



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2021 – 12:16 PM EDT

PDB ID : 7LJS  
Title : Porcine Dihydropyrimidine dehydrogenase (DPD) complexed with 5-Ethynyluracil (5EU) - Open Form  
Authors : Butrin, A.; Forouzesh, D.; Beaupre, B.; Wawrzak, Z.; Liu, D.; Moran, G.  
Deposited on : 2021-01-30  
Resolution : 2.00 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

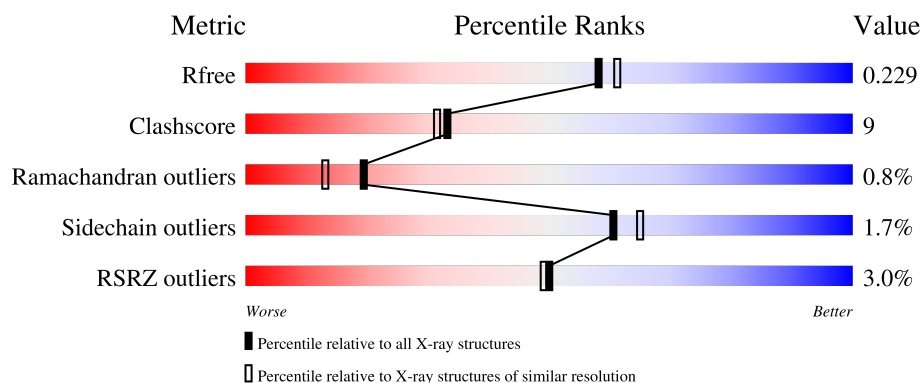
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

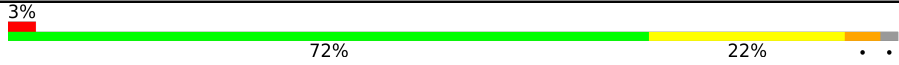



The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	
1	B	1025	
1	C	1025	
1	D	1025	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	A	1101	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33532 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.

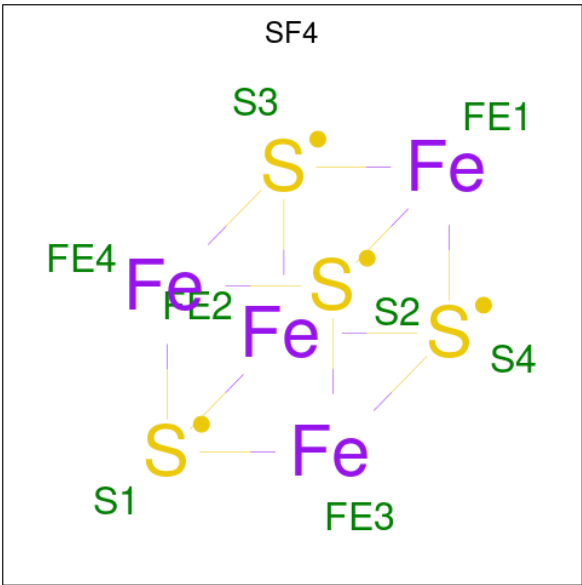
- Molecule 1 is a protein called Dihydropyrimidine dehydrogenase [NADP(+)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1005	Total	C	N	O	S	0	4	0
			7678	4869	1298	1456	55			
1	B	1004	Total	C	N	O	S	0	5	0
			7688	4874	1303	1456	55			
1	C	1010	Total	C	N	O	S	0	11	0
			7741	4915	1308	1464	54			
1	D	1014	Total	C	N	O	S	0	7	0
			7750	4914	1312	1468	56			

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>).



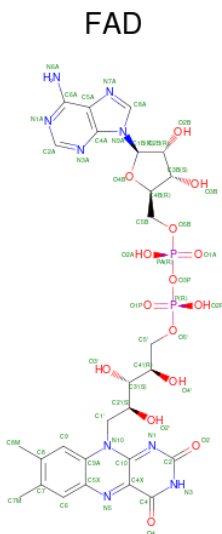
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2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

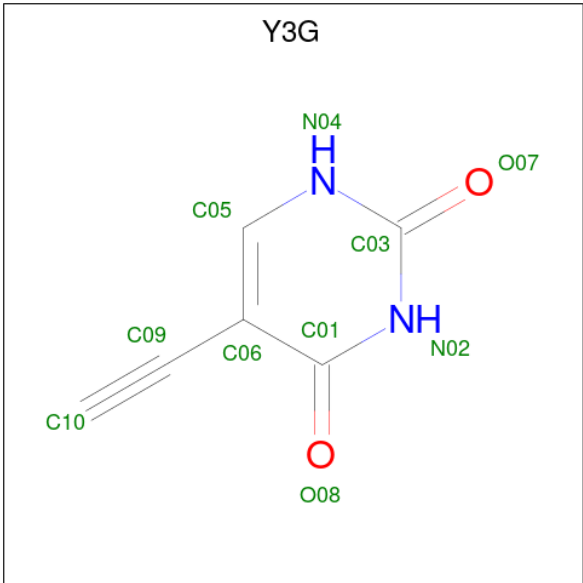
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- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a bicyclic structure with two nitrogen atoms, N1 and N5, and two carbonyl groups, C2=O2 and C4=O4) attached to a ribitol chain. The ribitol chain is a five-carbon chain (C1 to C5) with hydroxyl groups at C1, C2, C3, and C4. The C5 carbon is attached to a phosphate group (O1P, O2P, O3P, O4P). The ribitol chain is shown in a chair conformation with stereochemistry indicated by wedges and dashes. The phosphate group is shown as a phosphorus atom (P) bonded to four oxygen atoms (O1P, O2P, O3P, O4P). The ribitol chain is labeled with C1, C2, C3, C4, and C5. The phosphate group is labeled with O1P, O2P, O3P, and O4P. The isoalloxazine ring system is labeled with N1, N5, C2, C4, C5A, C8A, C9, C7M, C8, and C6. The ribitol chain is labeled with C1, C2, C3, C4, and C5. The phosphate group is labeled with O1P, O2P, O3P, and O4P.

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is 5-ethynylpyrimidine-2,4(1H,3H)-dione (three-letter code: Y3G) (formula:  $\text{C}_6\text{H}_4\text{N}_2\text{O}_2$ ) (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 water.

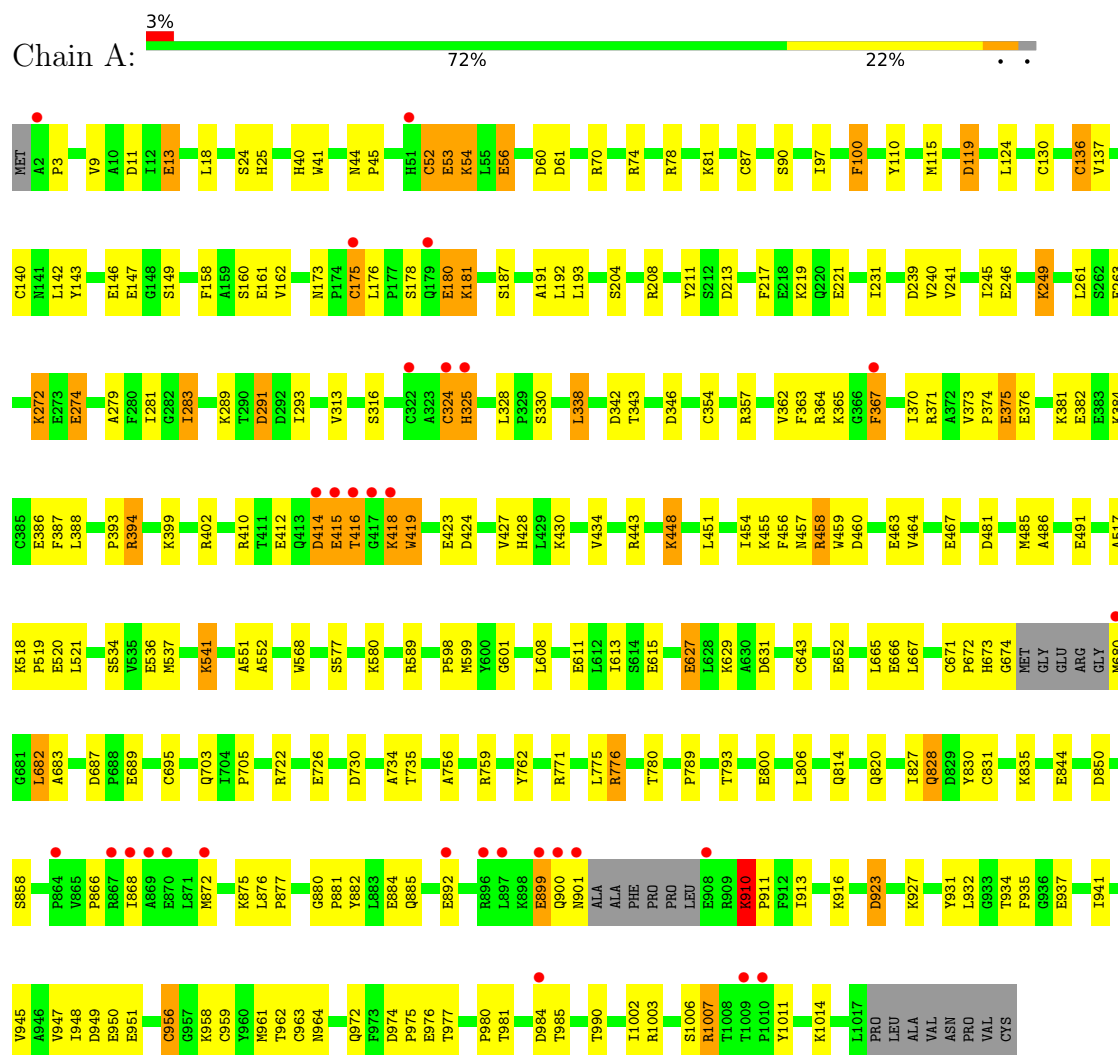
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	529	Total	O	0	0
			529	529		
6	B	490	Total	O	0	0
			490	490		
6	C	593	Total	O	0	0
			593	593		
6	D	559	Total	O	0	0
			559	559		



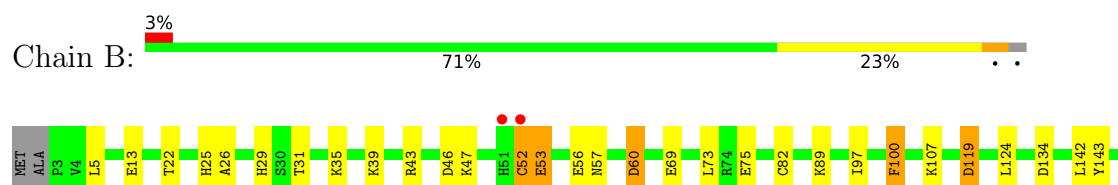
### 3 Residue-property plots

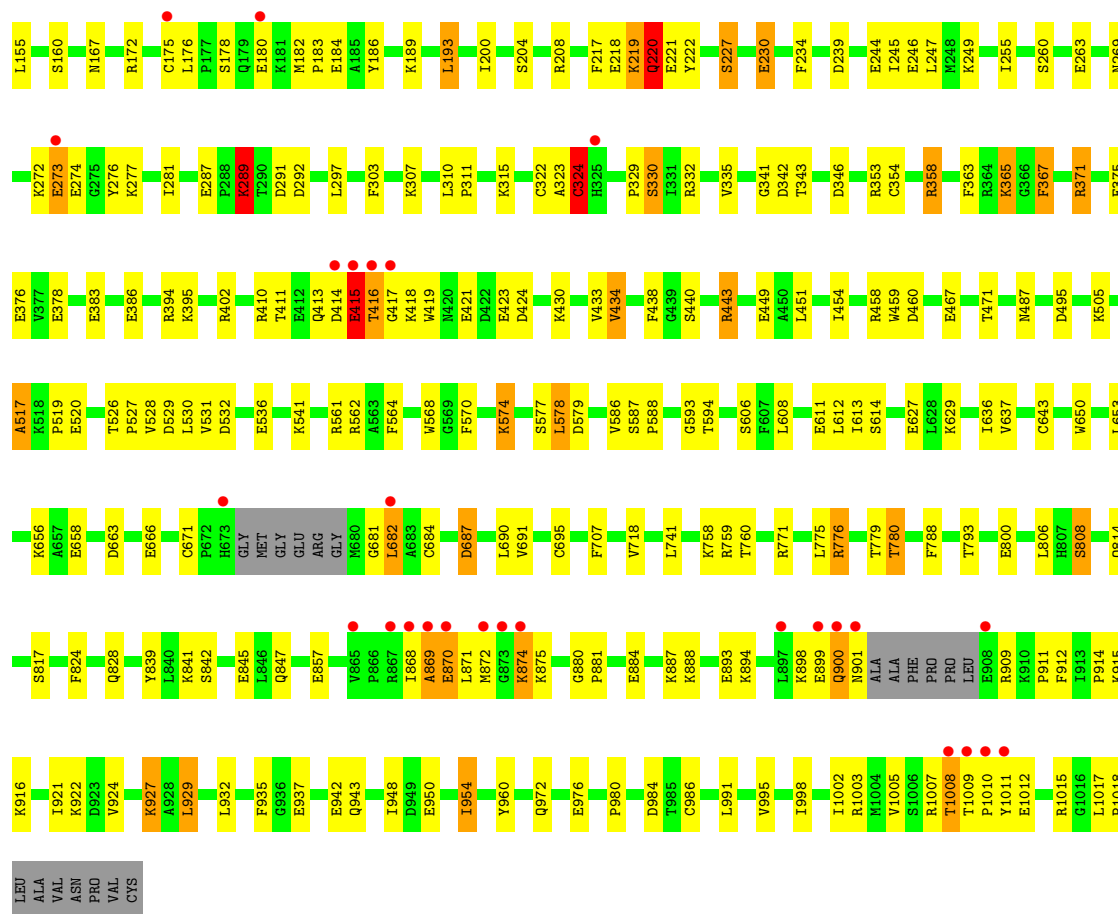
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 [NADP(+)]

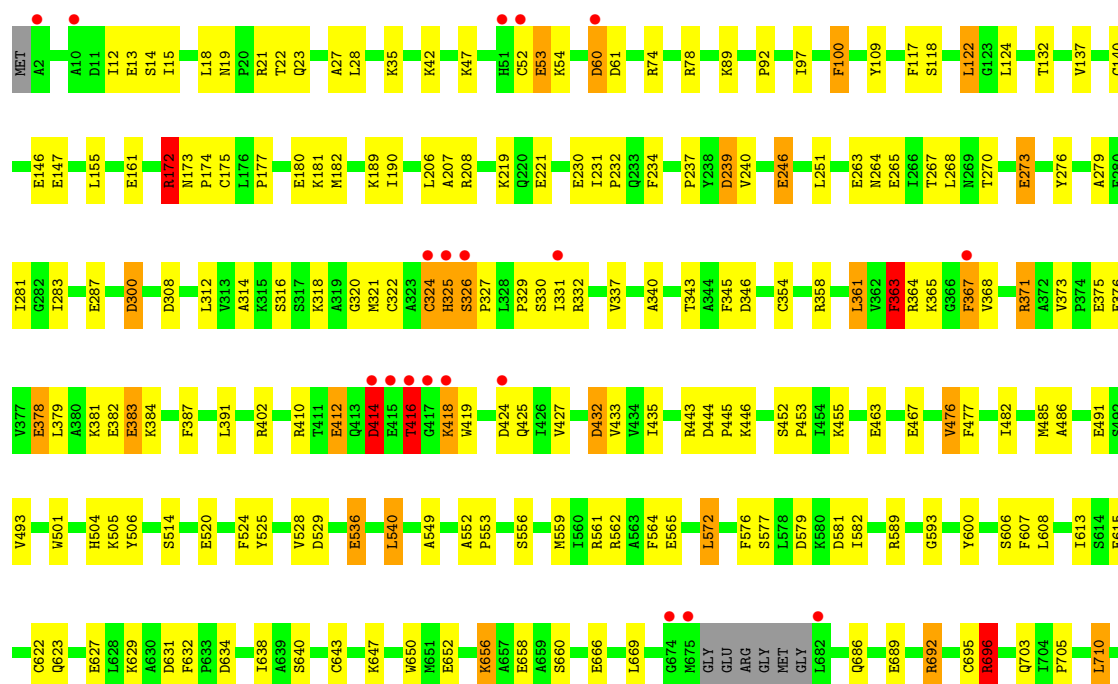


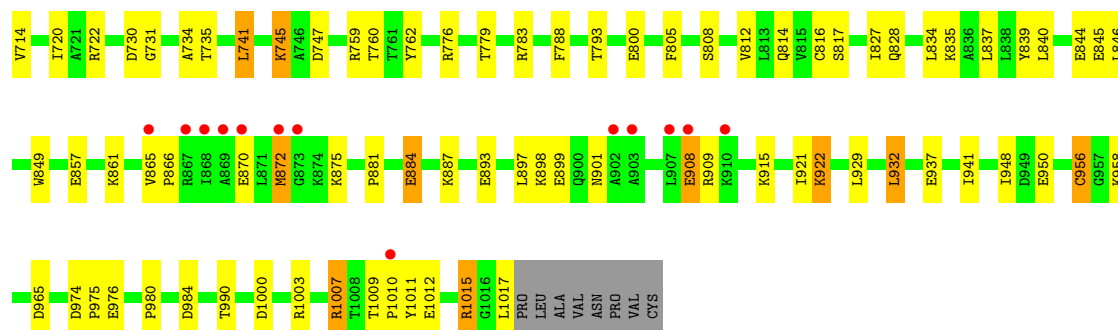
- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



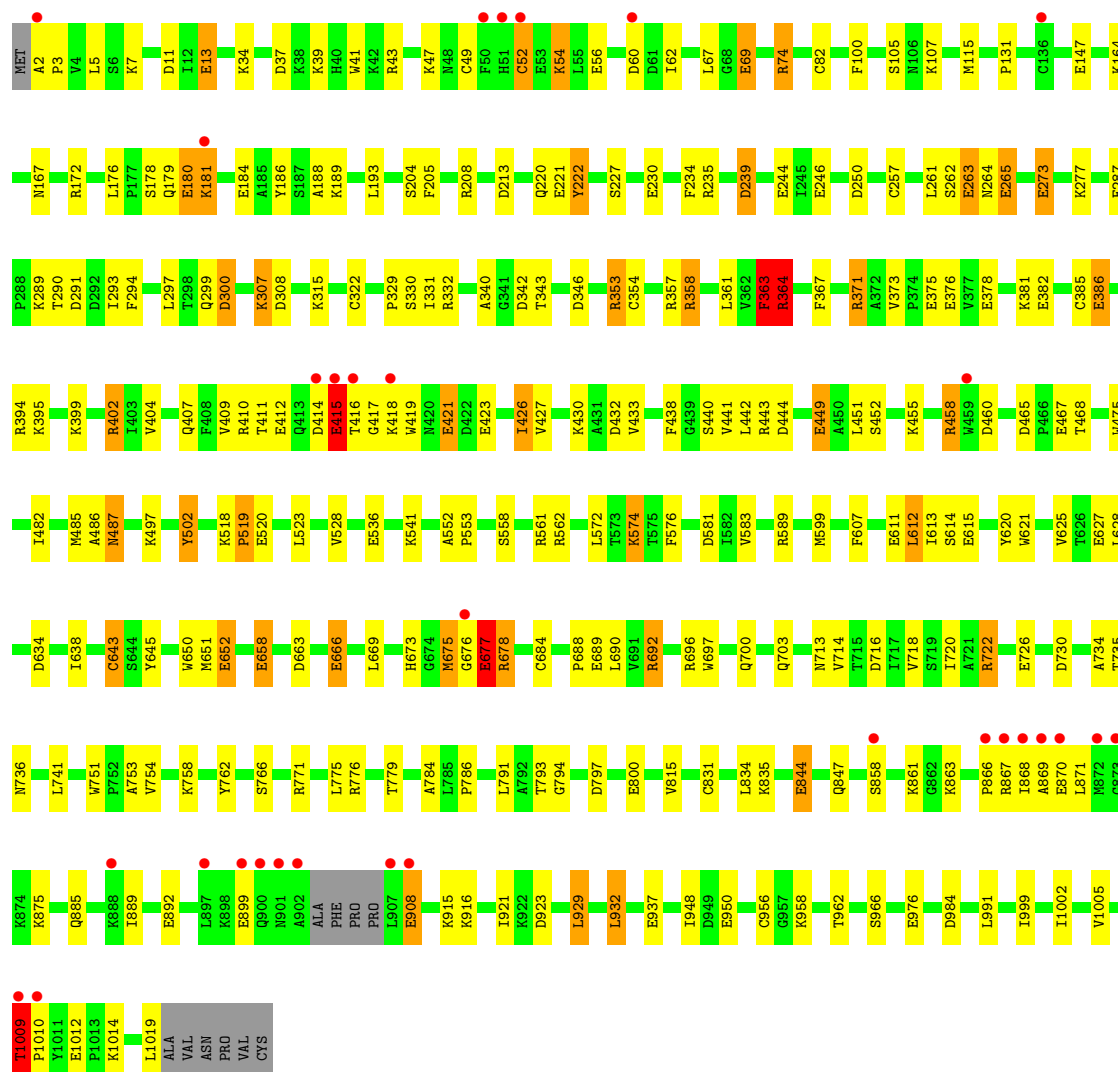


• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]





• 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, $\alpha$ , $\beta$ , $\gamma$	82.03Å 160.05Å 164.07Å 90.00° 95.95° 90.00°	Depositor
Resolution (Å)	45.62 – 2.00 45.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	77.1 (45.62-2.00) 77.1 (45.62-2.00)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, $R_{free}$	0.172 , 0.229 0.172 , 0.229	Depositor DCC
$R_{free}$ test set	10692 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	33532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: Y3G, SF4, FAD, FMN

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	1.43	96/7849 (1.2%)	1.20	47/10635 (0.4%)
1	B	1.43	98/7865 (1.2%)	1.23	62/10655 (0.6%)
1	C	1.50	129/7945 (1.6%)	1.25	70/10772 (0.6%)
1	D	1.55	129/7936 (1.6%)	1.28	66/10754 (0.6%)
All	All	1.48	452/31595 (1.4%)	1.24	245/42816 (0.6%)

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	A	0	3
1	B	0	3
1	C	0	3
1	D	0	5
All	All	0	14

The worst 5 of 452 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	519	PRO	N-CD	-20.33	1.19	1.47
1	D	265	GLU	CG-CD	18.56	1.79	1.51
1	A	956	CYS	CB-SG	14.74	2.07	1.82
1	D	265	GLU	CB-CG	12.59	1.76	1.52
1	C	60	ASP	CB-CG	11.67	1.76	1.51

The worst 5 of 245 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	11	ASP	CB-CG-OD2	-13.09	106.52	118.30
1	A	175	CYS	CA-CB-SG	-12.75	91.05	114.00
1	B	52	CYS	CA-CB-SG	-11.29	93.67	114.00
1	D	60	ASP	CB-CG-OD1	11.24	128.42	118.30
1	C	1015	ARG	NE-CZ-NH2	-10.93	114.84	120.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414	ASP	Peptide
1	A	418	LYS	Peptide
1	A	672	PRO	Peptide
1	B	324	CYS	Peptide
1	B	415	GLU	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	7678	0	7707	128	0
1	B	7688	0	7715	147	1
1	C	7741	0	7767	156	0
1	D	7750	0	7781	143	1
2	A	32	0	0	2	0
2	B	32	0	0	1	0
2	C	32	0	0	1	0
2	D	32	0	0	0	0
3	A	31	0	19	0	0
3	B	31	0	19	0	0
3	C	31	0	19	2	0
3	D	31	0	19	4	0
4	A	53	0	31	2	0
4	B	53	0	31	2	0
4	C	53	0	31	1	0
4	D	53	0	31	1	0
5	A	10	0	0	1	0
5	B	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	10	0	0	2	0
5	D	10	0	0	1	0
6	A	529	0	0	26	0
6	B	490	0	0	28	1
6	C	593	0	0	25	2
6	D	559	0	0	30	1
All	All	33532	0	31170	538	3

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 9.

The worst 5 of 538 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ARG:CG	1:B:371:ARG:CD	1.74	1.65
1:D:265:GLU:CG	1:D:265:GLU:CB	1.76	1.56
1:C:60:ASP:CG	1:C:60:ASP:CB	1.76	1.53
1:A:541:LYS:NZ	1:A:541:LYS:CE	1.70	1.52
1:D:265:GLU:CG	1:D:265:GLU:CD	1.79	1.50

All (3) 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)
1:B:219:LYS:O	1:D:677:GLU:OE1[2_746]	2.00	0.20
6:B:1634:HOH:O	6:C:1560:HOH:O[2_746]	2.15	0.05
6:C:1758:HOH:O	6:D:1728:HOH:O[1_655]	2.15	0.05

## 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	1003/1025 (98%)	955 (95%)	41 (4%)	7 (1%)	22	16
1	B	1003/1025 (98%)	942 (94%)	49 (5%)	12 (1%)	13	7
1	C	1017/1025 (99%)	972 (96%)	43 (4%)	2 (0%)	47	44
1	D	1017/1025 (99%)	964 (95%)	41 (4%)	12 (1%)	13	7
All	All	4040/4100 (98%)	3833 (95%)	174 (4%)	33 (1%)	19	13

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	GLU
1	A	416	THR
1	B	219	LYS
1	B	220	GLN
1	B	324	CYS

### 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	842/854 (99%)	828 (98%)	14 (2%)	60	65
1	B	845/854 (99%)	833 (99%)	12 (1%)	67	72
1	C	852/854 (100%)	833 (98%)	19 (2%)	52	55
1	D	851/854 (100%)	835 (98%)	16 (2%)	57	61
All	All	3390/3416 (99%)	3329 (98%)	61 (2%)	60	63

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	172	ARG
1	D	452	SER
1	C	367	PHE
1	D	364	ARG
1	D	867	ARG



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	C	420	ASN
1	C	901	ASN
1	A	859	HIS
1	B	23	GLN
1	B	648	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

28 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	FMN	A	1105	-	31,33,33	2.10	10 (32%)	40,50,50	2.49	11 (27%)
2	SF4	D	1103	1	0,12,12	0.00	-	-		
4	FAD	B	1106	-	51,58,58	1.41	5 (9%)	60,89,89	2.27	11 (18%)
2	SF4	D	1104	1	0,12,12	0.00	-	-		
2	SF4	A	1101	1	0,12,12	0.00	-	-		
2	SF4	D	1102	1	0,12,12	0.00	-	-		
2	SF4	B	1102	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FAD	A	1106	-	51,58,58	1.61	8 (15%)	60,89,89	2.39	11 (18%)
2	SF4	B	1104	1	0,12,12	0.00	-	-	-	-
5	Y3G	B	1107	-	9,10,10	2.38	3 (33%)	6,13,13	7.16	5 (83%)
2	SF4	A	1104	1	0,12,12	0.00	-	-	-	-
2	SF4	D	1101	1	0,12,12	0.00	-	-	-	-
5	Y3G	A	1107	-	9,10,10	2.82	3 (33%)	6,13,13	7.12	4 (66%)
2	SF4	C	1102	1	0,12,12	0.00	-	-	-	-
2	SF4	B	1103	1	0,12,12	0.00	-	-	-	-
5	Y3G	C	1107	-	9,10,10	2.49	1 (11%)	6,13,13	5.03	4 (66%)
4	FAD	D	1106	-	51,58,58	1.31	6 (11%)	60,89,89	2.26	9 (15%)
2	SF4	C	1101	1	0,12,12	0.00	-	-	-	-
5	Y3G	D	1107	-	9,10,10	3.27	3 (33%)	6,13,13	5.57	3 (50%)
3	FMN	B	1105	-	31,33,33	2.83	7 (22%)	40,50,50	2.52	12 (30%)
3	FMN	D	1105	-	31,33,33	1.98	7 (22%)	40,50,50	2.72	13 (32%)
2	SF4	C	1104	1	0,12,12	0.00	-	-	-	-
2	SF4	A	1103	1	0,12,12	0.00	-	-	-	-
2	SF4	A	1102	1	0,12,12	0.00	-	-	-	-
2	SF4	C	1103	1	0,12,12	0.00	-	-	-	-
2	SF4	B	1101	1	0,12,12	0.00	-	-	-	-
4	FAD	C	1106	-	51,58,58	1.44	6 (11%)	60,89,89	2.30	9 (15%)
3	FMN	C	1105	-	31,33,33	2.19	11 (35%)	40,50,50	1.87	10 (25%)

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

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1107	Y3G	O08-C01	8.34	1.45	1.24
3	B	1105	FMN	C1'-N10	8.30	1.56	1.48
3	B	1105	FMN	C4A-C10	8.00	1.46	1.38
5	A	1107	Y3G	O08-C01	7.03	1.42	1.24
5	C	1107	Y3G	O08-C01	6.67	1.41	1.24

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1107	Y3G	C06-C01-N02	-15.41	113.66	124.40
5	B	1107	Y3G	C06-C01-N02	-15.11	113.87	124.40
4	A	1106	FAD	C4-N3-C2	13.07	126.17	115.14
4	C	1106	FAD	C4-N3-C2	12.75	125.91	115.14
4	B	1106	FAD	C4-N3-C2	11.99	125.26	115.14

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1106	FAD	PA-O3P-P-O5'
3	B	1105	FMN	O3'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
3	B	1105	FMN	O3'-C3'-C4'-C5'
3	B	1105	FMN	C2'-C3'-C4'-O4'
4	B	1106	FAD	P-O3P-PA-O1A

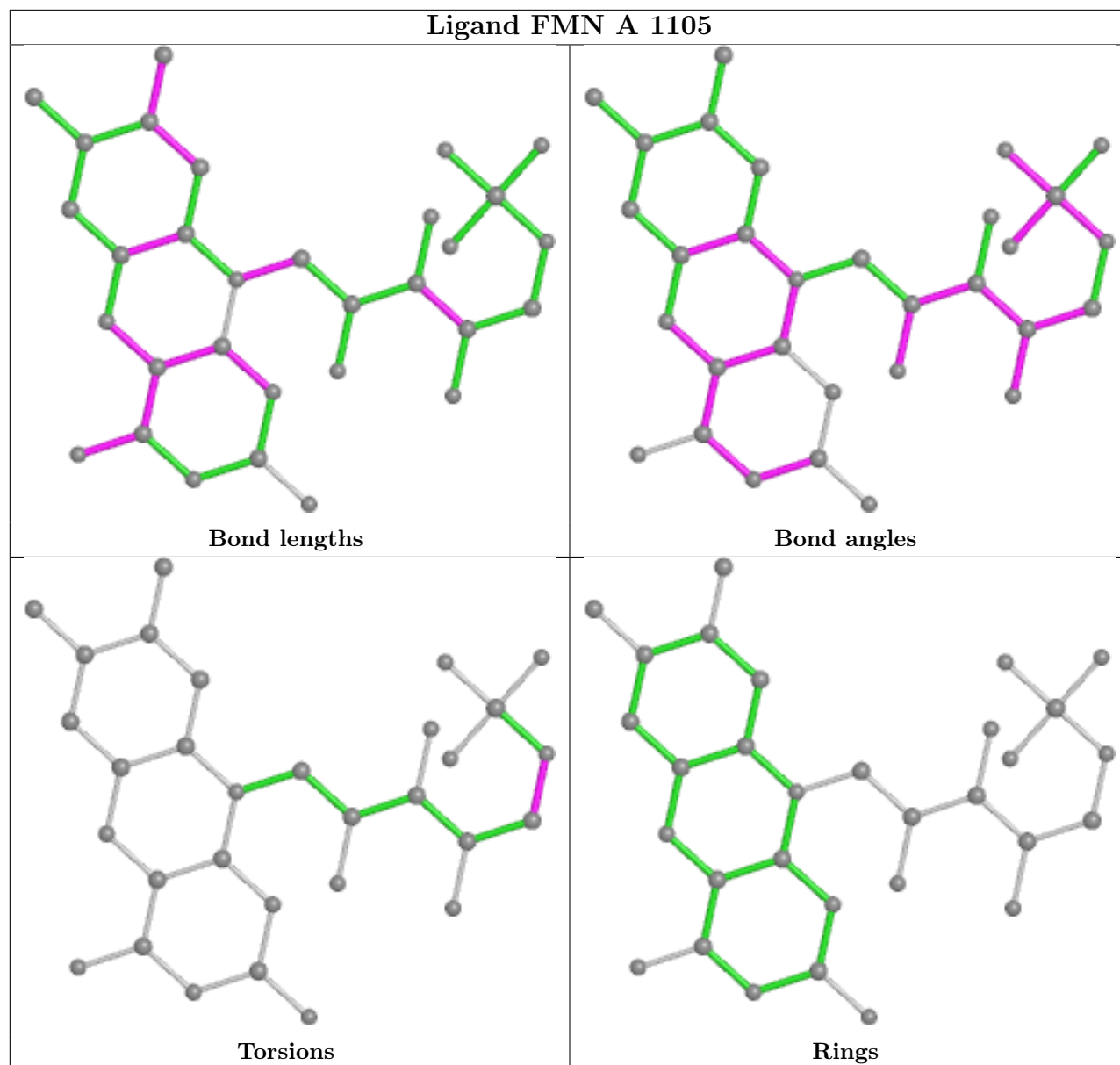
There are no ring outliers.

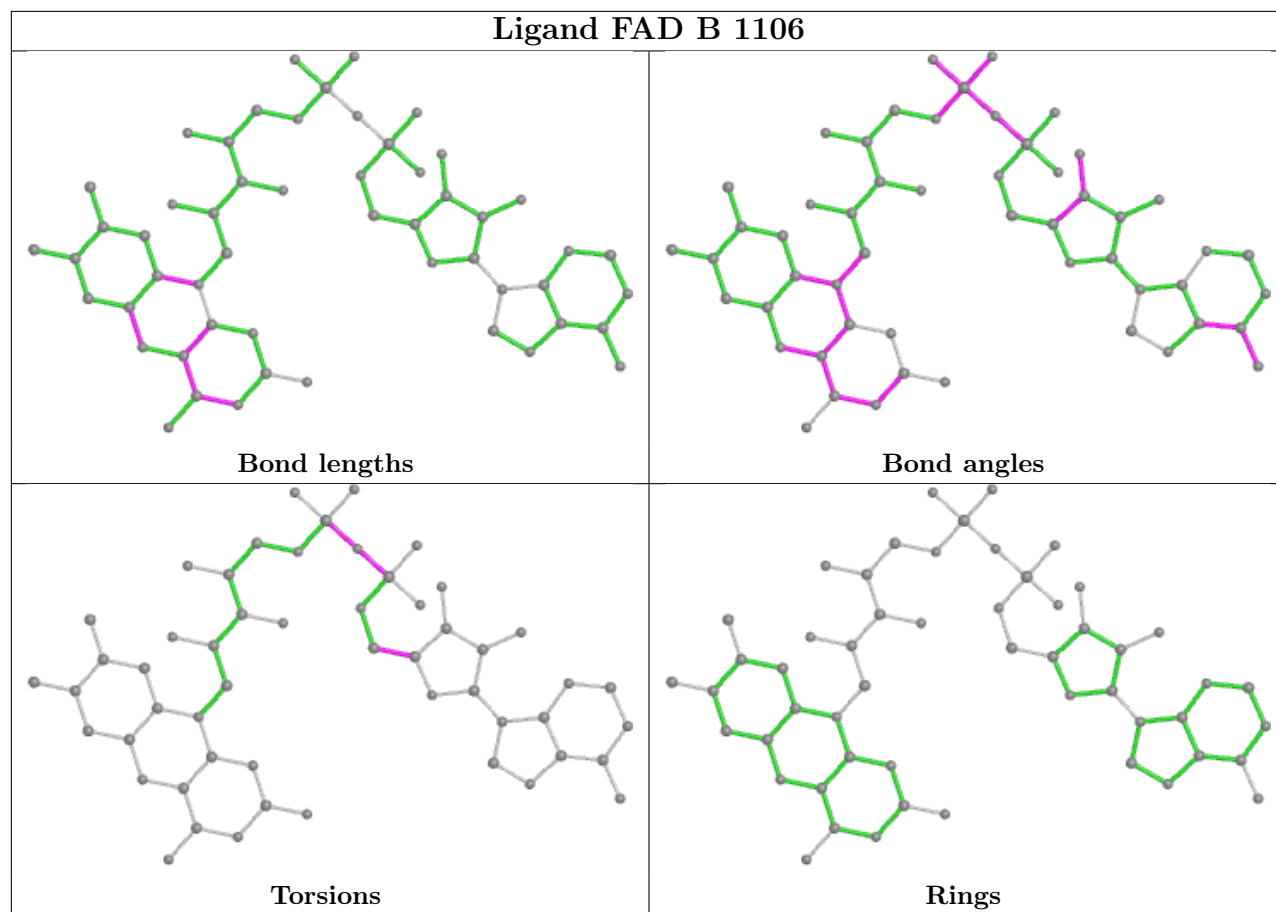
13 monomers are involved in 22 short contacts:

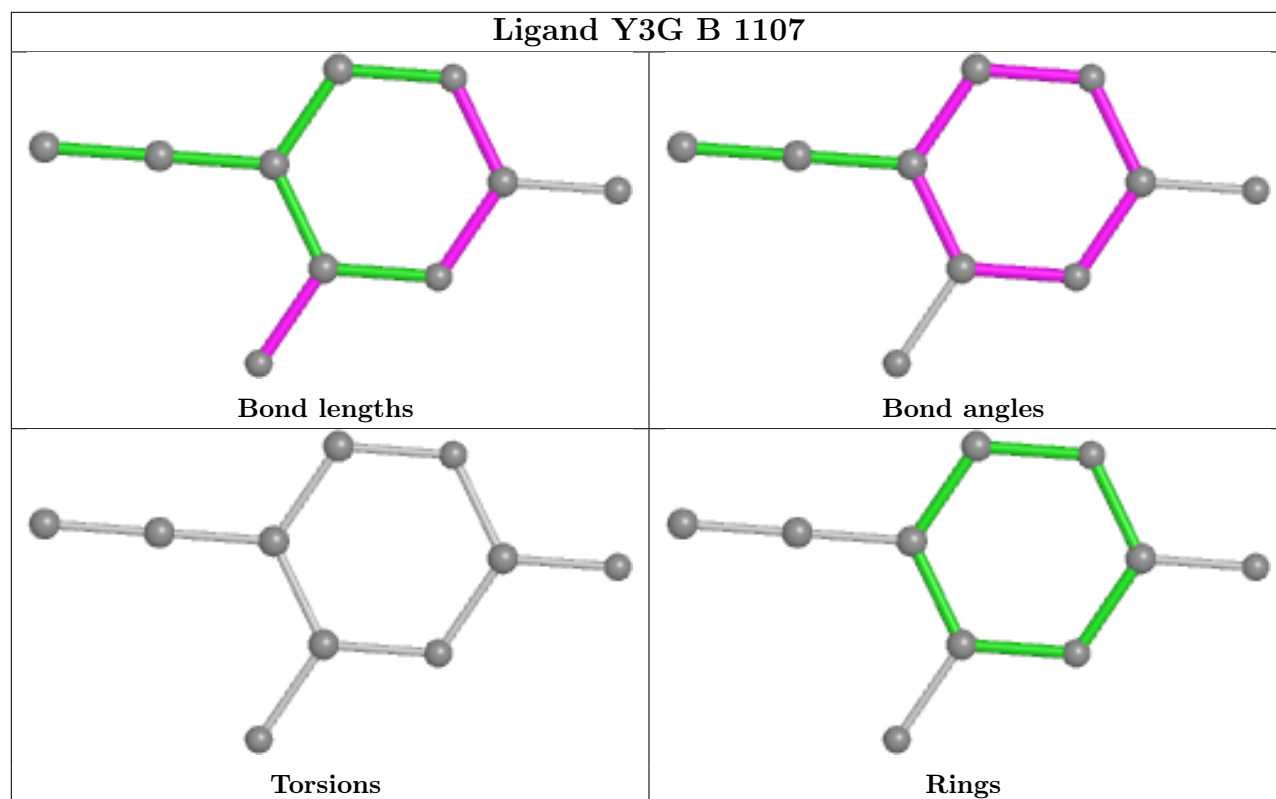
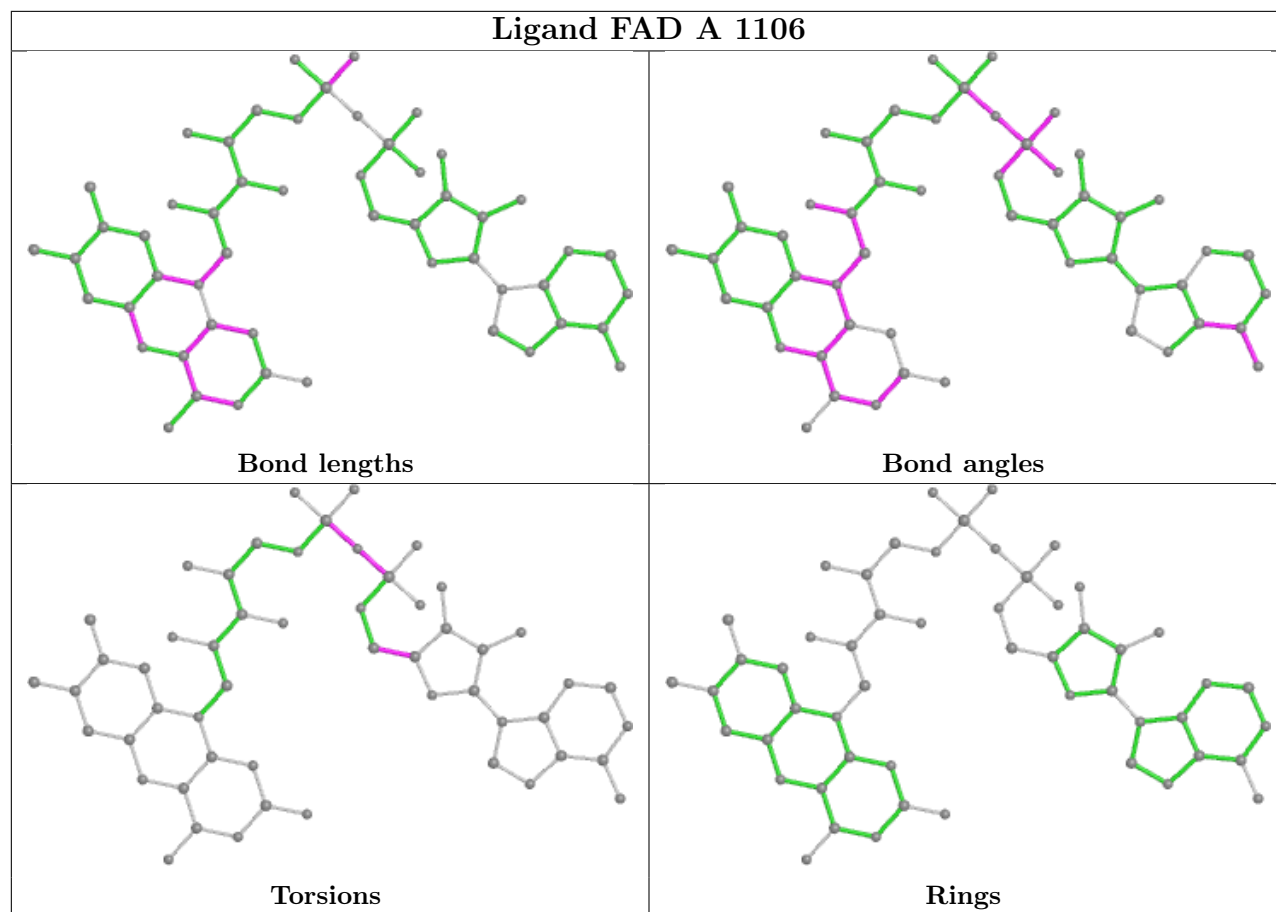
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1106	FAD	2	0
2	A	1101	SF4	2	0
4	A	1106	FAD	2	0
5	B	1107	Y3G	2	0
5	A	1107	Y3G	1	0
5	C	1107	Y3G	2	0
4	D	1106	FAD	1	0
2	C	1101	SF4	1	0
5	D	1107	Y3G	1	0
3	D	1105	FMN	4	0
2	B	1101	SF4	1	0
4	C	1106	FAD	1	0
3	C	1105	FMN	2	0

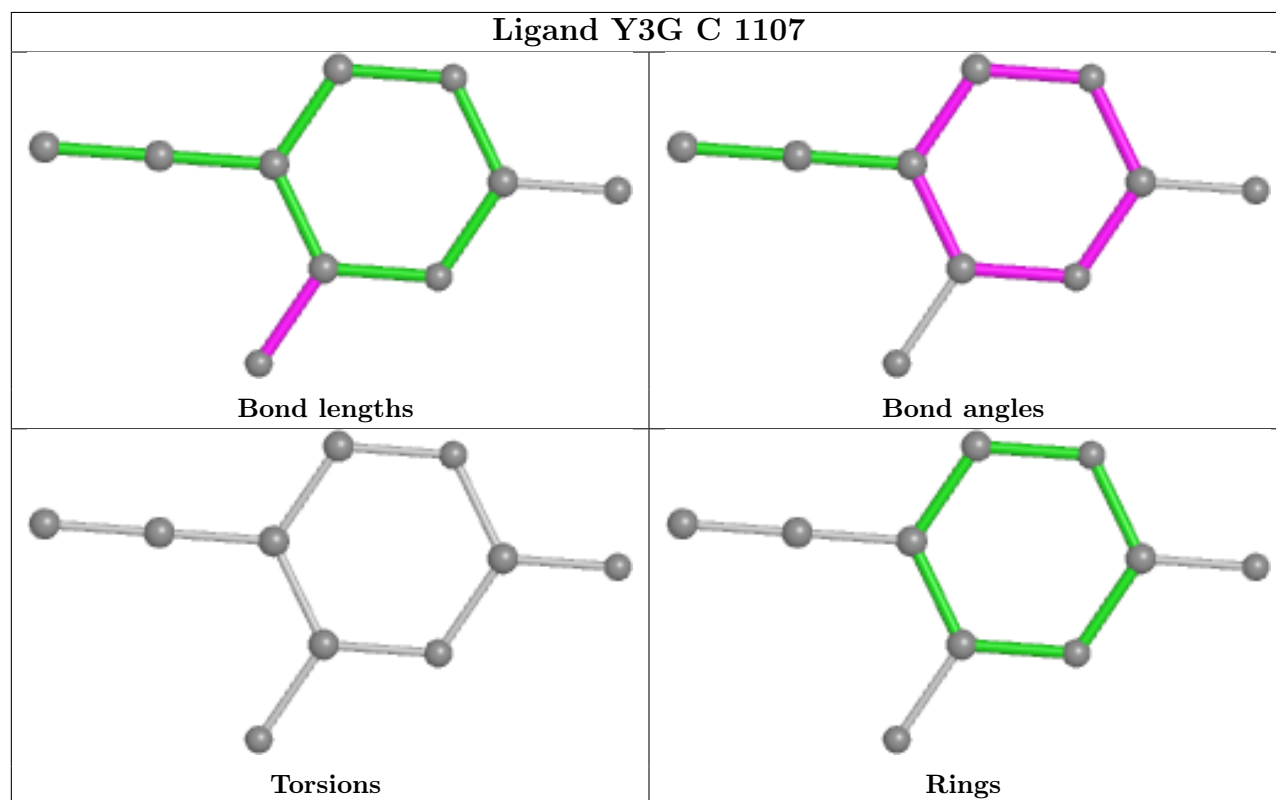
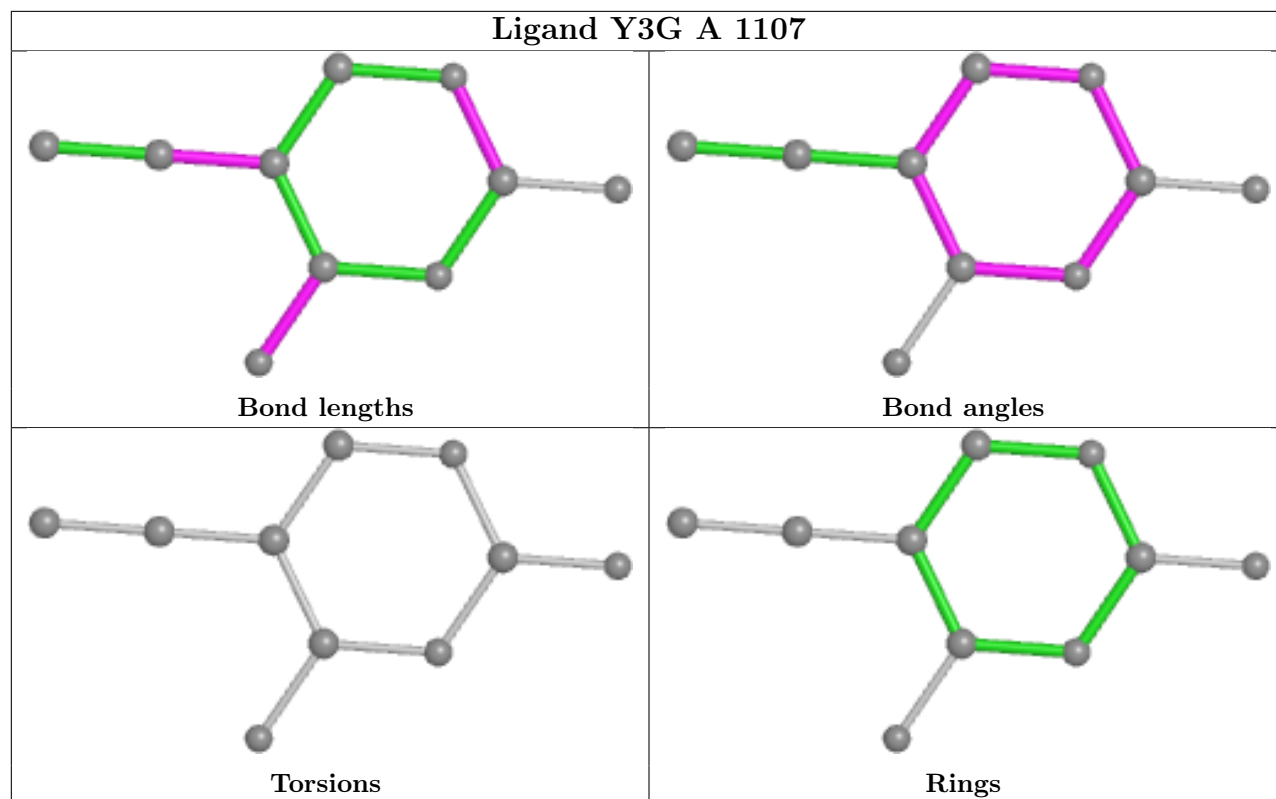
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand FMN A 1105

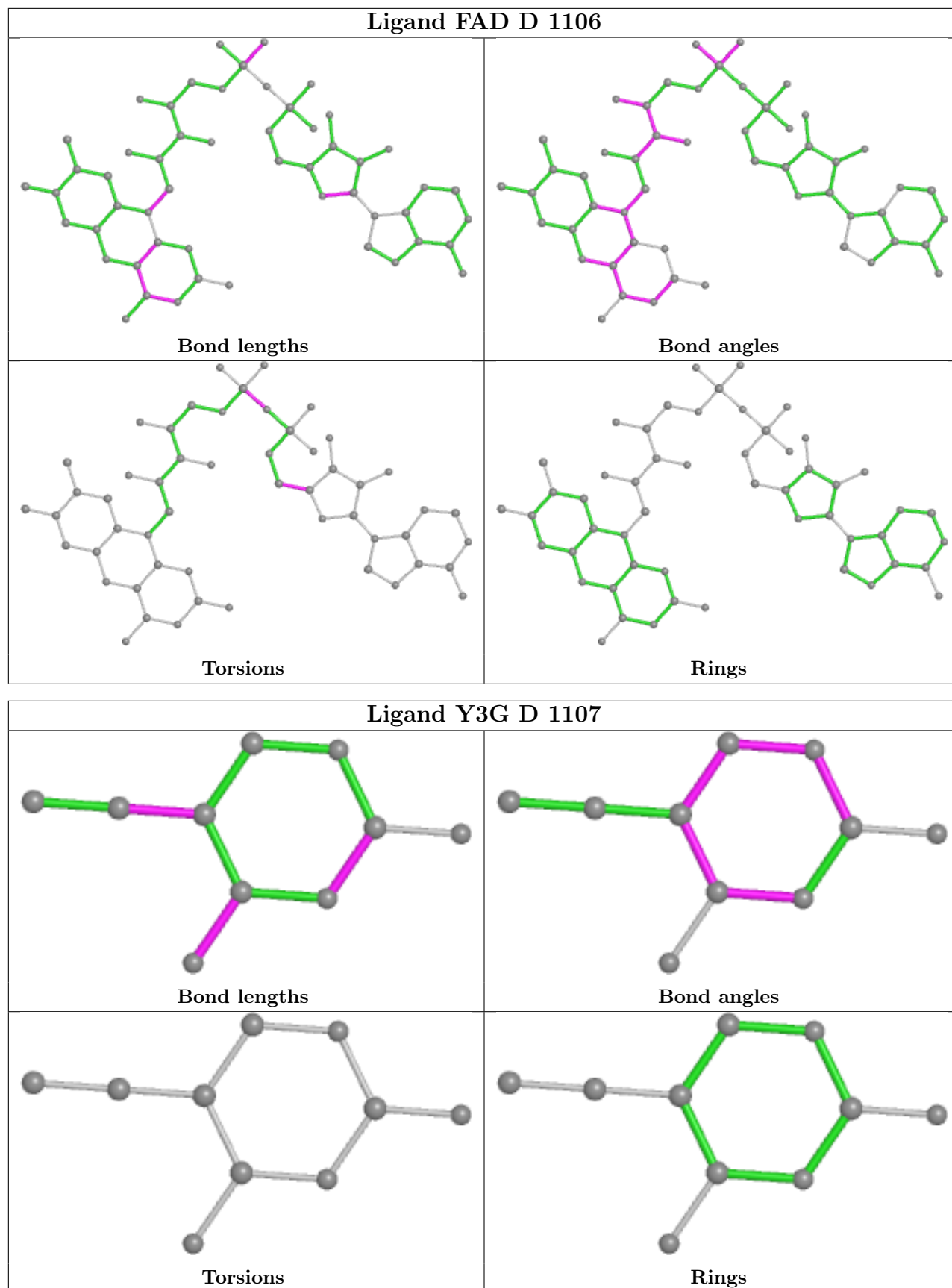




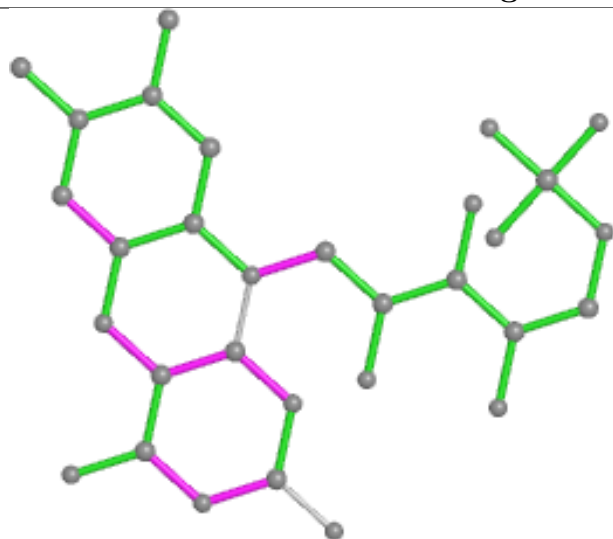




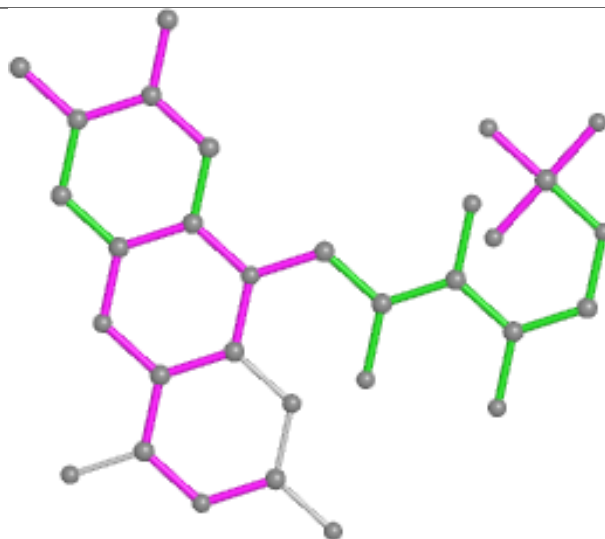




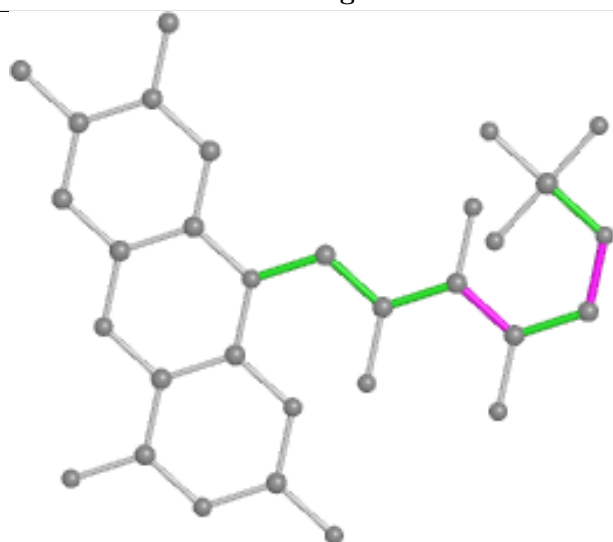
## Ligand FMN B 1105



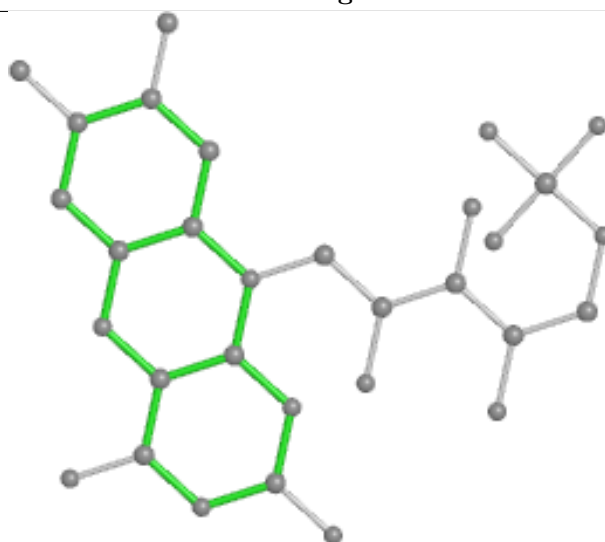
Bond lengths



Bond angles

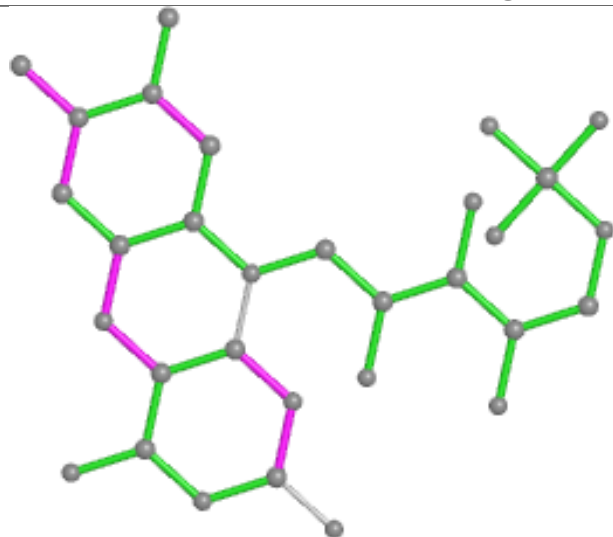


Torsions

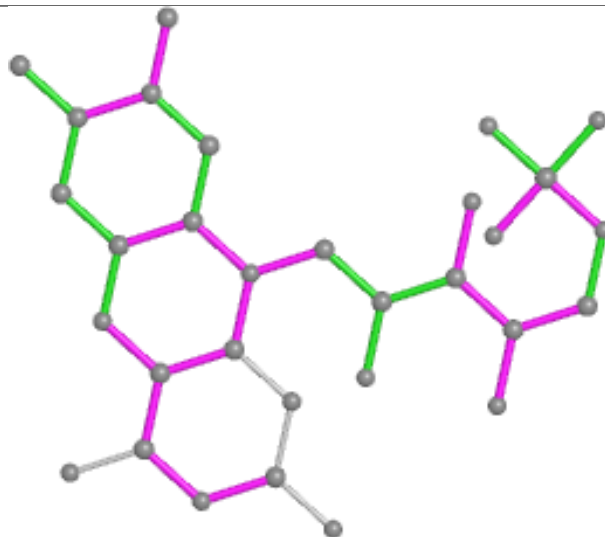


Rings

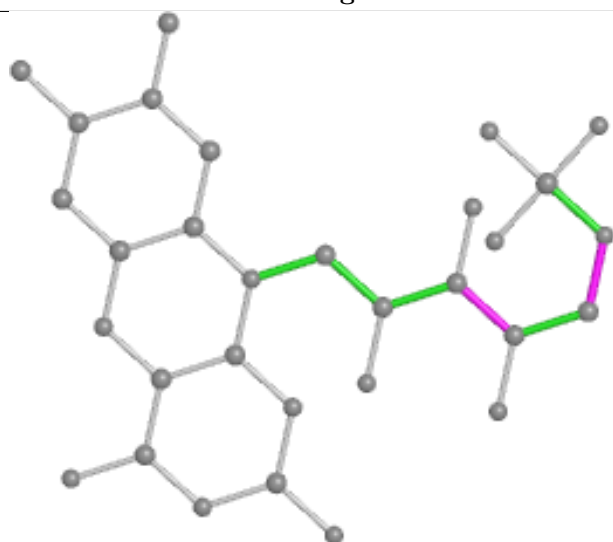
## Ligand FMN D 1105



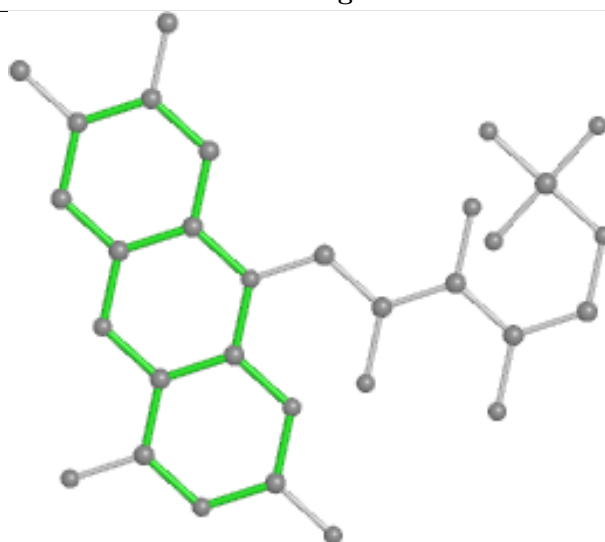
Bond lengths



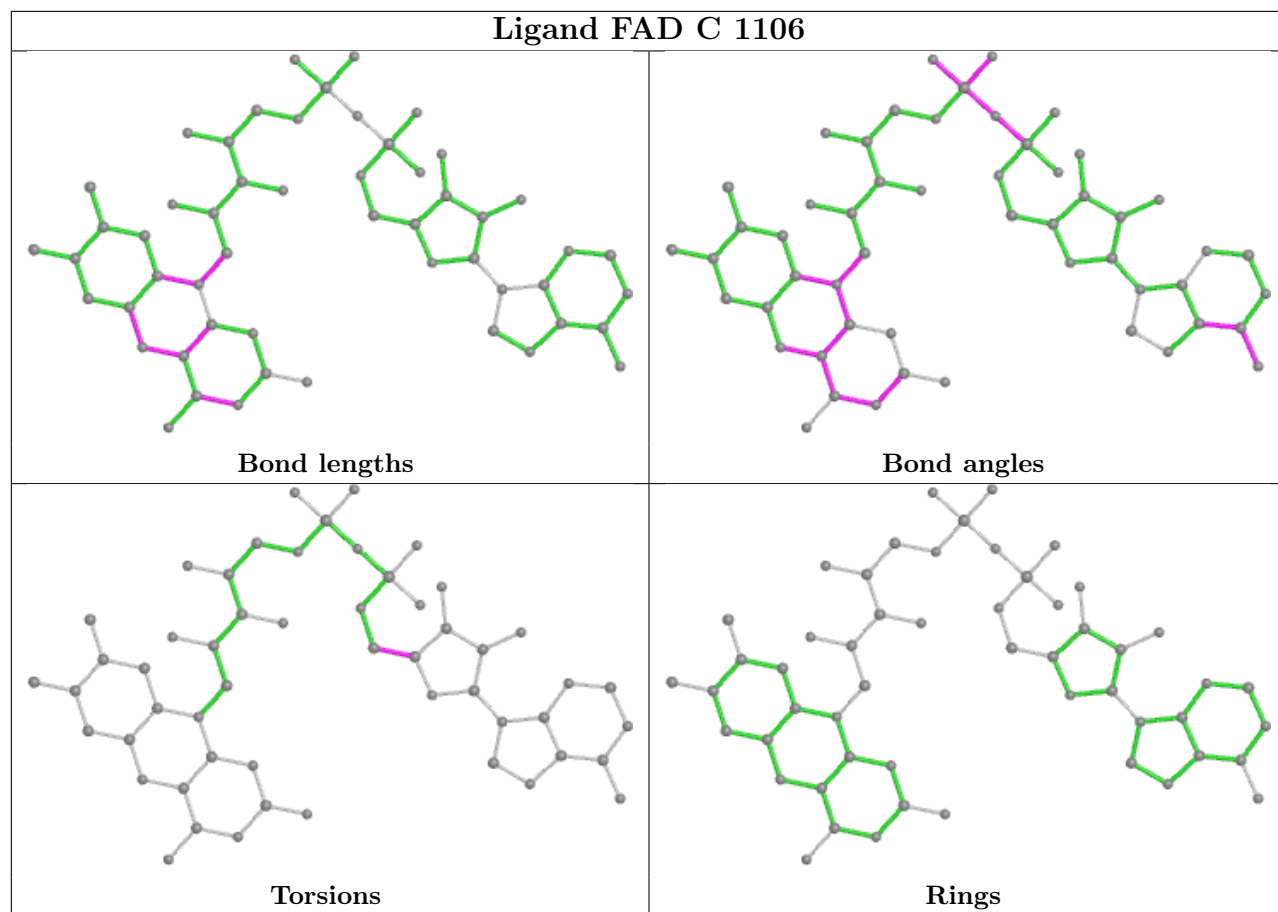
Bond angles

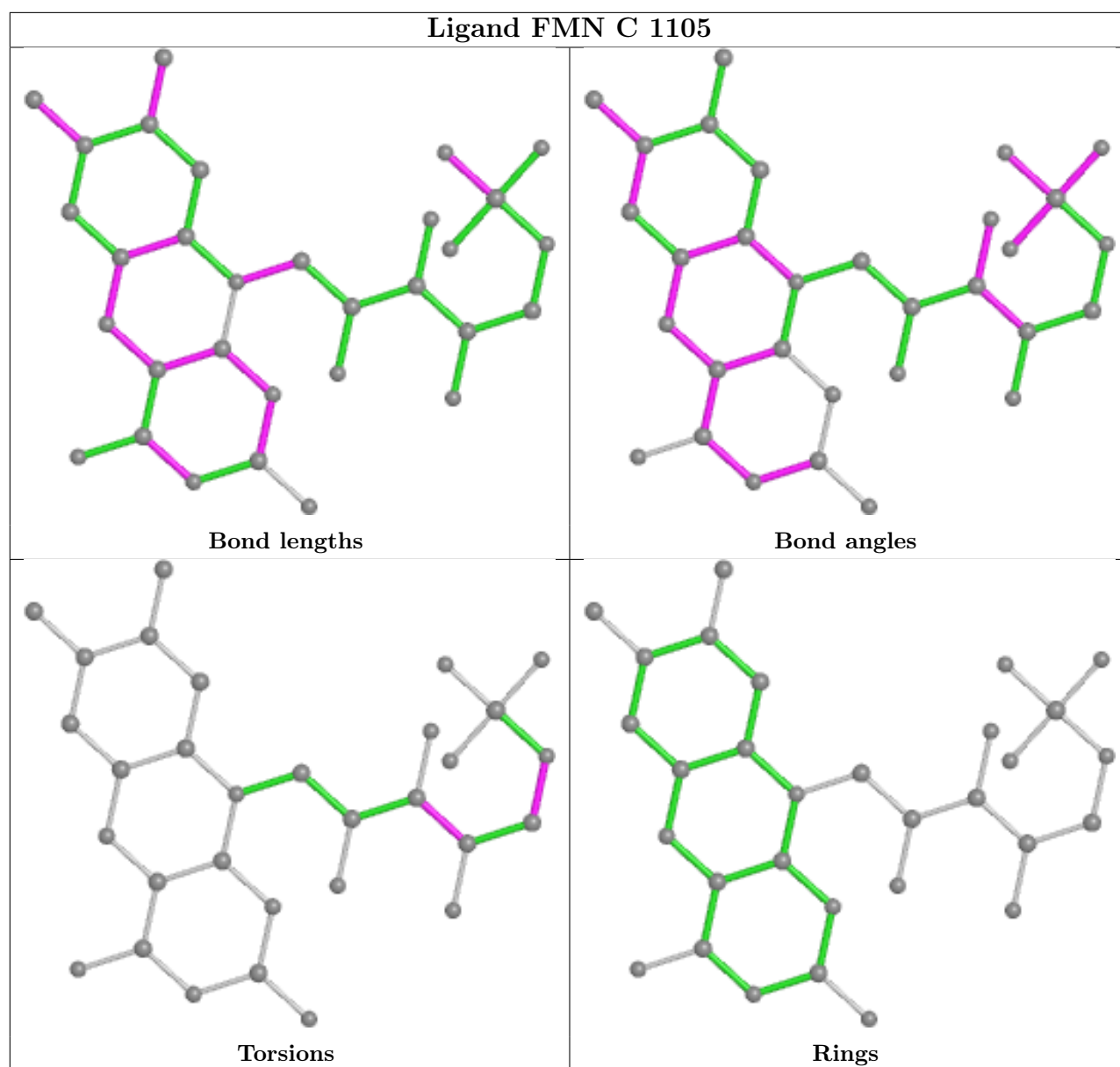


Torsions



Rings





## 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	1005/1025 (98%)	-0.06	30 (2%)	50	49	18, 29, 49, 71	0
1	B	1004/1025 (97%)	-0.13	29 (2%)	51	50	19, 29, 48, 66	0
1	C	1010/1025 (98%)	-0.13	32 (3%)	47	46	17, 26, 46, 70	0
1	D	1014/1025 (98%)	-0.11	31 (3%)	49	48	16, 26, 44, 63	0
All	All	4033/4100 (98%)	-0.11	122 (3%)	50	49	16, 28, 47, 71	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	12.4
1	D	676	GLY	8.8
1	D	902	ALA	7.0
1	C	2	ALA	7.0
1	A	417	GLY	6.4

### 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](#)

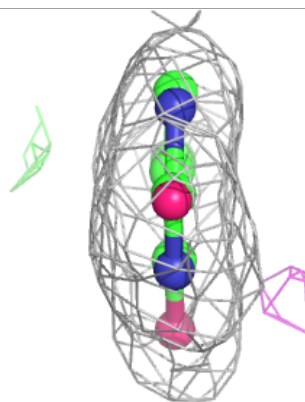
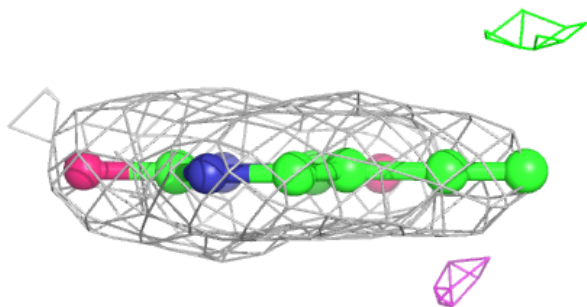
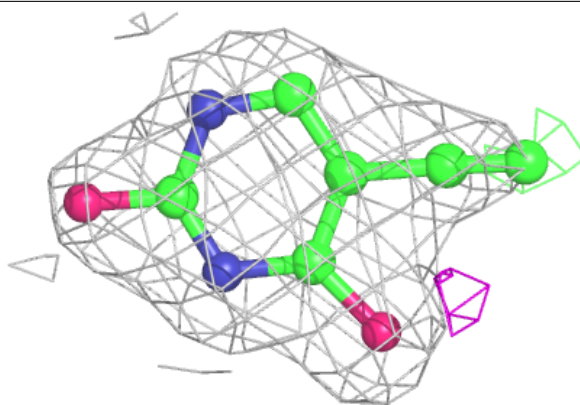
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 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
2	SF4	B	1103	8/8	0.90	0.08	20,21,21,21	0
5	Y3G	D	1107	10/10	0.90	0.15	32,33,34,34	0
2	SF4	C	1103	8/8	0.91	0.08	17,18,18,18	0
2	SF4	A	1104	8/8	0.92	0.07	22,22,23,23	0
5	Y3G	B	1107	10/10	0.92	0.17	36,36,37,37	0
5	Y3G	C	1107	10/10	0.92	0.12	32,32,32,32	0
2	SF4	B	1104	8/8	0.92	0.08	21,21,22,22	0
2	SF4	A	1103	8/8	0.93	0.07	19,20,20,21	0
2	SF4	B	1101	8/8	0.93	0.08	19,19,20,20	0
2	SF4	B	1102	8/8	0.93	0.08	17,17,17,18	0
2	SF4	C	1104	8/8	0.94	0.07	17,17,18,19	0
2	SF4	D	1103	8/8	0.94	0.08	18,19,20,20	0
5	Y3G	A	1107	10/10	0.94	0.11	39,39,40,40	0
2	SF4	C	1101	8/8	0.94	0.09	16,17,17,18	0
2	SF4	C	1102	8/8	0.94	0.09	16,16,17,17	0
2	SF4	A	1101	8/8	0.94	0.07	19,19,20,20	0
2	SF4	D	1102	8/8	0.95	0.10	15,16,17,17	0
2	SF4	D	1101	8/8	0.95	0.09	15,17,18,18	0
2	SF4	A	1102	8/8	0.96	0.09	17,18,18,18	0
2	SF4	D	1104	8/8	0.96	0.07	18,18,18,19	0
4	FAD	A	1106	53/53	0.97	0.10	22,24,24,24	0
4	FAD	B	1106	53/53	0.97	0.10	22,23,25,25	0
3	FMN	A	1105	31/31	0.97	0.12	22,22,23,23	0
4	FAD	D	1106	53/53	0.98	0.10	20,21,23,24	0
3	FMN	D	1105	31/31	0.98	0.12	17,18,18,18	0
3	FMN	B	1105	31/31	0.98	0.10	22,22,23,23	0
3	FMN	C	1105	31/31	0.98	0.12	18,19,21,22	0
4	FAD	C	1106	53/53	0.98	0.10	21,23,25,25	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 Y3G D 1107:**

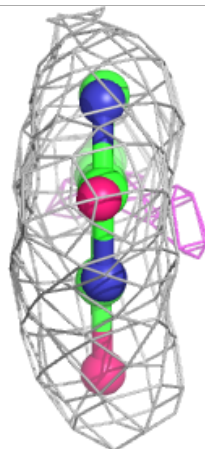
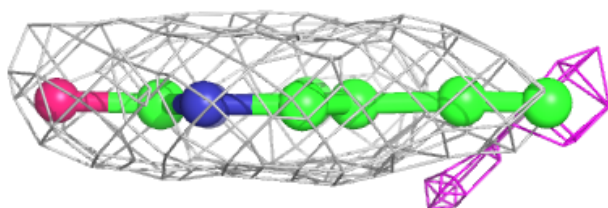
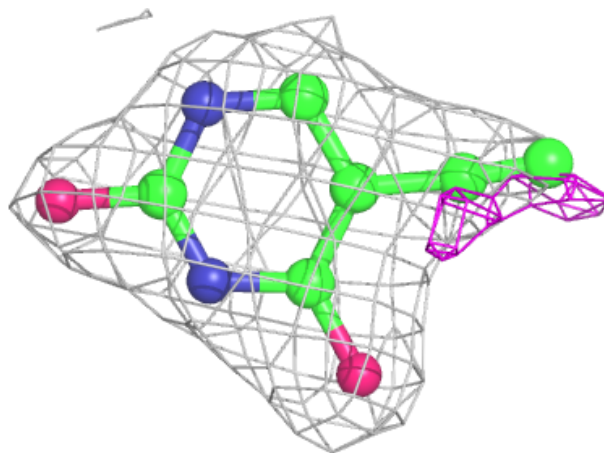
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





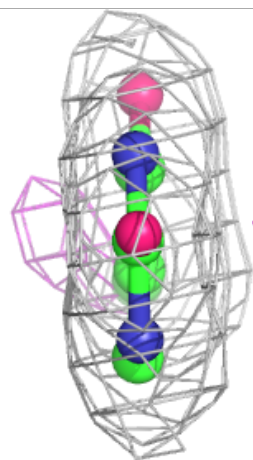
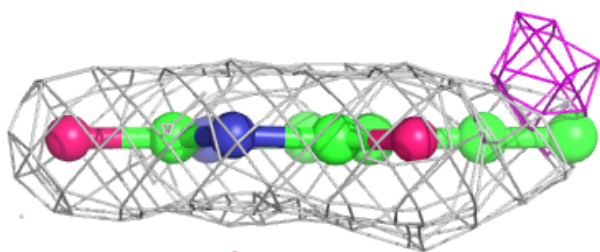
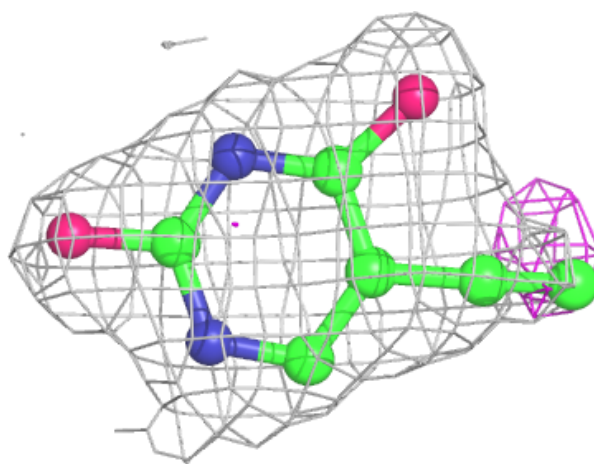
**Electron density around Y3G B 1107:**

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



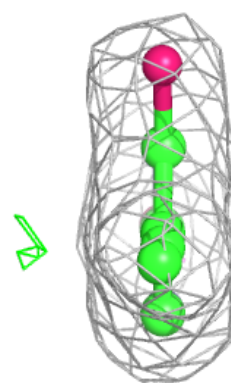
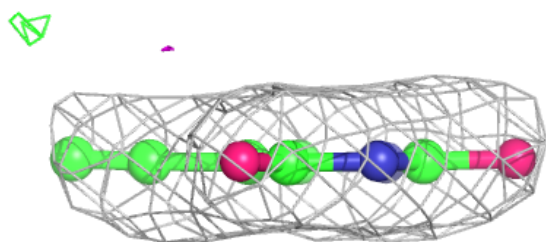
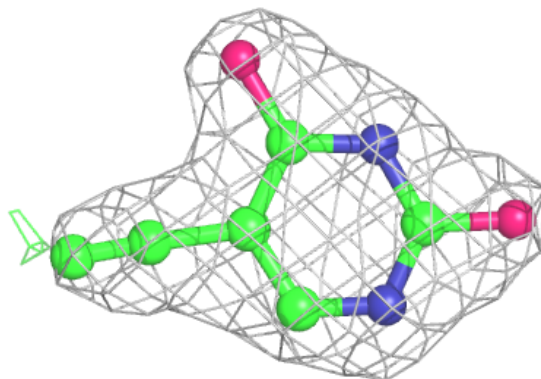
**Electron density around Y3G C 1107:**

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and green (positive)

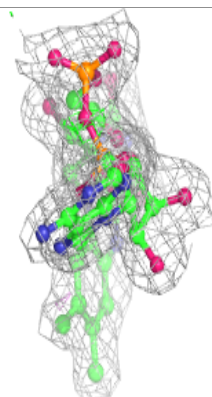
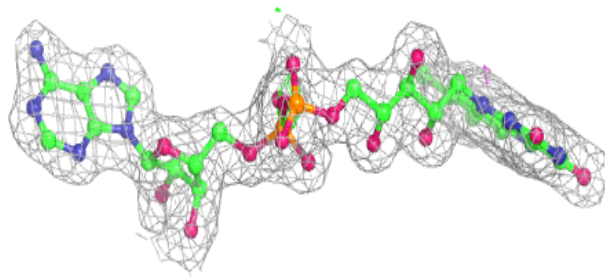
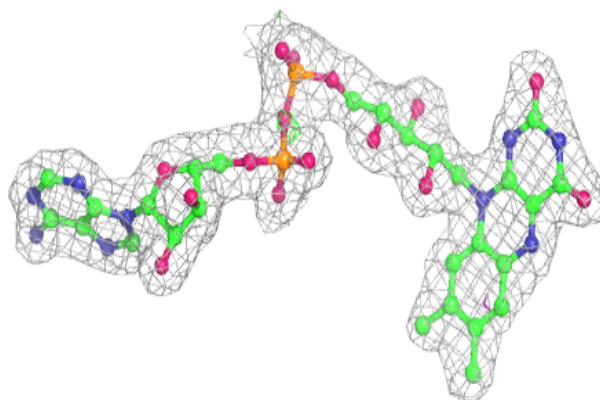


**Electron density around Y3G A 1107:**

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

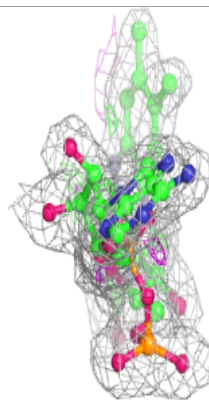
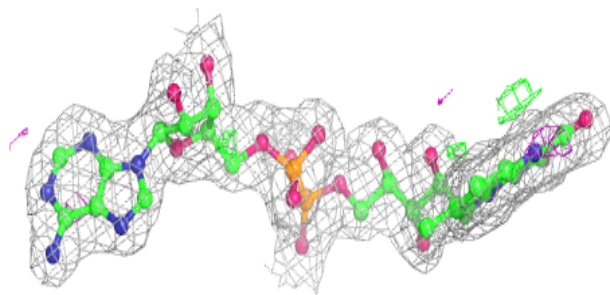
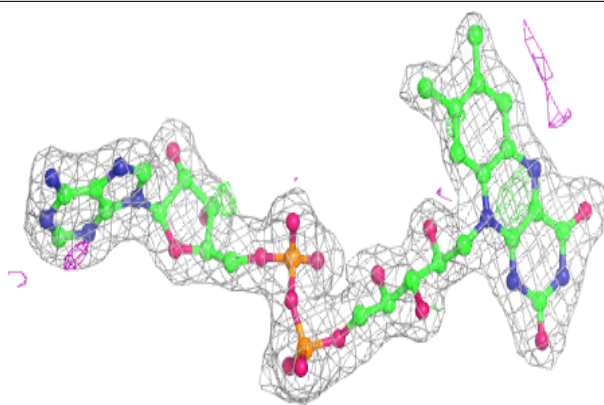
**Electron density around FAD A 1106:**

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



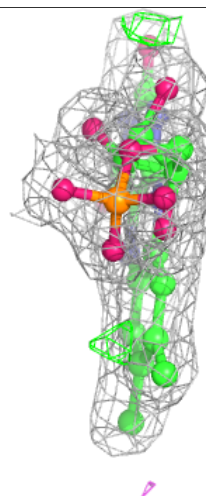
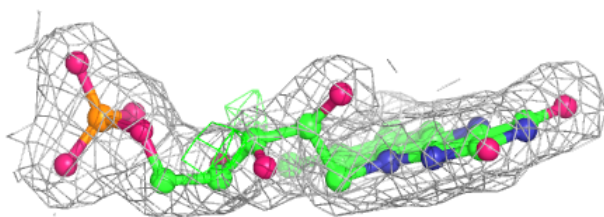
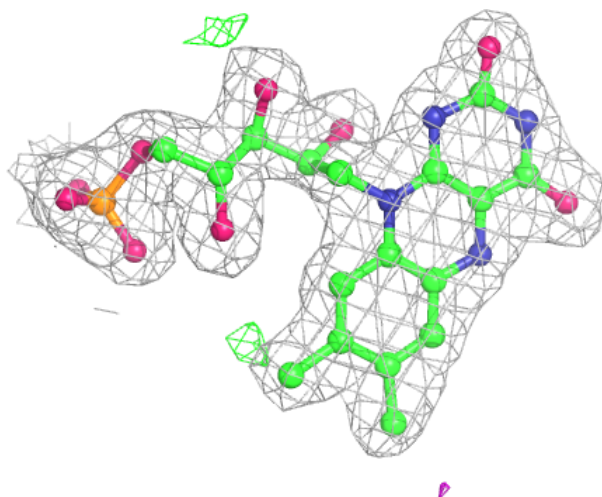
**Electron density around FAD B 1106:**

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



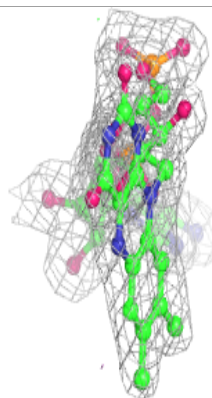
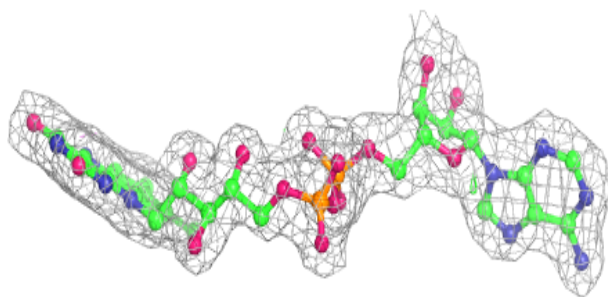
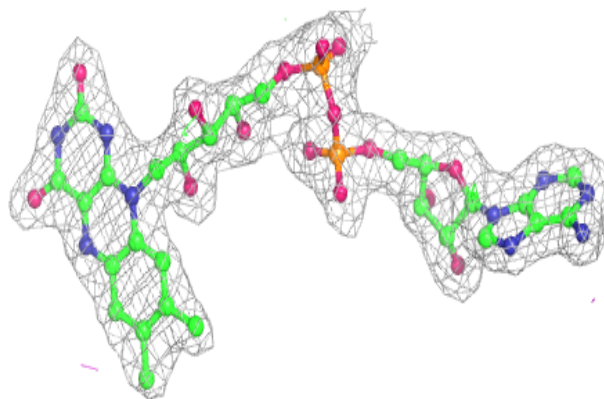
**Electron density around FMN A 1105:**

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and green (positive)

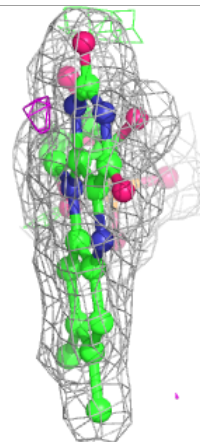
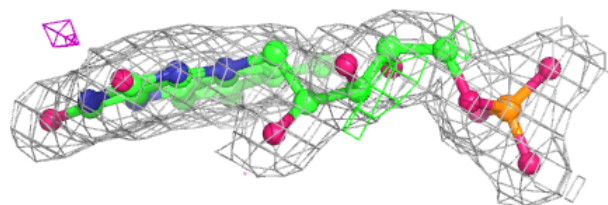
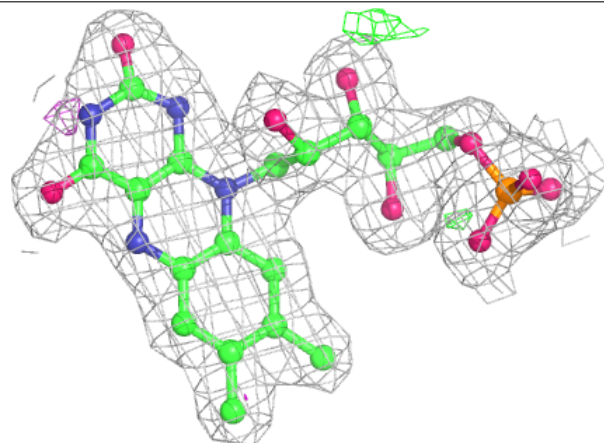


**Electron density around FAD D 1106:**

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

**Electron density around FMN D 1105:**

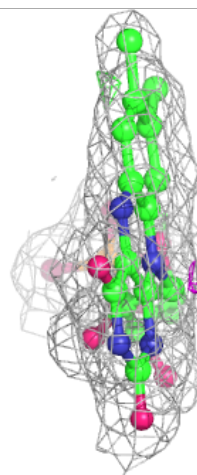
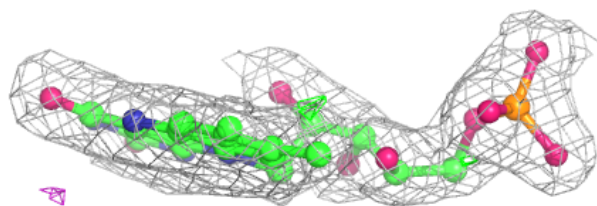
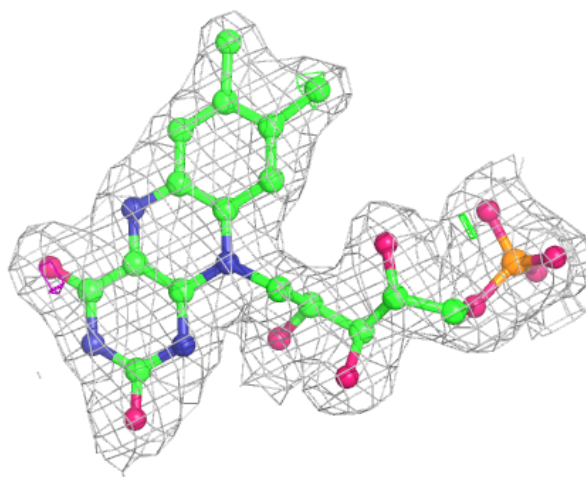
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





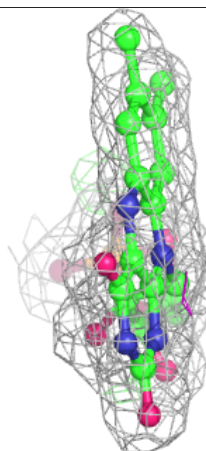
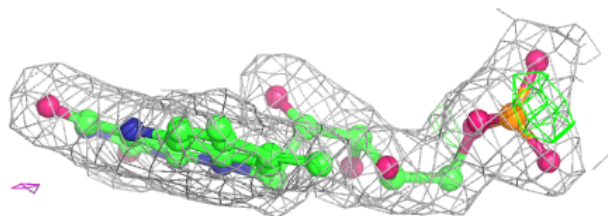
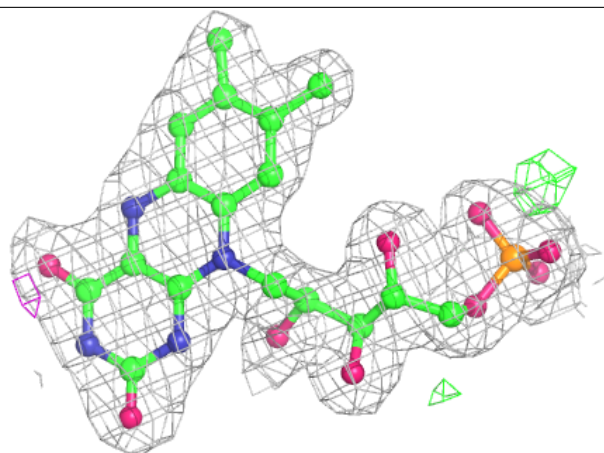
**Electron density around FMN B 1105:**

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

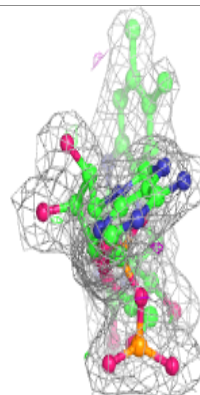
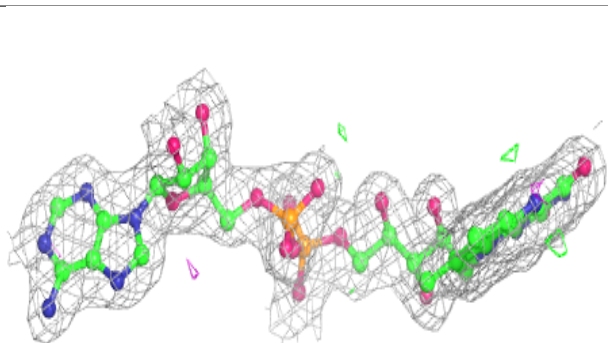
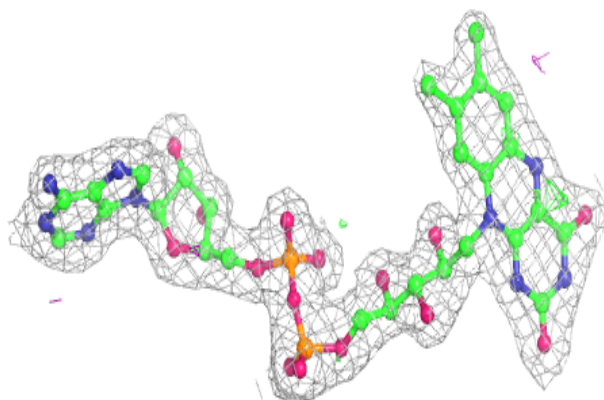


**Electron density around FMN C 1105:**

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

**Electron density around FAD 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.