



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2021 – 02:05 PM EST

PDB ID : 7L18  
Title : Crystal structure of a tandem deletion mutant of rat NADPH-cytochrome P450 reductase  
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Deposited on : 2020-12-14  
Resolution : 2.54 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](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 : 2.16  
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) : 2.16

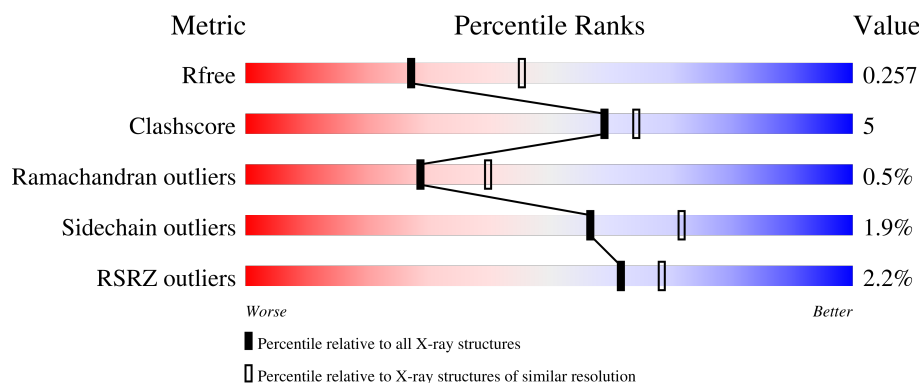
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	AAA	620	
1	BBB	620	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10291 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.

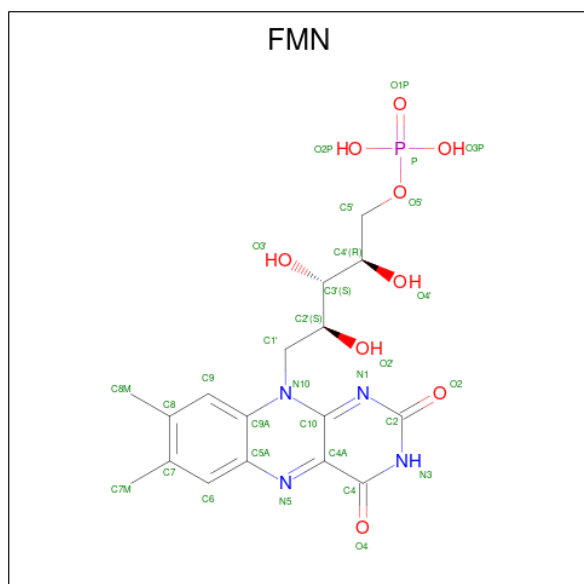
- Molecule 1 is a protein called NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	606	Total	C	N	O	S	0	0	0
			4865	3082	838	922	23			
1	BBB	605	Total	C	N	O	S	0	0	0
			4859	3078	837	921	23			

There are 4 discrepancies between the modelled and reference sequences:

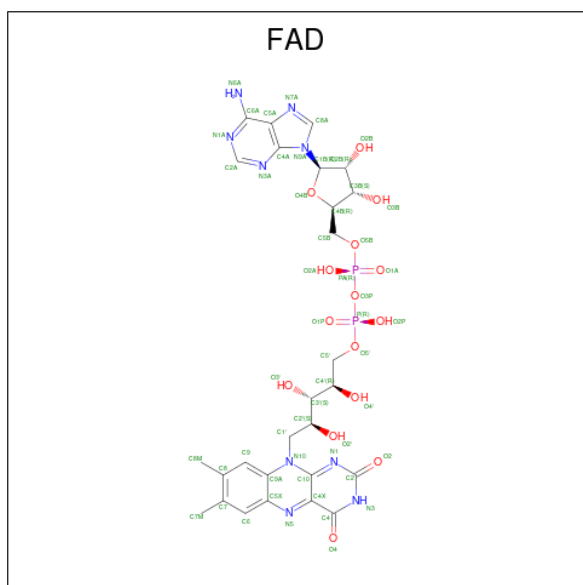
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	ASP	deletion	UNP P00388
AAA	?	-	VAL	deletion	UNP P00388
BBB	?	-	ASP	deletion	UNP P00388
BBB	?	-	VAL	deletion	UNP P00388

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	BBB	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	AAA	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	BBB	1	Total 31	C 10	N 5	O 13	P 3	0	0

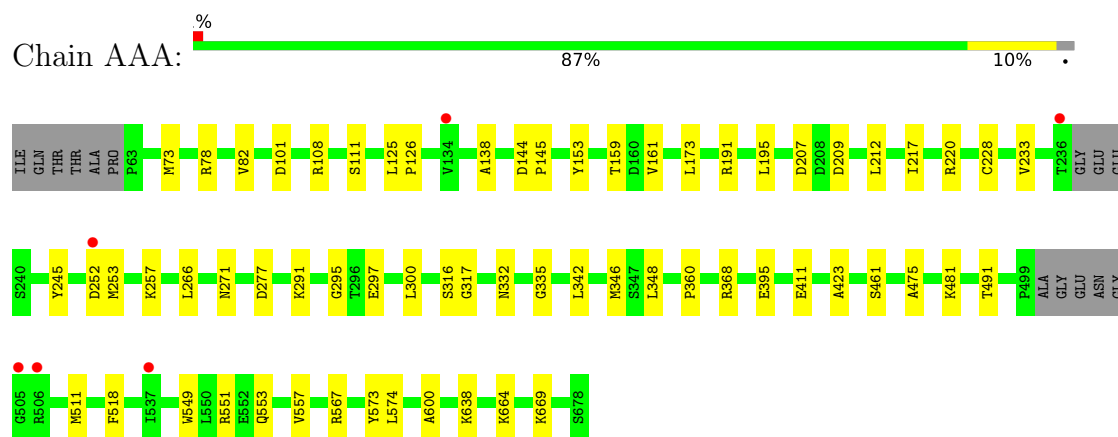
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	200	Total O 200 200	0	0
5	BBB	120	Total O 120 120	0	0

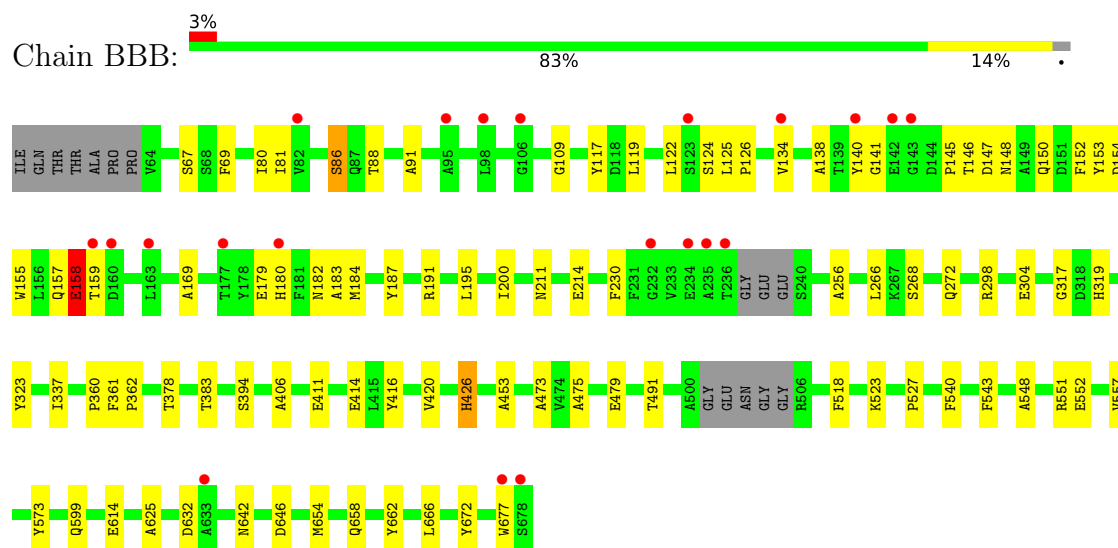
### 3 Residue-property plots

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

- Molecule 1: NADPH-cytochrome P450 reductase



- Molecule 1: NADPH-cytochrome P450 reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.06Å 114.82Å 120.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.54 29.77 – 2.54	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.79-2.54) 89.9 (29.77-2.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.69 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.181 , 0.254 0.185 , 0.257	Depositor DCC
$R_{free}$ test set	2143 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10291	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.52% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, NAP, 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	AAA	0.66	0/4981	0.79	0/6737
1	BBB	0.68	0/4974	0.79	0/6728
All	All	0.67	0/9955	0.79	0/13465

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

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	AAA	4865	0	4718	36	0
1	BBB	4859	0	4712	57	0
2	AAA	31	0	19	0	0
2	BBB	31	0	19	2	0
3	AAA	53	0	31	0	0
3	BBB	53	0	31	1	0
4	AAA	48	0	25	0	0
4	BBB	31	0	11	1	0
5	AAA	200	0	0	4	0
5	BBB	120	0	0	4	0
All	All	10291	0	9566	92	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 5.

All (92) 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:BBB:191:ARG:O	1:BBB:195:LEU:HD12	1.73	0.87
1:BBB:614:GLU:HB2	5:BBB:851:HOH:O	1.94	0.67
1:AAA:300:LEU:HD22	1:AAA:574:LEU:HD21	1.77	0.67
1:BBB:86:SER:HB3	1:BBB:91:ALA:HB3	1.77	0.66
1:AAA:346:MET:HE1	1:AAA:348:LEU:HG	1.78	0.65
1:BBB:69:PHE:CZ	1:BBB:122:LEU:HD12	2.32	0.65
1:AAA:73:MET:HB2	1:AAA:78:ARG:HB2	1.79	0.64
1:AAA:78:ARG:HH21	1:AAA:78:ARG:HG3	1.62	0.64
1:BBB:256:ALA:O	1:BBB:266:LEU:HD21	1.97	0.64
1:AAA:551:ARG:NH1	5:AAA:803:HOH:O	2.29	0.64
1:AAA:346:MET:CE	1:AAA:348:LEU:HG	2.30	0.62
1:AAA:600:ALA:HB1	1:BBB:337:ILE:HB	1.82	0.62
1:BBB:154:ASP:O	1:BBB:158:GLU:HB2	2.00	0.62
1:BBB:86:SER:HB2	2:BBB:701:FMN:O3P	1.99	0.62
1:BBB:551:ARG:HG3	1:BBB:557:VAL:HG21	1.83	0.61
1:AAA:257:LYS:HA	1:AAA:266:LEU:HD21	1.82	0.61
1:BBB:69:PHE:HZ	1:BBB:122:LEU:HD12	1.64	0.61
1:AAA:475:ALA:HA	1:AAA:491:THR:HB	1.85	0.58
1:BBB:200:ILE:HD11	1:BBB:230:PHE:CD1	2.38	0.58
1:BBB:146:THR:O	1:BBB:148:ASN:N	2.38	0.57
1:BBB:319:HIS:CD2	1:BBB:677:TRP:CZ2	2.93	0.57
1:BBB:523:LYS:HE3	5:BBB:915:HOH:O	2.04	0.55
1:AAA:411:GLU:HB3	5:AAA:833:HOH:O	2.05	0.55
1:AAA:228:CYS:HA	1:AAA:233:VAL:HG22	1.89	0.55
1:BBB:155:TRP:HA	1:BBB:158:GLU:HB2	1.89	0.55
1:BBB:599:GLN:N	1:BBB:599:GLN:CD	2.60	0.55
1:AAA:191:ARG:NH1	1:AAA:195:LEU:HD21	2.23	0.54
1:BBB:268:SER:O	1:BBB:272:GLN:NE2	2.38	0.54
1:AAA:335:GLY:HA3	1:AAA:342:LEU:HD11	1.90	0.54
1:BBB:191:ARG:O	1:BBB:195:LEU:CD1	2.54	0.53
1:BBB:317:GLY:HA3	1:BBB:518:PHE:O	2.10	0.53
1:AAA:332:ASN:OD1	1:AAA:368:ARG:NH2	2.41	0.52
1:BBB:157:GLN:HG3	1:BBB:187:TYR:OH	2.09	0.52
1:BBB:155:TRP:CA	1:BBB:158:GLU:HB2	2.40	0.52
1:AAA:101:ASP:OD2	1:AAA:220:ARG:HD2	2.09	0.52
1:BBB:86:SER:CB	1:BBB:91:ALA:HB3	2.40	0.52
1:AAA:423:ALA:HA	1:AAA:481:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:245:TYR:CD2	1:AAA:360:PRO:HD3	2.45	0.51
1:BBB:140:TYR:CD2	1:BBB:146:THR:HG22	2.45	0.51
1:BBB:319:HIS:CD2	1:BBB:677:TRP:HZ2	2.29	0.51
1:BBB:69:PHE:HB3	1:BBB:117:TYR:CD2	2.46	0.50
1:BBB:304:GLU:OE1	5:BBB:801:HOH:O	2.20	0.50
1:AAA:291:LYS:NZ	1:AAA:295:GLY:O	2.44	0.50
1:AAA:551:ARG:HG3	1:AAA:557:VAL:HG21	1.93	0.50
1:BBB:80:ILE:O	1:BBB:109:GLY:HA2	2.11	0.50
1:BBB:211:ASN:OD1	1:BBB:214:GLU:N	2.34	0.50
1:AAA:297:GLU:OE1	1:AAA:567:ARG:NH1	2.41	0.49
1:BBB:138:ALA:O	1:BBB:146:THR:HG23	2.12	0.49
1:BBB:383:THR:HB	1:BBB:406:ALA:HA	1.94	0.49
1:AAA:173:LEU:HD23	1:AAA:212:LEU:HD21	1.96	0.48
1:BBB:272:GLN:HG3	5:BBB:829:HOH:O	2.13	0.48
1:AAA:549:TRP:O	1:AAA:553:GLN:HG2	2.14	0.48
1:BBB:323:TYR:CE1	1:BBB:453:ALA:HB2	2.49	0.48
1:BBB:642:ASN:O	1:BBB:646:ASP:HB2	2.14	0.48
1:BBB:662:TYR:O	1:BBB:666:LEU:HD13	2.14	0.47
1:AAA:395:GLU:HG3	5:AAA:879:HOH:O	2.14	0.47
1:AAA:317:GLY:HA3	1:AAA:518:PHE:O	2.15	0.47
1:AAA:145:PRO:HG3	1:AAA:153:TYR:CG	2.50	0.47
1:BBB:416:TYR:O	1:BBB:420:VAL:HB	2.15	0.46
1:BBB:125:LEU:N	1:BBB:126:PRO:CD	2.79	0.46
1:AAA:207:ASP:OD1	1:AAA:209:ASP:HB3	2.17	0.45
1:BBB:475:ALA:HA	1:BBB:491:THR:HB	1.98	0.45
1:AAA:159:THR:OG1	1:AAA:161:VAL:HG23	2.16	0.45
1:AAA:125:LEU:N	1:AAA:126:PRO:CD	2.80	0.44
1:BBB:540:PHE:HA	1:BBB:543:PHE:HB2	1.99	0.44
1:AAA:217:ILE:HD12	5:AAA:965:HOH:O	2.17	0.44
1:AAA:245:TYR:CE2	1:AAA:360:PRO:HD3	2.53	0.44
1:AAA:638:LYS:HD3	1:AAA:638:LYS:HA	1.84	0.43
1:BBB:145:PRO:HG3	1:BBB:153:TYR:CD2	2.54	0.43
1:AAA:138:ALA:HA	1:AAA:173:LEU:HB2	2.00	0.43
1:BBB:155:TRP:HA	1:BBB:158:GLU:CB	2.48	0.43
1:BBB:319:HIS:HD2	1:BBB:677:TRP:HZ2	1.65	0.42
1:BBB:119:LEU:HD22	1:BBB:152:PHE:CD1	2.54	0.42
1:AAA:78:ARG:HD3	1:AAA:108:ARG:HB3	2.00	0.42
1:BBB:180:HIS:HB3	1:BBB:183:ALA:HB2	2.02	0.42
1:BBB:145:PRO:HB3	1:BBB:184:MET:HE2	2.01	0.42
1:BBB:158:GLU:HB3	1:BBB:159:THR:H	1.55	0.42
1:AAA:316:SER:OG	1:AAA:461:SER:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:144:ASP:OD1	1:AAA:669:LYS:HE3	2.20	0.41
1:BBB:599:GLN:CD	1:BBB:599:GLN:H	2.23	0.41
1:BBB:378:THR:O	1:BBB:426:HIS:HB3	2.20	0.41
1:BBB:548:ALA:O	1:BBB:552:GLU:HG3	2.20	0.41
1:BBB:654:MET:HB2	1:BBB:658:GLN:HB2	2.02	0.41
1:BBB:654:MET:HB2	1:BBB:658:GLN:CB	2.51	0.41
1:AAA:82:VAL:O	1:AAA:111:SER:HA	2.21	0.41
1:BBB:134:VAL:HA	1:BBB:169:ALA:O	2.21	0.41
1:BBB:473:ALA:HA	3:BBB:702:FAD:O2	2.21	0.40
1:BBB:360:PRO:HG2	1:BBB:361:PHE:CE2	2.57	0.40
1:BBB:298:ARG:NH1	4:BBB:703:NAP:O1N	2.50	0.40
1:BBB:69:PHE:CD1	1:BBB:81:ILE:HD13	2.57	0.40
1:BBB:527:PRO:HD2	1:BBB:625:ALA:HA	2.04	0.40
1:BBB:88:THR:OG1	2:BBB:701:FMN:O1P	2.31	0.40

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	AAA	600/620 (97%)	581 (97%)	19 (3%)	0	100	100
1	BBB	599/620 (97%)	554 (92%)	39 (6%)	6 (1%)	15	22
All	All	1199/1240 (97%)	1135 (95%)	58 (5%)	6 (0%)	29	40

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	141	GLY
1	BBB	147	ASP
1	BBB	158	GLU
1	BBB	179	GLU

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Mol	Chain	Res	Type
1	BBB	632	ASP
1	BBB	362	PRO

### 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	AAA	520/529 (98%)	513 (99%)	7 (1%)	69	80
1	BBB	519/529 (98%)	506 (98%)	13 (2%)	47	62
All	All	1039/1058 (98%)	1019 (98%)	20 (2%)	57	72

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	252	ASP
1	AAA	253	MET
1	AAA	271	ASN
1	AAA	277	ASP
1	AAA	511	MET
1	AAA	573	TYR
1	AAA	664	LYS
1	BBB	67	SER
1	BBB	86	SER
1	BBB	124	SER
1	BBB	150	GLN
1	BBB	158	GLU
1	BBB	182	ASN
1	BBB	394	SER
1	BBB	411	GLU
1	BBB	414	GLU
1	BBB	426	HIS
1	BBB	479	GLU
1	BBB	573	TYR
1	BBB	672	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

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	FMN	AAA	701	-	31,33,33	1.33	2 (6%)	40,50,50	2.04	6 (15%)
4	NAP	BBB	703	-	27,33,52	1.04	2 (7%)	35,52,80	0.77	0
4	NAP	AAA	703	-	45,52,52	0.84	3 (6%)	56,80,80	0.88	2 (3%)
2	FMN	BBB	701	-	31,33,33	1.33	2 (6%)	40,50,50	2.02	5 (12%)
3	FAD	BBB	702	-	51,58,58	1.09	2 (3%)	60,89,89	1.73	7 (11%)
3	FAD	AAA	702	-	51,58,58	1.10	3 (5%)	60,89,89	1.83	6 (10%)

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	FMN	AAA	701	-	-	1/18/18/18	0/3/3/3
4	NAP	BBB	703	-	-	0/17/37/67	0/3/3/5
4	NAP	AAA	703	-	-	11/31/67/67	0/5/5/5
2	FMN	BBB	701	-	-	5/18/18/18	0/3/3/3
3	FAD	BBB	702	-	-	2/30/50/50	0/6/6/6
3	FAD	AAA	702	-	-	2/30/50/50	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	701	FMN	C4A-C10	6.00	1.44	1.38
2	BBB	701	FMN	C4A-C10	5.98	1.44	1.38
3	BBB	702	FAD	C4X-C10	5.52	1.44	1.38
3	AAA	702	FAD	C4X-C10	5.09	1.43	1.38
4	BBB	703	NAP	P2B-O2B	3.71	1.66	1.59
3	AAA	702	FAD	C2-N1	-3.17	1.31	1.38
3	BBB	702	FAD	C4-N3	3.09	1.38	1.33
4	AAA	703	NAP	C2N-N1N	2.88	1.38	1.35
2	BBB	701	FMN	C4-N3	2.75	1.37	1.33
2	AAA	701	FMN	C4-N3	2.72	1.37	1.33
3	AAA	702	FAD	C4-N3	2.54	1.37	1.33
4	BBB	703	NAP	C8A-N7A	-2.15	1.30	1.34
4	AAA	703	NAP	C8A-N7A	-2.07	1.31	1.34
4	AAA	703	NAP	P2B-O2B	2.02	1.63	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	702	FAD	C4-N3-C2	8.59	122.39	115.14
2	BBB	701	FMN	C4-N3-C2	8.10	121.98	115.14
2	AAA	701	FMN	C4-N3-C2	8.00	121.90	115.14
3	BBB	702	FAD	C4-N3-C2	7.54	121.51	115.14
3	AAA	702	FAD	C4-C4X-C10	-5.91	116.04	119.95
3	BBB	702	FAD	C4-C4X-C10	-5.22	116.50	119.95
2	BBB	701	FMN	C4-C4A-C10	-5.02	116.63	119.95
2	AAA	701	FMN	C10-C4A-N5	4.94	124.68	121.26
2	AAA	701	FMN	C4-C4A-C10	-4.94	116.68	119.95
3	BBB	702	FAD	C10-C4X-N5	4.76	124.55	121.26
3	AAA	702	FAD	C4X-C4-N3	-4.74	116.94	123.43
2	BBB	701	FMN	C10-C4A-N5	4.71	124.52	121.26
3	AAA	702	FAD	C10-C4X-N5	4.39	124.29	121.26
2	BBB	701	FMN	C4A-C4-N3	-4.34	117.50	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	702	FAD	C4X-C4-N3	-4.23	117.65	123.43
2	AAA	701	FMN	C4A-C4-N3	-4.23	117.65	123.43
2	AAA	701	FMN	C4A-C10-N10	-3.65	116.55	120.30
3	AAA	702	FAD	C4X-C10-N10	-3.64	116.56	120.30
2	BBB	701	FMN	C4A-C10-N10	-3.63	116.57	120.30
3	BBB	702	FAD	C4X-C10-N10	-3.62	116.59	120.30
3	BBB	702	FAD	P-O3P-PA	-2.88	122.96	132.83
4	AAA	703	NAP	C6N-N1N-C2N	-2.84	119.38	121.97
2	AAA	701	FMN	C1'-N10-C9A	2.53	120.29	118.29
4	AAA	703	NAP	O2B-P2B-O1X	-2.42	100.06	109.39
3	AAA	702	FAD	C5A-C6A-N6A	2.33	123.89	120.35
3	BBB	702	FAD	C5A-C6A-N6A	2.03	123.44	120.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	703	NAP	C5B-O5B-PA-O1A
4	AAA	703	NAP	C5D-O5D-PN-O3
2	BBB	701	FMN	C5'-O5'-P-O1P
2	BBB	701	FMN	C5'-O5'-P-O2P
2	BBB	701	FMN	C5'-O5'-P-O3P
4	AAA	703	NAP	O4D-C4D-C5D-O5D
4	AAA	703	NAP	C3D-C4D-C5D-O5D
3	AAA	702	FAD	PA-O3P-P-O1P
4	AAA	703	NAP	C2B-O2B-P2B-O1X
4	AAA	703	NAP	C5B-O5B-PA-O3
4	AAA	703	NAP	C5B-O5B-PA-O2A
4	AAA	703	NAP	C5D-O5D-PN-O1N
4	AAA	703	NAP	C5D-O5D-PN-O2N
2	BBB	701	FMN	O4'-C4'-C5'-O5'
2	AAA	701	FMN	C5'-O5'-P-O1P
3	AAA	702	FAD	PA-O3P-P-O2P
2	BBB	701	FMN	O2'-C2'-C3'-C4'
3	BBB	702	FAD	PA-O3P-P-O1P
3	BBB	702	FAD	PA-O3P-P-O2P
4	AAA	703	NAP	C2B-O2B-P2B-O3X
4	AAA	703	NAP	PN-O3-PA-O1A

There are no ring outliers.

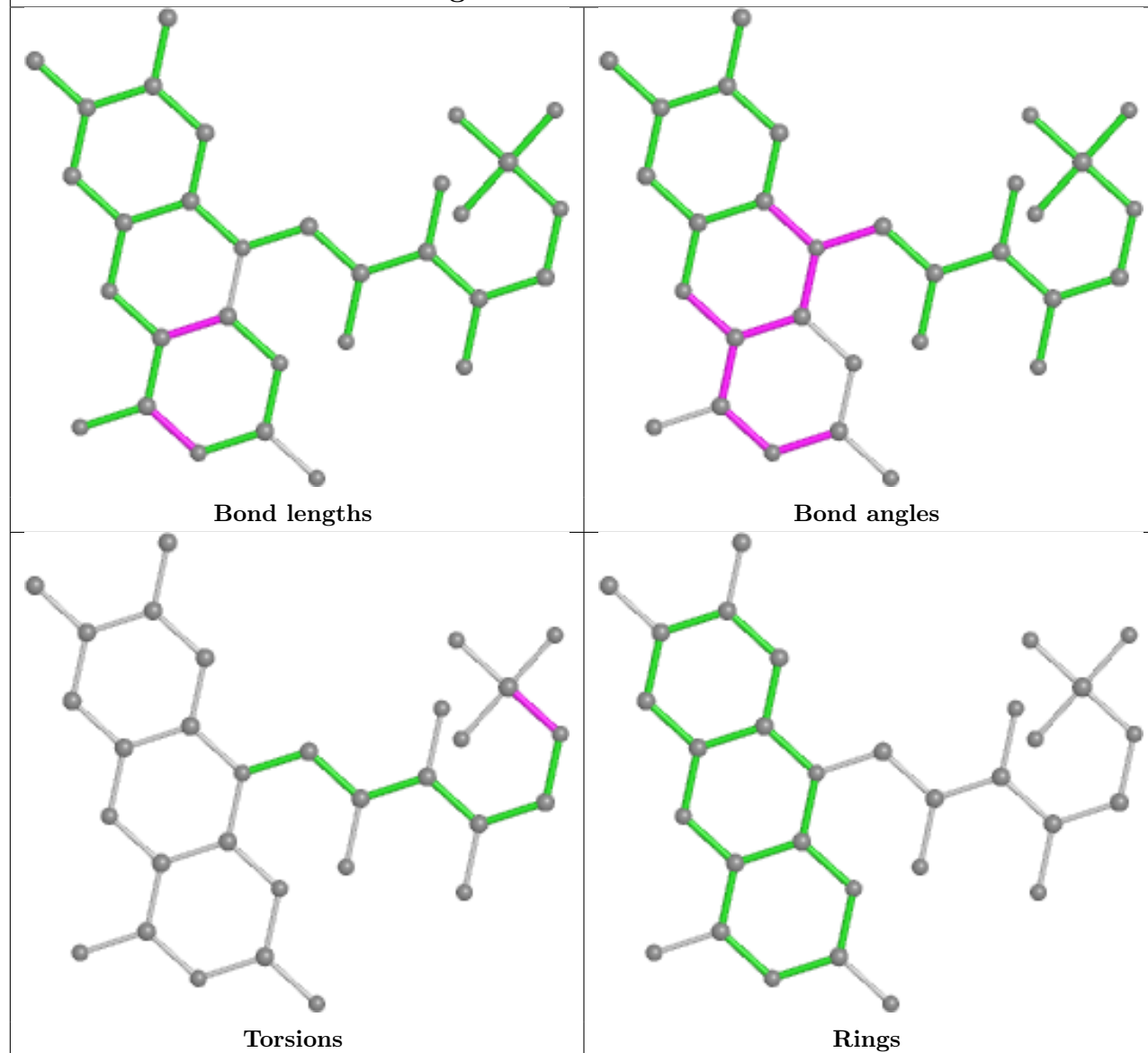
3 monomers are involved in 4 short contacts:

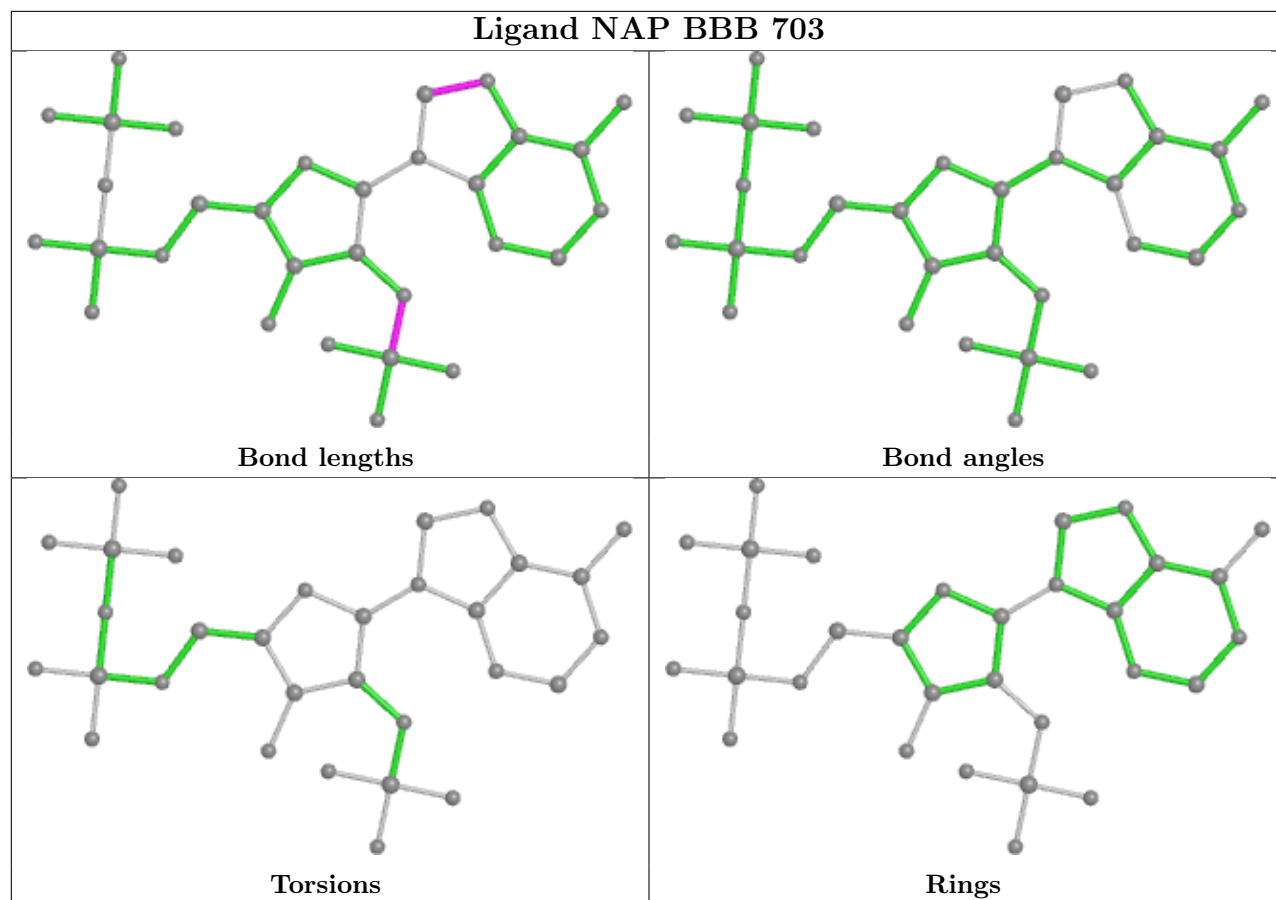
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	703	NAP	1	0
2	BBB	701	FMN	2	0
3	BBB	702	FAD	1	0

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.

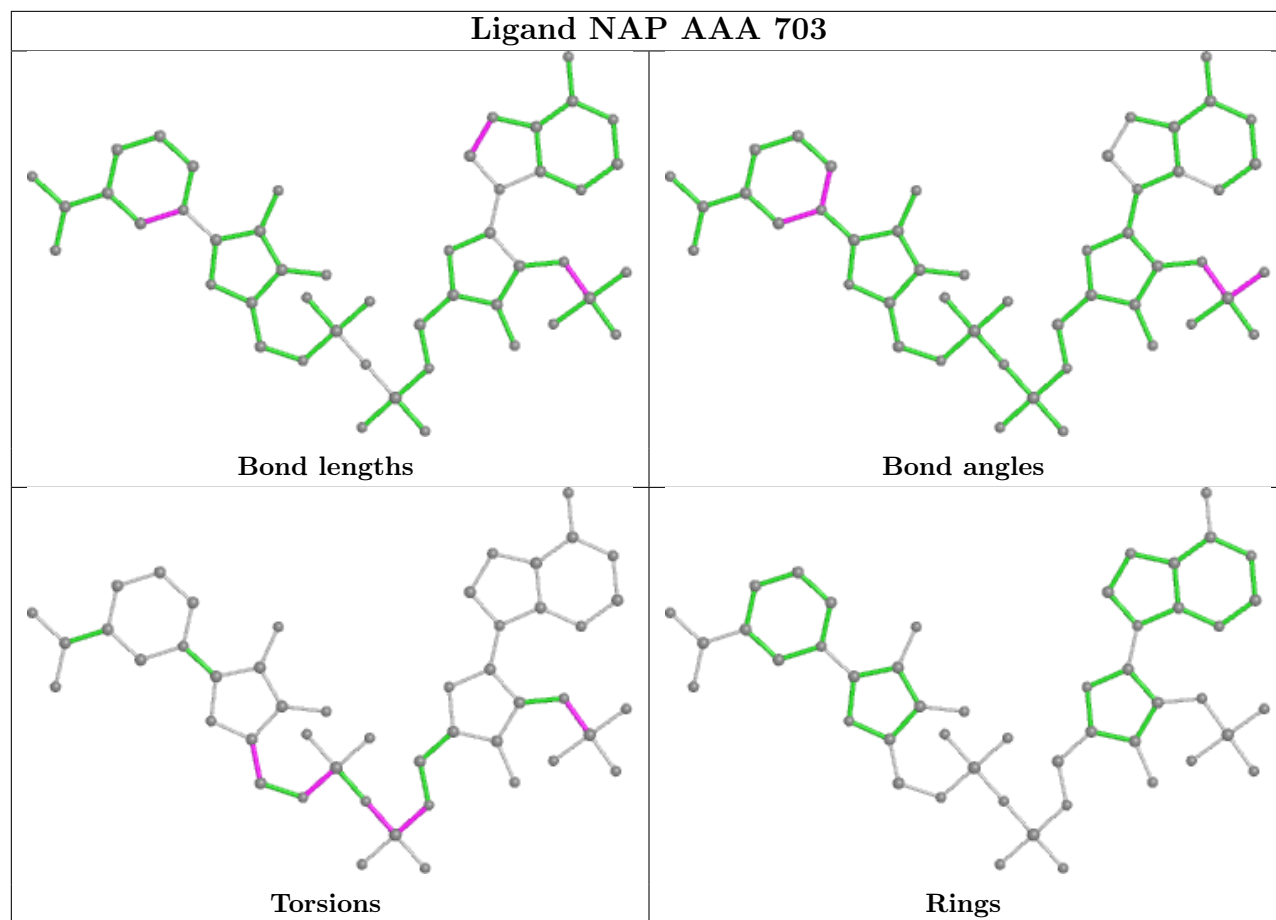


## Ligand FMN AAA 701

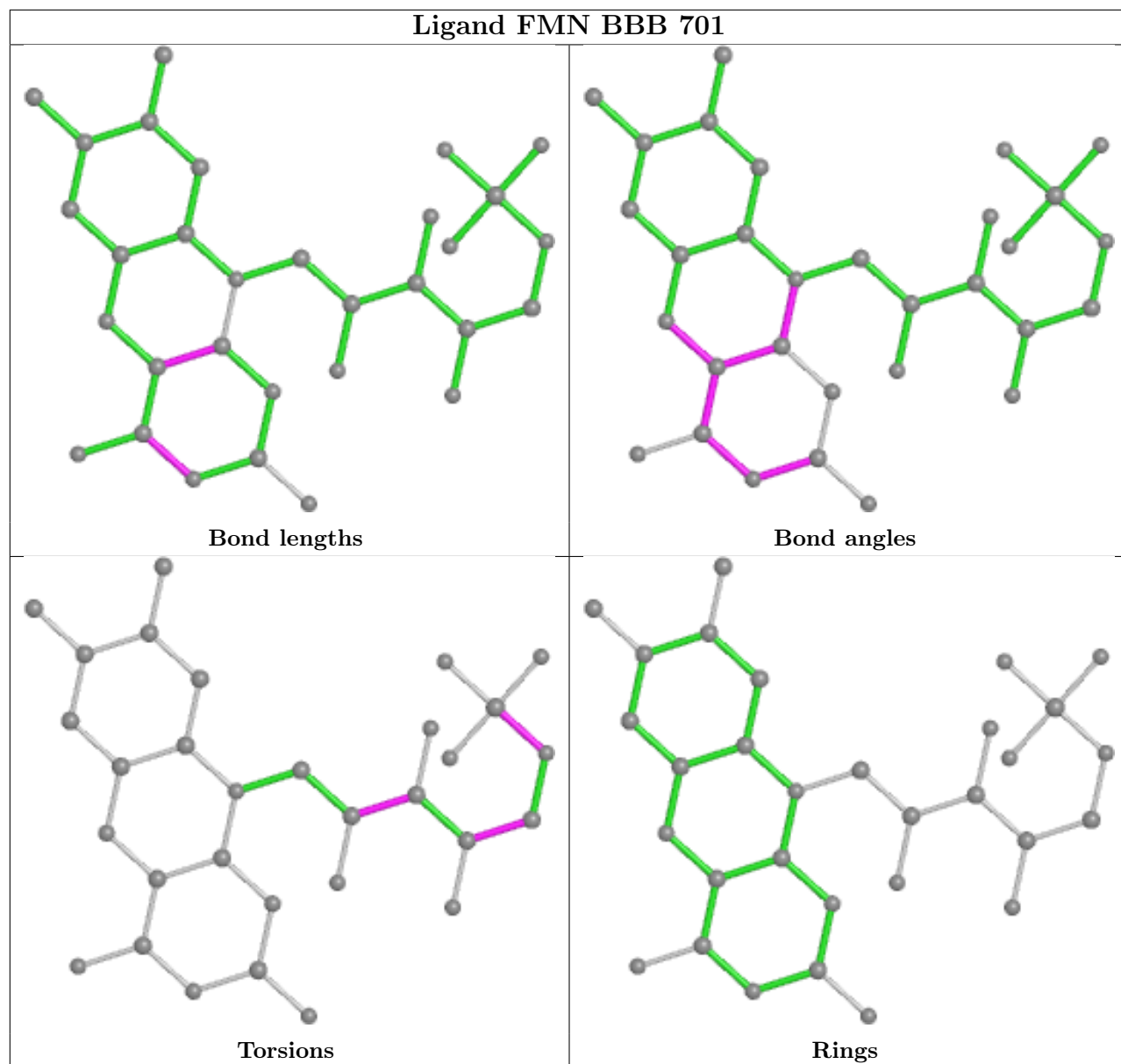


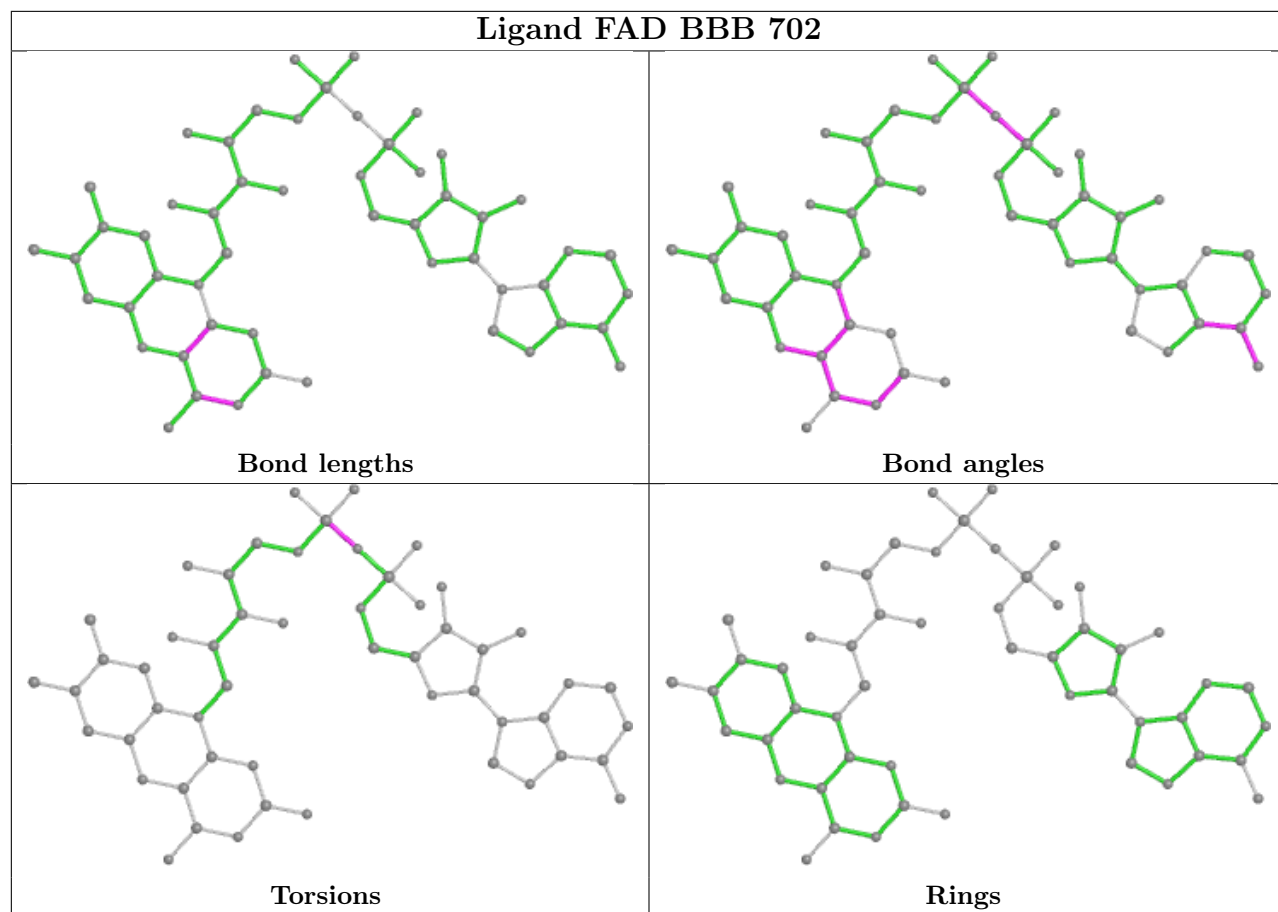


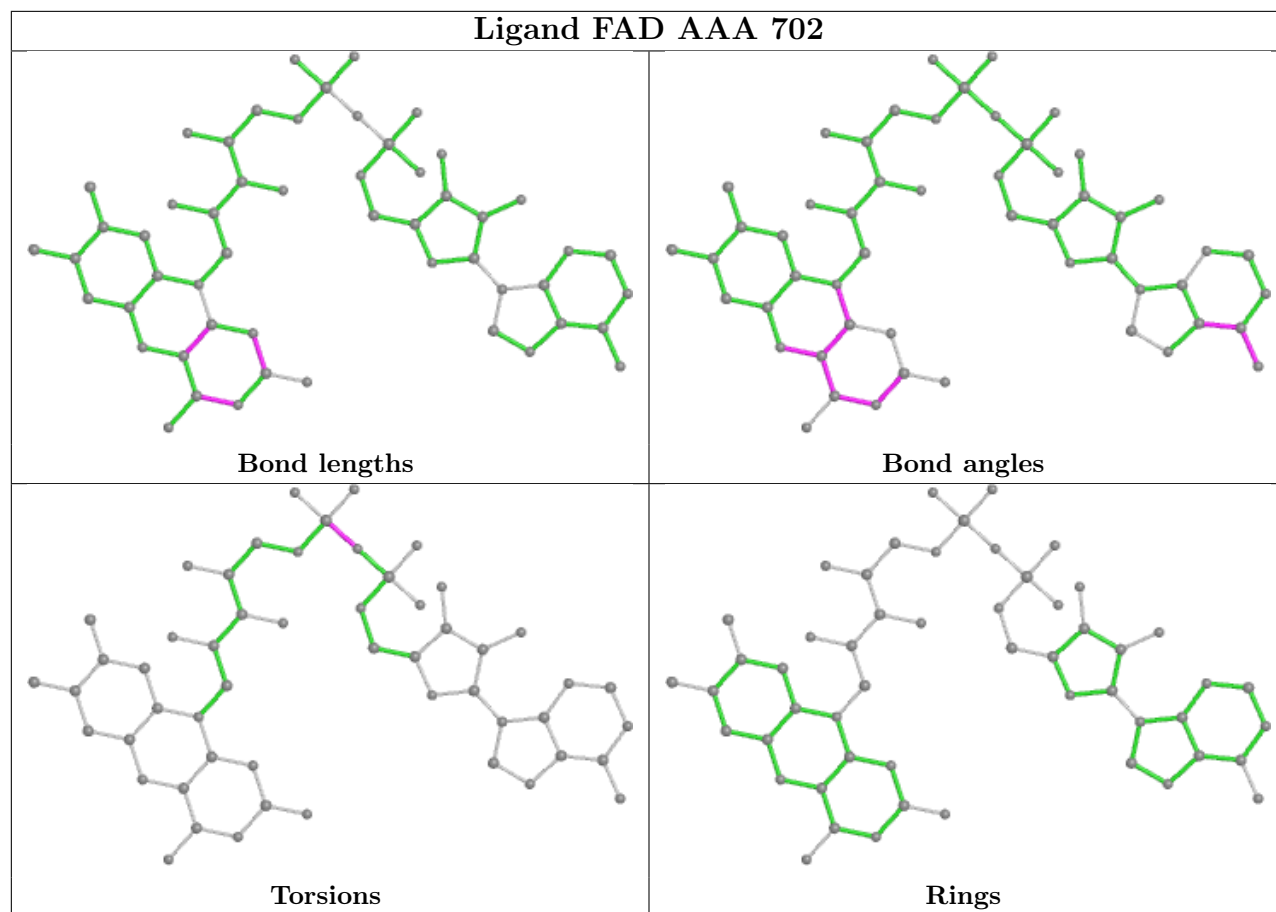
## Ligand NAP AAA 703



## Ligand FMN BBB 701







## 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

### 6.1 Protein, DNA and RNA chains

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	AAA	606/620 (97%)	-0.30	6 (0%) 82 86	28, 42, 65, 96	0
1	BBB	605/620 (97%)	0.02	21 (3%) 44 51	29, 54, 94, 133	0
All	All	1211/1240 (97%)	-0.14	27 (2%) 62 68	28, 46, 88, 133	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	82	VAL	3.7
1	BBB	633	ALA	3.4
1	BBB	677	TRP	3.4
1	BBB	159	THR	3.2
1	BBB	143	GLY	3.1
1	AAA	252	ASP	2.9
1	AAA	505	GLY	2.9
1	BBB	98	LEU	2.9
1	AAA	134	VAL	2.9
1	BBB	232	GLY	2.8
1	BBB	123	SER	2.8
1	BBB	180	HIS	2.8
1	BBB	236	THR	2.7
1	AAA	506	ARG	2.6
1	BBB	160	ASP	2.6
1	BBB	106	GLY	2.6
1	BBB	95	ALA	2.5
1	BBB	134	VAL	2.5
1	BBB	140	TYR	2.5
1	BBB	177	THR	2.3
1	BBB	142	GLU	2.3
1	BBB	234	GLU	2.3
1	BBB	235	ALA	2.2
1	BBB	678	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	537	ILE	2.1
1	BBB	163	LEU	2.1
1	AAA	236	THR	2.0

## 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.

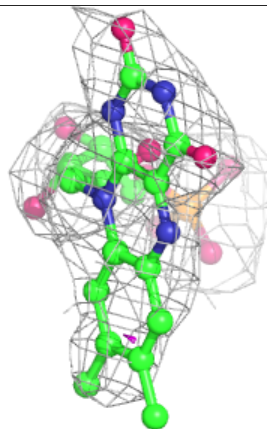
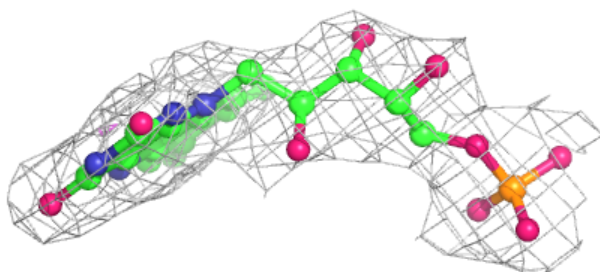
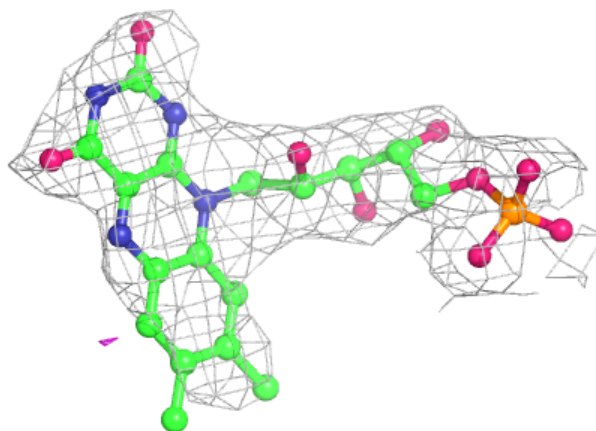
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FMN	BBB	701	31/31	0.90	0.21	63,84,91,91	0
4	NAP	AAA	703	48/48	0.97	0.14	30,48,125,128	0
2	FMN	AAA	701	31/31	0.97	0.11	31,43,50,56	0
3	FAD	AAA	702	53/53	0.97	0.12	24,33,44,48	0
3	FAD	BBB	702	53/53	0.98	0.09	29,34,40,43	0
4	NAP	BBB	703	31/48	0.98	0.08	28,33,51,54	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.



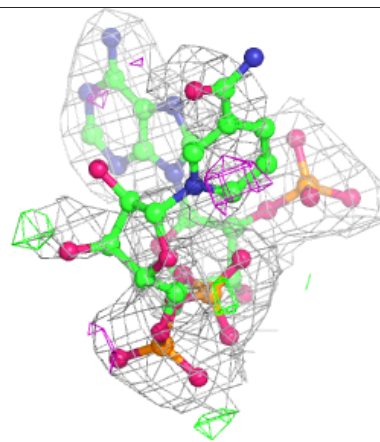
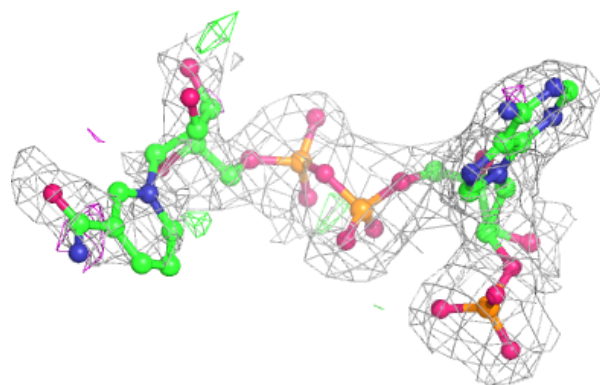
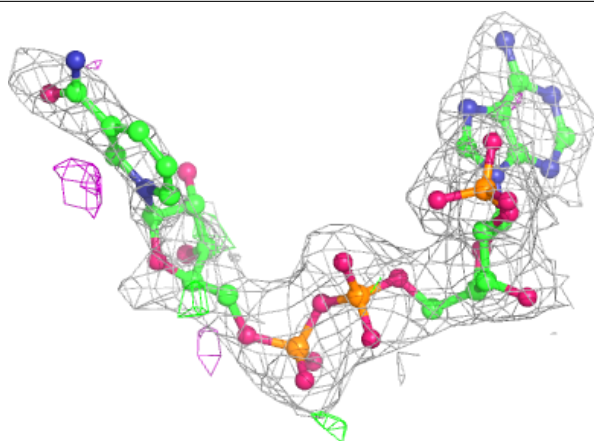
**Electron density around FMN BBB 701:**

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



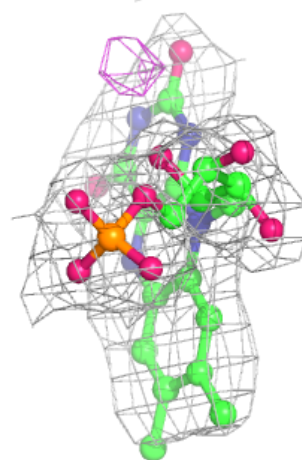
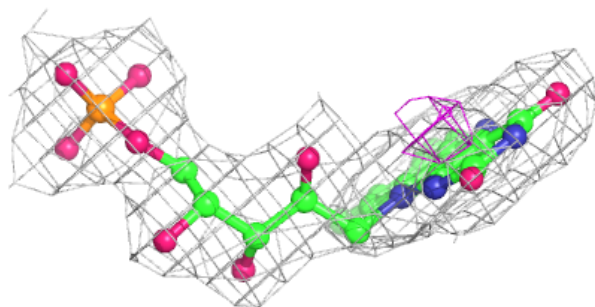
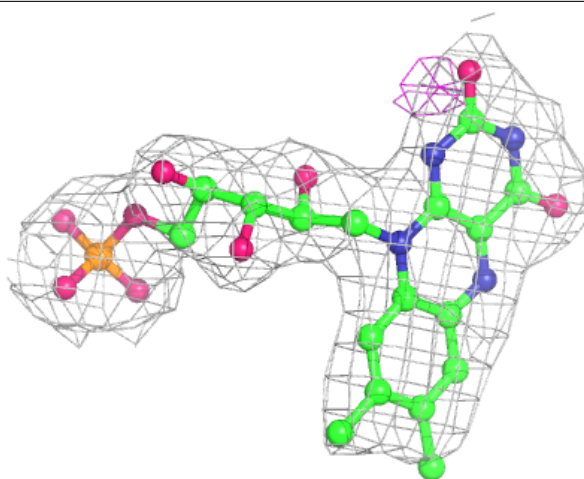
**Electron density around NAP AAA 703:**

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



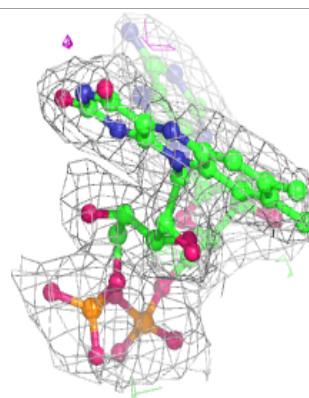
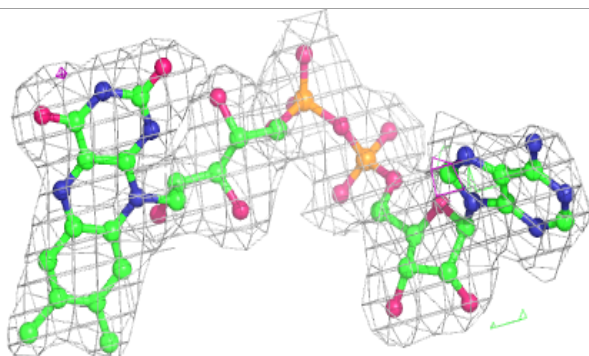
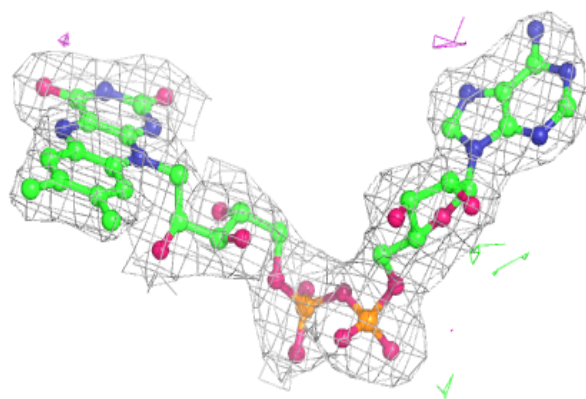
**Electron density around FMN AAA 701:**

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

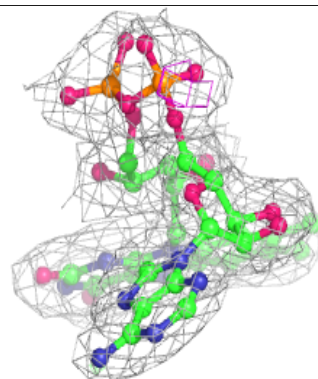
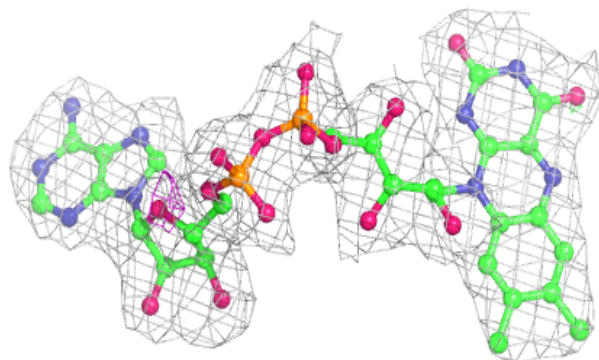
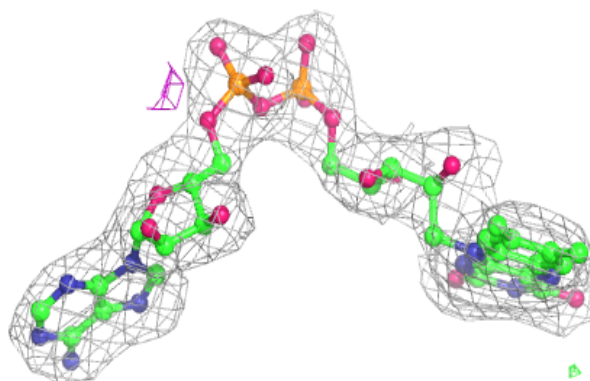


**Electron density around FAD AAA 702:**

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

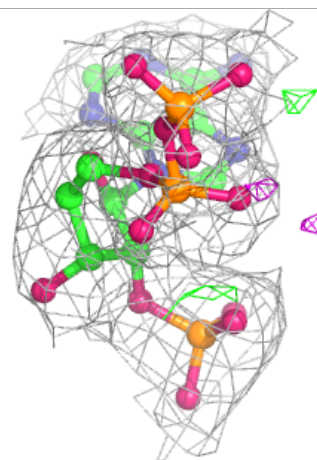
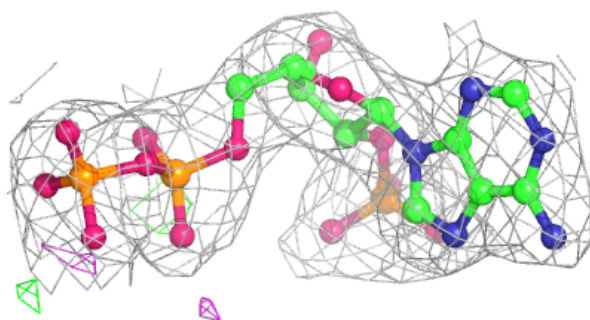
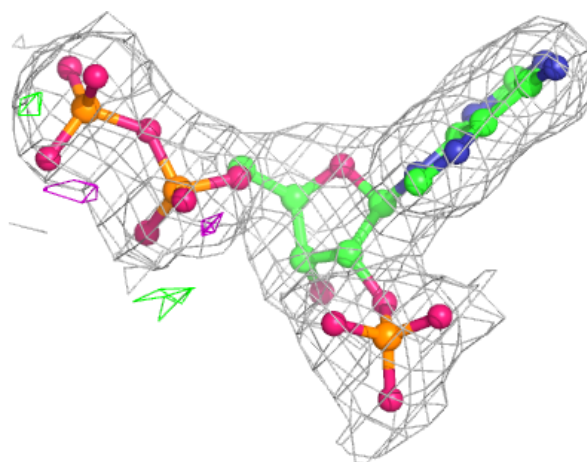
**Electron density around FAD BBB 702:**

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



**Electron density around NAP BBB 703:**

$2mF_o-DF_c$  (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.