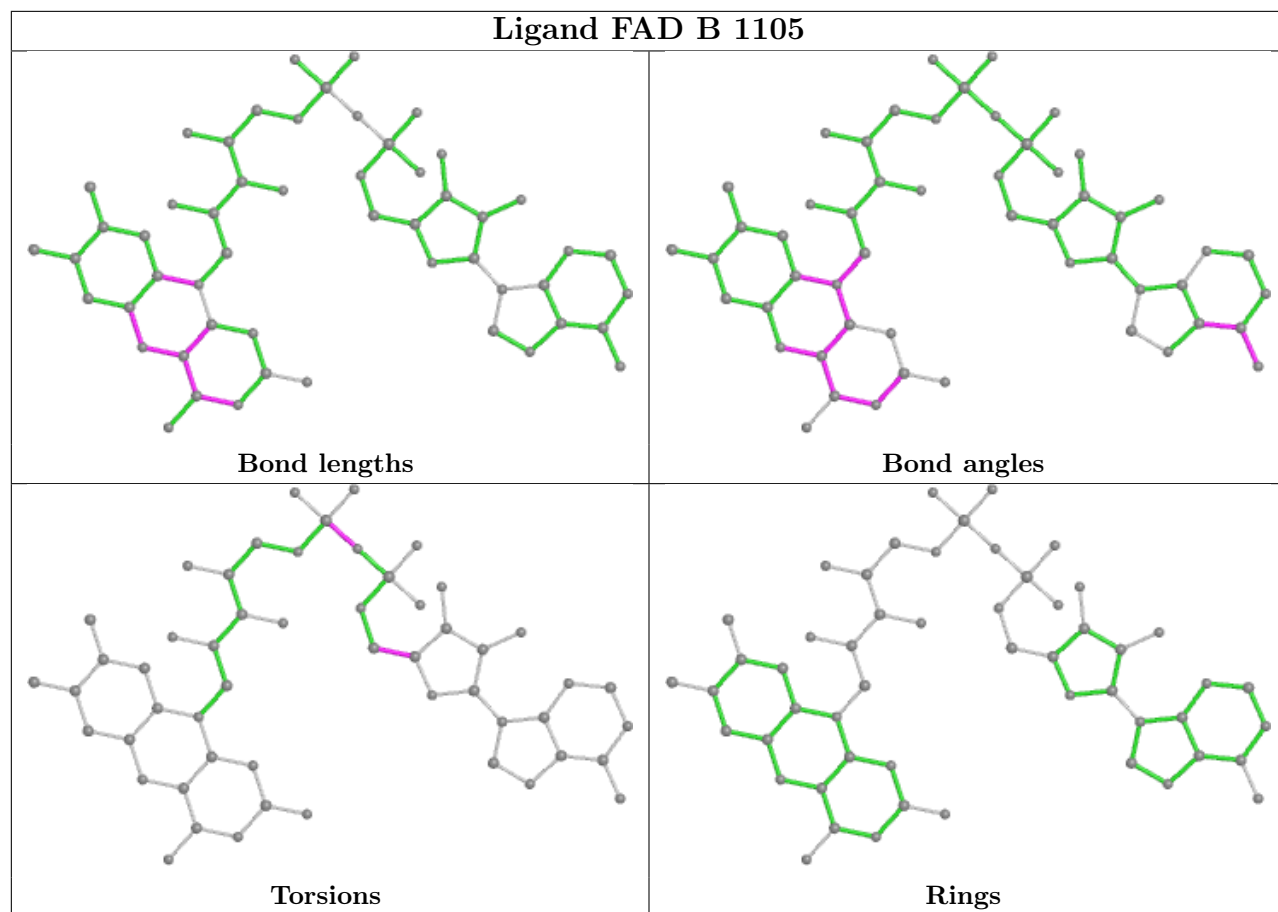


## Ligand FMN B 1106

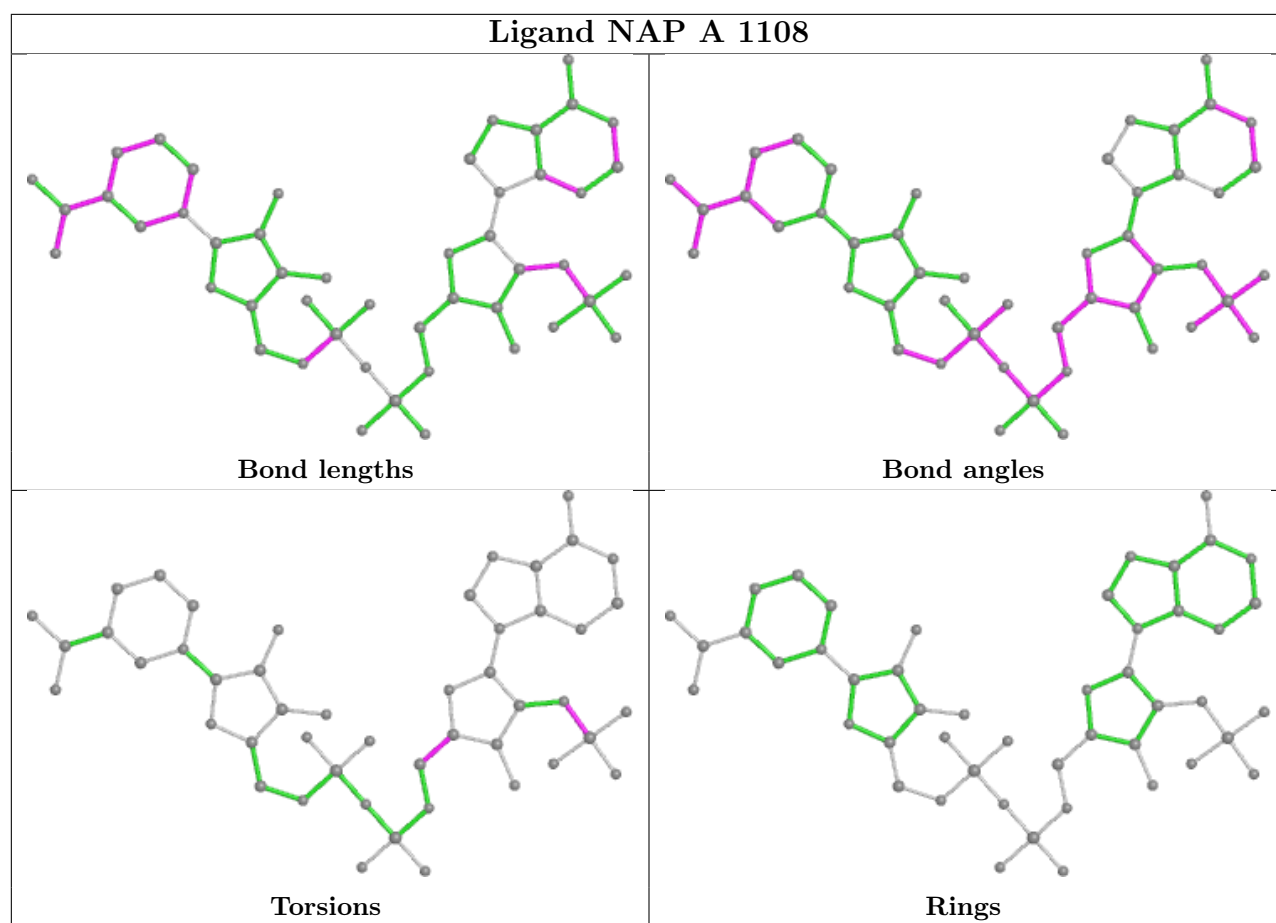


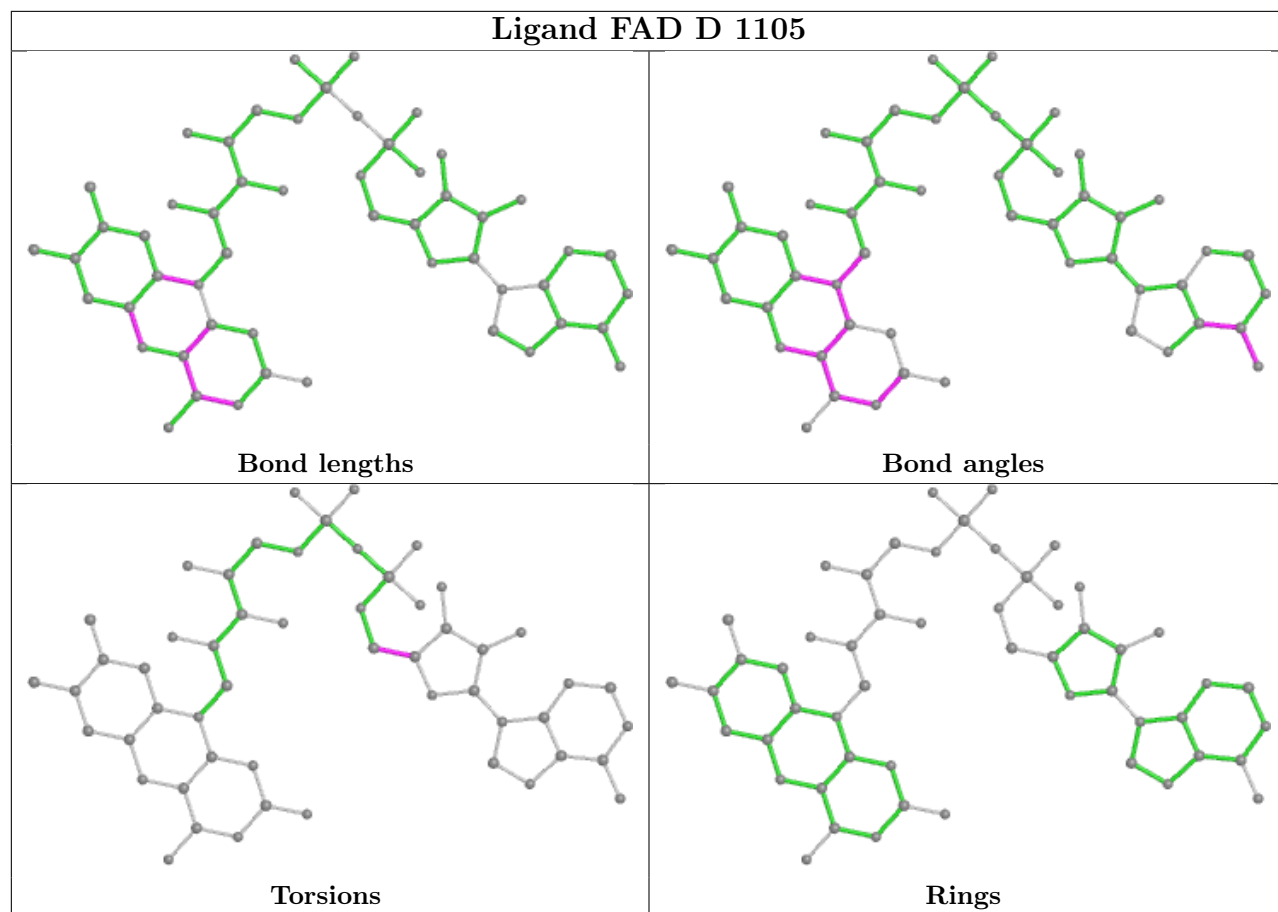




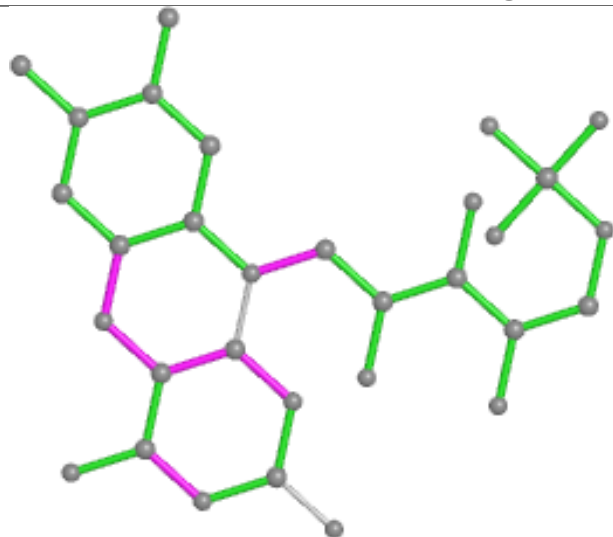




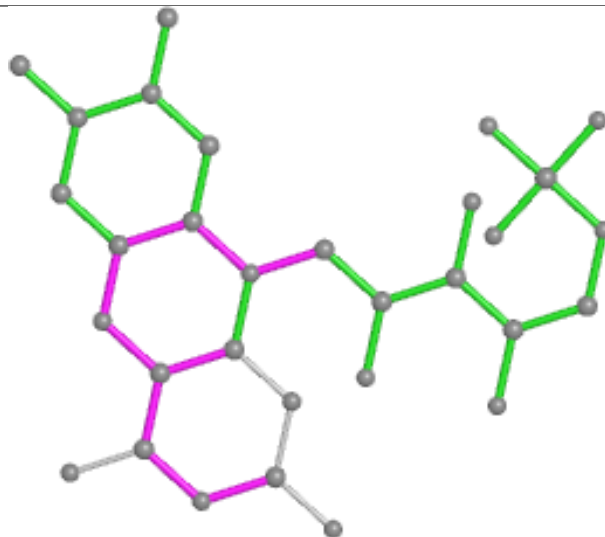




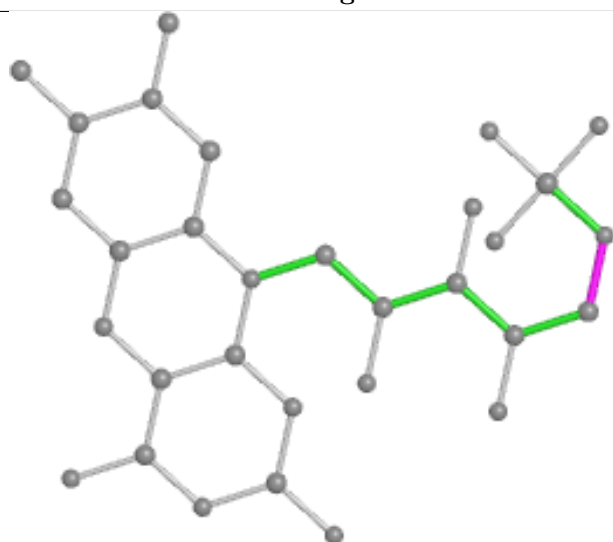
## Ligand FMN C 1106



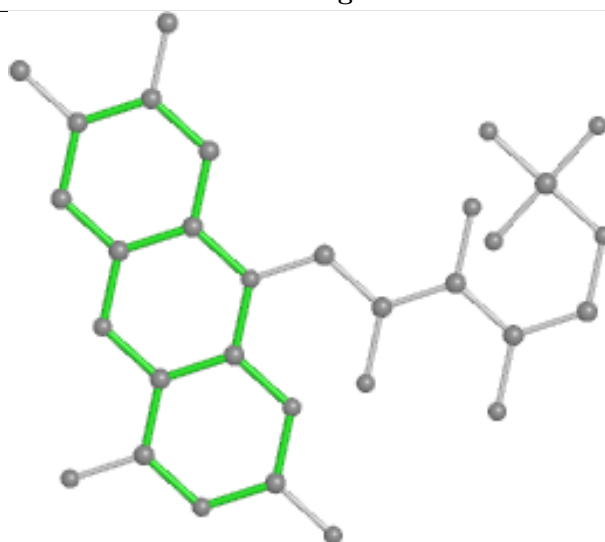
Bond lengths



Bond angles

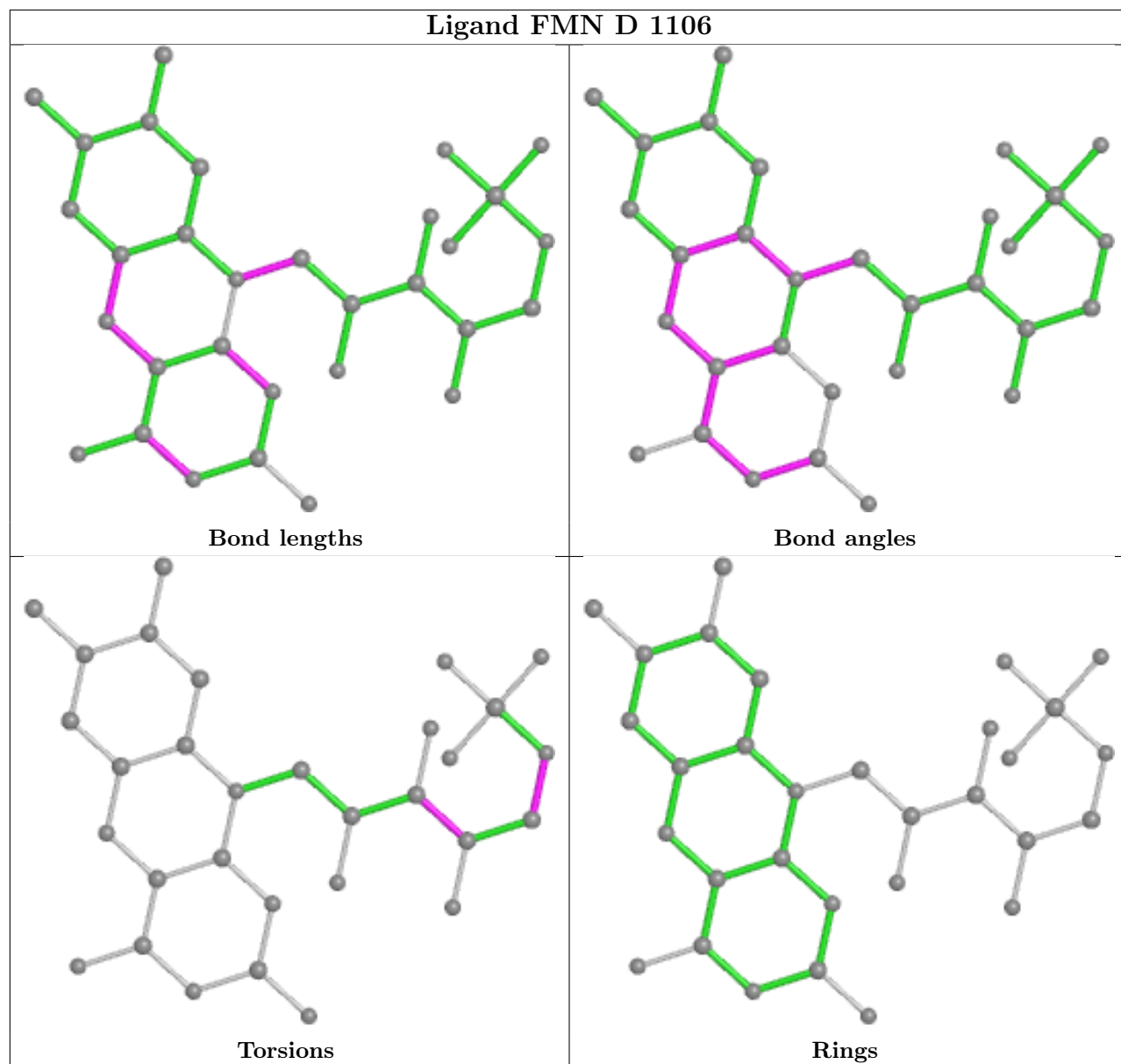


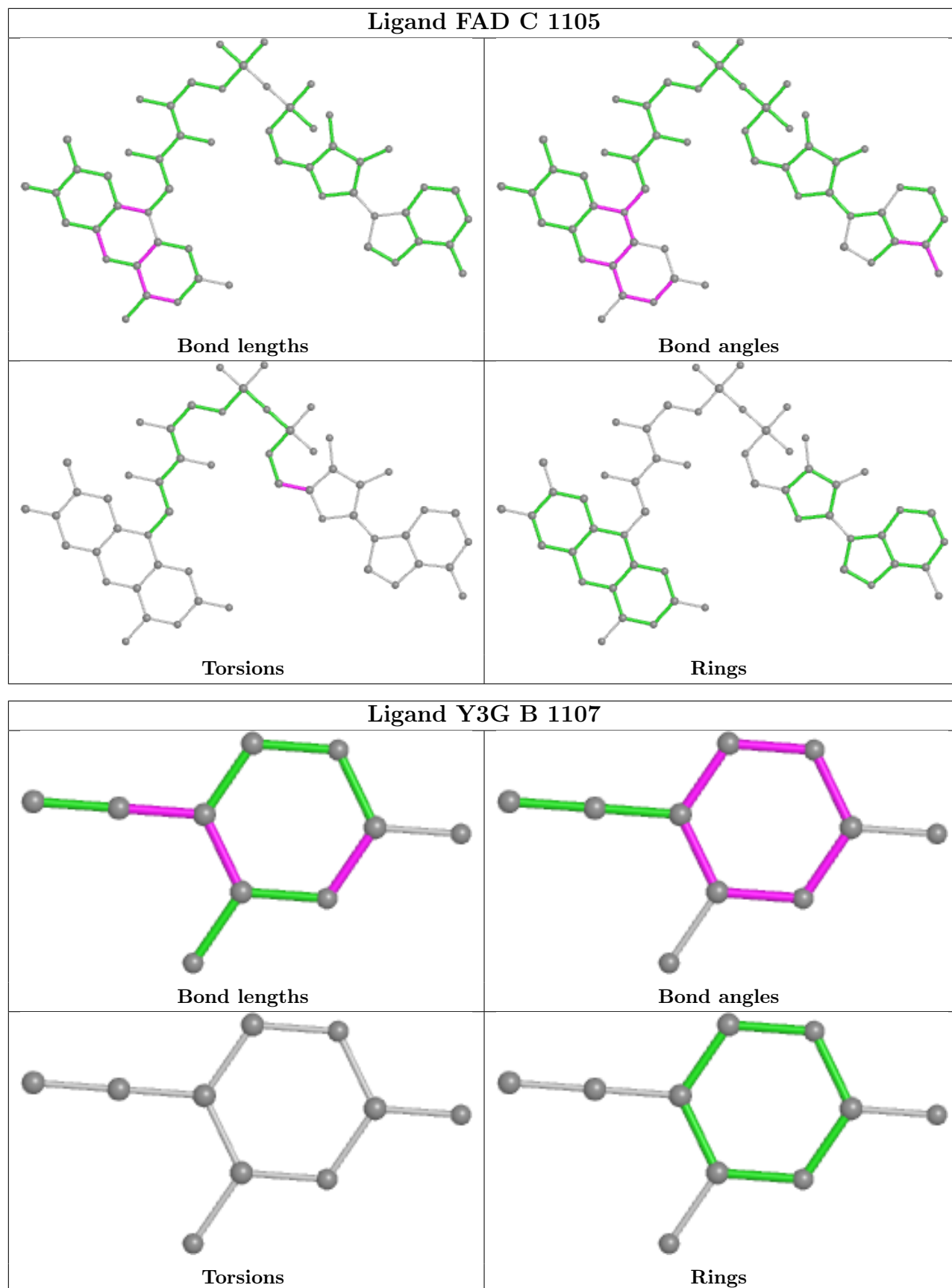
Torsions

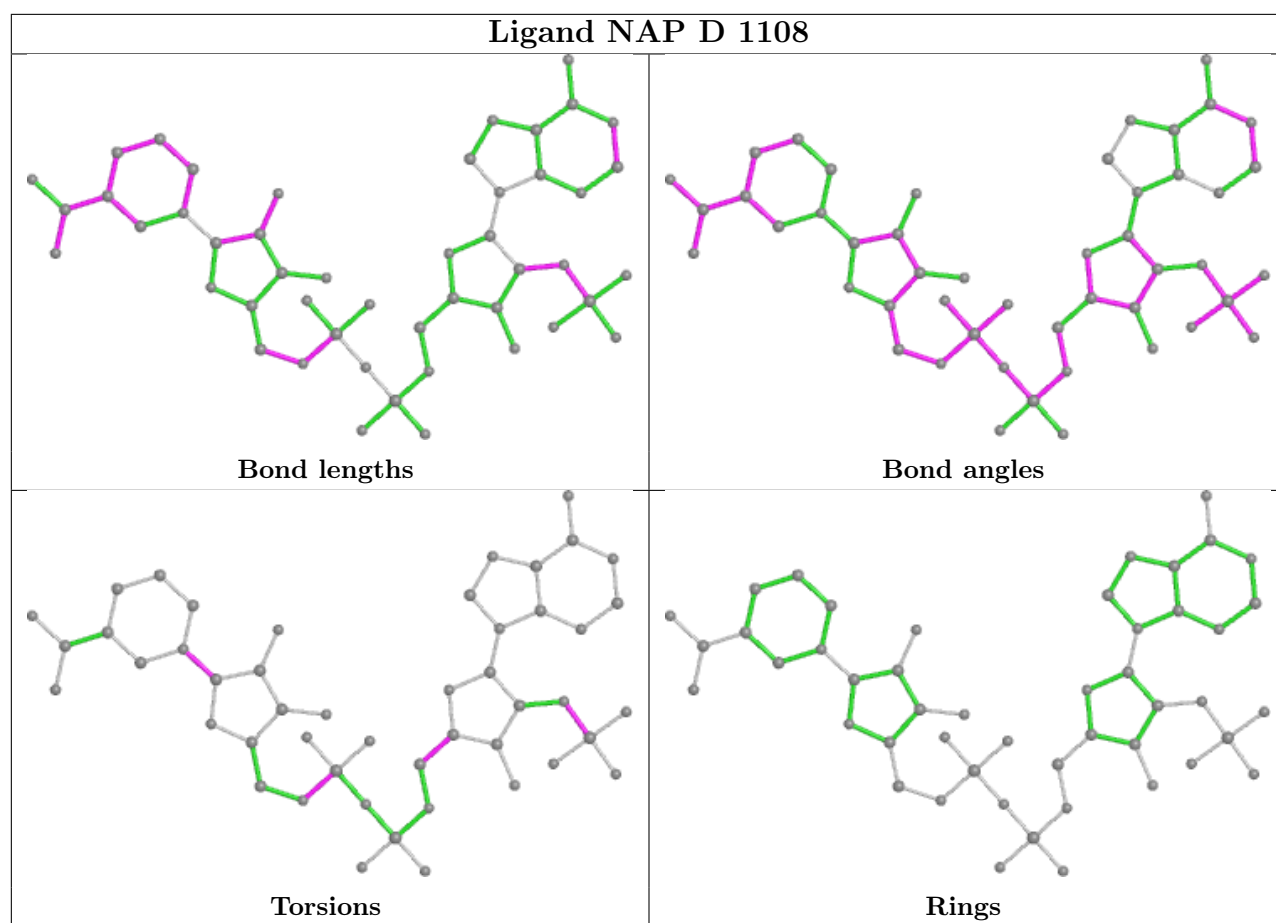


Rings

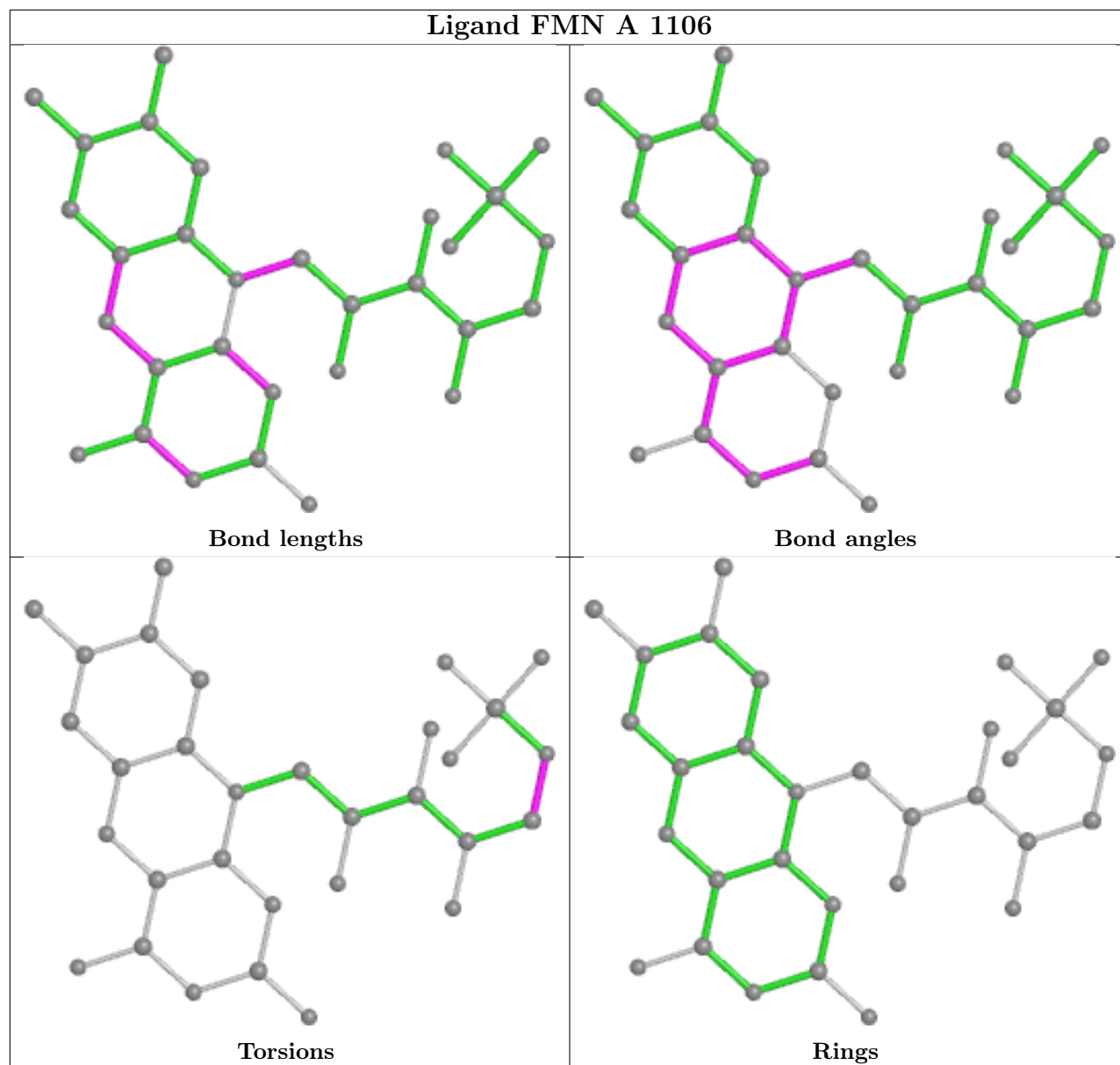
## Ligand FMN D 1106



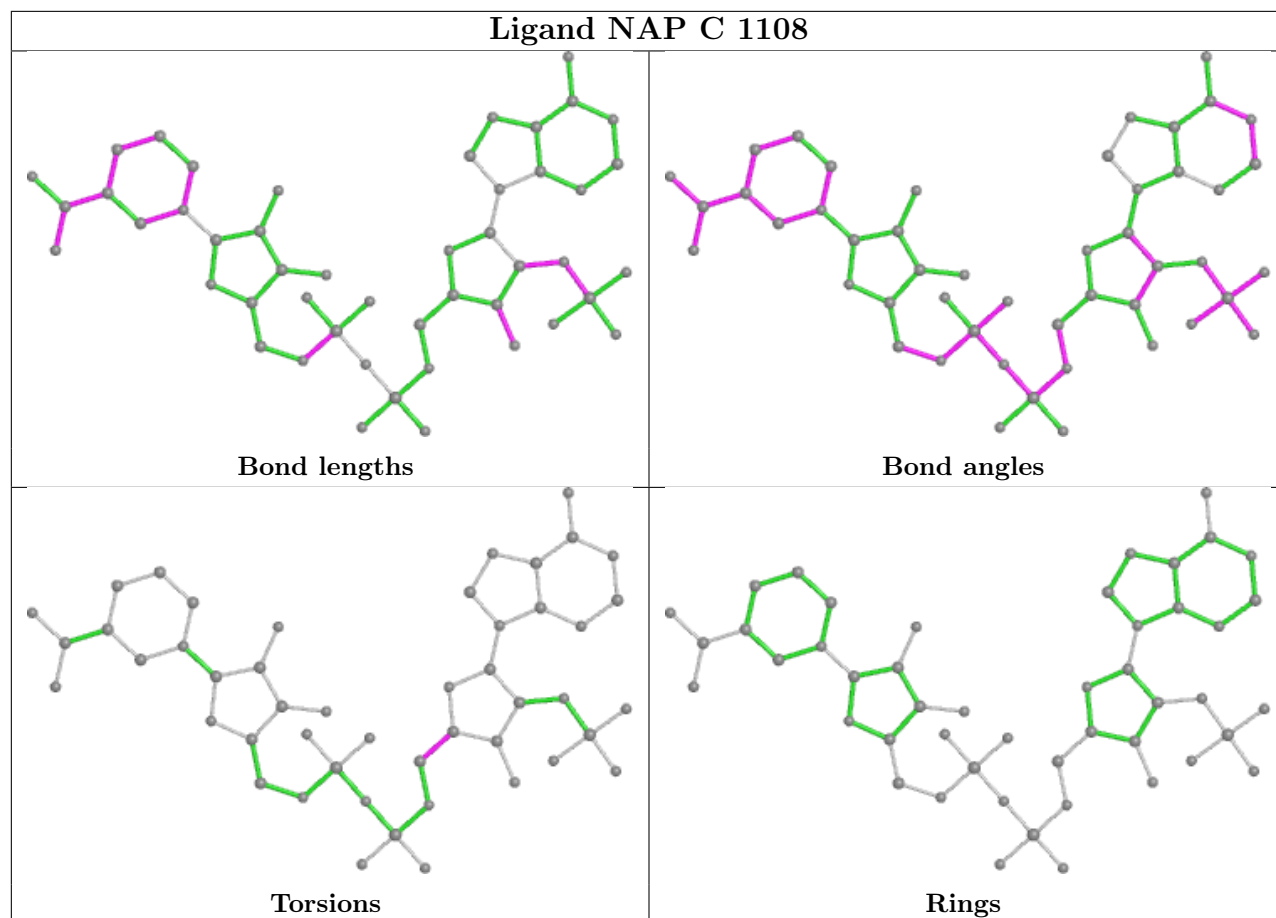




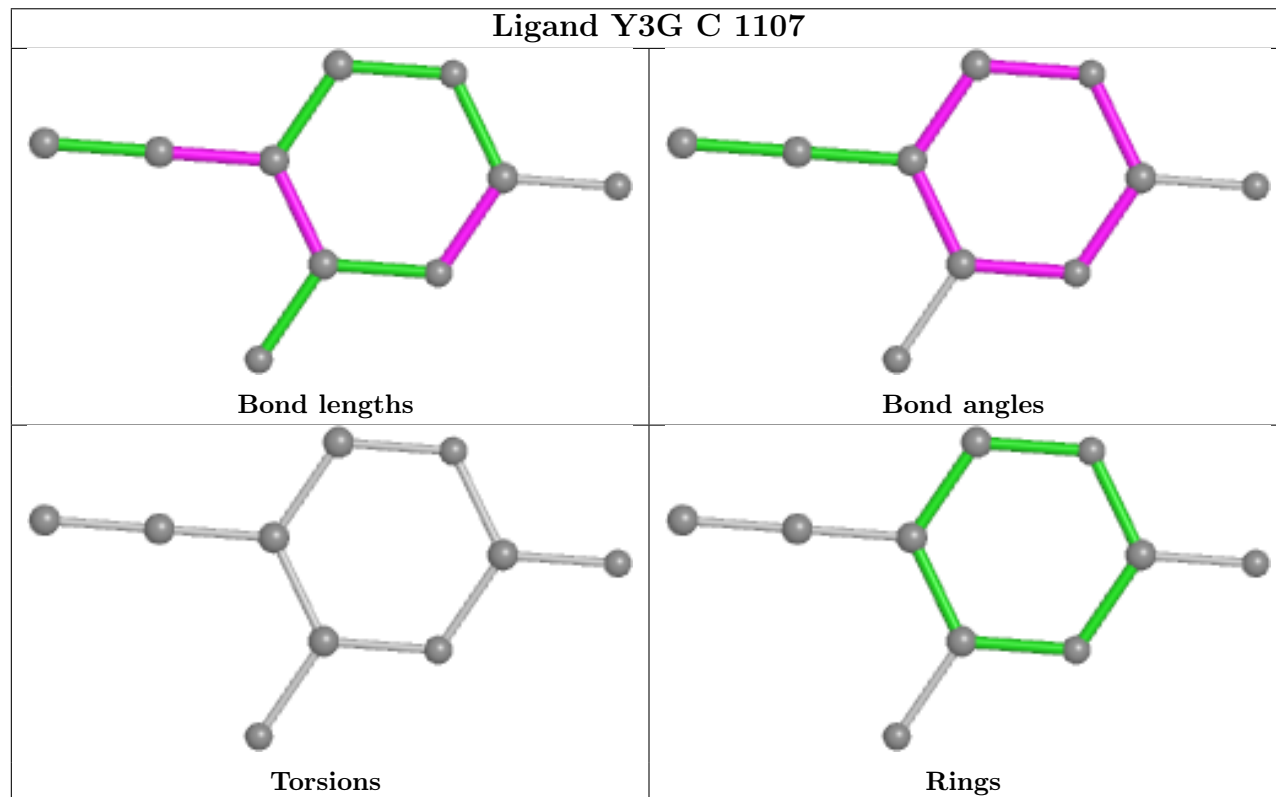
## Ligand FMN A 1106



## Ligand NAP C 1108



## Ligand Y3G C 1107





## 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, 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	1007/1025 (98%)	0.11	38 (3%)	40	43	11, 20, 30, 61	0
1	B	1006/1025 (98%)	0.13	48 (4%)	30	32	11, 21, 32, 53	0
1	C	1015/1025 (99%)	0.12	50 (4%)	29	32	9, 18, 36, 54	0
1	D	1011/1025 (98%)	0.05	34 (3%)	45	48	9, 18, 29, 56	0
All	All	4039/4100 (98%)	0.10	170 (4%)	36	38	9, 19, 32, 61	0

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	324	CYS	12.5
1	A	2	ALA	10.4
1	A	907	LEU	9.8
1	C	679	GLY	8.9
1	B	897	LEU	7.9

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

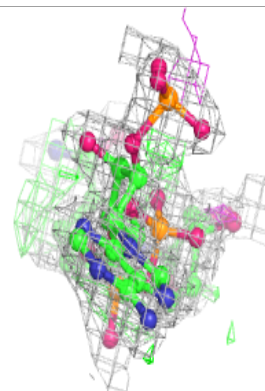
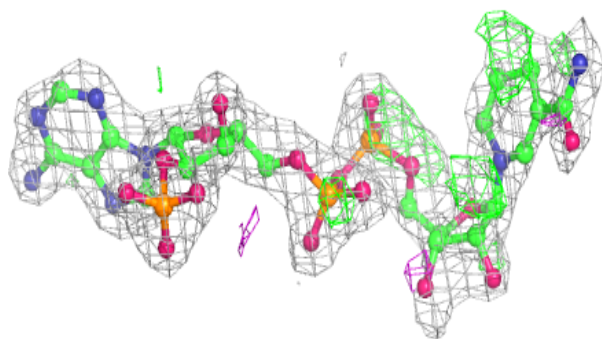
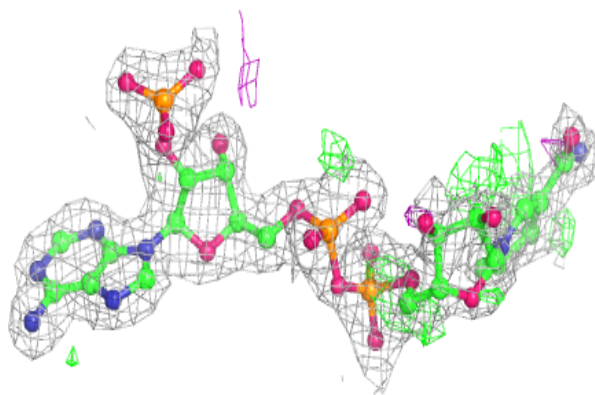
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
6	NAP	D	1108	48/48	0.90	0.14	20,20,20,20	48
6	NAP	A	1108	48/48	0.92	0.15	20,20,20,20	48
6	NAP	C	1108	48/48	0.92	0.13	20,20,20,20	48
5	Y3G	A	1107	10/10	0.92	0.11	14,17,20,23	0
6	NAP	B	1108	48/48	0.93	0.13	20,20,20,20	48
5	Y3G	B	1107	10/10	0.96	0.10	11,14,18,23	0
5	Y3G	C	1107	10/10	0.96	0.08	14,16,19,21	0
3	FAD	A	1105	53/53	0.97	0.10	8,15,20,24	0
3	FAD	B	1105	53/53	0.97	0.09	10,15,20,23	0
3	FAD	C	1105	53/53	0.97	0.09	11,15,22,25	0
4	FMN	A	1106	31/31	0.97	0.08	7,12,15,16	0
4	FMN	B	1106	31/31	0.97	0.09	10,13,17,19	0
4	FMN	C	1106	31/31	0.97	0.10	6,10,13,15	0
4	FMN	D	1106	31/31	0.97	0.10	7,11,12,15	0
3	FAD	D	1105	53/53	0.98	0.09	9,14,19,20	0
5	Y3G	D	1107	10/10	0.98	0.07	11,14,17,19	0
2	SF4	B	1103	8/8	0.99	0.05	13,14,14,14	0
2	SF4	B	1104	8/8	0.99	0.06	12,13,13,13	0
2	SF4	C	1102	8/8	0.99	0.06	11,11,12,12	0
2	SF4	D	1101	8/8	0.99	0.06	10,12,12,13	0
2	SF4	D	1104	8/8	0.99	0.06	10,10,11,11	0
2	SF4	A	1102	8/8	0.99	0.06	9,10,11,11	0
2	SF4	A	1103	8/8	0.99	0.05	11,11,11,12	0
2	SF4	D	1103	8/8	1.00	0.05	8,8,9,9	0
2	SF4	A	1101	8/8	1.00	0.04	10,11,12,12	0
2	SF4	A	1104	8/8	1.00	0.05	12,13,13,14	0
2	SF4	C	1101	8/8	1.00	0.06	10,10,11,11	0
2	SF4	B	1101	8/8	1.00	0.06	9,10,11,11	0
2	SF4	C	1103	8/8	1.00	0.06	9,9,10,10	0
2	SF4	C	1104	8/8	1.00	0.06	10,11,11,11	0
2	SF4	B	1102	8/8	1.00	0.06	11,11,11,11	0
2	SF4	D	1102	8/8	1.00	0.06	9,10,10,10	0

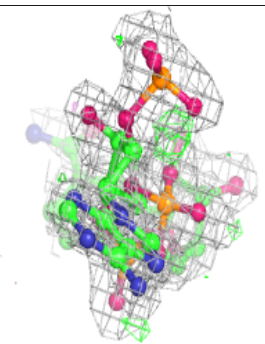
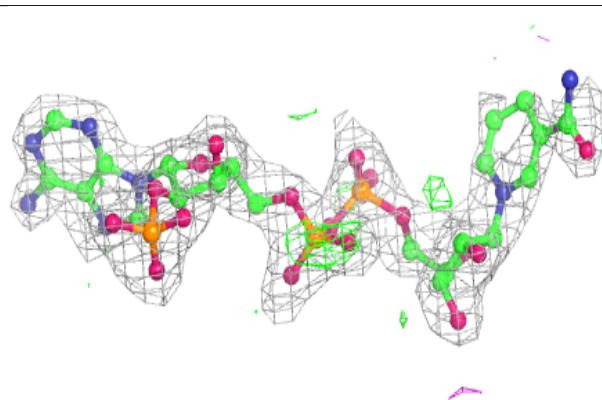
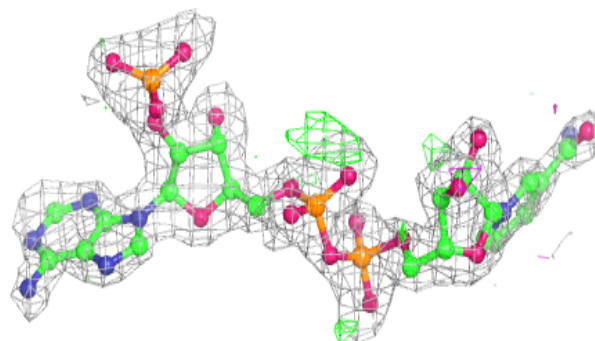
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP D 1108:**

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

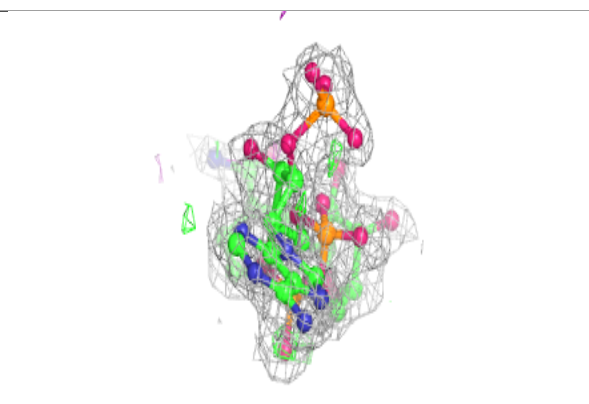
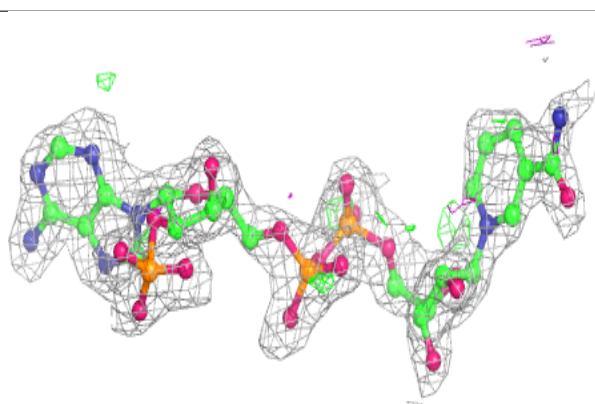
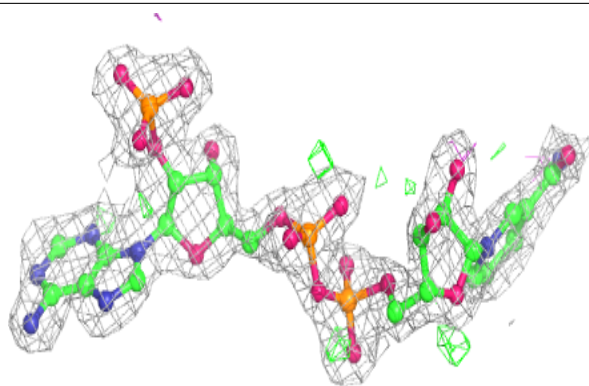
**Electron density around NAP A 1108:**

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

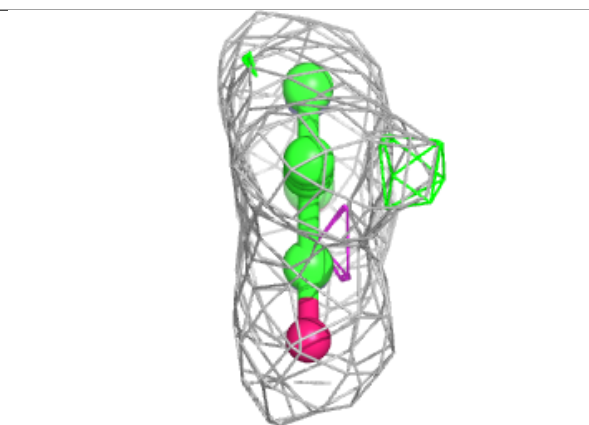
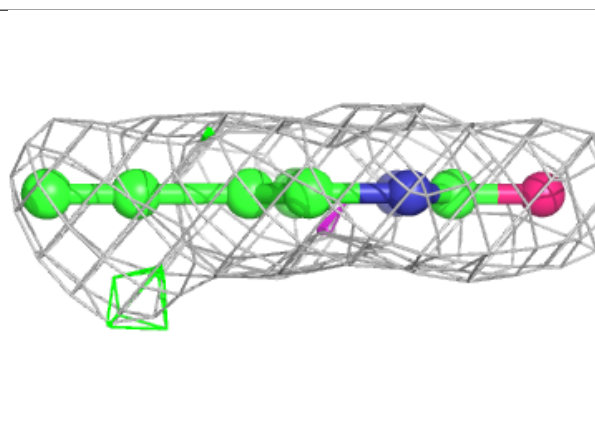
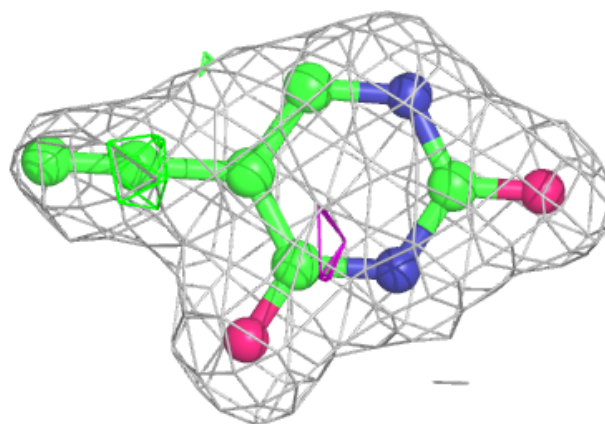


**Electron density around NAP C 1108:**

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

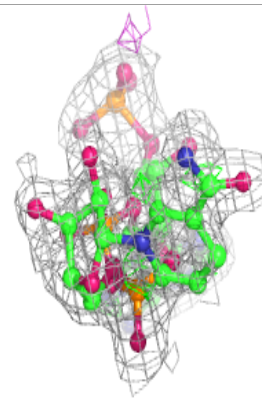
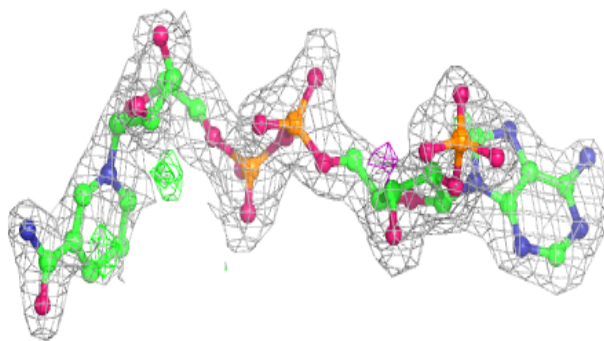
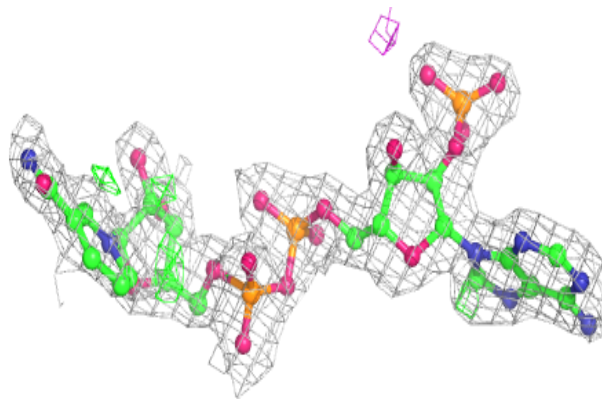
**Electron density around Y3G A 1107:**

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and green (positive)

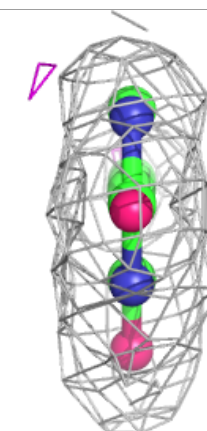
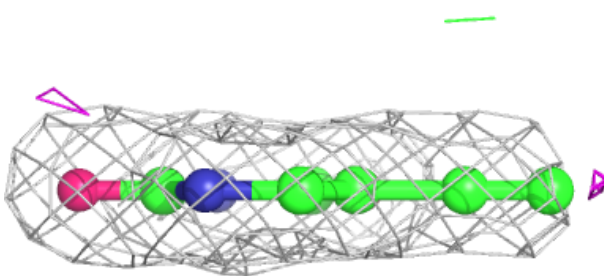
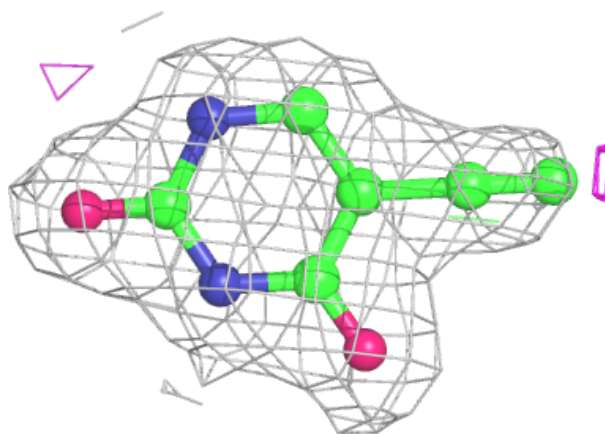


**Electron density around NAP B 1108:**

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

**Electron density around Y3G B 1107:**

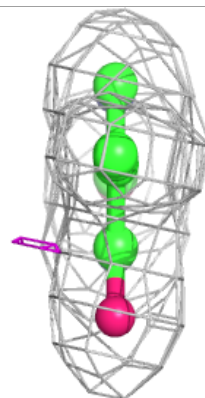
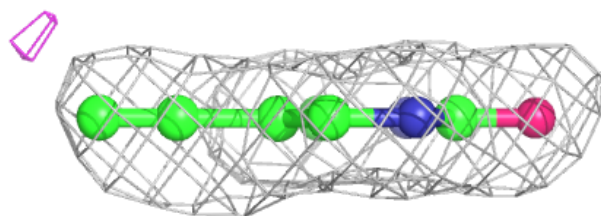
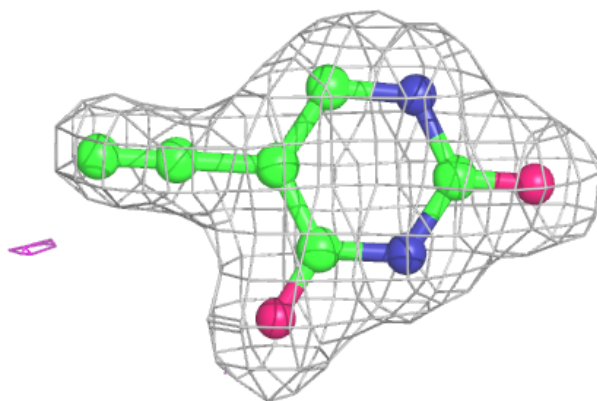
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



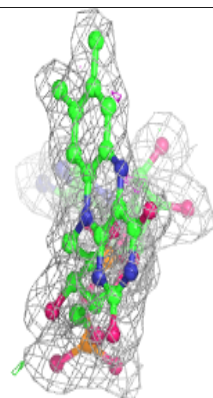
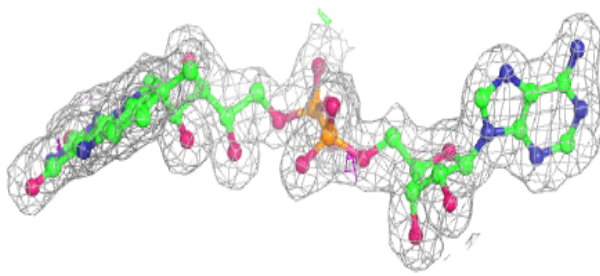
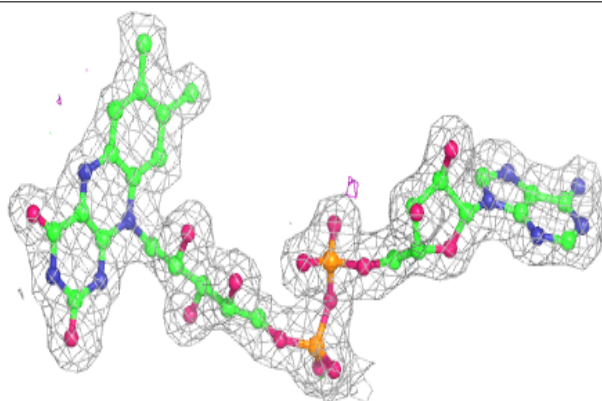


**Electron density around Y3G C 1107:**

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

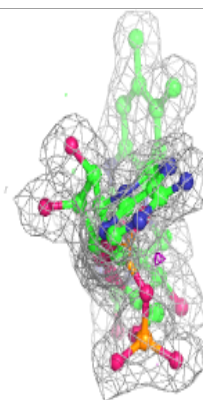
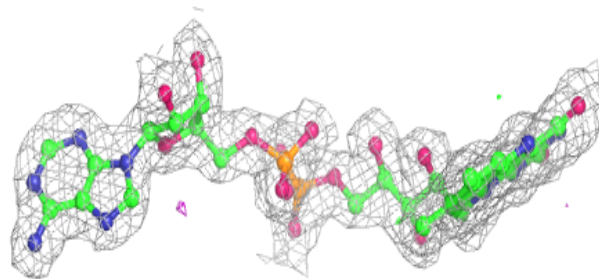
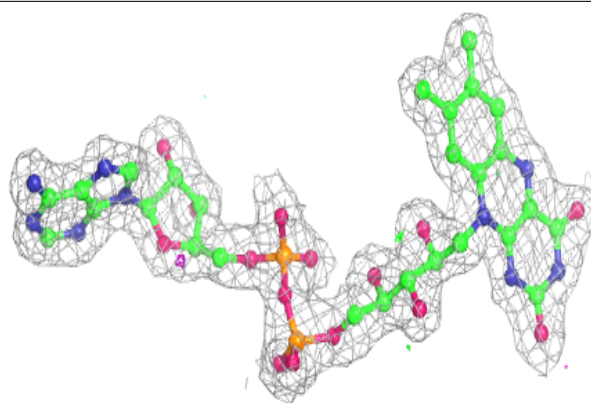
**Electron density around FAD A 1105:**

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

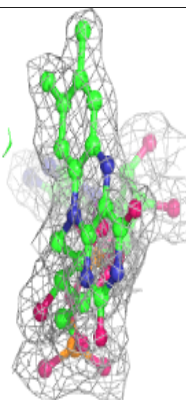
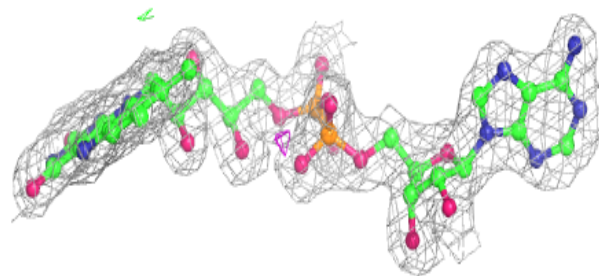
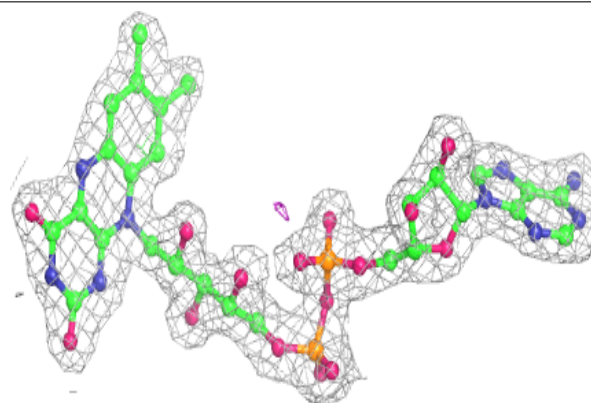


**Electron density around FAD B 1105:**

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

**Electron density around FAD C 1105:**

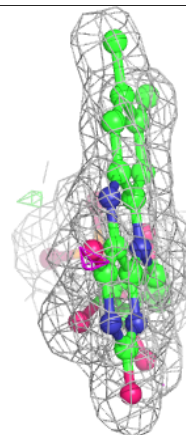
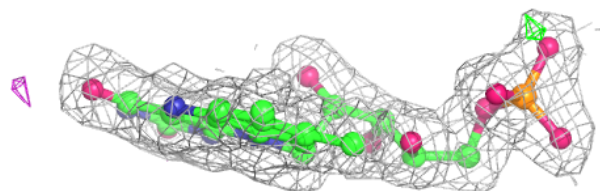
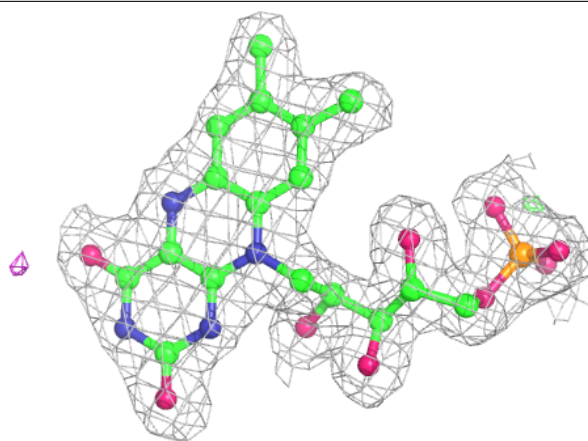
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





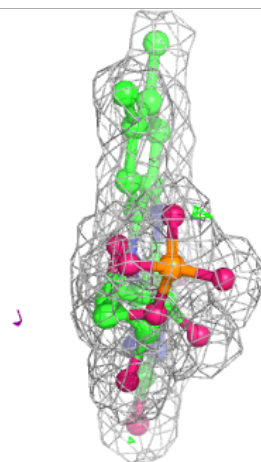
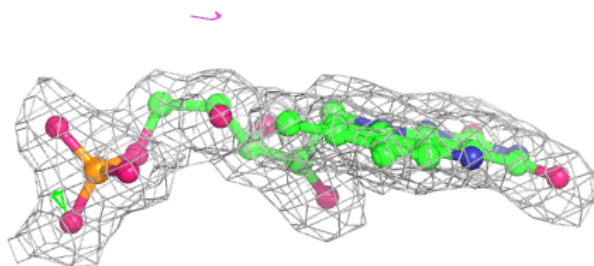
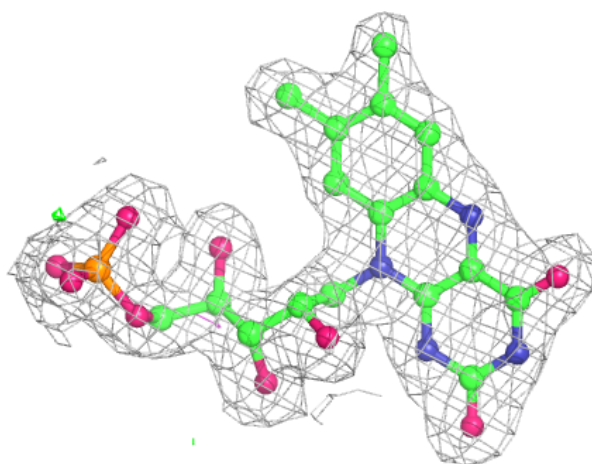
**Electron density around FMN A 1106:**

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



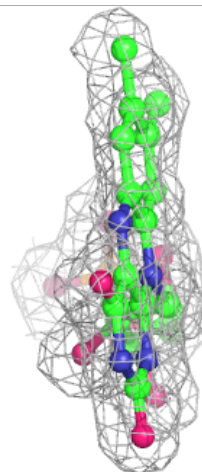
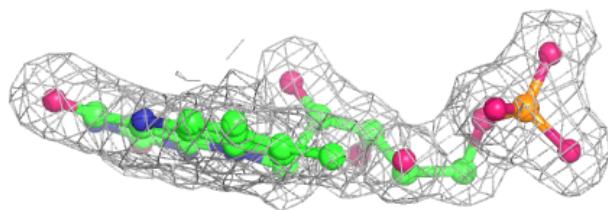
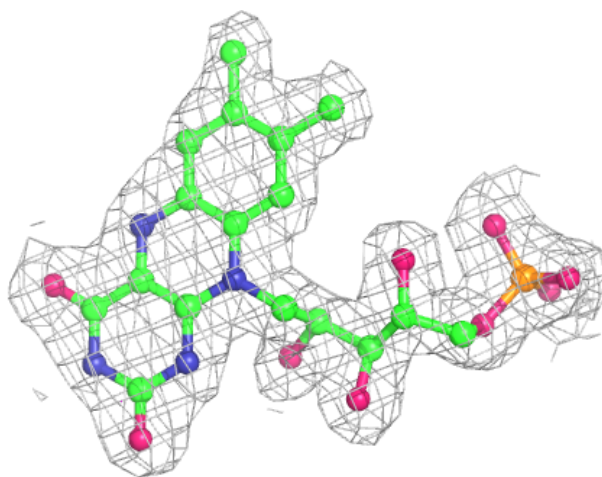
**Electron density around FMN B 1106:**

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



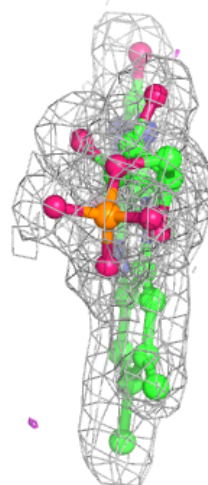
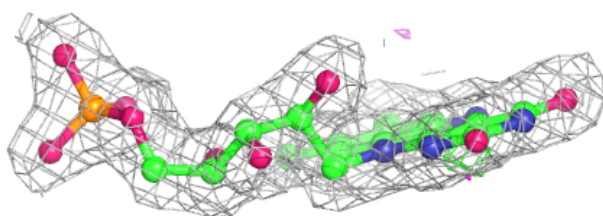
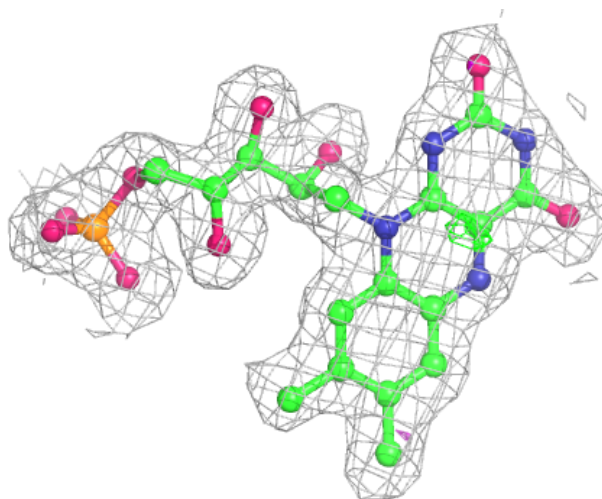
**Electron density around FMN C 1106:**

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



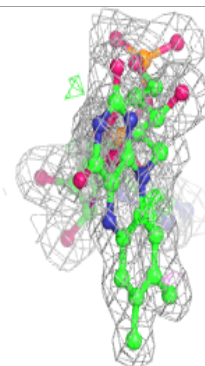
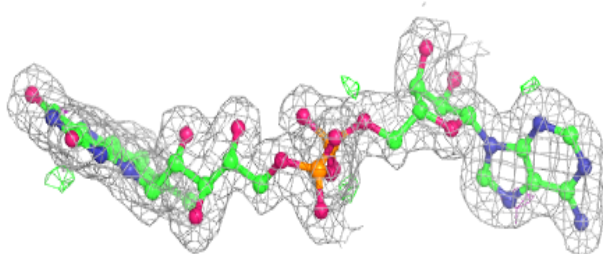
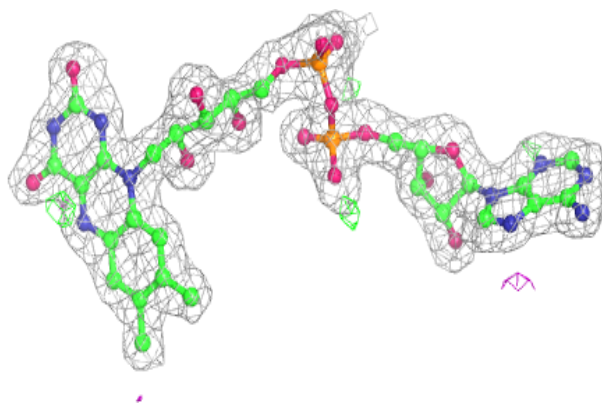
**Electron density around FMN D 1106:**

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

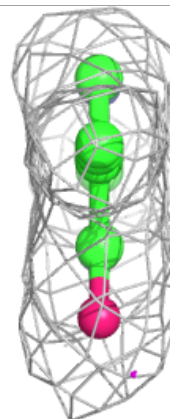
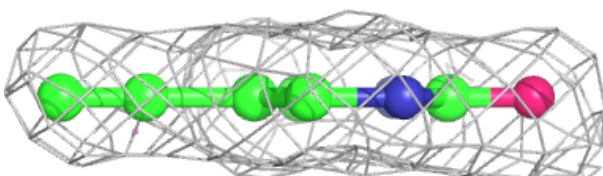
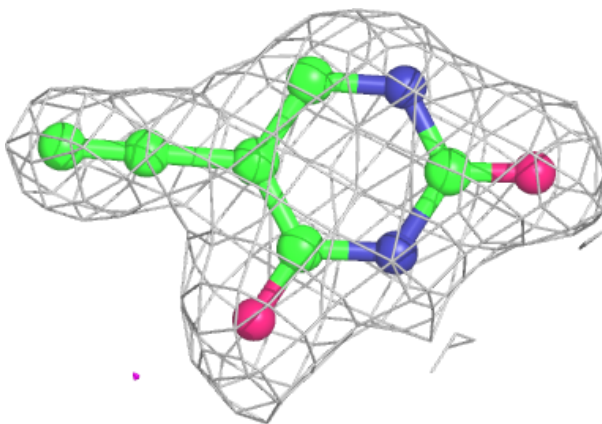


**Electron density around FAD D 1105:**

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

**Electron density around Y3G D 1107:**

$2mF_o-DF_c$  (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.