



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 11:19 AM UTC

PDB ID : 1AMO / pdb_00001amo
Title : THREE-DIMENSIONAL STRUCTURE OF NADPH-CYTOCHROME P450
REDUCTASE: PROTOTYPE FOR FMN-AND FAD-CONTAINING EN-
ZYMES
Authors : Wang, M.; Roberts, D.L.; Paschke, R.; Shea, T.M.; Masters, B.S.S.; Kim,
J.J.P.
Deposited on : 1997-06-17
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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>.

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.60 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

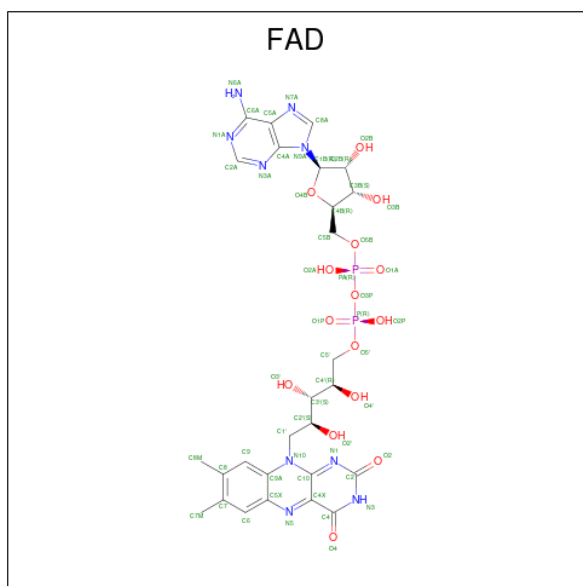
There are 5 unique types of molecules in this entry. The entry contains 10040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NADPH-CYTOCHROME P450 REDUCTASE.

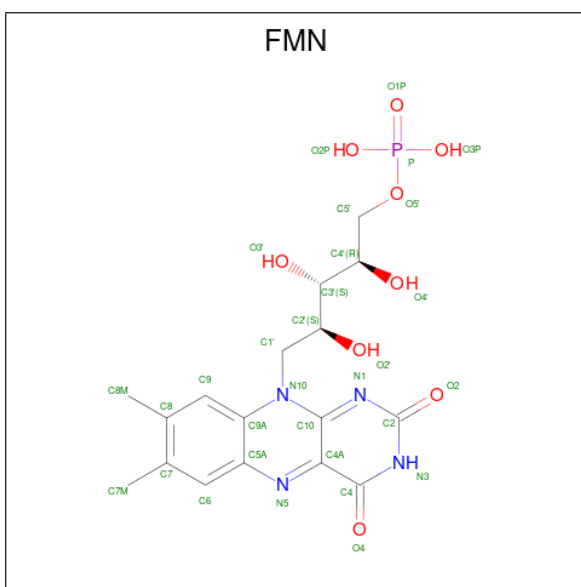
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4830	3062	830	915	23			
1	B	601	Total	C	N	O	S	0	0	0
			4830	3062	830	915	23			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



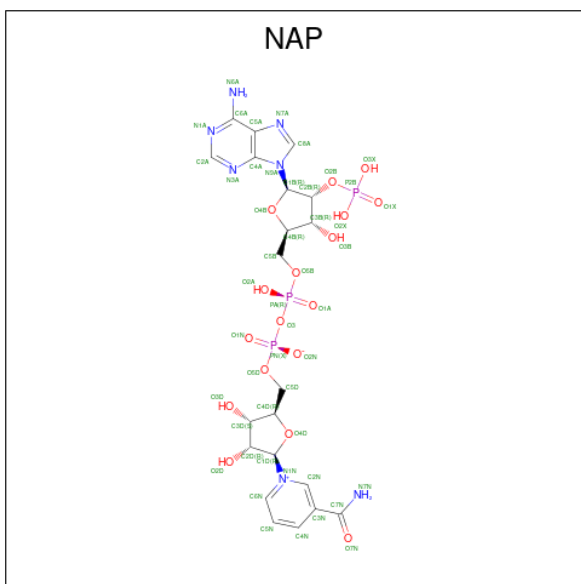
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			47	23	7	15	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	78	Total	O	0	0
			78	78		
5	B	78	Total	O	0	0
			78	78		

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

3 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.28Å 116.18Å 119.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	91.5 (10.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.200 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10040	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

6 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	750	-	43,46,58	2.64	6 (13%)	55,67,89	1.28	8 (14%)
3	FMN	B	751	-	33,33,33	1.39	5 (15%)	48,50,50	1.50	9 (18%)
4	NAP	A	752	-	32,33,52	1.24	3 (9%)	50,52,80	1.94	14 (28%)
2	FAD	A	750	-	58,58,58	1.64	7 (12%)	85,89,89	1.43	14 (16%)
4	NAP	B	752	-	32,33,52	1.24	3 (9%)	50,52,80	1.93	14 (28%)
3	FMN	A	751	-	33,33,33	1.39	5 (15%)	48,50,50	1.50	8 (16%)

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	750	-	-	4/34/50/50	0/3/4/6
3	FMN	B	751	-	-	0/18/18/18	0/3/3/3
4	NAP	A	752	-	-	9/21/37/67	0/3/3/5
2	FAD	A	750	-	-	4/34/50/50	0/6/6/6
4	NAP	B	752	-	-	9/21/37/67	0/3/3/5
3	FMN	A	751	-	-	0/18/18/18	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	FAD	C5X-N5	-10.11	1.36	1.46
2	B	750	FAD	C9-C9A	8.35	1.43	1.32
2	A	750	FAD	PA-O3P	-6.64	1.52	1.59
2	B	750	FAD	PA-O3P	-6.59	1.52	1.59
2	A	750	FAD	P-O3P	-6.06	1.53	1.59
2	B	750	FAD	P-O3P	-6.02	1.53	1.59
3	B	751	FMN	C9-C8	-4.33	1.33	1.39
3	A	751	FMN	C9-C8	-4.28	1.33	1.39
2	B	750	FAD	C10-C4X	-3.94	1.39	1.49
2	A	750	FAD	C4X-N5	3.27	1.37	1.30
4	B	752	NAP	C5A-N7A	-3.19	1.33	1.39
4	A	752	NAP	C5A-N7A	-3.19	1.33	1.39
3	B	751	FMN	C6-C7	-3.02	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	751	FMN	C6-C7	-3.02	1.35	1.39
2	A	750	FAD	C10-N10	2.99	1.43	1.37
2	A	750	FAD	C1B-N9A	2.52	1.53	1.46
2	B	750	FAD	C1B-N9A	2.51	1.53	1.46
2	A	750	FAD	C6-C7	-2.46	1.36	1.39
4	A	752	NAP	P2B-O2B	-2.33	1.55	1.59
4	A	752	NAP	C8A-N7A	2.32	1.36	1.31
4	B	752	NAP	C8A-N7A	2.31	1.36	1.31
3	A	751	FMN	C4A-N5	2.31	1.35	1.30
4	B	752	NAP	P2B-O2B	-2.30	1.55	1.59
3	B	751	FMN	C4A-N5	2.30	1.35	1.30
3	A	751	FMN	C10-N10	2.21	1.42	1.37
3	B	751	FMN	C10-N10	2.21	1.42	1.37
2	A	750	FAD	C9-C9A	2.09	1.43	1.39
3	A	751	FMN	P-O3P	-2.05	1.47	1.54
3	B	751	FMN	P-O3P	-2.03	1.47	1.54

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	752	NAP	C5A-C4A-N3A	-5.69	118.89	126.72
4	B	752	NAP	C5A-C4A-N3A	-5.66	118.92	126.72
4	A	752	NAP	N3A-C4A-N9A	4.89	135.48	127.17
4	B	752	NAP	N3A-C4A-N9A	4.87	135.45	127.17
2	A	750	FAD	C9A-C5X-N5	4.78	127.53	122.45
3	A	751	FMN	C9A-C5A-N5	4.66	127.40	122.45
3	B	751	FMN	C9A-C5A-N5	4.62	127.36	122.45
3	B	751	FMN	C5A-N5-C4A	-4.11	111.43	118.09
3	A	751	FMN	C5A-N5-C4A	-4.11	111.44	118.09
2	B	750	FAD	C2B-C3B-C4B	-3.87	95.13	102.61
2	A	750	FAD	C2B-C3B-C4B	-3.85	95.18	102.61
4	A	752	NAP	C2B-C1B-N9A	3.63	119.73	113.75
4	B	752	NAP	C2B-C1B-N9A	3.63	119.73	113.75
2	A	750	FAD	C5X-N5-C4X	-3.32	112.71	118.09
4	A	752	NAP	N3A-C2A-N1A	-3.25	123.66	128.58
4	B	752	NAP	N3A-C2A-N1A	-3.24	123.68	128.58
4	A	752	NAP	C6A-C5A-C4A	3.13	121.45	117.18
4	B	752	NAP	C6A-C5A-C4A	3.13	121.45	117.18
4	A	752	NAP	C4A-N9A-C1B	-3.13	119.32	126.63
4	B	752	NAP	C4A-N9A-C1B	-3.12	119.33	126.63
2	A	750	FAD	C2B-C1B-N9A	3.06	120.92	113.30
2	B	750	FAD	C2B-C1B-N9A	3.05	120.88	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	752	NAP	O2N-PN-O1N	2.91	122.17	110.83
4	B	752	NAP	O2N-PN-O1N	2.90	122.12	110.83
3	B	751	FMN	O2-C2-N3	2.89	124.12	118.58
3	A	751	FMN	O2-C2-N3	2.89	124.12	118.58
2	A	750	FAD	O2-C2-N3	2.87	124.08	118.58
2	B	750	FAD	C5X-N5-C4X	-2.79	112.72	117.30
4	B	752	NAP	C6A-C5A-N7A	-2.74	126.81	132.09
2	A	750	FAD	C10-N1-C2	2.73	122.76	116.85
4	A	752	NAP	C6A-C5A-N7A	-2.73	126.83	132.09
4	A	752	NAP	C2A-N3A-C4A	2.69	118.39	111.83
2	B	750	FAD	C4A-N9A-C8A	-2.68	102.92	105.74
4	B	752	NAP	C2A-N3A-C4A	2.68	118.36	111.83
2	A	750	FAD	C4A-N9A-C8A	-2.65	102.95	105.74
3	B	751	FMN	C10-N1-C2	2.62	122.51	116.85
3	A	751	FMN	C10-N1-C2	2.61	122.49	116.85
4	A	752	NAP	O5D-PN-O3	-2.59	95.95	104.64
4	B	752	NAP	O5D-PN-O3	-2.58	95.99	104.64
2	B	750	FAD	O3'-C3'-C2'	2.46	114.53	108.93
2	A	750	FAD	C5X-C9A-N10	-2.45	115.75	117.97
2	A	750	FAD	N3-C2-N1	-2.45	114.30	119.50
2	A	750	FAD	O3'-C3'-C2'	2.45	114.49	108.93
4	B	752	NAP	C1B-N9A-C8A	2.37	132.36	127.09
4	A	752	NAP	C1B-N9A-C8A	2.36	132.34	127.09
3	A	751	FMN	O3P-P-O2P	2.29	116.40	107.80
3	B	751	FMN	O3P-P-O2P	2.29	116.39	107.80
4	A	752	NAP	O2A-PA-O3	2.26	113.38	107.27
4	B	752	NAP	O2A-PA-O3	2.25	113.37	107.27
3	A	751	FMN	O3'-C3'-C4'	-2.16	104.01	108.93
4	B	752	NAP	O3B-C3B-C4B	-2.16	104.87	111.08
3	B	751	FMN	O3'-C3'-C4'	-2.16	104.02	108.93
4	A	752	NAP	O3B-C3B-C4B	-2.16	104.88	111.08
2	B	750	FAD	O5'-C5'-C4'	2.13	115.06	109.36
3	B	751	FMN	N3-C2-N1	-2.13	114.98	119.50
2	A	750	FAD	O5'-C5'-C4'	2.13	115.04	109.36
3	A	751	FMN	N3-C2-N1	-2.12	114.98	119.50
4	A	752	NAP	N9A-C8A-N7A	-2.10	110.96	113.94
2	A	750	FAD	C8M-C8-C9	2.08	123.24	119.57
4	B	752	NAP	N9A-C8A-N7A	-2.08	110.98	113.94
2	B	750	FAD	O2A-PA-O1A	2.08	122.10	112.44
2	A	750	FAD	O2A-PA-O1A	2.07	122.06	112.44
2	A	750	FAD	O2B-C2B-C3B	-2.05	105.26	111.82
2	B	750	FAD	O2B-C2B-C3B	-2.04	105.28	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	751	FMN	C2'-C1'-N10	2.02	119.74	110.20
3	B	751	FMN	C2'-C1'-N10	2.02	119.73	110.20
3	B	751	FMN	C4-C4A-N5	-2.00	115.44	118.21

There are no chirality outliers.

All (26) torsion outliers are listed below:

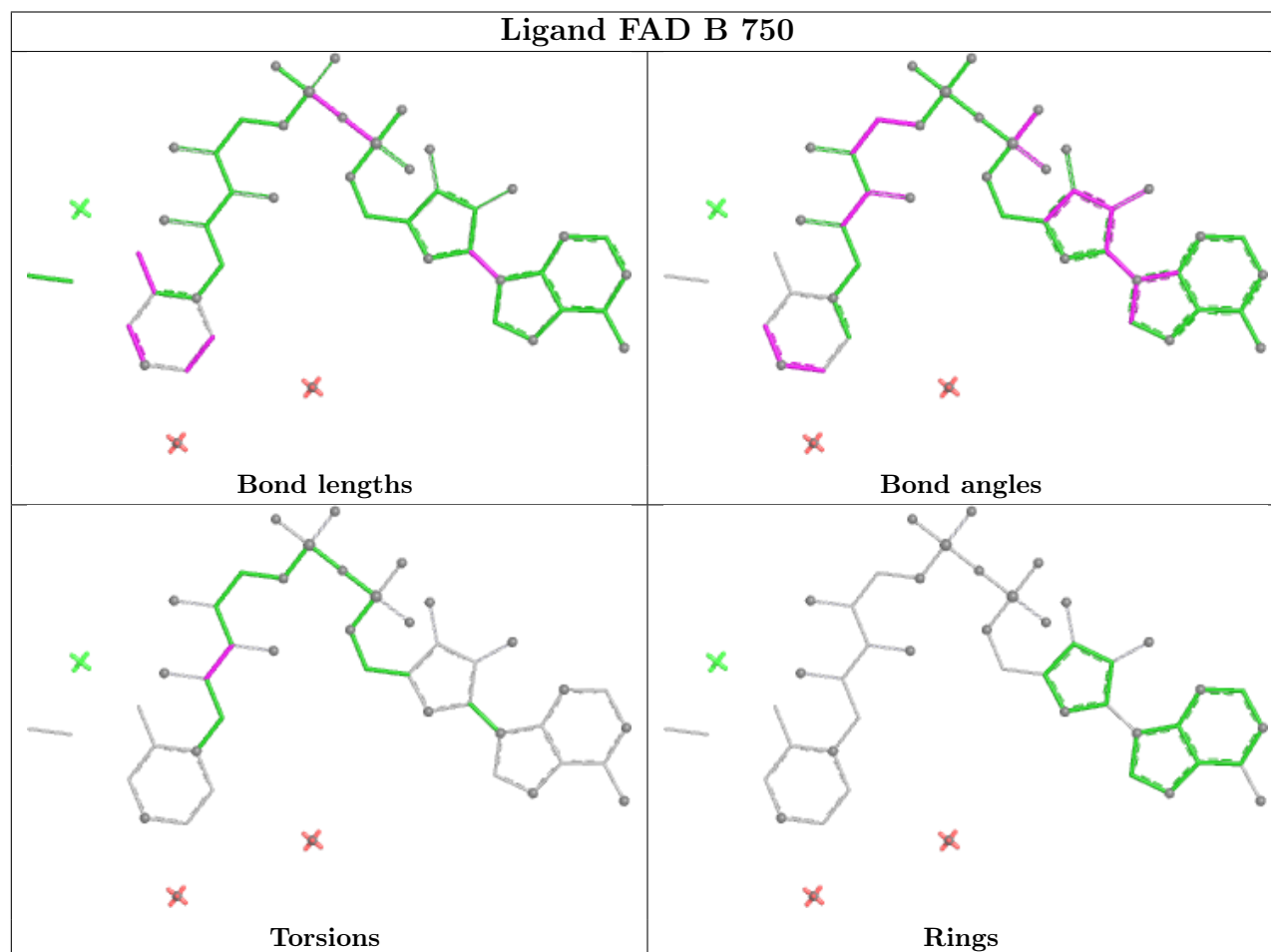
Mol	Chain	Res	Type	Atoms
2	A	750	FAD	C1'-C2'-C3'-C4'
2	B	750	FAD	C1'-C2'-C3'-C4'
4	A	752	NAP	C5B-O5B-PA-O1A
4	A	752	NAP	C5B-O5B-PA-O2A
4	A	752	NAP	C5B-O5B-PA-O3
4	A	752	NAP	C2B-C1B-N9A-C8A
4	B	752	NAP	C5B-O5B-PA-O1A
4	B	752	NAP	C5B-O5B-PA-O2A
4	B	752	NAP	C5B-O5B-PA-O3
4	B	752	NAP	C2B-C1B-N9A-C8A
4	A	752	NAP	C2B-C1B-N9A-C4A
4	B	752	NAP	C2B-C1B-N9A-C4A
2	A	750	FAD	O2'-C2'-C3'-C4'
2	B	750	FAD	O2'-C2'-C3'-C4'
4	A	752	NAP	PN-O3-PA-O1A
4	B	752	NAP	PN-O3-PA-O1A
2	A	750	FAD	O2'-C2'-C3'-O3'
2	B	750	FAD	O2'-C2'-C3'-O3'
4	A	752	NAP	C2B-O2B-P2B-O1X
4	B	752	NAP	C2B-O2B-P2B-O1X
2	A	750	FAD	C1'-C2'-C3'-O3'
2	B	750	FAD	C1'-C2'-C3'-O3'
4	A	752	NAP	C2B-O2B-P2B-O3X
4	B	752	NAP	C2B-O2B-P2B-O3X
4	A	752	NAP	PN-O3-PA-O2A
4	B	752	NAP	PN-O3-PA-O2A

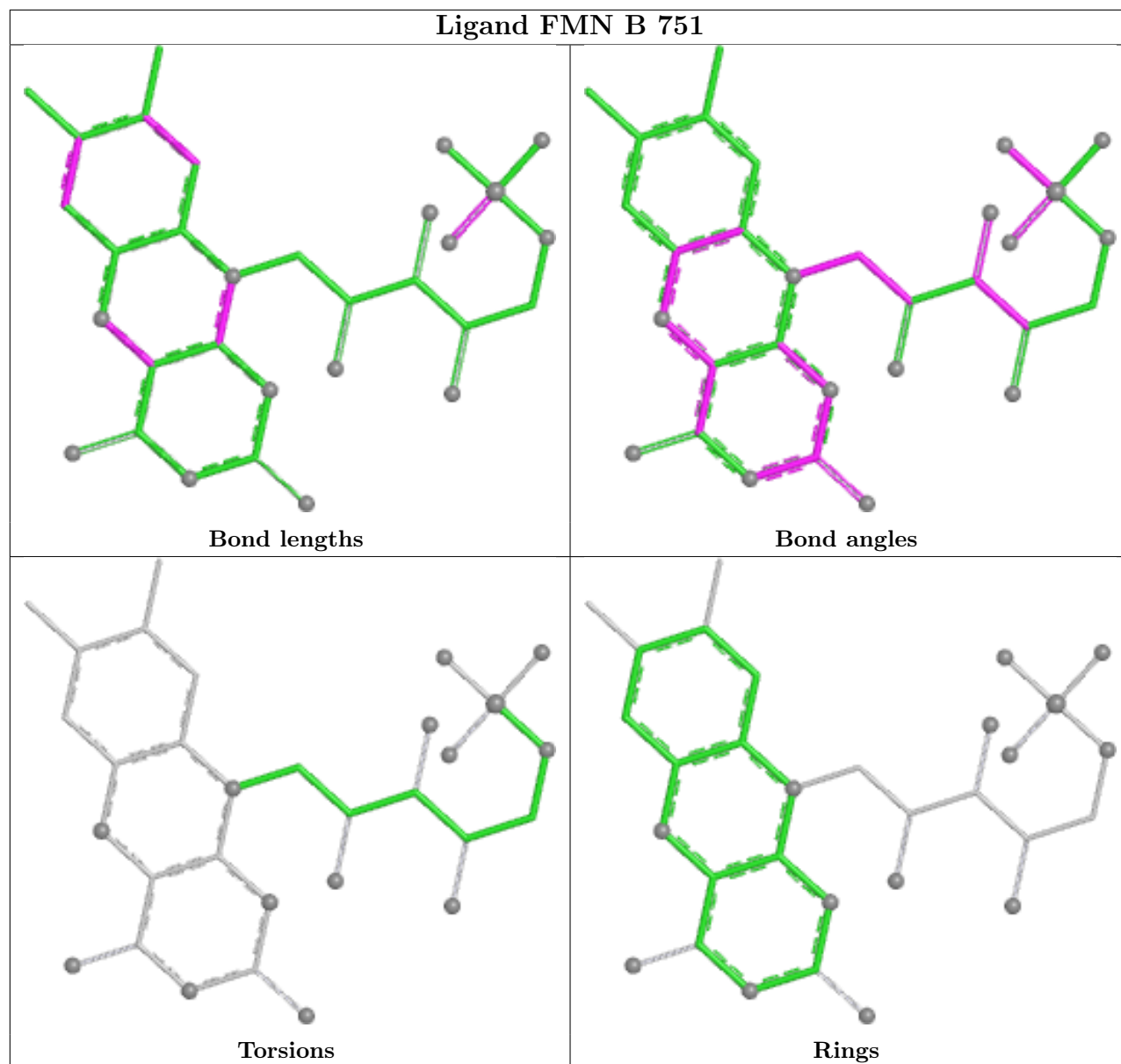
There are no ring outliers.

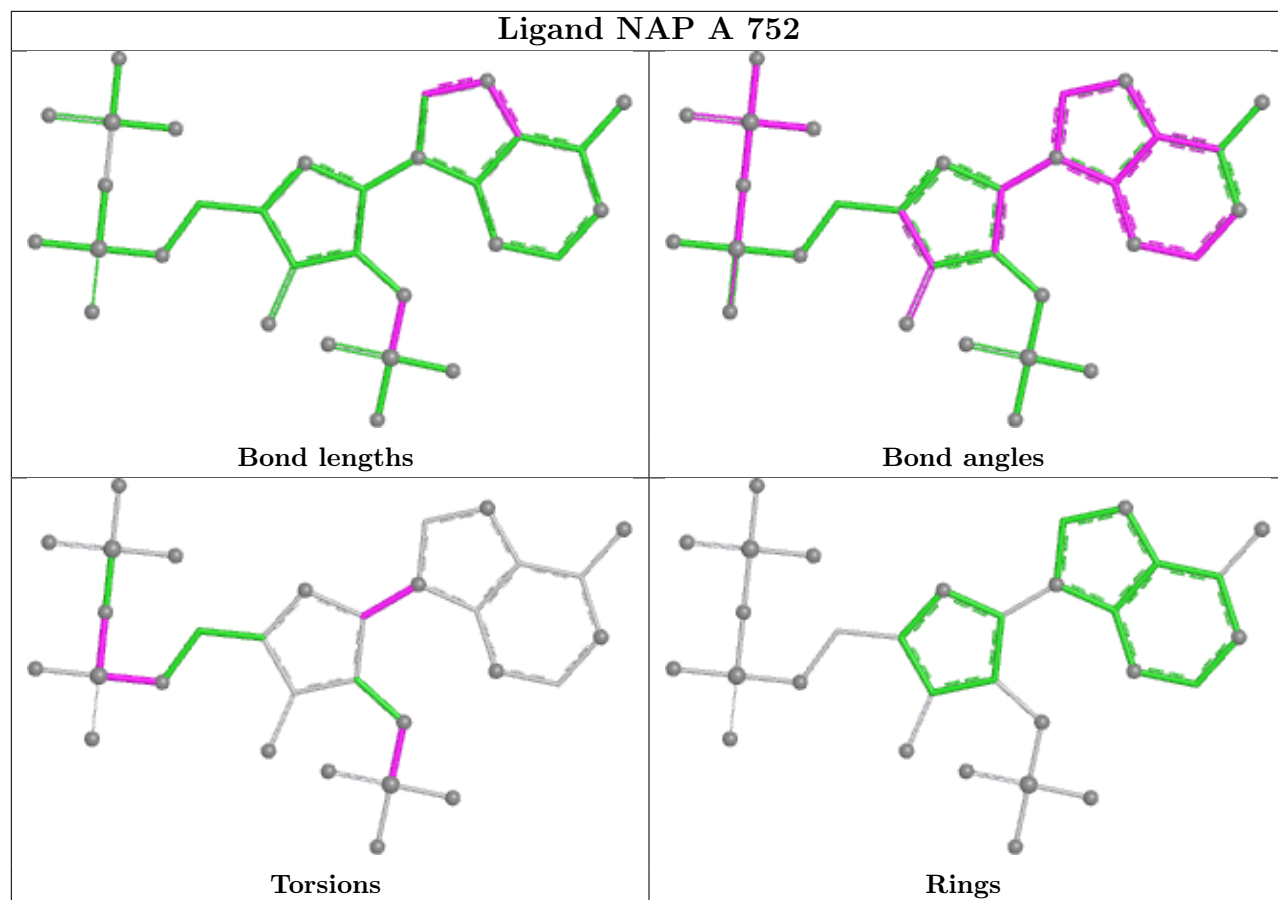
No monomer is involved in short contacts.

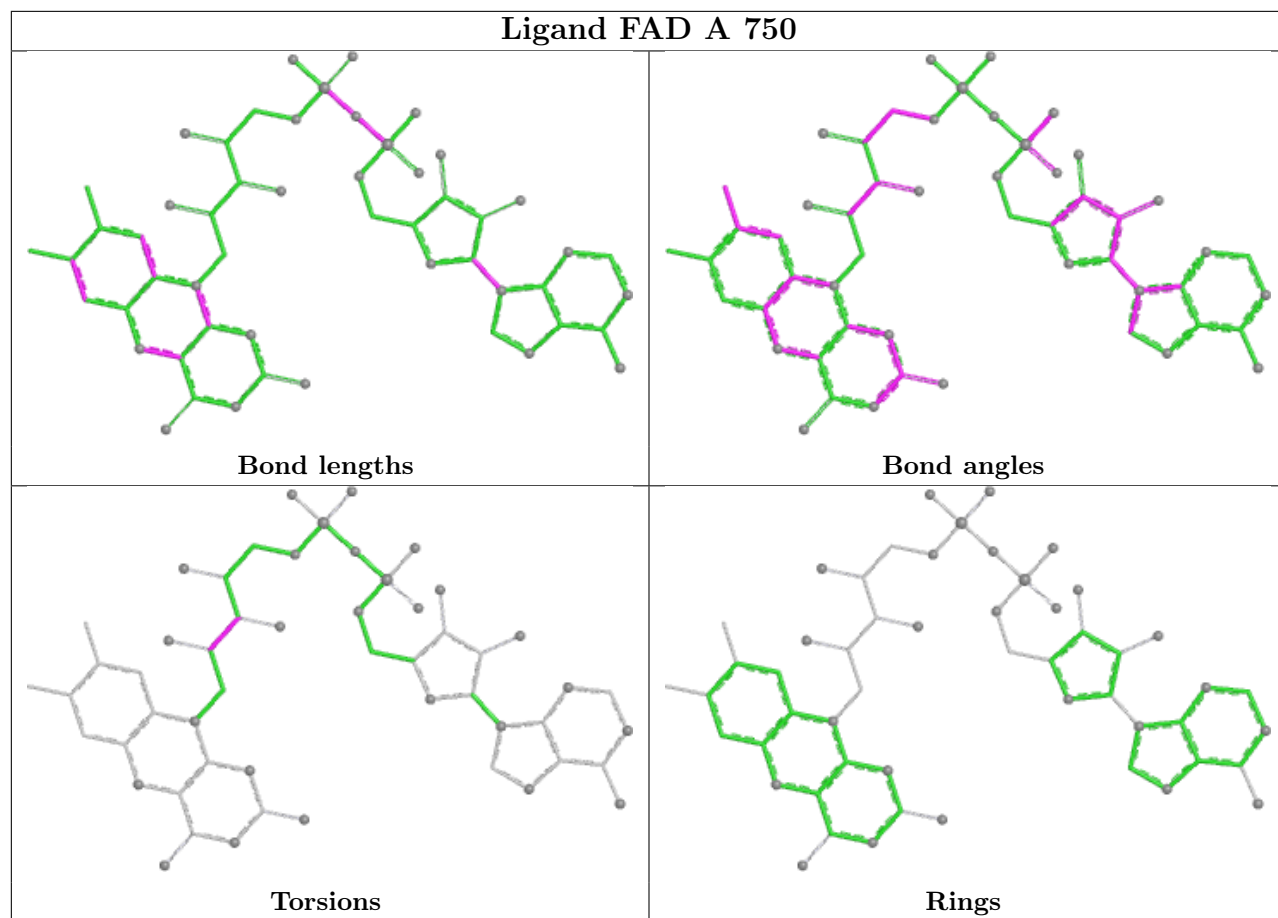
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

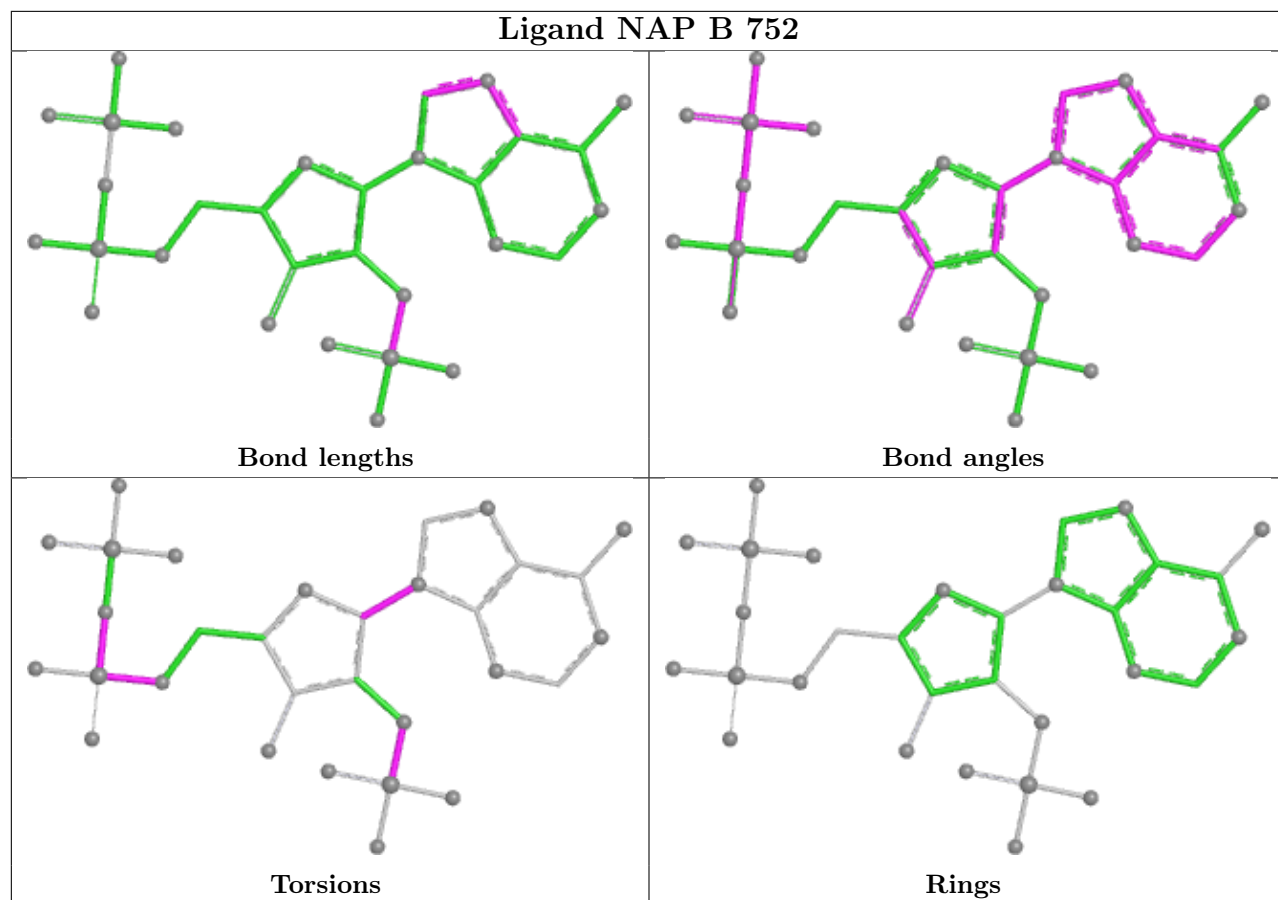
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

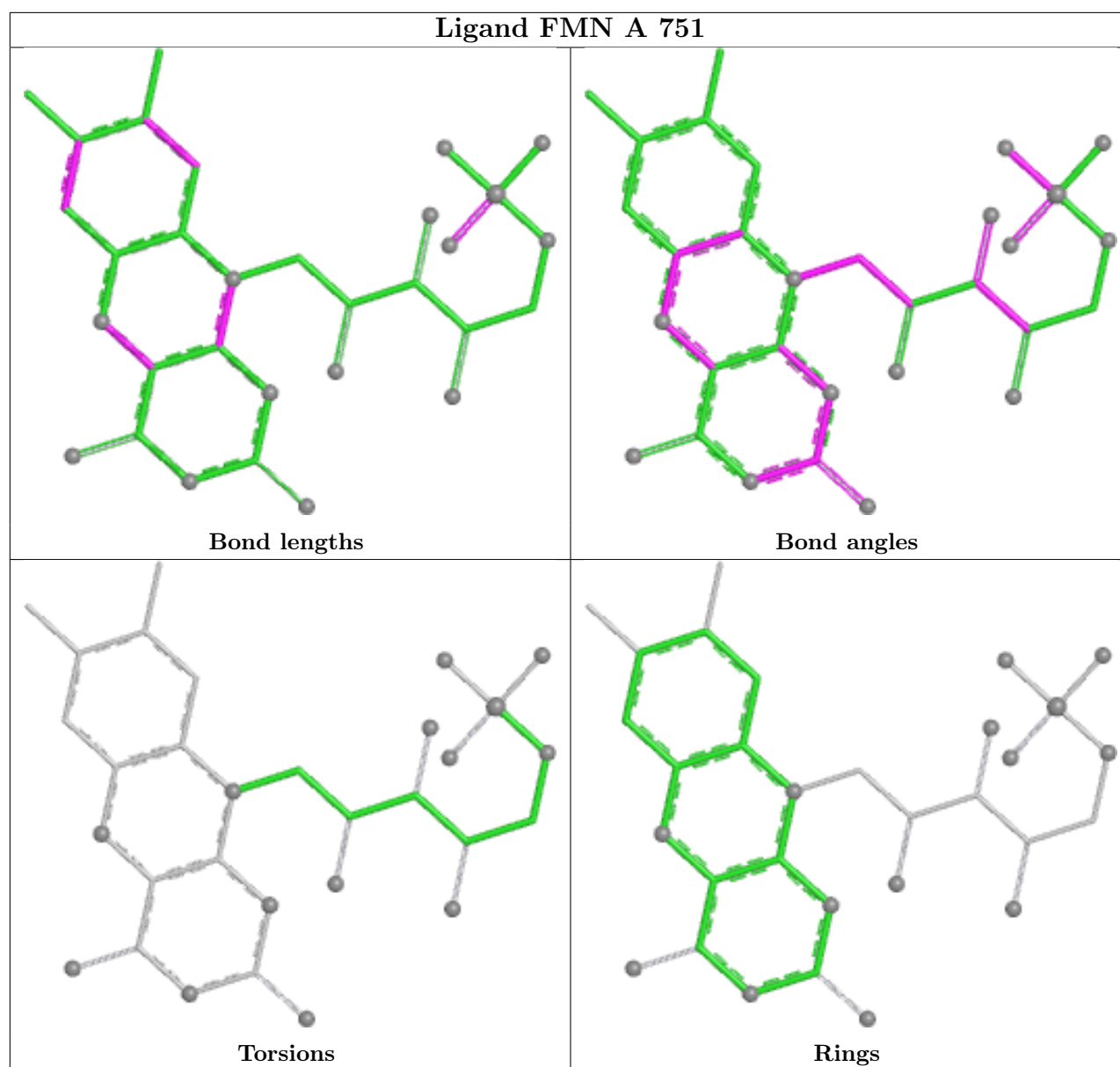












4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.