



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 26, 2024 – 04:13 AM EDT

PDB ID : 6RVB  
Title : NADH-dependent Coenzyme A Disulfide Reductase soaked with NADH  
Authors : Koepke, J.; Preu, J.  
Deposited on : 2019-05-31  
Resolution : 2.90 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

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

---

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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

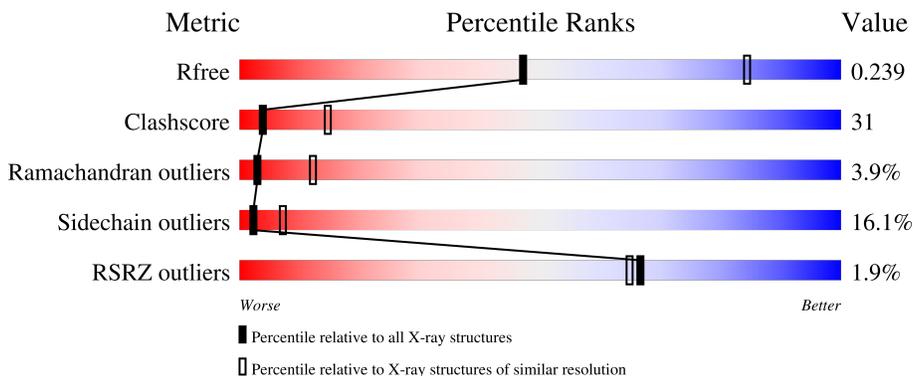
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	443	 2% 59% 28% 9% .
1	B	443	 2% 53% 32% 11% .
1	C	443	 2% 58% 27% 12% .
1	D	443	 % 56% 30% 12% .

## 2 Entry composition [i](#)

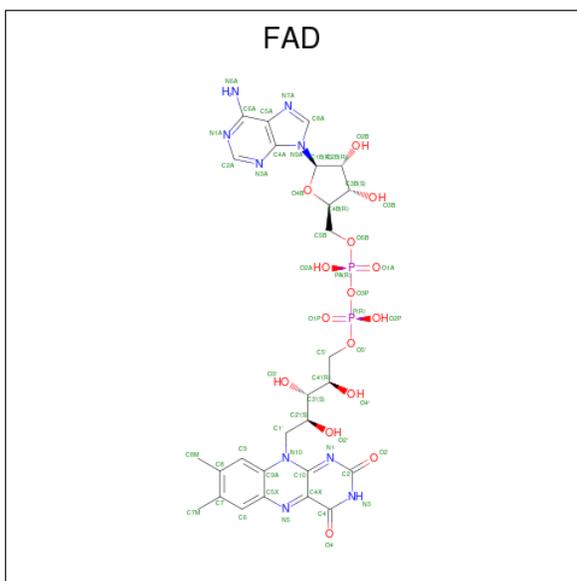
There are 5 unique types of molecules in this entry. The entry contains 14205 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NADH oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	443	Total 3379	C 2147	N 608	O 617	S 7	0	0	0
1	B	443	Total 3379	C 2147	N 608	O 617	S 7	0	0	0
1	C	443	Total 3378	C 2146	N 608	O 617	S 7	0	0	0
1	D	443	Total 3377	C 2146	N 608	O 616	S 7	0	0	0

- Molecule 2 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).



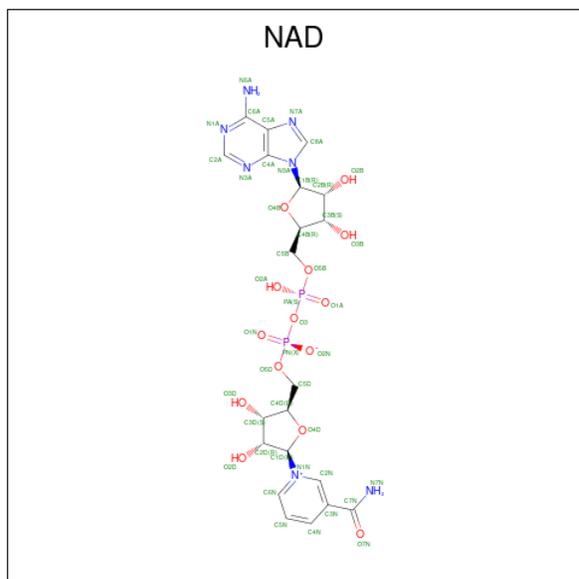
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

*Continued on next page...*

Continued from previous page...

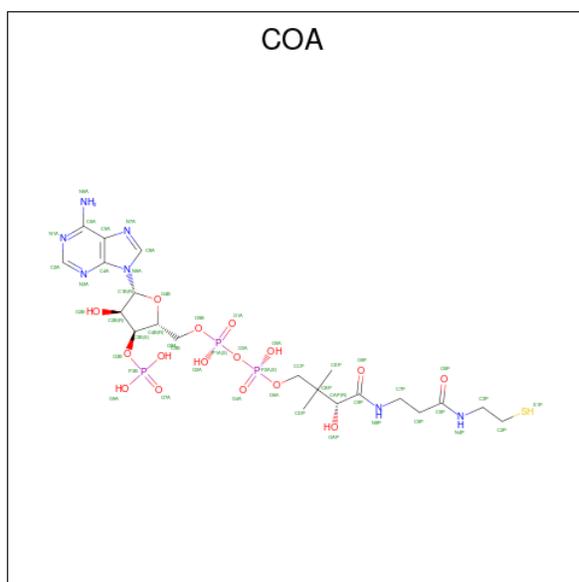
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



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

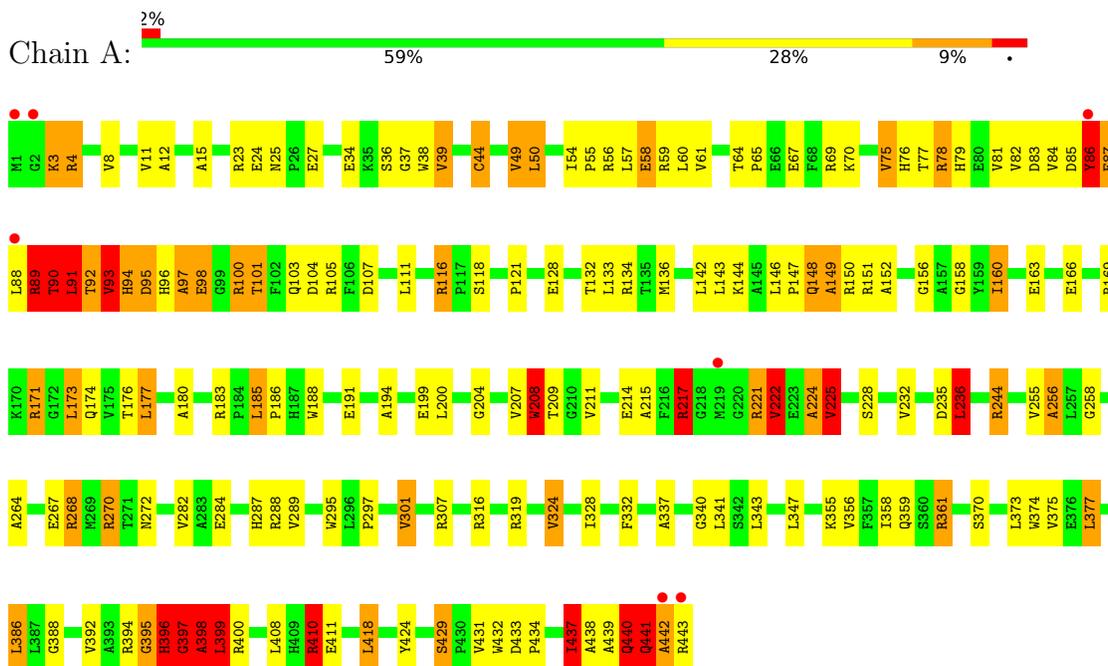
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	27	Total	O	0	0
			27	27		
5	C	27	Total	O	0	0
			27	27		
5	D	26	Total	O	0	0
			26	26		

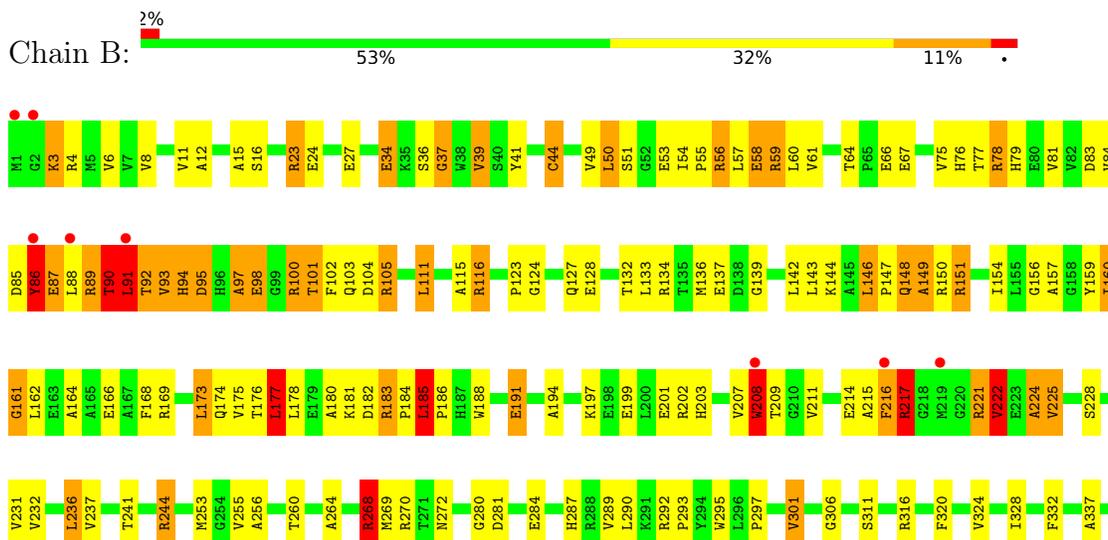
### 3 Residue-property plots

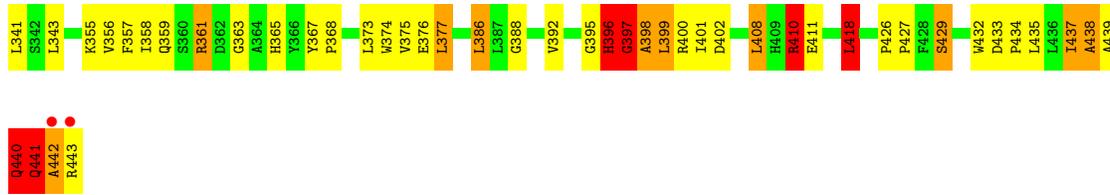
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

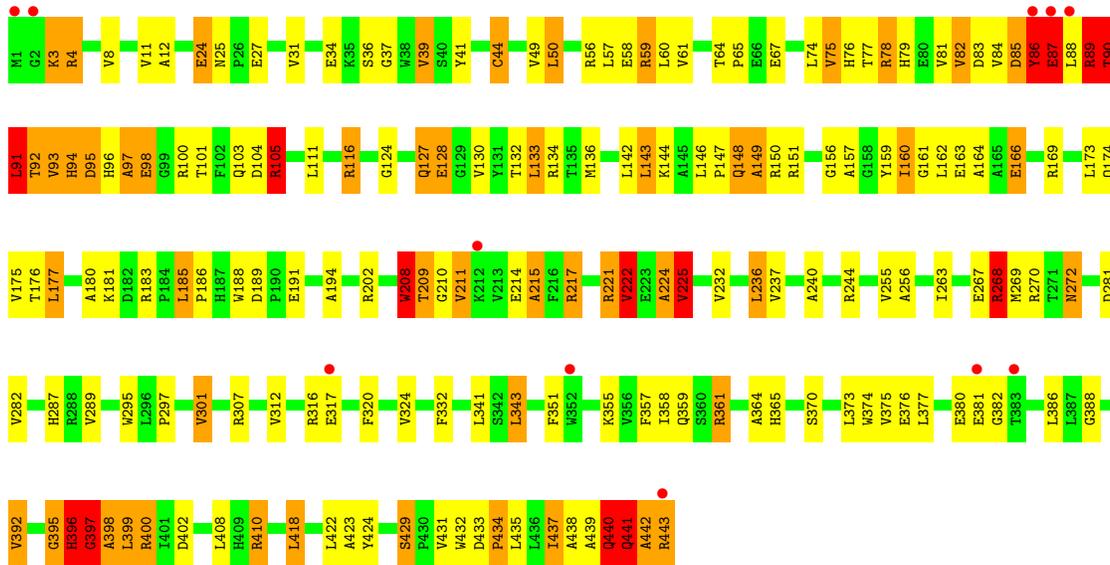


- Molecule 1: NADH oxidase

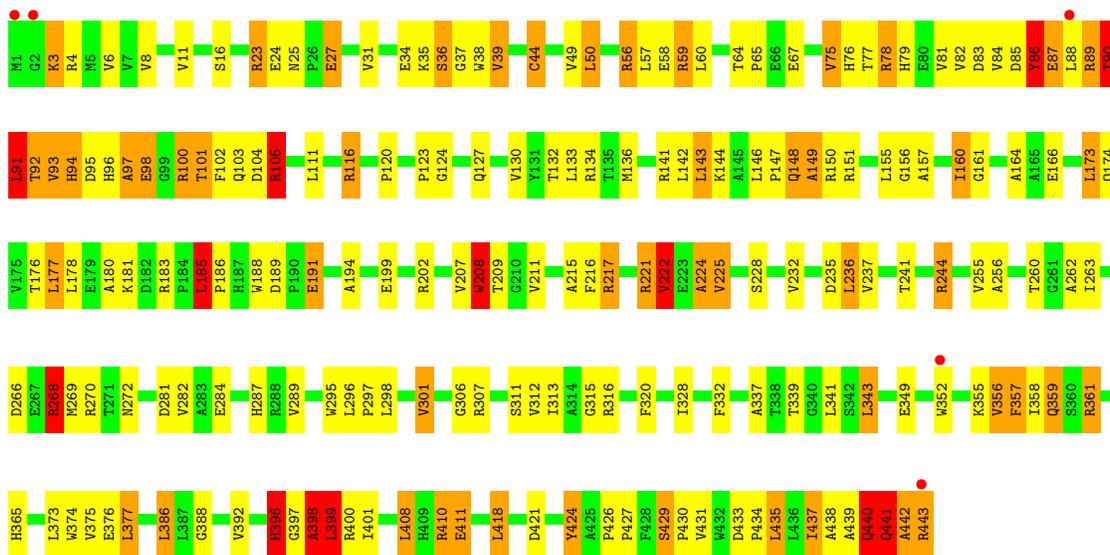




● Molecule 1: NADH oxidase



● Molecule 1: NADH oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.75Å 160.75Å 256.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.90 – 2.90 47.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.90-2.90) 100.0 (47.90-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.27	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, $R_{free}$	0.201 , 0.246 0.193 , 0.239	Depositor DCC
$R_{free}$ test set	2000 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtrriage
Anisotropy	0.084	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: COA, NAD, 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	1.55	36/3451 (1.0%)	1.39	37/4686 (0.8%)
1	B	1.50	28/3451 (0.8%)	1.38	31/4686 (0.7%)
1	C	1.48	32/3450 (0.9%)	1.37	29/4683 (0.6%)
1	D	1.49	25/3449 (0.7%)	1.38	36/4683 (0.8%)
All	All	1.51	121/13801 (0.9%)	1.38	133/18738 (0.7%)

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	6
1	B	0	4
1	C	0	6
1	D	0	3
All	All	0	19

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLU	CG-CD	11.35	1.69	1.51
1	D	396	HIS	C-O	9.65	1.41	1.23
1	C	440	GLN	C-O	9.27	1.41	1.23
1	B	208	TRP	CG-CD1	9.14	1.49	1.36
1	D	440	GLN	CD-NE2	9.05	1.55	1.32

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	397	GLY	N-CA-C	14.29	148.83	113.10
1	D	268	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	D	396	HIS	CA-C-N	-10.42	95.36	116.20
1	D	396	HIS	O-C-N	10.28	140.67	123.20
1	C	396	HIS	CA-C-N	-9.77	96.66	116.20

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	396	HIS	Peptide
1	A	398	ALA	Peptide
1	A	399	LEU	Peptide
1	A	91	LEU	Peptide
1	A	93	VAL	Peptide

## 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	3379	0	3407	215	0
1	B	3379	0	3407	257	0
1	C	3378	0	3402	191	0
1	D	3377	0	3402	201	0
2	A	53	0	31	7	0
2	B	53	0	31	11	0
2	C	53	0	31	7	0
2	D	53	0	31	6	0
3	A	44	0	26	11	0
3	B	44	0	26	10	0
3	C	44	0	26	9	0
3	D	44	0	26	12	0
4	A	48	0	31	3	0
4	B	48	0	31	5	0
4	C	48	0	31	0	0
4	D	48	0	31	3	0
5	A	32	0	0	10	1
5	B	27	0	0	17	1

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	27	0	0	17	0
5	D	26	0	0	13	0
All	All	14205	0	13970	862	1

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 31.

The worst 5 of 862 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:CD1	1:A:160:ILE:CG1	1.77	1.61
1:D:160:ILE:CD1	1:D:160:ILE:CG1	1.77	1.54
1:B:160:ILE:CD1	1:B:160:ILE:CG1	1.80	1.53
1:C:160:ILE:CD1	1:C:160:ILE:CG1	1.83	1.52
1:A:149:ALA:CB	1:A:150:ARG:HA	1.62	1.28

All (1) 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)
5:A:614:HOH:O	5:B:624:HOH:O[2_655]	2.01	0.19

## 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	441/443 (100%)	392 (89%)	31 (7%)	18 (4%)	3	11
1	B	441/443 (100%)	392 (89%)	31 (7%)	18 (4%)	3	11
1	C	441/443 (100%)	390 (88%)	35 (8%)	16 (4%)	3	14
1	D	441/443 (100%)	388 (88%)	36 (8%)	17 (4%)	3	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1764/1772 (100%)	1562 (88%)	133 (8%)	69 (4%)	3	12

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	TYR
1	A	89	ARG
1	A	90	THR
1	A	91	LEU
1	A	92	THR

### 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	338/338 (100%)	284 (84%)	54 (16%)	2	7
1	B	338/338 (100%)	283 (84%)	55 (16%)	2	7
1	C	337/338 (100%)	286 (85%)	51 (15%)	3	9
1	D	337/338 (100%)	280 (83%)	57 (17%)	2	6
All	All	1350/1352 (100%)	1133 (84%)	217 (16%)	2	7

5 of 217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	75	VAL
1	C	272	ASN
1	D	268	ARG
1	C	90	THR
1	C	143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	396	HIS
1	D	272	ASN
1	C	96	HIS
1	D	409	HIS
1	D	103	GLN

### 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](#)

12 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
2	FAD	B	501	-	53,58,58	2.25	16 (30%)	68,89,89	1.89	18 (26%)
4	COA	D	503	1	41,50,50	1.28	4 (9%)	52,75,75	2.13	19 (36%)
3	NAD	D	502	-	42,48,48	2.48	12 (28%)	50,73,73	2.68	20 (40%)
2	FAD	A	501	-	53,58,58	2.20	16 (30%)	68,89,89	1.79	15 (22%)
2	FAD	D	501	-	53,58,58	2.13	18 (33%)	68,89,89	1.74	19 (27%)
3	NAD	A	502	-	42,48,48	2.47	11 (26%)	50,73,73	2.71	22 (44%)
4	COA	A	503	1	41,50,50	1.21	4 (9%)	52,75,75	2.05	16 (30%)
3	NAD	C	502	-	42,48,48	2.55	9 (21%)	50,73,73	2.68	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	COA	B	503	1	41,50,50	1.31	4 (9%)	52,75,75	1.96	14 (26%)
4	COA	C	503	1	41,50,50	1.23	5 (12%)	52,75,75	2.14	17 (32%)
2	FAD	C	501	-	53,58,58	2.05	16 (30%)	68,89,89	1.74	15 (22%)
3	NAD	B	502	-	42,48,48	2.42	9 (21%)	50,73,73	2.46	19 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	501	-	-	8/30/50/50	0/6/6/6
4	COA	D	503	1	-	19/44/64/64	0/3/3/3
3	NAD	D	502	-	-	6/26/62/62	0/5/5/5
2	FAD	A	501	-	-	6/30/50/50	0/6/6/6
2	FAD	D	501	-	-	8/30/50/50	0/6/6/6
3	NAD	A	502	-	-	6/26/62/62	0/5/5/5
4	COA	A	503	1	-	17/44/64/64	0/3/3/3
3	NAD	C	502	-	-	5/26/62/62	0/5/5/5
4	COA	B	503	1	-	18/44/64/64	0/3/3/3
4	COA	C	503	1	-	19/44/64/64	0/3/3/3
2	FAD	C	501	-	-	5/30/50/50	0/6/6/6
3	NAD	B	502	-	-	5/26/62/62	0/5/5/5

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	NAD	O7N-C7N	10.20	1.43	1.24
3	C	502	NAD	O7N-C7N	9.31	1.42	1.24
3	B	502	NAD	O7N-C7N	9.15	1.41	1.24
3	A	502	NAD	O7N-C7N	9.04	1.41	1.24
2	B	501	FAD	C9A-C5X	8.71	1.55	1.41

The worst 5 of 214 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAD	O4B-C4B-C5B	8.22	136.41	109.37
3	C	502	NAD	O4B-C4B-C5B	8.02	135.75	109.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	NAD	O4B-C4B-C5B	7.89	135.32	109.37
3	B	502	NAD	O4B-C4B-C5B	7.51	134.08	109.37
4	A	503	COA	C7P-C6P-C5P	-6.70	101.21	112.36

There are no chirality outliers.

5 of 122 torsion outliers are listed below:

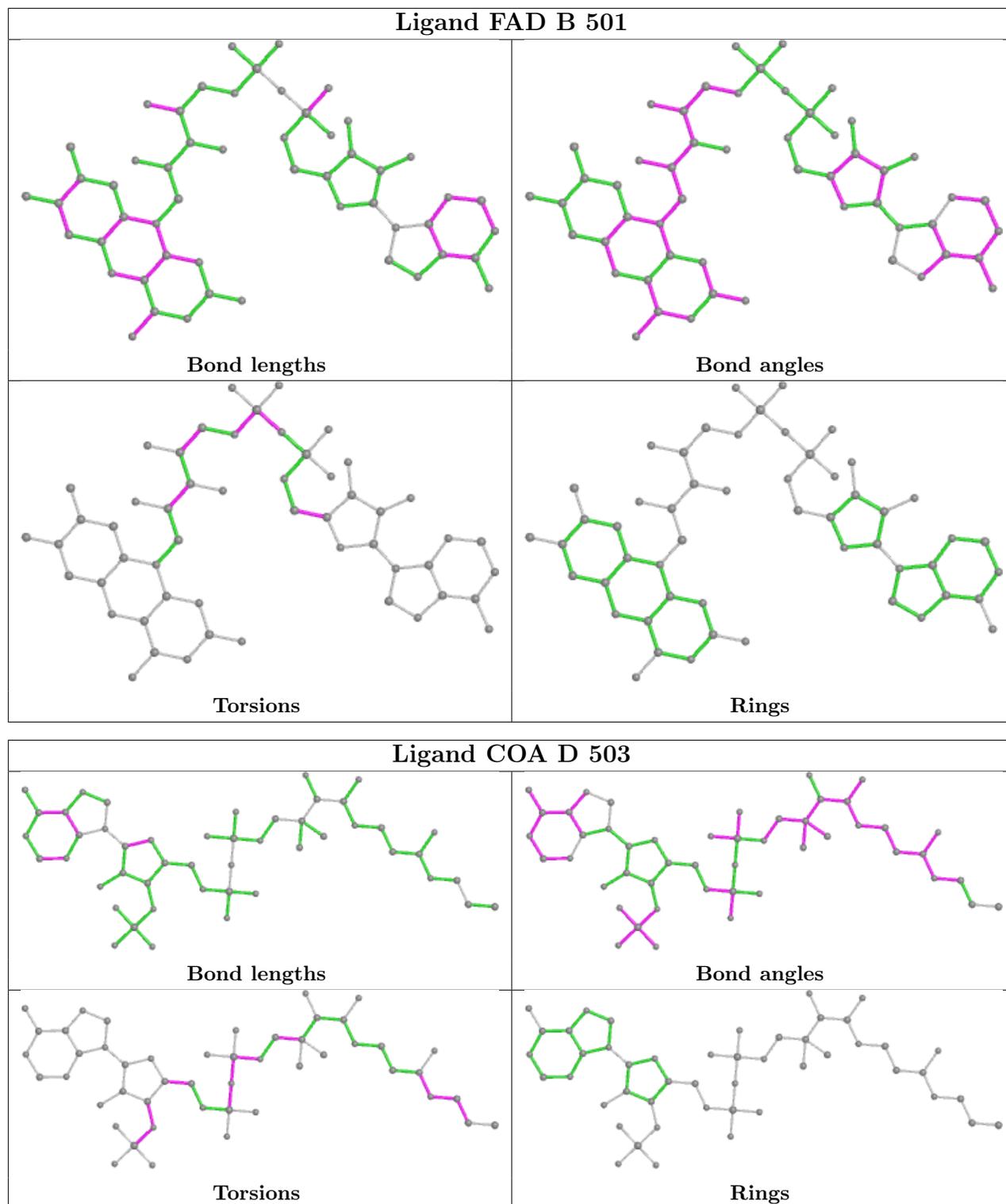
Mol	Chain	Res	Type	Atoms
2	A	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C3'-C4'-C5'-O5'
2	B	501	FAD	C1'-C2'-C3'-C4'
2	C	501	FAD	C3'-C4'-C5'-O5'
2	D	501	FAD	C3'-C4'-C5'-O5'

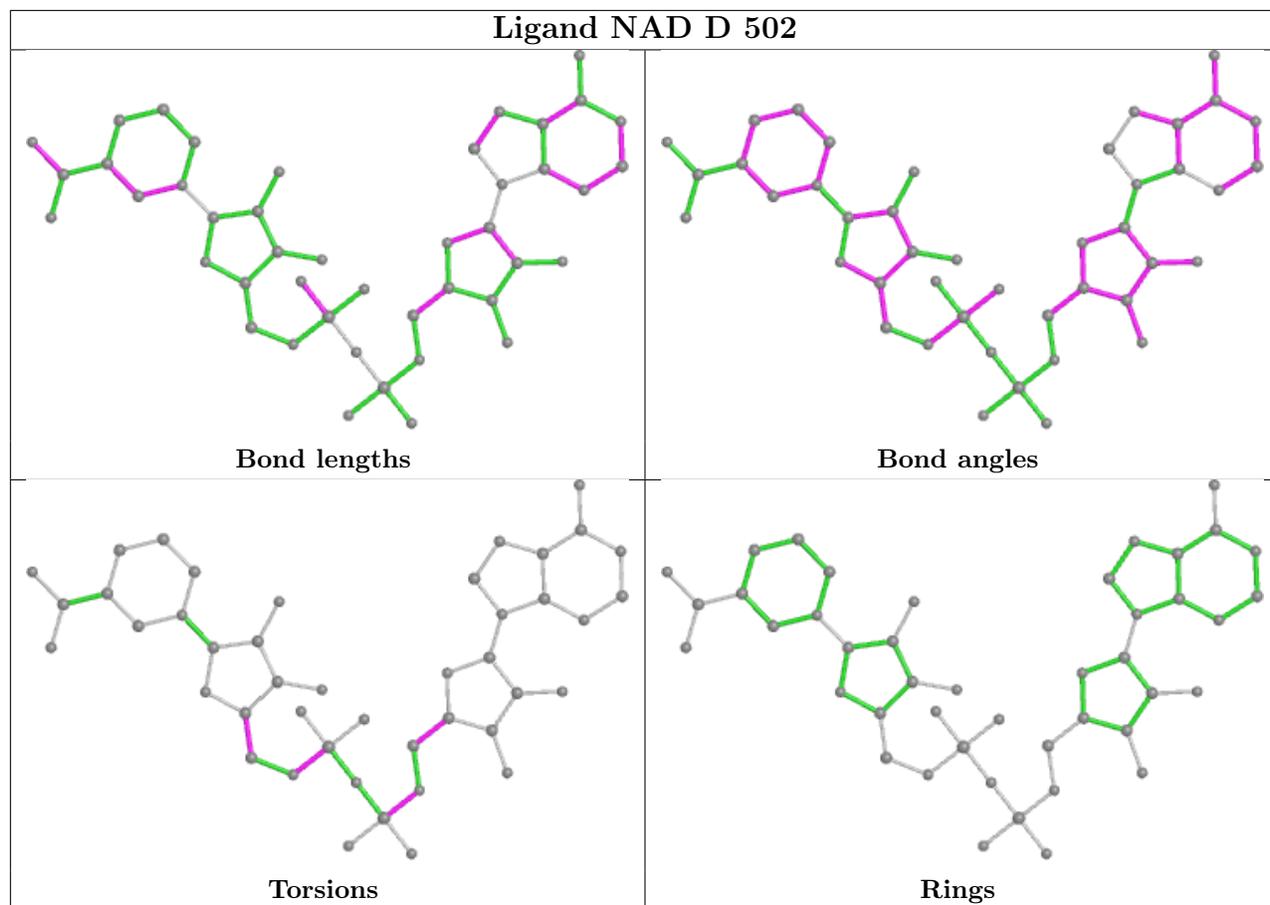
There are no ring outliers.

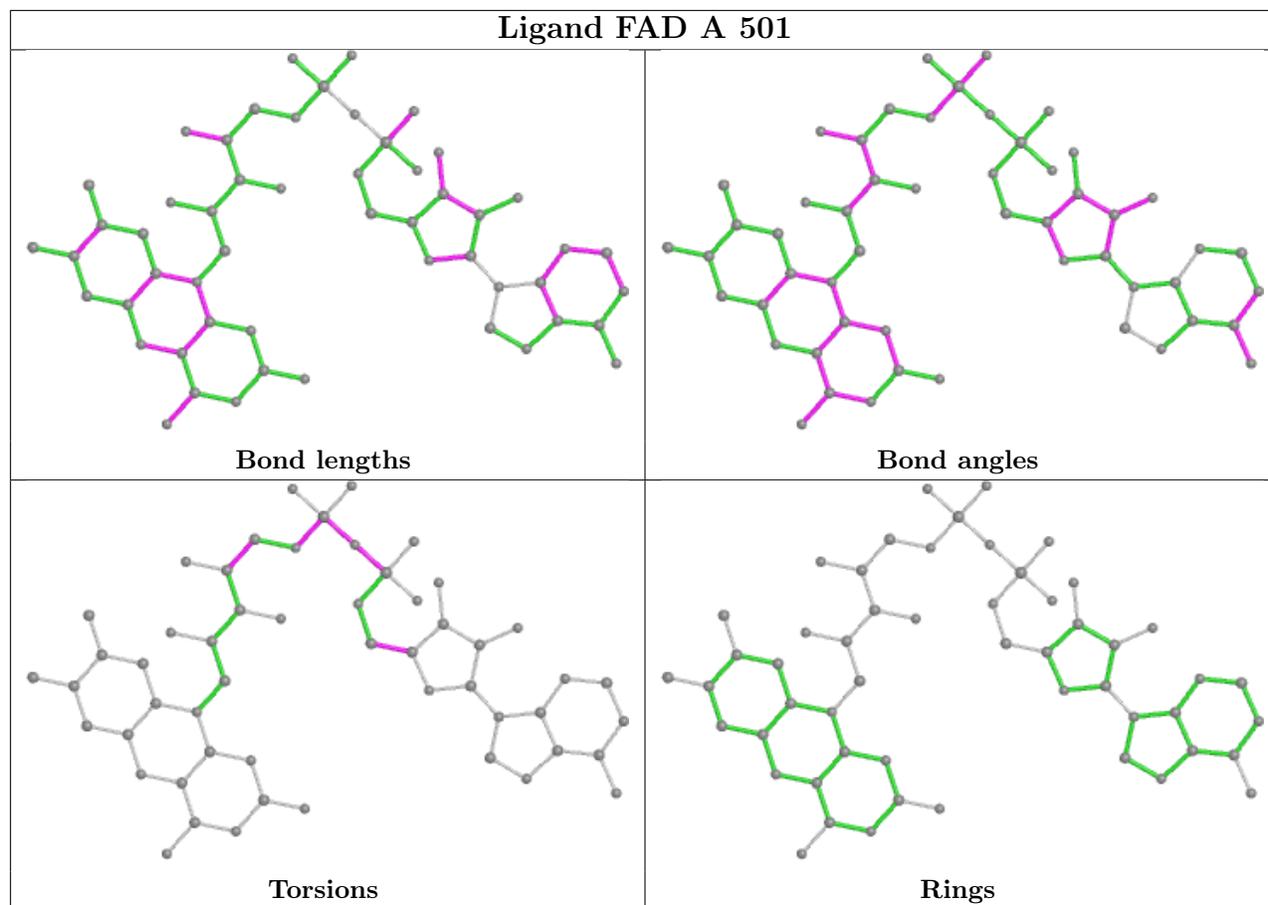
11 monomers are involved in 81 short contacts:

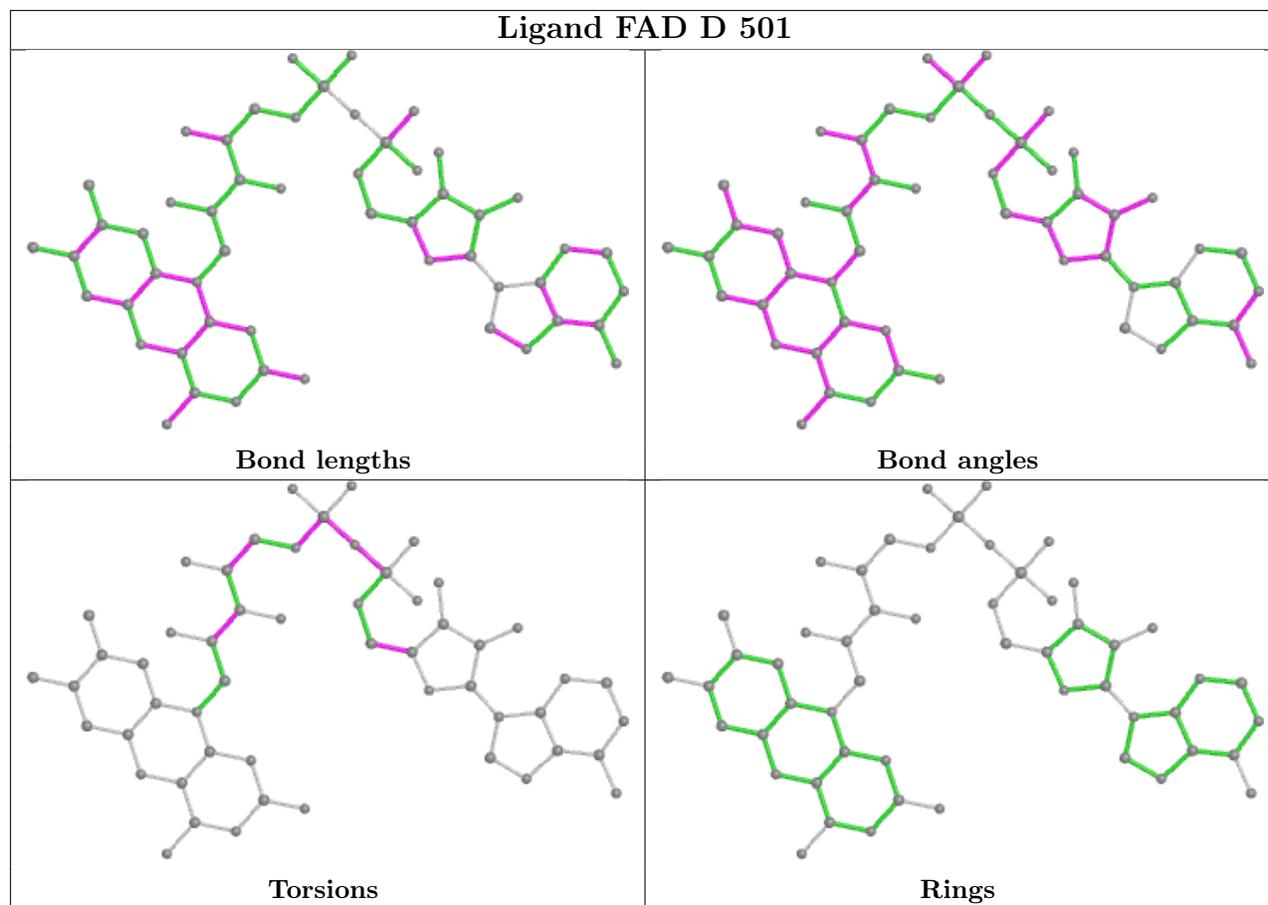
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FAD	11	0
4	D	503	COA	3	0
3	D	502	NAD	12	0
2	A	501	FAD	7	0
2	D	501	FAD	6	0
3	A	502	NAD	11	0
4	A	503	COA	3	0
3	C	502	NAD	9	0
4	B	503	COA	5	0
2	C	501	FAD	7	0
3	B	502	NAD	10	0

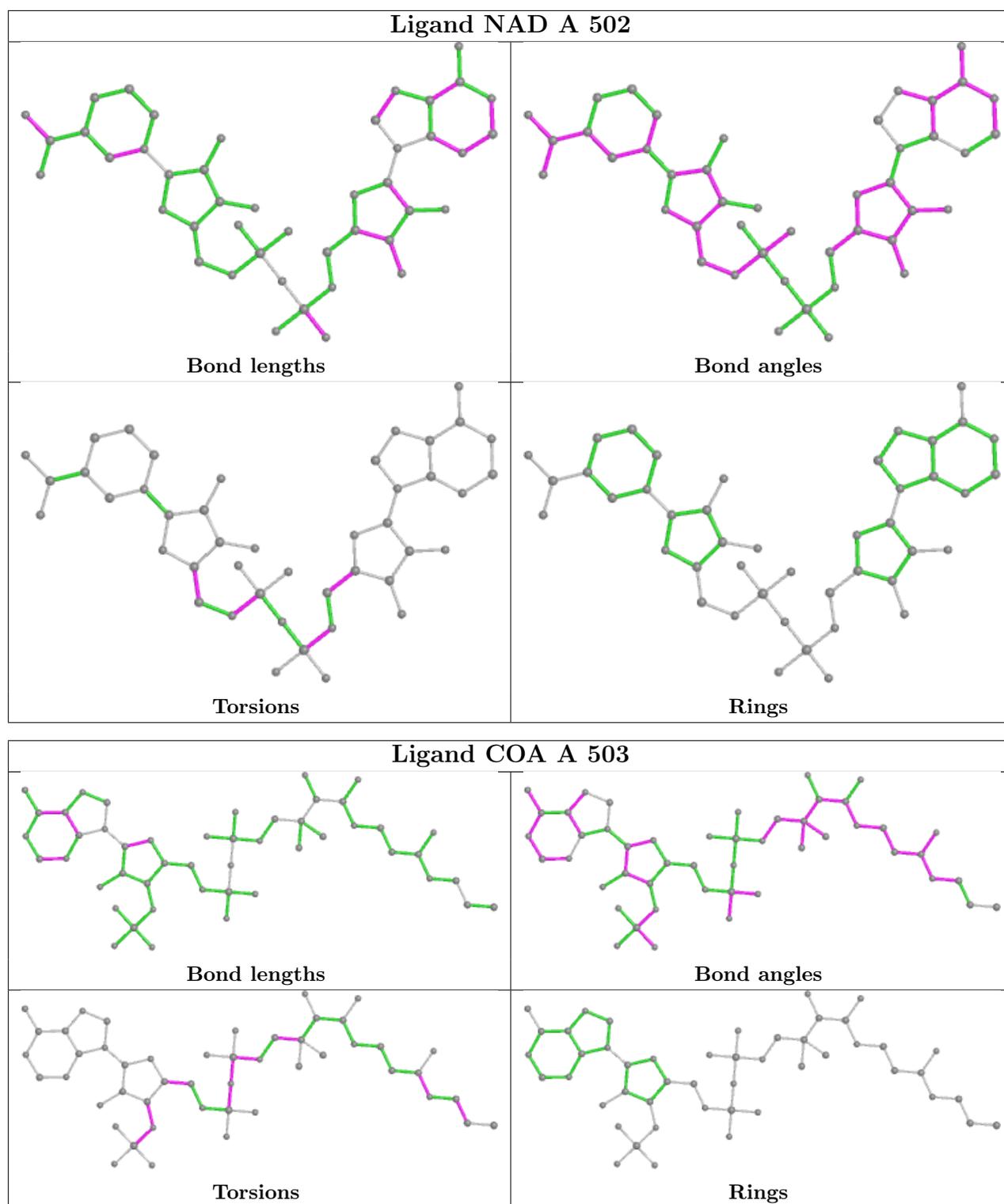
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

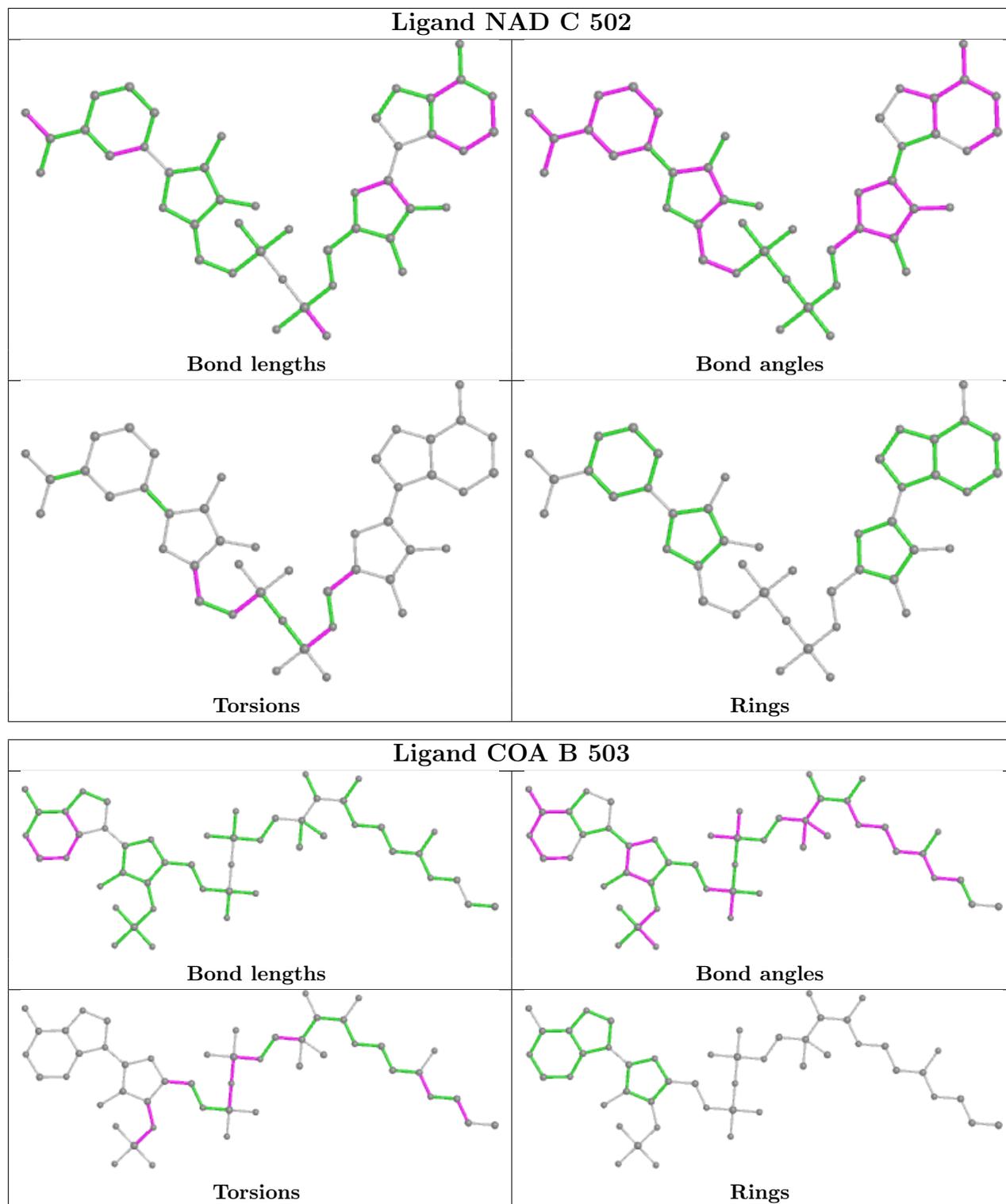


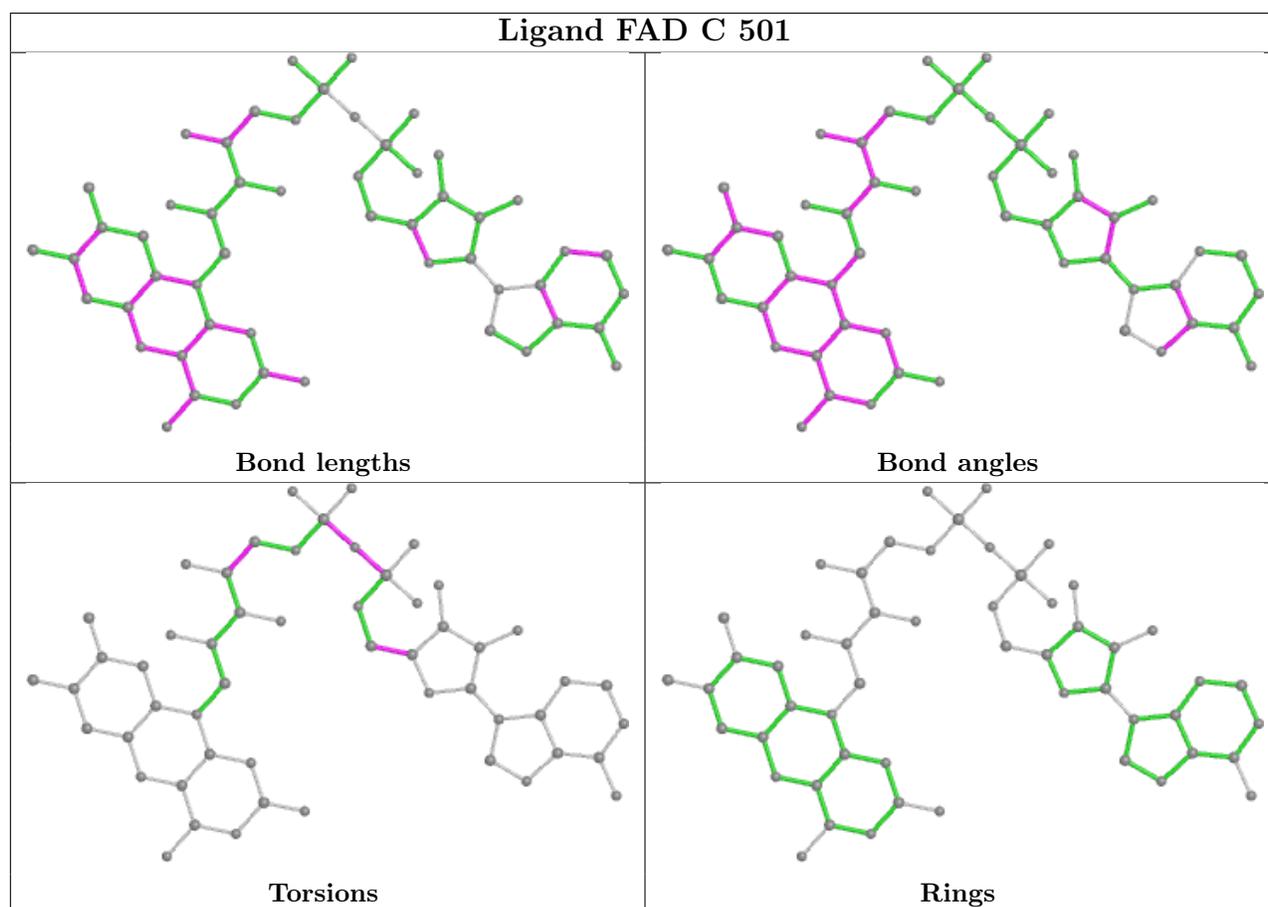
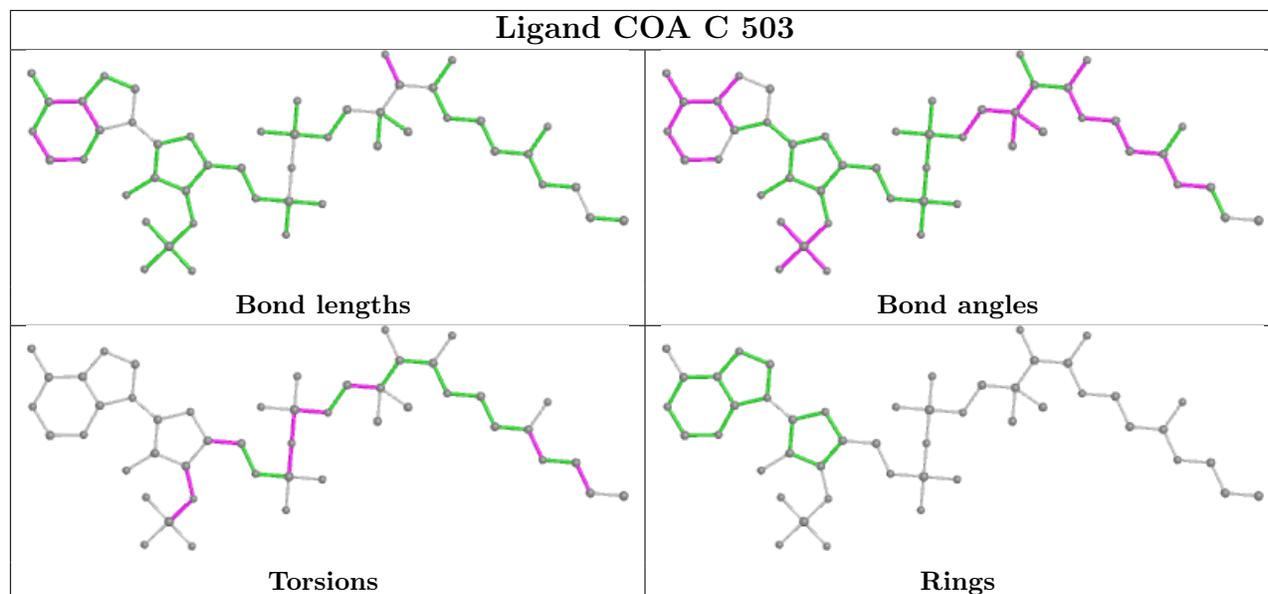


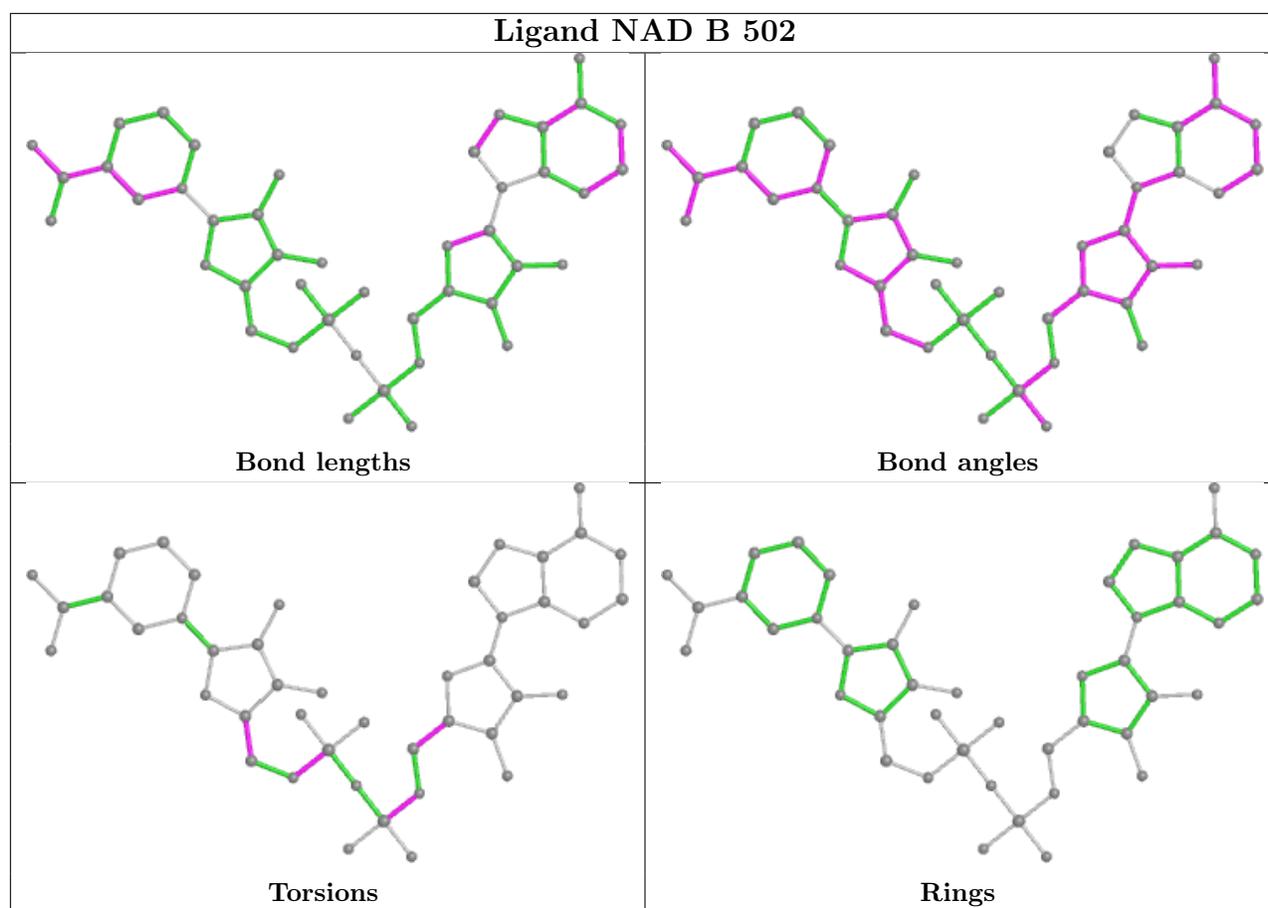












## 5.7 Other polymers [i](#)

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	443/443 (100%)	-0.21	7 (1%) 72 71	30, 47, 75, 130	0
1	B	443/443 (100%)	-0.06	10 (2%) 60 58	31, 49, 77, 129	0
1	C	443/443 (100%)	-0.16	11 (2%) 57 55	31, 48, 76, 132	0
1	D	443/443 (100%)	-0.18	5 (1%) 80 80	29, 49, 78, 132	0
All	All	1772/1772 (100%)	-0.15	33 (1%) 66 65	29, 48, 77, 132	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	10.5
1	B	443	ARG	8.5
1	B	1	MET	8.5
1	A	1	MET	8.2
1	C	1	MET	7.7

### 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](#)

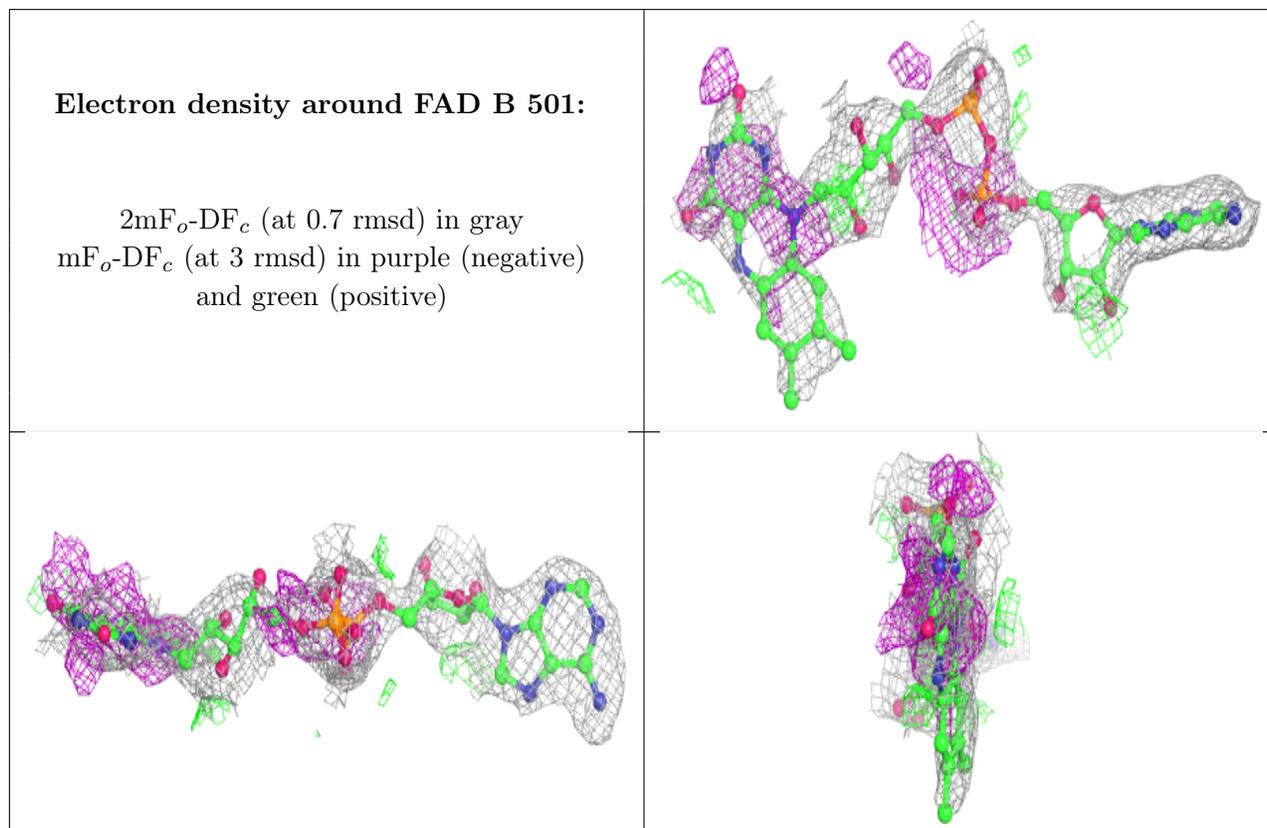
There are no monosaccharides in this entry.

### 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.

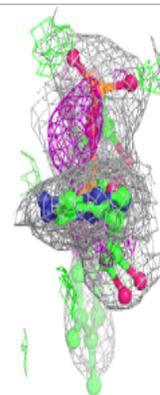
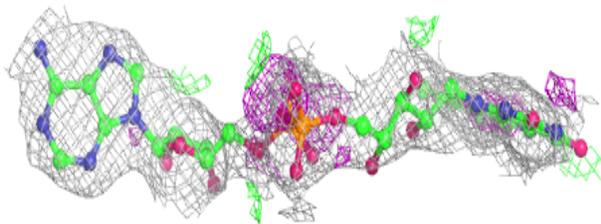
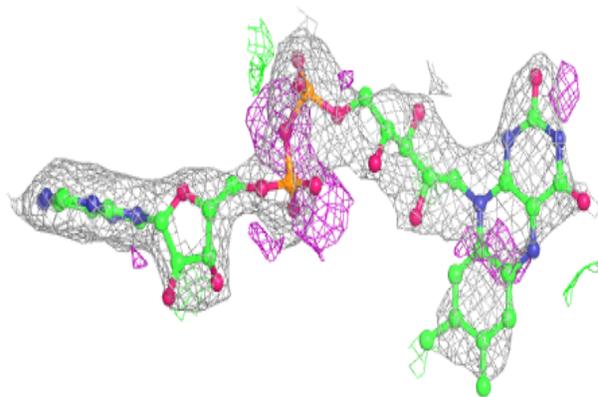
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	B	501	53/53	0.92	0.26	57,76,96,111	0
2	FAD	D	501	53/53	0.92	0.20	49,74,93,109	0
3	NAD	B	502	44/44	0.93	0.20	43,64,82,87	0
2	FAD	A	501	53/53	0.94	0.24	53,71,92,117	0
3	NAD	D	502	44/44	0.94	0.18	45,62,79,82	0
2	FAD	C	501	53/53	0.95	0.19	51,73,93,97	0
4	COA	A	503	48/48	0.95	0.23	54,72,85,110	0
4	COA	C	503	48/48	0.95	0.15	54,71,80,116	0
4	COA	D	503	48/48	0.95	0.17	51,71,81,111	0
4	COA	B	503	48/48	0.96	0.16	54,70,80,103	0
3	NAD	A	502	44/44	0.96	0.17	39,58,76,83	0
3	NAD	C	502	44/44	0.96	0.17	39,57,78,82	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.

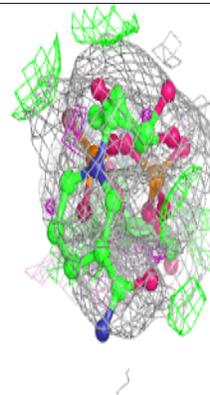
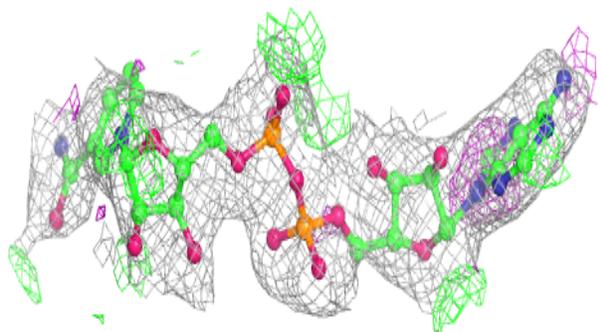
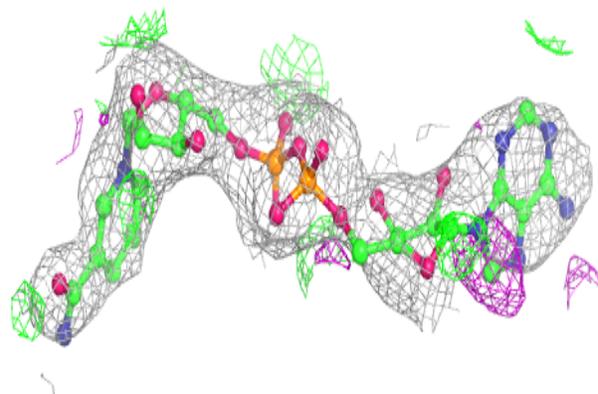


**Electron density around FAD D 501:**

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

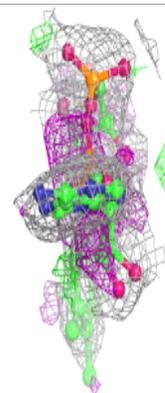
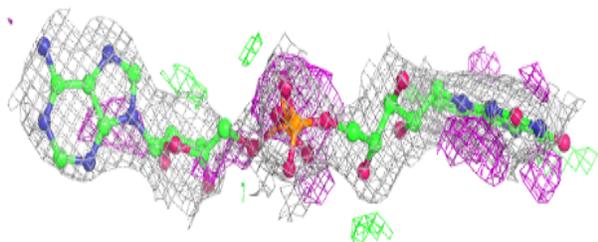
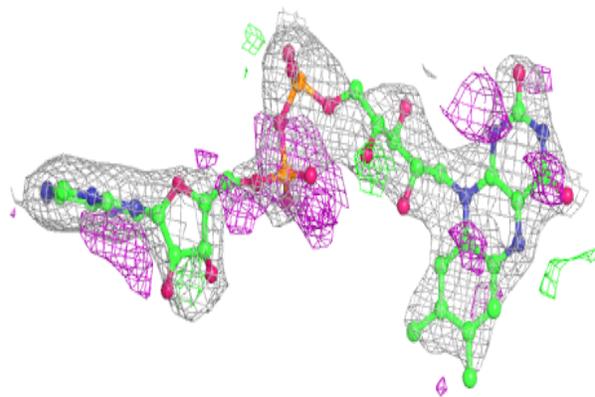
**Electron density around NAD B 502:**

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

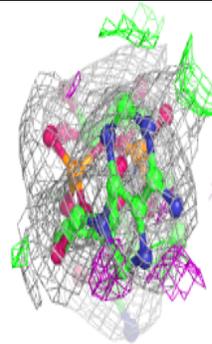
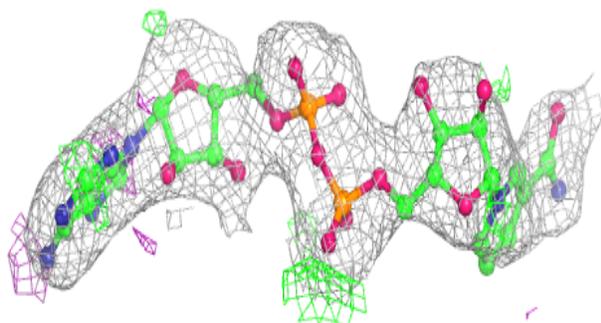
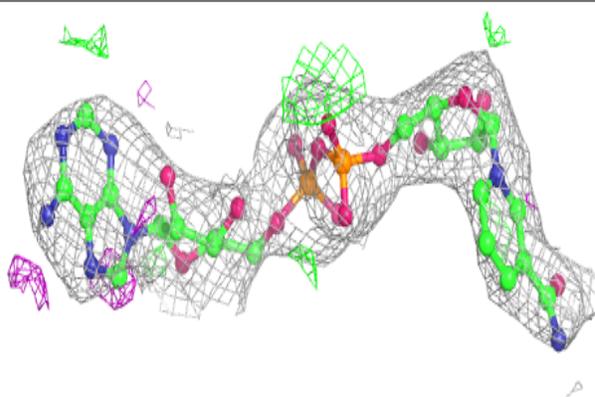


**Electron density around FAD A 501:**

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

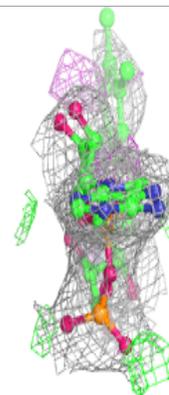
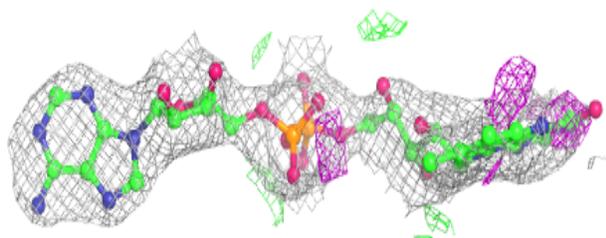
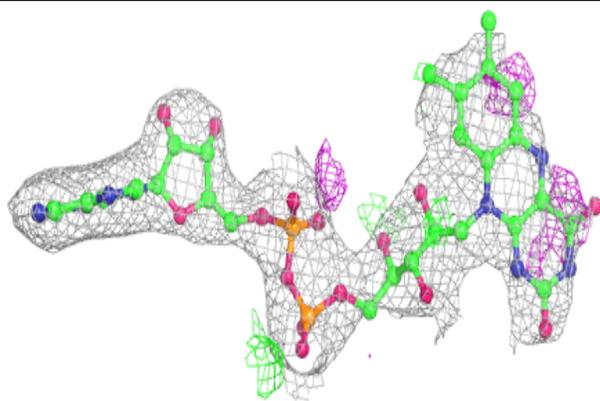
**Electron density around NAD D 502:**

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

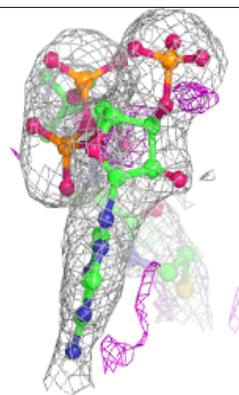
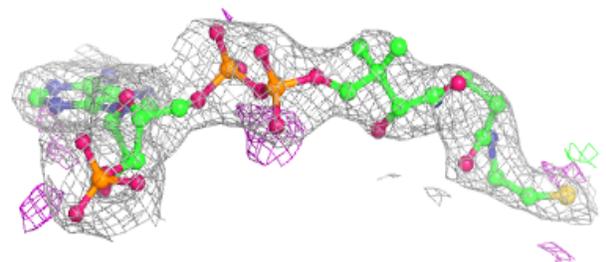
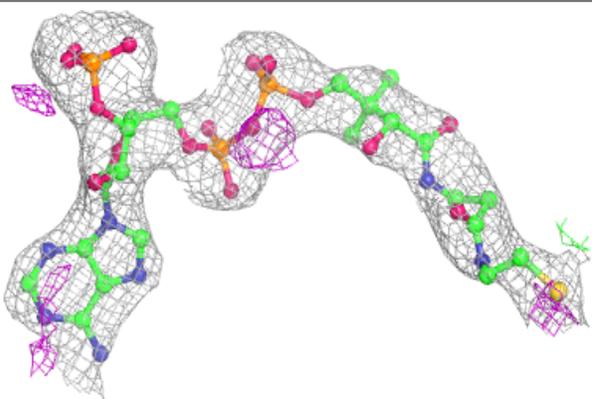


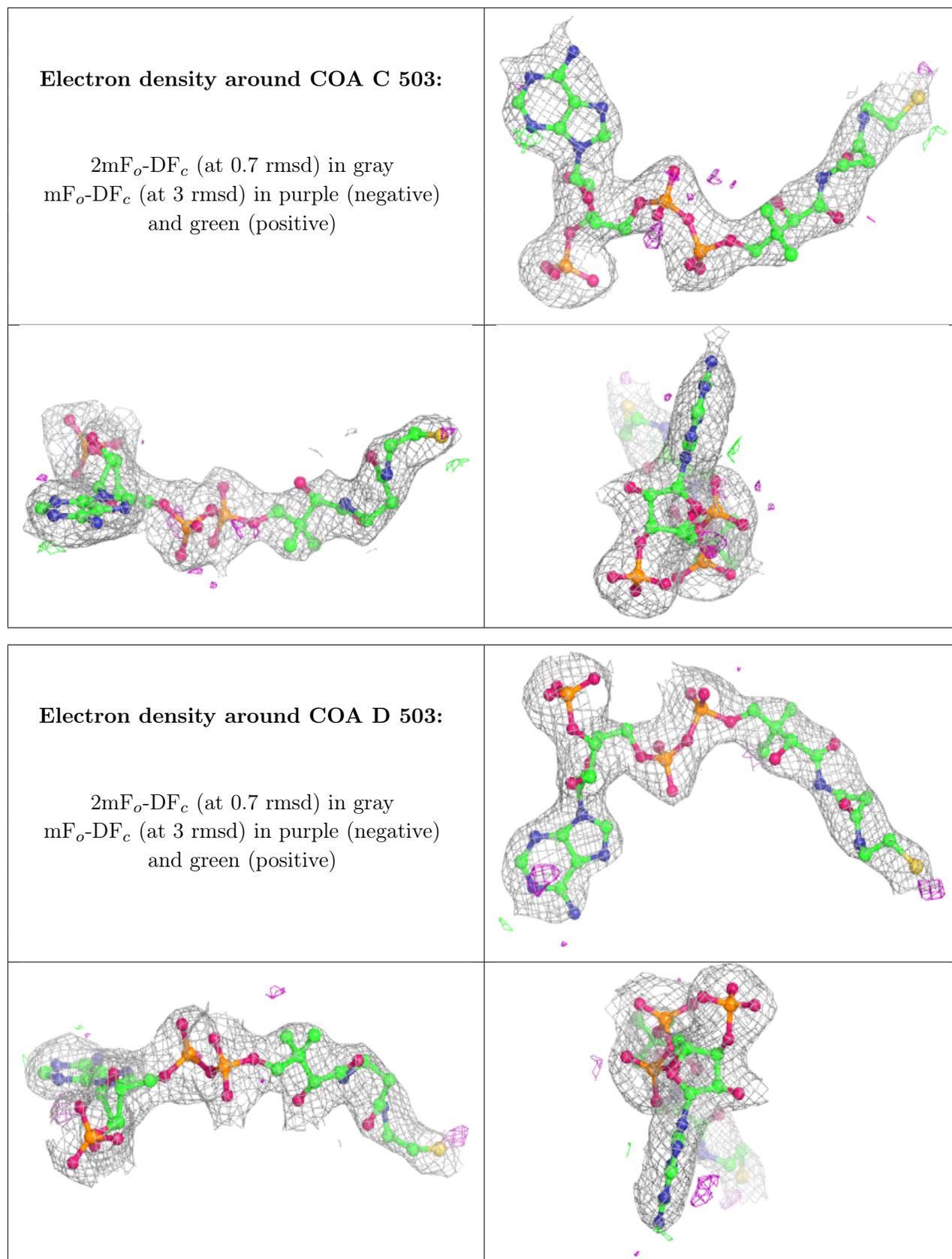
**Electron density around FAD C 501:**

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

**Electron density around COA A 503:**

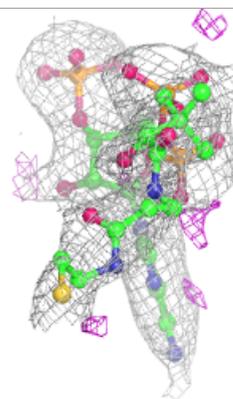
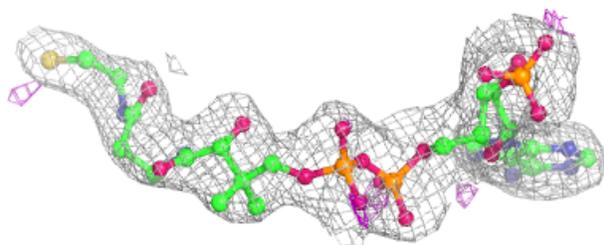
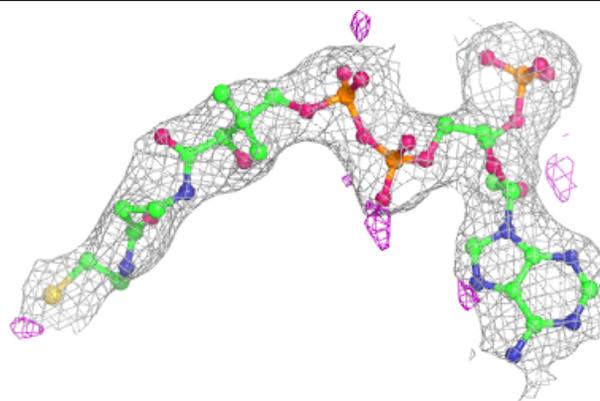
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



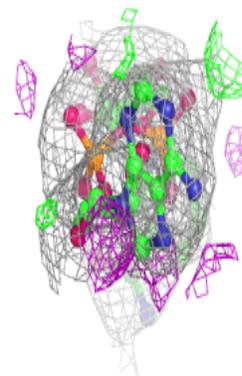
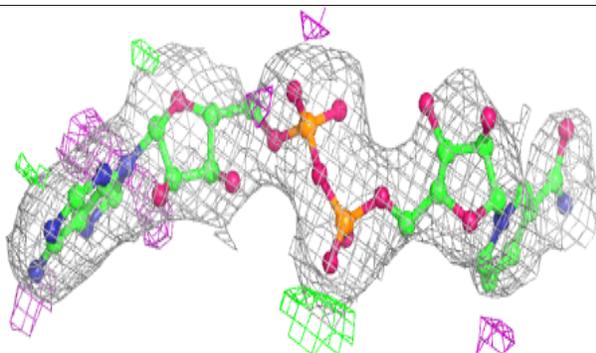
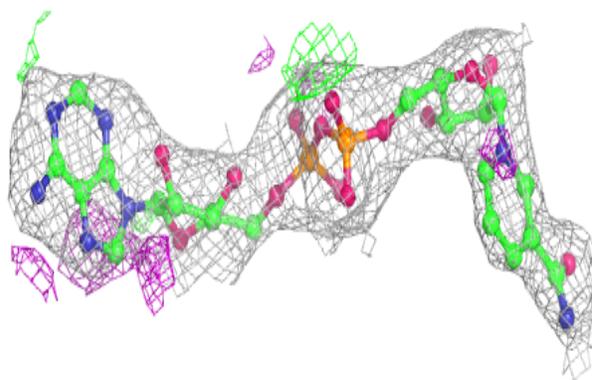


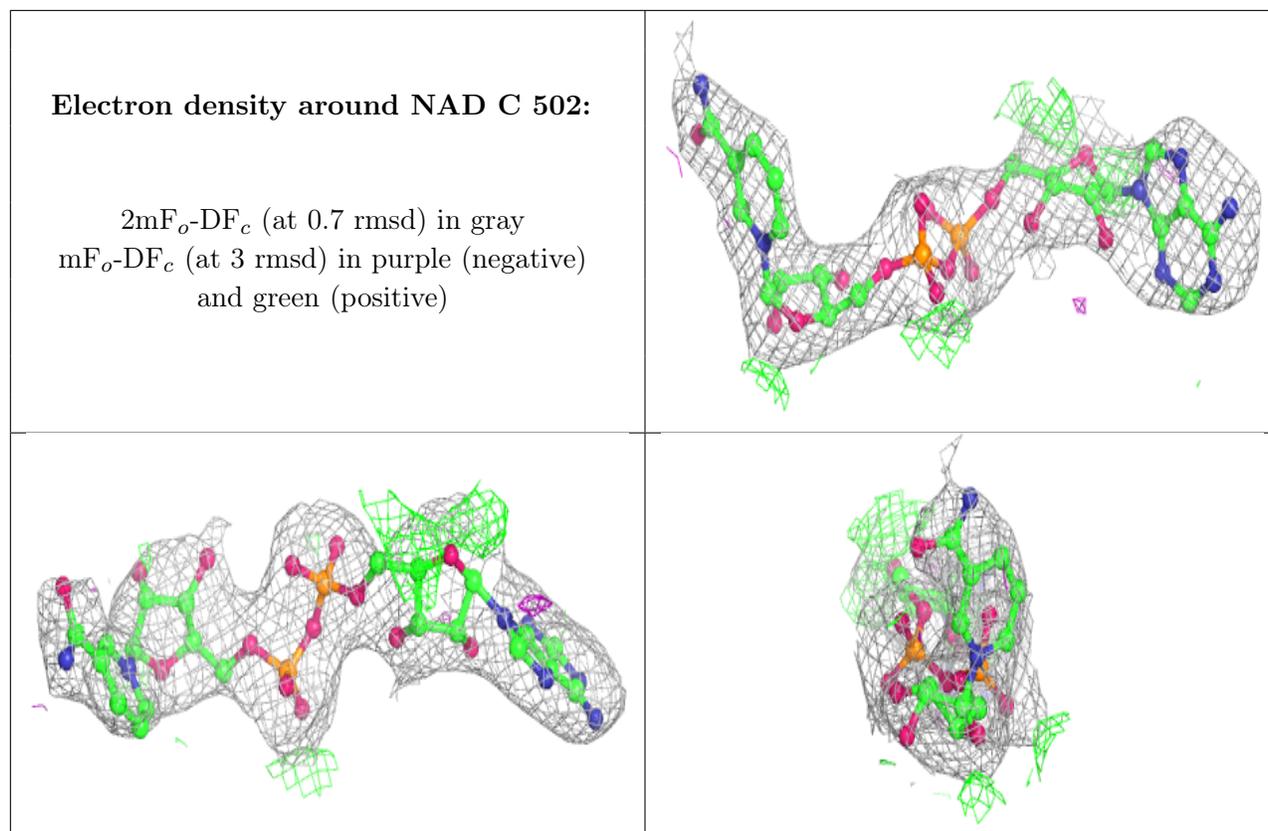
**Electron density around COA B 503:**

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

**Electron density around NAD 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.