



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 8, 2025 – 12:09 PM JST

PDB ID : 9UDD / pdb\_00009udd  
Title : Crystal structure of MonCI in complex with monoepoxidized farnesyl acetate  
Authors : Xiao, H.L.; Guan, Y.Z.; Chen, X.  
Deposited on : 2025-04-06  
Resolution : 2.10 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

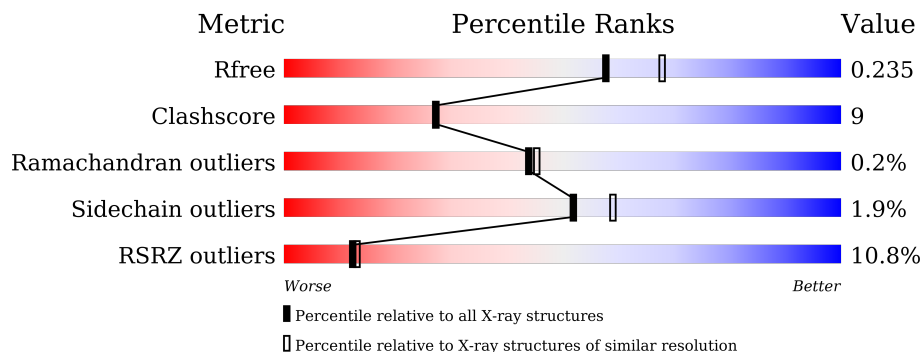
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	511	<div> <div>3%</div> <div>83%</div> <div>10%</div> <div>8%</div> </div>
1	B	511	<div> <div>17%</div> <div>71%</div> <div>20%</div> <div>8%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7526 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 MonCI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	1	0
			3592	2245	663	675	9			
1	B	472	Total	C	N	O	S	0	0	0
			3580	2236	662	673	9			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP Q846W9
A	-13	ASN	-	expression tag	UNP Q846W9
A	-12	HIS	-	expression tag	UNP Q846W9
A	-11	LYS	-	expression tag	UNP Q846W9
A	-10	VAL	-	expression tag	UNP Q846W9
A	-9	HIS	-	expression tag	UNP Q846W9
A	-8	HIS	-	expression tag	UNP Q846W9
A	-7	HIS	-	expression tag	UNP Q846W9
A	-6	HIS	-	expression tag	UNP Q846W9
A	-5	HIS	-	expression tag	UNP Q846W9
A	-4	HIS	-	expression tag	UNP Q846W9
A	-3	ILE	-	expression tag	UNP Q846W9
A	-2	GLU	-	expression tag	UNP Q846W9
A	-1	GLY	-	expression tag	UNP Q846W9
A	0	ARG	-	expression tag	UNP Q846W9
B	-14	MET	-	initiating methionine	UNP Q846W9
B	-13	ASN	-	expression tag	UNP Q846W9
B	-12	HIS	-	expression tag	UNP Q846W9
B	-11	LYS	-	expression tag	UNP Q846W9
B	-10	VAL	-	expression tag	UNP Q846W9
B	-9	HIS	-	expression tag	UNP Q846W9
B	-8	HIS	-	expression tag	UNP Q846W9
B	-7	HIS	-	expression tag	UNP Q846W9
B	-6	HIS	-	expression tag	UNP Q846W9
B	-5	HIS	-	expression tag	UNP Q846W9

*Continued on next page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP Q846W9
B	-3	ILE	-	expression tag	UNP Q846W9
B	-2	GLU	-	expression tag	UNP Q846W9
B	-1	GLY	-	expression tag	UNP Q846W9
B	0	ARG	-	expression tag	UNP Q846W9

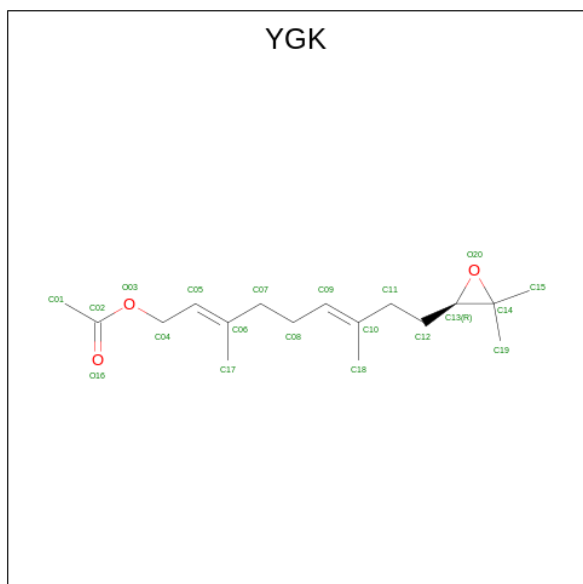
- # FAD
- 
- The image displays the chemical structure of Flavin Adenine Dinucleotide (FAD), a crucial coenzyme. The structure is composed of several interconnected parts:
- Flavin Mononucleotide (FMN) moiety:** Located at the top, it features an isoalloxazine ring system (a tricyclic aromatic system with two nitrogen atoms) substituted with an amino group (NH<sub>2</sub>) and a ribityl side chain. The ribityl chain is a three-carbon chain ending in a carboxylate group (COO<sup>-</sup>).
  - Ribitol linker:** A five-carbon chain (ribitol) connects the FMN moiety to the adenine moiety. It is shown in a zig-zag conformation with hydroxyl groups (OH) at specific positions.
  - Adenine moiety:** Located at the bottom, it consists of a purine ring system (a fused bicyclic aromatic system with two nitrogen atoms) substituted with an amino group (NH<sub>2</sub>) and a ribityl side chain. The ribityl chain is a three-carbon chain ending in a carboxylate group (COO<sup>-</sup>).
- The structure is rendered in a 3D ball-and-stick model, with atoms represented by colored spheres (carbon in grey, oxygen in red, nitrogen in blue, and hydrogen in white) and bonds shown as sticks. The overall structure is highly complex and detailed, showing the spatial arrangement of atoms and the connectivity of the various functional groups.

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is Monoepoxidized farnesyl acetate (CCD ID: YGK) (formula:  $C_{17}H_{28}O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	17	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	187	Total 187	O 187	0	0
6	B	28	Total 28	O 28	0	0



- Molecule 1: MonCl



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.83Å 52.44Å 145.51Å 90.00° 92.62° 90.00°	Depositor
Resolution (Å)	36.34 – 2.10 36.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.34-2.10) 99.4 (36.34-2.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, $R_{free}$	0.196 , 0.231 0.198 , 0.235	Depositor DCC
$R_{free}$ test set	2884 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: GOL, YGK, CL, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.49	0/3663	0.66	0/4990
1	B	0.40	0/3650	0.63	0/4972
All	All	0.45	0/7313	0.65	0/9962

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	3592	0	3578	42	0
1	B	3580	0	3570	89	0
2	A	53	0	31	4	0
2	B	53	0	31	6	0
3	A	12	0	16	1	0
4	A	20	0	0	6	0
5	A	1	0	0	0	0
6	A	187	0	0	3	0
6	B	28	0	0	1	0
All	All	7526	0	7226	131	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 9.

The worst 5 of 131 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:184:ARG:HB2	1:B:188:TRP:CZ2	2.07	0.88
1:B:211:ARG:HH21	1:B:291:PRO:HB2	1.41	0.84
1:B:362:ARG:HE	1:B:362:ARG:HA	1.48	0.79
1:B:184:ARG:O	1:B:188:TRP:CD2	2.38	0.77
1:A:208[A]:TYR:OH	1:A:331:ILE:HG13	1.87	0.75

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	469/511 (92%)	458 (98%)	10 (2%)	1 (0%)	44	45
1	B	468/511 (92%)	456 (97%)	11 (2%)	1 (0%)	44	45
All	All	937/1022 (92%)	914 (98%)	21 (2%)	2 (0%)	44	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	ARG
1	B	165	GLY

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/401 (92%)	363 (99%)	5 (1%)	62	70
1	B	367/401 (92%)	358 (98%)	9 (2%)	42	47
All	All	735/802 (92%)	721 (98%)	14 (2%)	52	59

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	189	LEU
1	B	231	ASP
1	B	362	ARG
1	B	298	SER
1	B	304	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	B	167	GLN
1	B	187	GLN
1	B	45	GLN
1	B	46	HIS
1	B	124	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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z  > 2$
3	GOL	A	504	-	5,5,5	0.73	0	5,5,5	1.05	1 (20%)
2	FAD	B	700	-	53,58,58	0.48	0	68,89,89	0.55	1 (1%)
4	YGK	A	503	-	20,20,20	2.01	2 (10%)	27,27,27	2.54	5 (18%)
2	FAD	A	501	-	53,58,58	0.55	0	68,89,89	0.66	2 (2%)
3	GOL	A	502	-	5,5,5	0.92	0	5,5,5	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	504	-	-	3/4/4/4	-
2	FAD	B	700	-	-	7/30/50/50	0/6/6/6
4	YGK	A	503	-	-	6/17/25/25	0/1/1/1
2	FAD	A	501	-	-	5/30/50/50	0/6/6/6
3	GOL	A	502	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	YGK	O20-C14	8.30	1.60	1.46
4	A	503	YGK	O20-C13	-2.15	1.41	1.45

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	YGK	O20-C13-C14	10.96	68.55	59.91
4	A	503	YGK	C14-O20-C13	-4.03	56.69	60.77
4	A	503	YGK	O20-C13-C12	-3.89	111.08	117.74
4	A	503	YGK	O20-C14-C13	-3.56	54.76	58.89
2	A	501	FAD	C5A-C6A-N6A	2.30	123.84	120.35

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

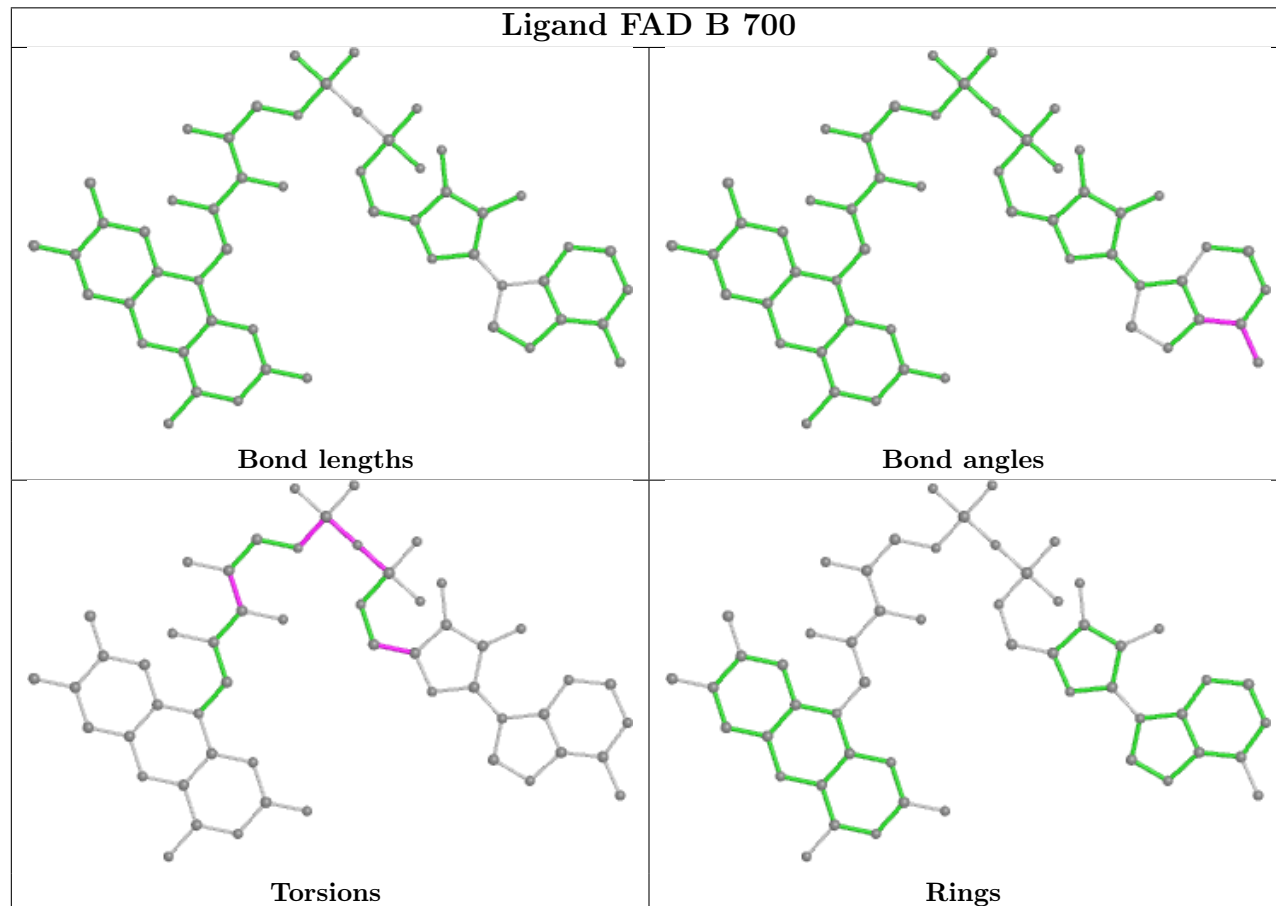
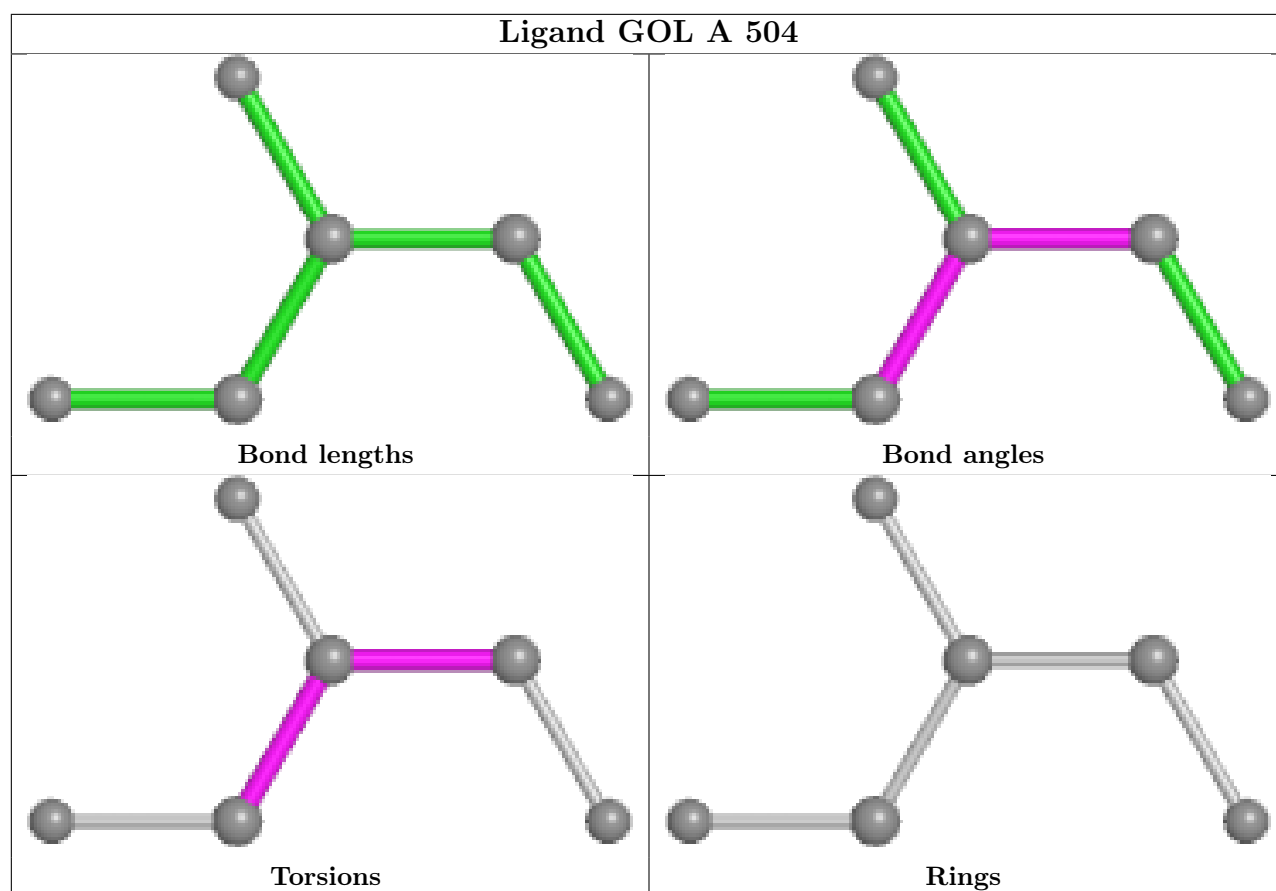
Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5'-O5'-P-O2P
2	A	501	FAD	C5'-O5'-P-O3P
3	A	504	GOL	O1-C1-C2-O2
3	A	504	GOL	O1-C1-C2-C3
4	A	503	YGK	C11-C12-C13-C14

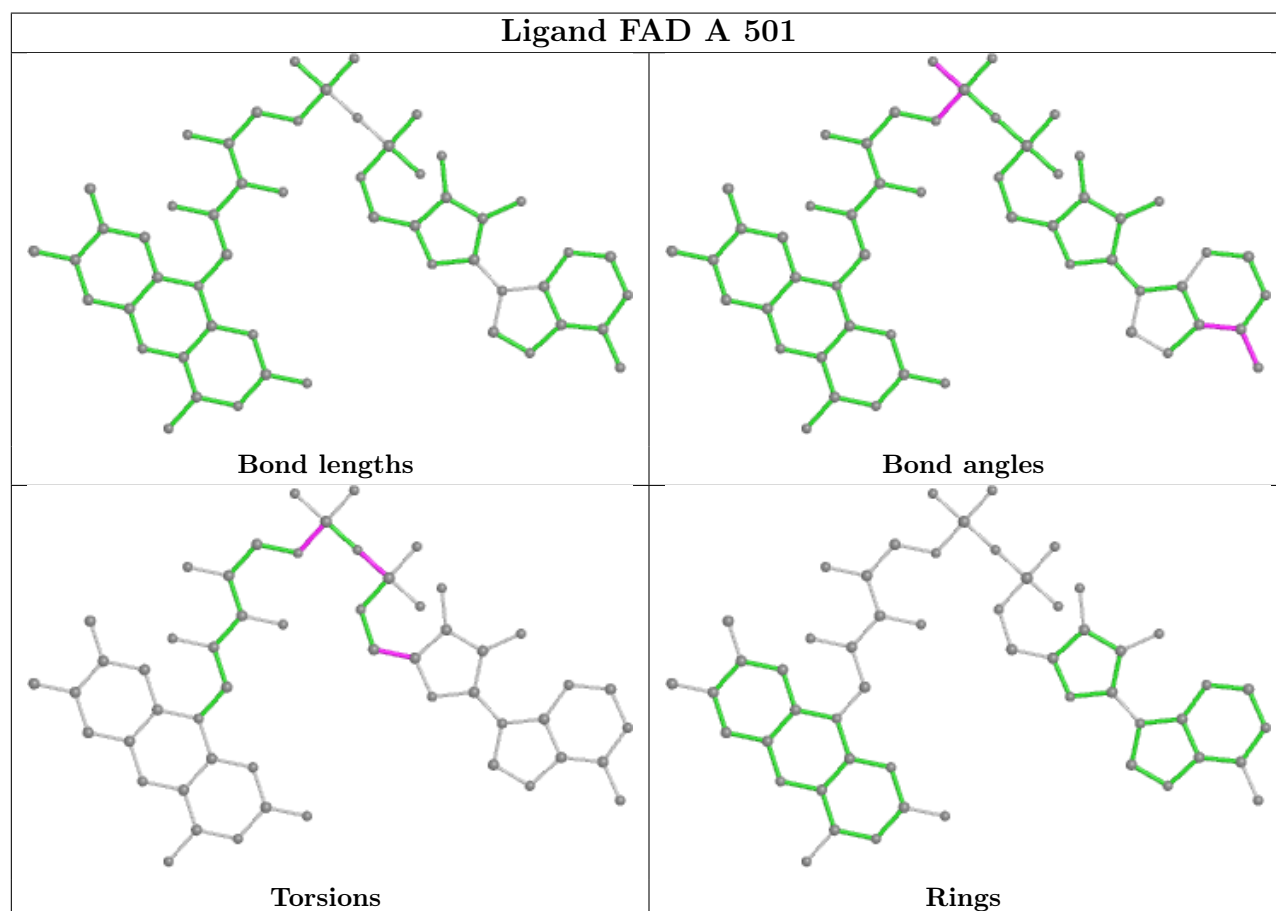
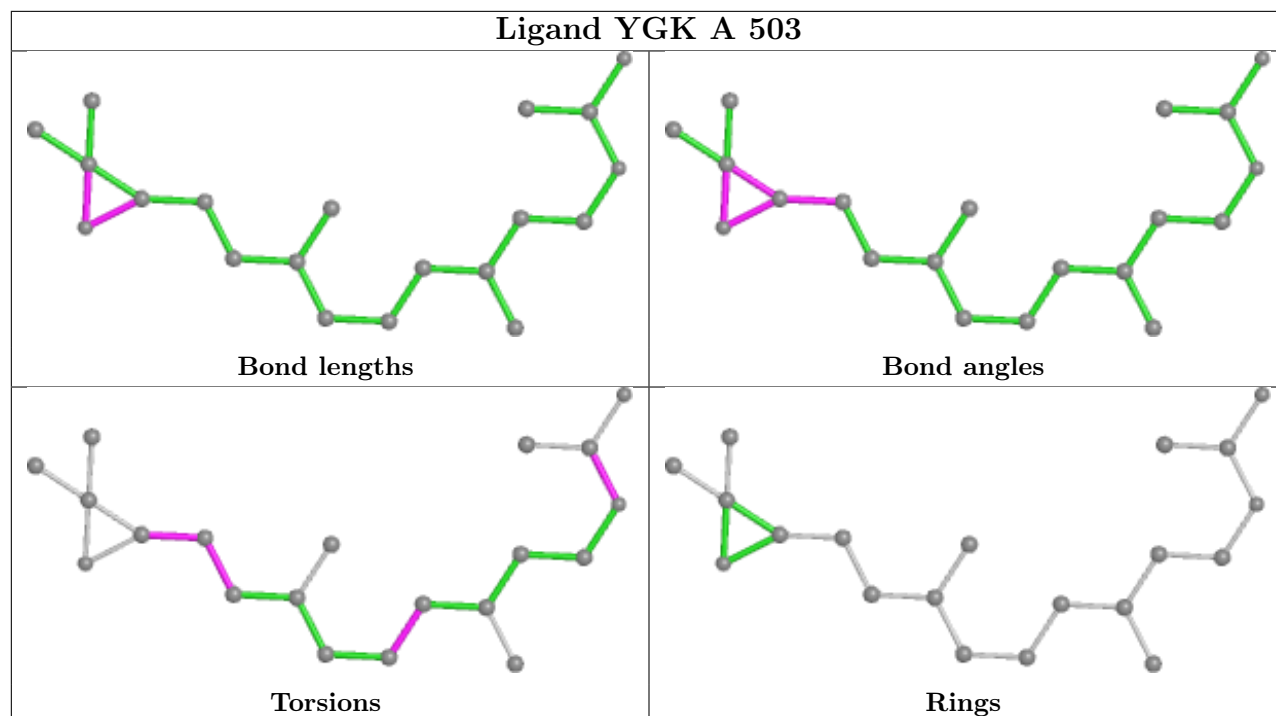
There are no ring outliers.

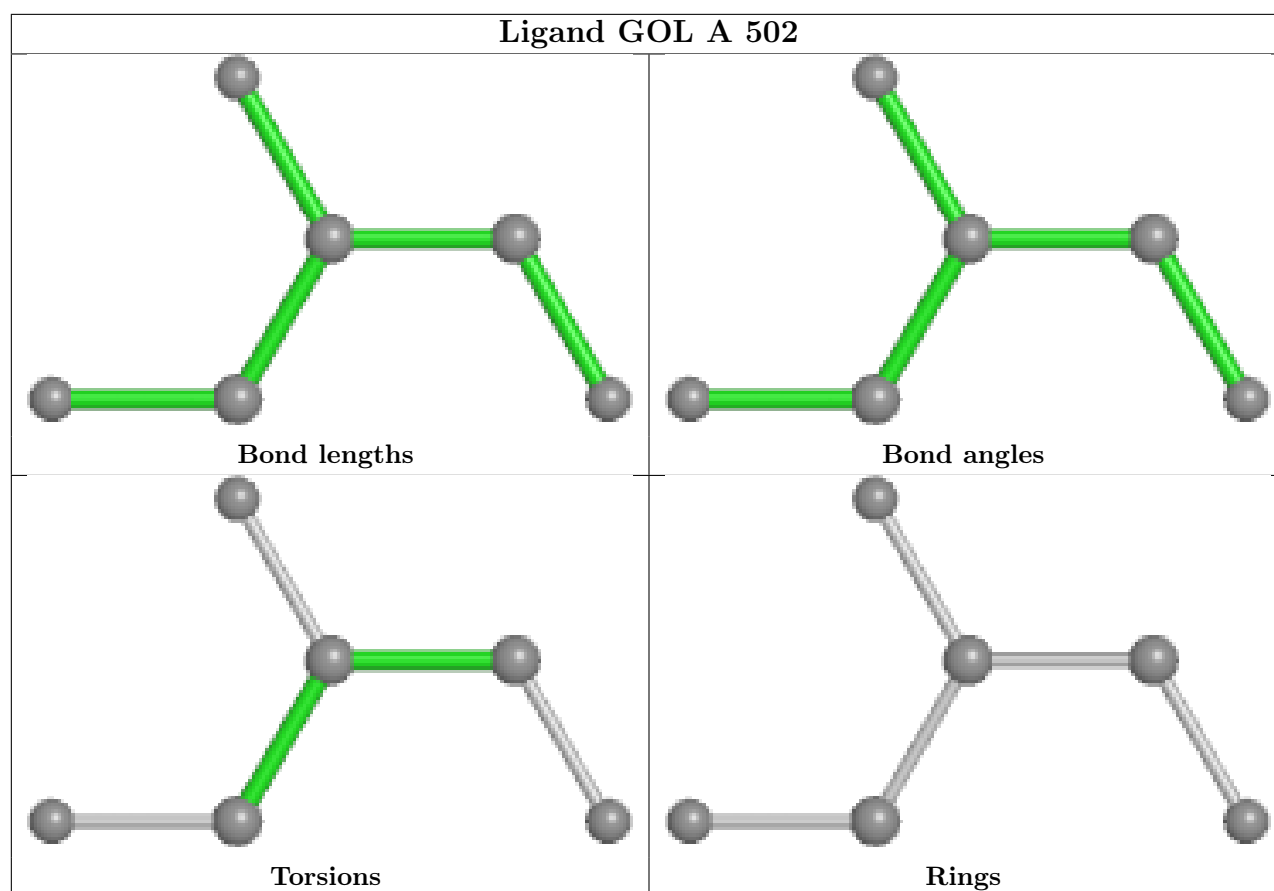
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	700	FAD	6	0
4	A	503	YGK	6	0
2	A	501	FAD	4	0
3	A	502	GOL	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.







## 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	472/511 (92%)	0.01	16 (3%)	48 50	18, 39, 67, 125	1 (0%)
1	B	472/511 (92%)	1.12	86 (18%)	4 5	36, 77, 120, 152	0
All	All	944/1022 (92%)	0.56	102 (10%)	12 13	18, 53, 112, 152	1 (0%)

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	ALA	6.7
1	A	479	ALA	5.5
1	B	363	ALA	5.3
1	B	230	ALA	5.0
1	A	361	ALA	4.7

### 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](#)

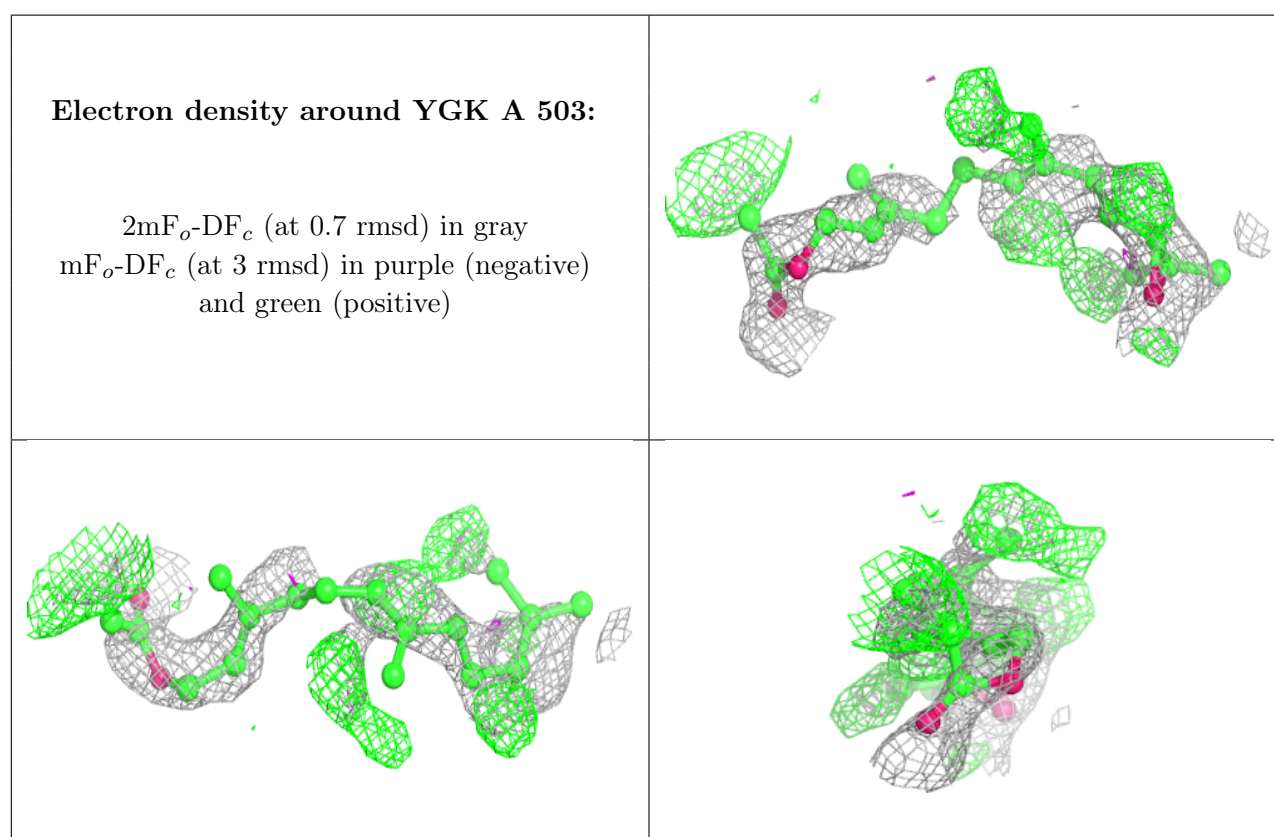
There are no monosaccharides in this entry.

### 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.

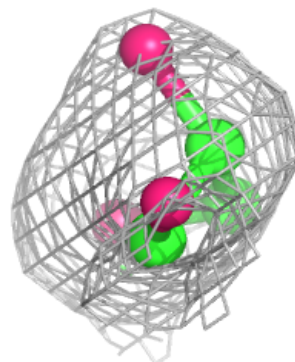
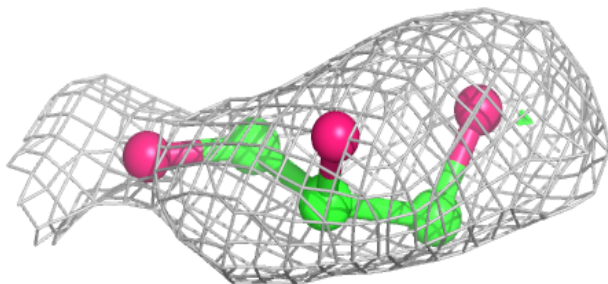
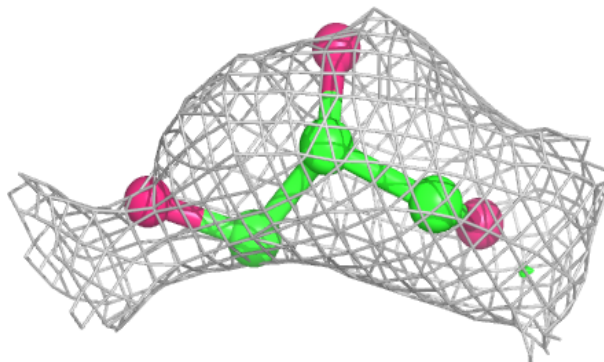
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	YGK	A	503	20/20	0.73	0.31	93,98,104,104	0
3	GOL	A	502	6/6	0.86	0.17	70,77,82,84	0
3	GOL	A	504	6/6	0.88	0.16	75,76,78,81	0
2	FAD	B	700	53/53	0.90	0.11	62,73,96,100	0
2	FAD	A	501	53/53	0.97	0.06	24,31,35,36	0
5	CL	A	505	1/1	0.98	0.08	42,42,42,42	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.



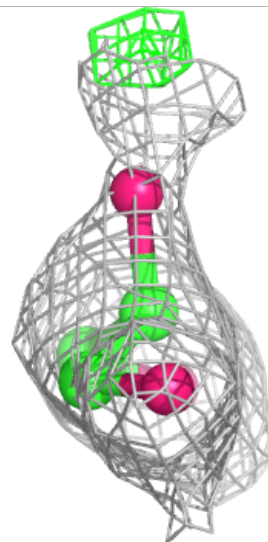
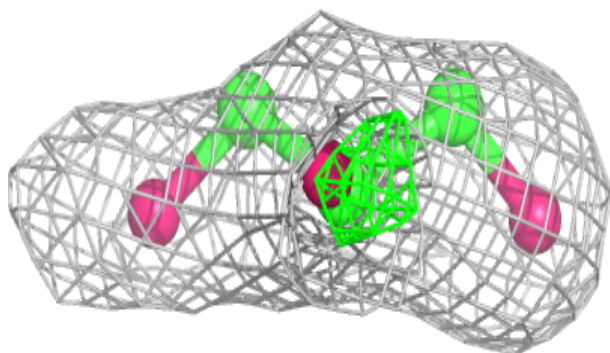
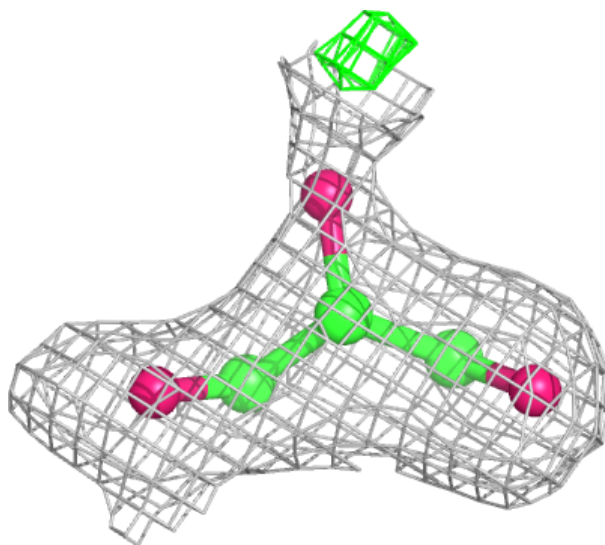
**Electron density around GOL A 502:**

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



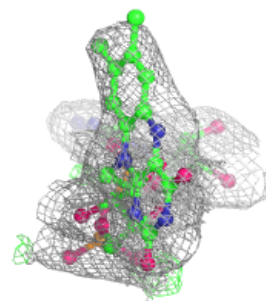
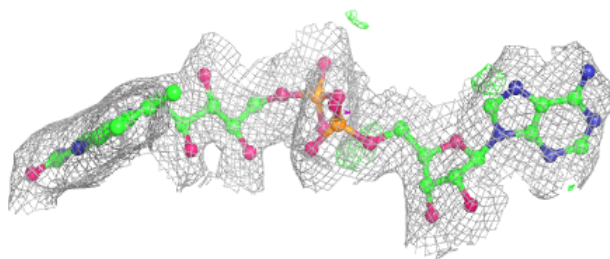
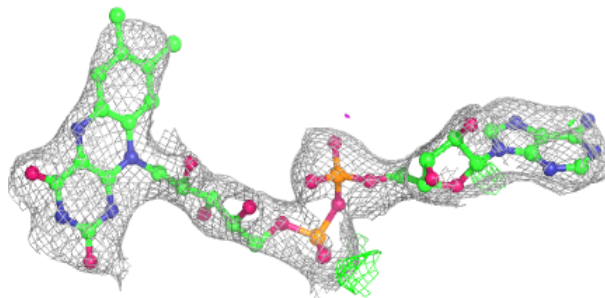
**Electron density around GOL A 504:**

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

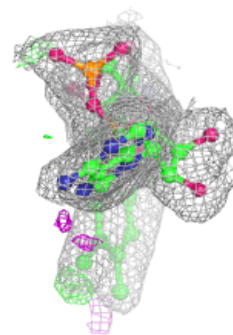
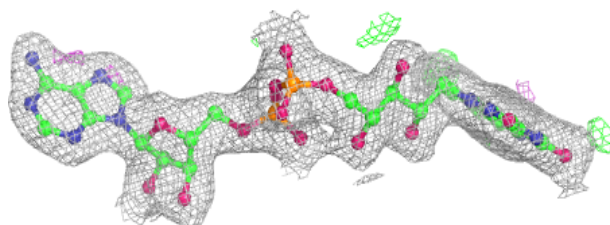
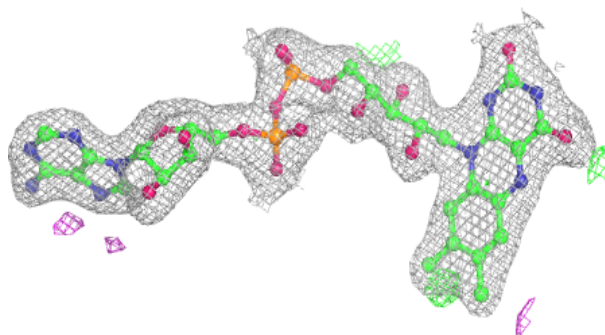


**Electron density around FAD B 700:**

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

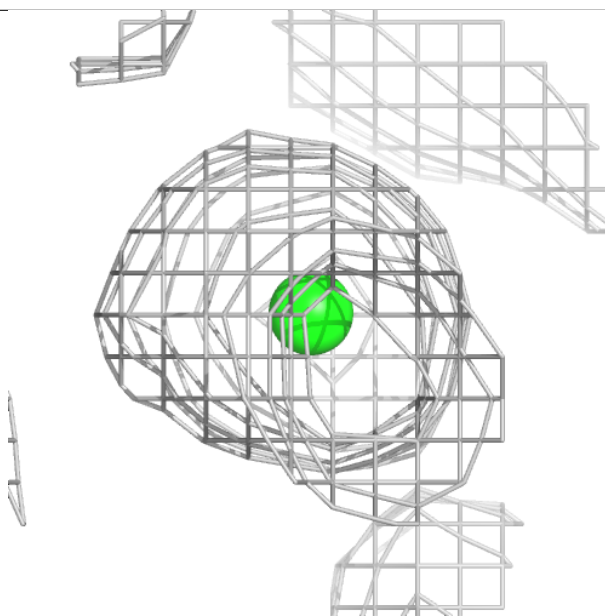
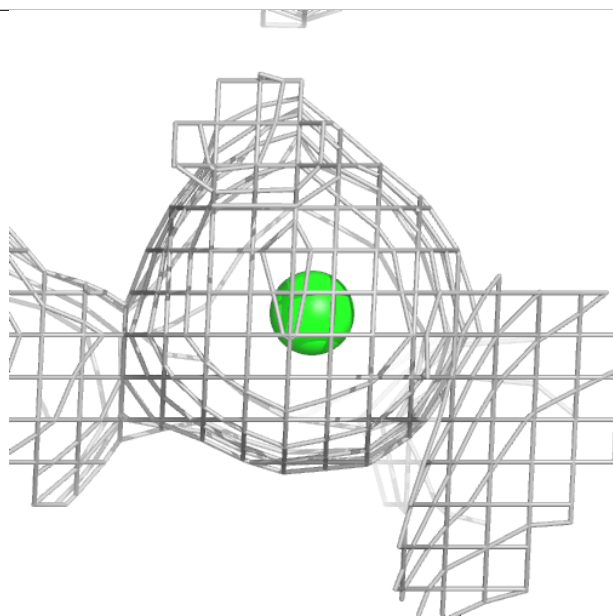
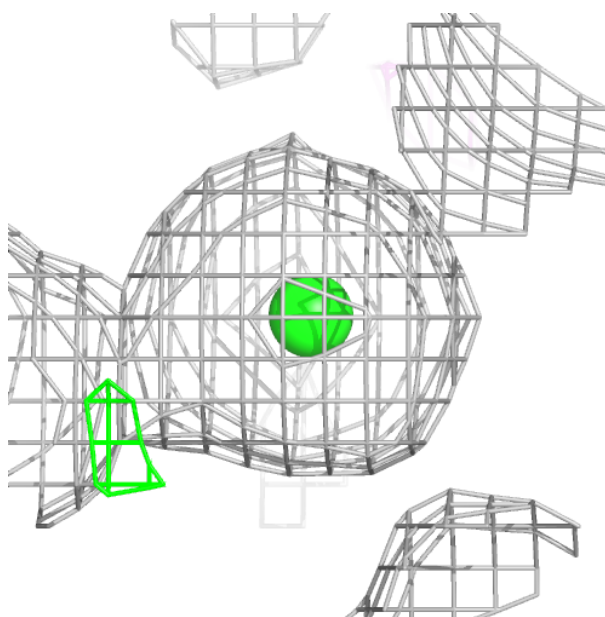
**Electron density around FAD A 501:**

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



**Electron density around CL A 505:**

$2mF_o-DF_c$  (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.