



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 08:16 PM BST

PDB ID : 6X0I  
Title : Structure of oxidized SidA ornithine hydroxylase with the FAD "in" and complexed with NADP  
Authors : Tanner, J.J.; Campbell, A.C.  
Deposited on : 2020-05-15  
Resolution : 1.95 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 : 2.13.1  
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) : 2.13.1

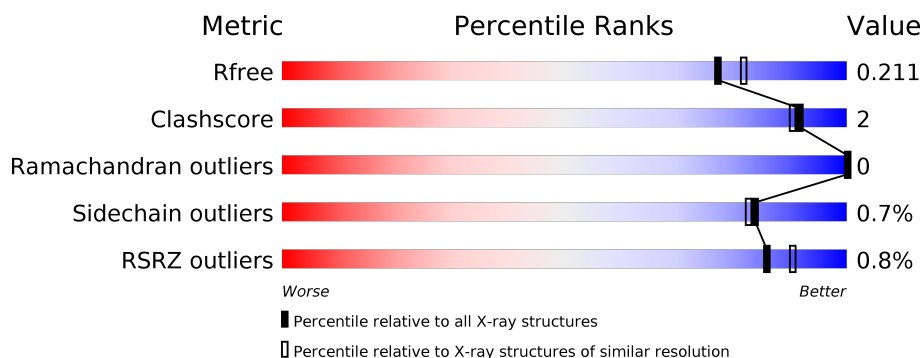
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 on 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	501	
1	B	501	
1	C	501	
1	D	501	

## 2 Entry composition [i](#)

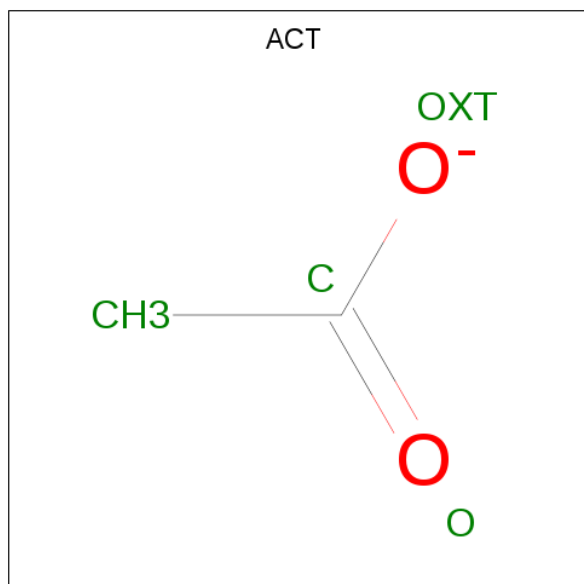
There are 6 unique types of molecules in this entry. The entry contains 15579 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-ornithine N(5)-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	4	0
			3514	2213	633	650	18			
1	B	443	Total	C	N	O	S	0	6	0
			3528	2223	633	654	18			
1	C	443	Total	C	N	O	S	0	6	0
			3518	2217	632	651	18			
1	D	442	Total	C	N	O	S	0	3	0
			3473	2188	623	644	18			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



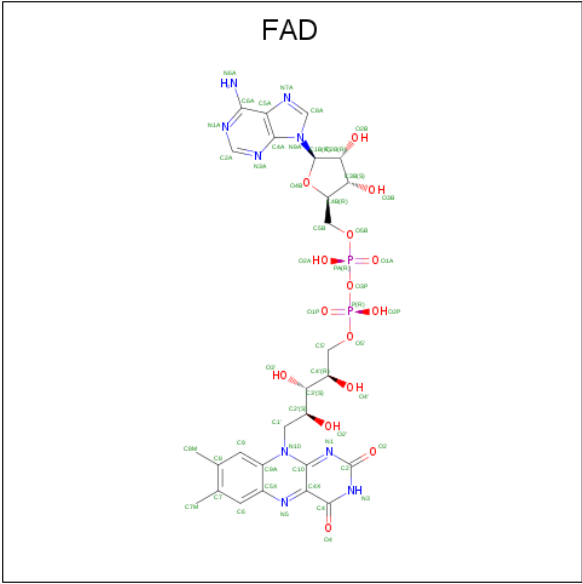
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 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 author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	1
			106	54	18	30	4		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	267	Total	O	0	0
			267	267		

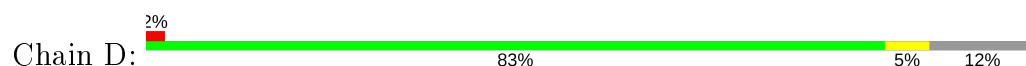
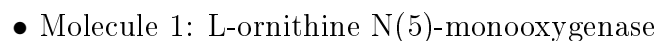
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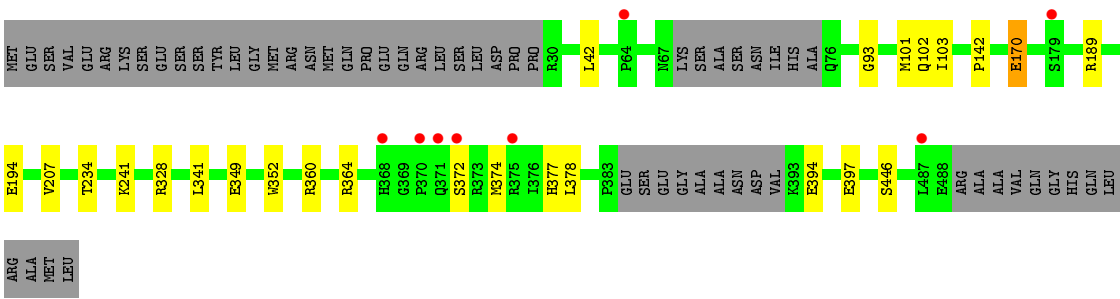
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	310	Total 310	O 310	0	0
6	C	256	Total 256	O 256	0	0
6	D	236	Total 236	O 236	0	0



- Molecule 1: L-ornithine N(5)-monooxygenase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.51Å 154.87Å 90.48Å 90.00° 109.25° 90.00°	Depositor
Resolution (Å)	63.21 – 1.95 63.21 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (63.21-1.95) 99.4 (63.21-1.95)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, $R_{free}$	0.168 , 0.211 0.168 , 0.211	Depositor DCC
$R_{free}$ test set	7476 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: CA, NAP, FAD, ACT

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	0.37	0/3602	0.53	0/4875
1	B	0.38	0/3622	0.55	0/4900
1	C	0.35	0/3612	0.53	0/4891
1	D	0.34	0/3558	0.52	0/4823
All	All	0.36	0/14394	0.53	0/19489

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	3514	0	3461	11	0
1	B	3528	0	3497	10	0
1	C	3518	0	3466	12	0
1	D	3473	0	3391	14	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	53	0	31	1	0
3	C	106	0	62	1	0
3	D	53	0	31	1	0
4	A	48	0	24	0	0
4	B	48	0	23	0	0
4	C	48	0	23	0	0
4	D	48	0	23	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	267	0	0	0	0
6	B	310	0	0	0	0
6	C	256	0	0	1	0
6	D	236	0	0	1	0
All	All	15579	0	14075	47	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 2.

All (47) 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:C:172[B]:ILE:HG12	1:C:187:THR:HB	1.76	0.68
1:A:42:LEU:HD11	1:A:207:VAL:HG23	1.80	0.63
1:C:103:ILE:HD11	1:C:107:LYS:HD2	1.83	0.60
1:C:101[B]:MET:SD	1:C:142:PRO:HD2	2.45	0.56
1:D:101[B]:MET:SD	1:D:142:PRO:HD2	2.46	0.56
1:D:360:ARG:NE	1:D:394:GLU:OE2	2.38	0.56
1:B:245:LYS:HG3	1:B:246:PRO:HD2	1.89	0.55
1:D:378:LEU:HB2	1:D:394:GLU:HG3	1.88	0.54
1:A:103:ILE:HD11	1:A:107:LYS:HD2	1.90	0.53
1:D:170:GLU:OE1	1:D:189:ARG:NH1	2.42	0.52
1:A:65:ARG:NH1	1:A:116:ARG:O	2.37	0.51
1:B:101[B]:MET:SD	1:B:142:PRO:HD2	2.52	0.49
1:C:242:ASP:HB3	1:C:245:LYS:HD2	1.94	0.48
1:D:93:GLY:HA2	1:D:234:THR:HG23	1.96	0.47
1:B:38:GLU:OE2	1:B:78:LYS:NZ	2.27	0.47
1:A:134:PHE:O	1:A:137:LEU:HB2	2.15	0.47
1:B:35:PRO:HD2	1:B:38:GLU:OE1	2.15	0.47
1:A:44:CYS:HB2	1:A:81:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:GLN:HB3	1:D:328:ARG:HH21	1.81	0.46
1:D:42:LEU:HD11	1:D:207:VAL:HG23	1.96	0.46
1:A:101[B]:MET:SD	1:A:142:PRO:HD2	2.55	0.46
1:D:241:LYS:HD2	6:D:924:HOH:O	2.16	0.45
1:C:288:ASP:HB3	6:C:767:HOH:O	2.16	0.45
1:B:102:GLN:HG2	1:B:328:ARG:NE	2.32	0.45
1:D:349[B]:GLU:HG3	1:D:352:TRP:CE3	2.51	0.44
1:C:266:GLN:HG2	1:C:354:HIS:CE1	2.51	0.44
1:A:375:ARG:NH1	1:A:397:GLU:OE1	2.50	0.44
1:C:134:PHE:O	1:C:137:LEU:HB2	2.17	0.44
1:C:173:PRO:HG3	1:C:419:VAL:HG12	2.00	0.44
1:C:407:TYR:CD1	3:C:602[B]:FAD:O4	2.73	0.42
1:A:103:ILE:HG22	3:A:602:FAD:HN3	1.85	0.42
1:A:225:ARG:HG2	1:A:239:LEU:HD11	2.01	0.42
1:B:124:TYR:O	1:B:128:LYS:HG2	2.20	0.42
1:D:349[B]:GLU:HG3	1:D:352:TRP:CZ3	2.54	0.42
1:B:349[A]:GLU:HG3	1:B:352:TRP:CE3	2.55	0.41
1:D:102:GLN:HB3	1:D:328:ARG:NH2	2.36	0.41
1:A:49:PRO:HD2	3:A:602:FAD:O1A	2.20	0.41
1:B:207:VAL:HG22	1:B:452:TRP:HB2	2.02	0.41
1:A:285:PRO:HA	1:A:327:VAL:O	2.21	0.41
1:B:252:LEU:HD22	1:B:362:ILE:HD12	2.03	0.41
1:C:44:CYS:HB2	1:C:81:PHE:CD2	2.55	0.41
1:D:374:MET:O	1:D:397:GLU:HA	2.21	0.41
1:D:364:ARG:HB3	1:D:377:HIS:HB2	2.03	0.41
1:C:436:TYR:CZ	1:C:474:ARG:HD2	2.57	0.40
1:C:96:VAL:HG22	1:C:99:SER:HB3	2.03	0.40
1:B:103:ILE:HG22	3:B:602:FAD:HN3	1.85	0.40
1:D:103:ILE:HG22	3:D:602:FAD:HN3	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	441/501 (88%)	429 (97%)	12 (3%)	0	100	100
1	B	443/501 (88%)	430 (97%)	13 (3%)	0	100	100
1	C	443/501 (88%)	430 (97%)	13 (3%)	0	100	100
1	D	439/501 (88%)	427 (97%)	12 (3%)	0	100	100
All	All	1766/2004 (88%)	1716 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/442 (87%)	379 (99%)	4 (1%)	76	74
1	B	389/442 (88%)	389 (100%)	0	100	100
1	C	384/442 (87%)	382 (100%)	2 (0%)	88	88
1	D	375/442 (85%)	370 (99%)	5 (1%)	69	65
All	All	1531/1768 (87%)	1520 (99%)	11 (1%)	84	82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	65	ARG
1	A	87	GLN
1	A	409	ARG
1	C	30	ARG
1	C	315	SER
1	D	170	GLU
1	D	194	GLU
1	D	341	LEU
1	D	372	SER
1	D	446	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\# Z  > 2$
2	ACT	C	601	-	1,3,3	7.46	1 (100%)	0,3,3	0.00	-
2	ACT	D	601	-	1,3,3	7.03	1 (100%)	0,3,3	0.00	-
4	NAP	D	603	-	45,52,52	4.43	15 (33%)	56,80,80	1.83	8 (14%)
3	FAD	B	602	-	51,58,58	2.19	17 (33%)	60,89,89	1.75	10 (16%)
3	FAD	D	602	-	51,58,58	2.28	18 (35%)	60,89,89	1.77	9 (15%)
4	NAP	B	603	-	45,52,52	4.32	15 (33%)	56,80,80	1.75	5 (8%)
3	FAD	C	602[A]	-	51,58,58	2.19	18 (35%)	60,89,89	1.78	10 (16%)
3	FAD	A	602	-	51,58,58	2.25	19 (37%)	60,89,89	1.87	12 (20%)
3	FAD	C	602[B]	-	51,58,58	2.24	19 (37%)	60,89,89	1.77	11 (18%)
4	NAP	C	603	-	45,52,52	4.33	14 (31%)	56,80,80	1.83	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAP	A	603	-	45,52,52	4.29	14 (31%)	56,80,80	1.94	5 (8%)
2	ACT	A	601	-	1,3,3	8.54	1 (100%)	0,3,3	0.00	-
2	ACT	B	601	-	1,3,3	5.66	1 (100%)	0,3,3	0.00	-

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
4	NAP	D	603	-	-	2/31/67/67	0/5/5/5
3	FAD	B	602	-	-	1/30/50/50	0/6/6/6
3	FAD	D	602	-	-	2/30/50/50	0/6/6/6
4	NAP	B	603	-	-	1/31/67/67	0/5/5/5
3	FAD	C	602[A]	-	-	4/30/50/50	0/6/6/6
3	FAD	A	602	-	-	1/30/50/50	0/6/6/6
3	FAD	C	602[B]	-	-	3/30/50/50	0/6/6/6
4	NAP	C	603	-	-	4/31/67/67	0/5/5/5
4	NAP	A	603	-	-	1/31/67/67	0/5/5/5

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	NAP	O4D-C1D	15.21	1.62	1.41
4	D	603	NAP	C2D-C1D	-15.04	1.30	1.53
4	C	603	NAP	O4D-C1D	14.91	1.61	1.41
4	B	603	NAP	C2D-C1D	-14.82	1.31	1.53
4	D	603	NAP	O4B-C1B	14.70	1.61	1.41
4	A	603	NAP	O4D-C1D	14.61	1.61	1.41
4	B	603	NAP	O4D-C1D	14.55	1.61	1.41
4	A	603	NAP	C2D-C1D	-14.50	1.31	1.53
4	C	603	NAP	C2D-C1D	-14.43	1.31	1.53
4	B	603	NAP	O4B-C1B	14.25	1.61	1.41
4	A	603	NAP	O4B-C1B	14.20	1.60	1.41
4	C	603	NAP	O4B-C1B	14.11	1.60	1.41
2	A	601	ACT	CH3-C	8.54	1.59	1.48
2	C	601	ACT	CH3-C	7.46	1.58	1.48
4	A	603	NAP	C7N-N7N	7.12	1.46	1.33
2	D	601	ACT	CH3-C	7.03	1.57	1.48
4	D	603	NAP	C7N-N7N	6.90	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	NAP	C7N-N7N	6.64	1.45	1.33
4	B	603	NAP	C7N-N7N	6.53	1.45	1.33
4	C	603	NAP	O4B-C4B	-6.28	1.31	1.45
4	D	603	NAP	O4B-C4B	-5.96	1.31	1.45
4	D	603	NAP	O4D-C4D	-5.96	1.31	1.45
4	A	603	NAP	O4B-C4B	-5.81	1.32	1.45
4	B	603	NAP	O4D-C4D	-5.81	1.32	1.45
4	B	603	NAP	O4B-C4B	-5.77	1.32	1.45
4	C	603	NAP	O4D-C4D	-5.76	1.32	1.45
4	A	603	NAP	O4D-C4D	-5.70	1.32	1.45
2	B	601	ACT	CH3-C	5.66	1.56	1.48
3	C	602[B]	FAD	C4X-C10	5.54	1.44	1.38
3	C	602[B]	FAD	C4-C4X	5.53	1.50	1.41
3	A	602	FAD	O4-C4	5.41	1.38	1.24
3	D	602	FAD	C4X-C10	5.28	1.44	1.38
3	A	602	FAD	C4X-C10	5.24	1.44	1.38
3	B	602	FAD	C4-C4X	5.22	1.50	1.41
3	D	602	FAD	O4-C4	5.13	1.37	1.24
3	B	602	FAD	O4-C4	5.08	1.37	1.24
3	D	602	FAD	C9A-N10	5.00	1.45	1.38
3	C	602[A]	FAD	C10-N1	5.00	1.39	1.33
3	B	602	FAD	C4X-C10	4.96	1.43	1.38
3	C	602[A]	FAD	C4X-N5	4.91	1.40	1.33
3	D	602	FAD	C10-N1	4.90	1.39	1.33
3	D	602	FAD	C4-C4X	4.89	1.49	1.41
3	B	602	FAD	C9A-N10	4.83	1.45	1.38
3	C	602[A]	FAD	O4-C4	4.82	1.36	1.24
3	C	602[B]	FAD	O4-C4	4.81	1.36	1.24
3	A	602	FAD	C9A-N10	4.80	1.45	1.38
3	A	602	FAD	C10-N1	4.78	1.39	1.33
3	A	602	FAD	C4X-N5	4.78	1.40	1.33
3	C	602[B]	FAD	C4X-N5	4.78	1.40	1.33
3	C	602[A]	FAD	C9A-N10	4.75	1.44	1.38
3	A	602	FAD	C4-C4X	4.74	1.49	1.41
3	C	602[B]	FAD	C10-N1	4.72	1.39	1.33
3	D	602	FAD	C4X-N5	4.63	1.40	1.33
3	B	602	FAD	C4X-N5	4.63	1.39	1.33
3	C	602[A]	FAD	C4X-C10	4.46	1.43	1.38
3	C	602[A]	FAD	C4-C4X	4.42	1.49	1.41
3	A	602	FAD	C2B-C1B	-3.89	1.47	1.53
3	B	602	FAD	C10-N1	3.63	1.37	1.33
3	D	602	FAD	C4-N3	3.51	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602[B]	FAD	C9A-N10	3.48	1.43	1.38
3	C	602[B]	FAD	C2-N1	3.37	1.44	1.38
3	C	602[A]	FAD	C4-N3	3.34	1.38	1.33
3	A	602	FAD	C4-N3	3.30	1.38	1.33
4	B	603	NAP	O3D-C3D	-3.28	1.35	1.43
4	C	603	NAP	P2B-O2B	3.20	1.65	1.59
4	C	603	NAP	C6A-N6A	3.17	1.45	1.34
4	C	603	NAP	O3D-C3D	-3.17	1.35	1.43
3	D	602	FAD	C2B-C1B	-3.17	1.48	1.53
3	C	602[B]	FAD	C5X-N5	3.15	1.40	1.35
3	D	602	FAD	C5X-N5	3.12	1.40	1.35
4	B	603	NAP	C6A-N6A	3.08	1.45	1.34
3	B	602	FAD	C5X-N5	3.07	1.40	1.35
3	D	602	FAD	C6A-N6A	3.05	1.45	1.34
4	D	603	NAP	C6A-N6A	3.02	1.45	1.34
3	C	602[A]	FAD	C2A-N3A	3.00	1.36	1.32
3	C	602[B]	FAD	C2A-N3A	2.99	1.36	1.32
4	D	603	NAP	O3D-C3D	-2.98	1.36	1.43
3	A	602	FAD	C5X-N5	2.97	1.40	1.35
3	B	602	FAD	C2B-C1B	-2.97	1.49	1.53
4	A	603	NAP	O3D-C3D	-2.97	1.36	1.43
4	C	603	NAP	O2D-C2D	2.95	1.49	1.43
4	D	603	NAP	O3B-C3B	-2.94	1.36	1.43
3	C	602[B]	FAD	C6A-N6A	2.93	1.44	1.34
4	D	603	NAP	P2B-O2B	2.93	1.64	1.59
3	C	602[A]	FAD	C6A-N6A	2.92	1.44	1.34
3	A	602	FAD	C6A-N6A	2.92	1.44	1.34
3	B	602	FAD	C6A-N6A	2.88	1.44	1.34
4	A	603	NAP	P2B-O2B	2.88	1.64	1.59
4	A	603	NAP	C6A-N6A	2.85	1.44	1.34
4	B	603	NAP	C2A-N3A	2.83	1.36	1.32
3	B	602	FAD	C4-N3	2.82	1.37	1.33
4	A	603	NAP	O2D-C2D	2.81	1.49	1.43
4	B	603	NAP	O3B-C3B	-2.79	1.36	1.43
4	C	603	NAP	O7N-C7N	-2.77	1.18	1.24
3	B	602	FAD	C2A-N3A	2.76	1.36	1.32
3	C	602[B]	FAD	C2B-C1B	-2.73	1.49	1.53
3	C	602[A]	FAD	C2B-C1B	-2.73	1.49	1.53
4	D	603	NAP	C5A-C4A	-2.70	1.33	1.40
3	D	602	FAD	C2A-N3A	2.70	1.36	1.32
4	B	603	NAP	C5A-C4A	-2.69	1.33	1.40
3	B	602	FAD	O4'-C4'	-2.66	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602[A]	FAD	C5X-N5	2.65	1.39	1.35
4	B	603	NAP	P2B-O2B	2.64	1.64	1.59
4	D	603	NAP	O7N-C7N	-2.62	1.19	1.24
4	C	603	NAP	O3B-C3B	-2.62	1.36	1.43
4	B	603	NAP	O2D-C2D	2.59	1.49	1.43
4	C	603	NAP	C5A-C4A	-2.59	1.34	1.40
3	C	602[B]	FAD	PA-O5B	-2.57	1.48	1.59
3	C	602[A]	FAD	O4'-C4'	-2.56	1.37	1.43
3	B	602	FAD	O2'-C2'	-2.55	1.37	1.43
4	B	603	NAP	O7N-C7N	-2.54	1.19	1.24
4	A	603	NAP	O3B-C3B	-2.53	1.37	1.43
4	C	603	NAP	C2A-N3A	2.52	1.36	1.32
3	C	602[A]	FAD	PA-O5B	-2.52	1.49	1.59
4	A	603	NAP	C5A-C4A	-2.51	1.34	1.40
4	D	603	NAP	C2A-N3A	2.48	1.36	1.32
3	C	602[A]	FAD	C2-N1	2.47	1.43	1.38
3	C	602[B]	FAD	O4'-C4'	-2.46	1.38	1.43
3	D	602	FAD	O2'-C2'	-2.44	1.38	1.43
4	D	603	NAP	O2D-C2D	2.44	1.48	1.43
4	A	603	NAP	C2A-N3A	2.43	1.36	1.32
3	D	602	FAD	PA-O2A	-2.43	1.43	1.55
3	A	602	FAD	C2A-N3A	2.41	1.36	1.32
3	D	602	FAD	O2B-C2B	-2.40	1.37	1.43
3	D	602	FAD	O4'-C4'	-2.38	1.38	1.43
3	C	602[B]	FAD	PA-O2A	-2.35	1.44	1.55
3	D	602	FAD	C2-N1	2.33	1.42	1.38
3	C	602[A]	FAD	PA-O2A	-2.33	1.44	1.55
3	A	602	FAD	C2-N1	2.32	1.42	1.38
3	C	602[B]	FAD	C4-N3	2.30	1.37	1.33
3	A	602	FAD	O4'-C4'	-2.29	1.38	1.43
4	B	603	NAP	C3N-C7N	2.29	1.54	1.50
4	D	603	NAP	C3N-C7N	2.29	1.54	1.50
3	A	602	FAD	O4B-C4B	-2.28	1.39	1.45
3	A	602	FAD	O2'-C2'	-2.27	1.38	1.43
3	A	602	FAD	PA-O5B	-2.25	1.50	1.59
3	C	602[B]	FAD	O4B-C4B	-2.24	1.40	1.45
3	B	602	FAD	PA-O5B	-2.22	1.50	1.59
4	A	603	NAP	O7N-C7N	-2.21	1.19	1.24
3	C	602[A]	FAD	O4B-C4B	-2.21	1.40	1.45
3	B	602	FAD	P-O1P	2.18	1.58	1.50
3	C	602[B]	FAD	O2'-C2'	-2.18	1.38	1.43
3	A	602	FAD	O2B-C2B	-2.18	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	FAD	PA-O5B	-2.17	1.50	1.59
3	D	602	FAD	P-O1P	2.12	1.58	1.50
3	B	602	FAD	O4B-C4B	-2.10	1.40	1.45
3	A	602	FAD	P-O1P	2.10	1.58	1.50
3	A	602	FAD	PA-O2A	-2.09	1.45	1.55
3	C	602[B]	FAD	P-O1P	2.04	1.58	1.50
3	C	602[A]	FAD	O2'-C2'	-2.04	1.39	1.43
3	C	602[B]	FAD	O3'-C3'	-2.01	1.38	1.43
3	C	602[A]	FAD	P-O1P	2.01	1.58	1.50
3	B	602	FAD	O3'-C3'	-2.01	1.38	1.43

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	NAP	C5A-C6A-N6A	9.26	134.42	120.35
4	C	603	NAP	C5A-C6A-N6A	8.54	133.33	120.35
4	D	603	NAP	C5A-C6A-N6A	8.18	132.79	120.35
4	B	603	NAP	C5A-C6A-N6A	7.87	132.32	120.35
3	A	602	FAD	C4-N3-C2	6.86	120.93	115.14
4	A	603	NAP	N6A-C6A-N1A	-6.53	105.01	118.57
3	D	602	FAD	C4-N3-C2	6.35	120.51	115.14
4	A	603	NAP	N3A-C2A-N1A	-6.03	119.26	128.68
3	A	602	FAD	N3A-C2A-N1A	-5.92	119.42	128.68
3	C	602[A]	FAD	N3A-C2A-N1A	-5.90	119.45	128.68
3	C	602[B]	FAD	N3A-C2A-N1A	-5.90	119.45	128.68
3	C	602[A]	FAD	C4-N3-C2	5.80	120.04	115.14
4	D	603	NAP	N3A-C2A-N1A	-5.75	119.69	128.68
4	C	603	NAP	N6A-C6A-N1A	-5.71	106.73	118.57
4	D	603	NAP	N6A-C6A-N1A	-5.68	106.78	118.57
3	D	602	FAD	N3A-C2A-N1A	-5.60	119.92	128.68
3	B	602	FAD	N3A-C2A-N1A	-5.60	119.93	128.68
4	C	603	NAP	N3A-C2A-N1A	-5.58	119.95	128.68
4	B	603	NAP	N3A-C2A-N1A	-5.57	119.98	128.68
3	B	602	FAD	C4-N3-C2	5.55	119.83	115.14
4	B	603	NAP	N6A-C6A-N1A	-5.50	107.15	118.57
3	C	602[B]	FAD	C4-N3-C2	5.16	119.50	115.14
3	C	602[A]	FAD	C4-C4X-C10	-4.91	116.70	119.95
3	C	602[B]	FAD	C4-C4X-C10	-4.69	116.85	119.95
3	B	602	FAD	C4X-N5-C5X	4.36	121.13	116.77
3	A	602	FAD	C4-C4X-C10	-4.26	117.13	119.95
3	D	602	FAD	C4-C4X-C10	-4.20	117.17	119.95
3	A	602	FAD	C4X-N5-C5X	4.09	120.86	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602[A]	FAD	C4X-N5-C5X	3.96	120.72	116.77
3	B	602	FAD	C4-C4X-C10	-3.92	117.36	119.95
3	B	602	FAD	C4-C4X-N5	3.83	122.97	118.60
3	D	602	FAD	C4X-N5-C5X	3.83	120.59	116.77
3	A	602	FAD	P-O3P-PA	-3.81	119.74	132.83
3	C	602[B]	FAD	C4-C4X-N5	3.80	122.94	118.60
3	C	602[B]	FAD	C4X-N5-C5X	3.79	120.56	116.77
3	D	602	FAD	C4-C4X-N5	3.55	122.65	118.60
3	B	602	FAD	P-O3P-PA	-3.44	121.04	132.83
3	A	602	FAD	C4-C4X-N5	3.33	122.41	118.60
3	C	602[B]	FAD	C5X-C9A-N10	3.23	120.06	117.72
3	C	602[A]	FAD	C4-C4X-N5	3.12	122.16	118.60
3	C	602[A]	FAD	C5X-C9A-N10	2.87	119.79	117.72
4	D	603	NAP	C6N-N1N-C2N	-2.80	119.42	121.97
4	C	603	NAP	C6N-N1N-C2N	-2.78	119.44	121.97
3	D	602	FAD	C1'-N10-C9A	2.78	120.48	118.29
4	B	603	NAP	PN-O3-PA	-2.72	123.48	132.83
4	A	603	NAP	C1B-N9A-C4A	-2.67	121.95	126.64
4	D	603	NAP	C3N-C7N-N7N	2.53	120.79	117.75
3	D	602	FAD	C4A-C5A-N7A	-2.52	106.78	109.40
3	A	602	FAD	C4X-C4-N3	-2.43	120.10	123.43
3	B	602	FAD	C1'-N10-C9A	2.43	120.20	118.29
4	B	603	NAP	C3N-C7N-N7N	2.42	120.65	117.75
3	A	602	FAD	C5X-C9A-N10	2.41	119.46	117.72
4	C	603	NAP	C3N-C7N-N7N	2.38	120.61	117.75
3	B	602	FAD	C10-C4X-N5	-2.38	119.61	121.26
3	A	602	FAD	C1'-N10-C9A	2.36	120.15	118.29
3	A	602	FAD	O2P-P-O5'	-2.30	97.05	107.75
4	A	603	NAP	C2N-C3N-C4N	2.29	120.85	118.26
3	C	602[B]	FAD	C1'-N10-C9A	2.28	120.08	118.29
3	D	602	FAD	C4X-C4-N3	-2.27	120.32	123.43
3	C	602[A]	FAD	C1'-N10-C9A	2.26	120.07	118.29
3	C	602[A]	FAD	C4X-C10-N10	-2.21	118.03	120.30
3	C	602[A]	FAD	O2P-P-O5'	-2.14	97.80	107.75
4	C	603	NAP	C3D-C2D-C1D	2.14	104.20	100.98
4	D	603	NAP	PN-O3-PA	-2.14	125.50	132.83
4	C	603	NAP	C2N-C3N-C4N	2.13	120.68	118.26
4	D	603	NAP	C5B-C4B-C3B	-2.13	107.21	115.18
3	B	602	FAD	C4X-C4-N3	-2.12	120.53	123.43
3	A	602	FAD	C4A-C5A-N7A	-2.10	107.21	109.40
3	A	602	FAD	C2A-N1A-C6A	2.08	122.31	118.75
3	C	602[A]	FAD	O2P-P-O1P	2.05	122.40	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602[B]	FAD	O5B-PA-O1A	2.05	117.08	109.07
3	D	602	FAD	C2A-N1A-C6A	2.04	122.24	118.75
3	B	602	FAD	C1'-N10-C10	2.04	120.23	118.41
4	D	603	NAP	C3D-C2D-C1D	2.03	104.03	100.98
3	C	602[B]	FAD	O2P-P-O5'	-2.02	98.35	107.75
3	C	602[B]	FAD	O2P-P-O1P	2.02	122.22	112.24
3	C	602[B]	FAD	C1'-N10-C10	2.01	120.20	118.41

There are no chirality outliers.

All (19) torsion outliers are listed below:

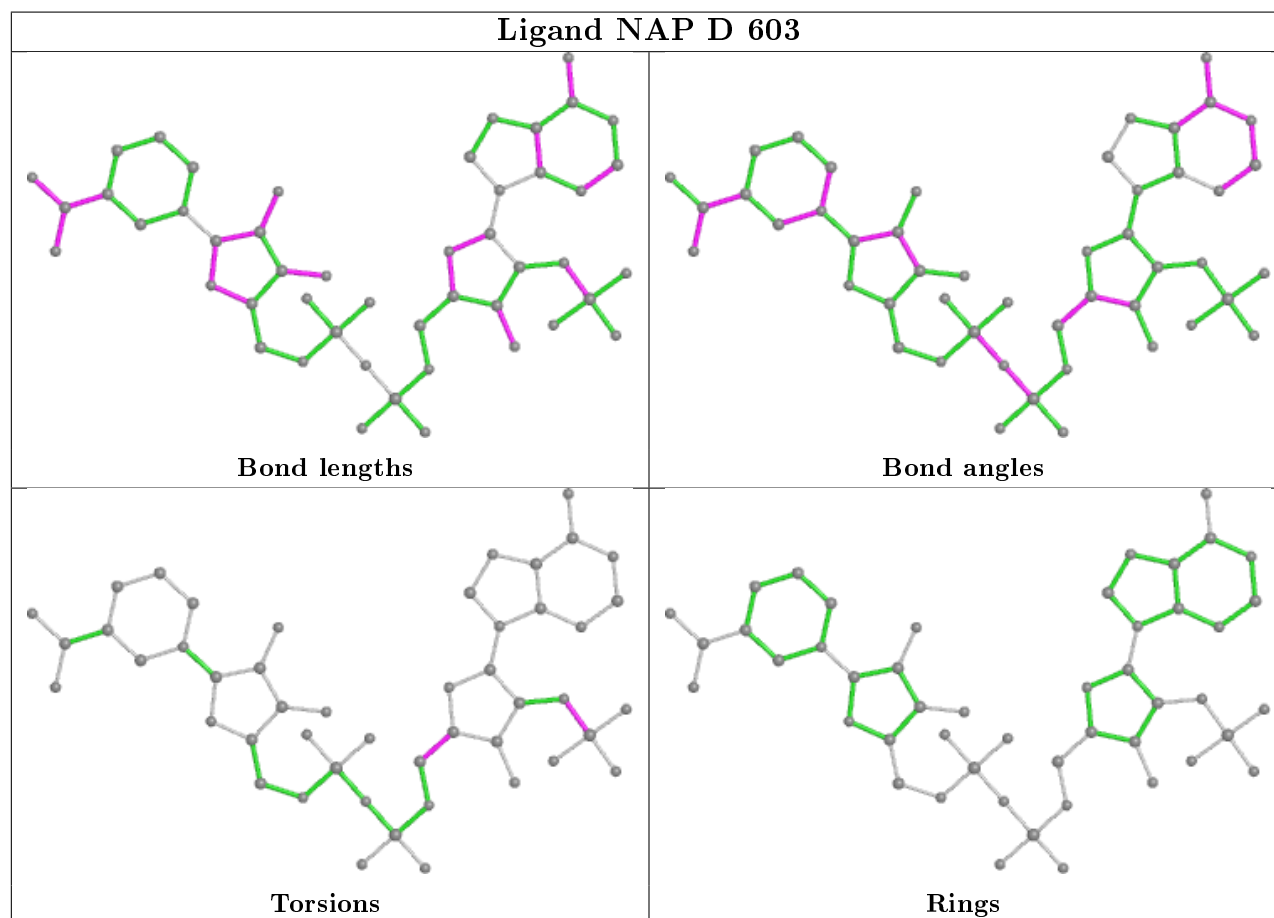
Mol	Chain	Res	Type	Atoms
3	C	602[A]	FAD	PA-O3P-P-O5'
4	C	603	NAP	C2B-O2B-P2B-O3X
3	D	602	FAD	PA-O3P-P-O5'
3	C	602[B]	FAD	PA-O3P-P-O5'
4	C	603	NAP	C2B-O2B-P2B-O1X
4	C	603	NAP	C5D-O5D-PN-O3
3	C	602[B]	FAD	O4B-C4B-C5B-O5B
3	C	602[A]	FAD	C2'-C3'-C4'-C5'
3	A	602	FAD	O4B-C4B-C5B-O5B
3	C	602[A]	FAD	O4B-C4B-C5B-O5B
4	D	603	NAP	C2B-O2B-P2B-O3X
4	D	603	NAP	O4B-C4B-C5B-O5B
3	B	602	FAD	O4B-C4B-C5B-O5B
4	B	603	NAP	O4B-C4B-C5B-O5B
4	C	603	NAP	O4B-C4B-C5B-O5B
4	A	603	NAP	O4B-C4B-C5B-O5B
3	C	602[B]	FAD	C5B-O5B-PA-O1A
3	D	602	FAD	O4B-C4B-C5B-O5B
3	C	602[A]	FAD	O3'-C3'-C4'-C5'

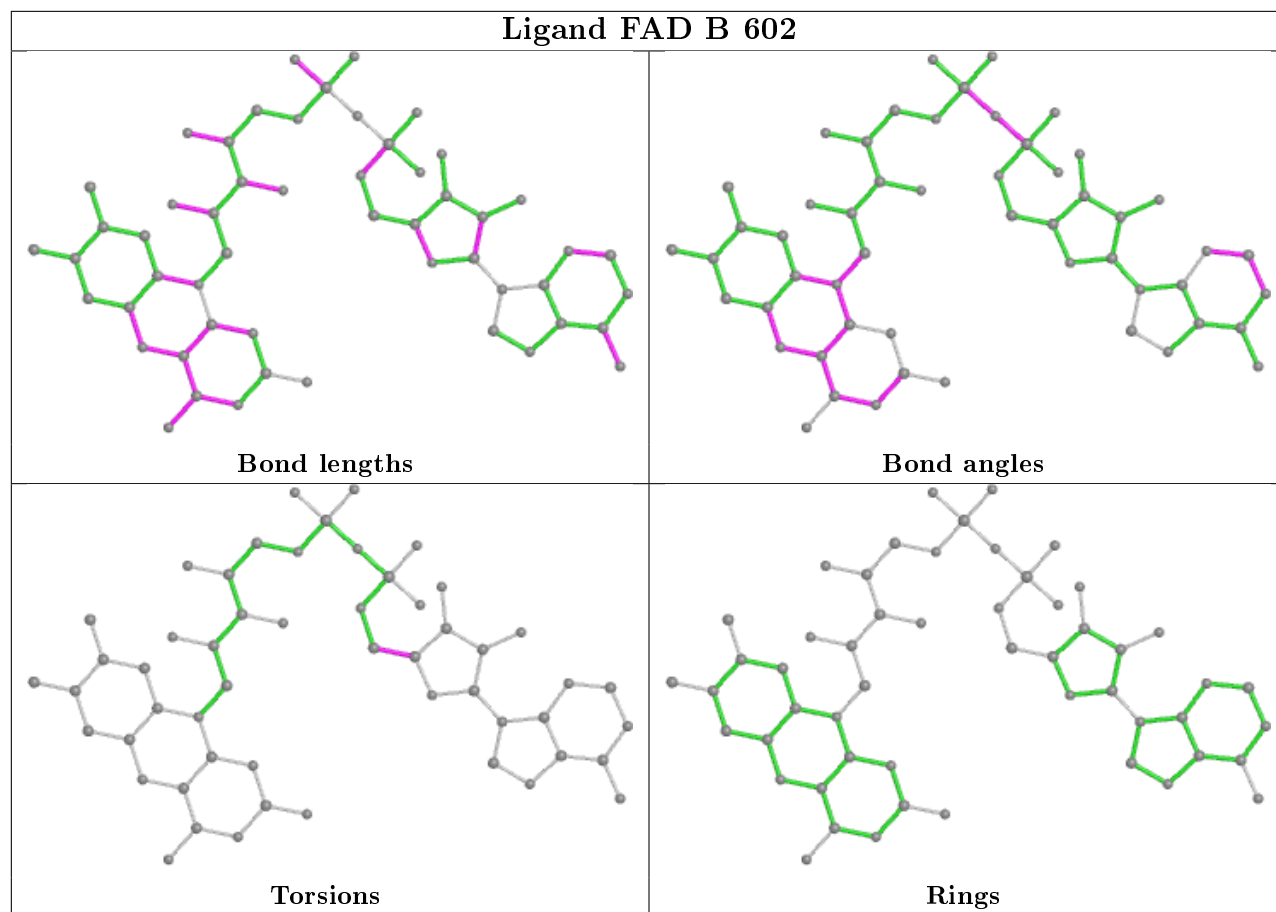
There are no ring outliers.

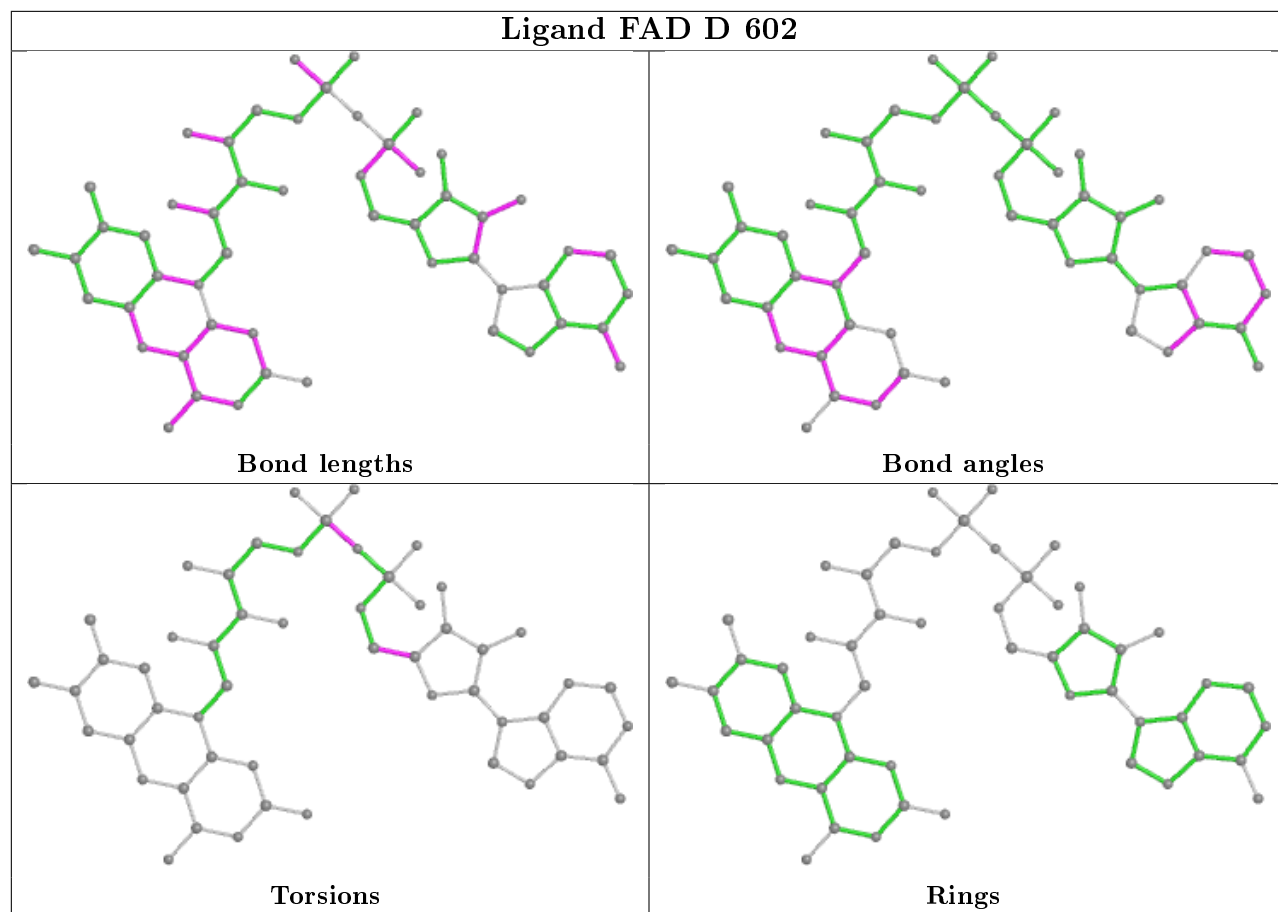
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	FAD	1	0
3	D	602	FAD	1	0
3	A	602	FAD	2	0
3	C	602[B]	FAD	1	0

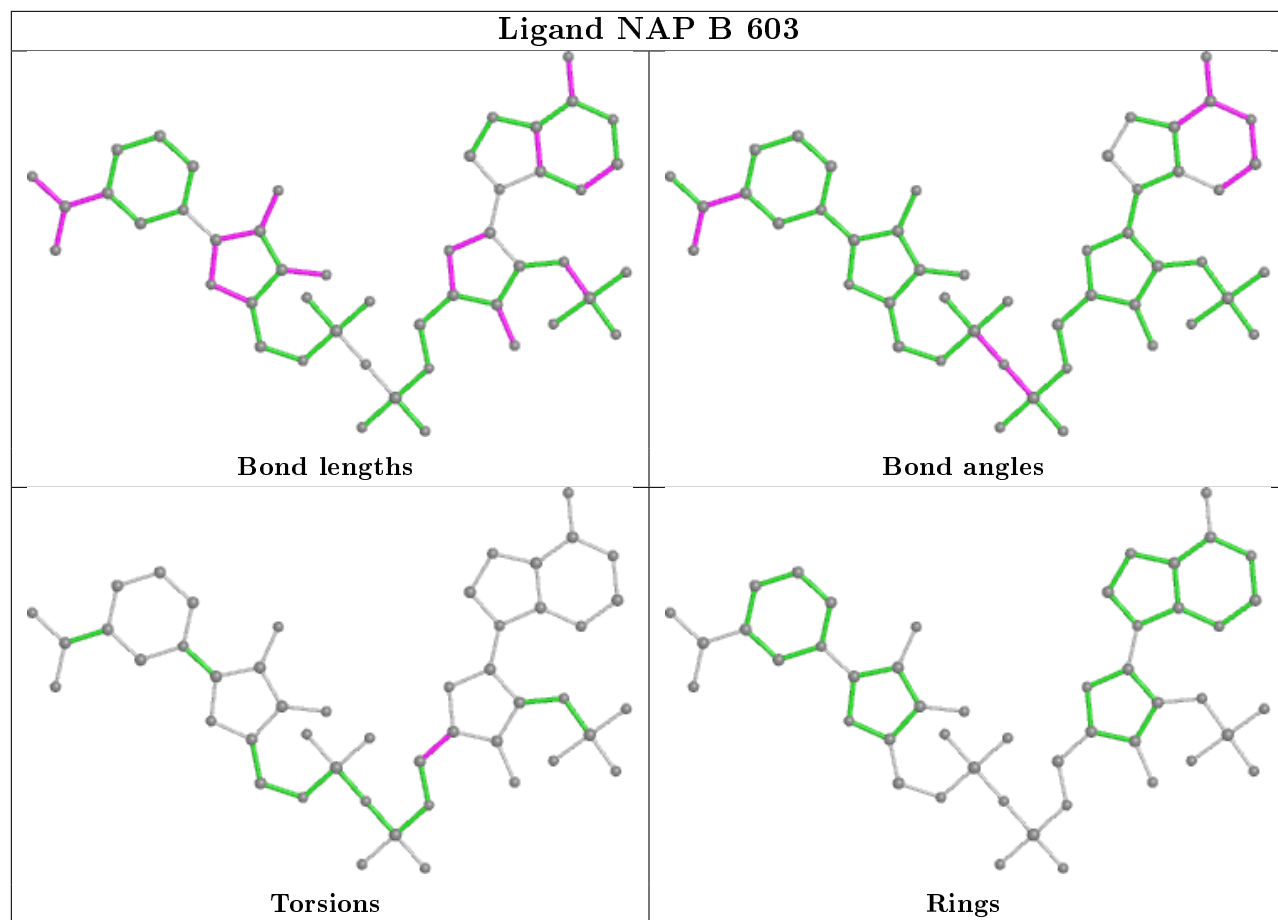
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



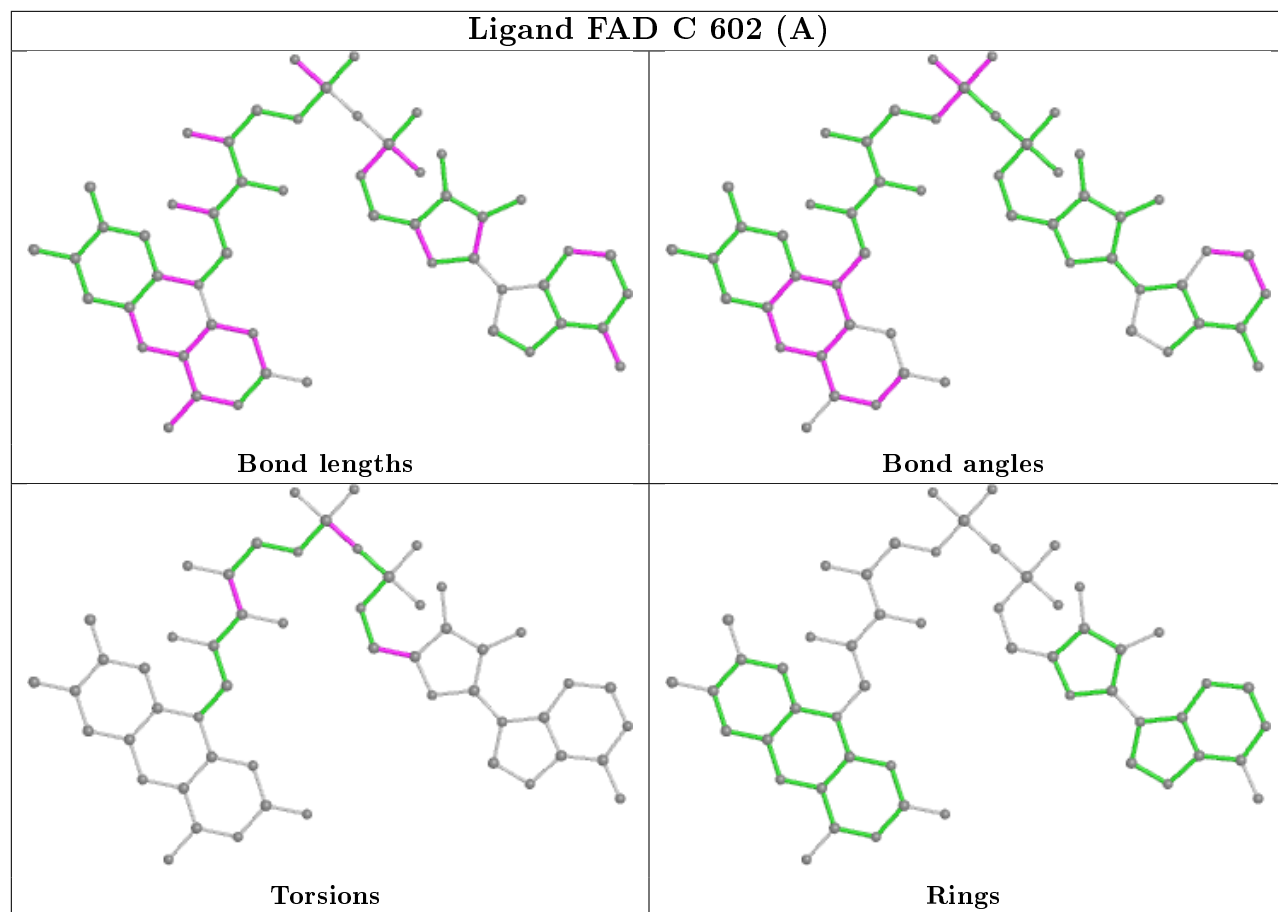


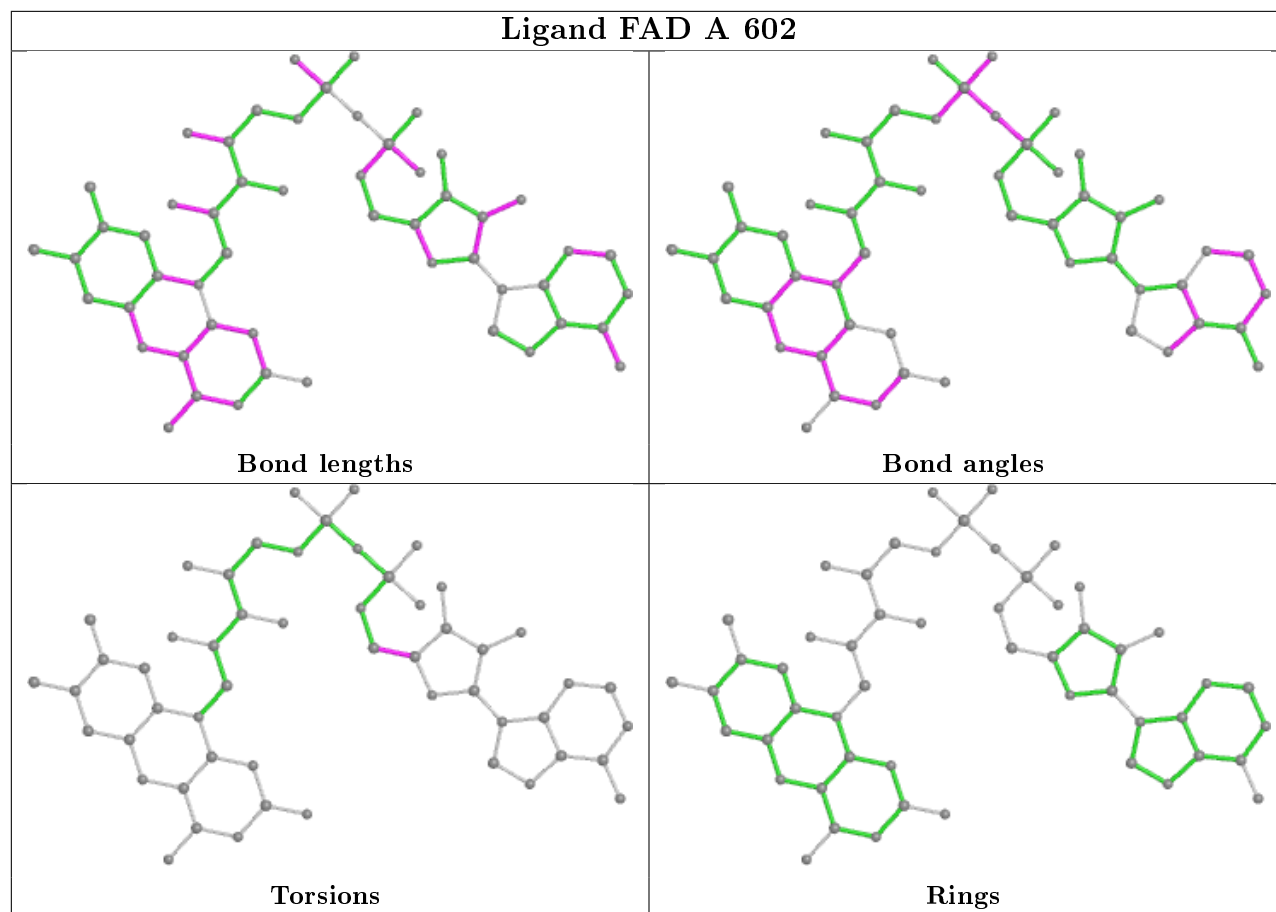




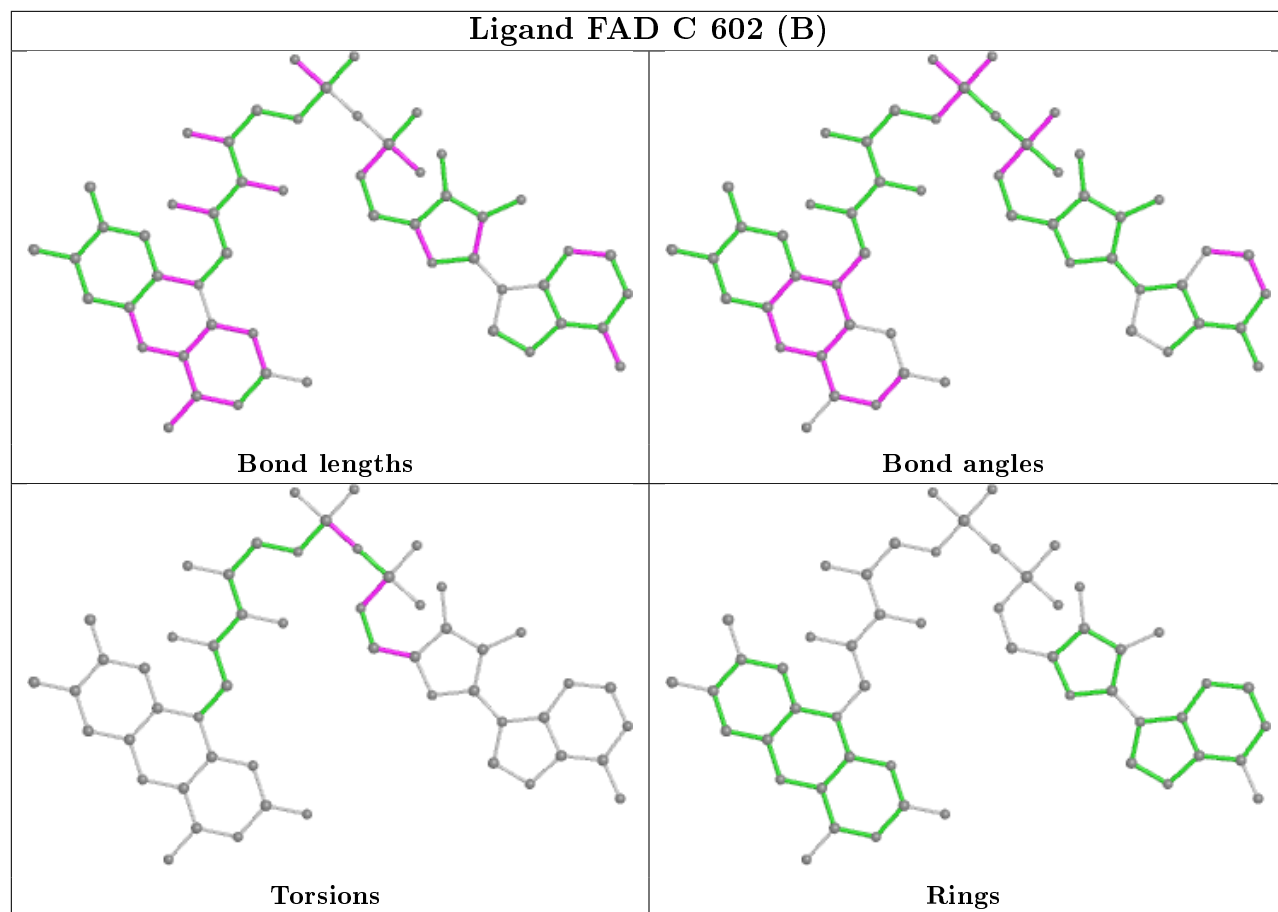


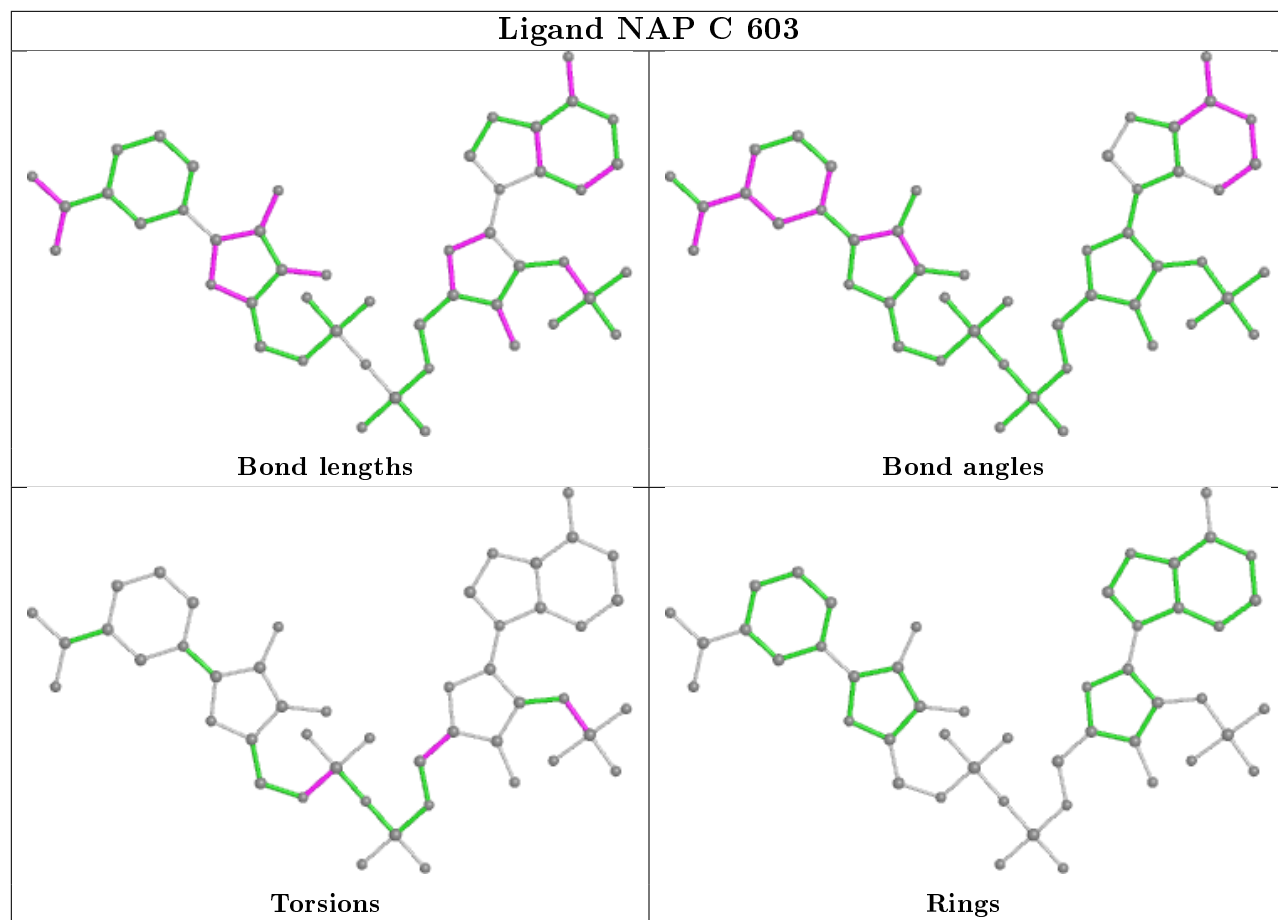
## Ligand FAD C 602 (A)

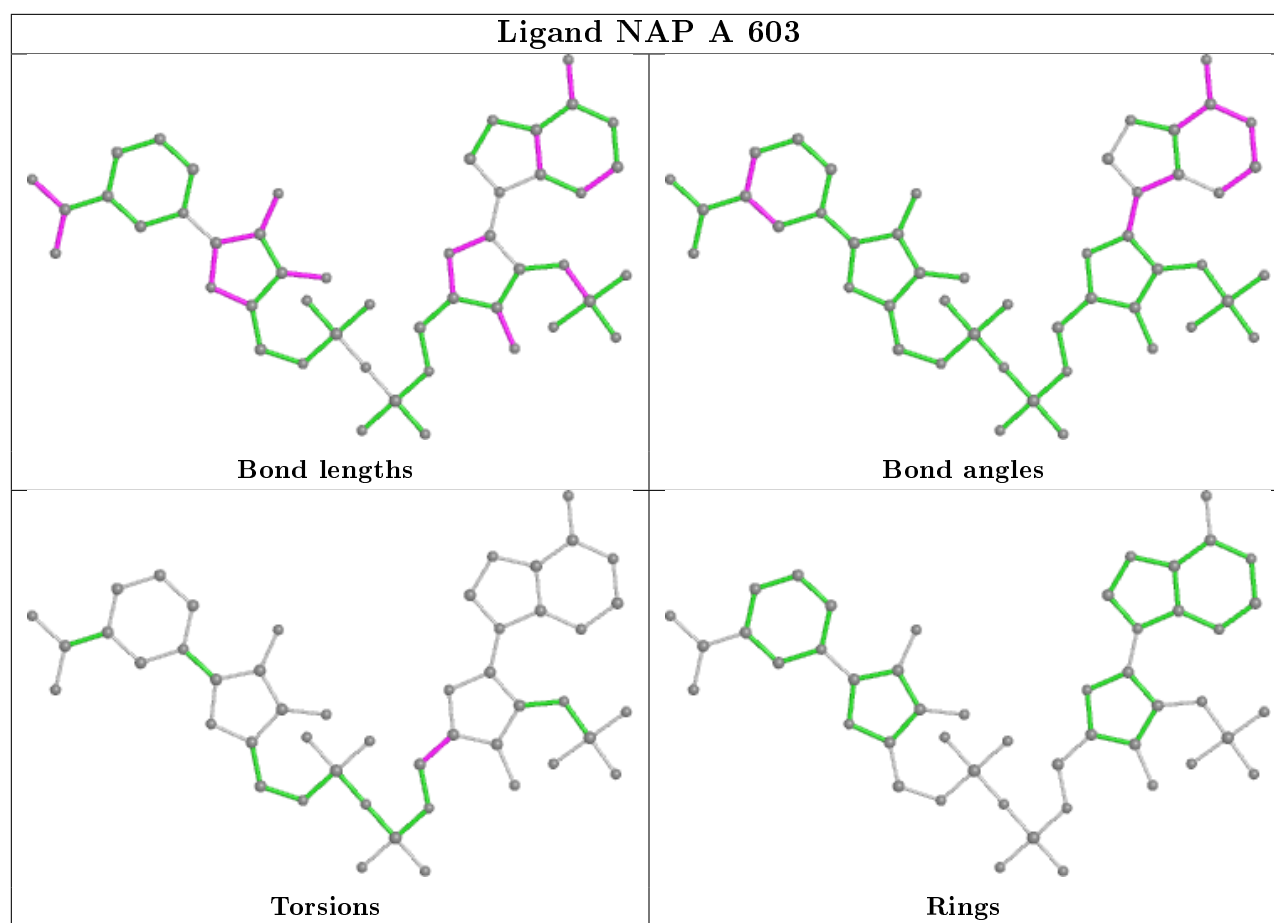




## Ligand FAD C 602 (B)







## 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	A	443/501 (88%)	-0.45	1 (0%) 95 97	14, 26, 48, 75	0
1	B	443/501 (88%)	-0.47	1 (0%) 95 97	13, 24, 45, 69	0
1	C	443/501 (88%)	-0.32	4 (0%) 84 89	15, 29, 55, 76	0
1	D	442/501 (88%)	-0.29	8 (1%) 68 76	17, 31, 57, 78	0
All	All	1771/2004 (88%)	-0.38	14 (0%) 86 90	13, 28, 53, 78	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	179	SER	4.4
1	D	487	LEU	3.3
1	D	64	PRO	3.2
1	C	179	SER	2.9
1	D	368	HIS	2.9
1	D	370	PRO	2.7
1	C	426	GLY	2.6
1	A	178	PRO	2.5
1	D	372	SER	2.5
1	D	375	ARG	2.5
1	C	178	PRO	2.5
1	B	30	ARG	2.4
1	D	371	GLN	2.2
1	C	64	PRO	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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.

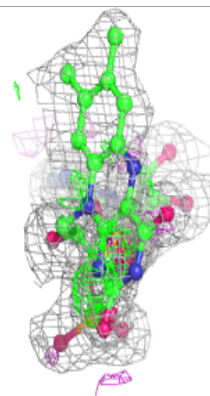
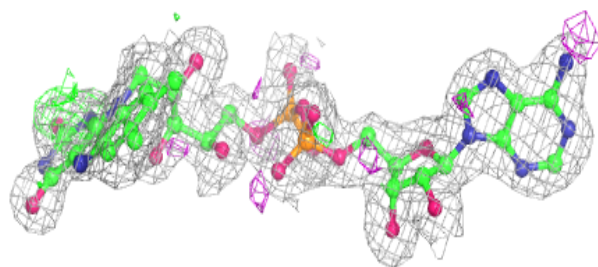
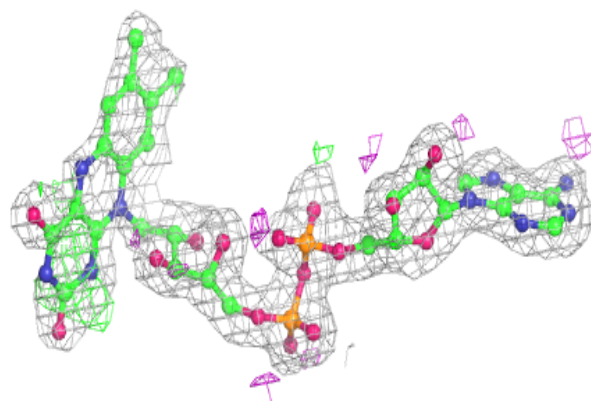
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACT	D	601	4/4	0.93	0.08	20,28,31,37	0
2	ACT	C	601	4/4	0.95	0.13	32,32,36,39	0
3	FAD	C	602[A]	53/53	0.95	0.13	6,21,25,30	53
3	FAD	C	602[B]	53/53	0.95	0.13	13,21,27,45	53
2	ACT	A	601	4/4	0.95	0.11	25,27,30,31	0
3	FAD	D	602	53/53	0.96	0.08	16,26,40,42	0
2	ACT	B	601	4/4	0.96	0.09	24,27,32,45	0
3	FAD	A	602	53/53	0.97	0.09	13,21,38,46	0
5	CA	D	604	1/1	0.97	0.09	52,52,52,52	0
4	NAP	C	603	48/48	0.97	0.09	17,26,36,41	0
5	CA	A	604	1/1	0.97	0.07	42,42,42,42	0
4	NAP	D	603	48/48	0.97	0.09	19,31,42,51	0
3	FAD	B	602	53/53	0.97	0.09	12,19,36,40	0
5	CA	B	604	1/1	0.98	0.09	36,36,36,36	0
4	NAP	A	603	48/48	0.98	0.08	15,24,38,46	0
4	NAP	B	603	48/48	0.98	0.08	13,23,34,41	0
5	CA	C	604	1/1	0.98	0.11	56,56,56,56	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.

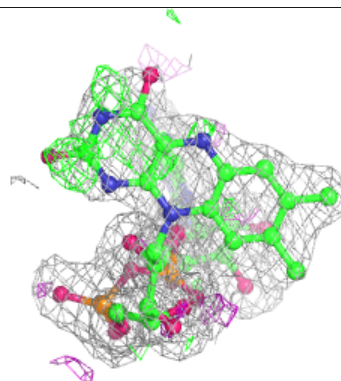
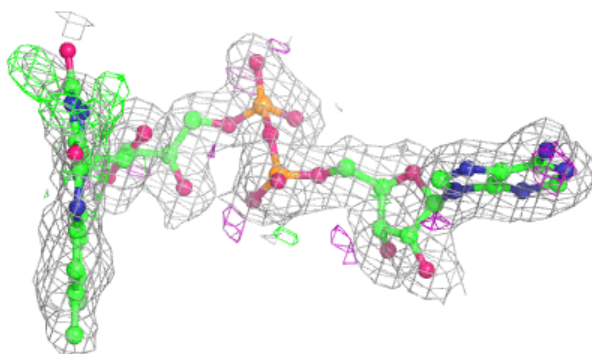
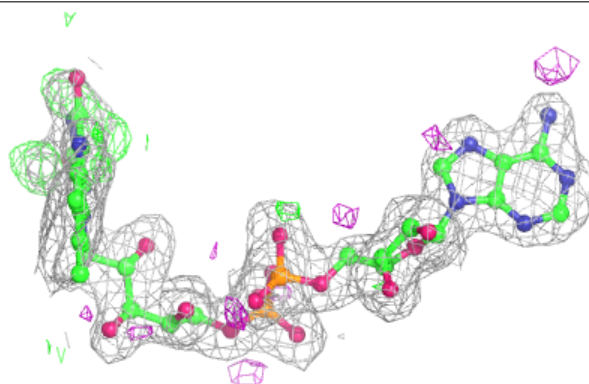


**Electron density around FAD C 602 (A):**

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

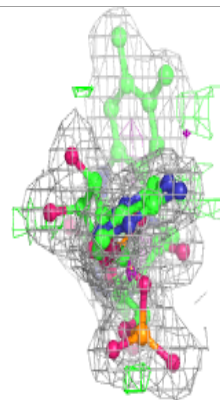
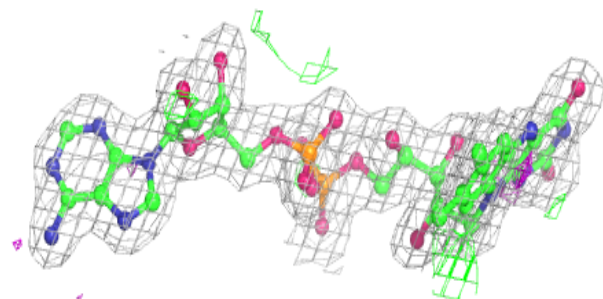
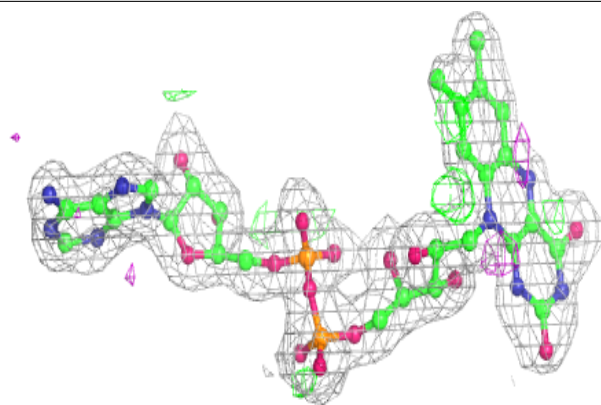
**Electron density around FAD C 602 (B):**

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

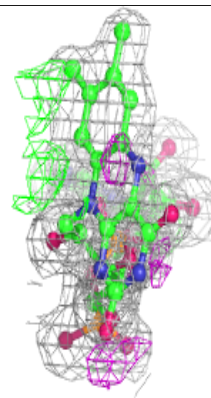
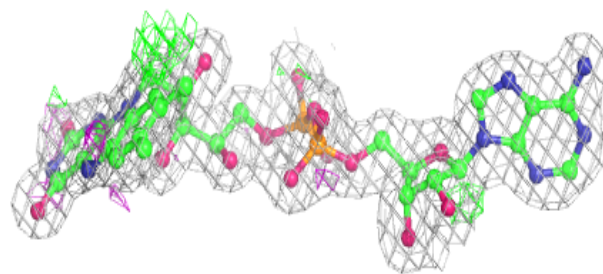
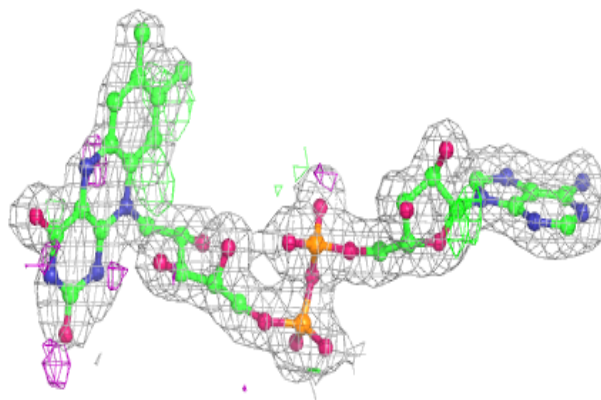


**Electron density around FAD D 602:**

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

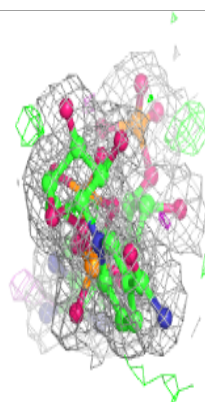
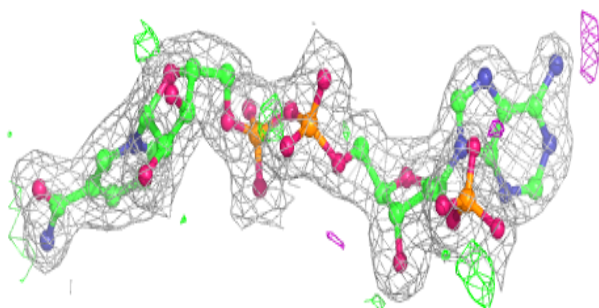
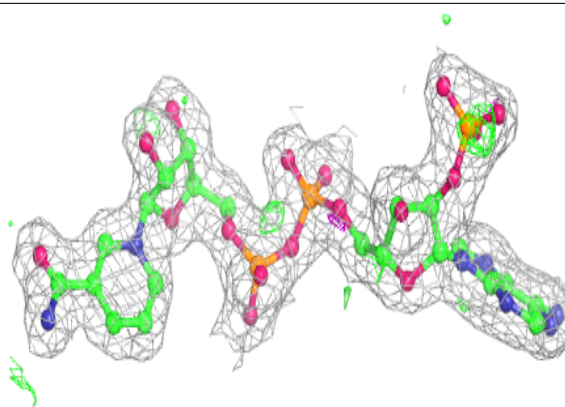
**Electron density around FAD A 602:**

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

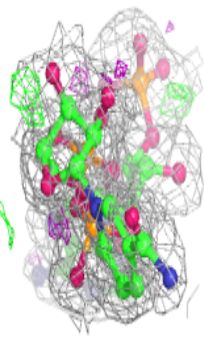
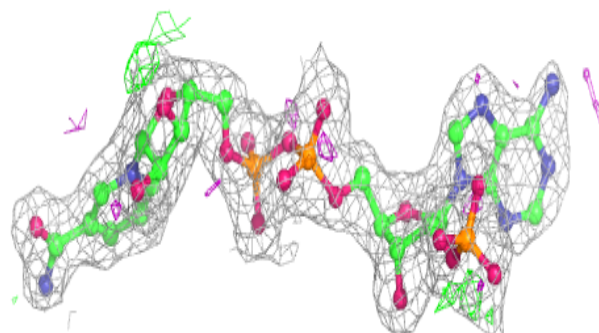
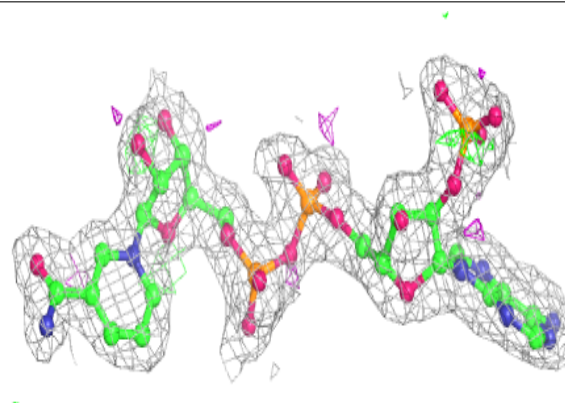


**Electron density around NAP C 603:**

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

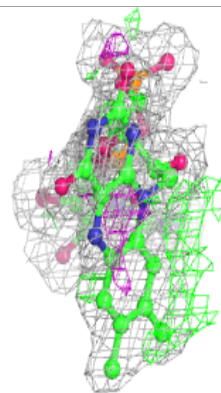
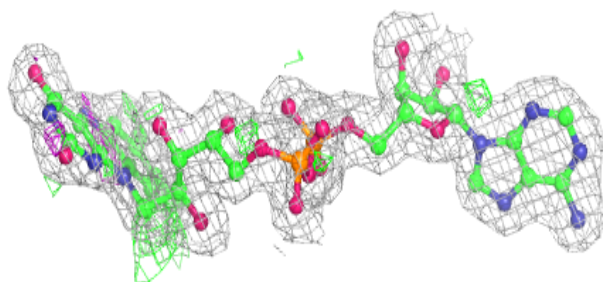
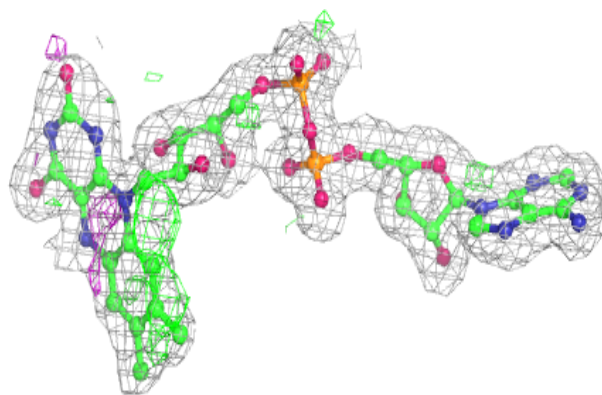
**Electron density around NAP D 603:**

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

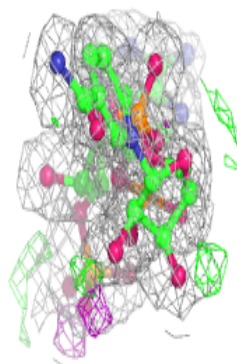
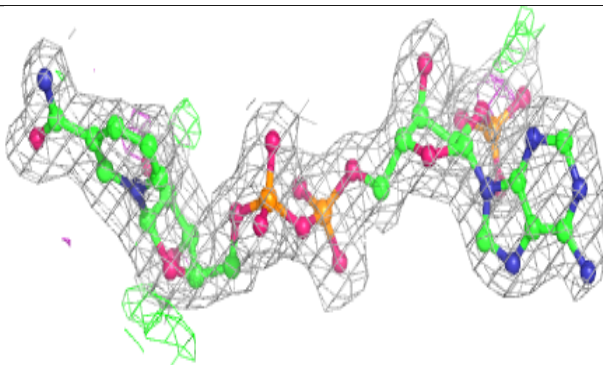
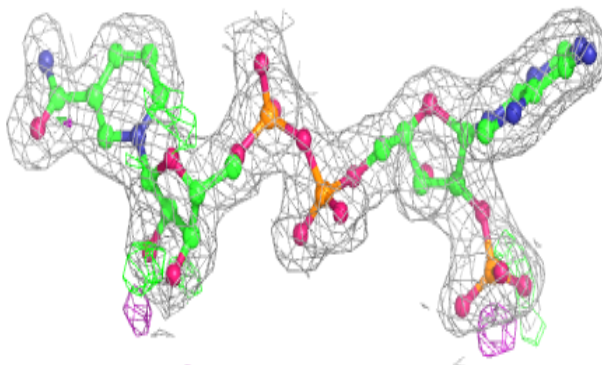


**Electron density around FAD B 602:**

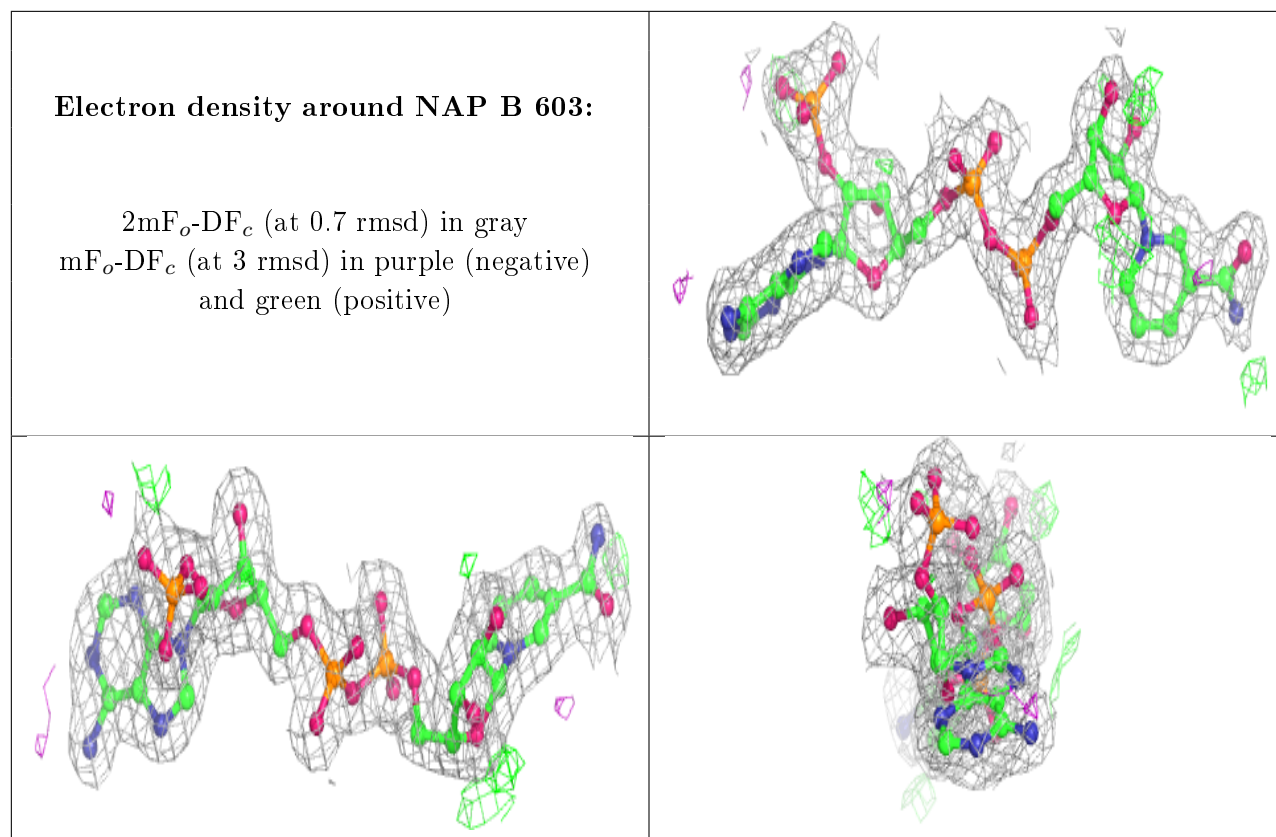
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAP A 603:**

$2mF_o - DF_c$  (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.