Full wwPDB X-ray Structure Validation Report (i)

Mar 14, 2026 – 11:40 AM UTC

PDB ID	:	9FD6 / pdb_00009fd6
Title	:	flavin reductase ThdF in complex with NAD and FAD
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Deposited on	:	2024-05-16
Resolution	:	1.43 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 (i) 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 (i)) were used in the production of this report:

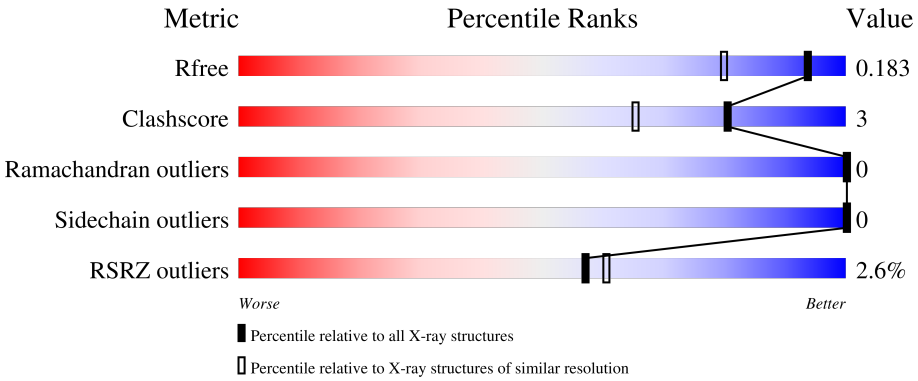
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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}	180053	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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 >=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 <=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	195	80% · 18%
1	B	195	3% 79% · 18%
1	C	195	3% 78% 5% 17%
1	D	195	3% 77% 5% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11750 atoms, of which 5376 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.

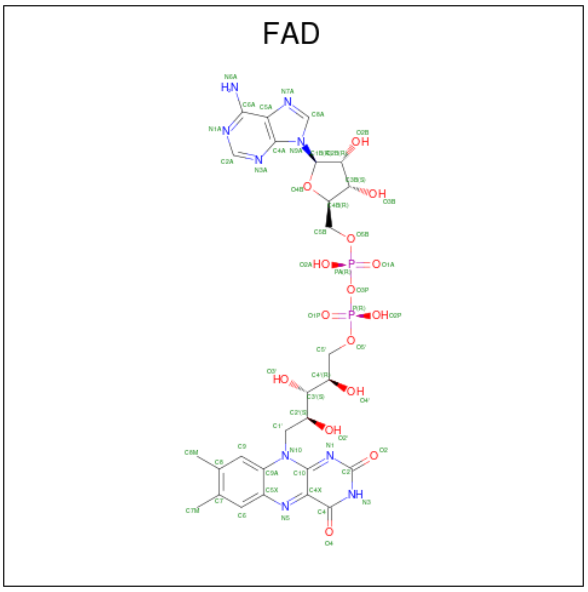
- Molecule 1 is a protein called Flavin reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	160	Total	C	H	N	O	S	0	14	0
			2535	798	1250	230	250	7			
1	C	162	Total	C	H	N	O	S	0	13	0
			2574	809	1280	234	243	8			
1	B	160	Total	C	H	N	O	S	0	11	0
			2532	798	1256	230	241	7			
1	D	160	Total	C	H	N	O	S	0	11	0
			2521	797	1251	225	241	7			

There are 16 discrepancies between the modelled and reference sequences:

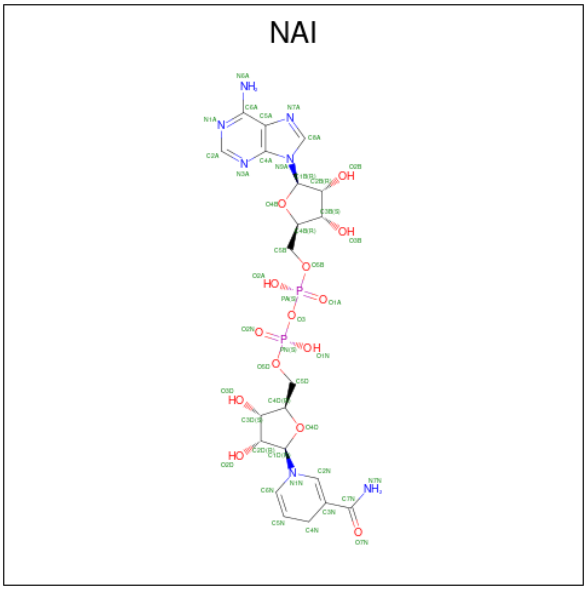
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A1B1V585
A	0	ALA	-	expression tag	UNP A0A1B1V585
A	1	MET	-	expression tag	UNP A0A1B1V585
A	2	ALA	-	expression tag	UNP A0A1B1V585
C	-1	GLY	-	expression tag	UNP A0A1B1V585
C	0	ALA	-	expression tag	UNP A0A1B1V585
C	1	MET	-	expression tag	UNP A0A1B1V585
C	2	ALA	-	expression tag	UNP A0A1B1V585
B	-1	GLY	-	expression tag	UNP A0A1B1V585
B	0	ALA	-	expression tag	UNP A0A1B1V585
B	1	MET	-	expression tag	UNP A0A1B1V585
B	2	ALA	-	expression tag	UNP A0A1B1V585
D	-1	GLY	-	expression tag	UNP A0A1B1V585
D	0	ALA	-	expression tag	UNP A0A1B1V585
D	1	MET	-	expression tag	UNP A0A1B1V585
D	2	ALA	-	expression tag	UNP A0A1B1V585

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	C	1	Total	C	H	N	O	P	0	1
			166	54	60	18	30	4		
2	B	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	D	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	C	1	Total	C	H	N	O	P	0	1
			142	42	54	14	28	4		
3	B	1	Total	C	H	N	O	P	0	1
			142	42	54	14	28	4		
3	D	1	Total	C	H	N	O	P	0	1
			142	42	54	14	28	4		

- Molecule 4 is water.

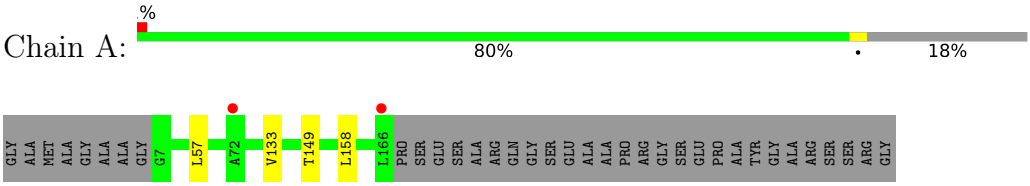
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	6
			178	178		
4	C	157	Total	O	0	4
			161	161		
4	B	173	Total	O	0	2
			175	175		
4	D	156	Total	O	0	6
			162	162		

3 Residue-property plots (i)

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.

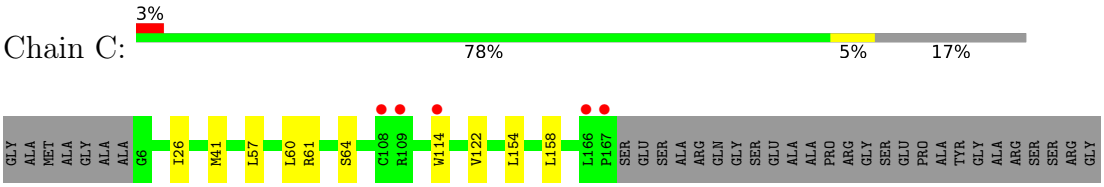
• Molecule 1: Flavin reductase

Chain A:



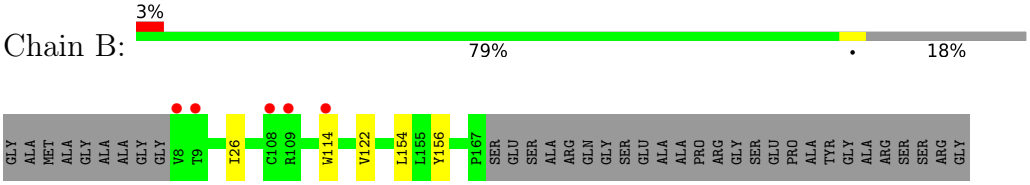
• Molecule 1: Flavin reductase

Chain C:



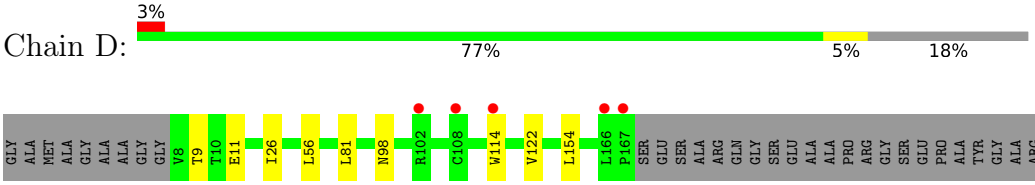
• Molecule 1: Flavin reductase

Chain B:



• Molecule 1: Flavin reductase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	47.76Å 83.48Å 159.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.74 – 1.43 45.74 – 1.43	Depositor EDS
% Data completeness (in resolution range)	80.3 (45.74-1.43) 81.1 (45.74-1.43)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.42Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.146 , 0.182 0.152 , 0.183	Depositor DCC
R_{free} test set	4919 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11750	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FAD, NAI

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	0.23	0/1335	0.45	0/1819
1	B	0.21	0/1316	0.45	0/1794
1	C	0.22	0/1340	0.48	0/1825
1	D	0.22	0/1313	0.45	0/1791
All	All	0.22	0/5304	0.46	0/7229

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	A	1285	1250	1213	5	0
1	B	1276	1256	1235	3	0
1	C	1294	1280	1261	9	0
1	D	1270	1251	1232	9	0
2	A	53	30	31	0	0
2	B	53	30	31	0	0
2	C	106	60	62	3	0
2	D	53	30	31	0	0
3	A	44	27	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	88	54	54	1	0
3	C	88	54	54	2	0
3	D	88	54	54	0	0
4	A	178	0	0	2	0
4	B	175	0	0	1	0
4	C	161	0	0	1	0
4	D	162	0	0	2	0
All	All	6374	5376	5285	29	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 3.

All (29) 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:D:26[B]:ILE:HD11	1:D:154:LEU:HD23	1.30	1.06
1:D:26[B]:ILE:HD12	1:D:81:LEU:HD12	1.48	0.96
1:B:114:TRP:CD1	1:B:122[B]:VAL:HG21	2.10	0.87
1:C:114:TRP:CD1	1:C:122[B]:VAL:HG21	2.16	0.81
1:D:114:TRP:CD1	1:D:122[B]:VAL:HG21	2.20	0.75
1:D:26[B]:ILE:CD1	1:D:81:LEU:HD12	2.17	0.73
1:A:149[B]:THR:HG22	4:A:384:HOH:O	1.91	0.71
1:C:61[A]:ARG:NH2	2:C:201[A]:FAD:O2A	2.27	0.68
4:C:347:HOH:O	1:D:9:THR:HG23	1.97	0.63
1:B:26[B]:ILE:HD11	1:B:156:TYR:HB2	1.81	0.62
1:C:64:SER:HB2	2:C:201[B]:FAD:O2P	1.99	0.61
1:C:41[B]:MET:HE3	2:C:201[B]:FAD:H5'2	1.82	0.61
1:A:149[B]:THR:HG23	4:A:443:HOH:O	2.00	0.60
3:B:202[A]:NAI:N7N	4:B:303:HOH:O	2.28	0.58
1:D:26[B]:ILE:HD11	1:D:154:LEU:CD2	2.22	0.57
1:C:57:LEU:C	1:C:57:LEU:HD12	2.38	0.47
1:C:26[B]:ILE:HD12	1:C:154:LEU:CD2	2.46	0.45
1:A:57:LEU:HD12	1:A:57:LEU:C	2.42	0.45
1:C:158[B]:LEU:HD22	1:C:158[B]:LEU:N	2.32	0.44
1:C:41[B]:MET:SD	1:C:60:LEU:HD22	2.58	0.44
1:D:11[B]:GLU:OE1	4:D:301:HOH:O	2.21	0.44
3:C:202[A]:NAI:O2A	3:C:202[A]:NAI:H3D	2.18	0.44
3:C:202[A]:NAI:H42N	3:C:202[A]:NAI:H2B	2.01	0.43
1:D:56:LEU:C	1:D:56:LEU:HD12	2.44	0.42
1:A:158[A]:LEU:HD22	1:A:158[A]:LEU:N	2.35	0.42
1:C:26[B]:ILE:HD12	1:C:154:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:O	1:A:133:VAL:HG13	2.21	0.41
1:D:98:ASN:HB3	4:D:414:HOH:O	2.21	0.41
1:B:26[B]:ILE:HD12	1:B:154:LEU:CD2	2.51	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/195 (88%)	168 (98%)	4 (2%)	0	100	100
1	B	169/195 (87%)	166 (98%)	3 (2%)	0	100	100
1	C	173/195 (89%)	171 (99%)	2 (1%)	0	100	100
1	D	169/195 (87%)	163 (96%)	6 (4%)	0	100	100
All	All	683/780 (88%)	668 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	142/147 (97%)	142 (100%)	0	100	100
1	B	140/147 (95%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	142/147 (97%)	142 (100%)	0	100	100
1	D	140/147 (95%)	140 (100%)	0	100	100
All	All	564/588 (96%)	564 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	GLN
1	B	98	ASN
1	B	131	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 oligosaccharides 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	C	201[B]	-	58,58,58	1.14	3 (5%)	85,89,89	0.78	3 (3%)
3	NAI	D	202[B]	-	47,48,48	1.02	2 (4%)	64,73,73	0.90	2 (3%)
2	FAD	D	201	-	58,58,58	1.09	2 (3%)	85,89,89	0.90	3 (3%)
3	NAI	C	202[A]	-	47,48,48	1.12	2 (4%)	64,73,73	0.84	2 (3%)
3	NAI	B	202[A]	-	47,48,48	1.02	2 (4%)	64,73,73	0.84	2 (3%)
2	FAD	B	201	-	58,58,58	1.01	2 (3%)	85,89,89	0.90	3 (3%)
3	NAI	D	202[A]	-	47,48,48	1.10	2 (4%)	64,73,73	0.96	3 (4%)
3	NAI	A	202	-	47,48,48	1.00	2 (4%)	64,73,73	0.99	5 (7%)
2	FAD	C	201[A]	-	58,58,58	1.13	2 (3%)	85,89,89	0.86	1 (1%)
2	FAD	A	201	-	58,58,58	1.04	3 (5%)	85,89,89	0.93	2 (2%)
3	NAI	B	202[B]	-	47,48,48	1.09	2 (4%)	64,73,73	0.81	2 (3%)
3	NAI	C	202[B]	-	47,48,48	1.05	2 (4%)	64,73,73	0.92	3 (4%)

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	C	201[B]	-	-	7/34/50/50	0/6/6/6
3	NAI	D	202[B]	-	-	5/29/72/72	0/5/5/5
2	FAD	D	201	-	-	2/34/50/50	0/6/6/6
3	NAI	C	202[A]	-	-	7/29/72/72	0/5/5/5
3	NAI	B	202[A]	-	-	6/29/72/72	0/5/5/5
2	FAD	B	201	-	-	8/34/50/50	0/6/6/6
3	NAI	D	202[A]	-	-	5/29/72/72	0/5/5/5
3	NAI	A	202	-	-	5/29/72/72	0/5/5/5
2	FAD	C	201[A]	-	-	9/34/50/50	0/6/6/6
2	FAD	A	201	-	-	8/34/50/50	0/6/6/6
3	NAI	B	202[B]	-	-	3/29/72/72	0/5/5/5
3	NAI	C	202[B]	-	-	7/29/72/72	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201[A]	FAD	P-O3P	5.78	1.65	1.59
2	C	201[B]	FAD	P-O3P	5.44	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	FAD	P-O3P	5.01	1.64	1.59
3	C	202[A]	NAI	PN-O3	4.83	1.64	1.59
3	D	202[A]	NAI	PN-O3	4.80	1.64	1.59
3	B	202[B]	NAI	PN-O3	4.62	1.64	1.59
2	A	201	FAD	P-O3P	4.55	1.64	1.59
3	C	202[B]	NAI	PN-O3	4.51	1.64	1.59
3	D	202[B]	NAI	PN-O3	4.24	1.64	1.59
2	B	201	FAD	P-O3P	4.13	1.64	1.59
3	A	202	NAI	PN-O3	4.08	1.63	1.59
3	B	202[A]	NAI	PN-O3	4.08	1.63	1.59
3	C	202[A]	NAI	PA-O3	3.74	1.63	1.59
3	B	202[B]	NAI	PA-O3	3.68	1.63	1.59
3	D	202[A]	NAI	PA-O3	3.61	1.63	1.59
2	D	201	FAD	PA-O3P	3.53	1.63	1.59
2	C	201[B]	FAD	PA-O3P	3.51	1.63	1.59
3	A	202	NAI	PA-O3	3.26	1.63	1.59
3	C	202[B]	NAI	PA-O3	3.14	1.62	1.59
2	C	201[A]	FAD	PA-O3P	3.14	1.62	1.59
3	B	202[A]	NAI	PA-O3	3.05	1.62	1.59
2	B	201	FAD	PA-O3P	2.68	1.62	1.59
3	D	202[B]	NAI	PA-O3	2.60	1.62	1.59
2	A	201	FAD	C1'-C2'	2.38	1.56	1.52
2	A	201	FAD	PA-O3P	2.19	1.61	1.59
2	C	201[B]	FAD	C5X-N5	-2.04	1.35	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	202[B]	NAI	C2B-C3B-C4B	-3.29	96.26	102.61
3	B	202[A]	NAI	C2B-C3B-C4B	-2.86	97.08	102.61
3	D	202[A]	NAI	C3D-C2D-C1D	2.83	106.81	101.46
3	C	202[B]	NAI	C2B-C3B-C4B	-2.78	97.24	102.61
3	B	202[B]	NAI	C3B-C2B-C1B	2.64	106.46	101.46
2	D	201	FAD	O2P-P-O3P	-2.61	100.21	107.27
3	A	202	NAI	C2B-C3B-C4B	-2.52	97.75	102.61
3	A	202	NAI	O4D-C1D-N1N	2.50	112.85	108.08
3	D	202[A]	NAI	C3B-C2B-C1B	2.50	106.18	101.46
2	C	201[A]	FAD	C3B-C2B-C1B	2.49	106.18	101.46
3	C	202[A]	NAI	C3B-C2B-C1B	2.49	106.17	101.46
2	D	201	FAD	O2P-P-O1P	2.48	123.96	112.44
2	C	201[B]	FAD	O2P-P-O1P	2.47	123.93	112.44
3	D	202[B]	NAI	O1N-PN-O2N	2.40	123.59	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	202	NAI	O3-PN-O2N	-2.36	103.61	110.70
2	C	201[B]	FAD	O2P-P-O3P	-2.32	101.01	107.27
3	D	202[A]	NAI	O1N-PN-O2N	2.30	123.14	112.44
2	A	201	FAD	C9A-C5X-N5	-2.27	120.05	122.45
2	B	201	FAD	O2A-PA-O1A	2.24	122.85	112.44
3	A	202	NAI	O1N-PN-O2N	2.22	122.76	112.44
3	C	202[A]	NAI	O1N-PN-O2N	2.17	122.53	112.44
3	B	202[B]	NAI	O1N-PN-O2N	2.14	122.39	112.44
2	A	201	FAD	O2P-P-O1P	2.10	122.23	112.44
2	B	201	FAD	O2P-P-O3P	-2.09	101.64	107.27
2	B	201	FAD	O2P-P-O1P	2.08	122.10	112.44
3	C	202[B]	NAI	O2A-PA-O1A	2.05	122.00	112.44
3	C	202[B]	NAI	O1N-PN-O2N	2.05	122.00	112.44
3	B	202[A]	NAI	O2A-PA-O1A	2.04	121.93	112.44
3	A	202	NAI	C6N-N1N-C2N	-2.03	117.15	119.32
2	D	201	FAD	C2B-C3B-C4B	-2.01	98.73	102.61
2	C	201[B]	FAD	O4-C4-N3	2.00	123.88	120.11

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201[A]	FAD	C5B-O5B-PA-O1A
2	C	201[A]	FAD	C5B-O5B-PA-O3P
2	C	201[A]	FAD	C5'-O5'-P-O3P
2	C	201[B]	FAD	O4B-C4B-C5B-O5B
2	C	201[B]	FAD	C5'-O5'-P-O2P
2	C	201[B]	FAD	C5'-O5'-P-O3P
3	C	202[A]	NAI	C5D-O5D-PN-O2N
3	C	202[B]	NAI	C5B-O5B-PA-O1A
3	C	202[B]	NAI	C5B-O5B-PA-O3
3	C	202[B]	NAI	O4D-C1D-N1N-C2N
3	B	202[A]	NAI	C5D-O5D-PN-O2N
3	B	202[A]	NAI	O4D-C1D-N1N-C2N
3	D	202[B]	NAI	C5B-O5B-PA-O1A
3	D	202[B]	NAI	C5D-O5D-PN-O2N
3	A	202	NAI	O4D-C1D-N1N-C2N
3	C	202[A]	NAI	O4D-C1D-N1N-C2N
3	B	202[B]	NAI	O4D-C1D-N1N-C2N
3	D	202[A]	NAI	O4D-C1D-N1N-C2N
3	D	202[B]	NAI	O4D-C1D-N1N-C2N
2	C	201[B]	FAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	A	201	FAD	C2'-C3'-C4'-O4'
2	B	201	FAD	C2B-C1B-N9A-C8A
2	B	201	FAD	P-O3P-PA-O1A
3	C	202[A]	NAI	PA-O3-PN-O2N
3	B	202[A]	NAI	PN-O3-PA-O1A
2	A	201	FAD	O3'-C3'-C4'-O4'
2	C	201[A]	FAD	C2'-C3'-C4'-O4'
2	A	201	FAD	C2'-C3'-C4'-C5'
2	A	201	FAD	P-O3P-PA-O5B
2	C	201[A]	FAD	P-O3P-PA-O5B
2	B	201	FAD	P-O3P-PA-O5B
2	D	201	FAD	P-O3P-PA-O5B
3	A	202	NAI	PN-O3-PA-O5B
3	A	202	NAI	PA-O3-PN-O5D
3	C	202[A]	NAI	PN-O3-PA-O5B
3	C	202[B]	NAI	PN-O3-PA-O5B
3	B	202[A]	NAI	PA-O3-PN-O5D
3	B	202[B]	NAI	PN-O3-PA-O5B
3	B	202[B]	NAI	PA-O3-PN-O5D
3	D	202[A]	NAI	PA-O3-PN-O5D
3	D	202[B]	NAI	PN-O3-PA-O5B
2	C	201[A]	FAD	C2'-C3'-C4'-C5'
2	A	201	FAD	P-O3P-PA-O1A
2	B	201	FAD	PA-O3P-P-O1P
2	C	201[A]	FAD	O3'-C3'-C4'-O4'
2	B	201	FAD	C2B-C1B-N9A-C4A
3	D	202[A]	NAI	O4D-C4D-C5D-O5D
2	C	201[A]	FAD	C5B-O5B-PA-O2A
2	C	201[B]	FAD	C5'-O5'-P-O1P
2	B	201	FAD	C5B-O5B-PA-O2A
3	C	202[A]	NAI	C5D-O5D-PN-O3
3	C	202[A]	NAI	C5D-O5D-PN-O1N
3	C	202[B]	NAI	C5B-O5B-PA-O2A
2	C	201[B]	FAD	C2B-C1B-N9A-C8A
2	A	201	FAD	PA-O3P-P-O1P
3	D	202[B]	NAI	PN-O3-PA-O1A
3	D	202[A]	NAI	C3D-C4D-C5D-O5D
3	A	202	NAI	C2N-C3N-C7N-N7N
3	C	202[B]	NAI	C2N-C3N-C7N-N7N
3	B	202[A]	NAI	C2N-C3N-C7N-N7N
3	C	202[A]	NAI	PA-O3-PN-O5D
3	B	202[A]	NAI	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
2	A	201	FAD	O3'-C3'-C4'-C5'
2	C	201[B]	FAD	O4B-C1B-N9A-C8A
2	C	201[A]	FAD	PA-O3P-P-O1P
2	B	201	FAD	PA-O3P-P-O2P
2	D	201	FAD	P-O3P-PA-O2A
3	A	202	NAI	PN-O3-PA-O1A
3	D	202[A]	NAI	PA-O3-PN-O2N
2	B	201	FAD	O4B-C1B-N9A-C8A
2	A	201	FAD	PA-O3P-P-O2P
3	C	202[B]	NAI	PN-O3-PA-O2A

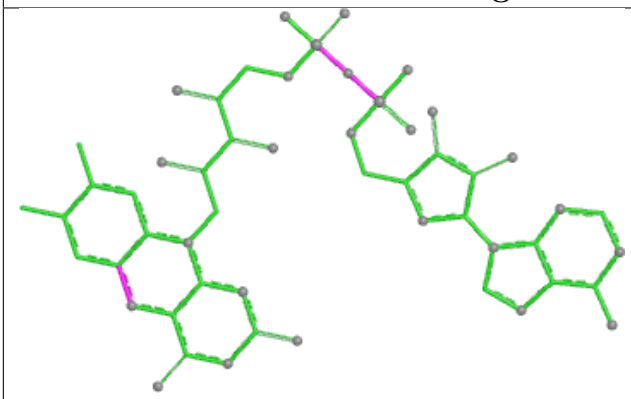
There are no ring outliers.

4 monomers are involved in 6 short contacts:

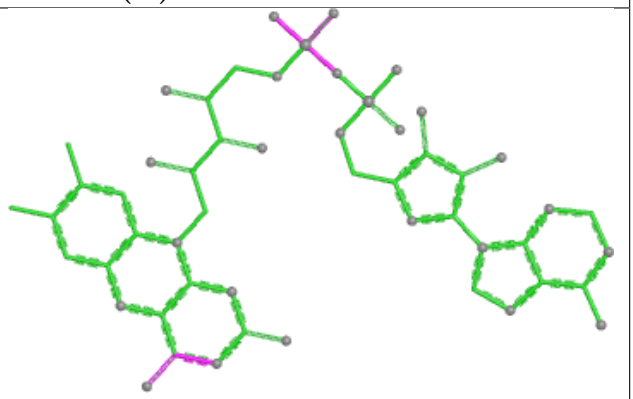
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201[B]	FAD	2	0
3	C	202[A]	NAI	2	0
3	B	202[A]	NAI	1	0
2	C	201[A]	FAD	1	0

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 then 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.

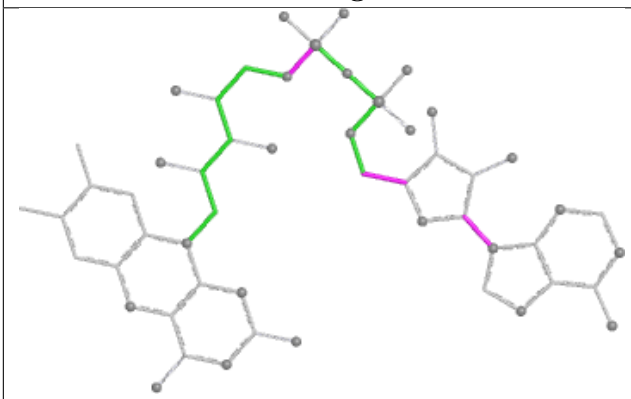
Ligand FAD C 201 (B)



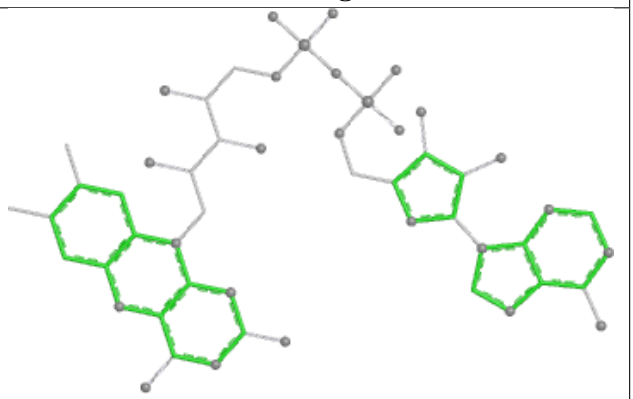
Bond lengths



Bond angles

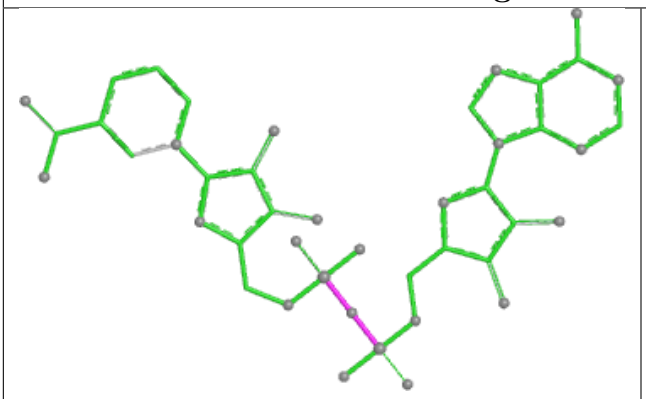


Torsions



Rings

Ligand NAI D 202 (B)



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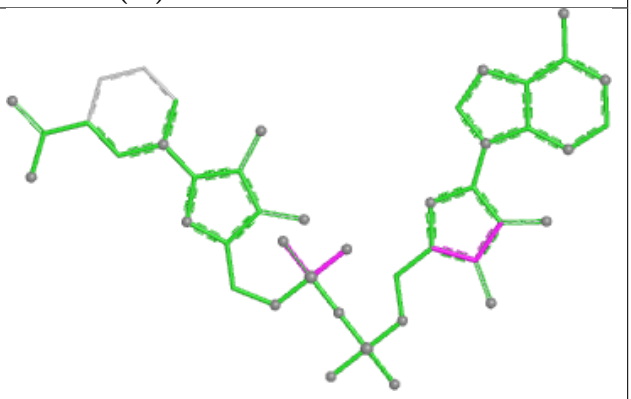

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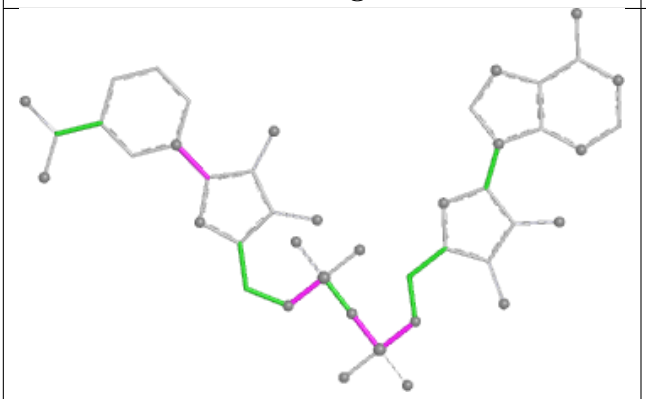

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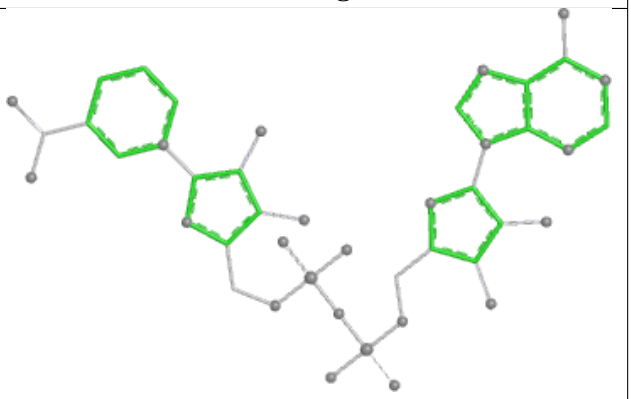

Rings

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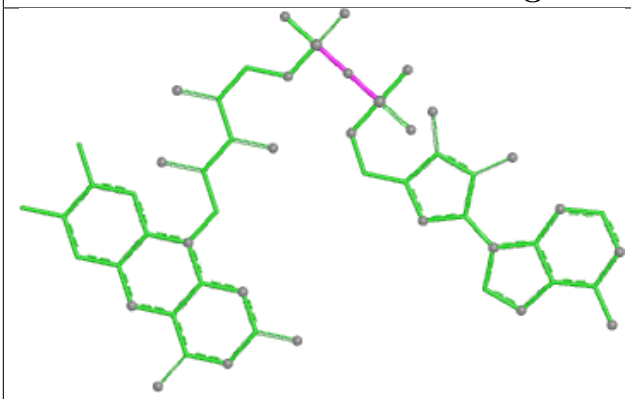

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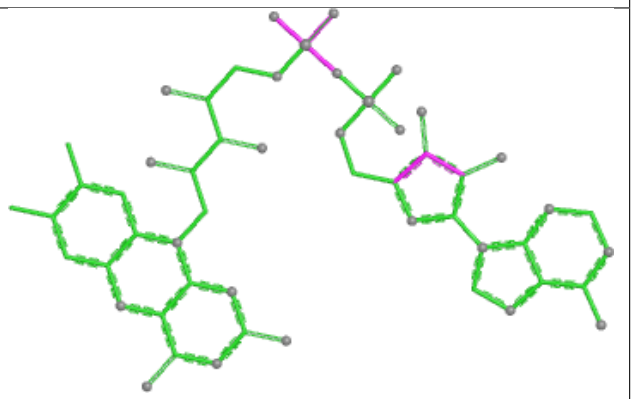

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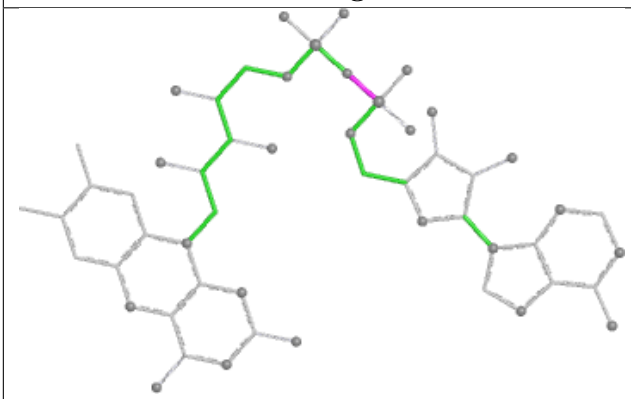

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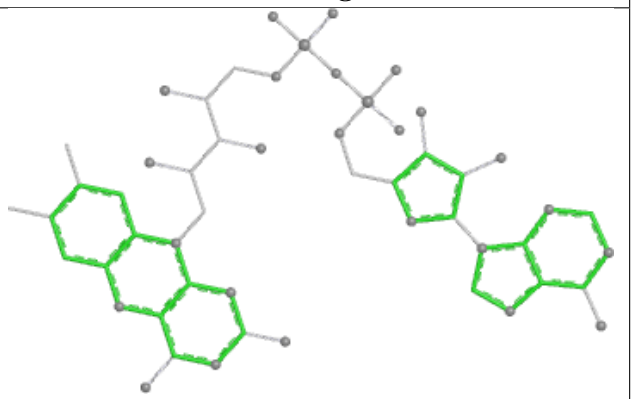
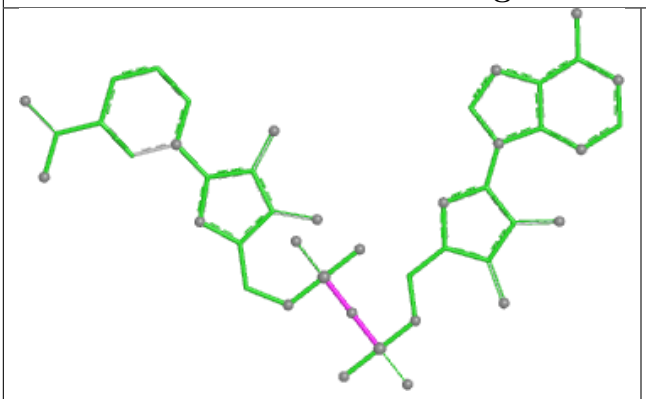


Rings

Ligand NAI C 202 (A)



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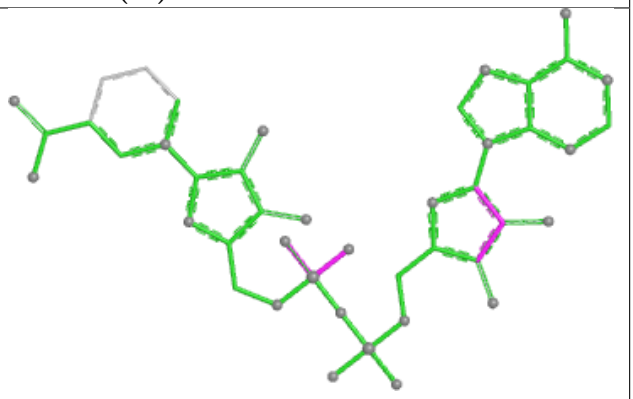

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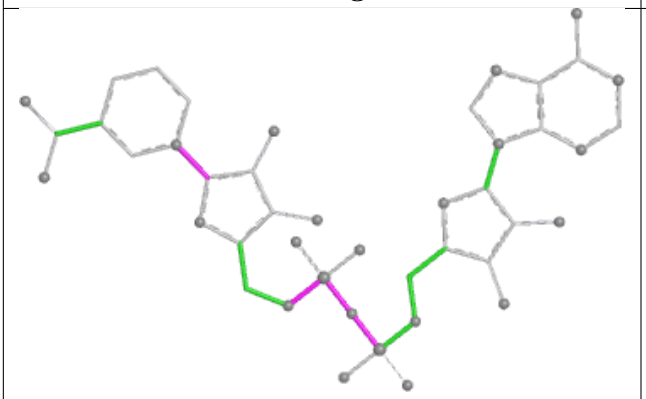

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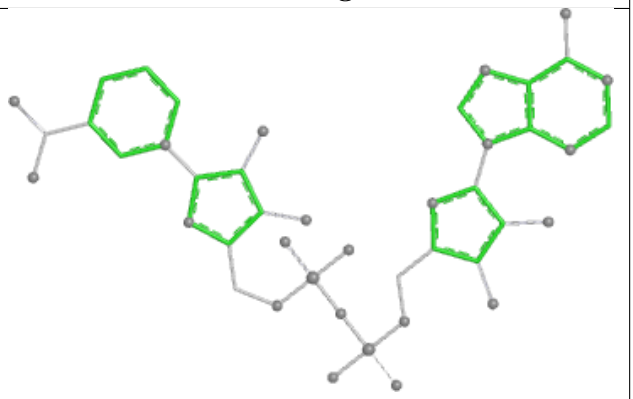
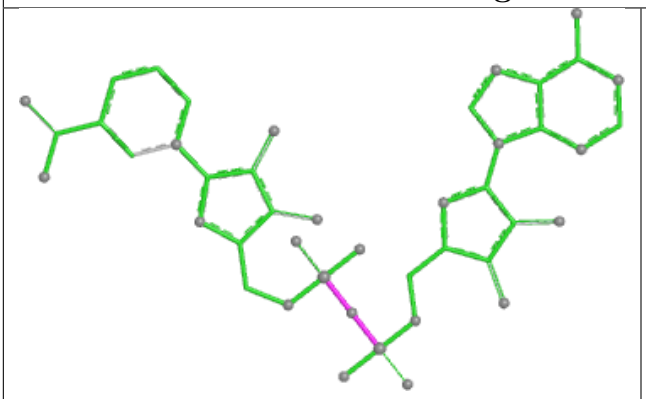


Rings

Ligand NAI B 202 (A)



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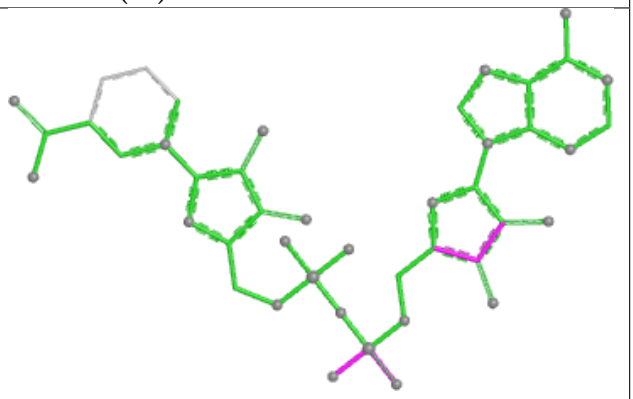
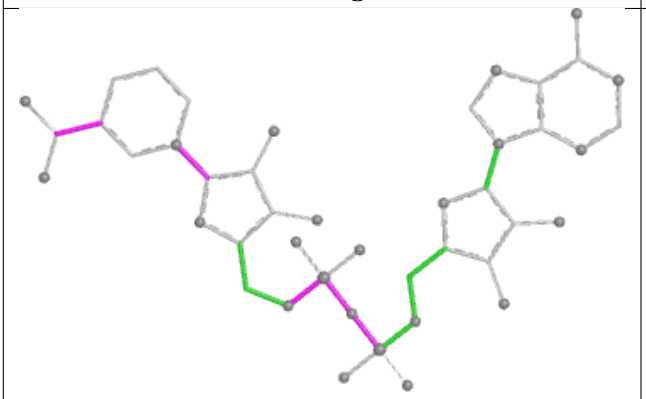


Bond angles



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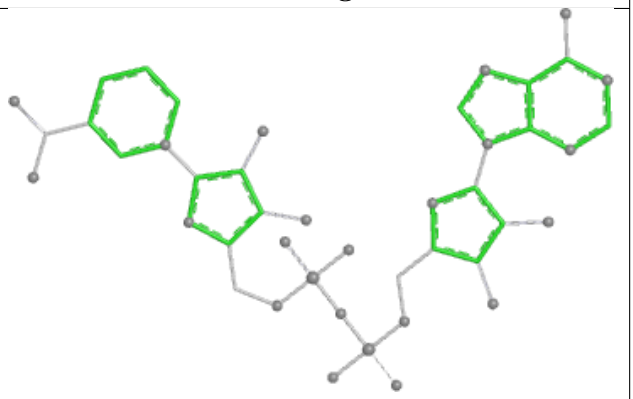
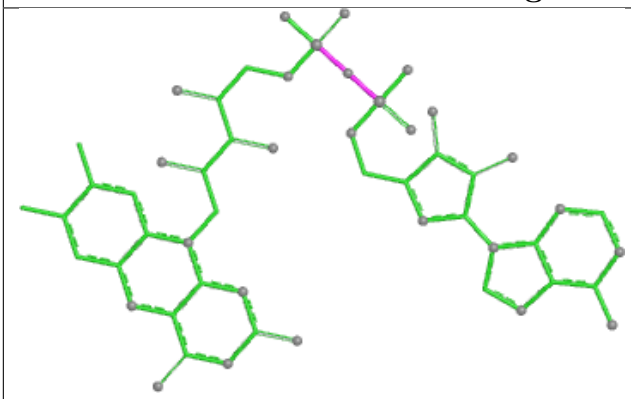


Rings

Ligand FAD B 201



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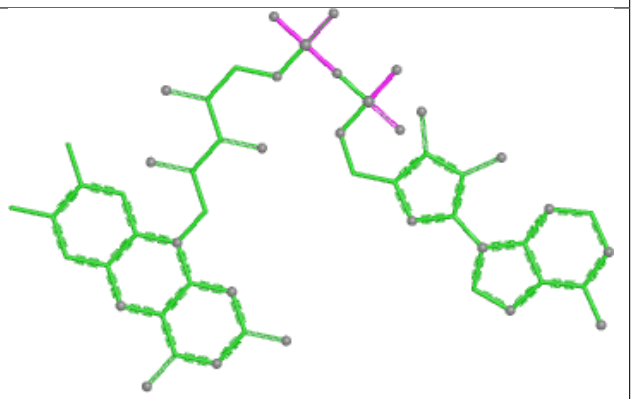

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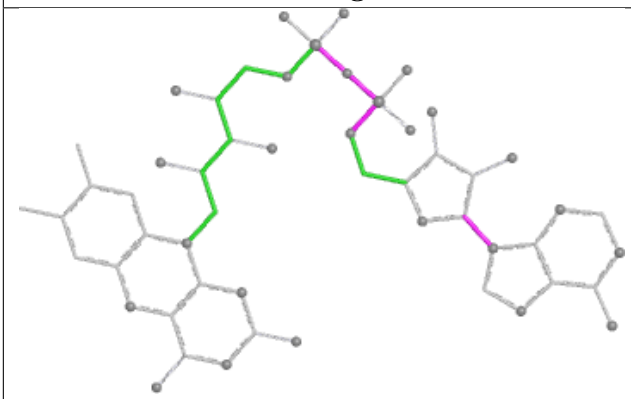

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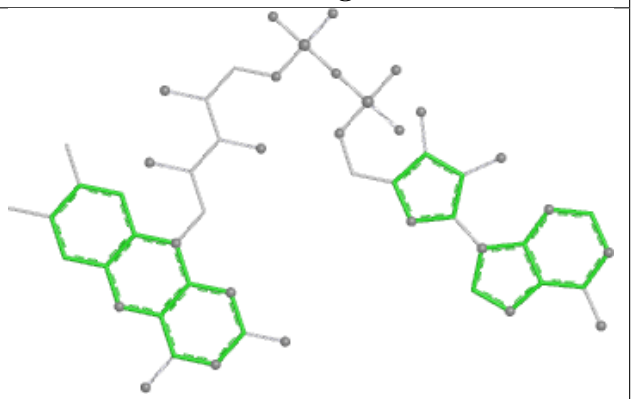
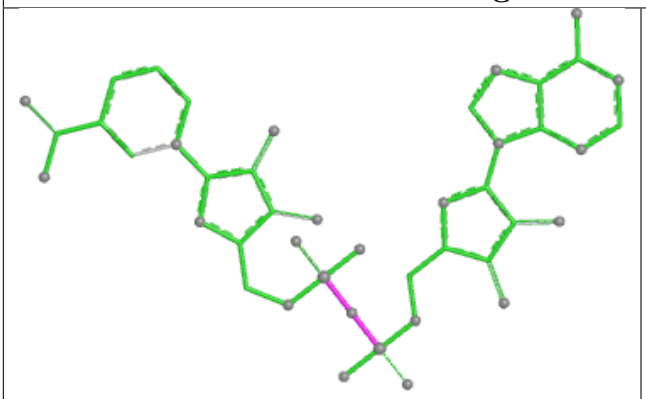


Rings

Ligand NAI D 202 (A)



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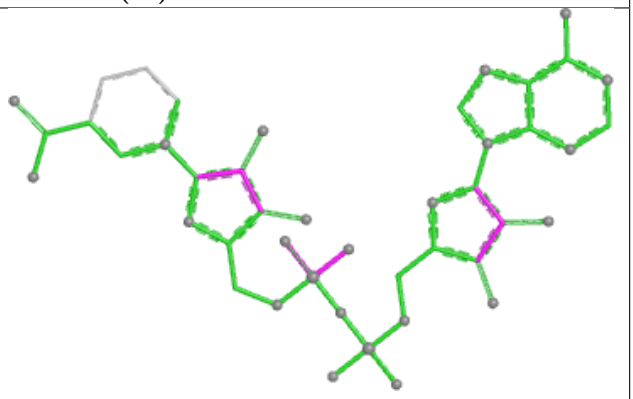
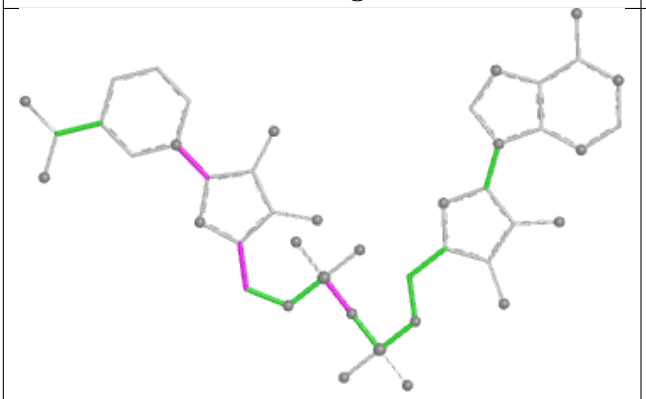


Bond angles



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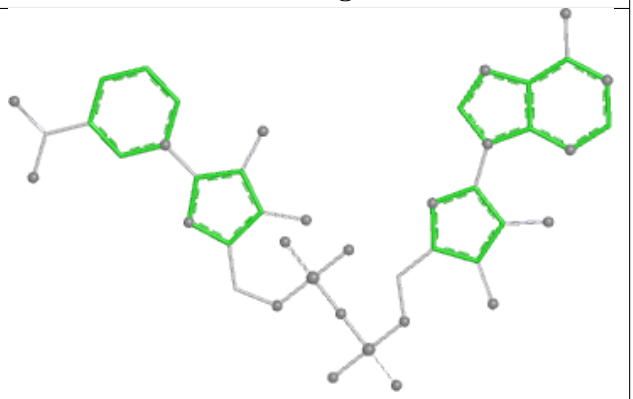
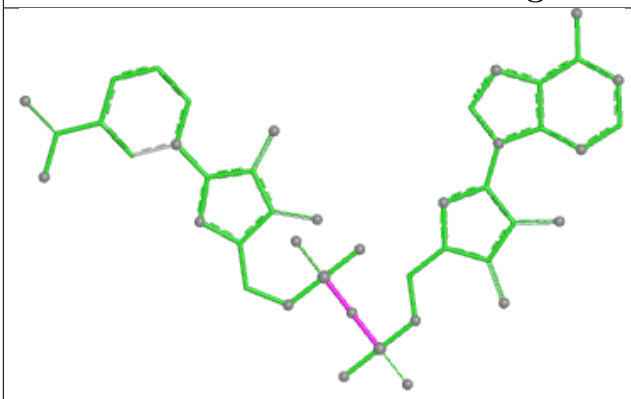
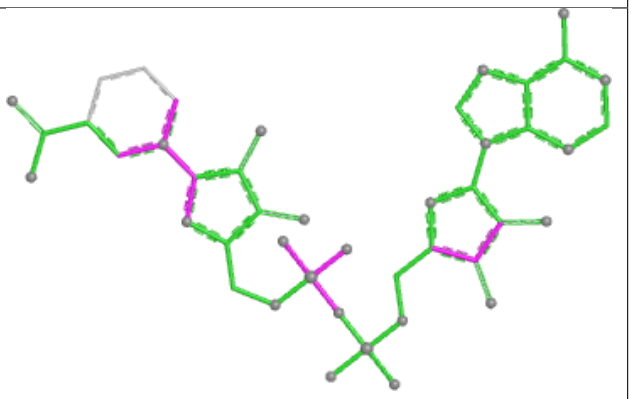


Rings

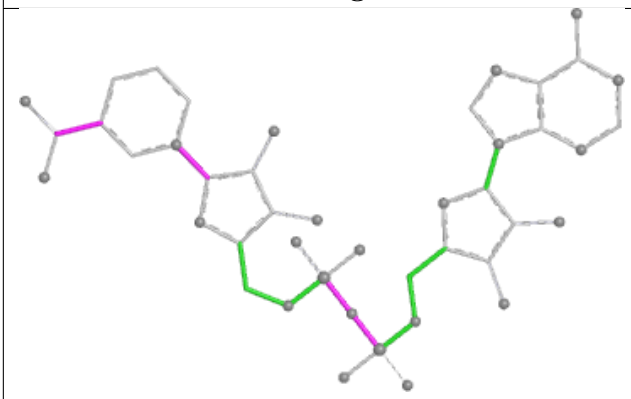
Ligand NAI A 202



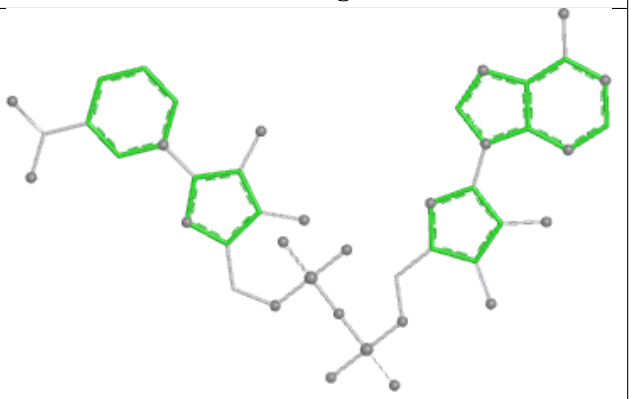
Bond lengths



Bond angles

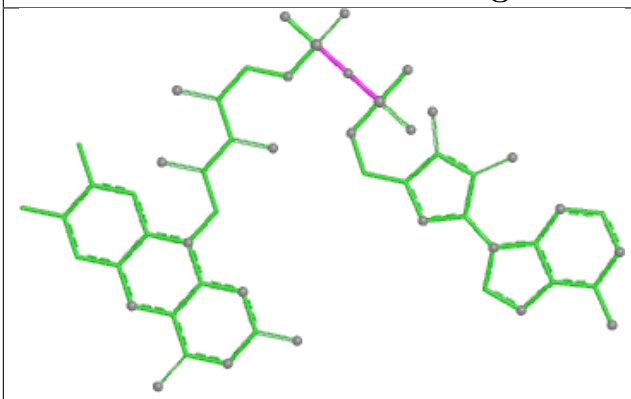


Torsions

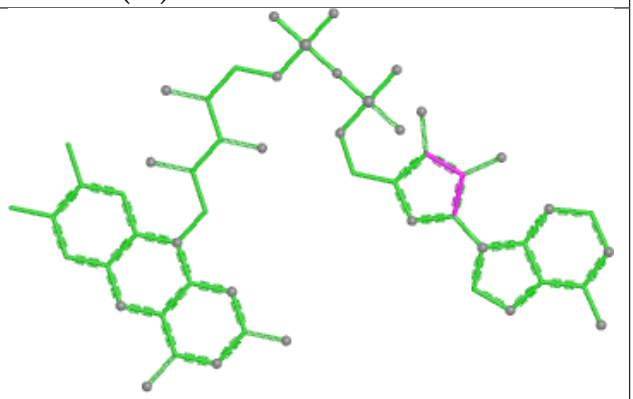


Rings

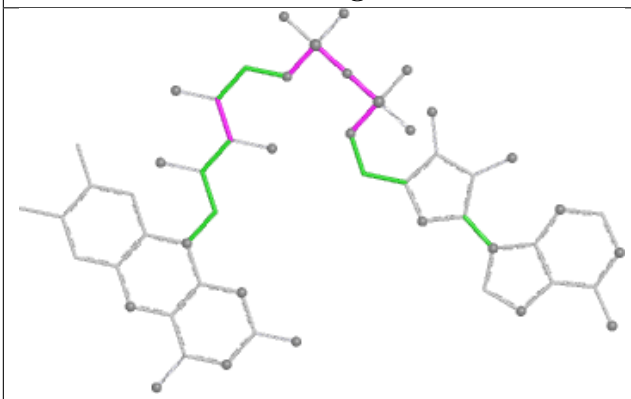
Ligand FAD C 201 (A)



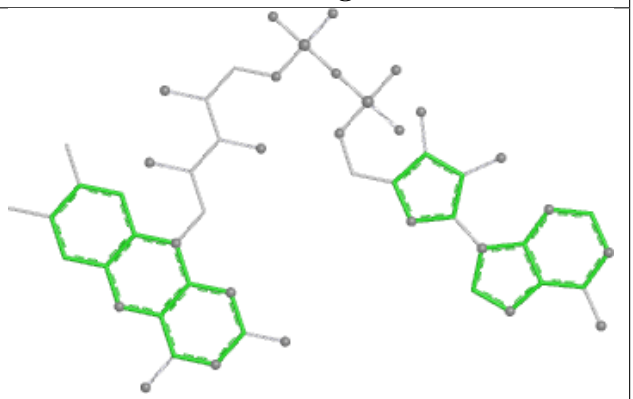
Bond lengths



Bond angles

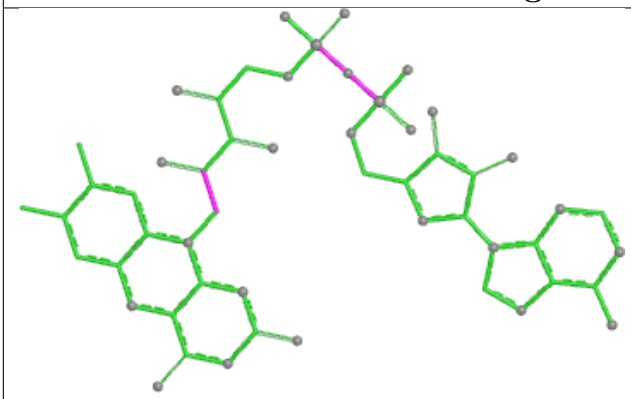


Torsions

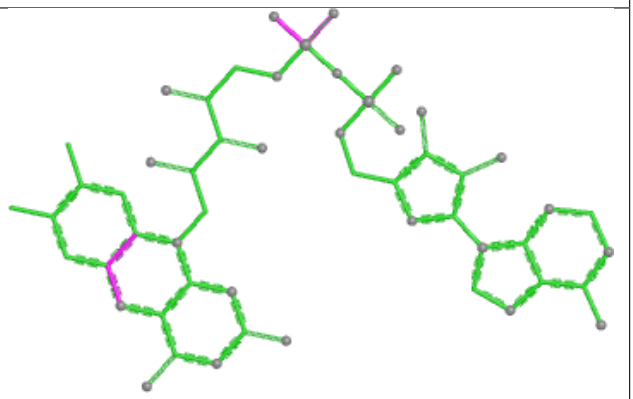


Rings

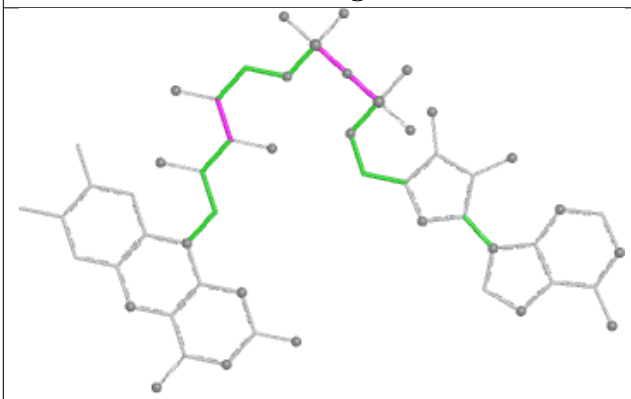
Ligand FAD A 201



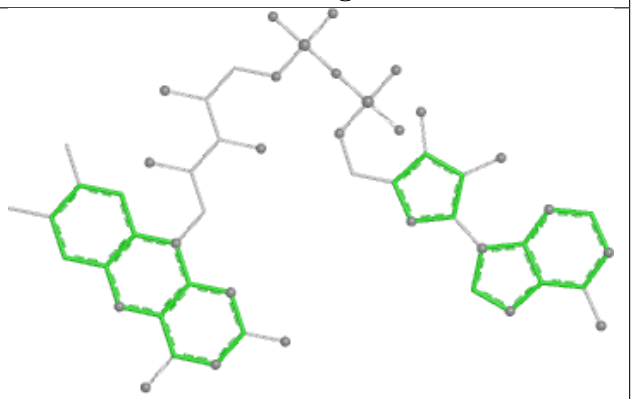
Bond lengths



Bond angles

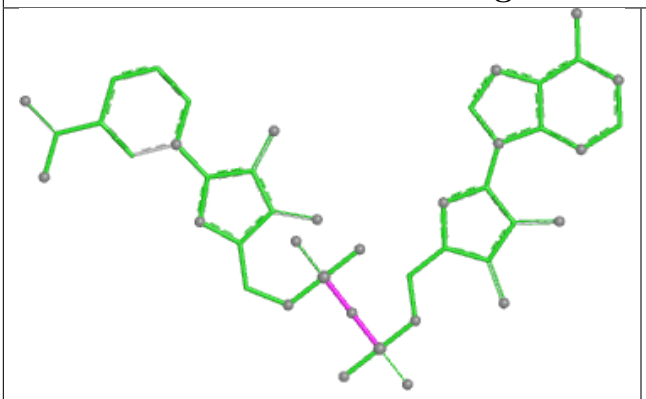


Torsions

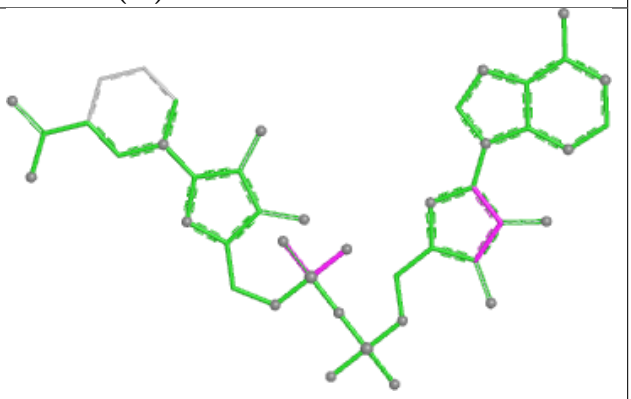


Rings

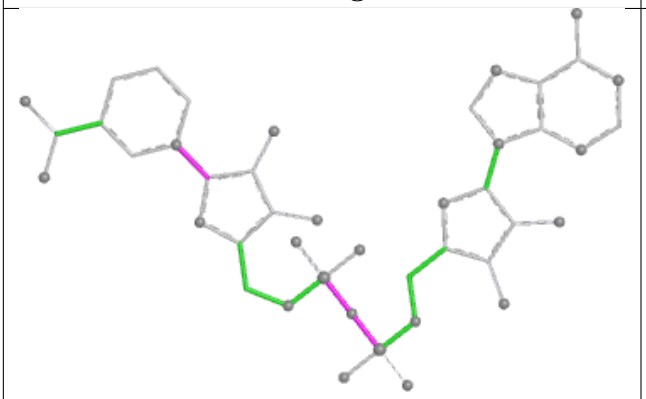
Ligand NAI B 202 (B)



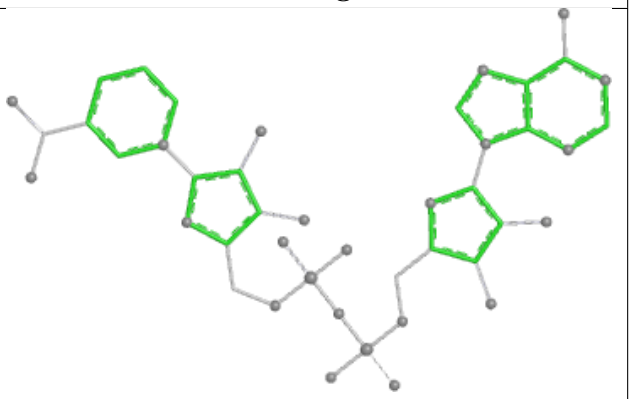
Bond lengths



Bond angles

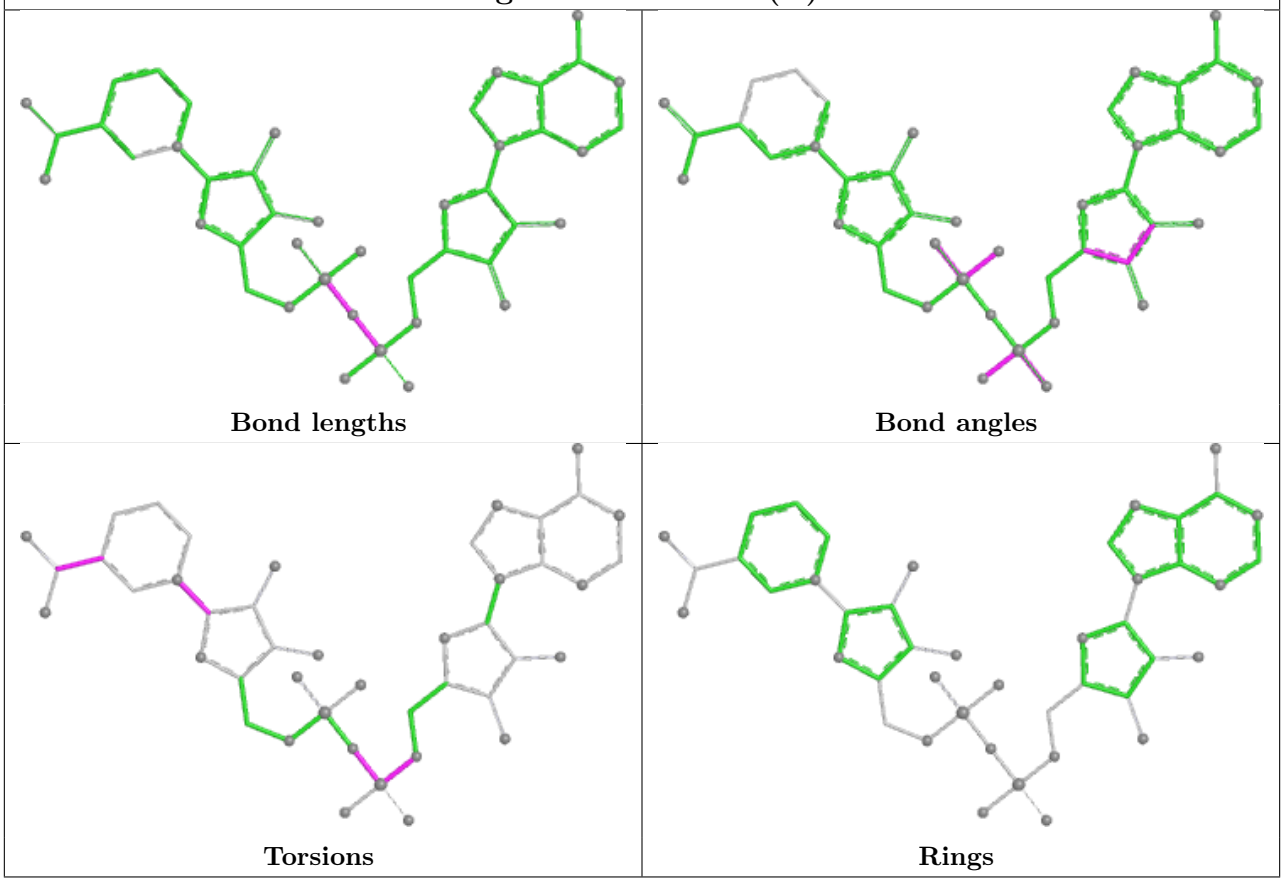


Torsions



Rings

Ligand NAI C 202 (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^{th} 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^2)	Q<0.9
1	A	160/195 (82%)	-0.46	2 (1%)	75	79	8, 19, 28, 38	12 (7%)
1	B	160/195 (82%)	-0.30	5 (3%)	51	54	8, 20, 38, 78	10 (6%)
1	C	162/195 (83%)	-0.28	5 (3%)	51	54	9, 21, 35, 69	12 (7%)
1	D	160/195 (82%)	-0.16	5 (3%)	51	54	8, 22, 45, 75	10 (6%)
All	All	642/780 (82%)	-0.30	17 (2%)	57	60	8, 20, 37, 78	44 (6%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	108	CYS	4.2
1	D	167	PRO	3.8
1	D	166	LEU	3.7
1	A	72	ALA	3.7
1	B	108	CYS	3.3
1	D	108	CYS	3.3
1	B	114	TRP	3.2
1	D	114	TRP	3.2
1	C	167	PRO	3.0
1	B	8	VAL	2.9
1	A	166	LEU	2.7
1	C	114	TRP	2.7
1	B	109	ARG	2.5
1	C	109	ARG	2.5
1	C	166	LEU	2.5
1	B	9	THR	2.4
1	D	102	ARG	2.2

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 (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

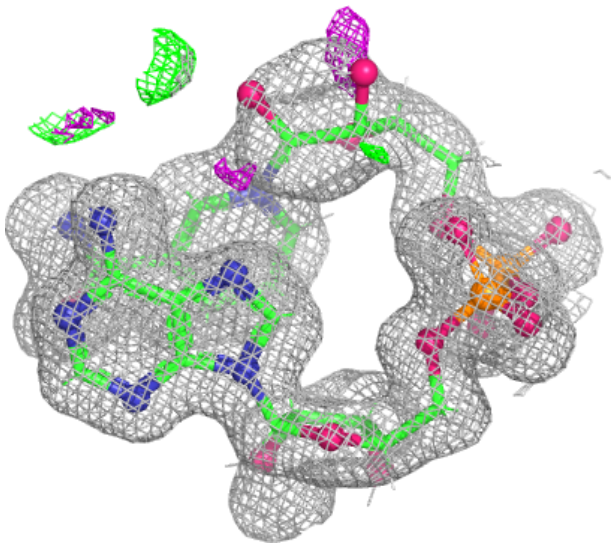
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

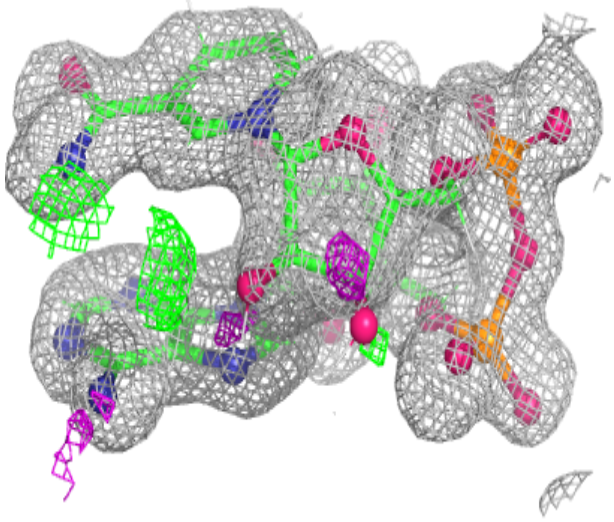
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAI	D	202[A]	44/44	0.94	0.07	16,21,26,28	71
3	NAI	D	202[B]	44/44	0.94	0.07	15,20,27,29	71
3	NAI	C	202[A]	44/44	0.95	0.07	19,24,30,30	71
3	NAI	C	202[B]	44/44	0.95	0.07	18,23,30,30	71
2	FAD	C	201[A]	53/53	0.96	0.09	13,23,56,61	83
2	FAD	C	201[B]	53/53	0.96	0.09	14,23,56,61	83
2	FAD	B	201	53/53	0.97	0.06	12,18,27,33	0
2	FAD	D	201	53/53	0.98	0.04	14,20,28,32	0
3	NAI	B	202[A]	44/44	0.98	0.05	15,21,28,30	71
3	NAI	B	202[B]	44/44	0.98	0.05	18,22,27,27	71
3	NAI	A	202	44/44	0.98	0.04	15,20,27,28	0
2	FAD	A	201	53/53	0.98	0.07	12,18,38,43	0

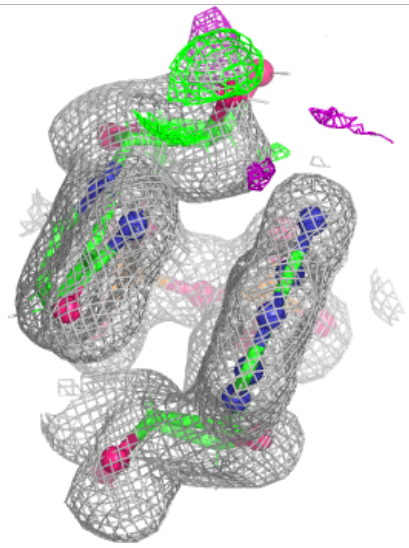
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAI D 202 (A):

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

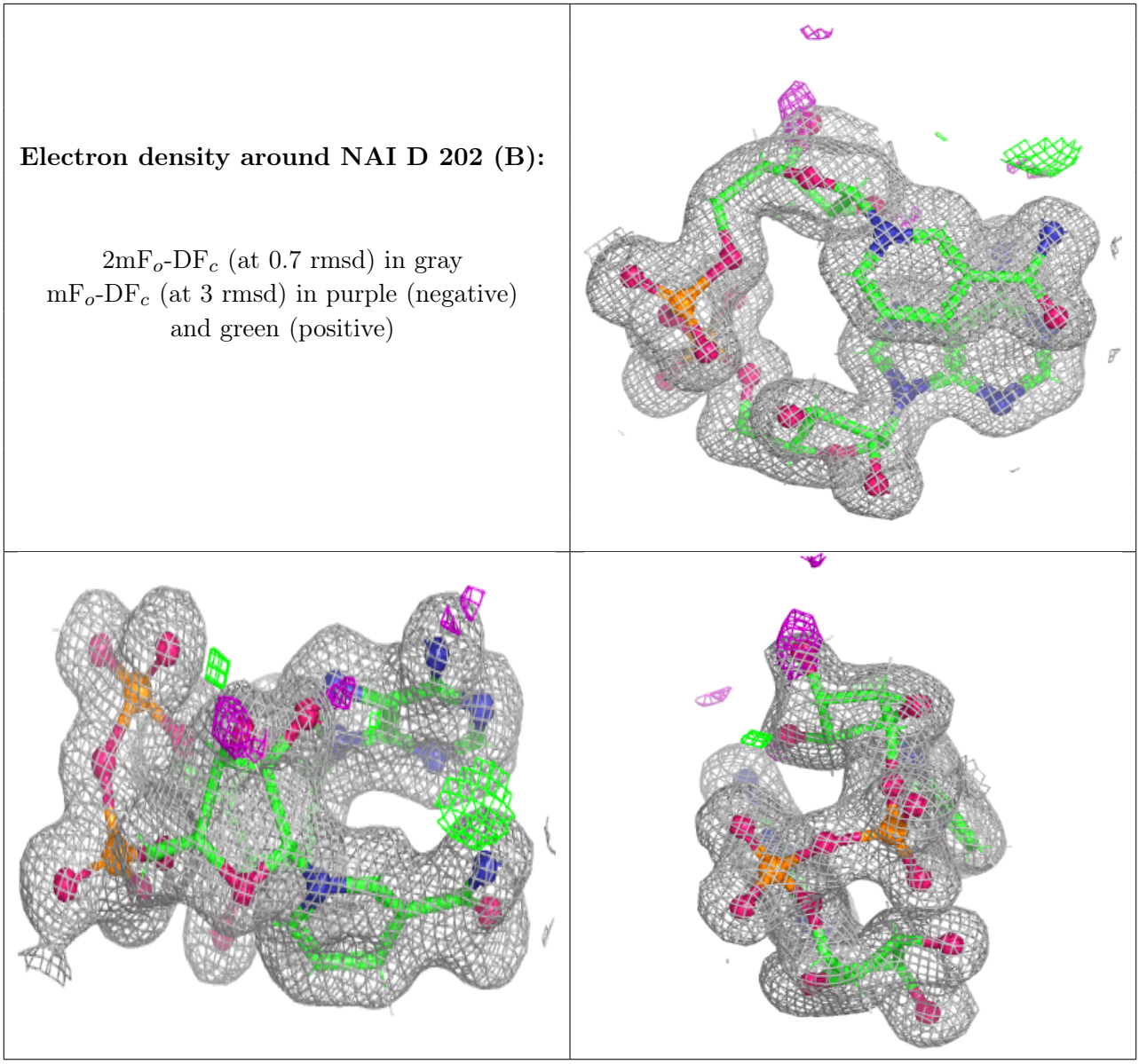






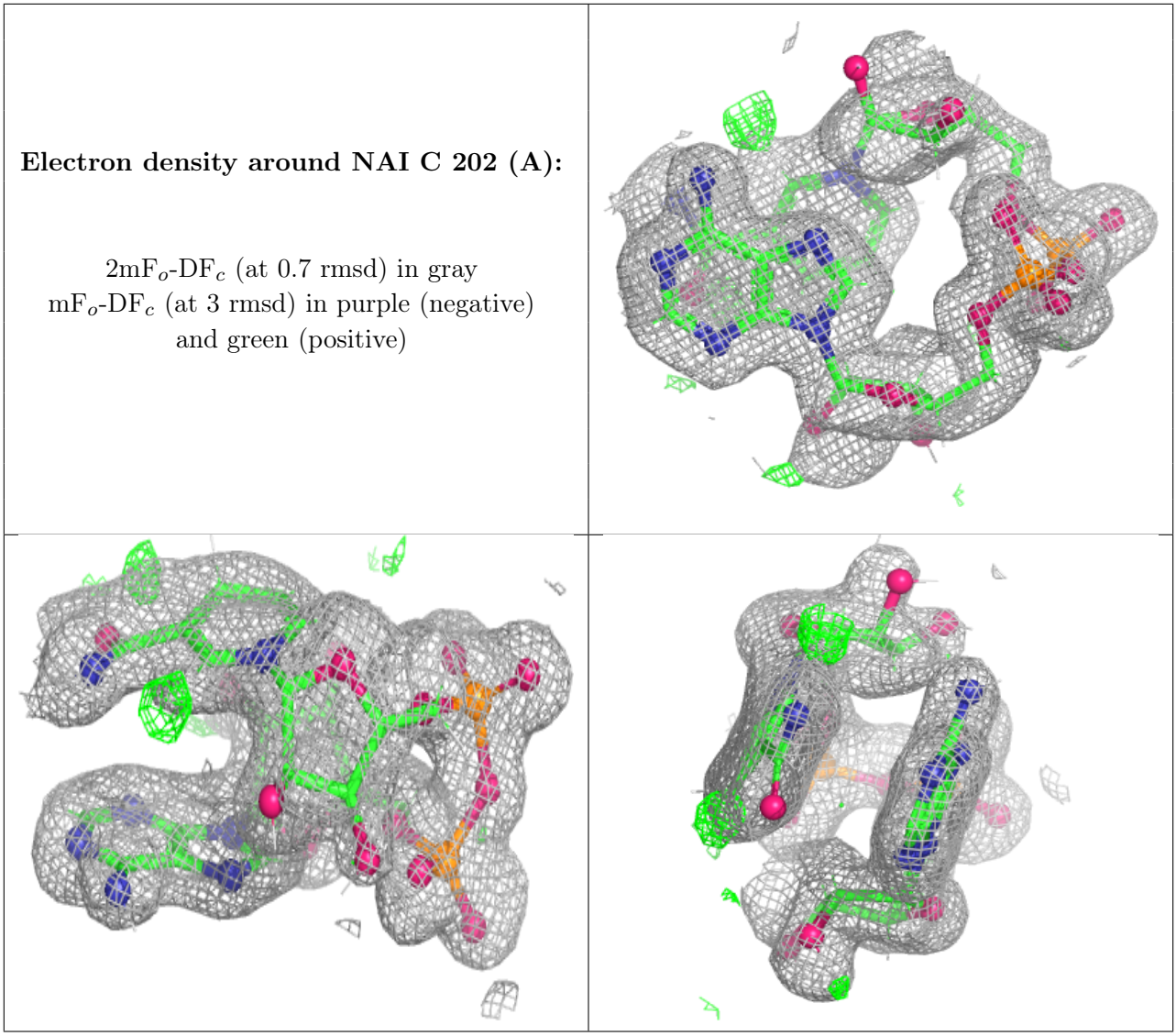
Electron density around NAI D 202 (B):

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



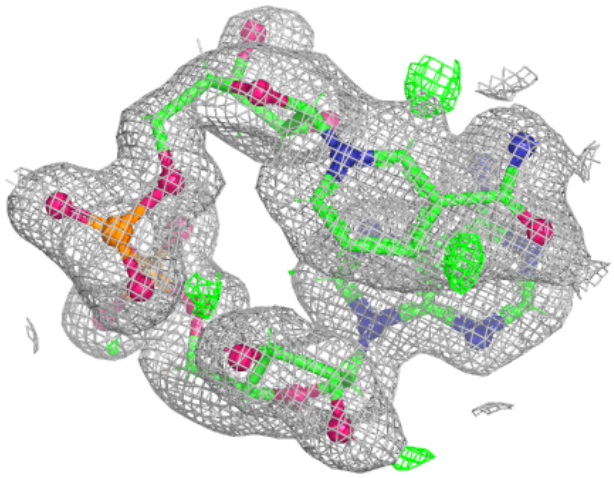
Electron density around NAI C 202 (A):

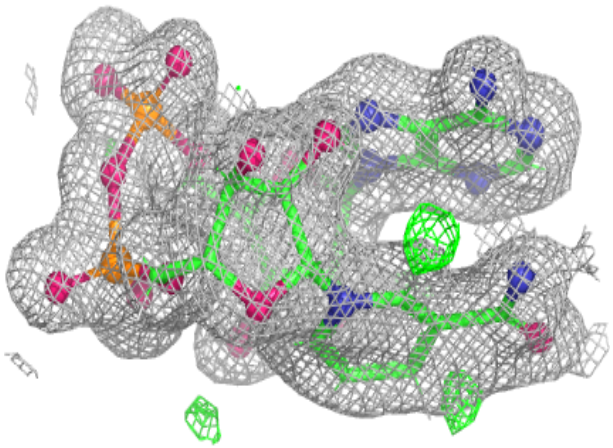
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

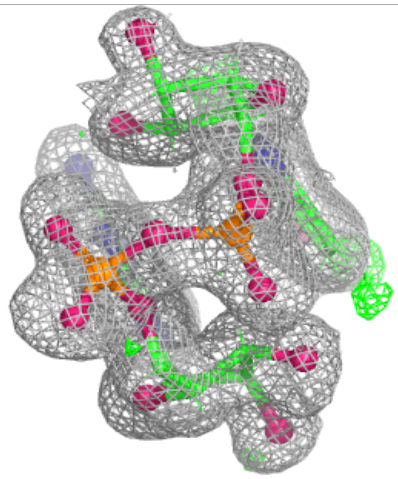


Electron density around NAI C 202 (B):

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

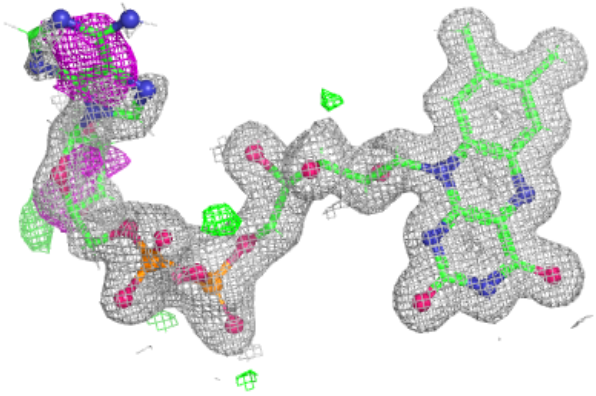


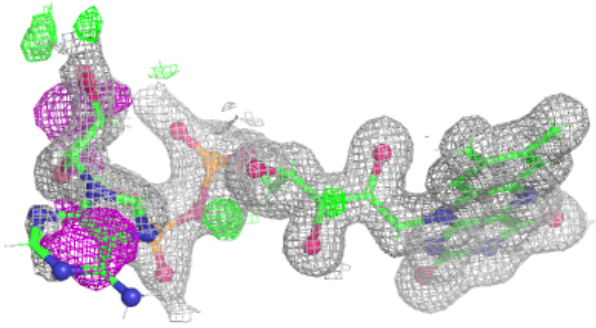


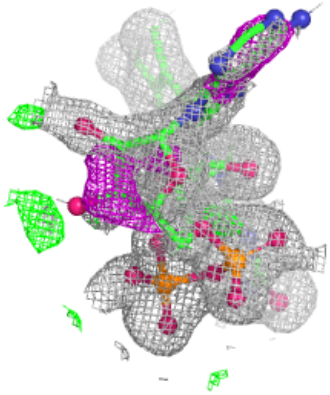


Electron density around FAD C 201 (A):

$2mF_o$-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 201 (B):

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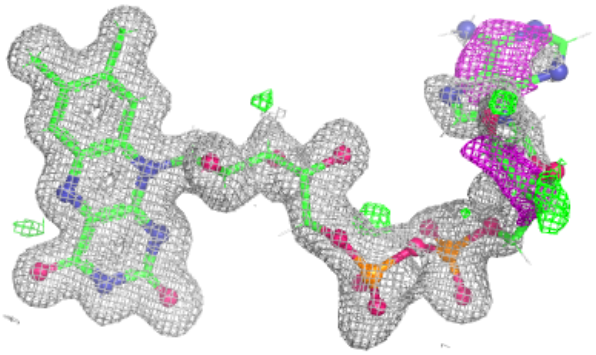
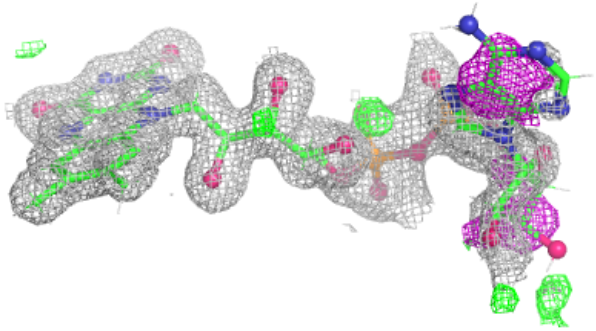
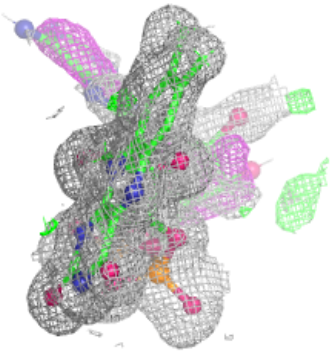
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

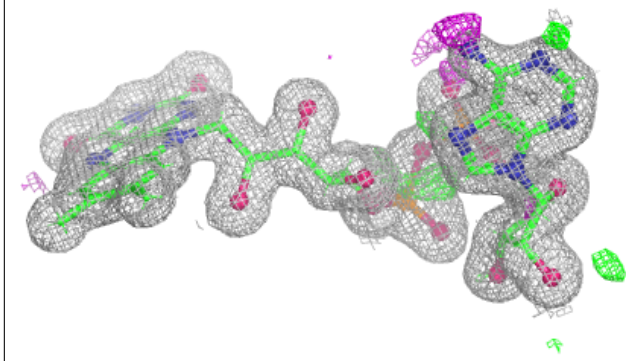


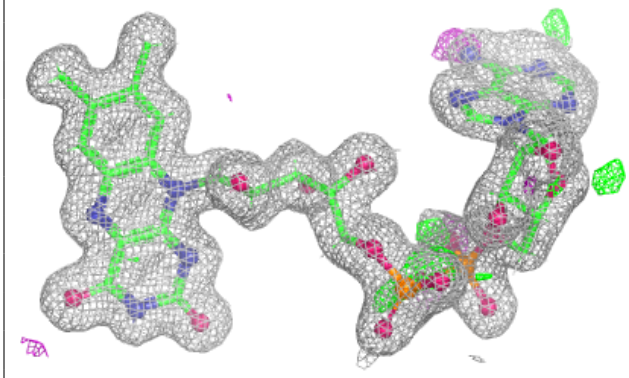


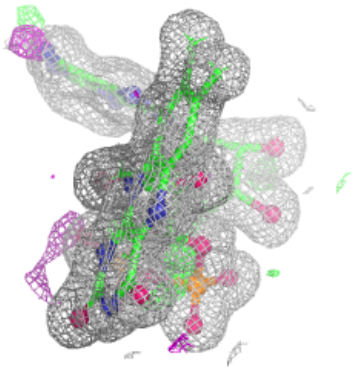


Electron density around FAD B 201:

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

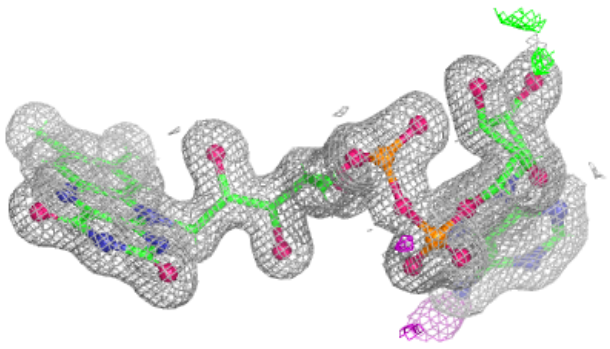


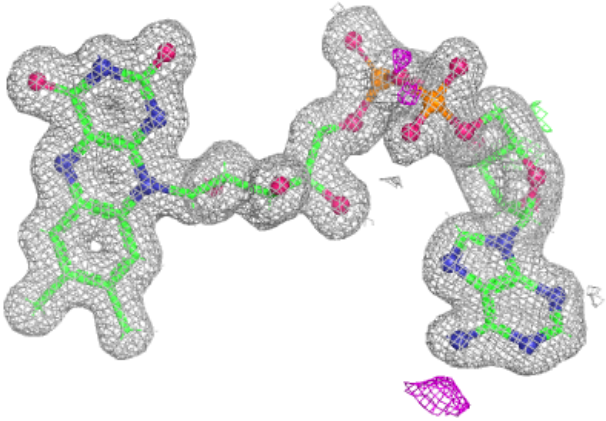


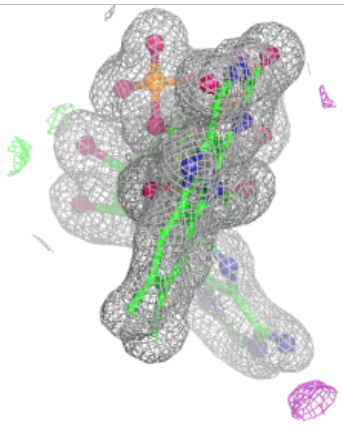


Electron density around FAD D 201:

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

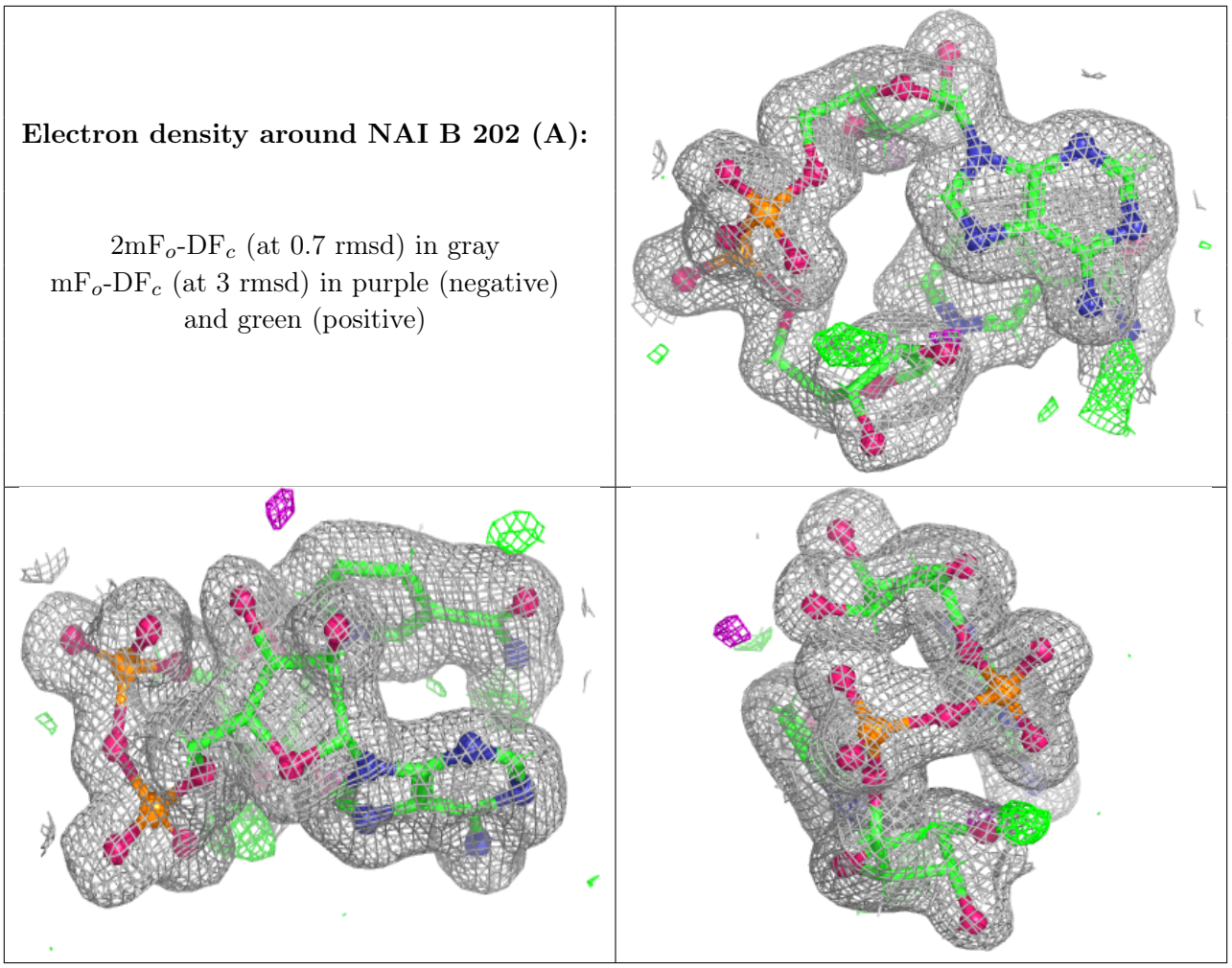






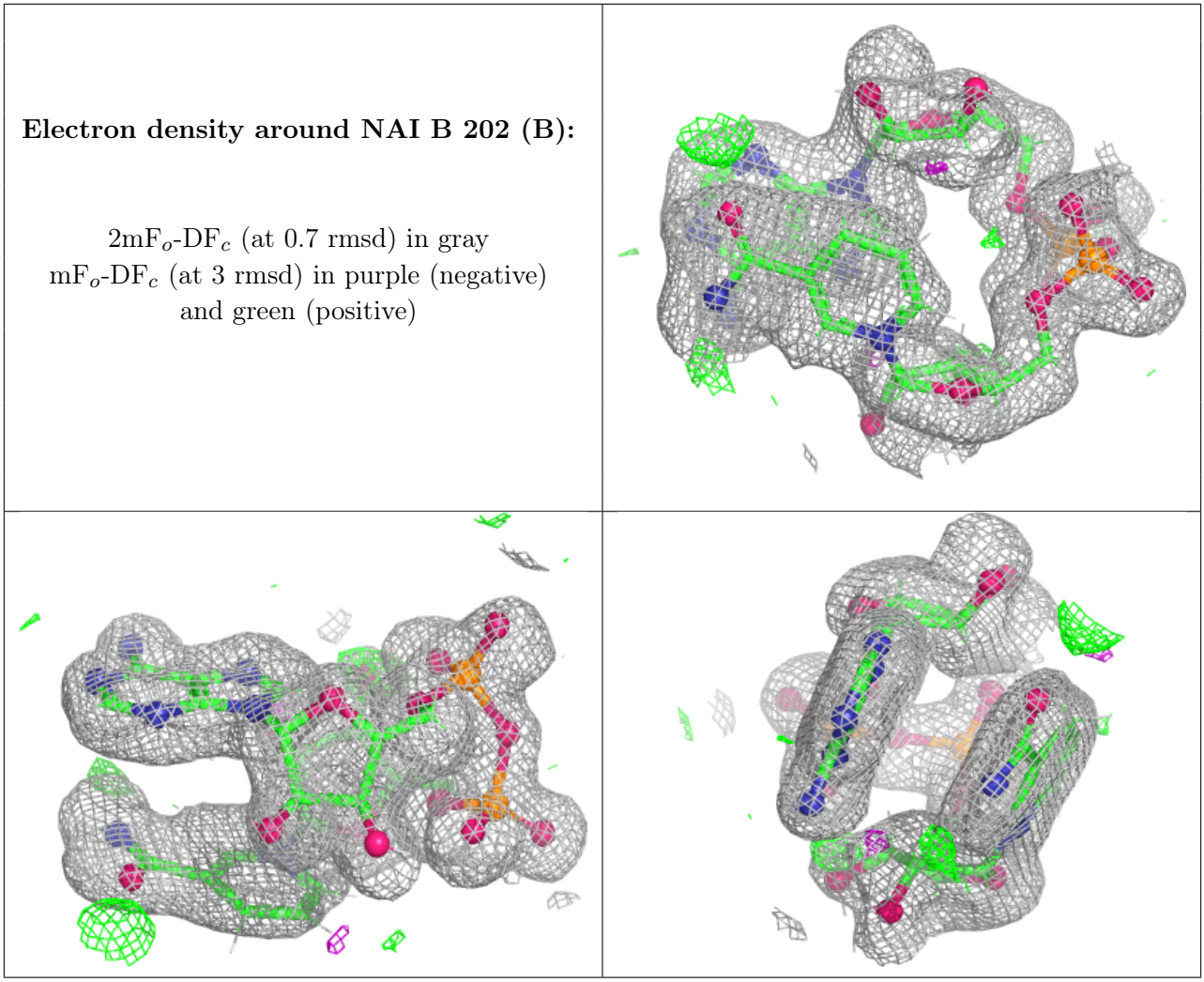
Electron density around NAI B 202 (A):

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



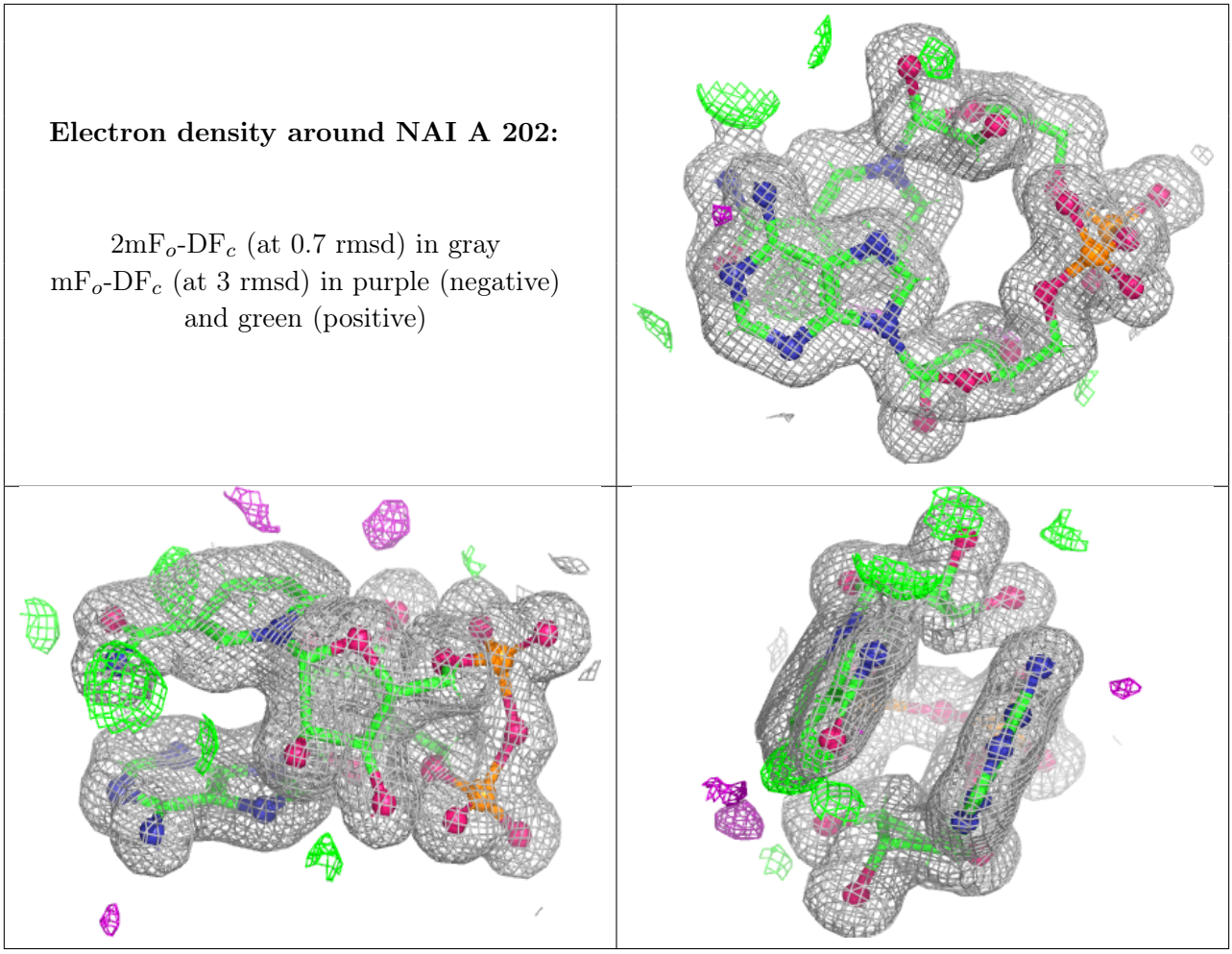
Electron density around NAI B 202 (B):

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



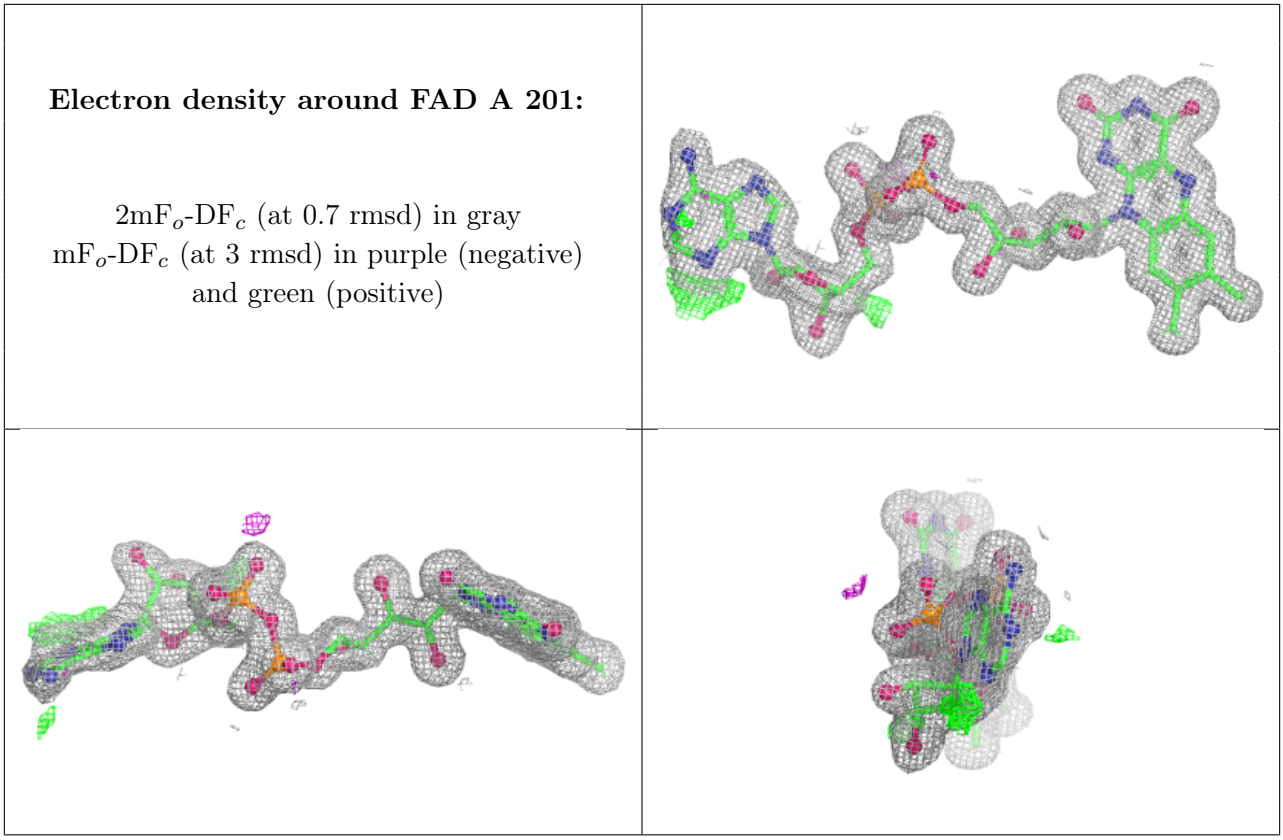
Electron density around NAI A 202:

$2mF_o$-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 201:

$2mF_o$-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.