wwPDB X-ray Structure Validation Summary Report (i)

Sep 4, 2023 – 04:39 PM EDT

PDB ID	:	3UIC
Title	:	Crystal Structure of FabI, an Enoyl Reductase from F. tularensis, in complex with a Novel and Potent Inhibitor
Authors	:	Mehboob, S.; Santarsiero, B.D.; Truong, K.; Johnson, M.E.
Deposited on	:	2011-11-04
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

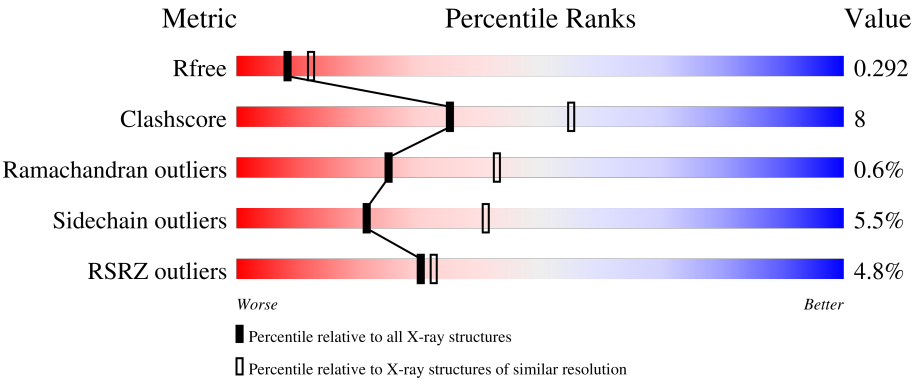
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	280	75% 15% • 8%
1	B	280	79% 12% • 8%
1	C	280	71% 20% • 8%
1	D	280	% 77% 13% • 9%
1	E	280	12% 71% 19% • 8%

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Mol	Chain	Length	Quality of chain
1	F	280	4% 76% 16% 8%
1	G	280	11% 76% 15% 8%
1	H	280	8% 79% 11% 8%
1	I	280	% 75% 16% 8%
1	J	280	2% 77% 14% 8%
1	K	280	73% 17% 8%
1	L	280	% 78% 13% 8%
1	M	280	9% 75% 16% 8%
1	N	280	5% 76% 15% 8%
1	O	280	11% 76% 15% 9%
1	P	280	5% 77% 14% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	09T	B	262	-	-	X	-
3	09T	M	262	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32732 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	B	257	Total	C	N	O	S	0	0	0
			1921	1219	322	364	16			
1	C	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	D	256	Total	C	N	O	S	0	0	0
			1913	1215	320	362	16			
1	E	258	Total	C	N	O	S	0	0	0
			1928	1224	323	365	16			
1	F	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	G	257	Total	C	N	O	S	0	0	0
			1921	1219	322	364	16			
1	H	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	I	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	J	257	Total	C	N	O	S	0	0	0
			1921	1219	322	364	16			
1	K	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	L	257	Total	C	N	O	S	0	0	0
			1921	1219	322	364	16			
1	M	257	Total	C	N	O	S	0	0	0
			1921	1219	322	364	16			
1	N	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	O	256	Total	C	N	O	S	0	0	0
			1913	1215	320	362	16			
1	P	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q5NGQ3
A	-18	GLY	-	expression tag	UNP Q5NGQ3
A	-17	SER	-	expression tag	UNP Q5NGQ3
A	-16	SER	-	expression tag	UNP Q5NGQ3
A	-15	HIS	-	expression tag	UNP Q5NGQ3
A	-14	HIS	-	expression tag	UNP Q5NGQ3
A	-13	HIS	-	expression tag	UNP Q5NGQ3
A	-12	HIS	-	expression tag	UNP Q5NGQ3
A	-11	HIS	-	expression tag	UNP Q5NGQ3
A	-10	HIS	-	expression tag	UNP Q5NGQ3
A	-9	SER	-	expression tag	UNP Q5NGQ3
A	-8	SER	-	expression tag	UNP Q5NGQ3
A	-7	GLY	-	expression tag	UNP Q5NGQ3
A	-6	LEU	-	expression tag	UNP Q5NGQ3
A	-5	VAL	-	expression tag	UNP Q5NGQ3
A	-4	PRO	-	expression tag	UNP Q5NGQ3
A	-3	ARG	-	expression tag	UNP Q5NGQ3
A	-2	GLY	-	expression tag	UNP Q5NGQ3
A	-1	SER	-	expression tag	UNP Q5NGQ3
A	0	HIS	-	expression tag	UNP Q5NGQ3
B	-19	MET	-	expression tag	UNP Q5NGQ3
B	-18	GLY	-	expression tag	UNP Q5NGQ3
B	-17	SER	-	expression tag	UNP Q5NGQ3
B	-16	SER	-	expression tag	UNP Q5NGQ3
B	-15	HIS	-	expression tag	UNP Q5NGQ3
B	-14	HIS	-	expression tag	UNP Q5NGQ3
B	-13	HIS	-	expression tag	UNP Q5NGQ3
B	-12	HIS	-	expression tag	UNP Q5NGQ3
B	-11	HIS	-	expression tag	UNP Q5NGQ3
B	-10	HIS	-	expression tag	UNP Q5NGQ3
B	-9	SER	-	expression tag	UNP Q5NGQ3
B	-8	SER	-	expression tag	UNP Q5NGQ3
B	-7	GLY	-	expression tag	UNP Q5NGQ3
B	-6	LEU	-	expression tag	UNP Q5NGQ3
B	-5	VAL	-	expression tag	UNP Q5NGQ3
B	-4	PRO	-	expression tag	UNP Q5NGQ3
B	-3	ARG	-	expression tag	UNP Q5NGQ3
B	-2	GLY	-	expression tag	UNP Q5NGQ3
B	-1	SER	-	expression tag	UNP Q5NGQ3
B	0	HIS	-	expression tag	UNP Q5NGQ3
C	-19	MET	-	expression tag	UNP Q5NGQ3
C	-18	GLY	-	expression tag	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP Q5NGQ3
C	-16	SER	-	expression tag	UNP Q5NGQ3
C	-15	HIS	-	expression tag	UNP Q5NGQ3
C	-14	HIS	-	expression tag	UNP Q5NGQ3
C	-13	HIS	-	expression tag	UNP Q5NGQ3
C	-12	HIS	-	expression tag	UNP Q5NGQ3
C	-11	HIS	-	expression tag	UNP Q5NGQ3
C	-10	HIS	-	expression tag	UNP Q5NGQ3
C	-9	SER	-	expression tag	UNP Q5NGQ3
C	-8	SER	-	expression tag	UNP Q5NGQ3
C	-7	GLY	-	expression tag	UNP Q5NGQ3
C	-6	LEU	-	expression tag	UNP Q5NGQ3
C	-5	VAL	-	expression tag	UNP Q5NGQ3
C	-4	PRO	-	expression tag	UNP Q5NGQ3
C	-3	ARG	-	expression tag	UNP Q5NGQ3
C	-2	GLY	-	expression tag	UNP Q5NGQ3
C	-1	SER	-	expression tag	UNP Q5NGQ3
C	0	HIS	-	expression tag	UNP Q5NGQ3
D	-19	MET	-	expression tag	UNP Q5NGQ3
D	-18	GLY	-	expression tag	UNP Q5NGQ3
D	-17	SER	-	expression tag	UNP Q5NGQ3
D	-16	SER	-	expression tag	UNP Q5NGQ3
D	-15	HIS	-	expression tag	UNP Q5NGQ3
D	-14	HIS	-	expression tag	UNP Q5NGQ3
D	-13	HIS	-	expression tag	UNP Q5NGQ3
D	-12	HIS	-	expression tag	UNP Q5NGQ3
D	-11	HIS	-	expression tag	UNP Q5NGQ3
D	-10	HIS	-	expression tag	UNP Q5NGQ3
D	-9	SER	-	expression tag	UNP Q5NGQ3
D	-8	SER	-	expression tag	UNP Q5NGQ3
D	-7	GLY	-	expression tag	UNP Q5NGQ3
D	-6	LEU	-	expression tag	UNP Q5NGQ3
D	-5	VAL	-	expression tag	UNP Q5NGQ3
D	-4	PRO	-	expression tag	UNP Q5NGQ3
D	-3	ARG	-	expression tag	UNP Q5NGQ3
D	-2	GLY	-	expression tag	UNP Q5NGQ3
D	-1	SER	-	expression tag	UNP Q5NGQ3
D	0	HIS	-	expression tag	UNP Q5NGQ3
E	-19	MET	-	expression tag	UNP Q5NGQ3
E	-18	GLY	-	expression tag	UNP Q5NGQ3
E	-17	SER	-	expression tag	UNP Q5NGQ3
E	-16	SER	-	expression tag	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	expression tag	UNP Q5NGQ3
E	-14	HIS	-	expression tag	UNP Q5NGQ3
E	-13	HIS	-	expression tag	UNP Q5NGQ3
E	-12	HIS	-	expression tag	UNP Q5NGQ3
E	-11	HIS	-	expression tag	UNP Q5NGQ3
E	-10	HIS	-	expression tag	UNP Q5NGQ3
E	-9	SER	-	expression tag	UNP Q5NGQ3
E	-8	SER	-	expression tag	UNP Q5NGQ3
E	-7	GLY	-	expression tag	UNP Q5NGQ3
E	-6	LEU	-	expression tag	UNP Q5NGQ3
E	-5	VAL	-	expression tag	UNP Q5NGQ3
E	-4	PRO	-	expression tag	UNP Q5NGQ3
E	-3	ARG	-	expression tag	UNP Q5NGQ3
E	-2	GLY	-	expression tag	UNP Q5NGQ3
E	-1	SER	-	expression tag	UNP Q5NGQ3
E	0	HIS	-	expression tag	UNP Q5NGQ3
F	-19	MET	-	expression tag	UNP Q5NGQ3
F	-18	GLY	-	expression tag	UNP Q5NGQ3
F	-17	SER	-	expression tag	UNP Q5NGQ3
F	-16	SER	-	expression tag	UNP Q5NGQ3
F	-15	HIS	-	expression tag	UNP Q5NGQ3
F	-14	HIS	-	expression tag	UNP Q5NGQ3
F	-13	HIS	-	expression tag	UNP Q5NGQ3
F	-12	HIS	-	expression tag	UNP Q5NGQ3
F	-11	HIS	-	expression tag	UNP Q5NGQ3
F	-10	HIS	-	expression tag	UNP Q5NGQ3
F	-9	SER	-	expression tag	UNP Q5NGQ3
F	-8	SER	-	expression tag	UNP Q5NGQ3
F	-7	GLY	-	expression tag	UNP Q5NGQ3
F	-6	LEU	-	expression tag	UNP Q5NGQ3
F	-5	VAL	-	expression tag	UNP Q5NGQ3
F	-4	PRO	-	expression tag	UNP Q5NGQ3
F	-3	ARG	-	expression tag	UNP Q5NGQ3
F	-2	GLY	-	expression tag	UNP Q5NGQ3
F	-1	SER	-	expression tag	UNP Q5NGQ3
F	0	HIS	-	expression tag	UNP Q5NGQ3
G	-19	MET	-	expression tag	UNP Q5NGQ3
G	-18	GLY	-	expression tag	UNP Q5NGQ3
G	-17	SER	-	expression tag	UNP Q5NGQ3
G	-16	SER	-	expression tag	UNP Q5NGQ3
G	-15	HIS	-	expression tag	UNP Q5NGQ3
G	-14	HIS	-	expression tag	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	expression tag	UNP Q5NGQ3
G	-12	HIS	-	expression tag	UNP Q5NGQ3
G	-11	HIS	-	expression tag	UNP Q5NGQ3
G	-10	HIS	-	expression tag	UNP Q5NGQ3
G	-9	SER	-	expression tag	UNP Q5NGQ3
G	-8	SER	-	expression tag	UNP Q5NGQ3
G	-7	GLY	-	expression tag	UNP Q5NGQ3
G	-6	LEU	-	expression tag	UNP Q5NGQ3
G	-5	VAL	-	expression tag	UNP Q5NGQ3
G	-4	PRO	-	expression tag	UNP Q5NGQ3
G	-3	ARG	-	expression tag	UNP Q5NGQ3
G	-2	GLY	-	expression tag	UNP Q5NGQ3
G	-1	SER	-	expression tag	UNP Q5NGQ3
G	0	HIS	-	expression tag	UNP Q5NGQ3
H	-19	MET	-	expression tag	UNP Q5NGQ3
H	-18	GLY	-	expression tag	UNP Q5NGQ3
H	-17	SER	-	expression tag	UNP Q5NGQ3
H	-16	SER	-	expression tag	UNP Q5NGQ3
H	-15	HIS	-	expression tag	UNP Q5NGQ3
H	-14	HIS	-	expression tag	UNP Q5NGQ3
H	-13	HIS	-	expression tag	UNP Q5NGQ3
H	-12	HIS	-	expression tag	UNP Q5NGQ3
H	-11	HIS	-	expression tag	UNP Q5NGQ3
H	-10	HIS	-	expression tag	UNP Q5NGQ3
H	-9	SER	-	expression tag	UNP Q5NGQ3
H	-8	SER	-	expression tag	UNP Q5NGQ3
H	-7	GLY	-	expression tag	UNP Q5NGQ3
H	-6	LEU	-	expression tag	UNP Q5NGQ3
H	-5	VAL	-	expression tag	UNP Q5NGQ3
H	-4	PRO	-	expression tag	UNP Q5NGQ3
H	-3	ARG	-	expression tag	UNP Q5NGQ3
H	-2	GLY	-	expression tag	UNP Q5NGQ3
H	-1	SER	-	expression tag	UNP Q5NGQ3
H	0	HIS	-	expression tag	UNP Q5NGQ3
I	-19	MET	-	expression tag	UNP Q5NGQ3
I	-18	GLY	-	expression tag	UNP Q5NGQ3
I	-17	SER	-	expression tag	UNP Q5NGQ3
I	-16	SER	-	expression tag	UNP Q5NGQ3
I	-15	HIS	-	expression tag	UNP Q5NGQ3
I	-14	HIS	-	expression tag	UNP Q5NGQ3
I	-13	HIS	-	expression tag	UNP Q5NGQ3
I	-12	HIS	-	expression tag	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	expression tag	UNP Q5NGQ3
I	-10	HIS	-	expression tag	UNP Q5NGQ3
I	-9	SER	-	expression tag	UNP Q5NGQ3
I	-8	SER	-	expression tag	UNP Q5NGQ3
I	-7	GLY	-	expression tag	UNP Q5NGQ3
I	-6	LEU	-	expression tag	UNP Q5NGQ3
I	-5	VAL	-	expression tag	UNP Q5NGQ3
I	-4	PRO	-	expression tag	UNP Q5NGQ3
I	-3	ARG	-	expression tag	UNP Q5NGQ3
I	-2	GLY	-	expression tag	UNP Q5NGQ3
I	-1	SER	-	expression tag	UNP Q5NGQ3
I	0	HIS	-	expression tag	UNP Q5NGQ3
J	-19	MET	-	expression tag	UNP Q5NGQ3
J	-18	GLY	-	expression tag	UNP Q5NGQ3
J	-17	SER	-	expression tag	UNP Q5NGQ3
J	-16	SER	-	expression tag	UNP Q5NGQ3
J	-15	HIS	-	expression tag	UNP Q5NGQ3
J	-14	HIS	-	expression tag	UNP Q5NGQ3
J	-13	HIS	-	expression tag	UNP Q5NGQ3
J	-12	HIS	-	expression tag	UNP Q5NGQ3
J	-11	HIS	-	expression tag	UNP Q5NGQ3
J	-10	HIS	-	expression tag	UNP Q5NGQ3
J	-9	SER	-	expression tag	UNP Q5NGQ3
J	-8	SER	-	expression tag	UNP Q5NGQ3
J	-7	GLY	-	expression tag	UNP Q5NGQ3
J	-6	LEU	-	expression tag	UNP Q5NGQ3
J	-5	VAL	-	expression tag	UNP Q5NGQ3
J	-4	PRO	-	expression tag	UNP Q5NGQ3
J	-3	ARG	-	expression tag	UNP Q5NGQ3
J	-2	GLY	-	expression tag	UNP Q5NGQ3
J	-1	SER	-	expression tag	UNP Q5NGQ3
J	0	HIS	-	expression tag	UNP Q5NGQ3
K	-19	MET	-	expression tag	UNP Q5NGQ3
K	-18	GLY	-	expression tag	UNP Q5NGQ3
K	-17	SER	-	expression tag	UNP Q5NGQ3
K	-16	SER	-	expression tag	UNP Q5NGQ3
K	-15	HIS	-	expression tag	UNP Q5NGQ3
K	-14	HIS	-	expression tag	UNP Q5NGQ3
K	-13	HIS	-	expression tag	UNP Q5NGQ3
K	-12	HIS	-	expression tag	UNP Q5NGQ3
K	-11	HIS	-	expression tag	UNP Q5NGQ3
K	-10	HIS	-	expression tag	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	SER	-	expression tag	UNP Q5NGQ3
K	-8	SER	-	expression tag	UNP Q5NGQ3
K	-7	GLY	-	expression tag	UNP Q5NGQ3
K	-6	LEU	-	expression tag	UNP Q5NGQ3
K	-5	VAL	-	expression tag	UNP Q5NGQ3
K	-4	PRO	-	expression tag	UNP Q5NGQ3
K	-3	ARG	-	expression tag	UNP Q5NGQ3
K	-2	GLY	-	expression tag	UNP Q5NGQ3
K	-1	SER	-	expression tag	UNP Q5NGQ3
K	0	HIS	-	expression tag	UNP Q5NGQ3
L	-19	MET	-	expression tag	UNP Q5NGQ3
L	-18	GLY	-	expression tag	UNP Q5NGQ3
L	-17	SER	-	expression tag	UNP Q5NGQ3
L	-16	SER	-	expression tag	UNP Q5NGQ3
L	-15	HIS	-	expression tag	UNP Q5NGQ3
L	-14	HIS	-	expression tag	UNP Q5NGQ3
L	-13	HIS	-	expression tag	UNP Q5NGQ3
L	-12	HIS	-	expression tag	UNP Q5NGQ3
L	-11	HIS	-	expression tag	UNP Q5NGQ3
L	-10	HIS	-	expression tag	UNP Q5NGQ3
L	-9	SER	-	expression tag	UNP Q5NGQ3
L	-8	SER	-	expression tag	UNP Q5NGQ3
L	-7	GLY	-	expression tag	UNP Q5NGQ3
L	-6	LEU	-	expression tag	UNP Q5NGQ3
L	-5	VAL	-	expression tag	UNP Q5NGQ3
L	-4	PRO	-	expression tag	UNP Q5NGQ3
L	-3	ARG	-	expression tag	UNP Q5NGQ3
L	-2	GLY	-	expression tag	UNP Q5NGQ3
L	-1	SER	-	expression tag	UNP Q5NGQ3
L	0	HIS	-	expression tag	UNP Q5NGQ3
M	-19	MET	-	expression tag	UNP Q5NGQ3
M	-18	GLY	-	expression tag	UNP Q5NGQ3
M	-17	SER	-	expression tag	UNP Q5NGQ3
M	-16	SER	-	expression tag	UNP Q5NGQ3
M	-15	HIS	-	expression tag	UNP Q5NGQ3
M	-14	HIS	-	expression tag	UNP Q5NGQ3
M	-13	HIS	-	expression tag	UNP Q5NGQ3
M	-12	HIS	-	expression tag	UNP Q5NGQ3
M	-11	HIS	-	expression tag	UNP Q5NGQ3
M	-10	HIS	-	expression tag	UNP Q5NGQ3
M	-9	SER	-	expression tag	UNP Q5NGQ3
M	-8	SER	-	expression tag	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	GLY	-	expression tag	UNP Q5NGQ3
M	-6	LEU	-	expression tag	UNP Q5NGQ3
M	-5	VAL	-	expression tag	UNP Q5NGQ3
M	-4	PRO	-	expression tag	UNP Q5NGQ3
M	-3	ARG	-	expression tag	UNP Q5NGQ3
M	-2	GLY	-	expression tag	UNP Q5NGQ3
M	-1	SER	-	expression tag	UNP Q5NGQ3
M	0	HIS	-	expression tag	UNP Q5NGQ3
N	-19	MET	-	expression tag	UNP Q5NGQ3
N	-18	GLY	-	expression tag	UNP Q5NGQ3
N	-17	SER	-	expression tag	UNP Q5NGQ3
N	-16	SER	-	expression tag	UNP Q5NGQ3
N	-15	HIS	-	expression tag	UNP Q5NGQ3
N	-14	HIS	-	expression tag	UNP Q5NGQ3
N	-13	HIS	-	expression tag	UNP Q5NGQ3
N	-12	HIS	-	expression tag	UNP Q5NGQ3
N	-11	HIS	-	expression tag	UNP Q5NGQ3
N	-10	HIS	-	expression tag	UNP Q5NGQ3
N	-9	SER	-	expression tag	UNP Q5NGQ3
N	-8	SER	-	expression tag	UNP Q5NGQ3
N	-7	GLY	-	expression tag	UNP Q5NGQ3
N	-6	LEU	-	expression tag	UNP Q5NGQ3
N	-5	VAL	-	expression tag	UNP Q5NGQ3
N	-4	PRO	-	expression tag	UNP Q5NGQ3
N	-3	ARG	-	expression tag	UNP Q5NGQ3
N	-2	GLY	-	expression tag	UNP Q5NGQ3
N	-1	SER	-	expression tag	UNP Q5NGQ3
N	0	HIS	-	expression tag	UNP Q5NGQ3
O	-19	MET	-	expression tag	UNP Q5NGQ3
O	-18	GLY	-	expression tag	UNP Q5NGQ3
O	-17	SER	-	expression tag	UNP Q5NGQ3
O	-16	SER	-	expression tag	UNP Q5NGQ3
O	-15	HIS	-	expression tag	UNP Q5NGQ3
O	-14	HIS	-	expression tag	UNP Q5NGQ3
O	-13	HIS	-	expression tag	UNP Q5NGQ3
O	-12	HIS	-	expression tag	UNP Q5NGQ3
O	-11	HIS	-	expression tag	UNP Q5NGQ3
O	-10	HIS	-	expression tag	UNP Q5NGQ3
O	-9	SER	-	expression tag	UNP Q5NGQ3
O	-8	SER	-	expression tag	UNP Q5NGQ3
O	-7	GLY	-	expression tag	UNP Q5NGQ3
O	-6	LEU	-	expression tag	UNP Q5NGQ3

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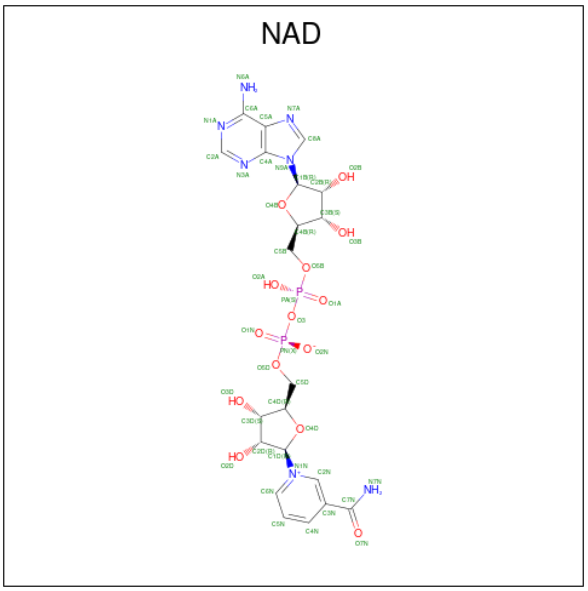
Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	VAL	-	expression tag	UNP Q5NGQ3
O	-4	PRO	-	expression tag	UNP Q5NGQ3
O	-3	ARG	-	expression tag	UNP Q5NGQ3
O	-2	GLY	-	expression tag	UNP Q5NGQ3
O	-1	SER	-	expression tag	UNP Q5NGQ3
O	0	HIS	-	expression tag	UNP Q5NGQ3
P	-19	MET	-	expression tag	UNP Q5NGQ3
P	-18	GLY	-	expression tag	UNP Q5NGQ3
P	-17	SER	-	expression tag	UNP Q5NGQ3
P	-16	SER	-	expression tag	UNP Q5NGQ3
P	-15	HIS	-	expression tag	UNP Q5NGQ3
P	-14	HIS	-	expression tag	UNP Q5NGQ3
P	-13	HIS	-	expression tag	UNP Q5NGQ3
P	-12	HIS	-	expression tag	UNP Q5NGQ3
P	-11	HIS	-	expression tag	UNP Q5NGQ3
P	-10	HIS	-	expression tag	UNP Q5NGQ3
P	-9	SER	-	expression tag	UNP Q5NGQ3
P	-8	SER	-	expression tag	UNP Q5NGQ3
P	-7	GLY	-	expression tag	UNP Q5NGQ3
P	-6	LEU	-	expression tag	UNP Q5NGQ3
P	-5	VAL	-	expression tag	UNP Q5NGQ3
P	-4	PRO	-	expression tag	UNP Q5NGQ3
P	-3	ARG	-	expression tag	UNP Q5NGQ3
P	-2	GLY	-	expression tag	UNP Q5NGQ3
P	-1	SER	-	expression tag	UNP Q5NGQ3
P	0	HIS	-	expression tag	UNP Q5NGQ3

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	M	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	N	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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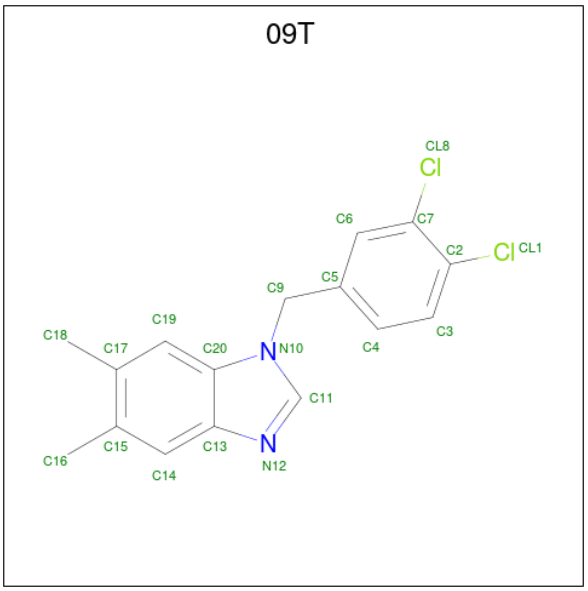
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 1-(3,4-dichlorobenzyl)-5,6-dimethyl-1H-benzimidazole (three-letter code: 09T) (formula: $C_{16}H_{14}Cl_2N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	B	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	C	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	D	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	E	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	F	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	G	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	H	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	I	1	Total	C	Cl	N	0	0
			20	16	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	K	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	L	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	M	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	N	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	O	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	P	1	Total	C	Cl	N	0	0
			20	16	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	55	Total	O	0	0
			55	55		
4	C	71	Total	O	0	0
			71	71		
4	D	77	Total	O	0	0
			77	77		
4	E	48	Total	O	0	0
			48	48		
4	F	48	Total	O	0	0
			48	48		
4	G	35	Total	O	0	0
			35	35		
4	H	33	Total	O	0	0
			33	33		
4	I	77	Total	O	0	0
			77	77		
4	J	63	Total	O	0	0
			63	63		
4	K	79	Total	O	0	0
			79	79		
4	L	56	Total	O	0	0
			56	56		

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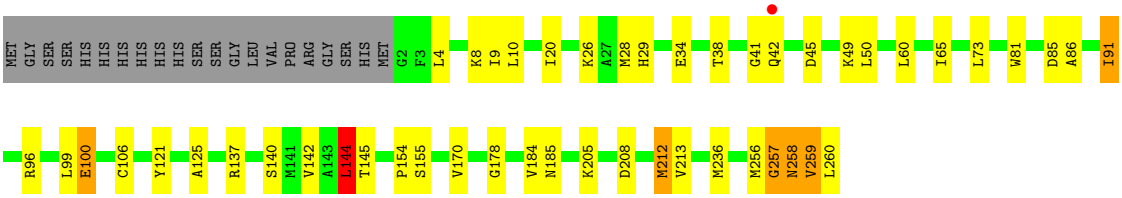
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	35	Total O 35 35	0	0
4	N	34	Total O 34 34	0	0
4	O	38	Total O 38 38	0	0
4	P	41	Total O 41 41	0	0

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.

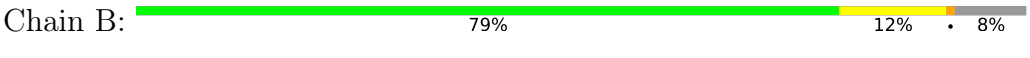
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

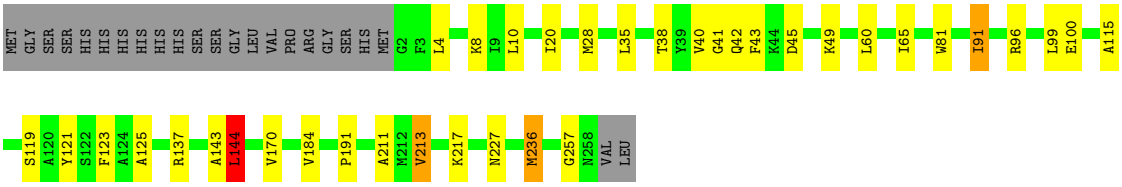
Chain A:



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

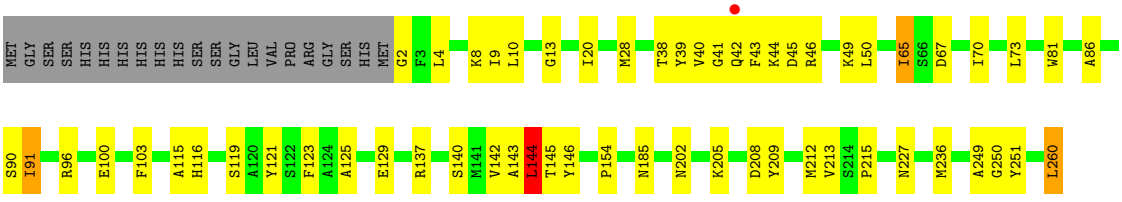
Chain B:





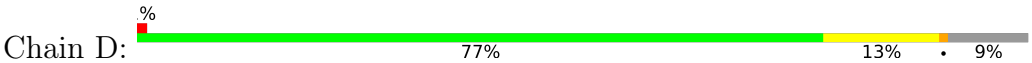
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

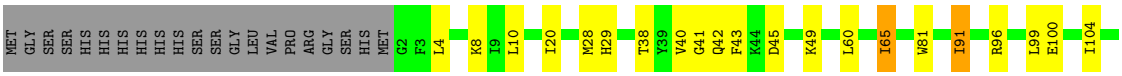
Chain C:

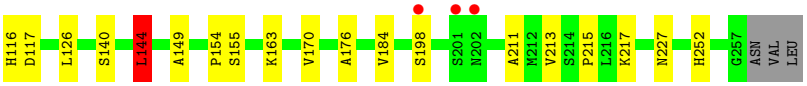


• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain D:

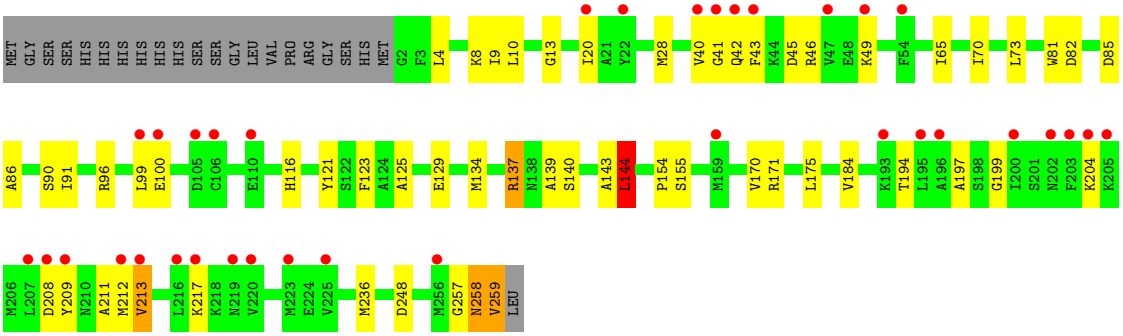






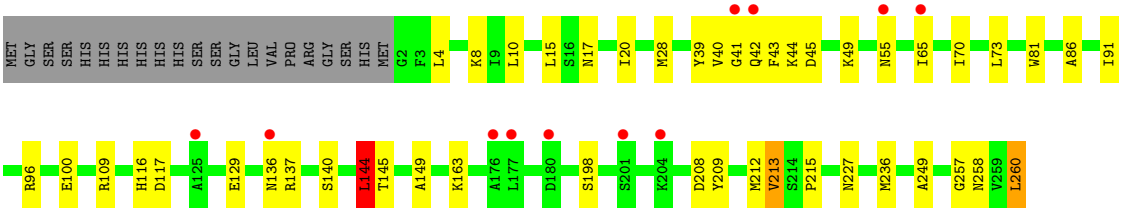
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain E:



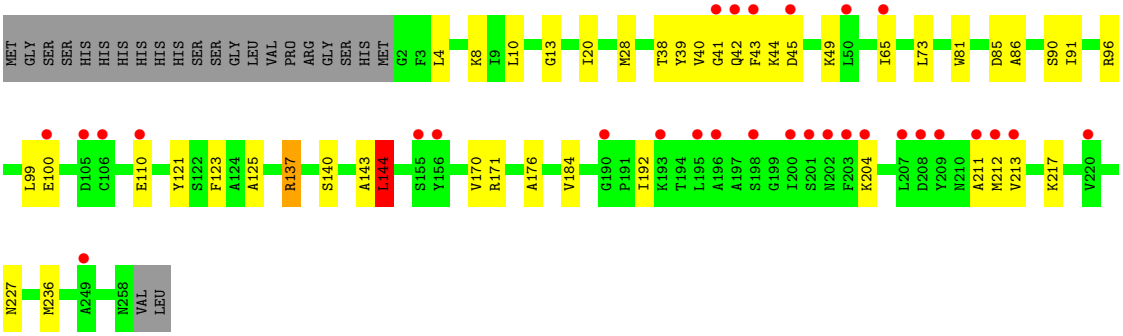
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain F:



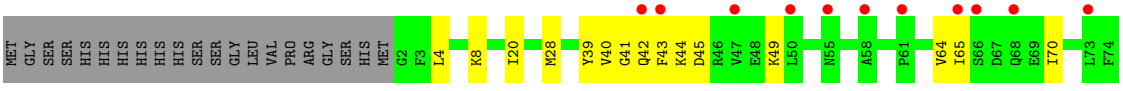
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain G:



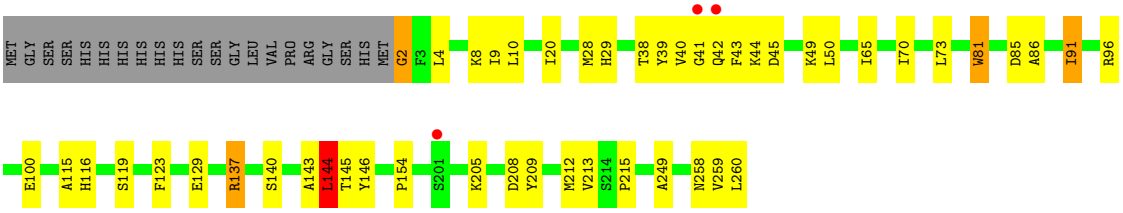
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain H:



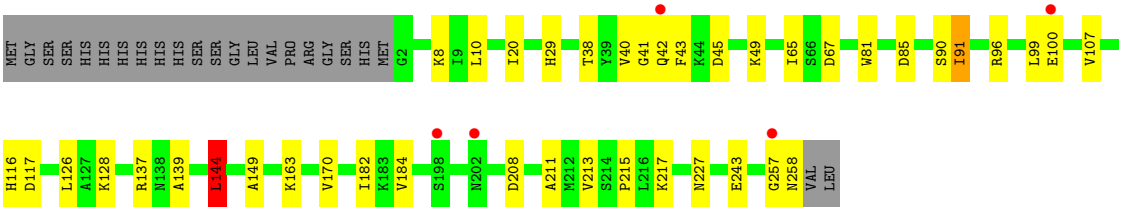
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain I:



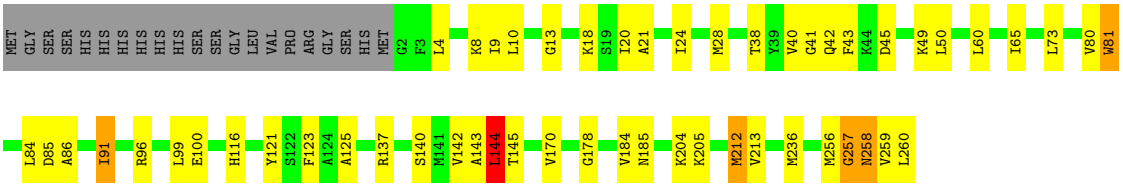
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain J:



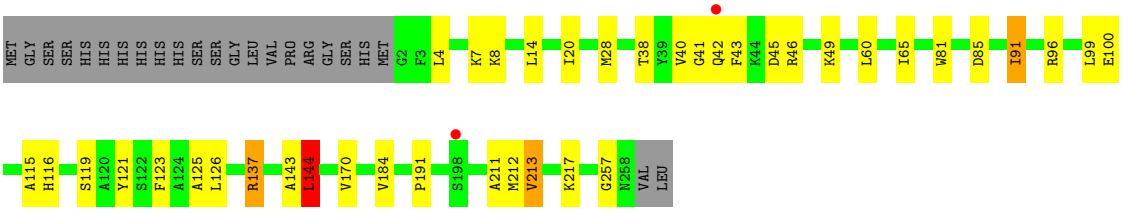
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain K:



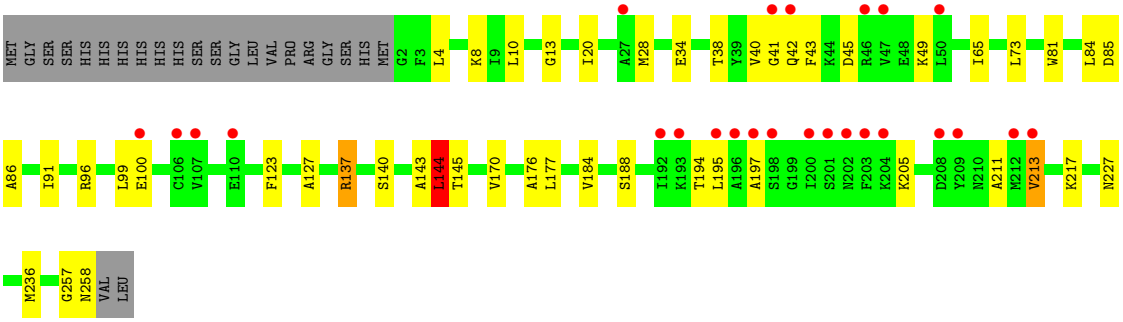
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain L:

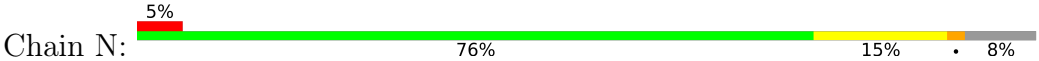


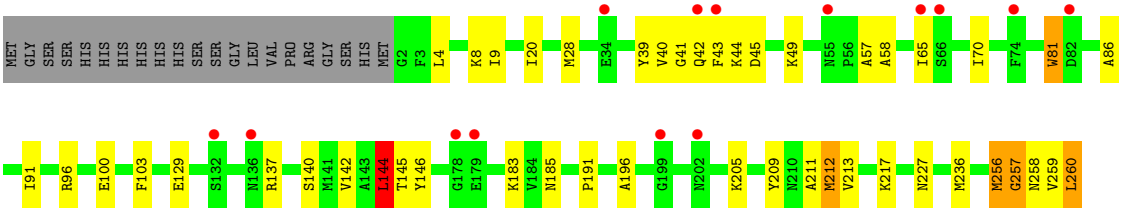
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain M:

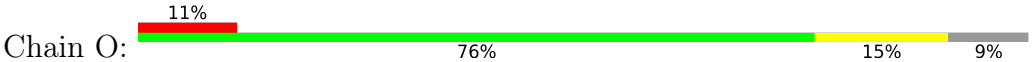


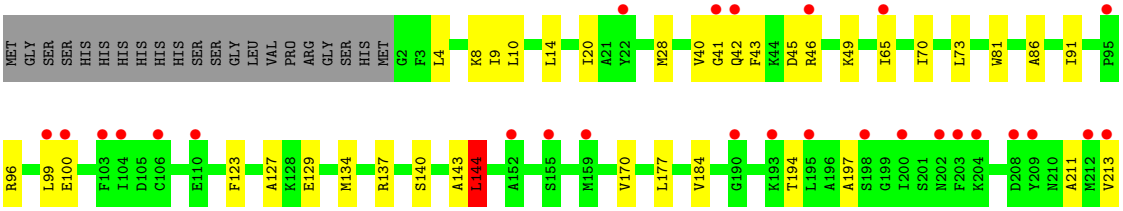
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



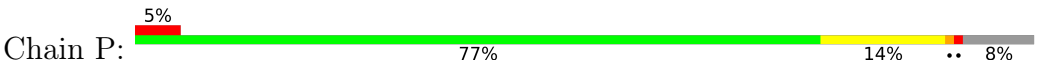


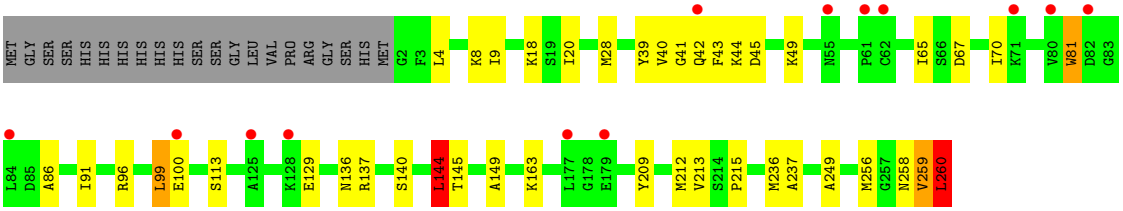
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]





• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.41Å 123.46Å 203.33Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.99-2.50) 99.7 (19.99-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.21 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.241 , 0.292 0.241 , 0.292	Depositor DCC
R_{free} test set	7281 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 10.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32732	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7847e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, 09T

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	0.97	0/1967	0.95	3/2655 (0.1%)
1	B	0.92	0/1952	0.88	2/2634 (0.1%)
1	C	0.95	0/1967	0.92	3/2655 (0.1%)
1	D	0.96	0/1944	0.91	2/2623 (0.1%)
1	E	0.73	0/1959	0.79	2/2644 (0.1%)
1	F	0.71	0/1967	0.79	1/2655 (0.0%)
1	G	0.70	0/1952	0.77	1/2634 (0.0%)
1	H	0.70	1/1967 (0.1%)	0.80	3/2655 (0.1%)
1	I	0.97	2/1967 (0.1%)	0.92	2/2655 (0.1%)
1	J	0.96	1/1952 (0.1%)	0.90	4/2634 (0.2%)
1	K	1.01	1/1967 (0.1%)	0.94	2/2655 (0.1%)
1	L	0.91	0/1952	0.88	1/2634 (0.0%)
1	M	0.71	0/1952	0.79	1/2634 (0.0%)
1	N	0.70	1/1967 (0.1%)	0.79	1/2655 (0.0%)
1	O	0.72	0/1944	0.80	3/2623 (0.1%)
1	P	0.70	1/1967 (0.1%)	0.82	5/2655 (0.2%)
All	All	0.84	7/31343 (0.0%)	0.86	36/42300 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	243	GLU	CD-OE1	5.36	1.31	1.25
1	I	2	GLY	N-CA	5.32	1.54	1.46
1	I	81	TRP	CD2-CE2	5.09	1.47	1.41
1	K	81	TRP	CD2-CE2	5.09	1.47	1.41
1	N	81	TRP	CD2-CE2	5.06	1.47	1.41

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	144	LEU	CA-CB-CG	-9.26	94.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	144	LEU	CA-CB-CG	-9.19	94.17	115.30
1	G	144	LEU	CA-CB-CG	-9.08	94.42	115.30
1	K	144	LEU	CA-CB-CG	-8.87	94.89	115.30
1	C	144	LEU	CA-CB-CG	-8.86	94.92	115.30

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	1936	0	1956	65	0
1	B	1921	0	1936	19	0
1	C	1936	0	1956	45	0
1	D	1913	0	1930	27	0
1	E	1928	0	1945	46	0
1	F	1936	0	1956	38	0
1	G	1921	0	1936	26	0
1	H	1936	0	1956	54	0
1	I	1936	0	1956	35	0
1	J	1921	0	1936	22	0
1	K	1936	0	1956	54	0
1	L	1921	0	1936	25	0
1	M	1921	0	1936	28	0
1	N	1936	0	1956	53	0
1	O	1913	0	1930	22	0
1	P	1936	0	1956	37	0
2	A	44	0	26	2	0
2	B	44	0	26	6	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	6	0
2	F	44	0	26	2	0
2	G	44	0	26	4	0
2	H	44	0	26	3	0
2	I	44	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	44	0	26	1	0
2	K	44	0	26	3	0
2	L	44	0	26	3	0
2	M	44	0	26	10	0
2	N	44	0	26	3	0
2	O	44	0	26	3	0
2	P	44	0	26	1	0
3	A	20	0	14	1	0
3	B	20	0	14	7	0
3	C	20	0	14	1	0
3	D	20	0	14	2	0
3	E	20	0	14	4	0
3	F	20	0	14	0	0
3	G	20	0	14	3	0
3	H	20	0	14	0	0
3	I	20	0	14	1	0
3	J	20	0	14	2	0
3	K	20	0	14	1	0
3	L	20	0	14	2	0
3	M	20	0	14	12	0
3	N	20	0	14	1	0
3	O	20	0	14	5	0
3	P	20	0	14	0	0
4	A	71	0	0	7	0
4	B	55	0	0	1	0
4	C	71	0	0	2	0
4	D	77	0	0	8	0
4	E	48	0	0	8	0
4	F	48	0	0	7	0
4	G	35	0	0	3	0
4	H	33	0	0	1	0
4	I	77	0	0	4	0
4	J	63	0	0	3	0
4	K	79	0	0	3	0
4	L	56	0	0	4	0
4	M	35	0	0	5	0
4	N	34	0	0	5	0
4	O	38	0	0	3	0
4	P	41	0	0	8	0
All	All	32732	0	31773	520	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 8.

The worst 5 of 520 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:E:70:ILE:HA	4:E:653:HOH:O	1.39	1.19
1:F:55:ASN:HB2	4:F:600:HOH:O	1.42	1.19
1:N:212:MET:CE	1:N:259:VAL:HG11	1.73	1.17
1:M:34:GLU:HG2	4:M:840:HOH:O	1.43	1.14
1:F:109:ARG:HA	4:F:613:HOH:O	1.45	1.13

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	257/280 (92%)	242 (94%)	13 (5%)	2 (1%)	19	35
1	B	255/280 (91%)	241 (94%)	13 (5%)	1 (0%)	34	54
1	C	257/280 (92%)	244 (95%)	12 (5%)	1 (0%)	34	54
1	D	254/280 (91%)	240 (94%)	13 (5%)	1 (0%)	34	54
1	E	256/280 (91%)	241 (94%)	13 (5%)	2 (1%)	19	35
1	F	257/280 (92%)	243 (95%)	13 (5%)	1 (0%)	34	54
1	G	255/280 (91%)	243 (95%)	11 (4%)	1 (0%)	34	54
1	H	257/280 (92%)	239 (93%)	14 (5%)	4 (2%)	9	17
1	I	257/280 (92%)	244 (95%)	12 (5%)	1 (0%)	34	54
1	J	255/280 (91%)	237 (93%)	17 (7%)	1 (0%)	34	54
1	K	257/280 (92%)	238 (93%)	17 (7%)	2 (1%)	19	35
1	L	255/280 (91%)	241 (94%)	13 (5%)	1 (0%)	34	54
1	M	255/280 (91%)	241 (94%)	13 (5%)	1 (0%)	34	54
1	N	257/280 (92%)	241 (94%)	13 (5%)	3 (1%)	13	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	254/280 (91%)	239 (94%)	14 (6%)	1 (0%)	34	54
1	P	257/280 (92%)	242 (94%)	14 (5%)	1 (0%)	34	54
All	All	4095/4480 (91%)	3856 (94%)	215 (5%)	24 (1%)	25	43

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	GLY
1	C	41	GLY
1	F	41	GLY
1	H	41	GLY
1	I	41	GLY

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	203/221 (92%)	190 (94%)	13 (6%)	17	33
1	B	201/221 (91%)	191 (95%)	10 (5%)	24	46
1	C	203/221 (92%)	192 (95%)	11 (5%)	22	42
1	D	200/221 (90%)	190 (95%)	10 (5%)	24	46
1	E	202/221 (91%)	191 (95%)	11 (5%)	22	42
1	F	203/221 (92%)	192 (95%)	11 (5%)	22	42
1	G	201/221 (91%)	191 (95%)	10 (5%)	24	46
1	H	203/221 (92%)	190 (94%)	13 (6%)	17	33
1	I	203/221 (92%)	191 (94%)	12 (6%)	19	37
1	J	201/221 (91%)	192 (96%)	9 (4%)	27	51
1	K	203/221 (92%)	192 (95%)	11 (5%)	22	42
1	L	201/221 (91%)	191 (95%)	10 (5%)	24	46
1	M	201/221 (91%)	190 (94%)	11 (6%)	21	41
1	N	203/221 (92%)	191 (94%)	12 (6%)	19	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	200/221 (90%)	189 (94%)	11 (6%)	21 41
1	P	203/221 (92%)	190 (94%)	13 (6%)	17 33
All	All	3231/3536 (91%)	3053 (94%)	178 (6%)	21 41

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	96	ARG
1	N	45	ASP
1	K	213	VAL
1	L	213	VAL
1	N	144	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	258	ASN
1	L	258	ASN
1	H	258	ASN
1	P	258	ASN
1	J	29	HIS

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)

32 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	NAD	A	261	-	42,48,48	2.23	9 (21%)	50,73,73	2.22	19 (38%)
2	NAD	I	261	-	42,48,48	2.22	8 (19%)	50,73,73	1.81	9 (18%)
3	09T	J	262	-	21,22,22	1.67	4 (19%)	28,32,32	1.76	7 (25%)
2	NAD	P	261	-	42,48,48	2.20	11 (26%)	50,73,73	2.25	15 (30%)
2	NAD	G	261	-	42,48,48	2.45	10 (23%)	50,73,73	2.11	14 (28%)
3	09T	C	262	-	21,22,22	2.28	4 (19%)	28,32,32	2.32	9 (32%)
2	NAD	K	261	-	42,48,48	2.35	8 (19%)	50,73,73	2.36	15 (30%)
2	NAD	M	261	-	42,48,48	2.45	9 (21%)	50,73,73	2.15	13 (26%)
3	09T	O	262	-	21,22,22	1.85	5 (23%)	28,32,32	1.22	3 (10%)
3	09T	F	262	-	21,22,22	1.64	3 (14%)	28,32,32	2.06	8 (28%)
2	NAD	H	261	-	42,48,48	2.61	12 (28%)	50,73,73	1.96	12 (24%)
3	09T	D	262	-	21,22,22	1.83	5 (23%)	28,32,32	1.77	6 (21%)
3	09T	A	262	-	21,22,22	1.36	4 (19%)	28,32,32	1.38	3 (10%)
2	NAD	F	261	-	42,48,48	2.41	9 (21%)	50,73,73	2.24	12 (24%)
2	NAD	B	261	-	42,48,48	2.26	12 (28%)	50,73,73	1.56	10 (20%)
3	09T	G	262	-	21,22,22	1.67	4 (19%)	28,32,32	1.10	1 (3%)
3	09T	N	262	-	21,22,22	1.71	5 (23%)	28,32,32	0.89	0
3	09T	P	262	-	21,22,22	1.59	3 (14%)	28,32,32	2.07	8 (28%)
3	09T	K	262	-	21,22,22	1.21	2 (9%)	28,32,32	1.98	3 (10%)
3	09T	M	262	-	21,22,22	1.45	3 (14%)	28,32,32	0.70	0
2	NAD	L	261	-	42,48,48	2.33	10 (23%)	50,73,73	1.74	13 (26%)
3	09T	B	262	-	21,22,22	1.37	2 (9%)	28,32,32	0.94	1 (3%)
3	09T	H	262	-	21,22,22	1.64	4 (19%)	28,32,32	0.87	1 (3%)
2	NAD	E	261	-	42,48,48	2.44	9 (21%)	50,73,73	2.22	16 (32%)
3	09T	E	262	-	21,22,22	1.72	4 (19%)	28,32,32	1.28	4 (14%)
2	NAD	C	261	-	42,48,48	2.10	10 (23%)	50,73,73	1.93	16 (32%)
2	NAD	J	261	-	42,48,48	2.53	6 (14%)	50,73,73	2.24	13 (26%)
3	09T	I	262	-	21,22,22	1.95	3 (14%)	28,32,32	1.92	7 (25%)
3	09T	L	262	-	21,22,22	1.24	2 (9%)	28,32,32	1.17	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	O	261	-	42,48,48	2.53	11 (26%)	50,73,73	2.32	13 (26%)
2	NAD	N	261	-	42,48,48	2.49	13 (30%)	50,73,73	2.09	13 (26%)
2	NAD	D	261	-	42,48,48	2.61	8 (19%)	50,73,73	2.19	14 (28%)

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	NAD	A	261	-	-	8/26/62/62	0/5/5/5
2	NAD	I	261	-	-	7/26/62/62	0/5/5/5
3	09T	J	262	-	-	0/4/4/4	0/3/3/3
2	NAD	P	261	-	-	5/26/62/62	0/5/5/5
2	NAD	G	261	-	-	11/26/62/62	0/5/5/5
3	09T	C	262	-	-	0/4/4/4	0/3/3/3
2	NAD	K	261	-	-	9/26/62/62	0/5/5/5
2	NAD	M	261	-	-	15/26/62/62	0/5/5/5
3	09T	O	262	-	-	0/4/4/4	0/3/3/3
3	09T	F	262	-	-	0/4/4/4	0/3/3/3
2	NAD	H	261	-	-	10/26/62/62	0/5/5/5
3	09T	D	262	-	-	0/4/4/4	0/3/3/3
3	09T	A	262	-	-	0/4/4/4	0/3/3/3
2	NAD	F	261	-	-	5/26/62/62	0/5/5/5
2	NAD	B	261	-	-	6/26/62/62	0/5/5/5
3	09T	G	262	-	-	0/4/4/4	0/3/3/3
3	09T	N	262	-	-	0/4/4/4	0/3/3/3
3	09T	P	262	-	-	0/4/4/4	0/3/3/3
3	09T	K	262	-	-	0/4/4/4	0/3/3/3
3	09T	M	262	-	-	0/4/4/4	0/3/3/3
2	NAD	L	261	-	-	6/26/62/62	0/5/5/5
3	09T	B	262	-	-	0/4/4/4	0/3/3/3
3	09T	H	262	-	-	0/4/4/4	0/3/3/3
2	NAD	E	261	-	-	17/26/62/62	0/5/5/5
3	09T	E	262	-	-	0/4/4/4	0/3/3/3
2	NAD	C	261	-	-	7/26/62/62	0/5/5/5
2	NAD	J	261	-	-	12/26/62/62	0/5/5/5
3	09T	I	262	-	-	0/4/4/4	0/3/3/3
3	09T	L	262	-	-	0/4/4/4	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	O	261	-	-	12/26/62/62	0/5/5/5
2	NAD	N	261	-	-	9/26/62/62	0/5/5/5
2	NAD	D	261	-	-	12/26/62/62	0/5/5/5

The worst 5 of 212 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	261	NAD	C2N-N1N	12.59	1.50	1.35
2	F	261	NAD	C2N-N1N	12.53	1.50	1.35
2	H	261	NAD	C2N-N1N	11.73	1.49	1.35
2	J	261	NAD	C2N-N1N	11.64	1.49	1.35
2	K	261	NAD	C2N-N1N	11.02	1.48	1.35

The worst 5 of 279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	261	NAD	O4D-C1D-C2D	-8.36	94.70	106.93
2	M	261	NAD	C1B-N9A-C4A	-8.23	112.18	126.64
2	G	261	NAD	C1B-N9A-C4A	-8.18	112.28	126.64
3	K	262	09T	C7-C6-C5	-8.03	114.98	120.46
2	J	261	NAD	C1B-N9A-C4A	-7.98	112.62	126.64

There are no chirality outliers.

5 of 151 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	261	NAD	C5B-O5B-PA-O1A
2	A	261	NAD	C5D-O5D-PN-O1N
2	A	261	NAD	C5D-O5D-PN-O2N
2	B	261	NAD	C5D-O5D-PN-O3
2	B	261	NAD	O4D-C1D-N1N-C2N

There are no ring outliers.

28 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	261	NAD	2	0
2	I	261	NAD	2	0
3	J	262	09T	2	0
2	P	261	NAD	1	0

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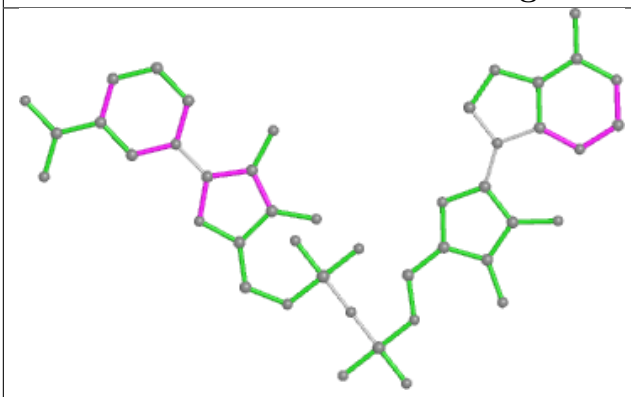
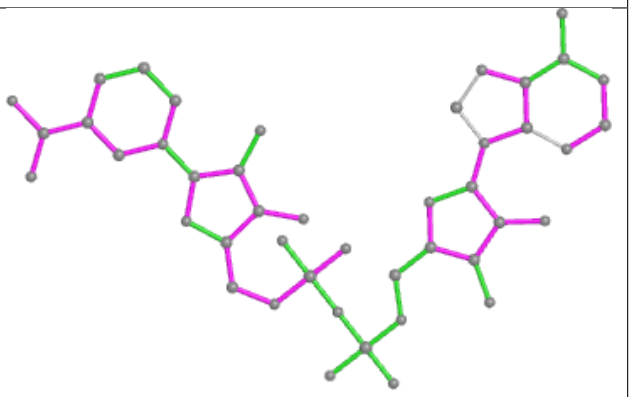
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	261	NAD	4	0
3	C	262	09T	1	0
2	K	261	NAD	3	0
2	M	261	NAD	10	0
3	O	262	09T	5	0
2	H	261	NAD	3	0
3	D	262	09T	2	0
3	A	262	09T	1	0
2	F	261	NAD	2	0
2	B	261	NAD	6	0
3	G	262	09T	3	0
3	N	262	09T	1	0
3	K	262	09T	1	0
3	M	262	09T	12	0
2	L	261	NAD	3	0
3	B	262	09T	7	0
2	E	261	NAD	6	0
3	E	262	09T	4	0
2	C	261	NAD	1	0
2	J	261	NAD	1	0
3	I	262	09T	1	0
3	L	262	09T	2	0
2	O	261	NAD	3	0
2	N	261	NAD	3	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.

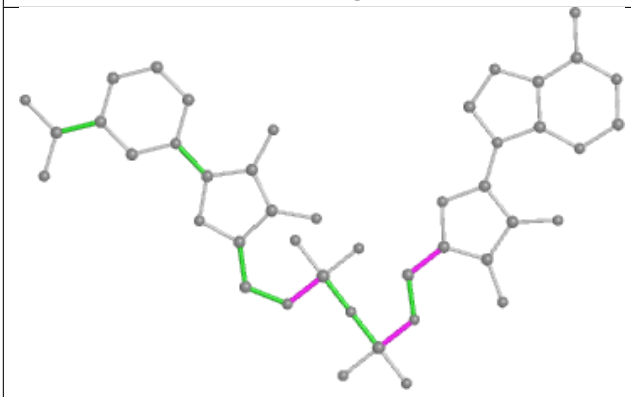
Ligand NAD A 261



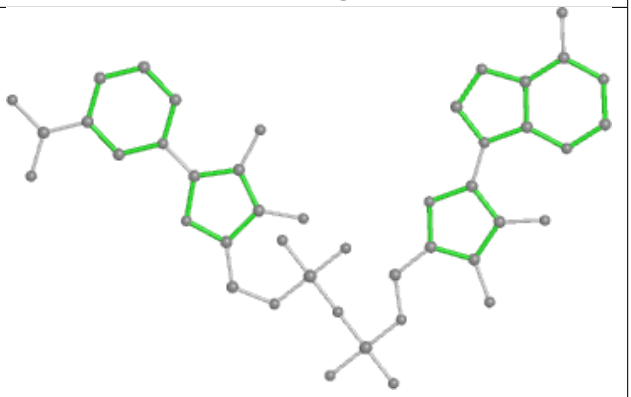
Bond lengths



Bond angles

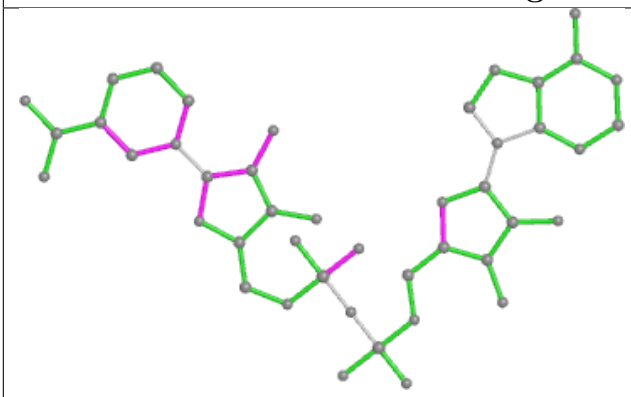


Torsions

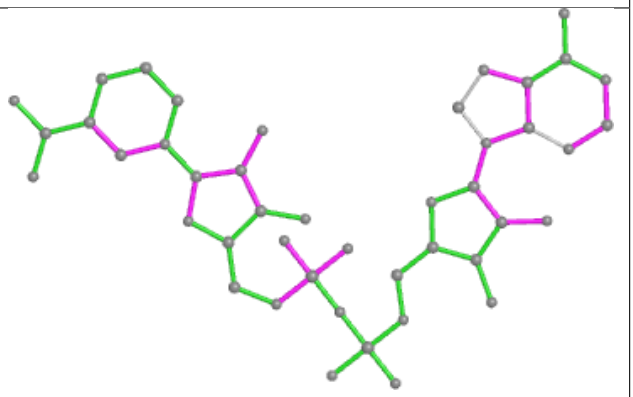


Rings

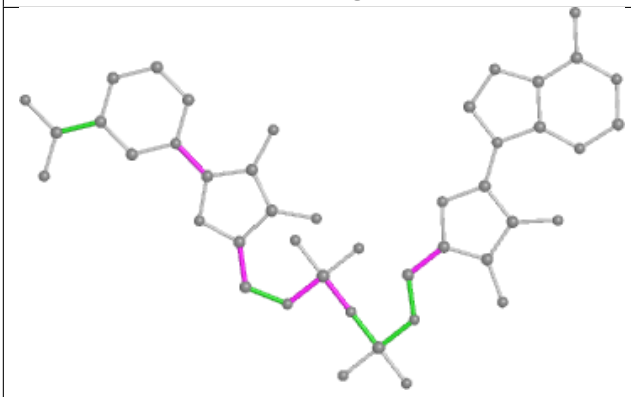
Ligand NAD I 261



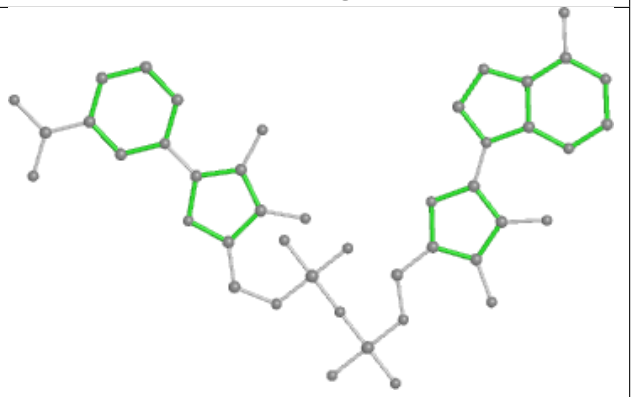
Bond lengths



Bond angles

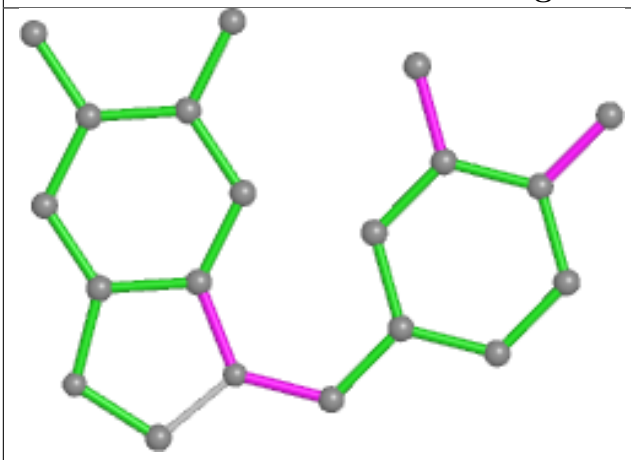


Torsions



Rings

Ligand 09T J 262



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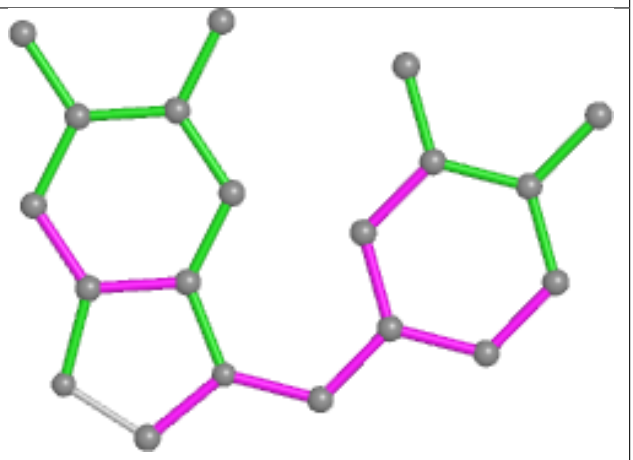

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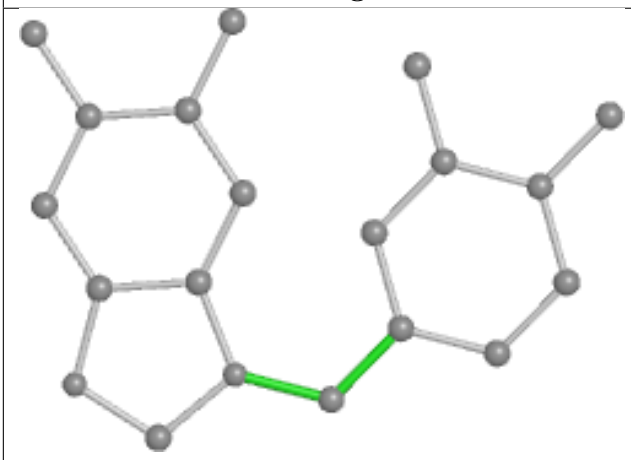

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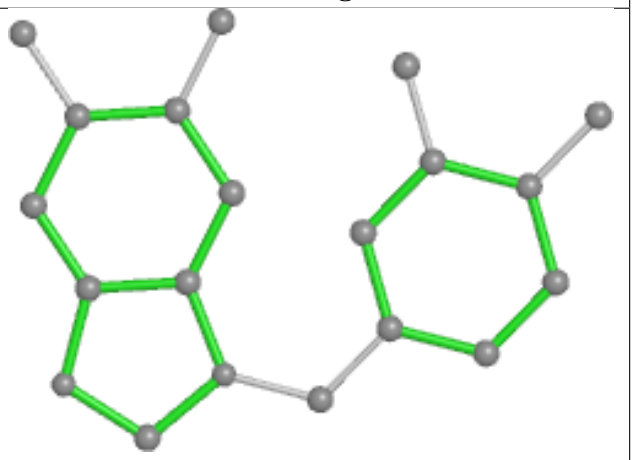
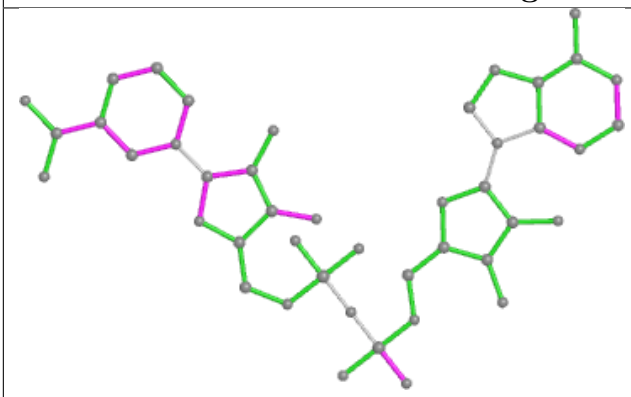


Rings

Ligand NAD P 261



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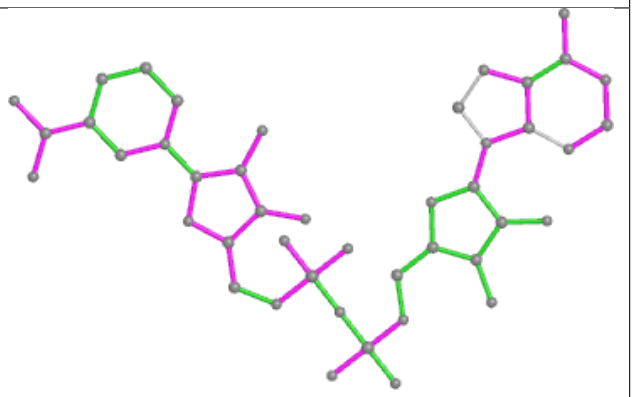
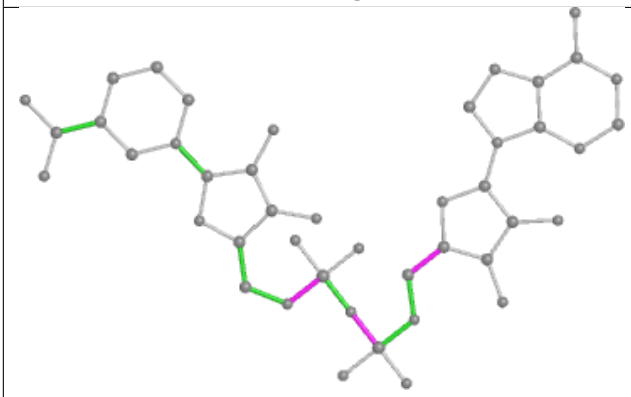


Bond angles



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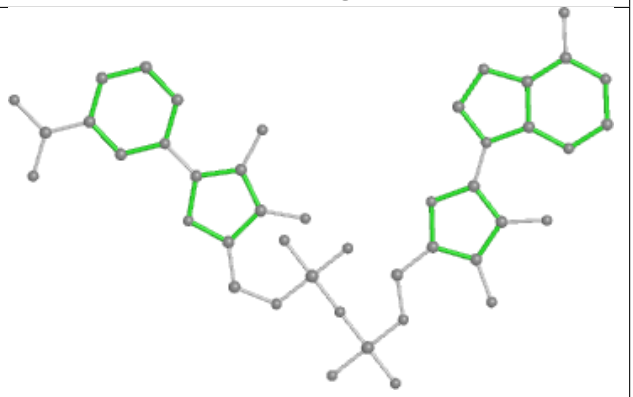
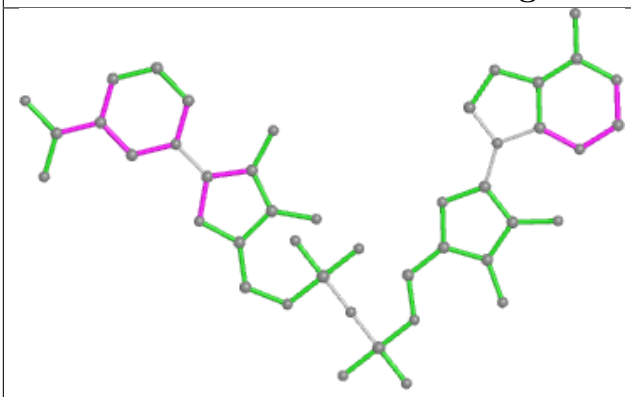
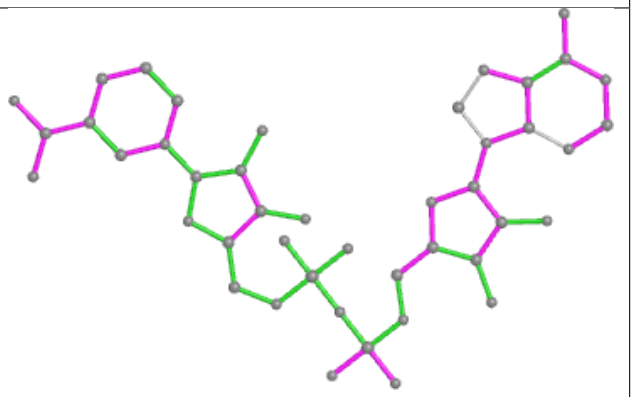


Rings

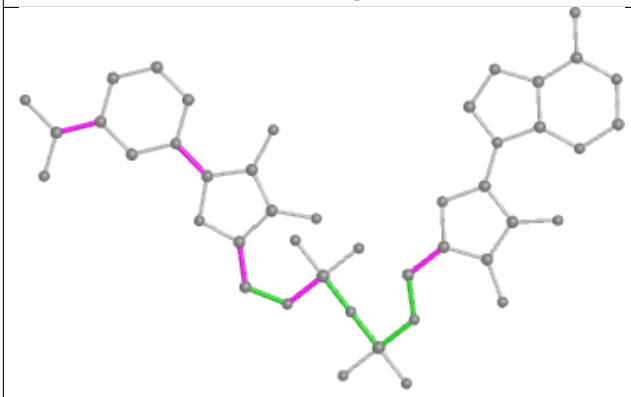
Ligand NAD G 261



Bond lengths



Bond angles



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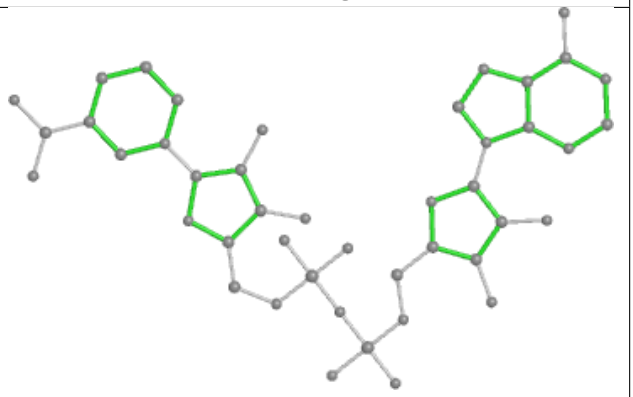
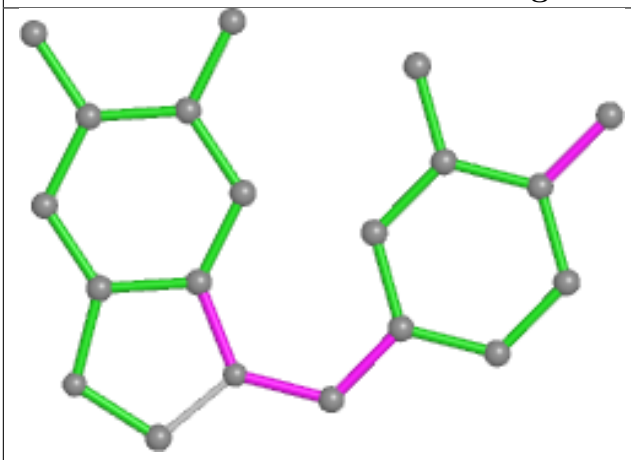


Rings

Ligand 09T C 262



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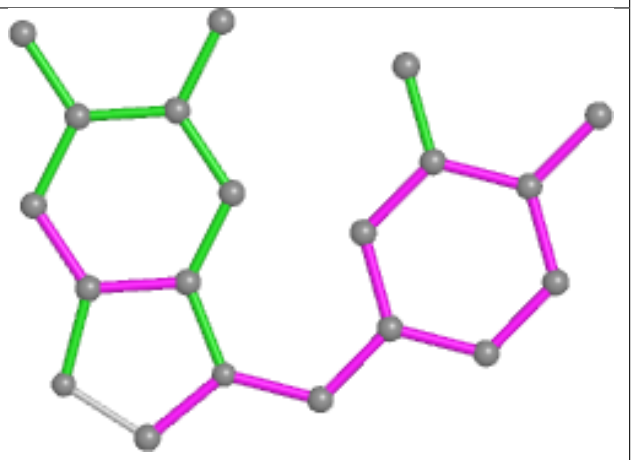
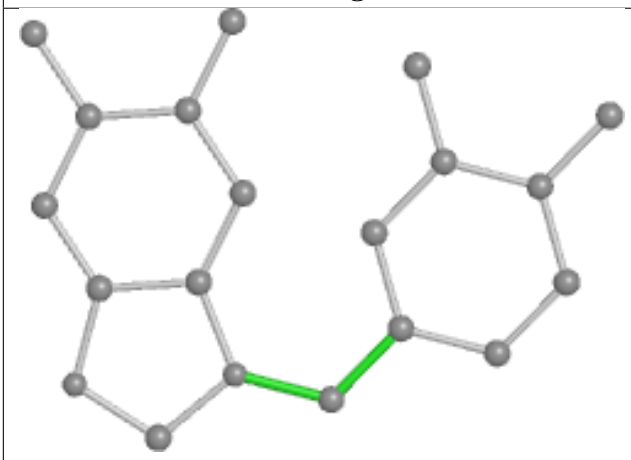


Bond angles



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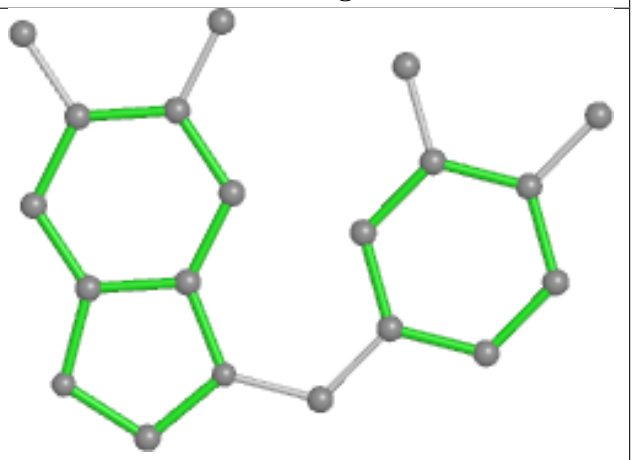
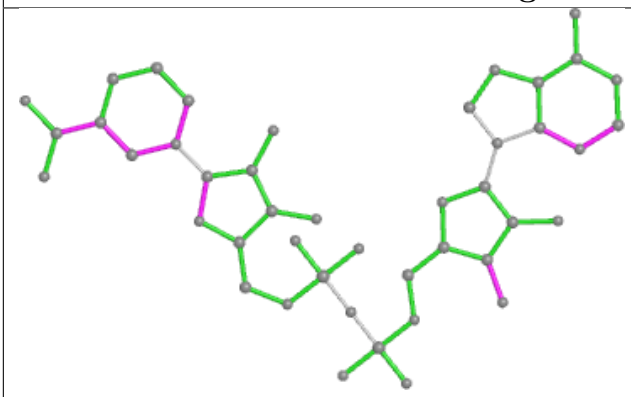


Rings

Ligand NAD K 261



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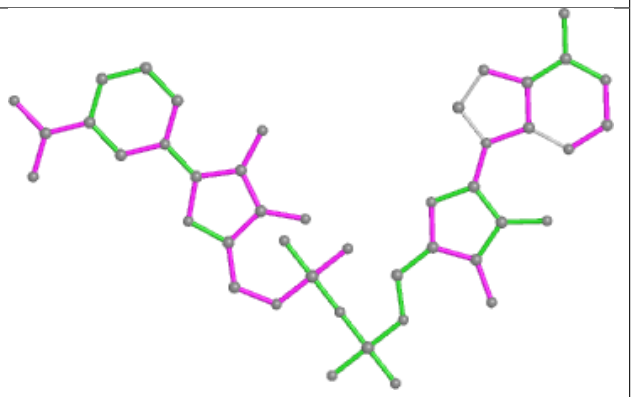
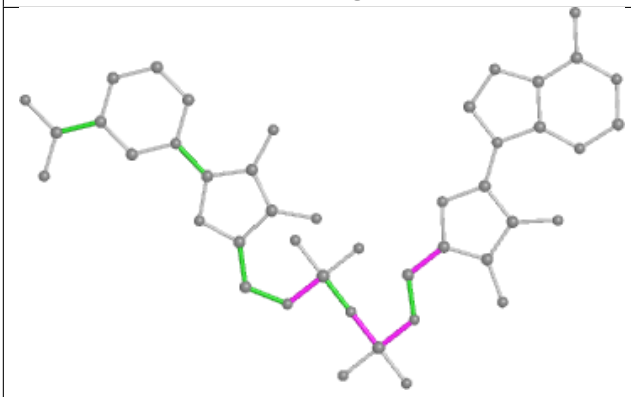


Bond angles



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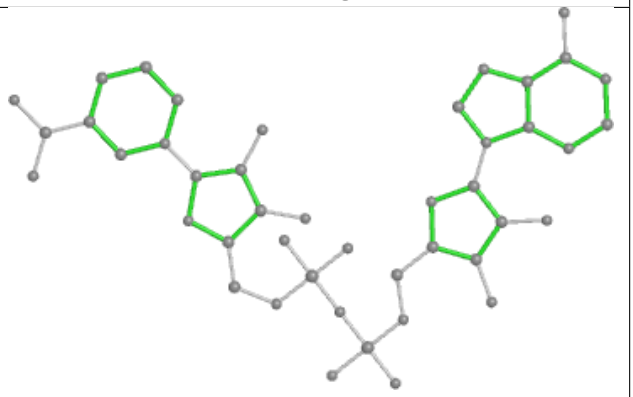
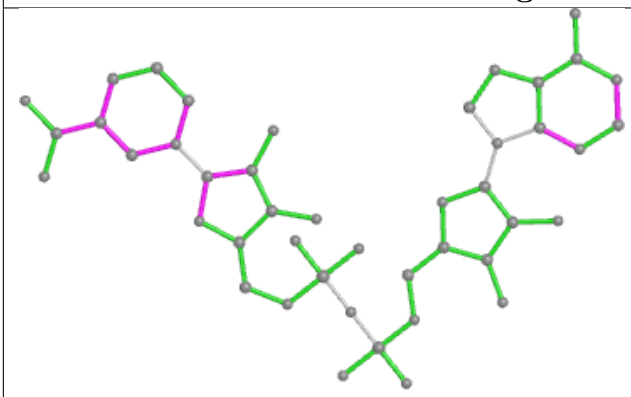
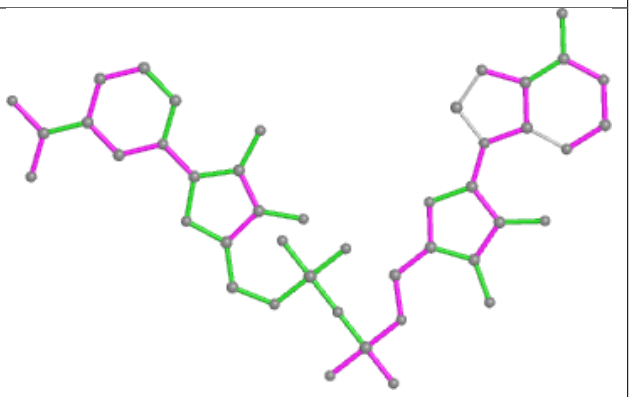


Rings

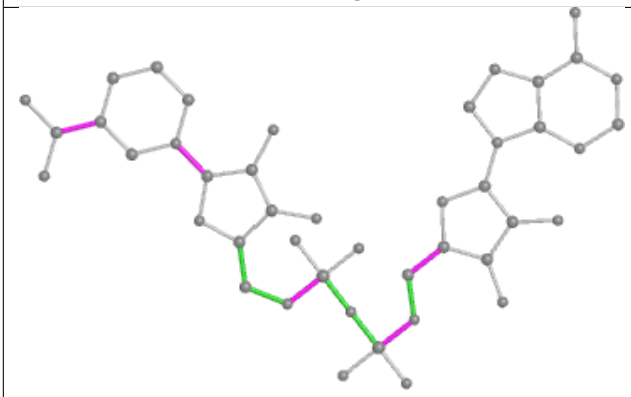
Ligand NAD M 261



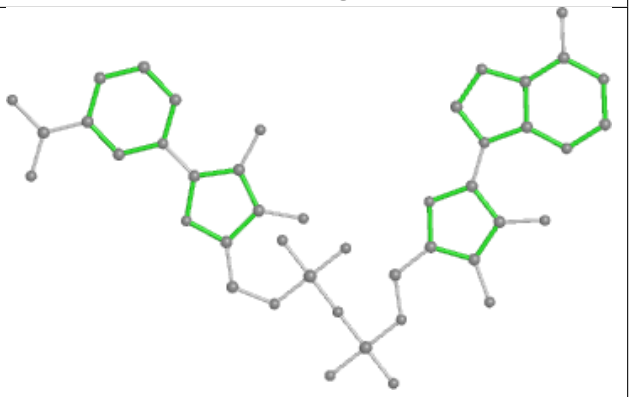
Bond lengths



Bond angles

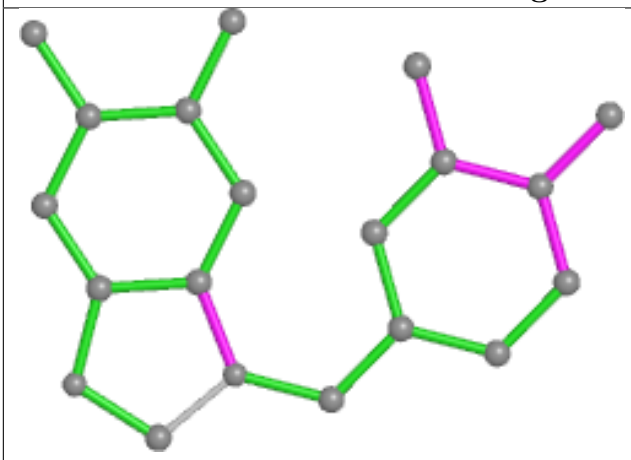


Torsions



Rings

Ligand 09T O 262



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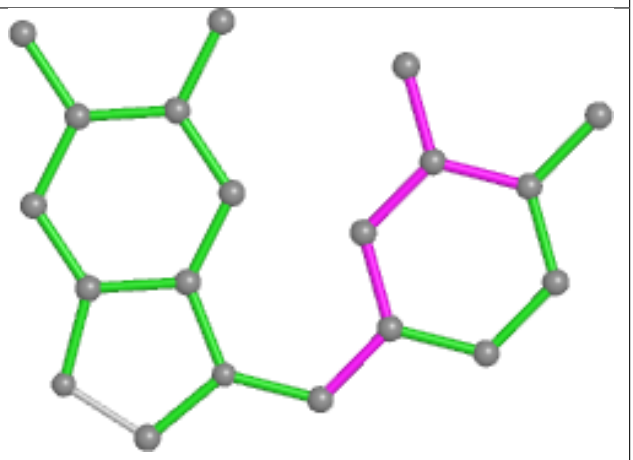

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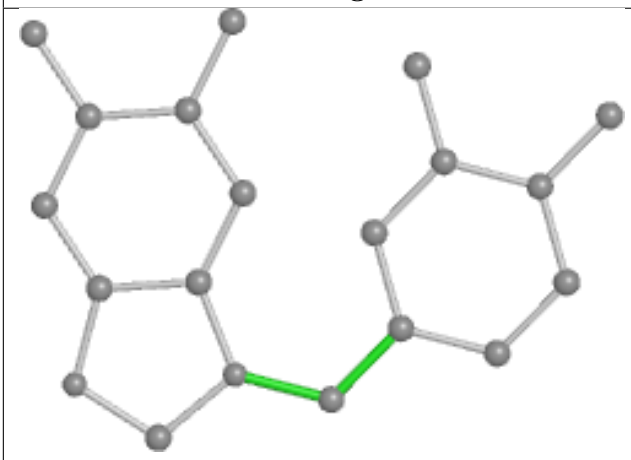

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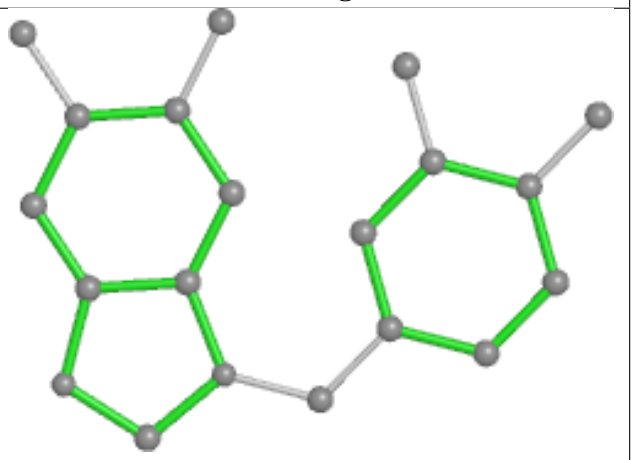
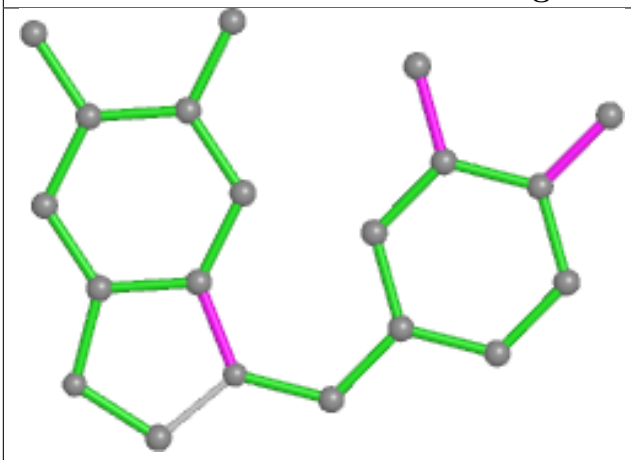


Rings

Ligand 09T F 262



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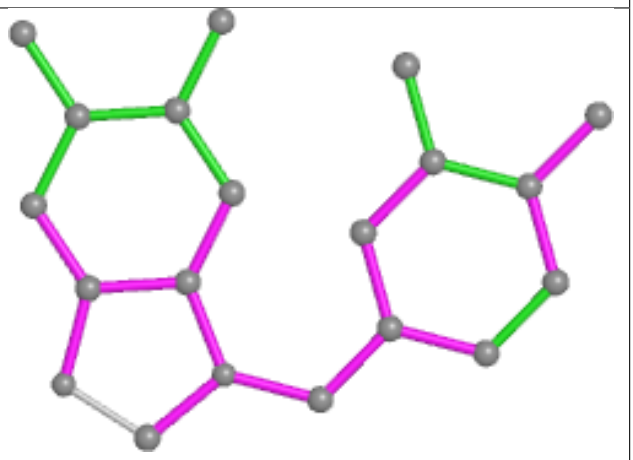
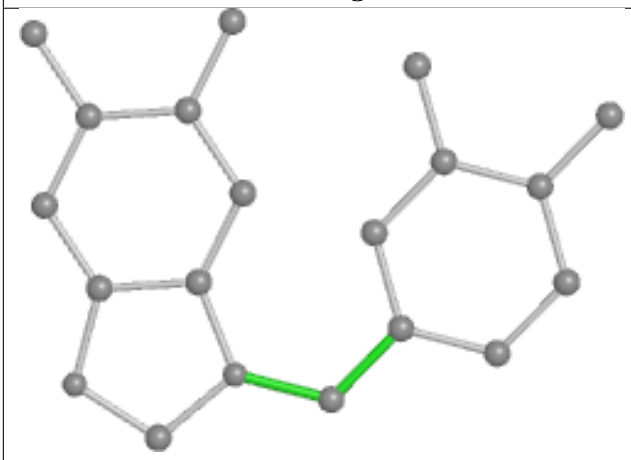
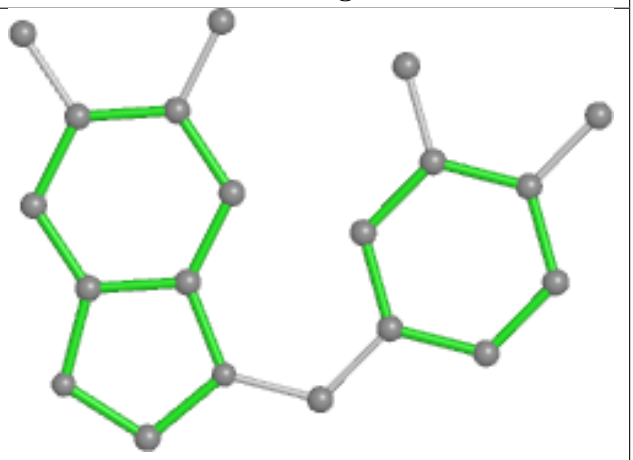


Bond angles

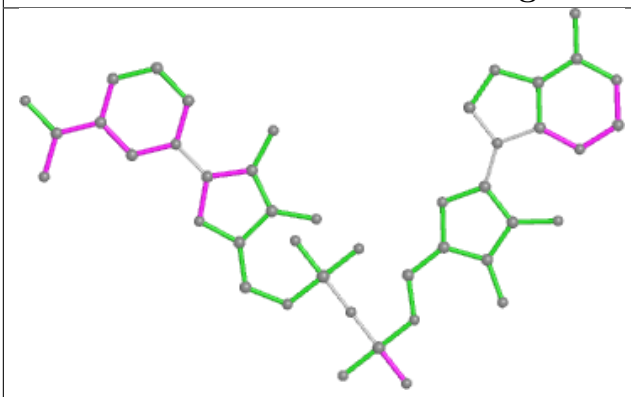


Torsions



Rings

Ligand NAD H 261



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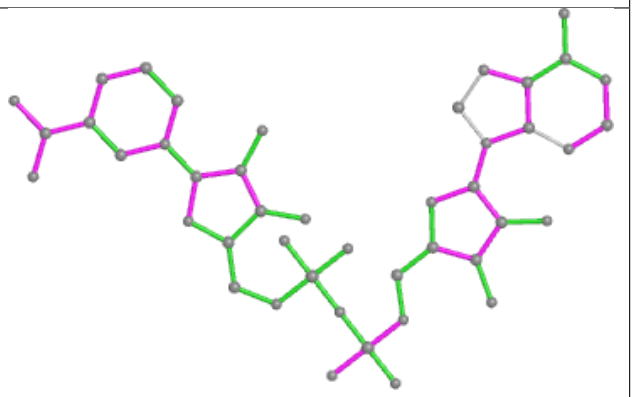
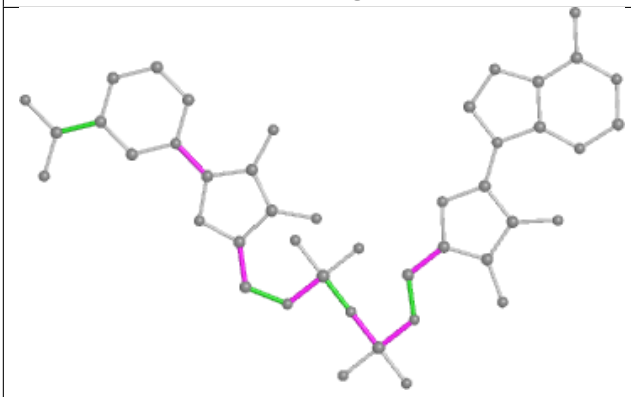


Bond angles



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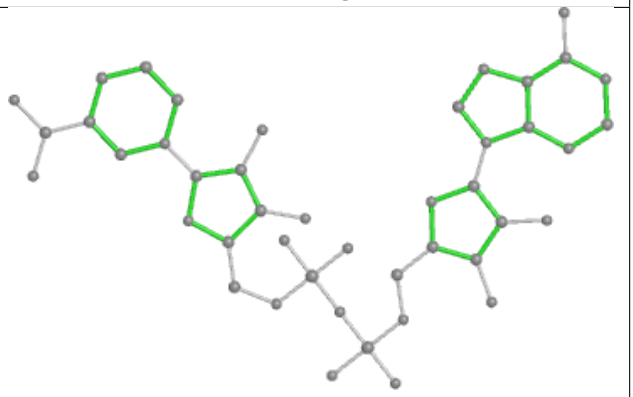
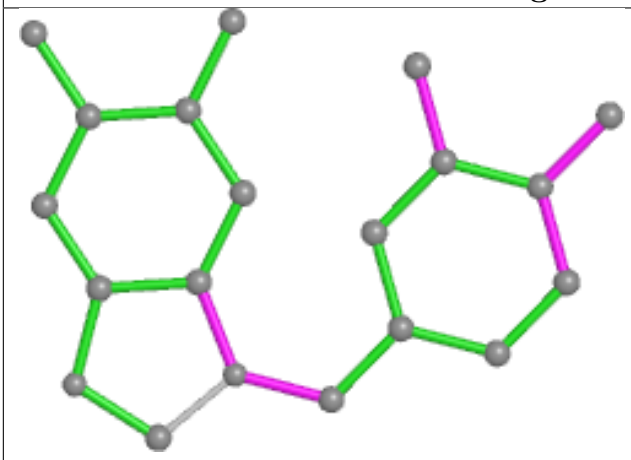


Rings

Ligand 09T D 262



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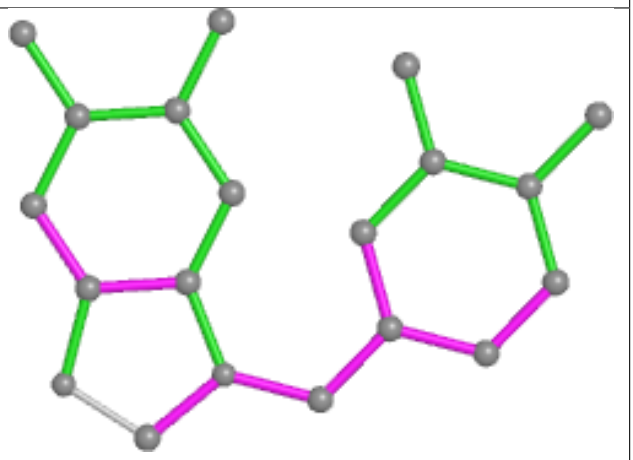
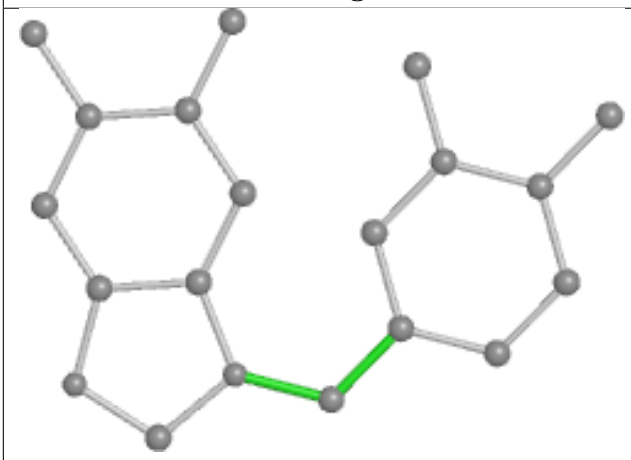
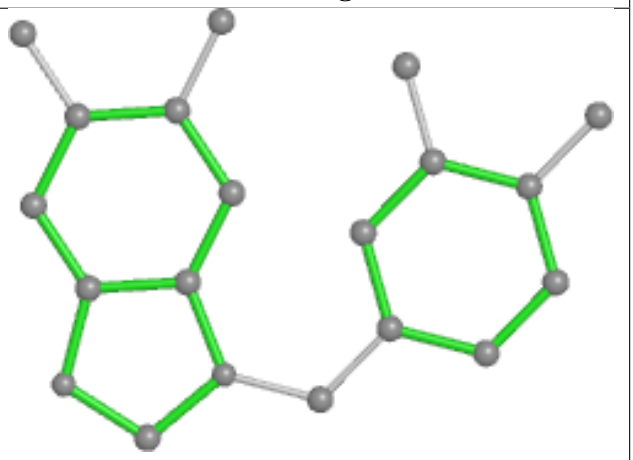


Bond angles

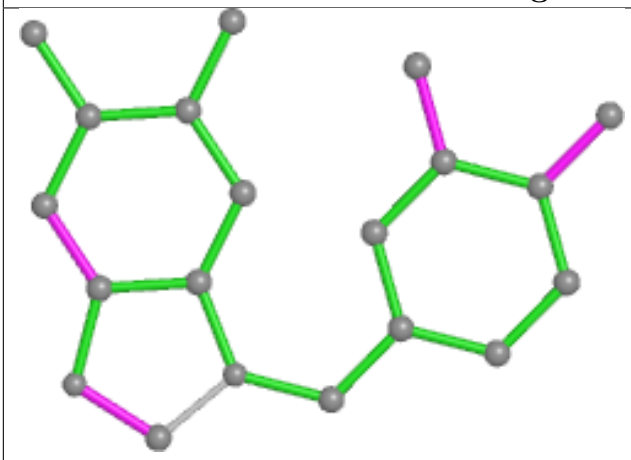


Torsions



Rings

Ligand 09T A 262



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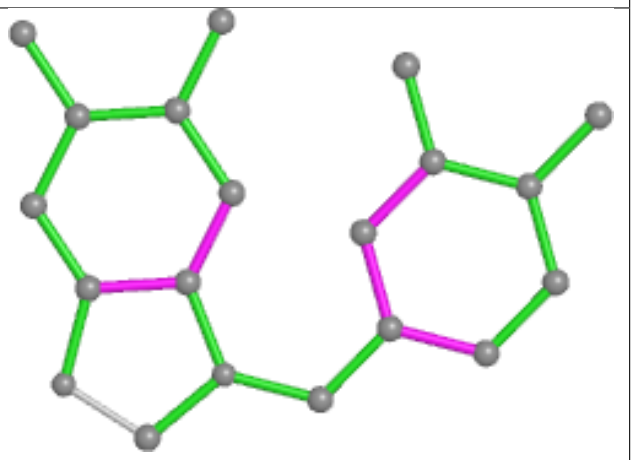
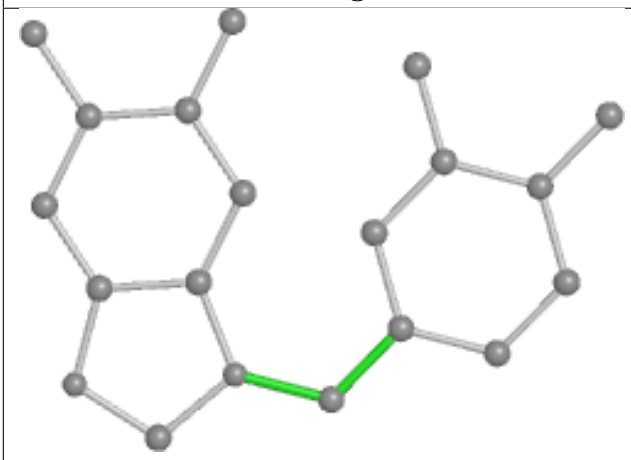


Bond angles



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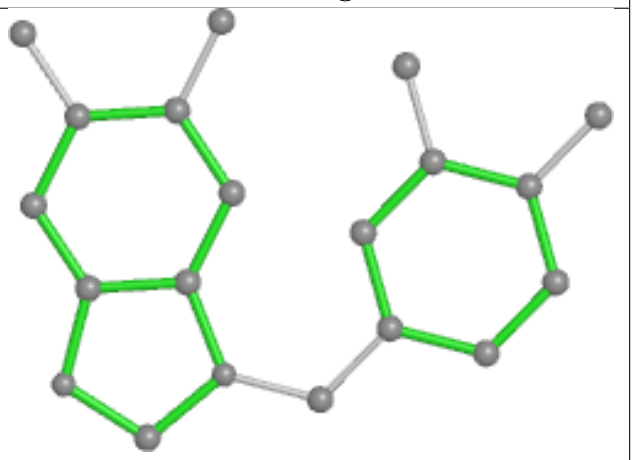
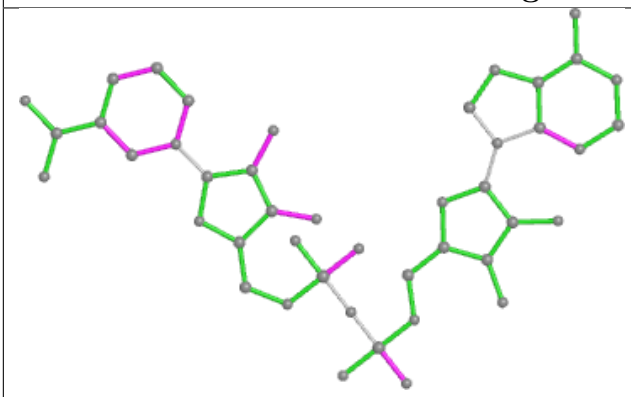


Rings

Ligand NAD F 261



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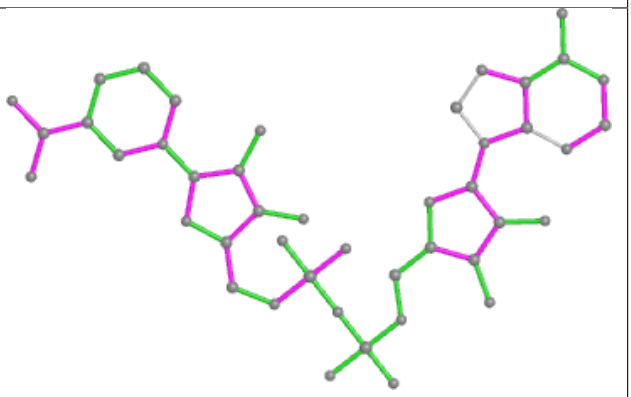
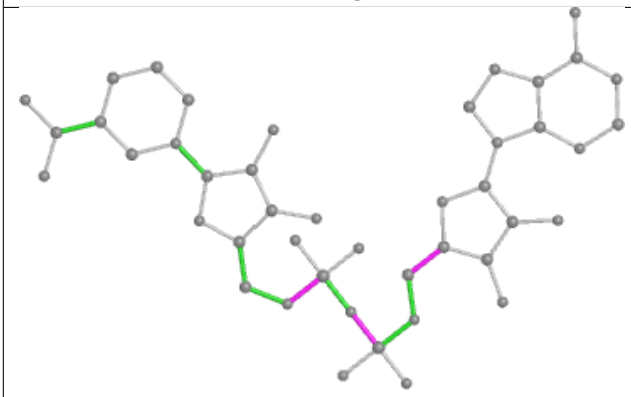


Bond angles



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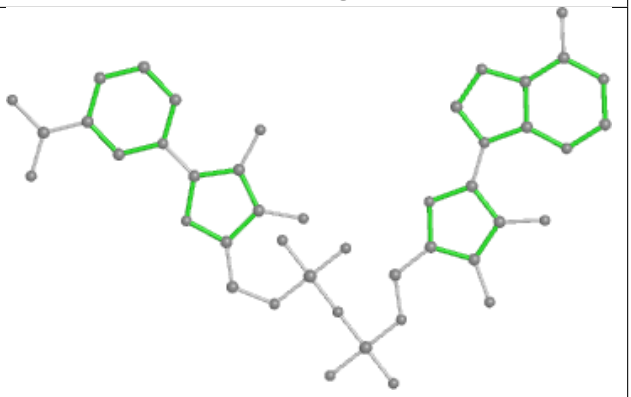
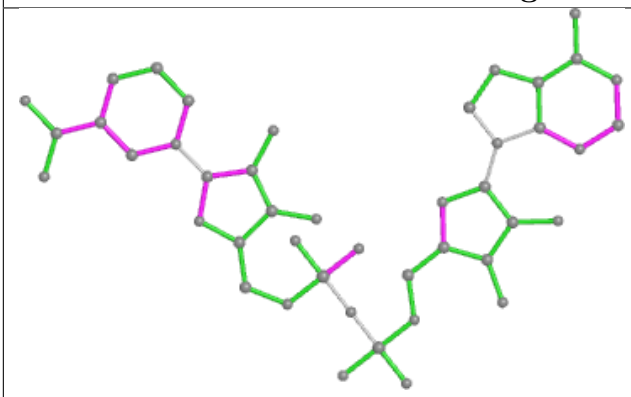
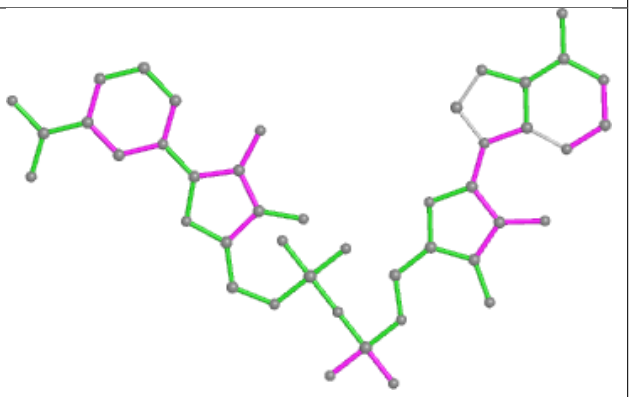


Rings

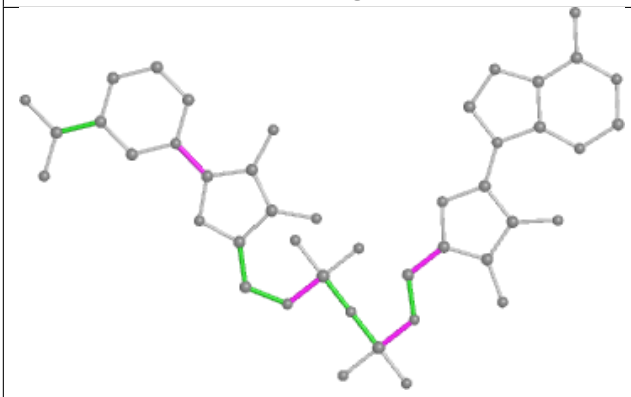
Ligand NAD B 261



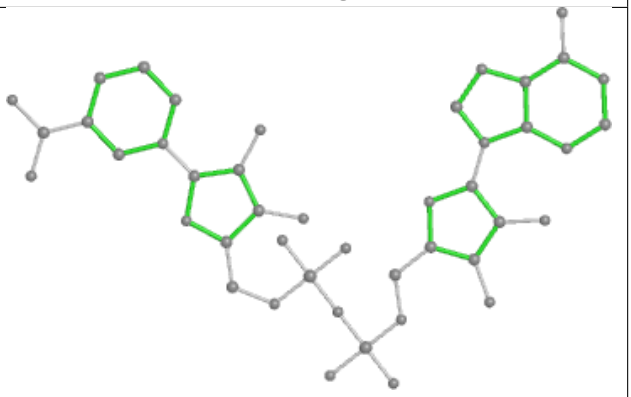
Bond lengths



Bond angles

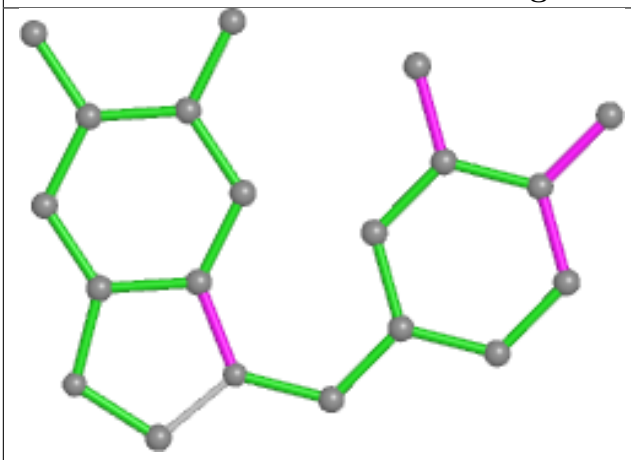


Torsions

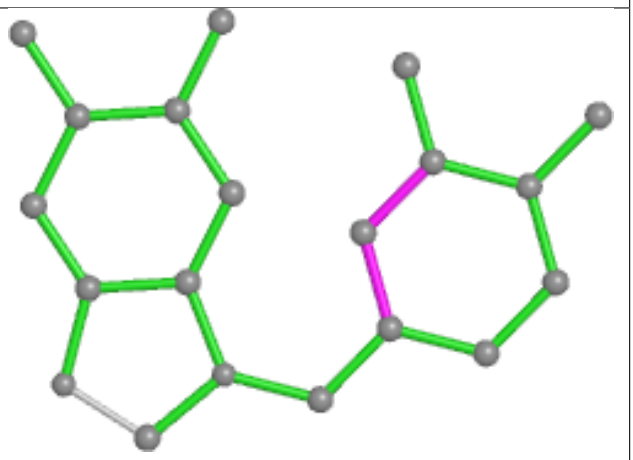


Rings

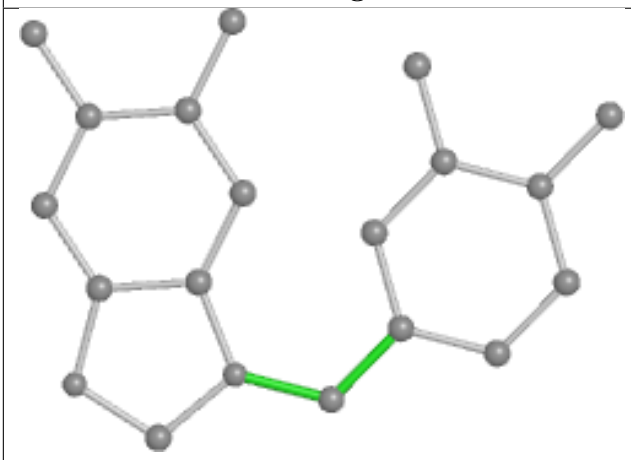
Ligand 09T G 262



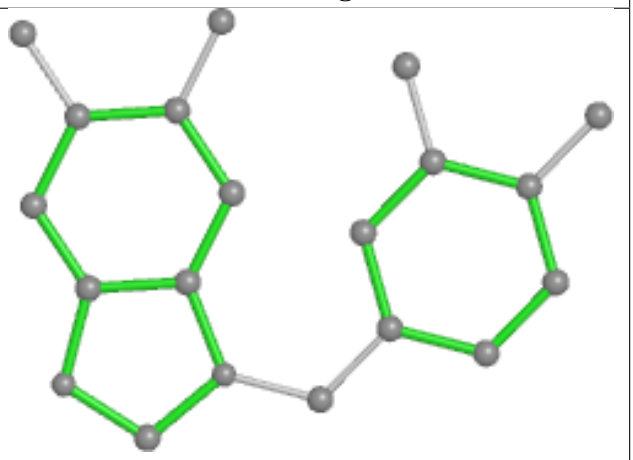
Bond lengths



Bond angles

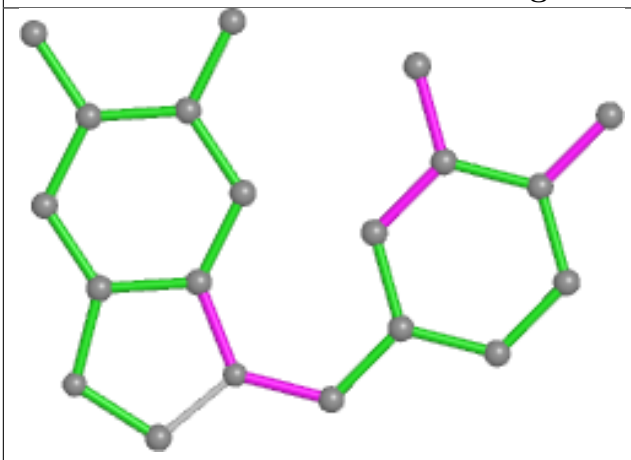


Torsions



Rings

Ligand 09T N 262



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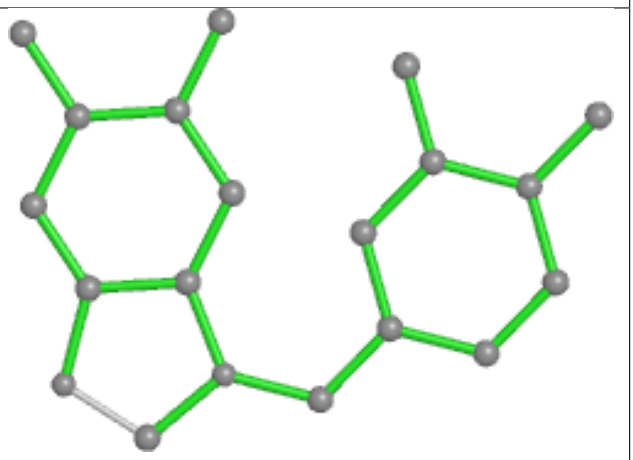
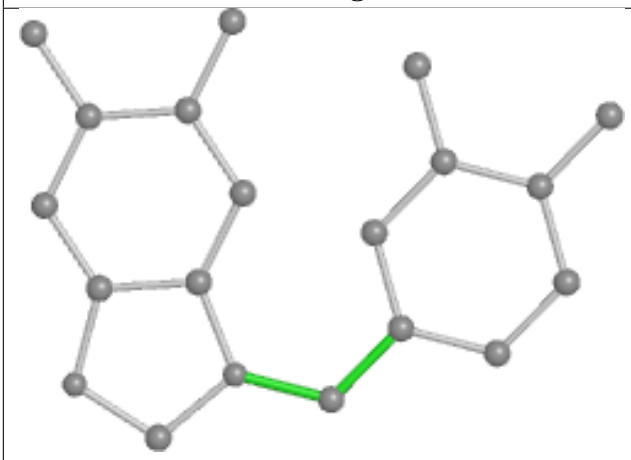
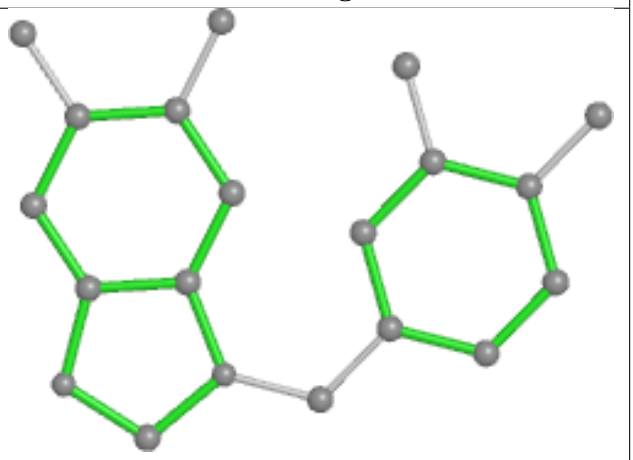


Bond angles

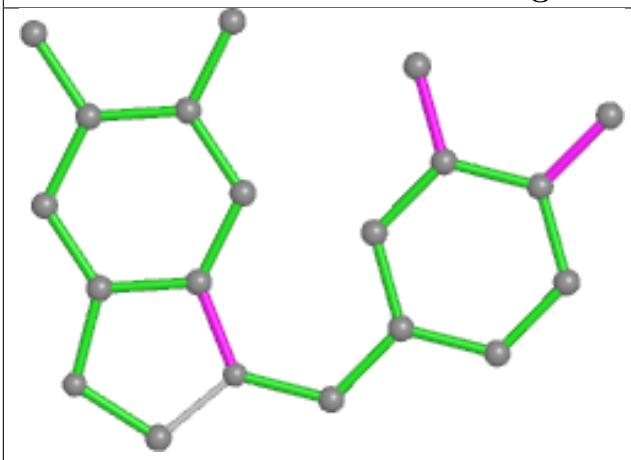


Torsions



Rings

Ligand 09T P 262



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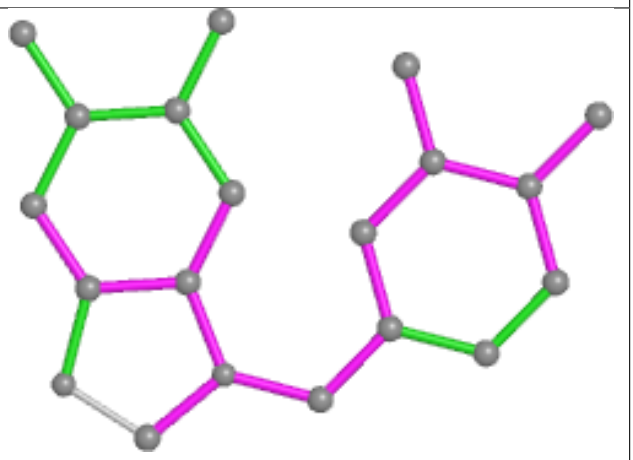
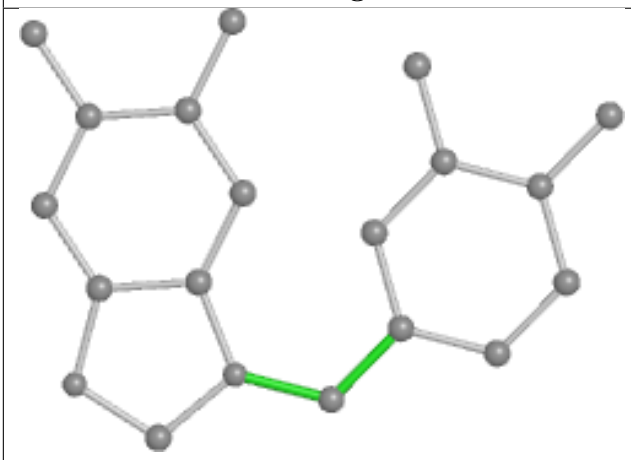
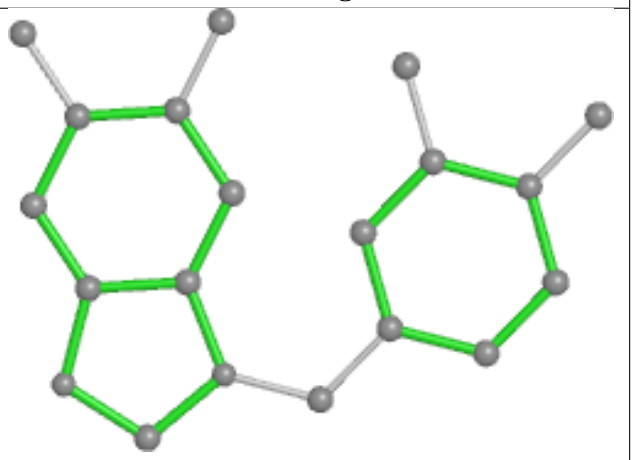


Bond angles

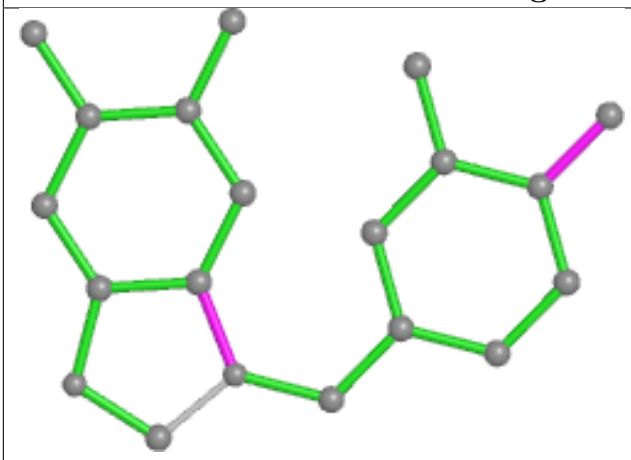


Torsions



Rings

Ligand 09T K 262



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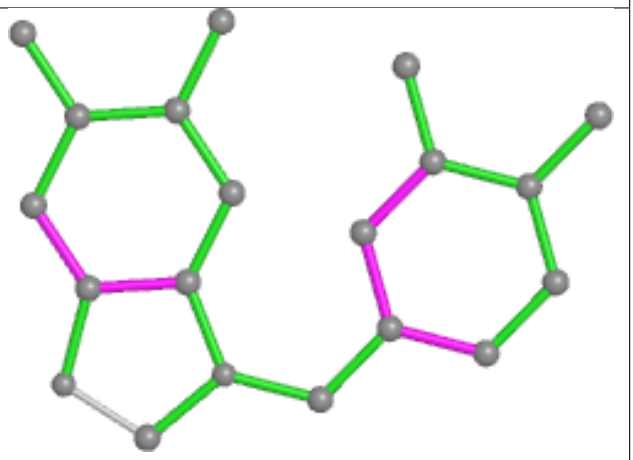
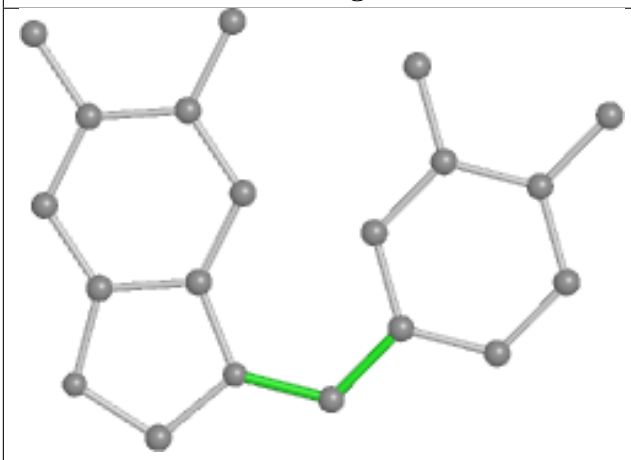
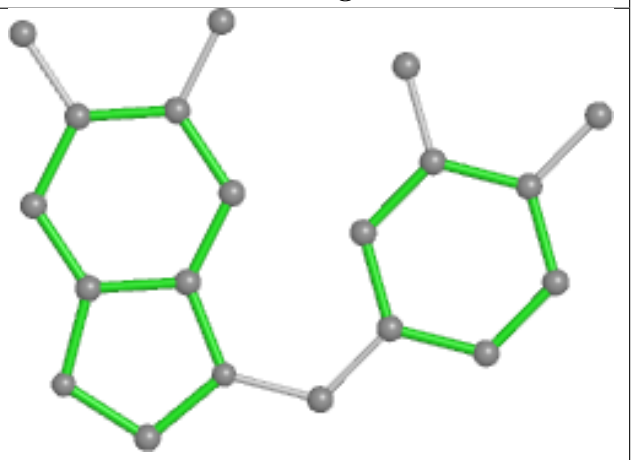


Bond angles

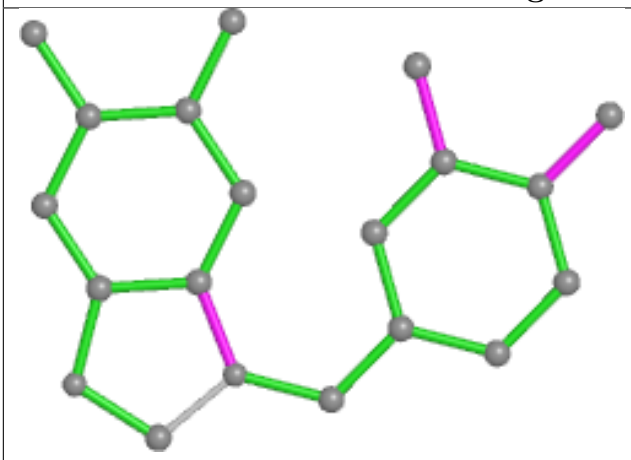


Torsions



Rings

Ligand 09T M 262



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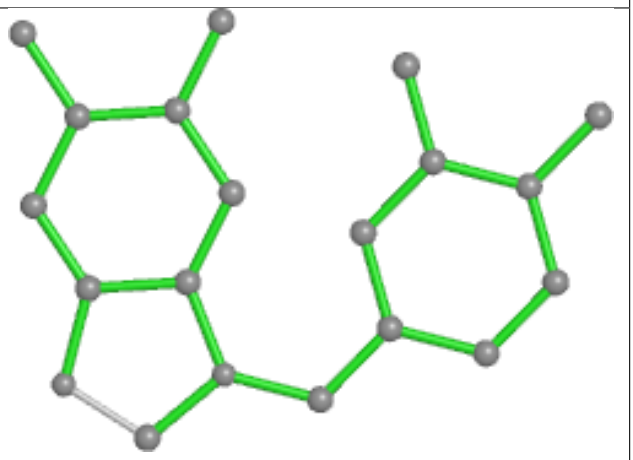
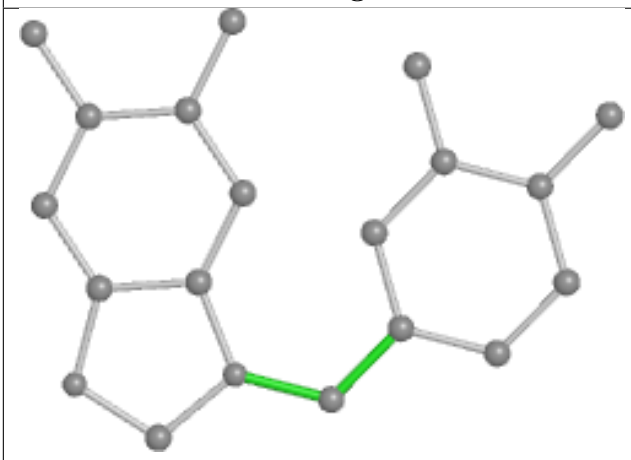


Bond angles



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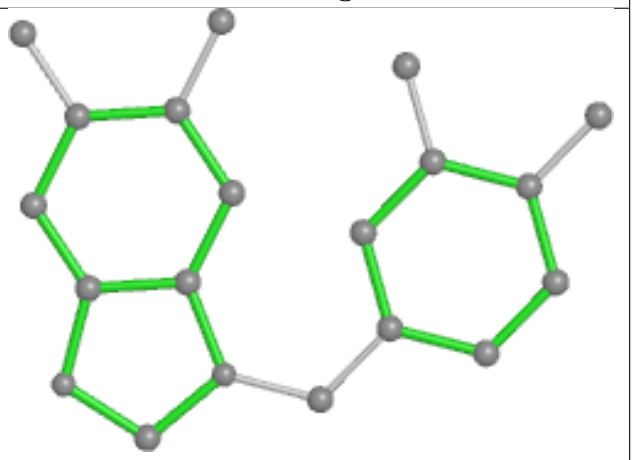
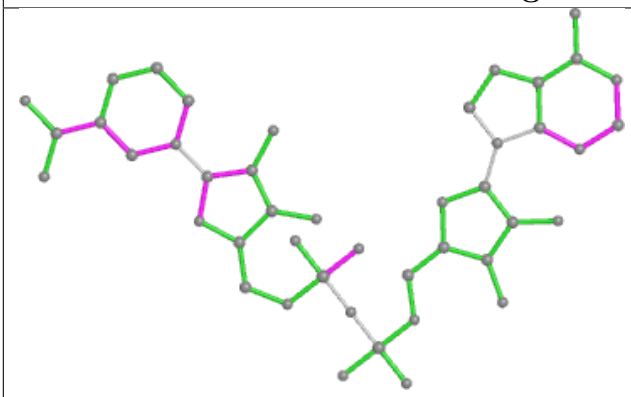


Rings

Ligand NAD L 261



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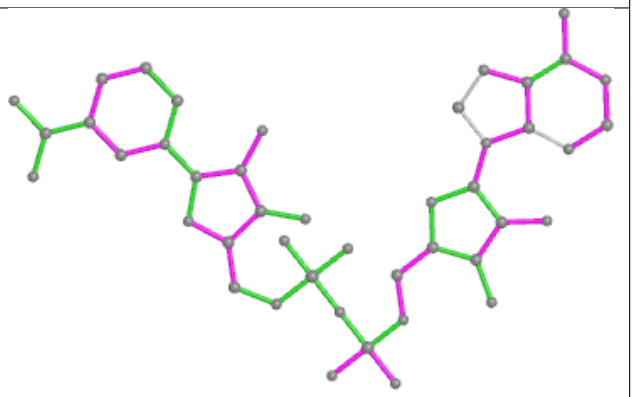

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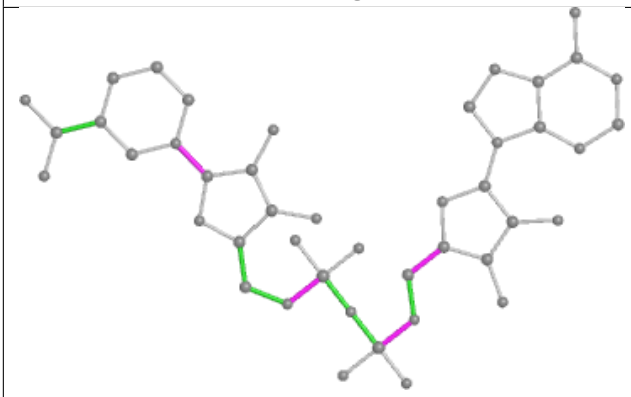

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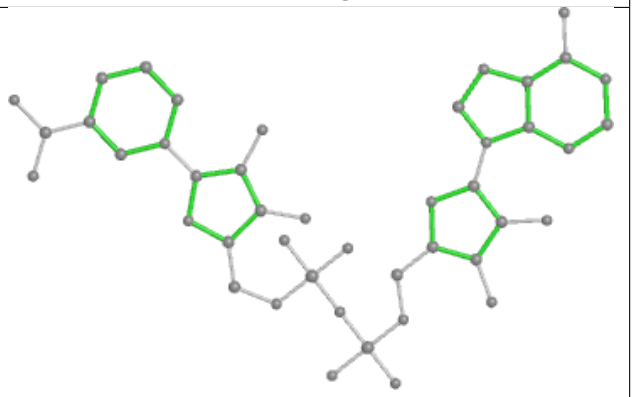
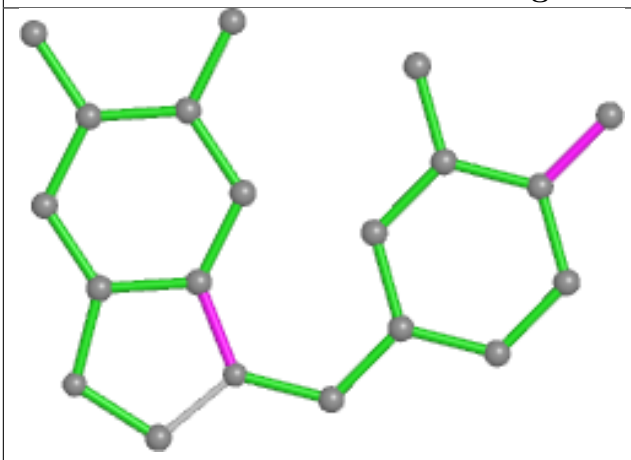


Rings

Ligand 09T B 262



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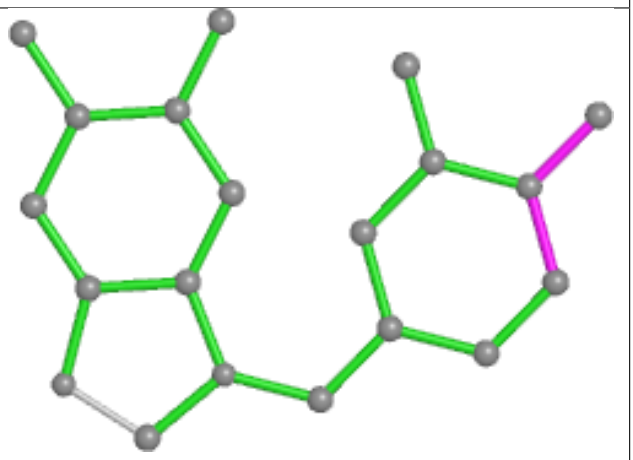
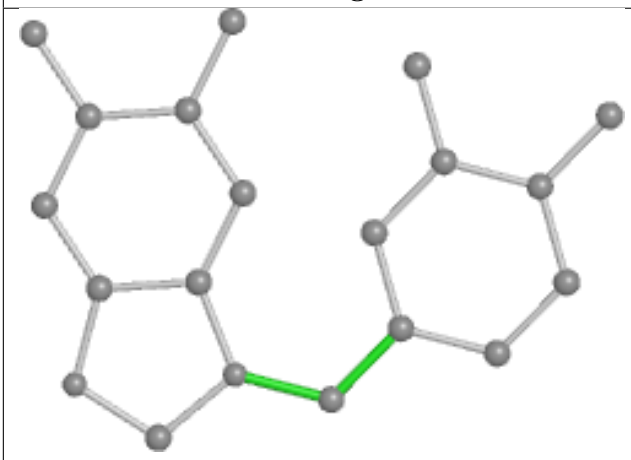


Bond angles



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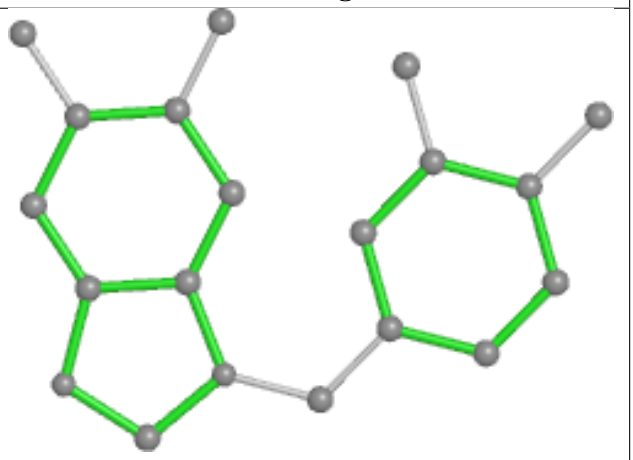
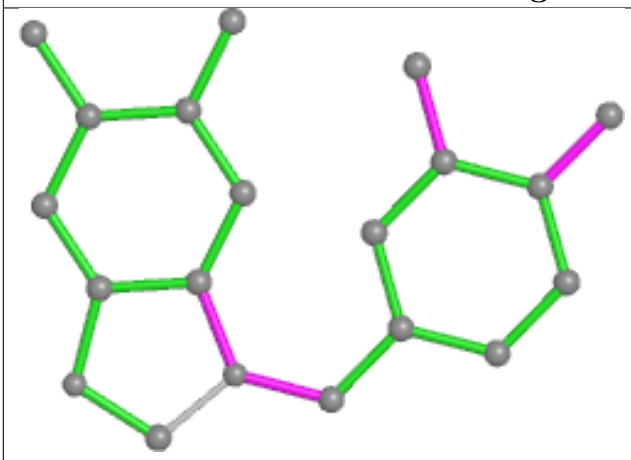


Rings

Ligand 09T H 262



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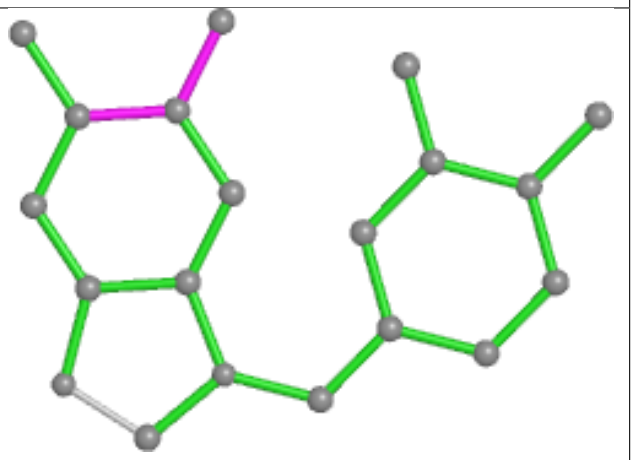
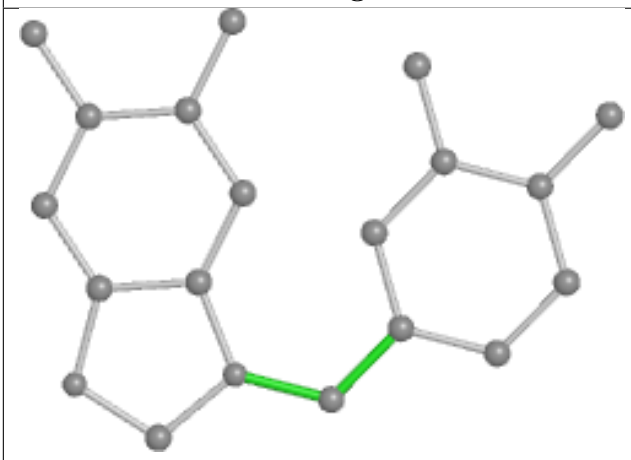


Bond angles



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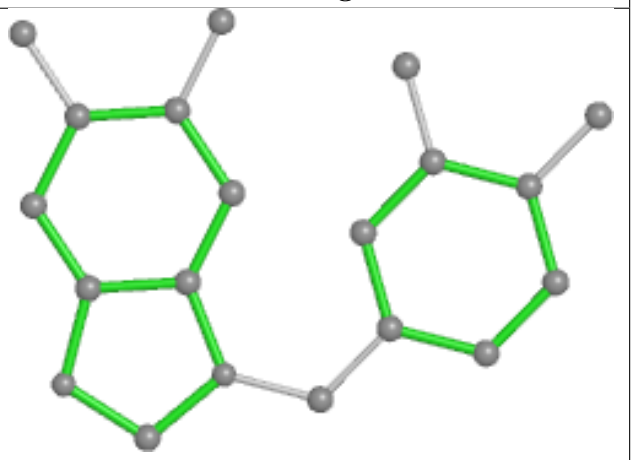
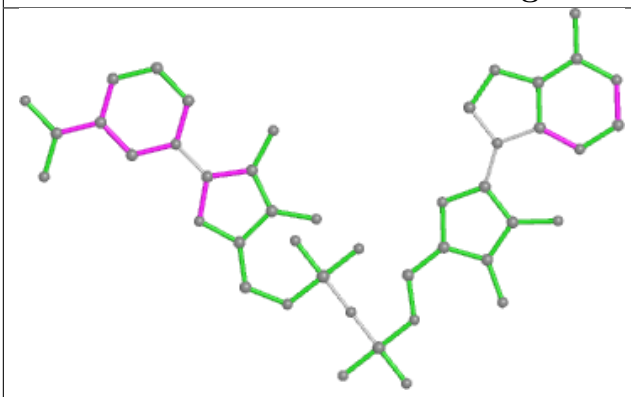


Rings

Ligand NAD E 261



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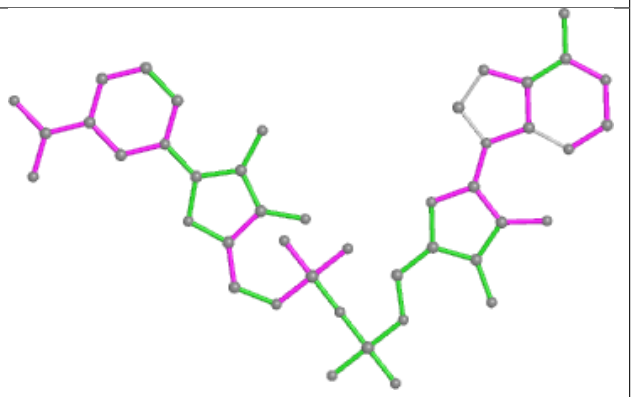
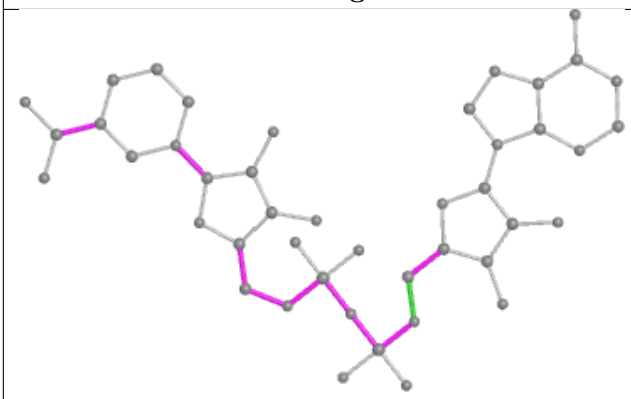


Bond angles



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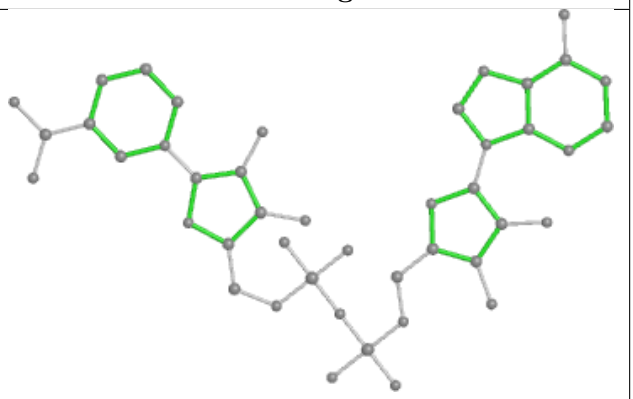
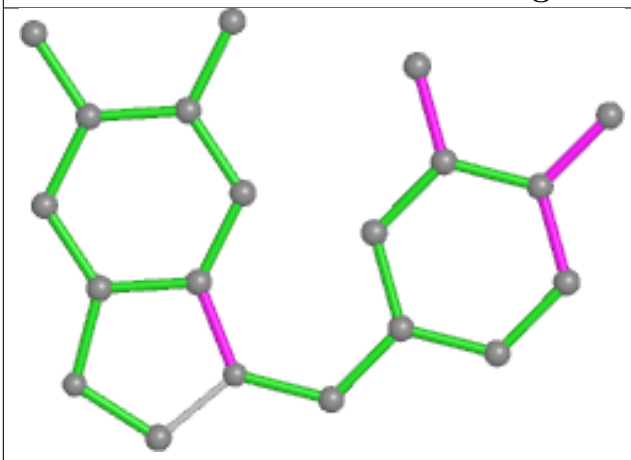


Rings

Ligand 09T E 262



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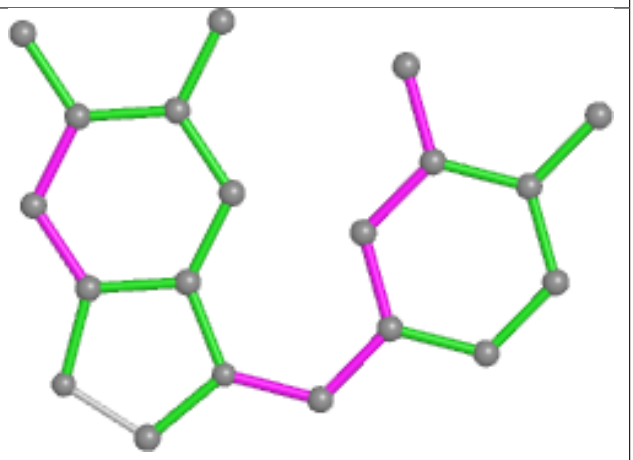
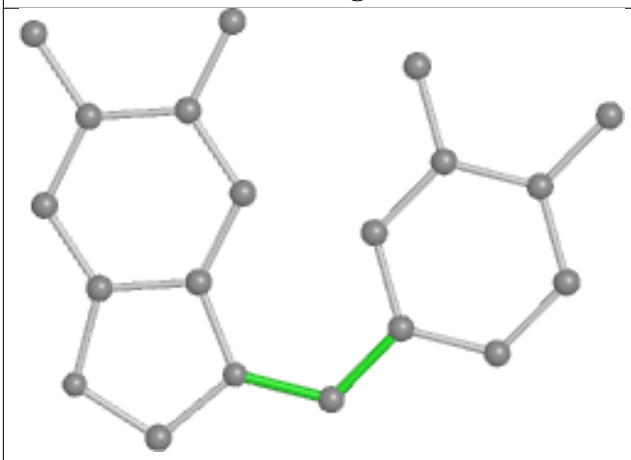


Bond angles



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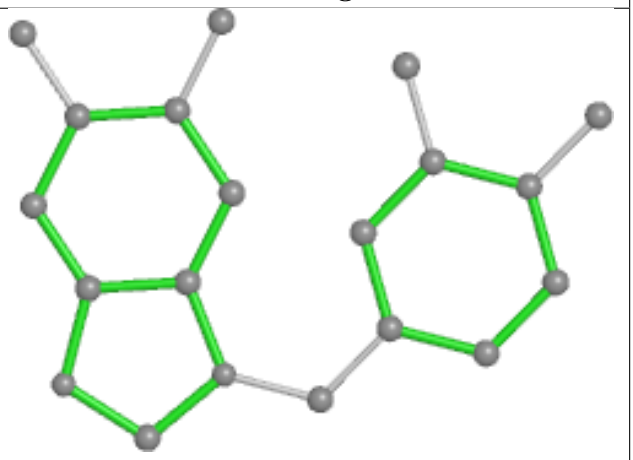
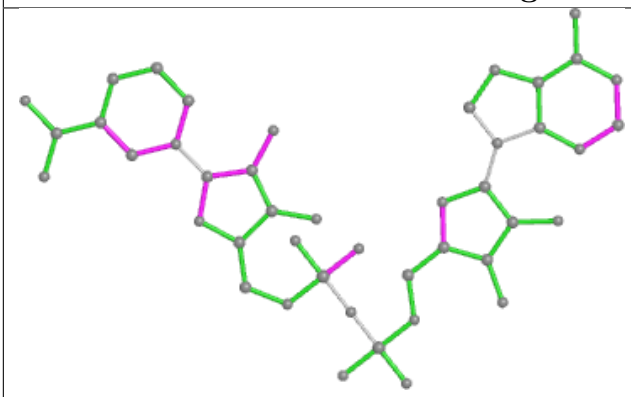


Rings

Ligand NAD C 261



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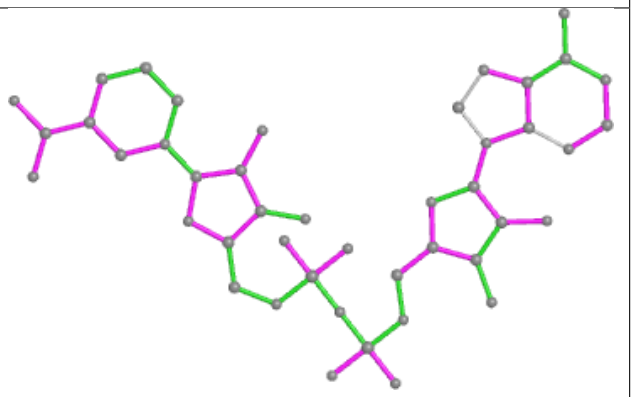
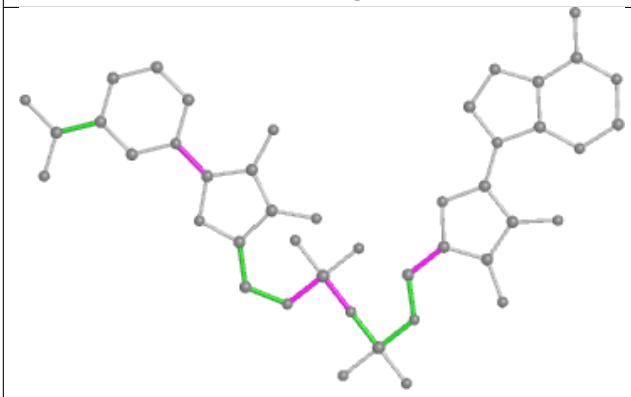


Bond angles



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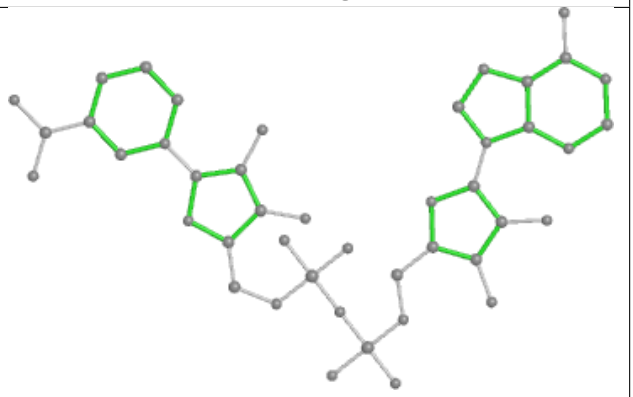
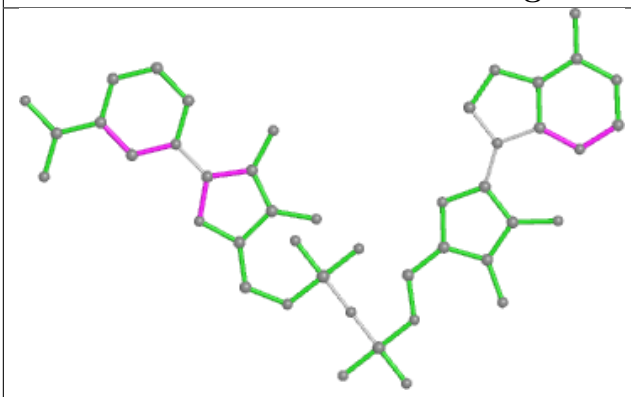


Rings

Ligand NAD J 261



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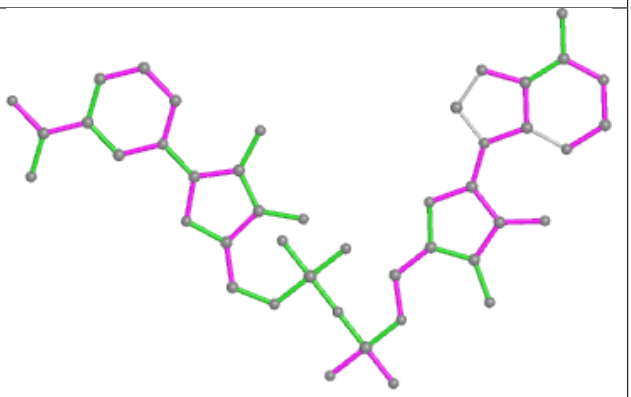
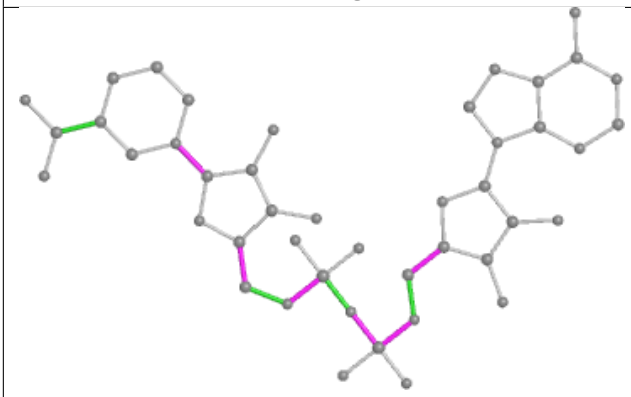


Bond angles



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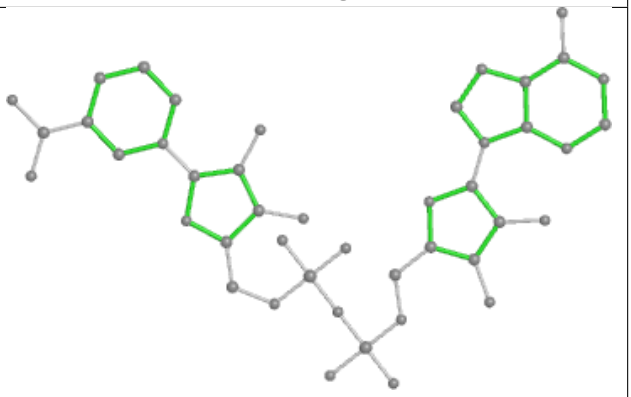
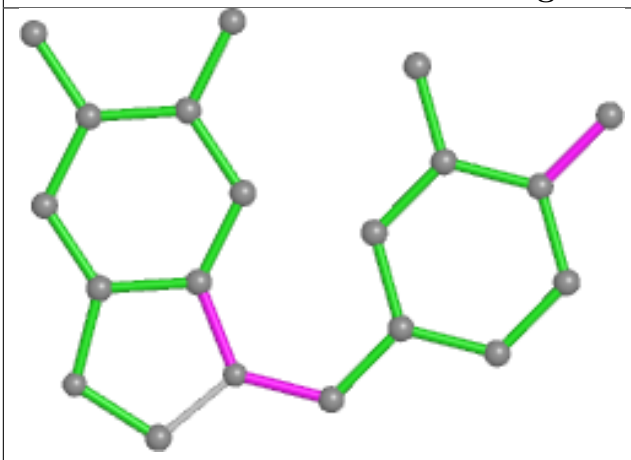


Rings

Ligand 09T I 262



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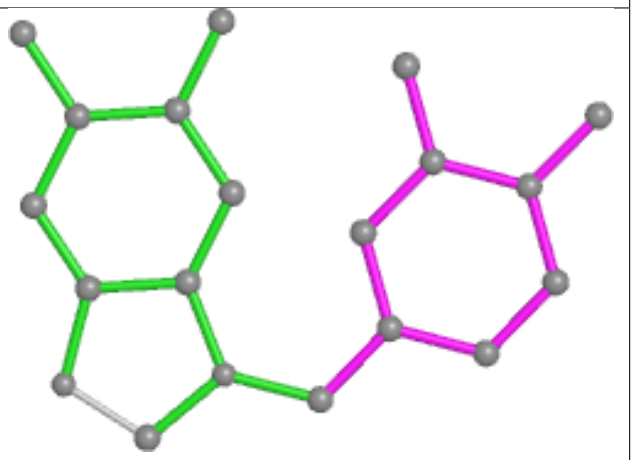
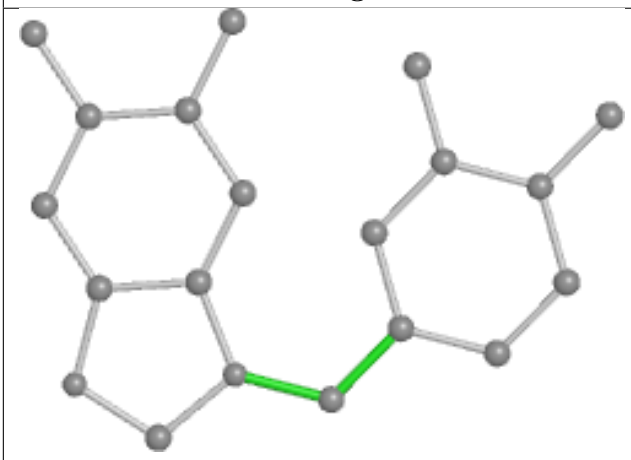
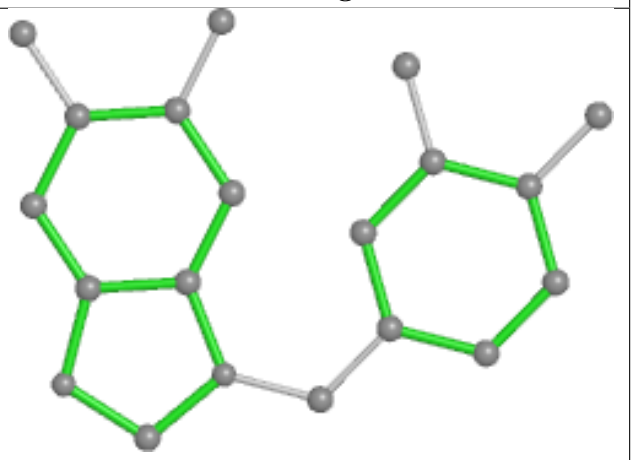


Bond angles

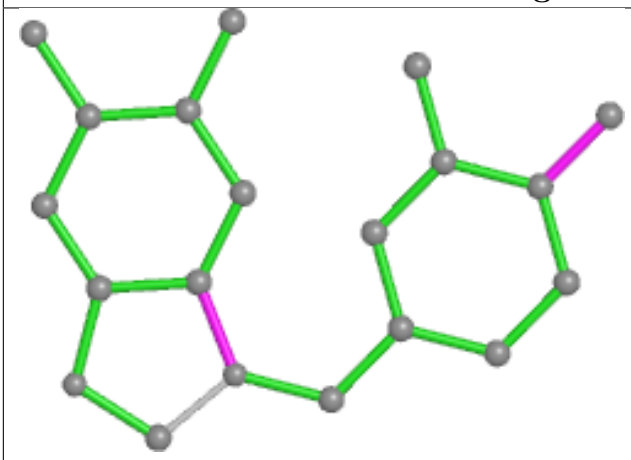


Torsions

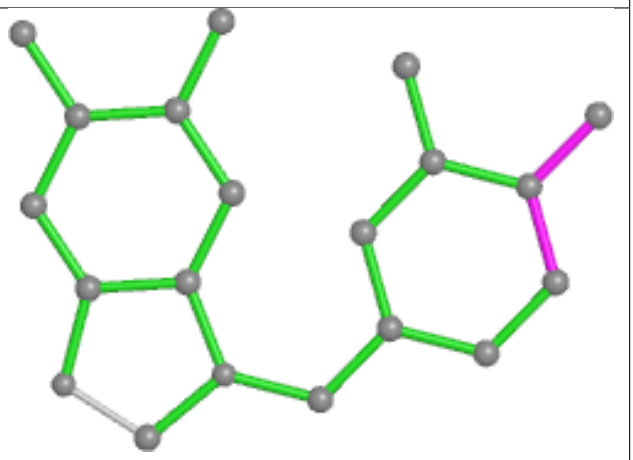


Rings

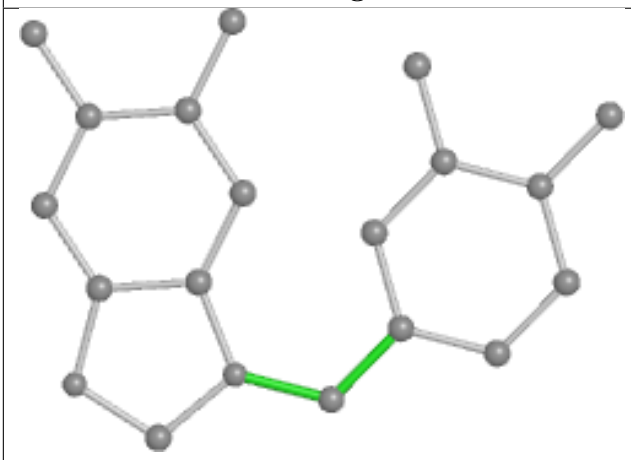
Ligand 09T L 262



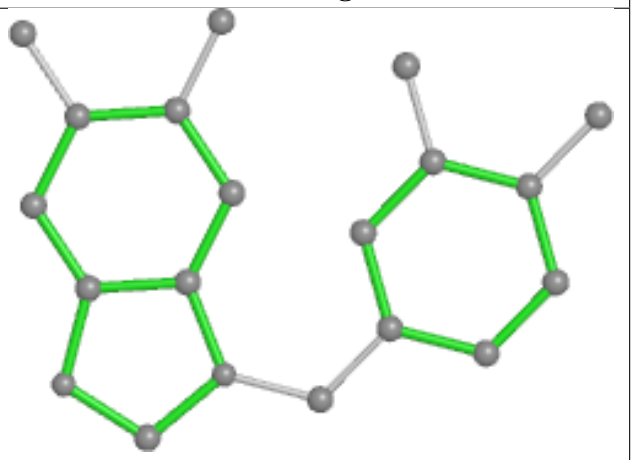
Bond lengths



Bond angles

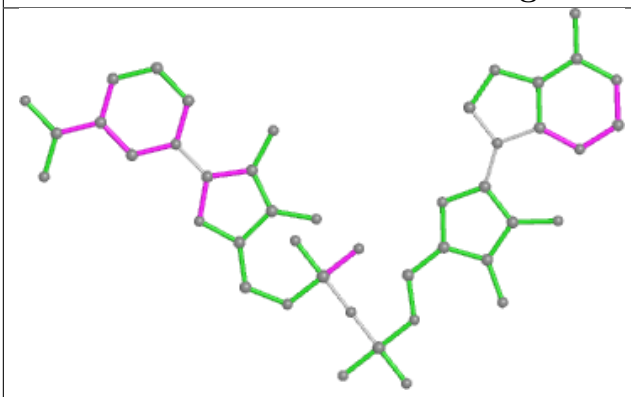


Torsions

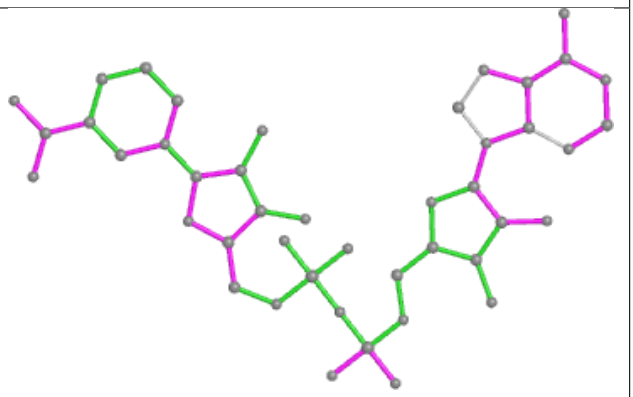


Rings

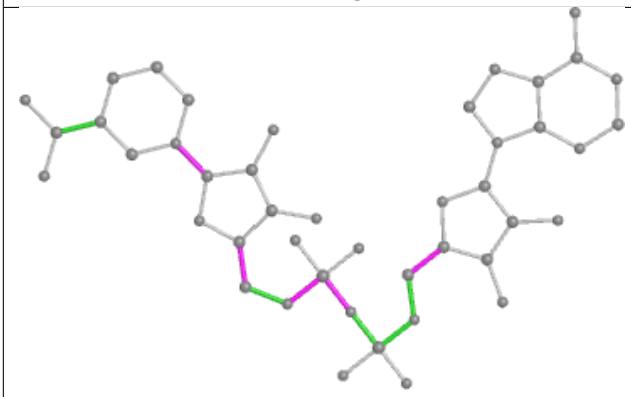
Ligand NAD O 261



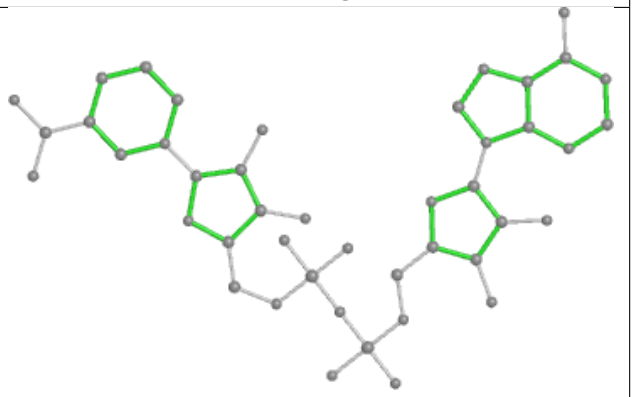
Bond lengths



Bond angles

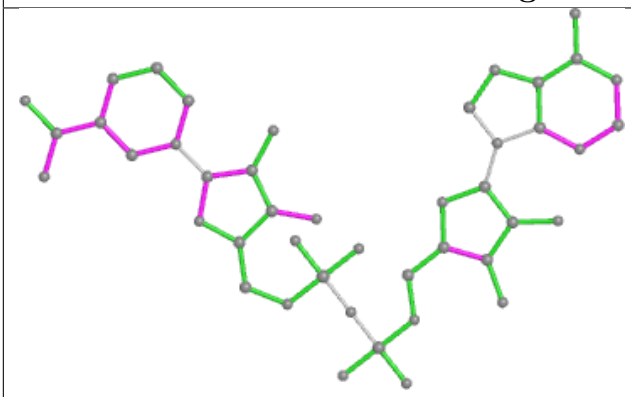


Torsions

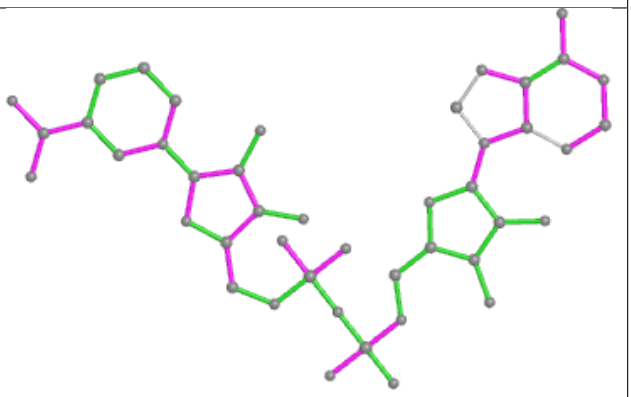


Rings

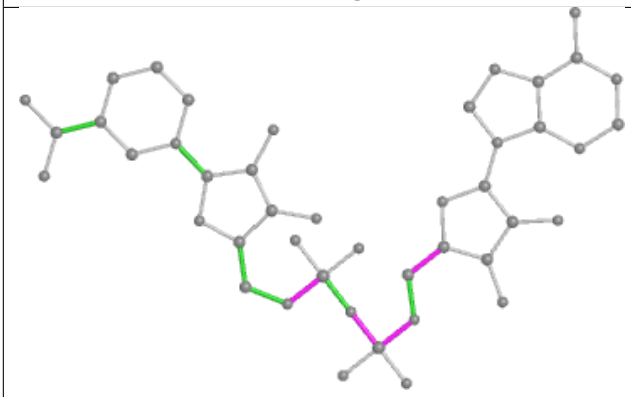
Ligand NAD N 261



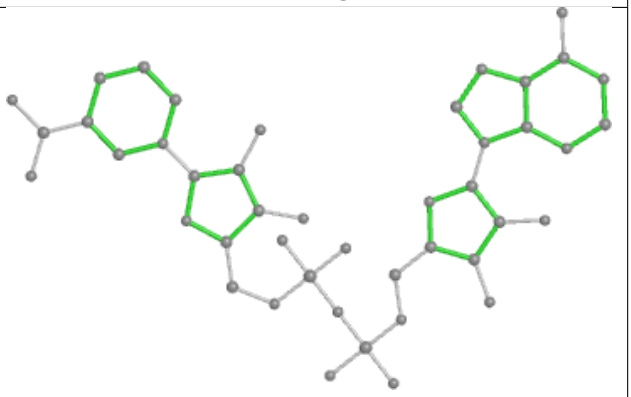
Bond lengths



Bond angles

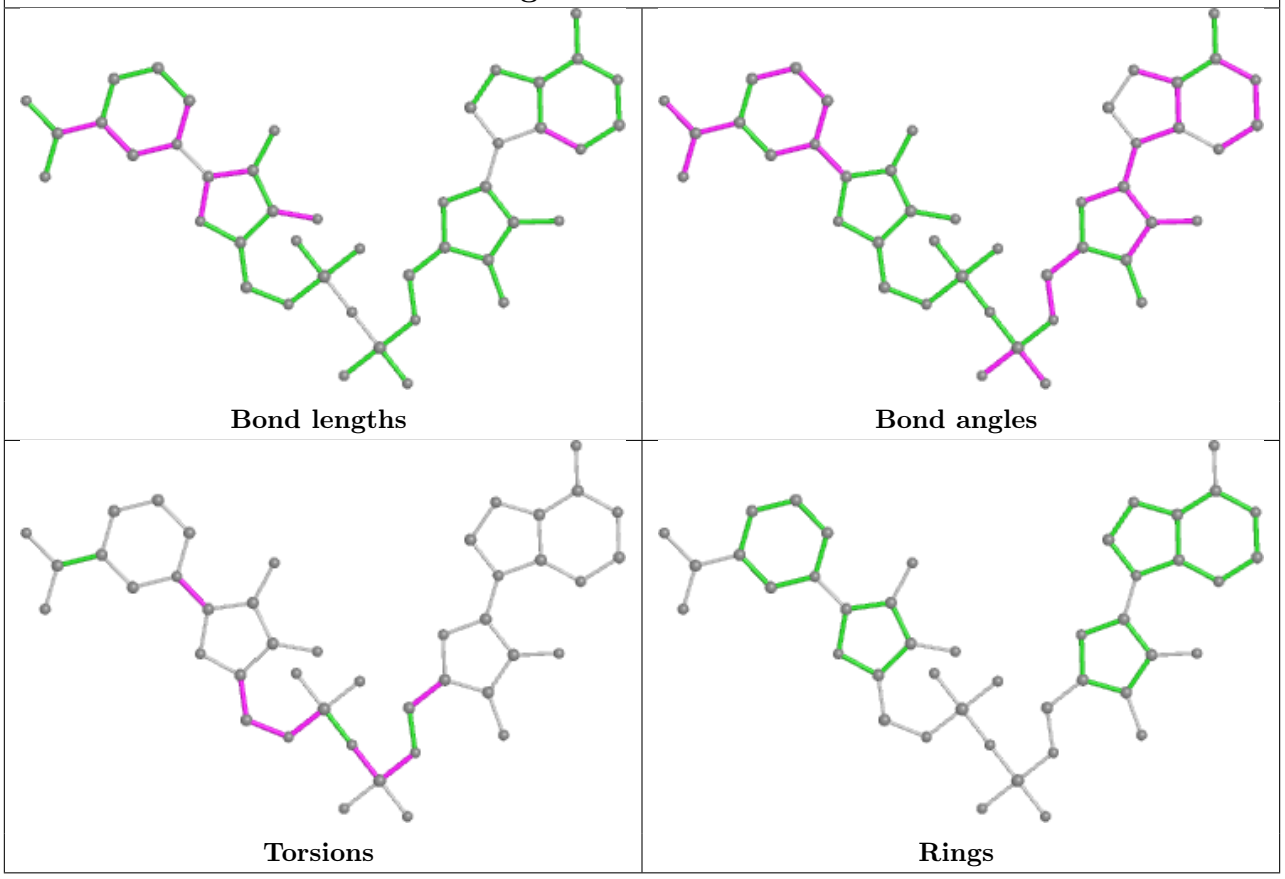


Torsions



Rings

Ligand NAD D 261



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	259/280 (92%)	-0.21	1 (0%) 92 93	6, 15, 37, 72	0
1	B	257/280 (91%)	-0.12	0 100 100	4, 17, 44, 71	0
1	C	259/280 (92%)	-0.24	1 (0%) 92 93	6, 15, 37, 96	0
1	D	256/280 (91%)	-0.17	3 (1%) 79 80	6, 17, 45, 70	0
1	E	258/280 (92%)	0.73	35 (13%) 3 2	17, 38, 75, 98	0
1	F	259/280 (92%)	0.42	11 (4%) 36 39	17, 36, 63, 89	0
1	G	257/280 (91%)	0.78	30 (11%) 4 4	15, 40, 78, 97	0
1	H	259/280 (92%)	0.61	22 (8%) 10 10	17, 39, 70, 106	0
1	I	259/280 (92%)	-0.27	3 (1%) 79 80	6, 15, 37, 88	0
1	J	257/280 (91%)	-0.19	5 (1%) 66 69	5, 17, 45, 76	0
1	K	259/280 (92%)	-0.24	0 100 100	6, 15, 41, 60	0
1	L	257/280 (91%)	-0.16	2 (0%) 86 87	5, 18, 47, 71	0
1	M	257/280 (91%)	0.75	25 (9%) 7 7	16, 39, 77, 110	0
1	N	259/280 (92%)	0.53	14 (5%) 25 27	17, 39, 70, 98	0
1	O	256/280 (91%)	0.75	32 (12%) 3 3	17, 39, 76, 99	0
1	P	259/280 (92%)	0.51	13 (5%) 28 30	14, 37, 66, 84	0
All	All	4127/4480 (92%)	0.22	197 (4%) 30 32	4, 27, 65, 110	0

The worst 5 of 197 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	42	GLN	5.7
1	M	41	GLY	5.1
1	O	208	ASP	4.9
1	O	217	LYS	4.9
1	M	200	ILE	4.9

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^{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	09T	G	262	20/20	0.82	0.27	42,48,94,98	0
3	09T	M	262	20/20	0.84	0.28	43,51,103,139	0
3	09T	O	262	20/20	0.84	0.23	37,41,58,74	0
3	09T	E	262	20/20	0.86	0.22	33,37,58,71	0
3	09T	N	262	20/20	0.88	0.22	36,47,72,94	0
3	09T	L	262	20/20	0.89	0.21	35,39,58,79	0
3	09T	A	262	20/20	0.89	0.17	20,23,35,54	0
3	09T	B	262	20/20	0.89	0.23	39,44,61,95	0
3	09T	H	262	20/20	0.89	0.21	39,54,68,87	0
2	NAD	G	261	44/44	0.90	0.18	23,42,66,75	0
3	09T	F	262	20/20	0.90	0.18	18,20,47,66	0
2	NAD	M	261	44/44	0.91	0.15	24,40,52,58	0
2	NAD	O	261	44/44	0.91	0.17	25,34,51,57	0
2	NAD	E	261	44/44	0.91	0.17	30,40,52,55	0
3	09T	J	262	20/20	0.92	0.18	22,28,52,94	0
3	09T	K	262	20/20	0.92	0.14	17,21,38,61	0
3	09T	D	262	20/20	0.92	0.19	25,30,48,91	0
3	09T	P	262	20/20	0.92	0.17	21,26,42,54	0
2	NAD	N	261	44/44	0.93	0.17	22,34,75,77	0
2	NAD	H	261	44/44	0.93	0.17	24,37,81,84	0
3	09T	I	262	20/20	0.94	0.14	11,12,27,53	0
3	09T	C	262	20/20	0.94	0.15	10,12,26,49	0
2	NAD	F	261	44/44	0.94	0.17	14,23,68,73	3
2	NAD	P	261	44/44	0.94	0.16	19,29,70,76	0
2	NAD	B	261	44/44	0.95	0.13	15,18,24,25	0
2	NAD	D	261	44/44	0.96	0.12	12,14,18,22	0
2	NAD	J	261	44/44	0.96	0.13	10,13,16,20	0

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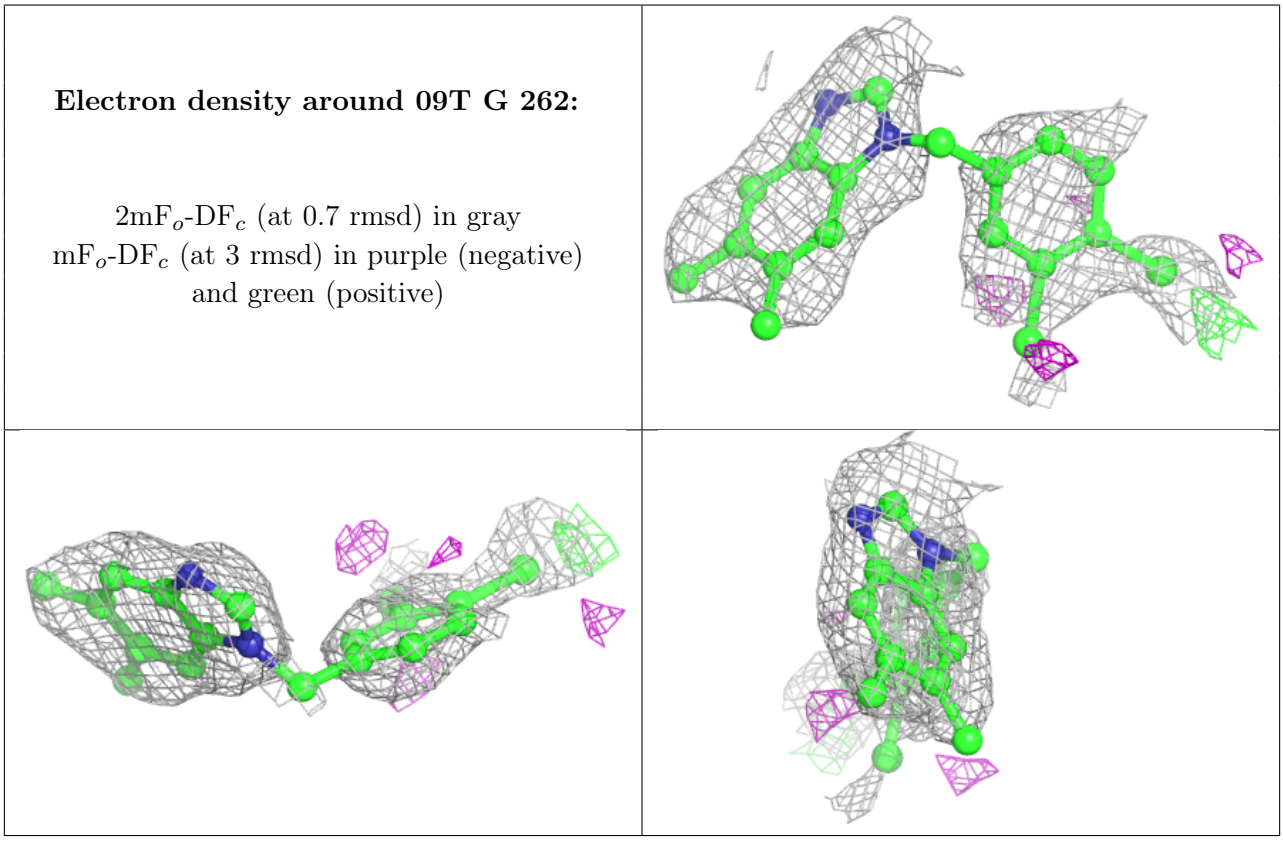
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	K	261	44/44	0.96	0.12	5,7,17,17	0
2	NAD	L	261	44/44	0.96	0.12	14,18,20,21	0
2	NAD	A	261	44/44	0.97	0.12	4,7,15,15	0
2	NAD	C	261	44/44	0.97	0.11	5,8,23,24	0
2	NAD	I	261	44/44	0.98	0.11	5,8,22,23	0

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.

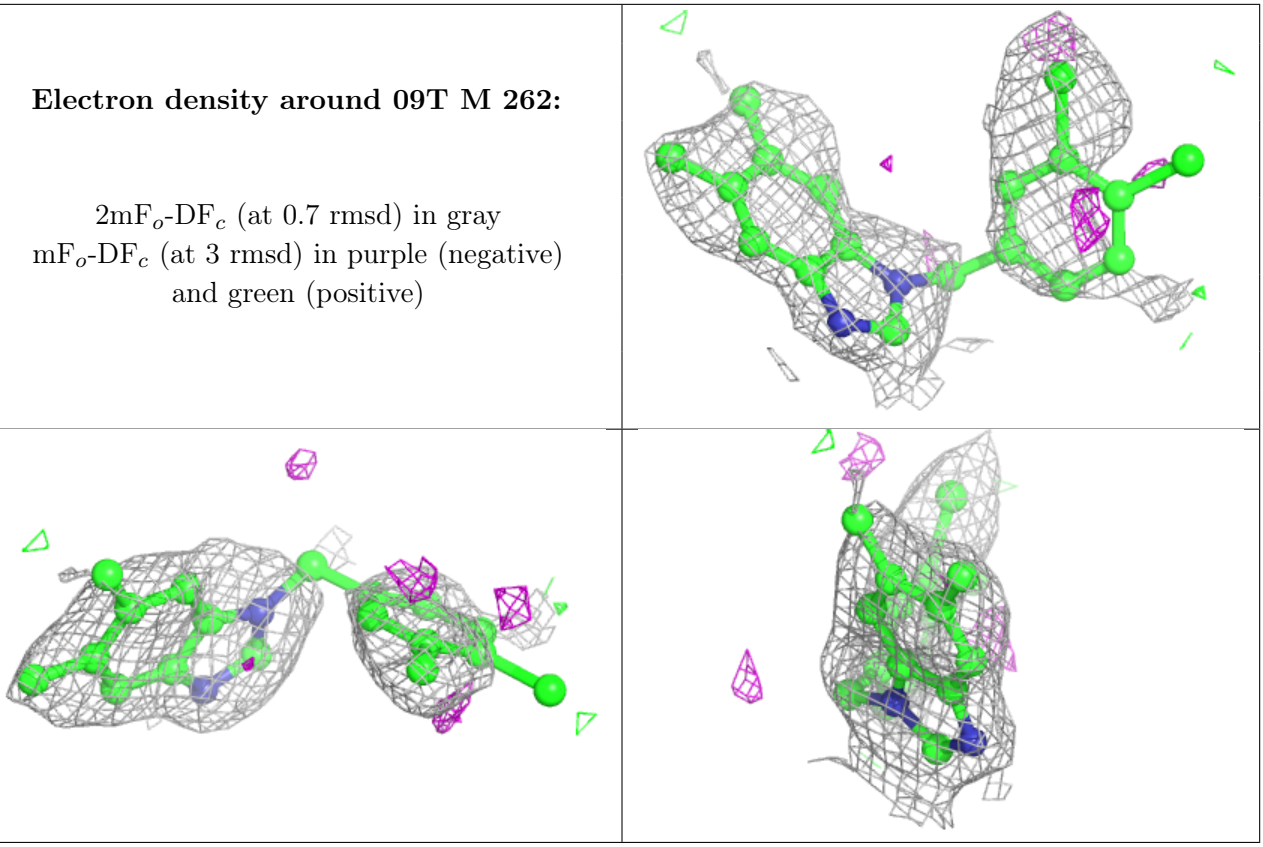
Electron density around 09T G 262:

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



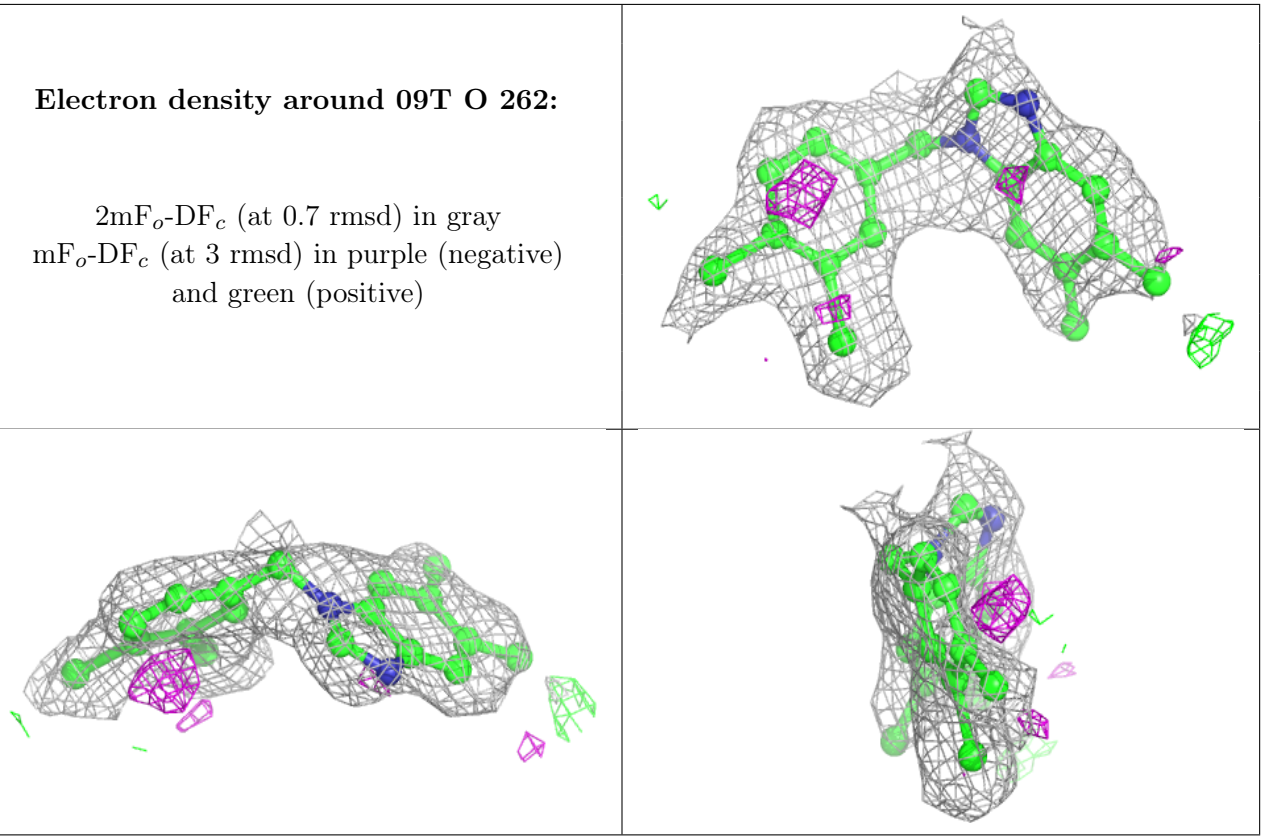
Electron density around 09T M 262:

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



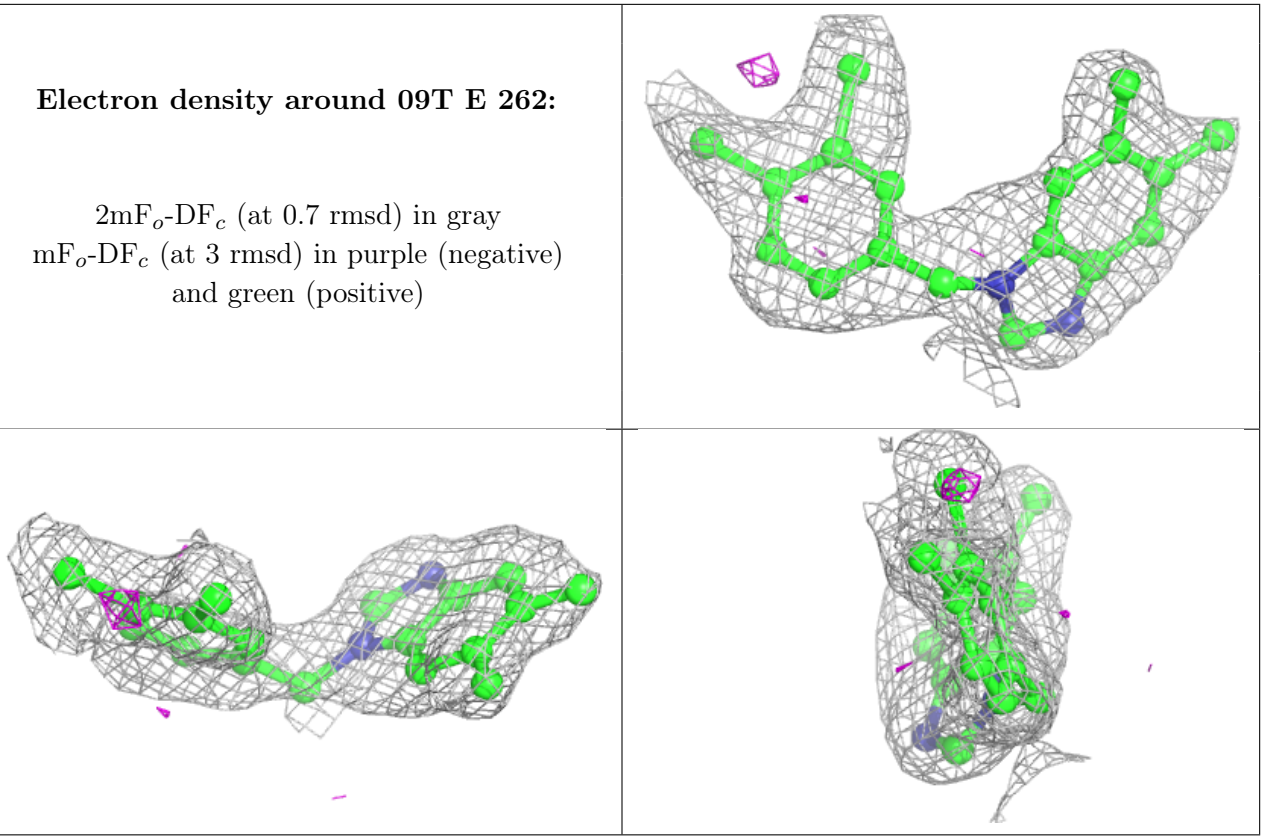
Electron density around 09T O 262:

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



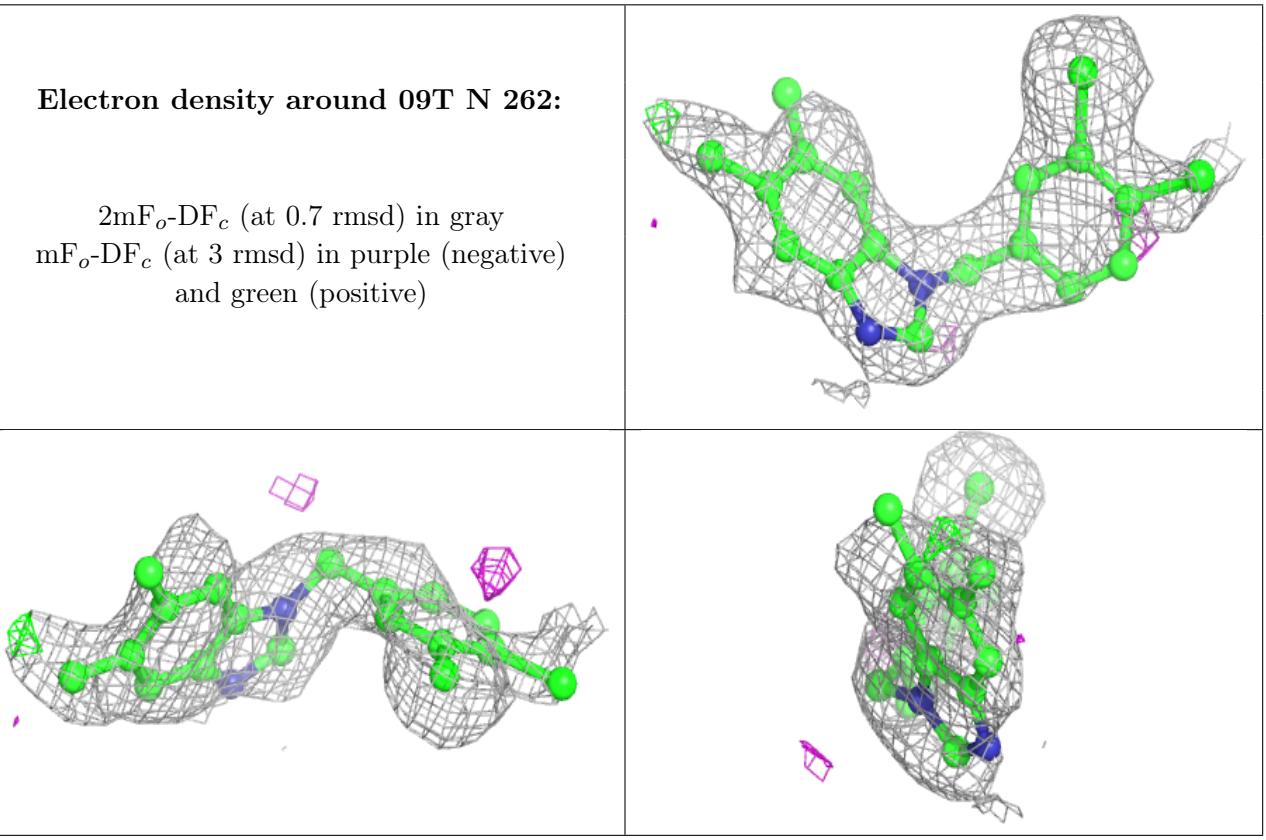
Electron density around 09T E 262:

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



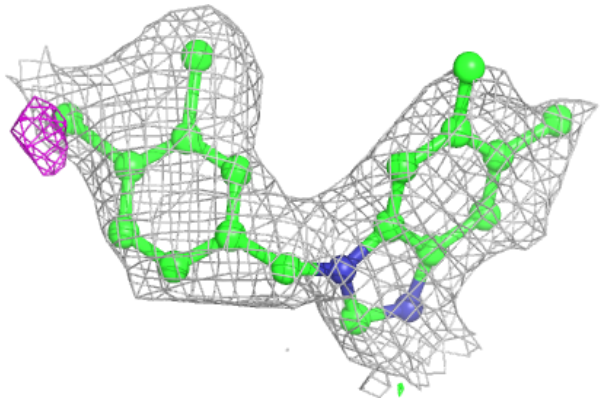
Electron density around 09T N 262:

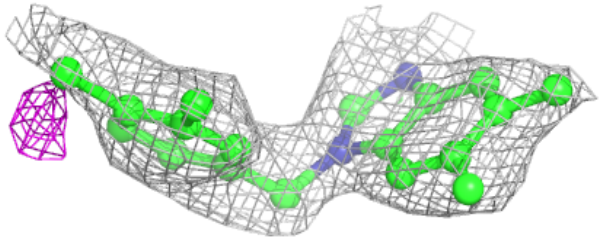
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

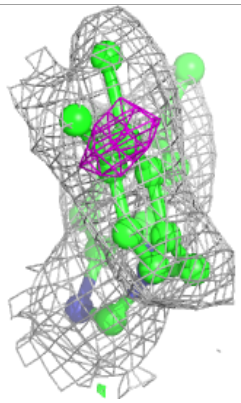


Electron density around 09T L 262:

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

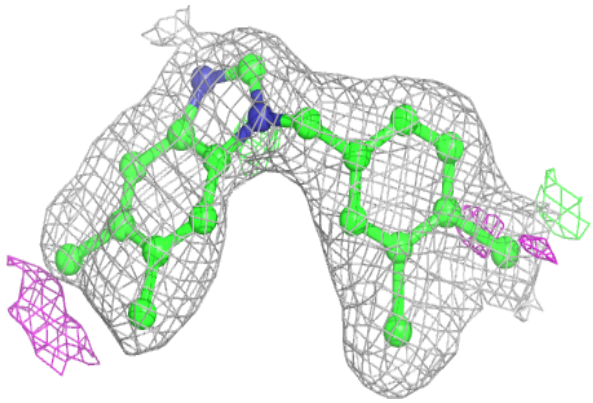


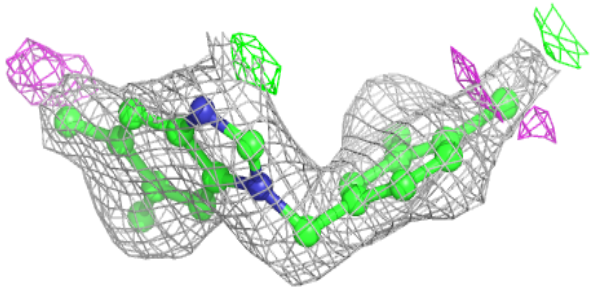


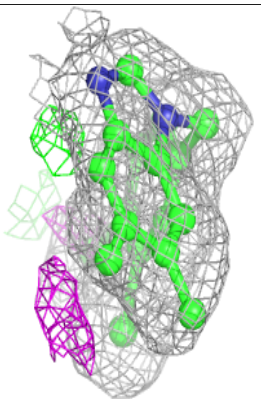


Electron density around 09T A 262:

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

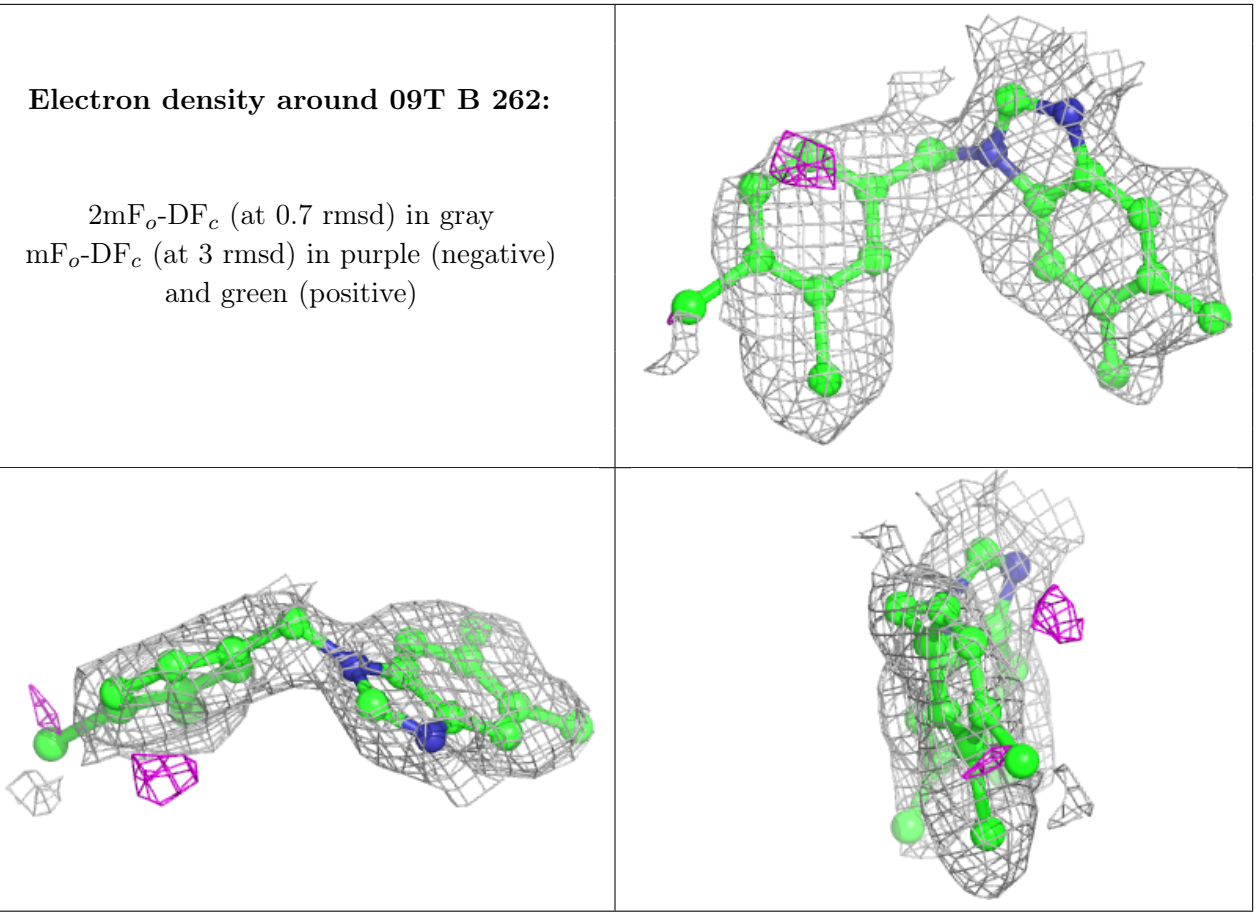






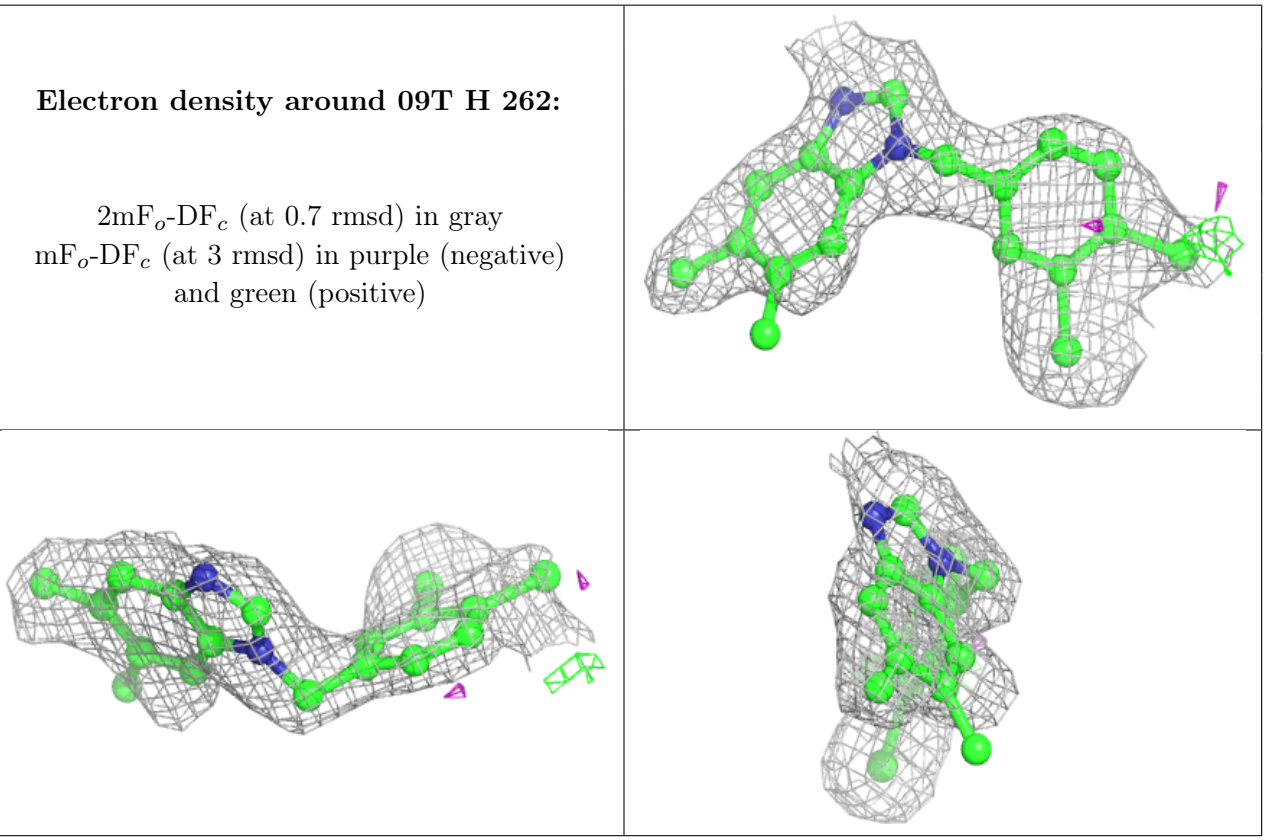
Electron density around 09T B 262:

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



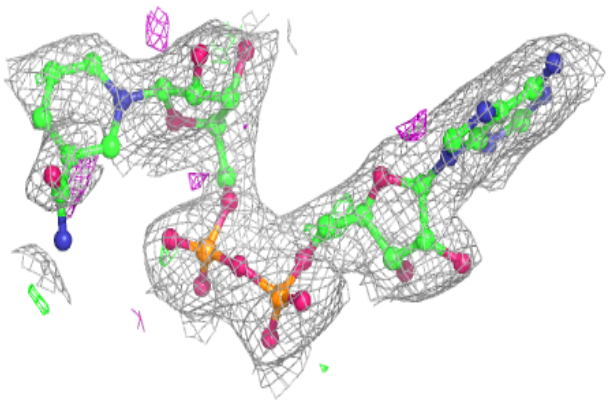
Electron density around 09T H 262:

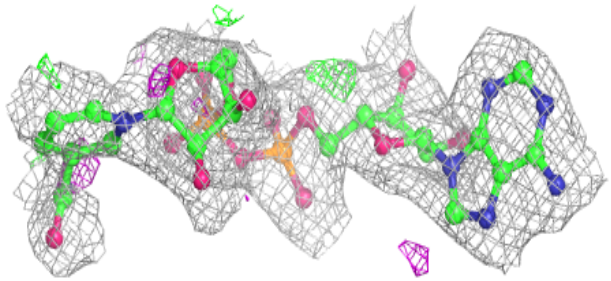
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

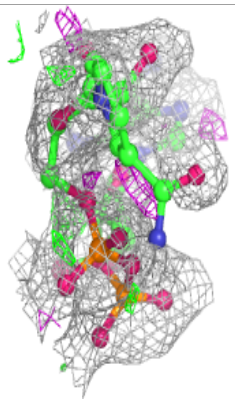


Electron density around NAD G 261:

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

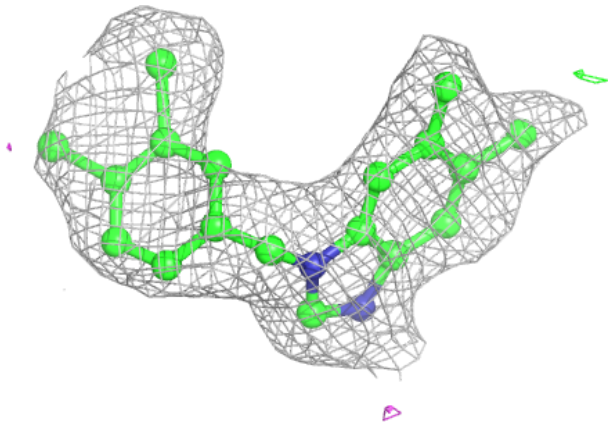


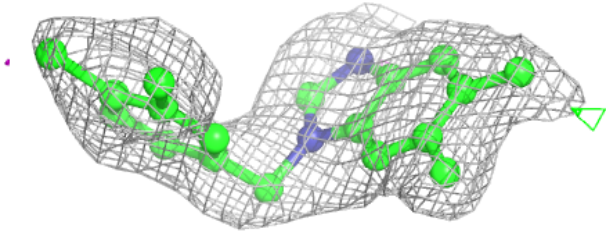


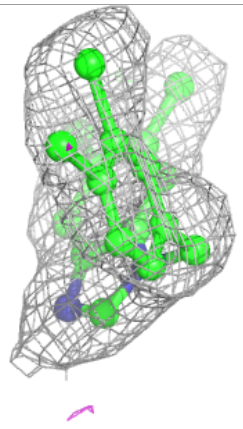


Electron density around 09T F 262:

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

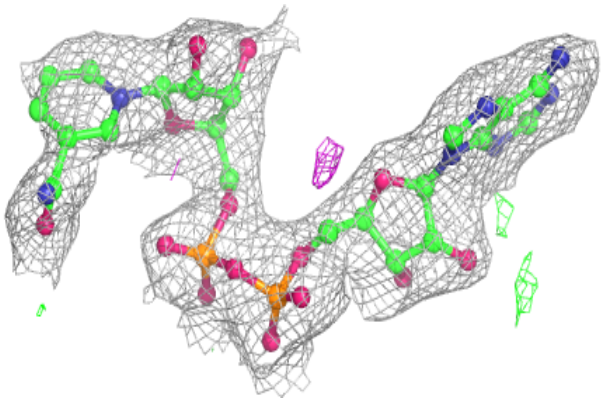


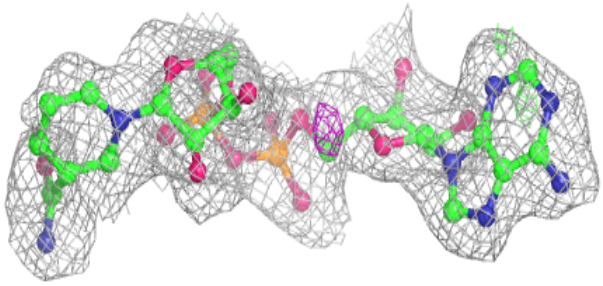


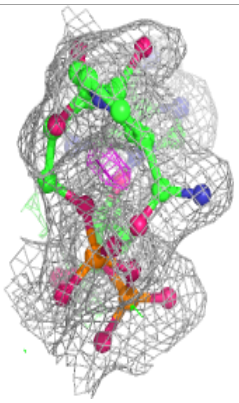


Electron density around NAD M 261:

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

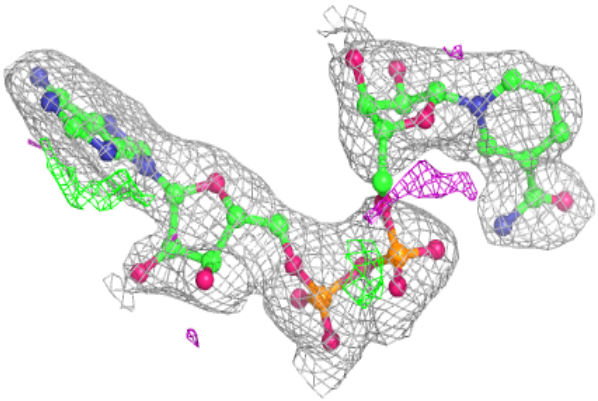


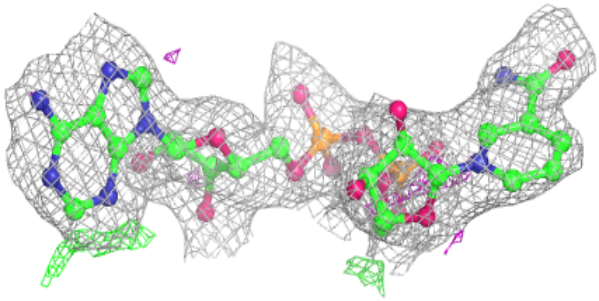


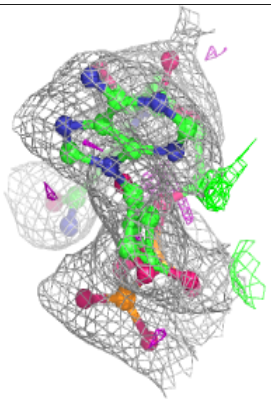


Electron density around NAD O 261:

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

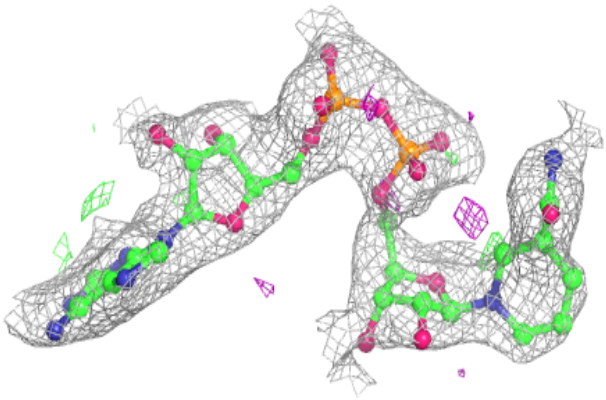


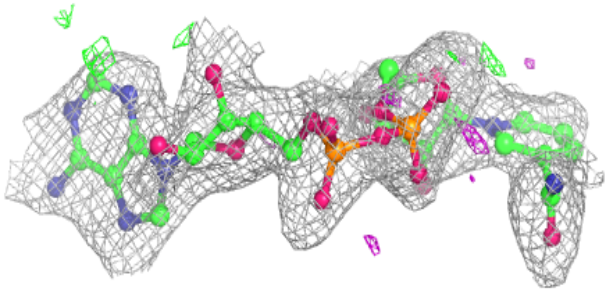


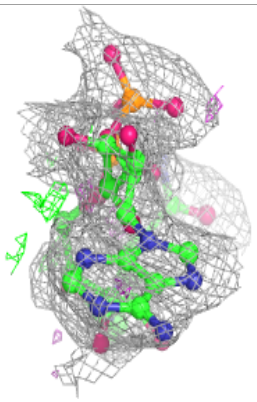


Electron density around NAD E 261:

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

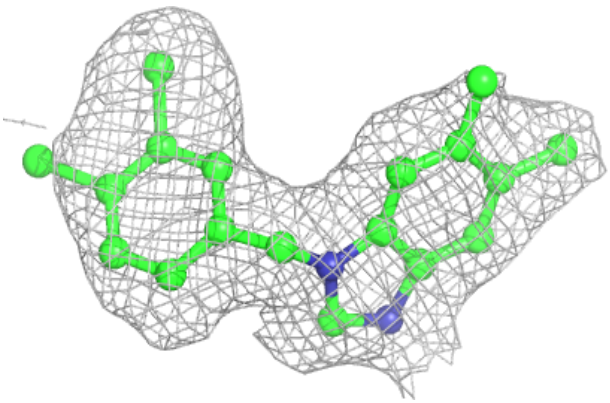


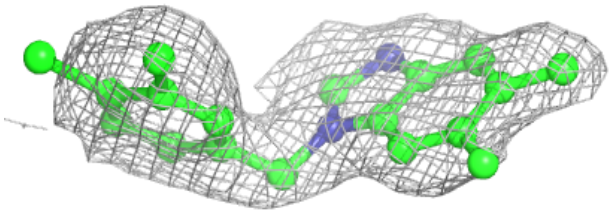


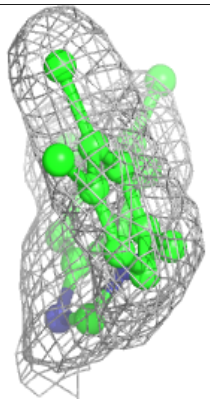


Electron density around 09T J 262:

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

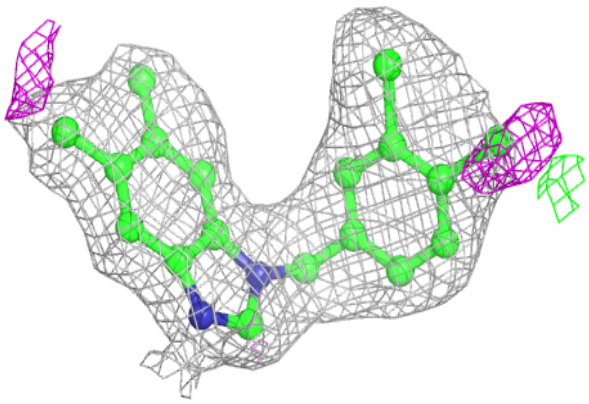


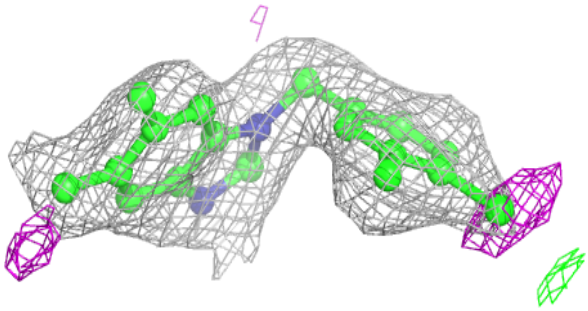


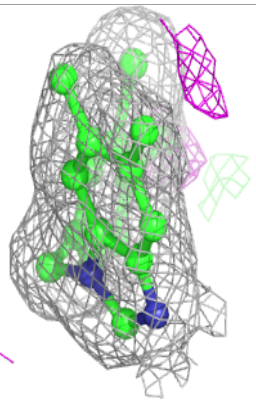


Electron density around 09T K 262:

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

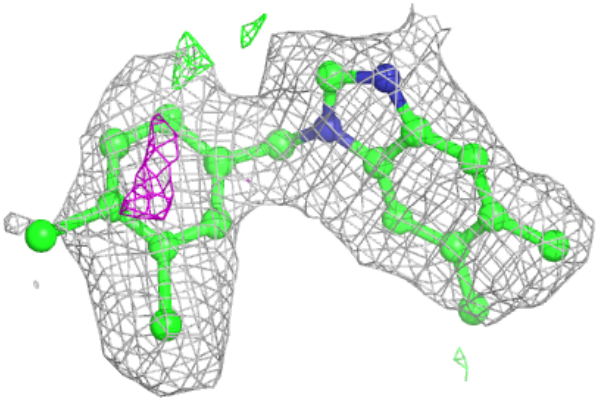


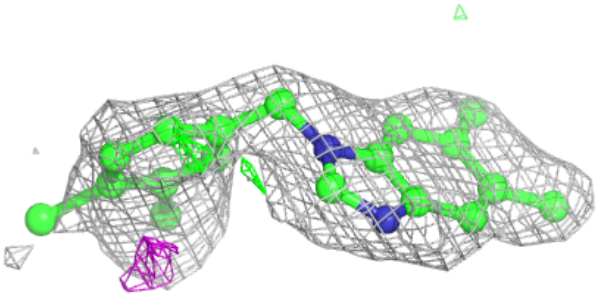


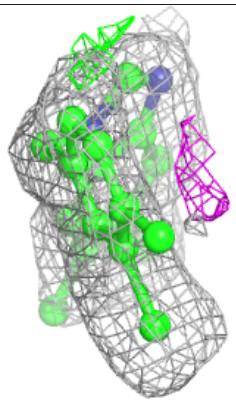


Electron density around 09T D 262:

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

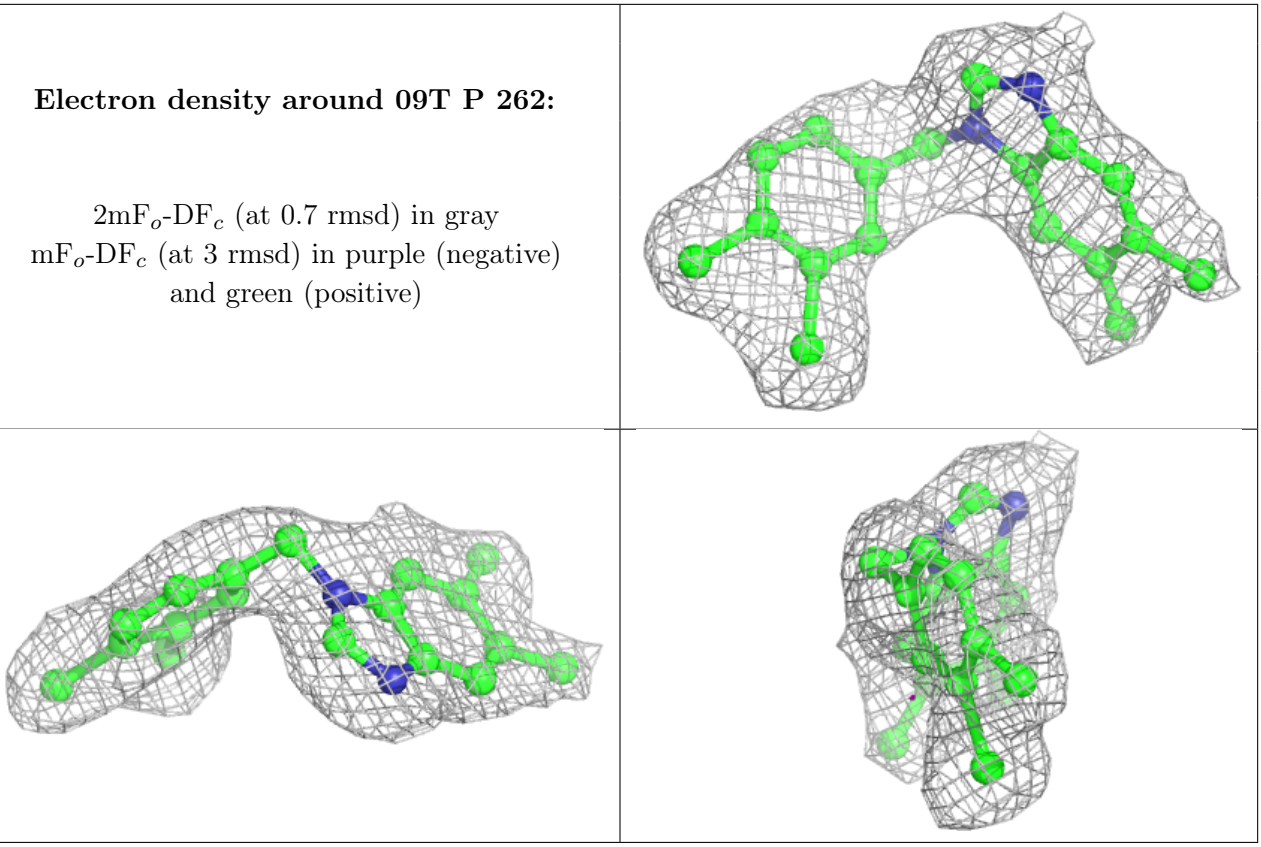






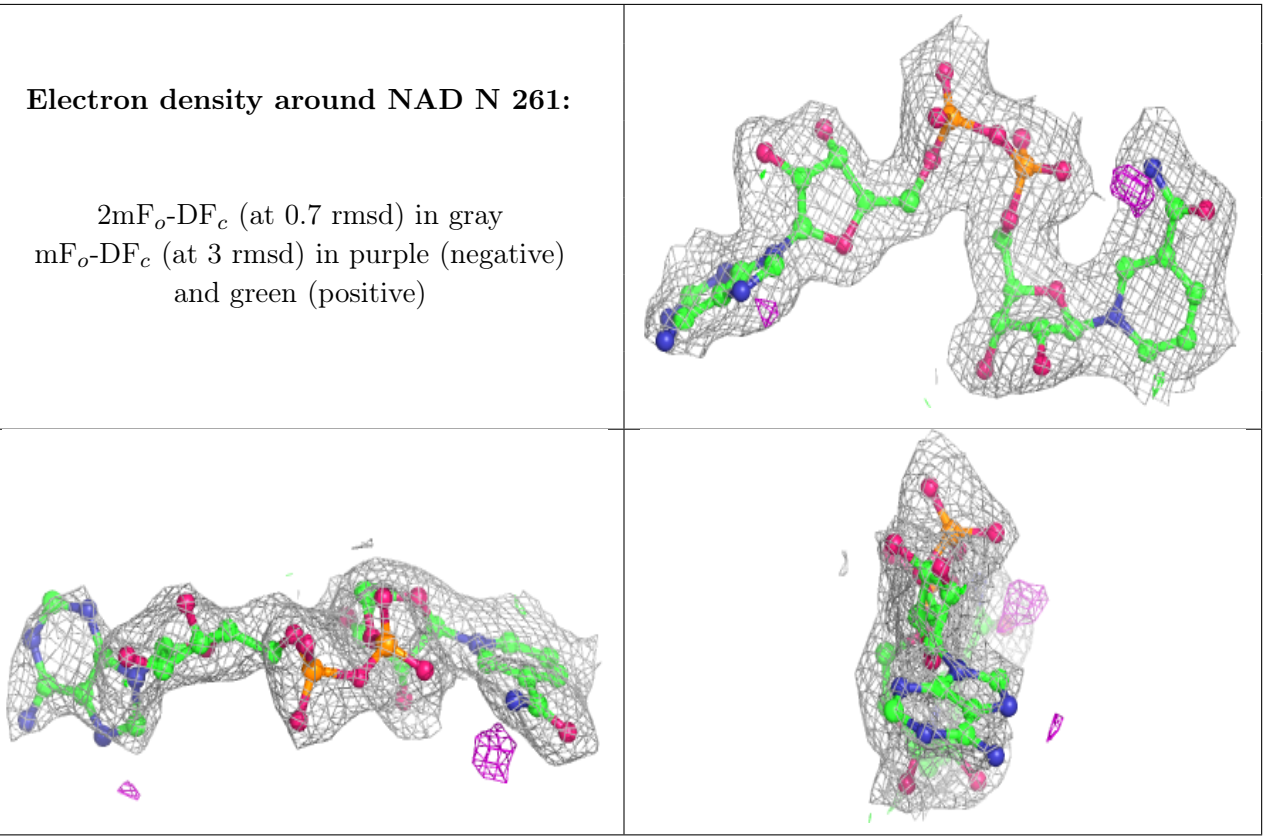
Electron density around 09T P 262:

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



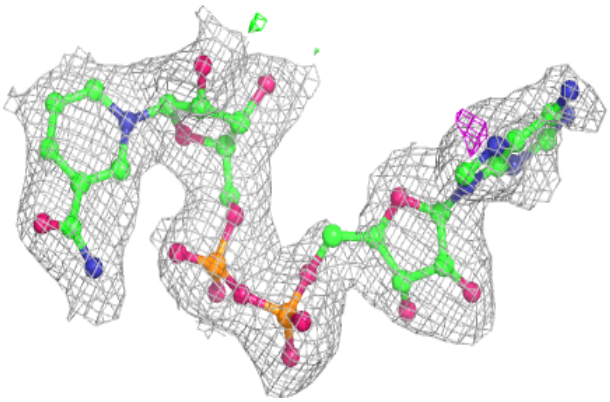
Electron density around NAD N 261:

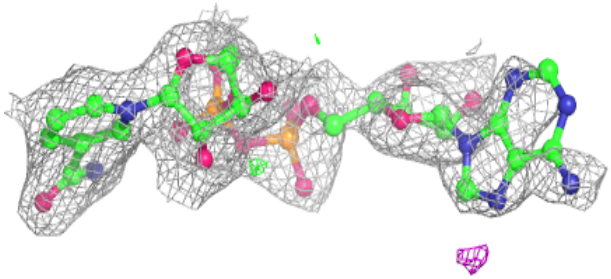
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

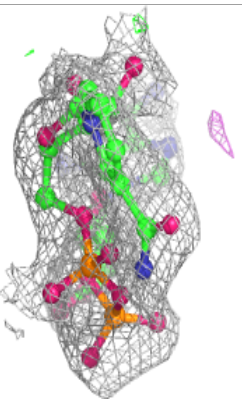


Electron density around NAD H 261:

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

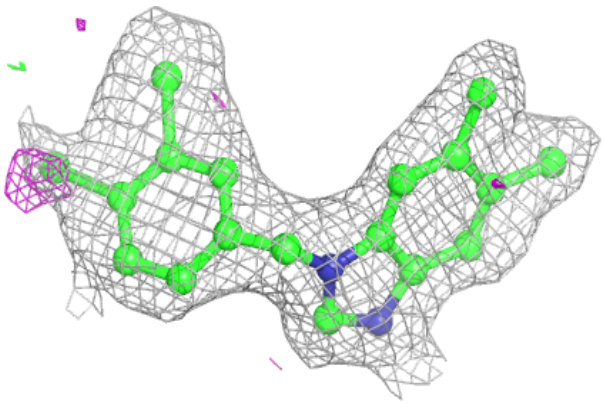


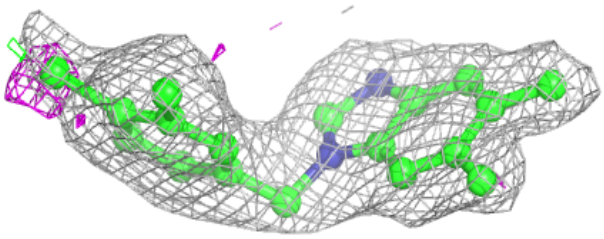


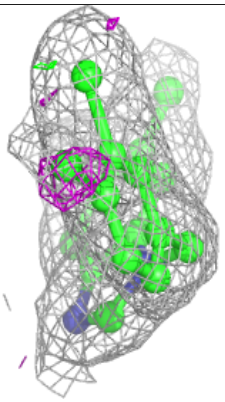


Electron density around 09T I 262:

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

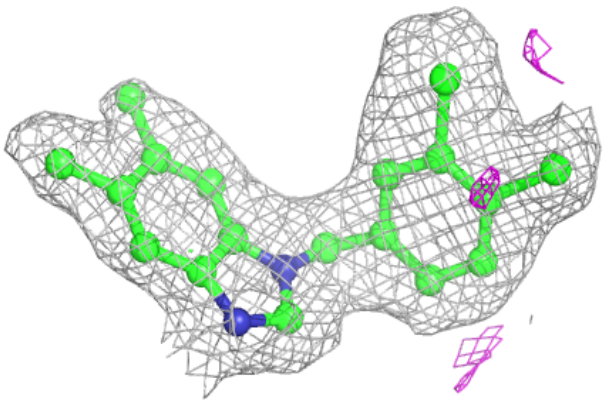


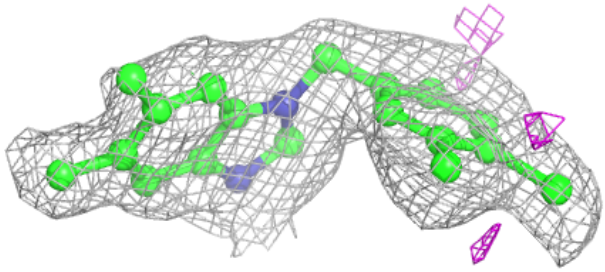


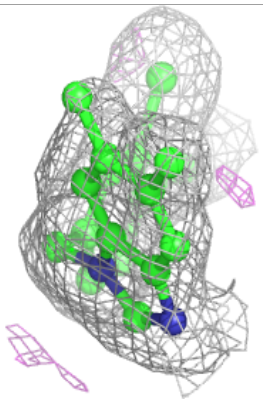


Electron density around 09T C 262:

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

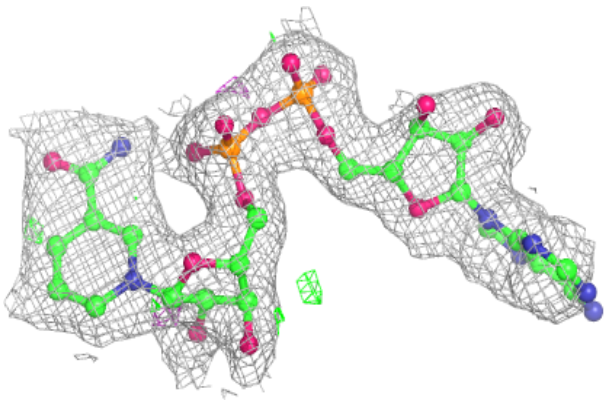


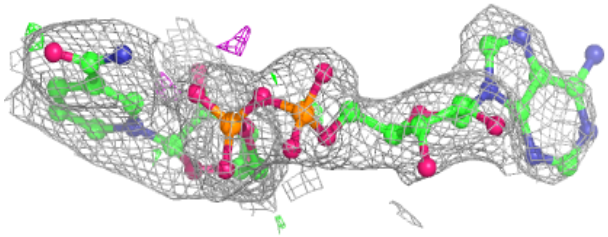


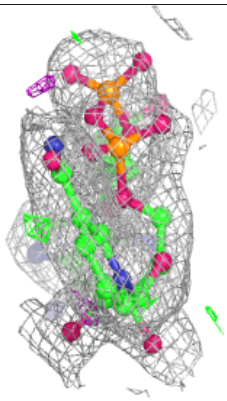


Electron density around NAD F 261:

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

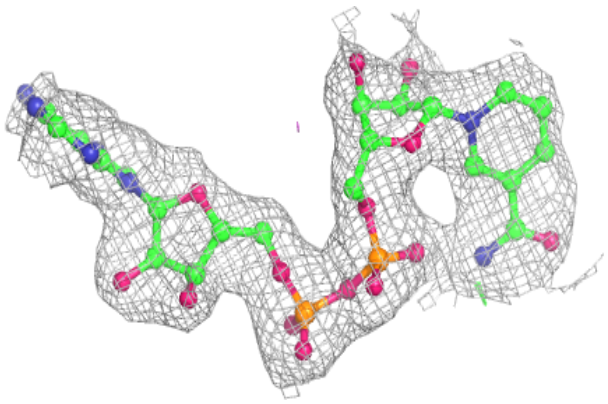


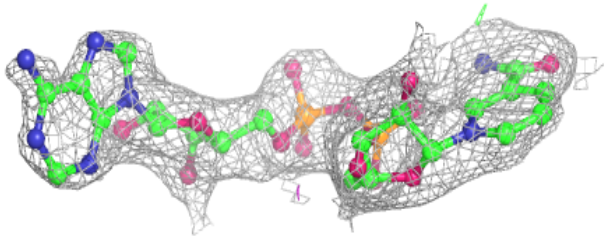


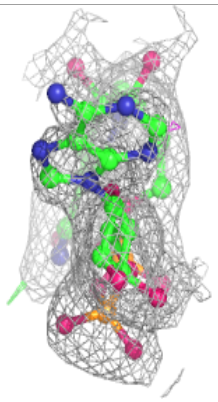


Electron density around NAD P 261:

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

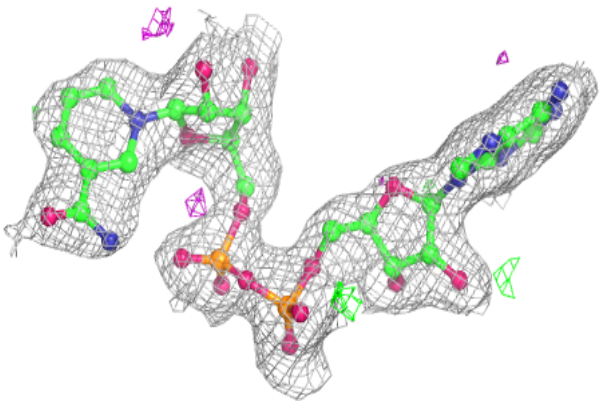


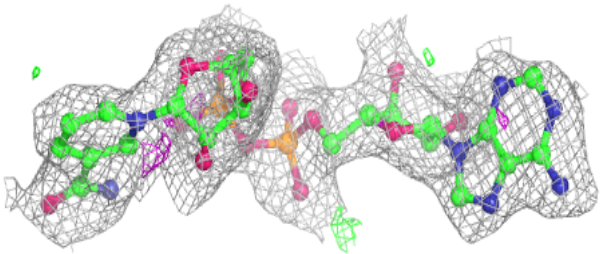


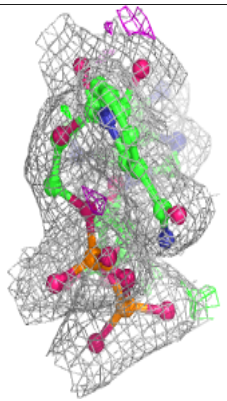


Electron density around NAD B 261:

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

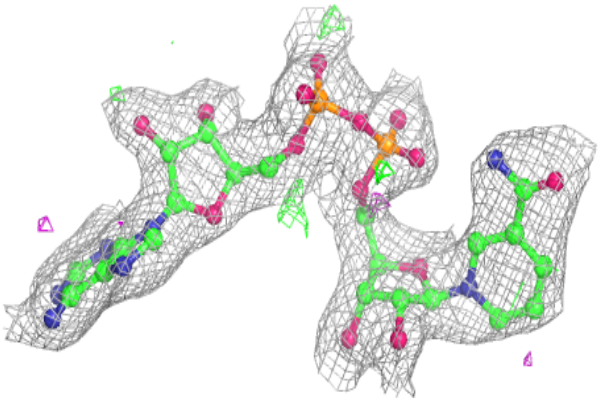


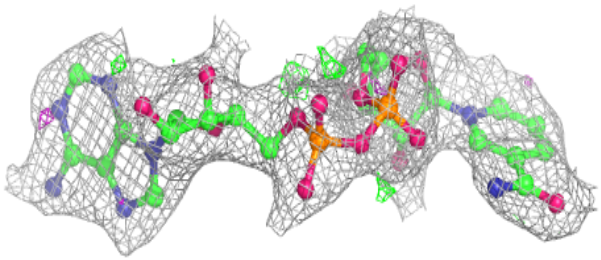


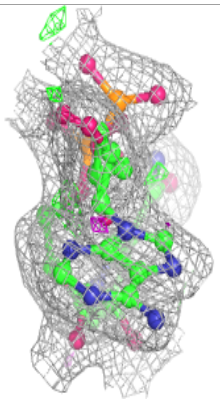


Electron density around NAD D 261:

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

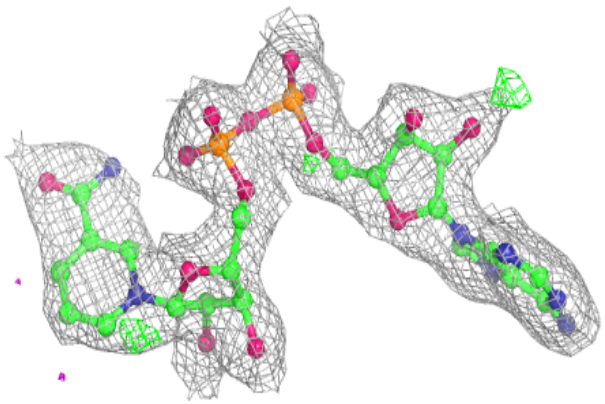


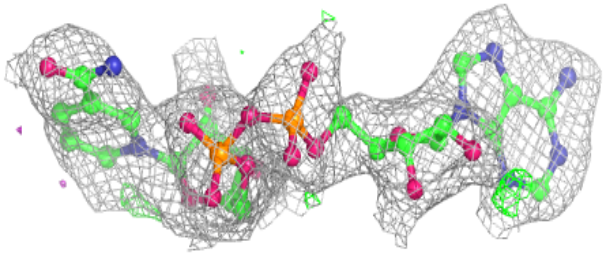


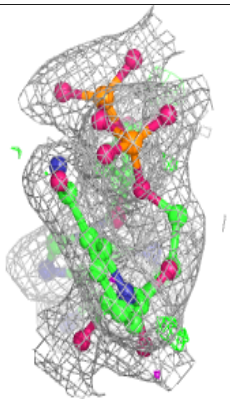


Electron density around NAD J 261:

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

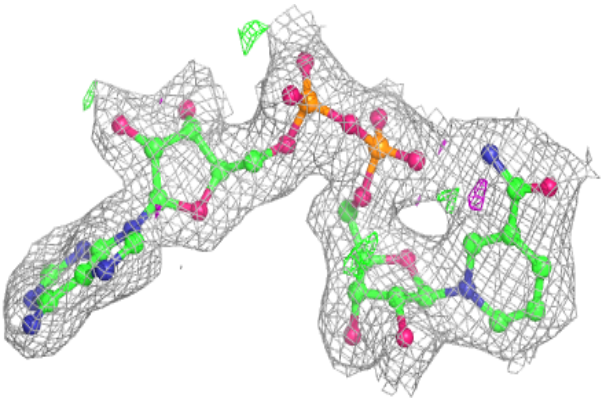


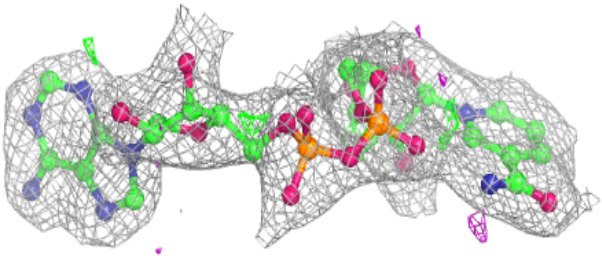


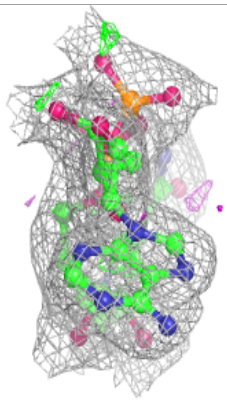


Electron density around NAD K 261:

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

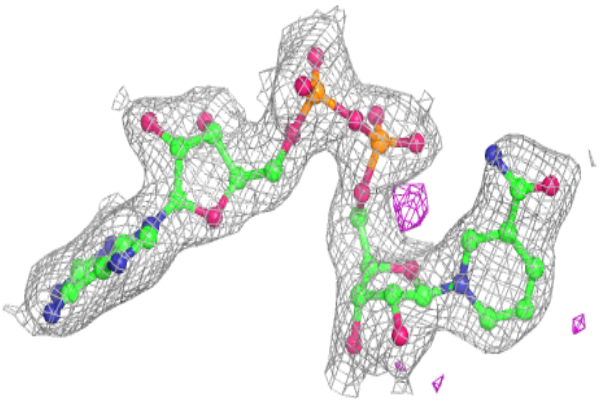


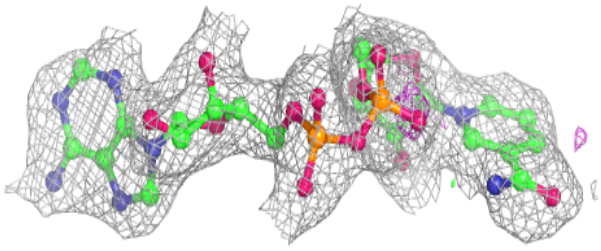


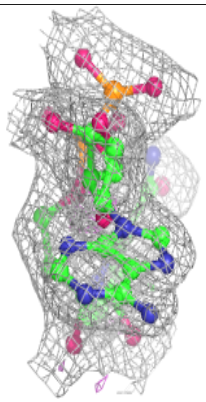


Electron density around NAD L 261:

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

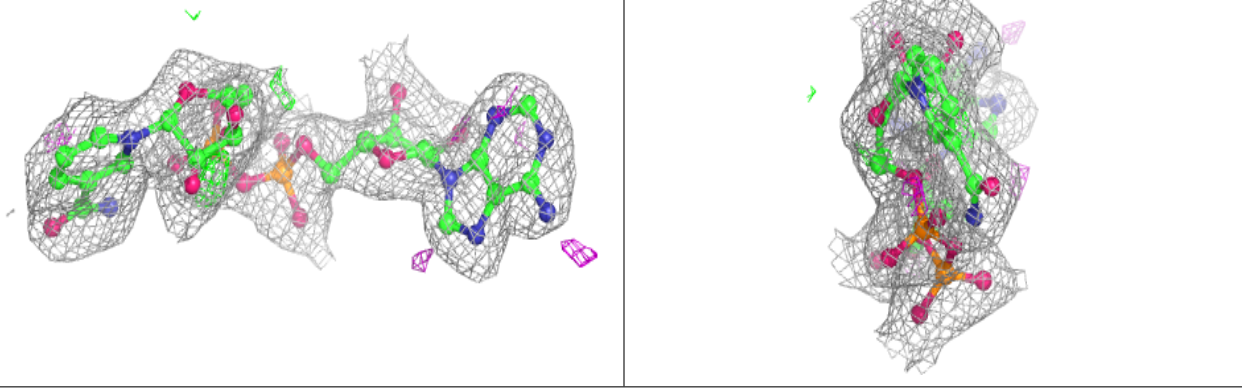






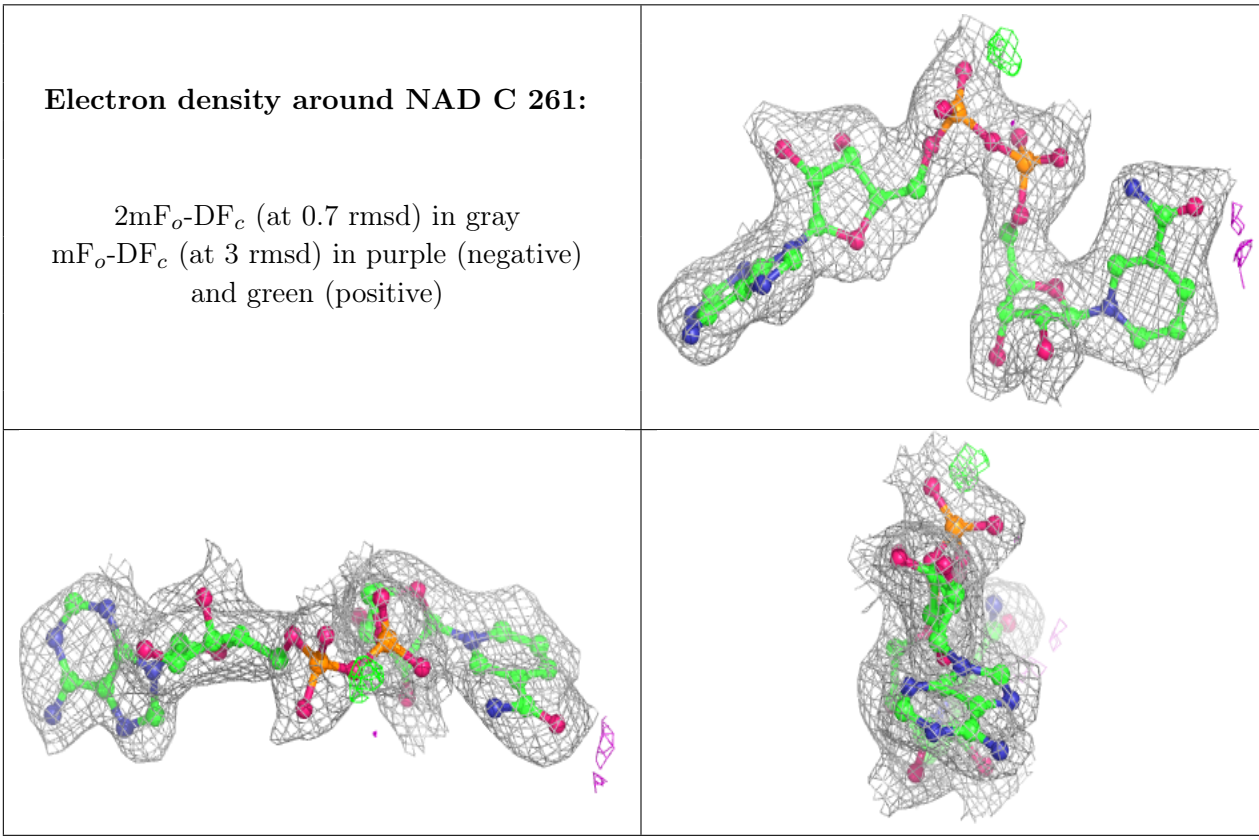
Electron density around NAD A 261:

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



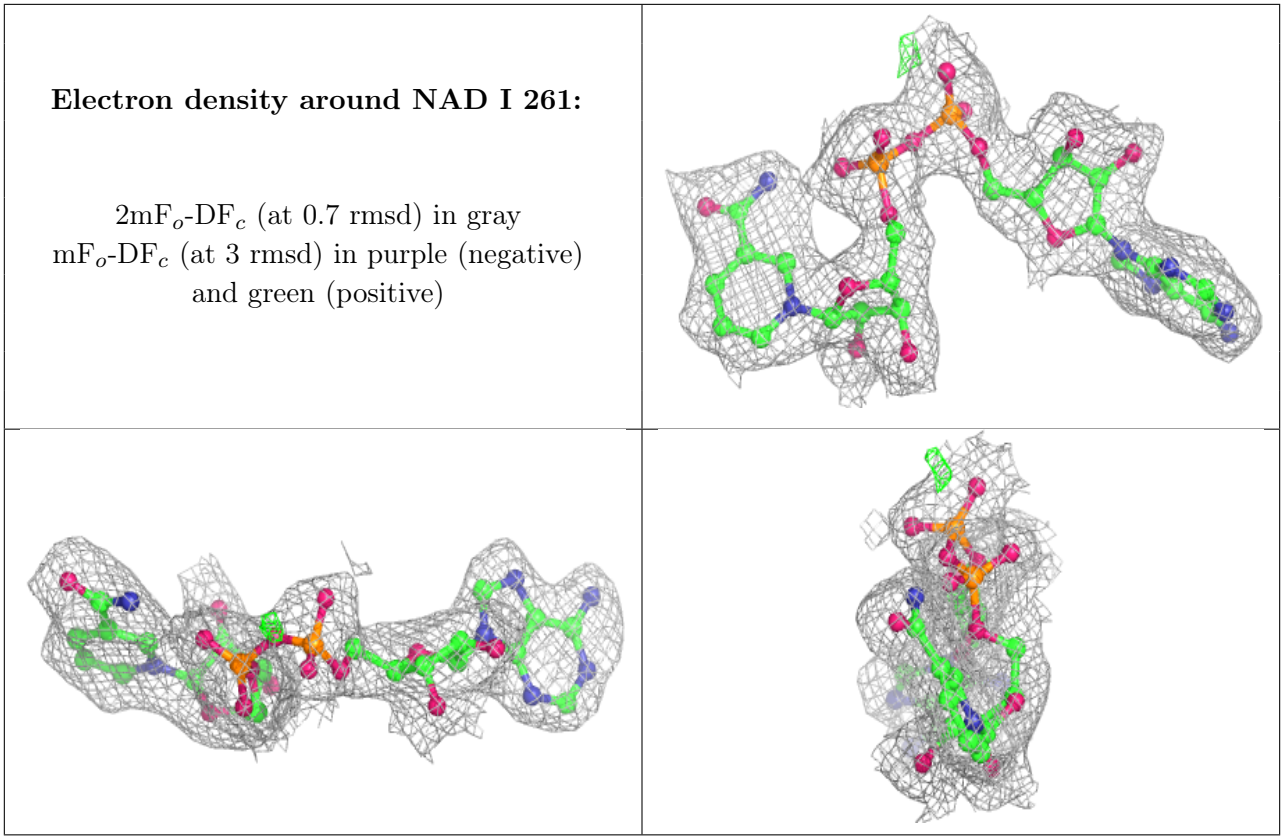
Electron density around NAD C 261:

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



Electron density around NAD I 261:

$2mF_o$-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.