



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 08:58 am BST

PDB ID : 5I7F
Title : Crystal structure of B. pseudomallei FabI in complex with NAD and PT405
Authors : Eltschkner, S.; Tonge, P.J.; Kisker, C.
Deposited on : 2016-02-17
Resolution : 2.70 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

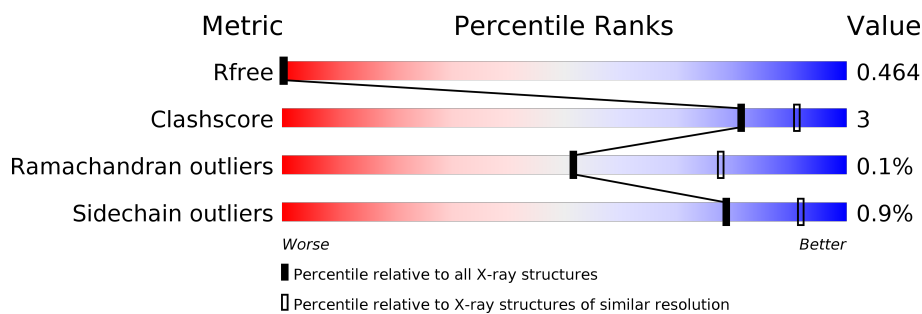
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	276	86% 7% 7%
1	B	276	86% 7% 7%
1	C	276	88% 5% 7%
1	D	276	87% 7% 7%
1	E	276	89% • 7%
1	F	276	89% • 7%
1	G	276	86% 7% 7%

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Mol	Chain	Length	Quality of chain
1	H	276	<div><div></div><div>84%</div><div>9%</div><div>7%</div></div>
1	I	276	<div><div></div><div>90%</div><div></div><div>7%</div></div>
1	J	276	<div><div></div><div>88%</div><div>5%</div><div>7%</div></div>
1	K	276	<div><div></div><div>89%</div><div></div><div>7%</div></div>
1	L	276	<div><div></div><div>86%</div><div>7%</div><div>7%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46664 atoms, of which 22715 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	B	257	Total	C	H	N	O	S	0	0	0
			3754	1218	1842	325	363	6			
1	E	257	Total	C	H	N	O	S	0	1	0
			3765	1221	1848	325	365	6			
1	H	257	Total	C	H	N	O	S	0	0	0
			3759	1218	1847	325	363	6			
1	C	257	Total	C	H	N	O	S	0	0	0
			3754	1218	1842	325	363	6			
1	A	257	Total	C	H	N	O	S	0	0	0
			3759	1218	1847	325	363	6			
1	F	257	Total	C	H	N	O	S	19	1	0
			3777	1223	1859	326	363	6			
1	G	257	Total	C	H	N	O	S	0	1	0
			3766	1221	1849	325	365	6			
1	D	257	Total	C	H	N	O	S	0	0	0
			3759	1218	1847	325	363	6			
1	I	257	Total	C	H	N	O	S	0	0	0
			3772	1218	1860	325	363	6			
1	K	257	Total	C	H	N	O	S	0	1	0
			3771	1223	1853	326	363	6			
1	L	257	Total	C	H	N	O	S	0	0	0
			3774	1218	1862	325	363	6			
1	J	257	Total	C	H	N	O	S	19	1	0
			3809	1223	1891	326	363	6			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	LYS	-	expression tag	UNP A0A069B9A4
B	265	LEU	-	expression tag	UNP A0A069B9A4
B	266	ALA	-	expression tag	UNP A0A069B9A4
B	267	ALA	-	expression tag	UNP A0A069B9A4
B	268	ALA	-	expression tag	UNP A0A069B9A4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	269	LEU	-	expression tag	UNP A0A069B9A4
B	270	GLU	-	expression tag	UNP A0A069B9A4
B	271	HIS	-	expression tag	UNP A0A069B9A4
B	272	HIS	-	expression tag	UNP A0A069B9A4
B	273	HIS	-	expression tag	UNP A0A069B9A4
B	274	HIS	-	expression tag	UNP A0A069B9A4
B	275	HIS	-	expression tag	UNP A0A069B9A4
B	276	HIS	-	expression tag	UNP A0A069B9A4
E	264	LYS	-	expression tag	UNP A0A069B9A4
E	265	LEU	-	expression tag	UNP A0A069B9A4
E	266	ALA	-	expression tag	UNP A0A069B9A4
E	267	ALA	-	expression tag	UNP A0A069B9A4
E	268	ALA	-	expression tag	UNP A0A069B9A4
E	269	LEU	-	expression tag	UNP A0A069B9A4
E	270	GLU	-	expression tag	UNP A0A069B9A4
E	271	HIS	-	expression tag	UNP A0A069B9A4
E	272	HIS	-	expression tag	UNP A0A069B9A4
E	273	HIS	-	expression tag	UNP A0A069B9A4
E	274	HIS	-	expression tag	UNP A0A069B9A4
E	275	HIS	-	expression tag	UNP A0A069B9A4
E	276	HIS	-	expression tag	UNP A0A069B9A4
H	264	LYS	-	expression tag	UNP A0A069B9A4
H	265	LEU	-	expression tag	UNP A0A069B9A4
H	266	ALA	-	expression tag	UNP A0A069B9A4
H	267	ALA	-	expression tag	UNP A0A069B9A4
H	268	ALA	-	expression tag	UNP A0A069B9A4
H	269	LEU	-	expression tag	UNP A0A069B9A4
H	270	GLU	-	expression tag	UNP A0A069B9A4
H	271	HIS	-	expression tag	UNP A0A069B9A4
H	272	HIS	-	expression tag	UNP A0A069B9A4
H	273	HIS	-	expression tag	UNP A0A069B9A4
H	274	HIS	-	expression tag	UNP A0A069B9A4
H	275	HIS	-	expression tag	UNP A0A069B9A4
H	276	HIS	-	expression tag	UNP A0A069B9A4
C	264	LYS	-	expression tag	UNP A0A069B9A4
C	265	LEU	-	expression tag	UNP A0A069B9A4
C	266	ALA	-	expression tag	UNP A0A069B9A4
C	267	ALA	-	expression tag	UNP A0A069B9A4
C	268	ALA	-	expression tag	UNP A0A069B9A4
C	269	LEU	-	expression tag	UNP A0A069B9A4
C	270	GLU	-	expression tag	UNP A0A069B9A4
C	271	HIS	-	expression tag	UNP A0A069B9A4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	272	HIS	-	expression tag	UNP A0A069B9A4
C	273	HIS	-	expression tag	UNP A0A069B9A4
C	274	HIS	-	expression tag	UNP A0A069B9A4
C	275	HIS	-	expression tag	UNP A0A069B9A4
C	276	HIS	-	expression tag	UNP A0A069B9A4
A	264	LYS	-	expression tag	UNP A0A069B9A4
A	265	LEU	-	expression tag	UNP A0A069B9A4
A	266	ALA	-	expression tag	UNP A0A069B9A4
A	267	ALA	-	expression tag	UNP A0A069B9A4
A	268	ALA	-	expression tag	UNP A0A069B9A4
A	269	LEU	-	expression tag	UNP A0A069B9A4
A	270	GLU	-	expression tag	UNP A0A069B9A4
A	271	HIS	-	expression tag	UNP A0A069B9A4
A	272	HIS	-	expression tag	UNP A0A069B9A4
A	273	HIS	-	expression tag	UNP A0A069B9A4
A	274	HIS	-	expression tag	UNP A0A069B9A4
A	275	HIS	-	expression tag	UNP A0A069B9A4
A	276	HIS	-	expression tag	UNP A0A069B9A4
F	264	LYS	-	expression tag	UNP A0A069B9A4
F	265	LEU	-	expression tag	UNP A0A069B9A4
F	266	ALA	-	expression tag	UNP A0A069B9A4
F	267	ALA	-	expression tag	UNP A0A069B9A4
F	268	ALA	-	expression tag	UNP A0A069B9A4
F	269	LEU	-	expression tag	UNP A0A069B9A4
F	270	GLU	-	expression tag	UNP A0A069B9A4
F	271	HIS	-	expression tag	UNP A0A069B9A4
F	272	HIS	-	expression tag	UNP A0A069B9A4
F	273	HIS	-	expression tag	UNP A0A069B9A4
F	274	HIS	-	expression tag	UNP A0A069B9A4
F	275	HIS	-	expression tag	UNP A0A069B9A4
F	276	HIS	-	expression tag	UNP A0A069B9A4
G	264	LYS	-	expression tag	UNP A0A069B9A4
G	265	LEU	-	expression tag	UNP A0A069B9A4
G	266	ALA	-	expression tag	UNP A0A069B9A4
G	267	ALA	-	expression tag	UNP A0A069B9A4
G	268	ALA	-	expression tag	UNP A0A069B9A4
G	269	LEU	-	expression tag	UNP A0A069B9A4
G	270	GLU	-	expression tag	UNP A0A069B9A4
G	271	HIS	-	expression tag	UNP A0A069B9A4
G	272	HIS	-	expression tag	UNP A0A069B9A4
G	273	HIS	-	expression tag	UNP A0A069B9A4
G	274	HIS	-	expression tag	UNP A0A069B9A4

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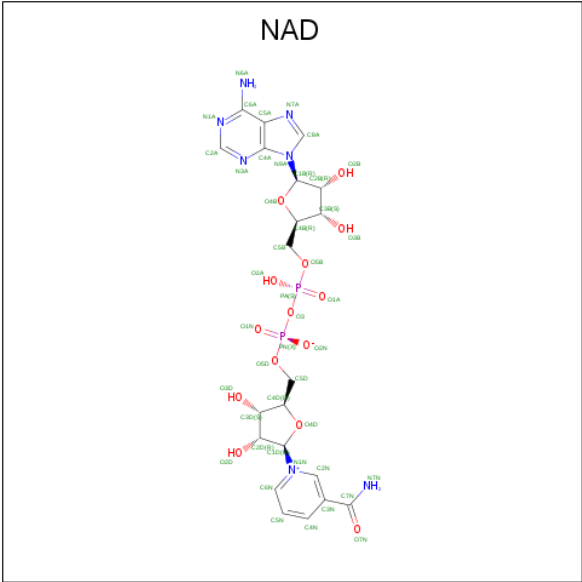
Chain	Residue	Modelled	Actual	Comment	Reference
G	275	HIS	-	expression tag	UNP A0A069B9A4
G	276	HIS	-	expression tag	UNP A0A069B9A4
D	264	LYS	-	expression tag	UNP A0A069B9A4
D	265	LEU	-	expression tag	UNP A0A069B9A4
D	266	ALA	-	expression tag	UNP A0A069B9A4
D	267	ALA	-	expression tag	UNP A0A069B9A4
D	268	ALA	-	expression tag	UNP A0A069B9A4
D	269	LEU	-	expression tag	UNP A0A069B9A4
D	270	GLU	-	expression tag	UNP A0A069B9A4
D	271	HIS	-	expression tag	UNP A0A069B9A4
D	272	HIS	-	expression tag	UNP A0A069B9A4
D	273	HIS	-	expression tag	UNP A0A069B9A4
D	274	HIS	-	expression tag	UNP A0A069B9A4
D	275	HIS	-	expression tag	UNP A0A069B9A4
D	276	HIS	-	expression tag	UNP A0A069B9A4
I	264	LYS	-	expression tag	UNP A0A069B9A4
I	265	LEU	-	expression tag	UNP A0A069B9A4
I	266	ALA	-	expression tag	UNP A0A069B9A4
I	267	ALA	-	expression tag	UNP A0A069B9A4
I	268	ALA	-	expression tag	UNP A0A069B9A4
I	269	LEU	-	expression tag	UNP A0A069B9A4
I	270	GLU	-	expression tag	UNP A0A069B9A4
I	271	HIS	-	expression tag	UNP A0A069B9A4
I	272	HIS	-	expression tag	UNP A0A069B9A4
I	273	HIS	-	expression tag	UNP A0A069B9A4
I	274	HIS	-	expression tag	UNP A0A069B9A4
I	275	HIS	-	expression tag	UNP A0A069B9A4
I	276	HIS	-	expression tag	UNP A0A069B9A4
K	264	LYS	-	expression tag	UNP A0A069B9A4
K	265	LEU	-	expression tag	UNP A0A069B9A4
K	266	ALA	-	expression tag	UNP A0A069B9A4
K	267	ALA	-	expression tag	UNP A0A069B9A4
K	268	ALA	-	expression tag	UNP A0A069B9A4
K	269	LEU	-	expression tag	UNP A0A069B9A4
K	270	GLU	-	expression tag	UNP A0A069B9A4
K	271	HIS	-	expression tag	UNP A0A069B9A4
K	272	HIS	-	expression tag	UNP A0A069B9A4
K	273	HIS	-	expression tag	UNP A0A069B9A4
K	274	HIS	-	expression tag	UNP A0A069B9A4
K	275	HIS	-	expression tag	UNP A0A069B9A4
K	276	HIS	-	expression tag	UNP A0A069B9A4
L	264	LYS	-	expression tag	UNP A0A069B9A4

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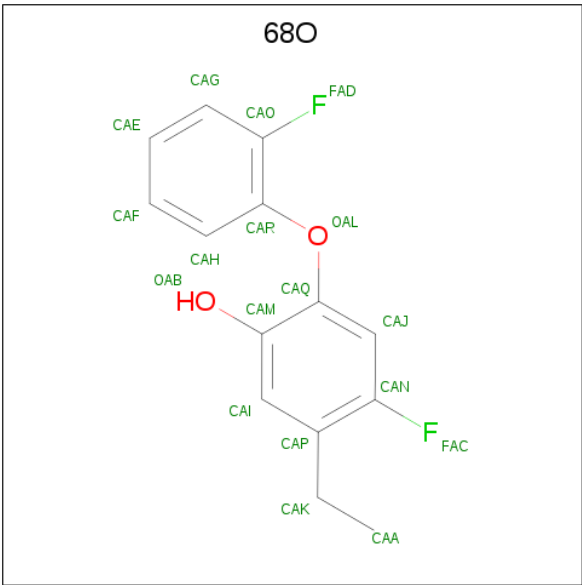
Chain	Residue	Modelled	Actual	Comment	Reference
L	265	LEU	-	expression tag	UNP A0A069B9A4
L	266	ALA	-	expression tag	UNP A0A069B9A4
L	267	ALA	-	expression tag	UNP A0A069B9A4
L	268	ALA	-	expression tag	UNP A0A069B9A4
L	269	LEU	-	expression tag	UNP A0A069B9A4
L	270	GLU	-	expression tag	UNP A0A069B9A4
L	271	HIS	-	expression tag	UNP A0A069B9A4
L	272	HIS	-	expression tag	UNP A0A069B9A4
L	273	HIS	-	expression tag	UNP A0A069B9A4
L	274	HIS	-	expression tag	UNP A0A069B9A4
L	275	HIS	-	expression tag	UNP A0A069B9A4
L	276	HIS	-	expression tag	UNP A0A069B9A4
J	264	LYS	-	expression tag	UNP A0A069B9A4
J	265	LEU	-	expression tag	UNP A0A069B9A4
J	266	ALA	-	expression tag	UNP A0A069B9A4
J	267	ALA	-	expression tag	UNP A0A069B9A4
J	268	ALA	-	expression tag	UNP A0A069B9A4
J	269	LEU	-	expression tag	UNP A0A069B9A4
J	270	GLU	-	expression tag	UNP A0A069B9A4
J	271	HIS	-	expression tag	UNP A0A069B9A4
J	272	HIS	-	expression tag	UNP A0A069B9A4
J	273	HIS	-	expression tag	UNP A0A069B9A4
J	274	HIS	-	expression tag	UNP A0A069B9A4
J	275	HIS	-	expression tag	UNP A0A069B9A4
J	276	HIS	-	expression tag	UNP A0A069B9A4

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	E	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	H	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	A	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	F	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	G	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	I	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	K	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	L	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
2	J	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		

- Molecule 3 is 5-ethyl-4-fluoro-2-(2-fluorophenoxy)phenol (three-letter code: 68O) (formula: C₁₄H₁₂F₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	E	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	H	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	C	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	A	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	F	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	G	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	D	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	I	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	K	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	L	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	J	1	Total	C	F	H	O	0	0
			30	14	2	12	2		

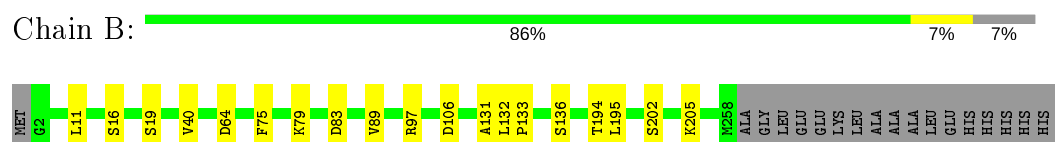
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	20	Total 20	O 20	0	0
4	E	22	Total 22	O 22	0	0
4	H	17	Total 17	O 17	0	0
4	C	13	Total 13	O 13	0	0
4	A	22	Total 22	O 22	0	0
4	F	24	Total 24	O 24	0	0
4	G	23	Total 23	O 23	0	0
4	D	32	Total 32	O 32	0	0
4	I	10	Total 10	O 10	0	0
4	K	18	Total 18	O 18	0	0
4	L	12	Total 12	O 12	0	0
4	J	20	Total 20	O 20	0	0

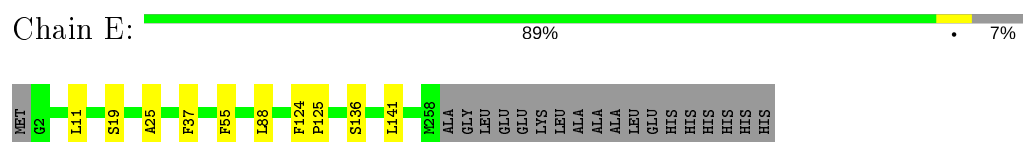
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

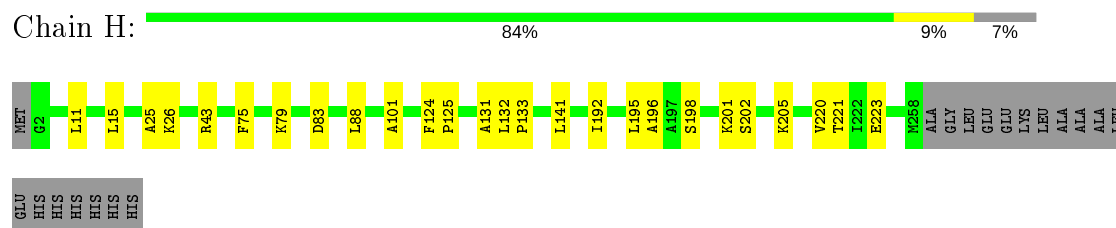
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



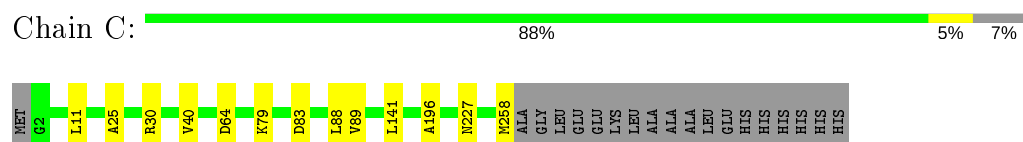
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



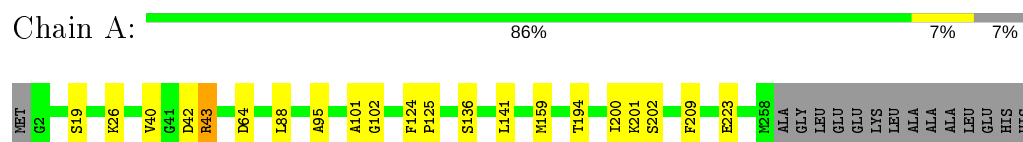
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



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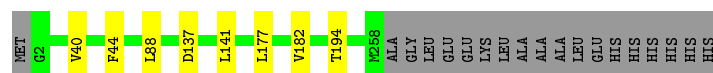
- Chain G: 86% 7% 7%



- Chain D:  87% 7% 7%



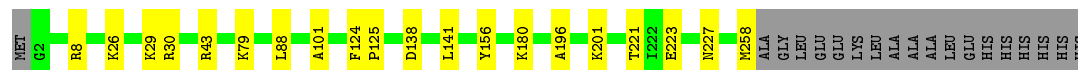
- Chain I:  90% • 7%

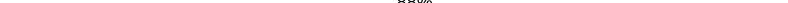


- Chain K: 89% • 7%



- Chain L:  86% 7% 7%



- Chain J:  88% 5% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.43 Å 109.78 Å 269.80 Å 90.00° 104.51° 90.00°	Depositor
Resolution (Å)	47.17 – 2.70 48.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.4 (47.17-2.70) 94.6 (48.99-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.69 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.192 , 0.223 0.445 , 0.464	Depositor DCC
R_{free} test set	4941 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	115.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.47$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	46664	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 52.58 % 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 4.7678e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 68O, NAD

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	0.36	2/1945 (0.1%)	0.68	2/2631 (0.1%)
1	B	0.27	0/1945	0.45	0/2631
1	C	0.26	0/1945	0.46	0/2631
1	D	0.28	0/1945	0.46	0/2631
1	E	0.28	0/1953	0.46	0/2642
1	F	0.28	0/1954	0.47	0/2642
1	G	0.27	0/1953	0.46	0/2642
1	H	0.27	0/1945	0.47	0/2631
1	I	0.26	0/1945	0.45	0/2631
1	J	0.28	0/1954	0.47	0/2642
1	K	0.29	0/1954	0.49	0/2642
1	L	0.27	0/1945	0.48	0/2631
All	All	0.28	2/23383 (0.0%)	0.49	2/31627 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	ARG	CZ-NH2	-6.43	1.24	1.33
1	A	43	ARG	CD-NE	-5.42	1.37	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	NE-CZ-NH2	-18.27	111.17	120.30
1	A	43	ARG	NE-CZ-NH1	16.36	128.48	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1912	1847	1919	15	0
1	B	1912	1842	1919	17	0
1	C	1912	1842	1919	7	0
1	D	1912	1847	1919	10	0
1	E	1917	1848	1923	7	0
1	F	1918	1859	1932	6	0
1	G	1917	1849	1923	10	0
1	H	1912	1847	1919	15	0
1	I	1912	1860	1919	4	0
1	J	1918	1891	1932	12	0
1	K	1918	1853	1932	7	0
1	L	1912	1862	1919	14	0
2	A	44	27	26	3	0
2	B	44	27	26	3	0
2	C	44	27	26	1	0
2	D	44	27	26	0	0
2	E	44	27	26	1	0
2	F	44	27	26	1	0
2	G	44	27	26	2	0
2	H	44	27	26	1	0
2	I	44	27	26	2	0
2	J	44	27	26	1	0
2	K	44	27	26	2	0
2	L	44	27	26	1	0
3	A	18	12	0	1	0
3	B	18	12	0	0	0
3	C	18	12	0	0	0
3	D	18	12	0	0	0
3	E	18	12	0	0	0
3	F	18	12	0	0	0
3	G	18	12	0	0	0
3	H	18	12	0	0	0
3	I	18	12	0	0	0
3	J	18	12	0	1	0
3	K	18	12	0	0	0
3	L	18	12	0	1	0
4	A	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	0	1	0
4	C	13	0	0	0	0
4	D	32	0	0	0	0
4	E	22	0	0	0	0
4	F	24	0	0	0	0
4	G	23	0	0	0	0
4	H	17	0	0	0	0
4	I	10	0	0	0	0
4	J	20	0	0	1	0
4	K	18	0	0	0	0
4	L	12	0	0	0	0
All	All	23949	22715	23387	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 120 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:L:101:ALA:HB1	1:L:201:LYS:HD2	1.50	0.91
1:H:101:ALA:HB1	1:H:201:LYS:HD2	1.56	0.87
1:G:97:ARG:NH1	1:L:138:ASP:OD2	2.15	0.79
1:C:30:ARG:NH2	1:C:227:ASN:OD1	2.18	0.76
1:A:101:ALA:HB1	1:A:201:LYS:HD2	1.67	0.76

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	255/276 (92%)	241 (94%)	13 (5%)	1 (0%)	34 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
1	C	255/276 (92%)	241 (94%)	14 (6%)	0	100	100
1	D	255/276 (92%)	244 (96%)	11 (4%)	0	100	100
1	E	256/276 (93%)	244 (95%)	12 (5%)	0	100	100
1	F	256/276 (93%)	243 (95%)	13 (5%)	0	100	100
1	G	256/276 (93%)	242 (94%)	13 (5%)	1 (0%)	34	60
1	H	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
1	I	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
1	J	256/276 (93%)	245 (96%)	11 (4%)	0	100	100
1	K	256/276 (93%)	245 (96%)	11 (4%)	0	100	100
1	L	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
All	All	3065/3312 (92%)	2917 (95%)	146 (5%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	202	SER
1	A	202	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/209 (93%)	193 (99%)	2 (1%)	76	91
1	B	195/209 (93%)	194 (100%)	1 (0%)	88	96
1	C	195/209 (93%)	194 (100%)	1 (0%)	88	96
1	D	195/209 (93%)	194 (100%)	1 (0%)	88	96
1	E	196/209 (94%)	195 (100%)	1 (0%)	88	96
1	F	196/209 (94%)	194 (99%)	2 (1%)	76	91
1	G	196/209 (94%)	194 (99%)	2 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/209 (93%)	194 (100%)	1 (0%)	88	96
1	I	195/209 (93%)	194 (100%)	1 (0%)	88	96
1	J	196/209 (94%)	193 (98%)	3 (2%)	65	86
1	K	196/209 (94%)	194 (99%)	2 (1%)	76	91
1	L	195/209 (93%)	191 (98%)	4 (2%)	53	80
All	All	2345/2508 (94%)	2324 (99%)	21 (1%)	78	92

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	176	SER
1	I	137	ASP
1	L	180	LYS
1	G	43	ARG
1	J	8	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 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	L	301	-	42,48,48	0.83	2 (4%)	50,73,73	1.37	3 (6%)
3	68O	F	302	-	19,19,19	1.22	1 (5%)	25,26,26	1.32	3 (12%)
2	NAD	H	301	-	42,48,48	0.96	2 (4%)	50,73,73	1.40	2 (4%)
2	NAD	E	301	-	42,48,48	0.94	2 (4%)	50,73,73	1.33	3 (6%)
3	68O	I	302	-	19,19,19	1.21	1 (5%)	25,26,26	1.29	3 (12%)
3	68O	K	302	-	19,19,19	1.23	1 (5%)	25,26,26	1.52	6 (24%)
2	NAD	K	301	-	42,48,48	0.92	2 (4%)	50,73,73	1.34	2 (4%)
2	NAD	G	301	-	42,48,48	0.82	2 (4%)	50,73,73	1.41	4 (8%)
3	68O	G	302	-	19,19,19	1.25	1 (5%)	25,26,26	1.33	3 (12%)
3	68O	J	302	-	19,19,19	1.23	1 (5%)	25,26,26	1.20	3 (12%)
2	NAD	C	301	-	42,48,48	0.94	2 (4%)	50,73,73	1.35	3 (6%)
2	NAD	A	301	-	42,48,48	0.88	2 (4%)	50,73,73	1.40	4 (8%)
3	68O	L	302	-	19,19,19	1.20	1 (5%)	25,26,26	1.32	3 (12%)
3	68O	A	302	-	19,19,19	1.23	1 (5%)	25,26,26	1.28	3 (12%)
3	68O	B	302	-	19,19,19	1.25	1 (5%)	25,26,26	1.26	3 (12%)
3	68O	C	302	-	19,19,19	1.33	2 (10%)	25,26,26	1.25	3 (12%)
3	68O	E	302	-	19,19,19	1.23	1 (5%)	25,26,26	1.27	3 (12%)
3	68O	H	302	-	19,19,19	1.26	1 (5%)	25,26,26	1.31	3 (12%)
2	NAD	F	301	-	42,48,48	0.93	2 (4%)	50,73,73	1.34	3 (6%)
2	NAD	B	301	-	42,48,48	0.87	2 (4%)	50,73,73	1.43	3 (6%)
2	NAD	J	301	-	42,48,48	0.94	2 (4%)	50,73,73	1.40	2 (4%)
3	68O	D	302	-	19,19,19	1.37	2 (10%)	25,26,26	1.35	5 (20%)
2	NAD	I	301	-	42,48,48	0.86	2 (4%)	50,73,73	1.38	2 (4%)
2	NAD	D	301	-	42,48,48	0.88	2 (4%)	50,73,73	1.37	3 (6%)

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	L	301	-	-	5/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	68O	F	302	-	-	0/6/6/6	0/2/2/2
2	NAD	H	301	-	-	6/26/62/62	0/5/5/5
2	NAD	E	301	-	-	6/26/62/62	0/5/5/5
3	68O	I	302	-	-	0/6/6/6	0/2/2/2
3	68O	K	302	-	-	2/6/6/6	0/2/2/2
2	NAD	K	301	-	-	7/26/62/62	0/5/5/5
2	NAD	G	301	-	-	4/26/62/62	0/5/5/5
3	68O	G	302	-	-	0/6/6/6	0/2/2/2
3	68O	J	302	-	-	0/6/6/6	0/2/2/2
2	NAD	C	301	-	-	7/26/62/62	0/5/5/5
2	NAD	A	301	-	-	5/26/62/62	0/5/5/5
3	68O	L	302	-	-	0/6/6/6	0/2/2/2
3	68O	A	302	-	-	0/6/6/6	0/2/2/2
3	68O	B	302	-	-	0/6/6/6	0/2/2/2
3	68O	C	302	-	-	0/6/6/6	0/2/2/2
3	68O	E	302	-	-	0/6/6/6	0/2/2/2
3	68O	H	302	-	-	0/6/6/6	0/2/2/2
2	NAD	F	301	-	-	7/26/62/62	0/5/5/5
2	NAD	B	301	-	-	6/26/62/62	0/5/5/5
2	NAD	J	301	-	-	14/26/62/62	0/5/5/5
3	68O	D	302	-	-	0/6/6/6	0/2/2/2
2	NAD	I	301	-	-	4/26/62/62	0/5/5/5
2	NAD	D	301	-	-	6/26/62/62	0/5/5/5

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	68O	CAK-CAP	-4.64	1.39	1.51
3	I	302	68O	CAK-CAP	-4.51	1.39	1.51
3	D	302	68O	CAK-CAP	-4.50	1.39	1.51
3	H	302	68O	CAK-CAP	-4.48	1.39	1.51
3	A	302	68O	CAK-CAP	-4.45	1.39	1.51

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAD	PN-O3-PA	8.27	161.22	132.83
2	H	301	NAD	PN-O3-PA	8.08	160.57	132.83
2	J	301	NAD	PN-O3-PA	8.04	160.41	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	NAD	PN-O3-PA	7.87	159.84	132.83
2	I	301	NAD	PN-O3-PA	7.79	159.55	132.83

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	301	NAD	PN-O3-PA-O5B
2	H	301	NAD	C5D-O5D-PN-O2N
2	E	301	NAD	C5D-O5D-PN-O2N
2	K	301	NAD	C5D-O5D-PN-O2N
2	K	301	NAD	O4D-C1D-N1N-C2N

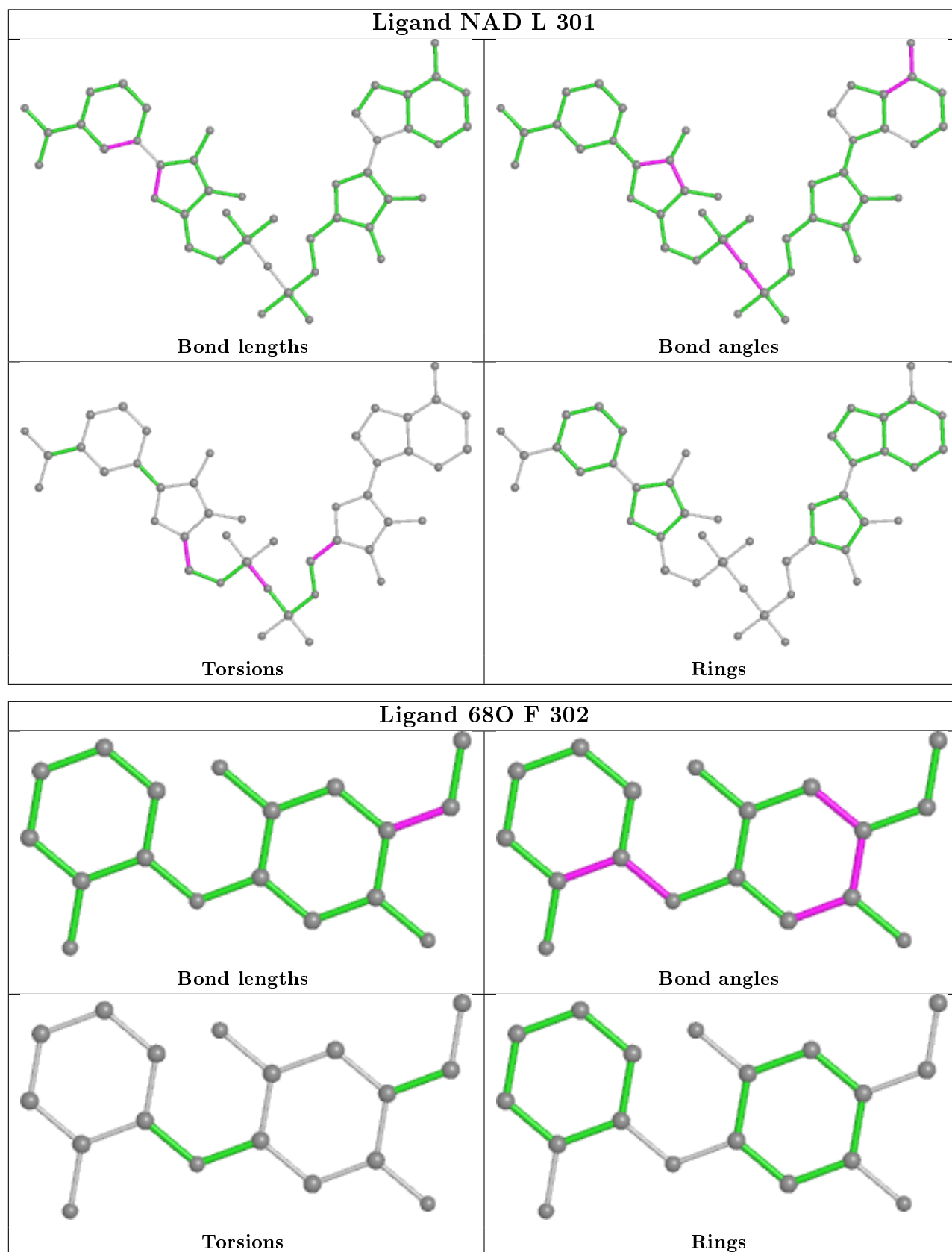
There are no ring outliers.

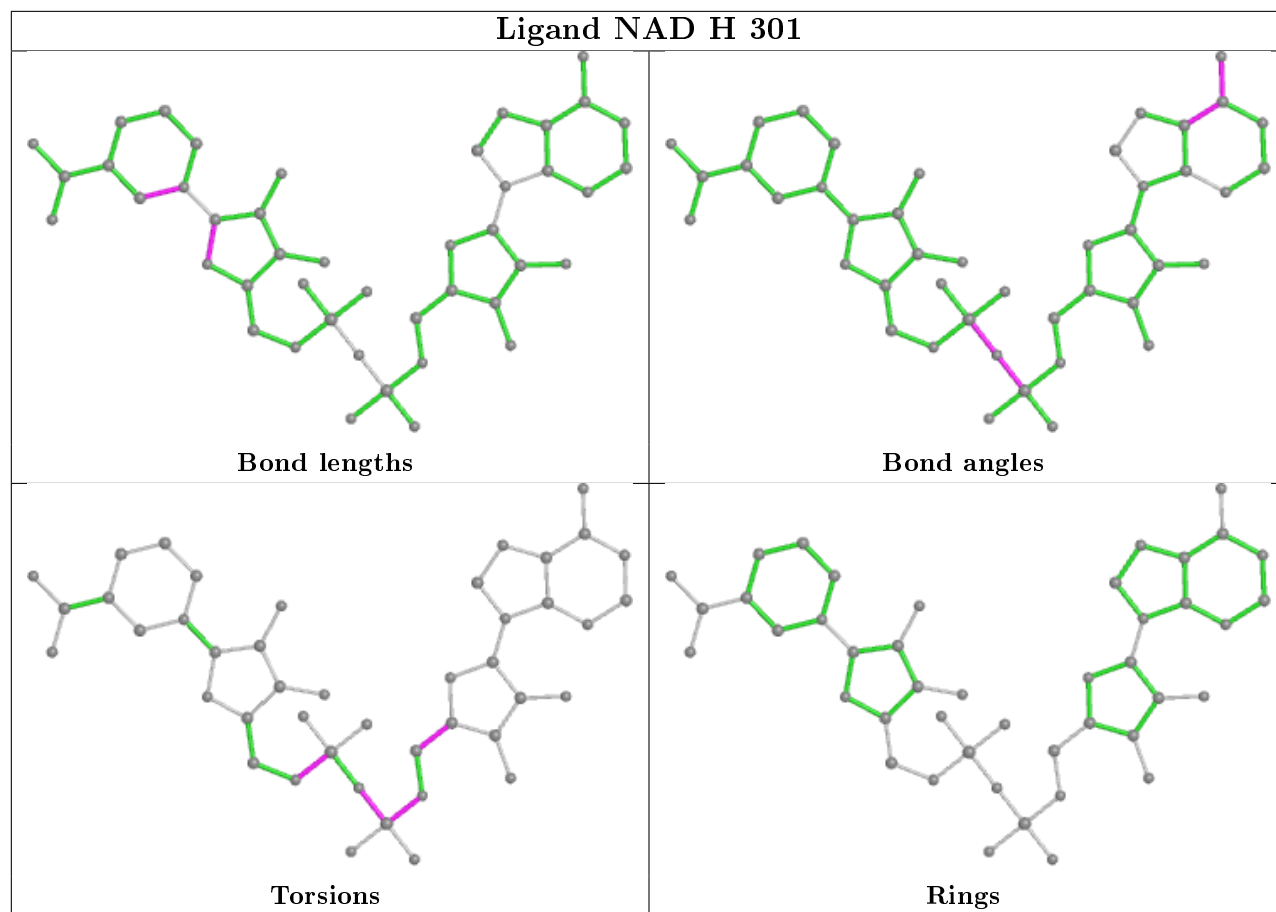
14 monomers are involved in 21 short contacts:

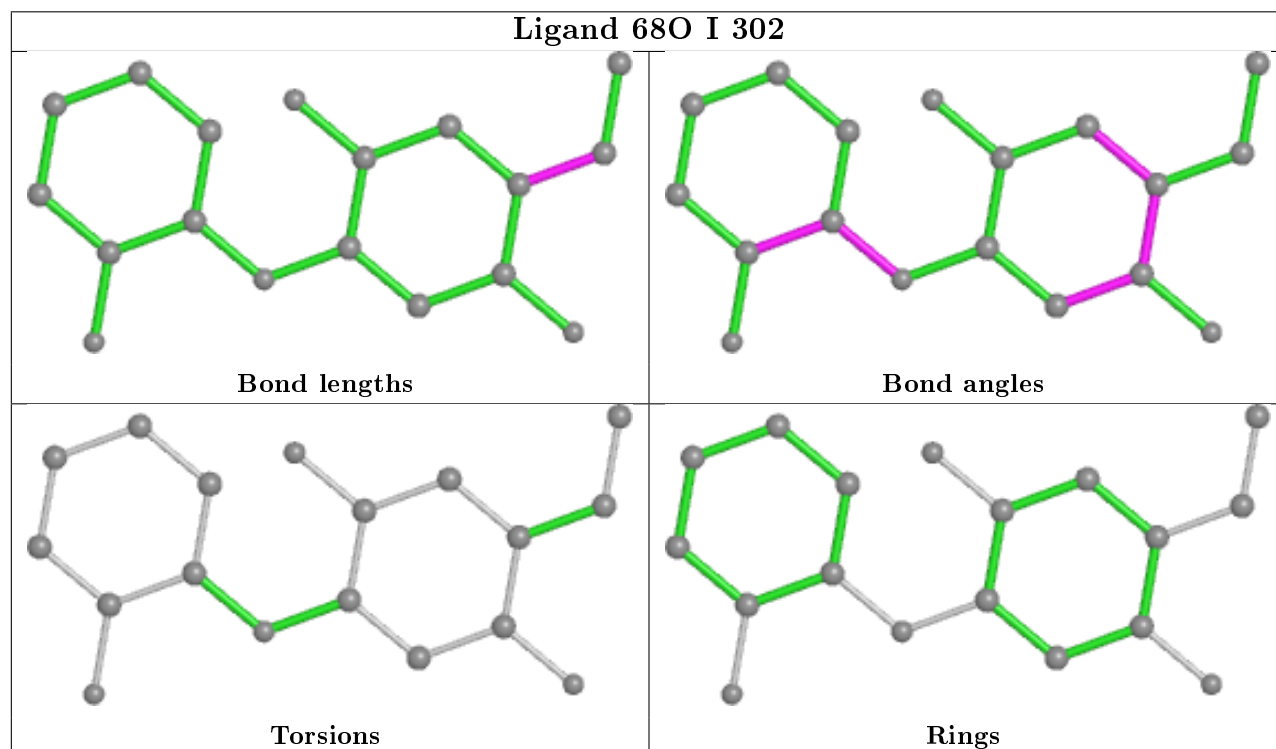
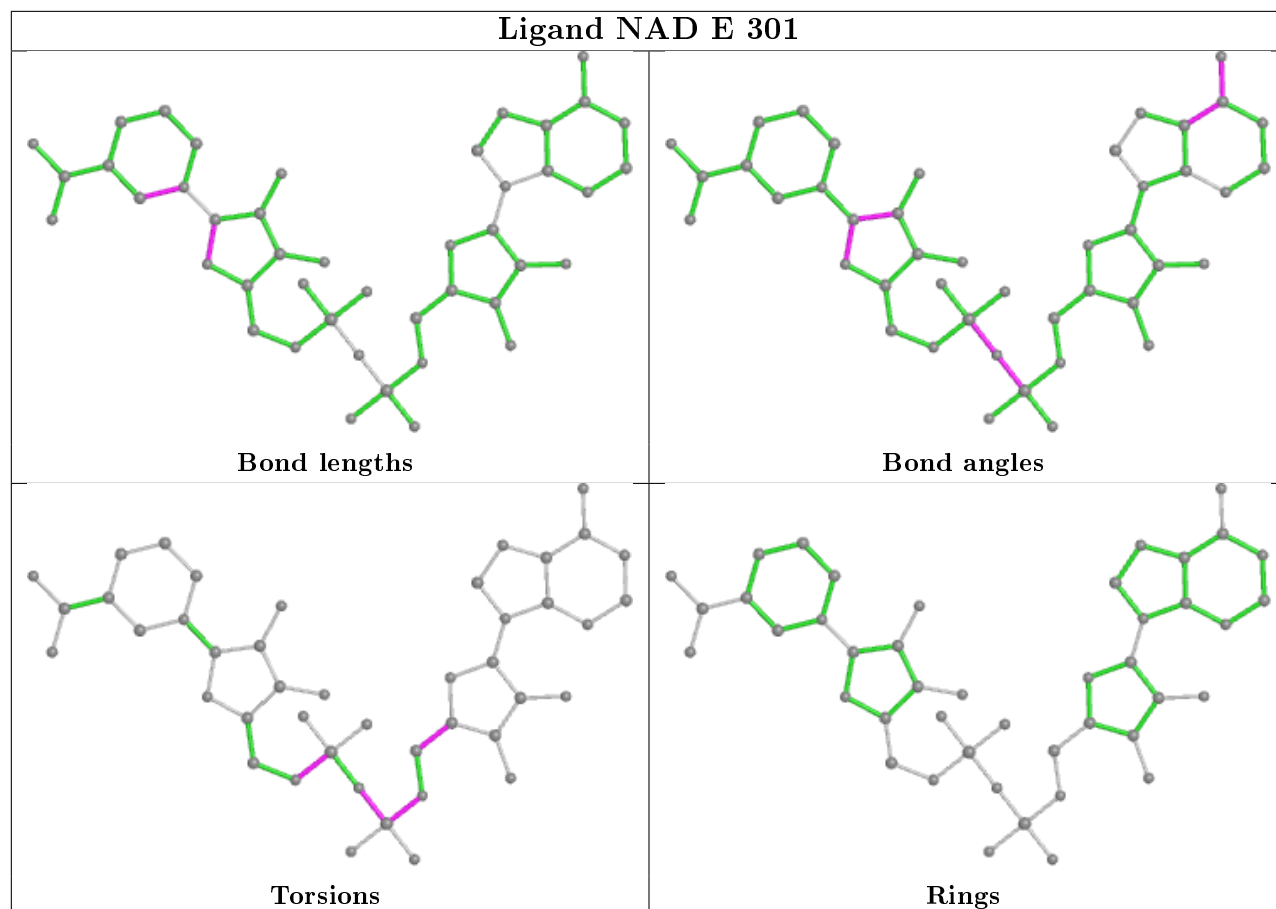
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	301	NAD	1	0
2	H	301	NAD	1	0
2	E	301	NAD	1	0
2	K	301	NAD	2	0
2	G	301	NAD	2	0
3	J	302	68O	1	0
2	C	301	NAD	1	0
2	A	301	NAD	3	0
3	L	302	68O	1	0
3	A	302	68O	1	0
2	F	301	NAD	1	0
2	B	301	NAD	3	0
2	J	301	NAD	1	0
2	I	301	NAD	2	0

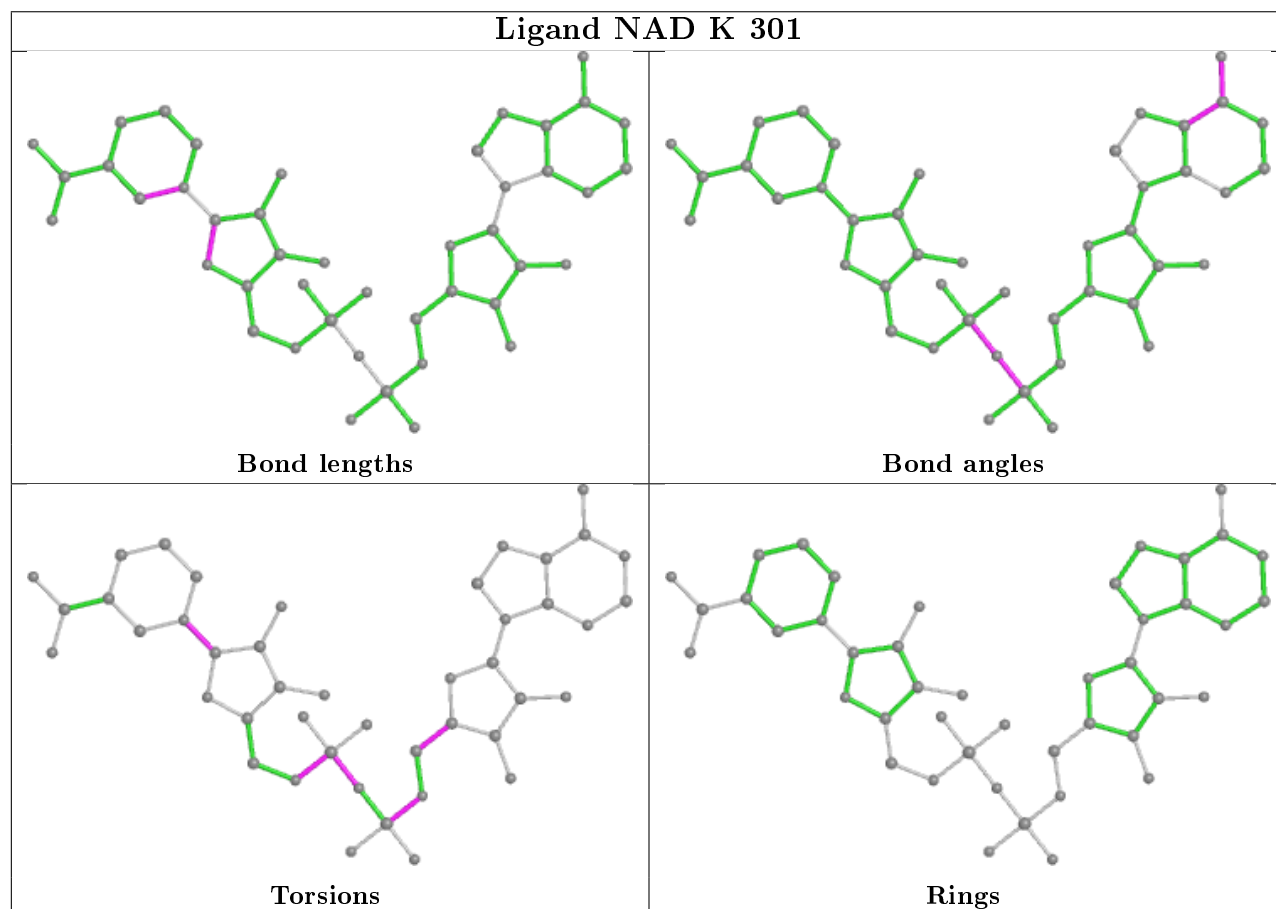
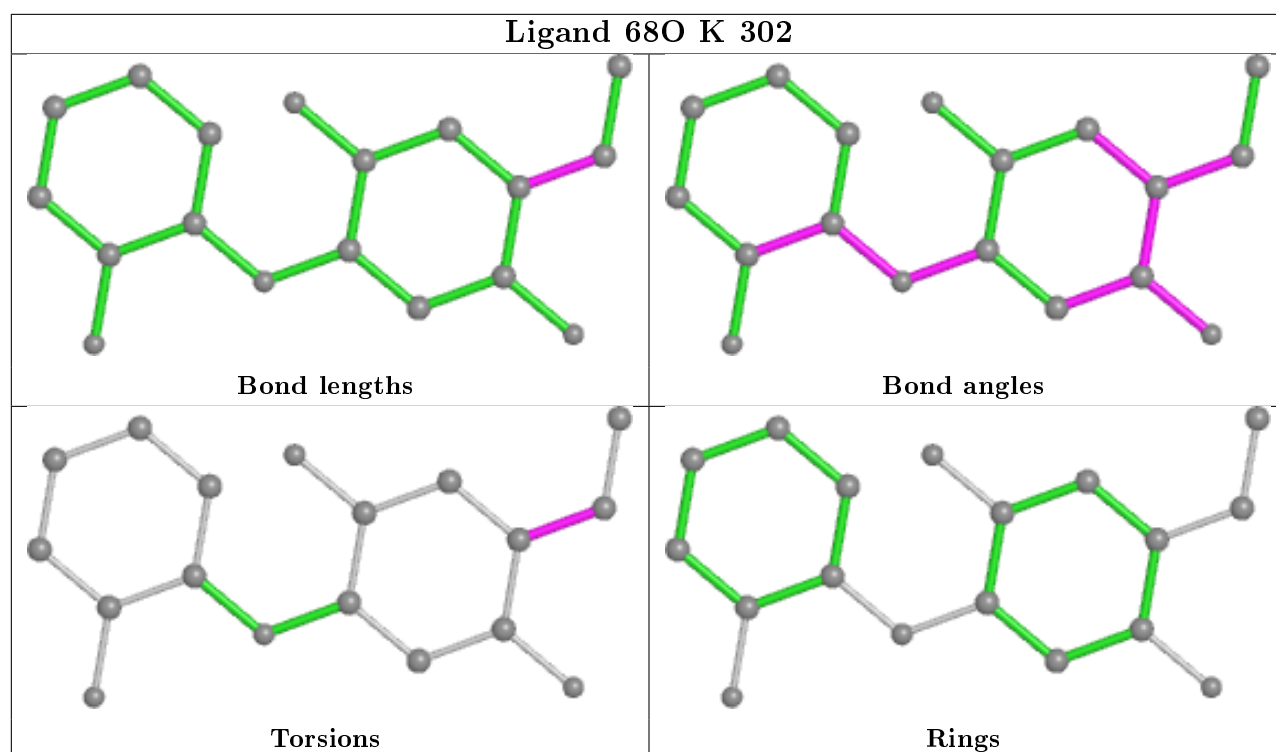
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

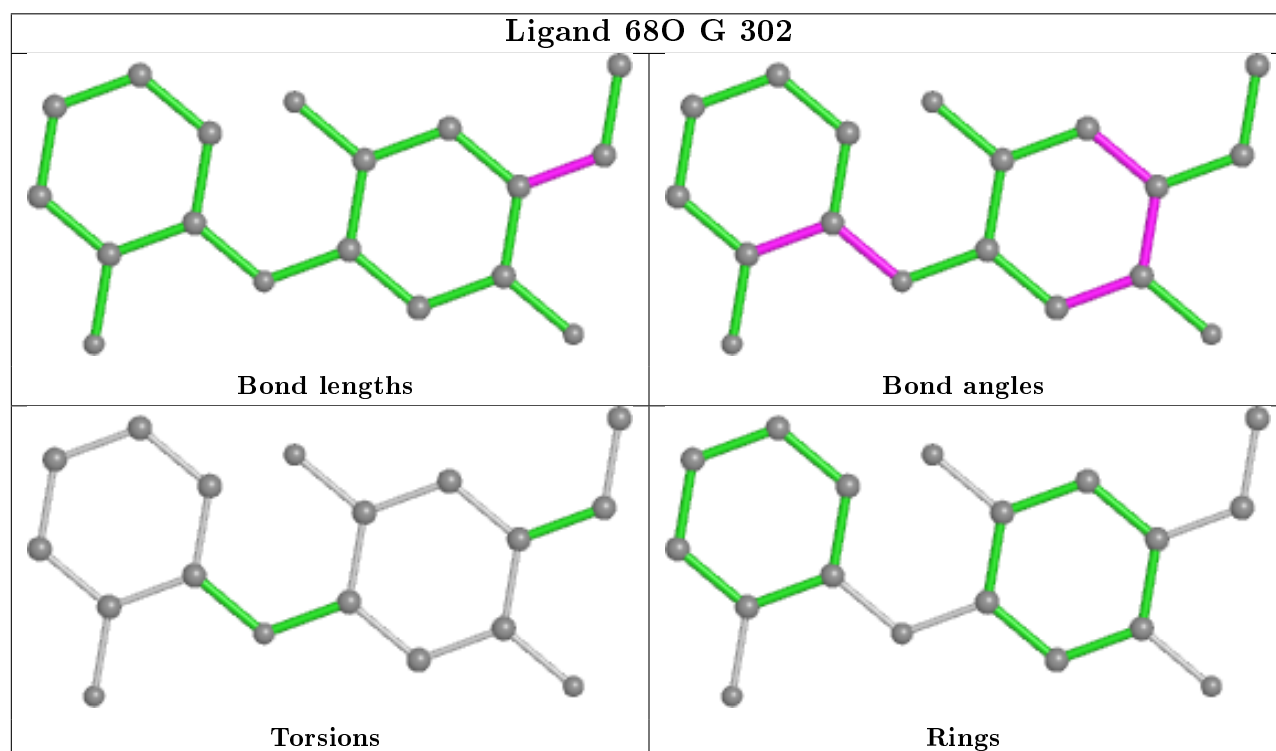
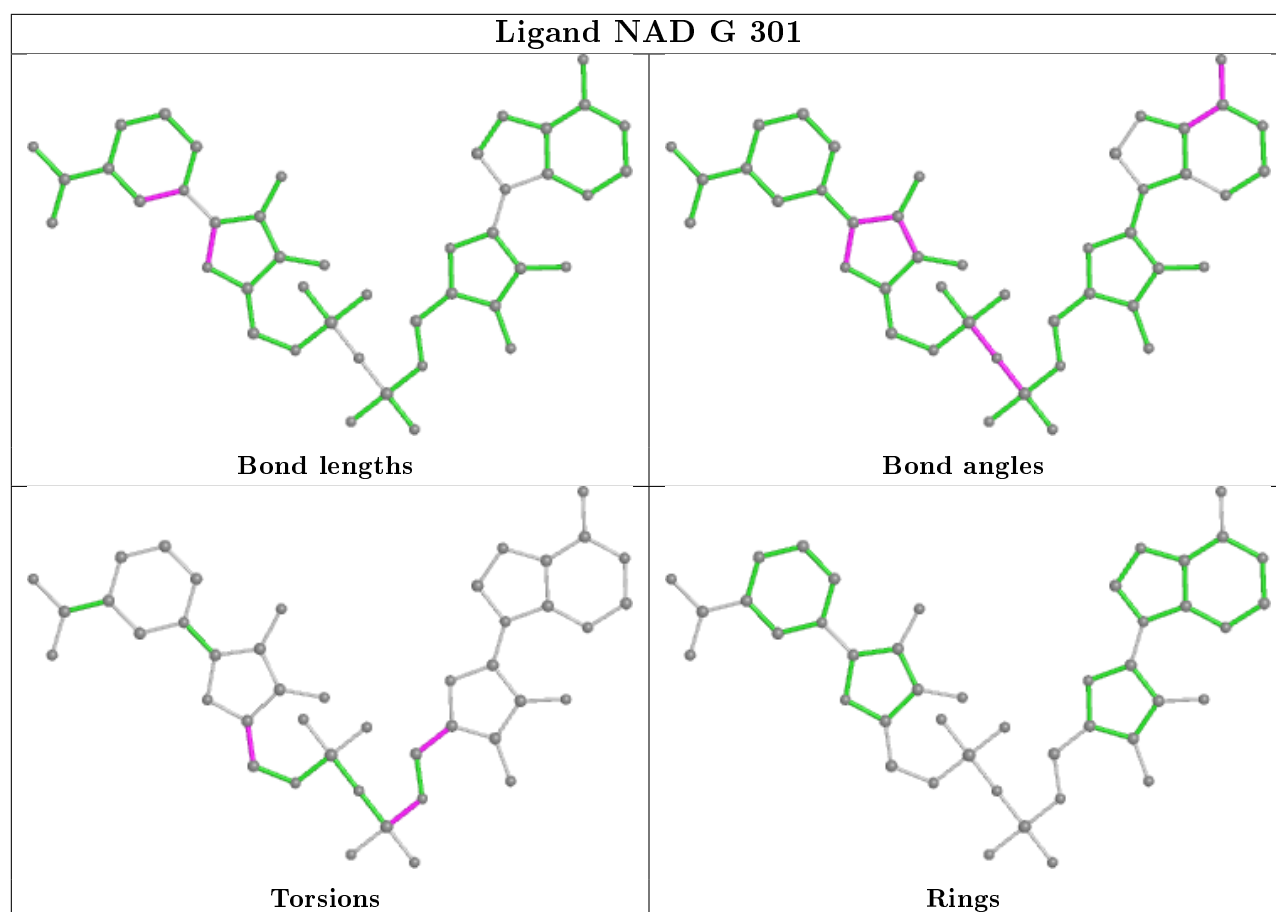
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



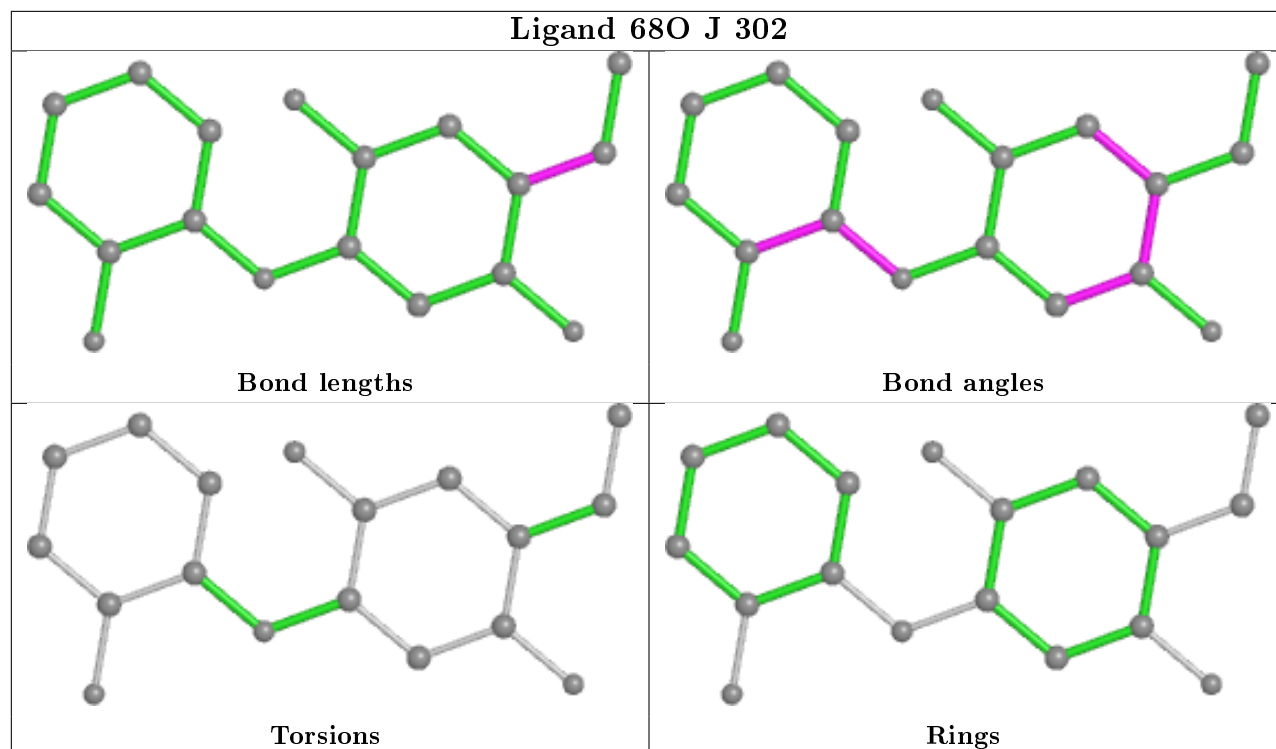




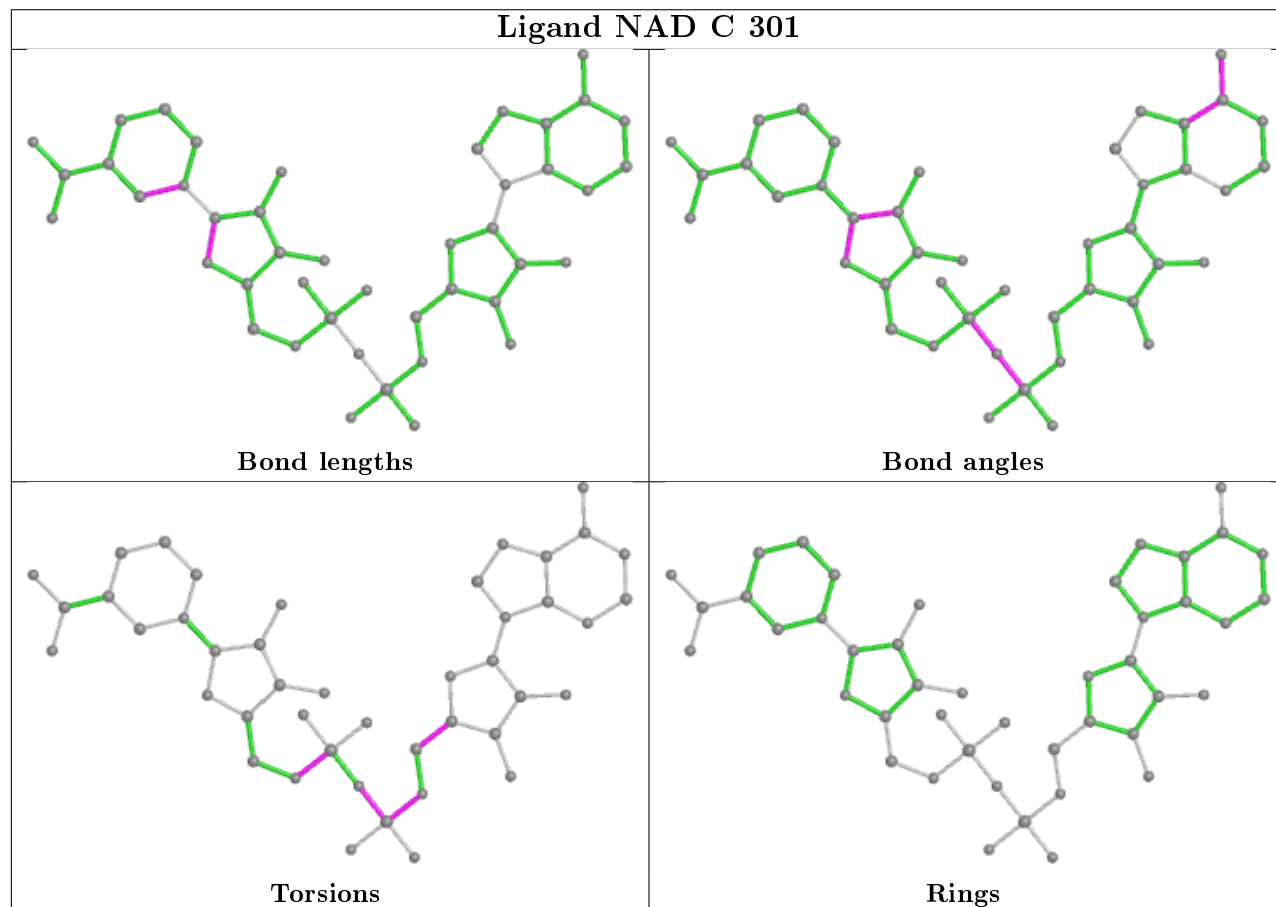


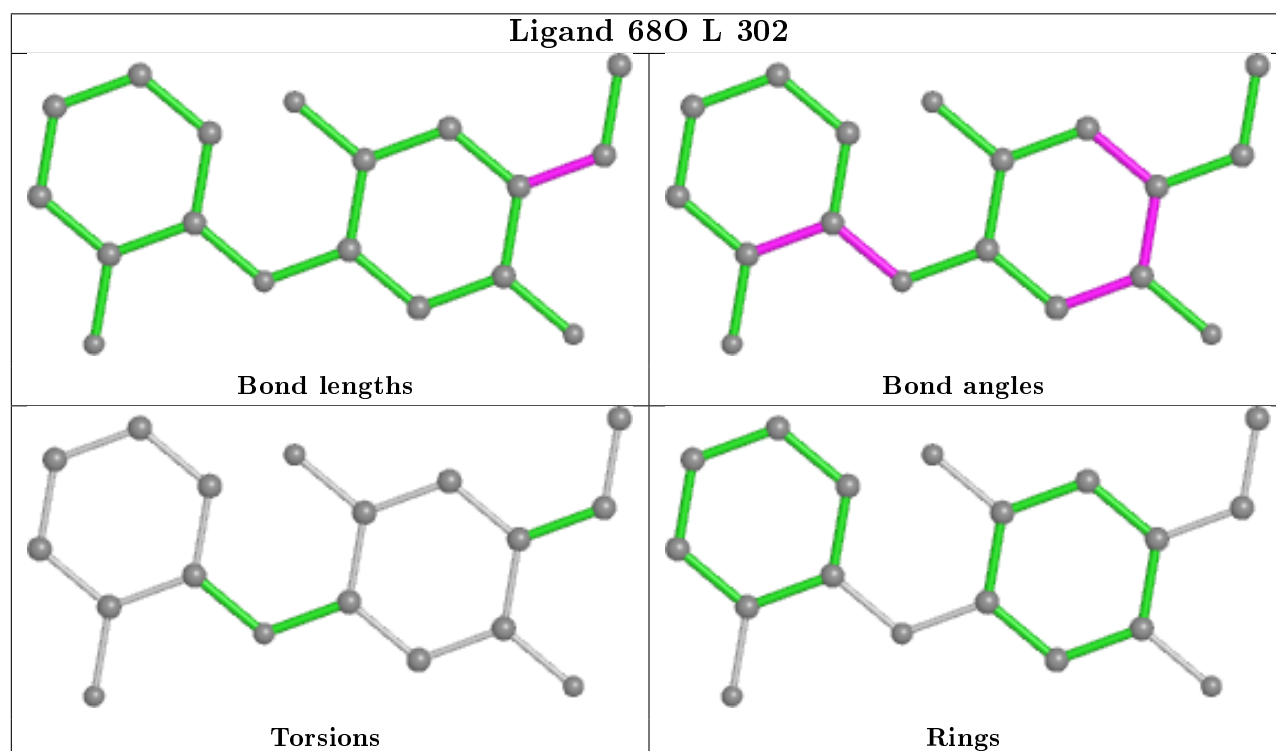
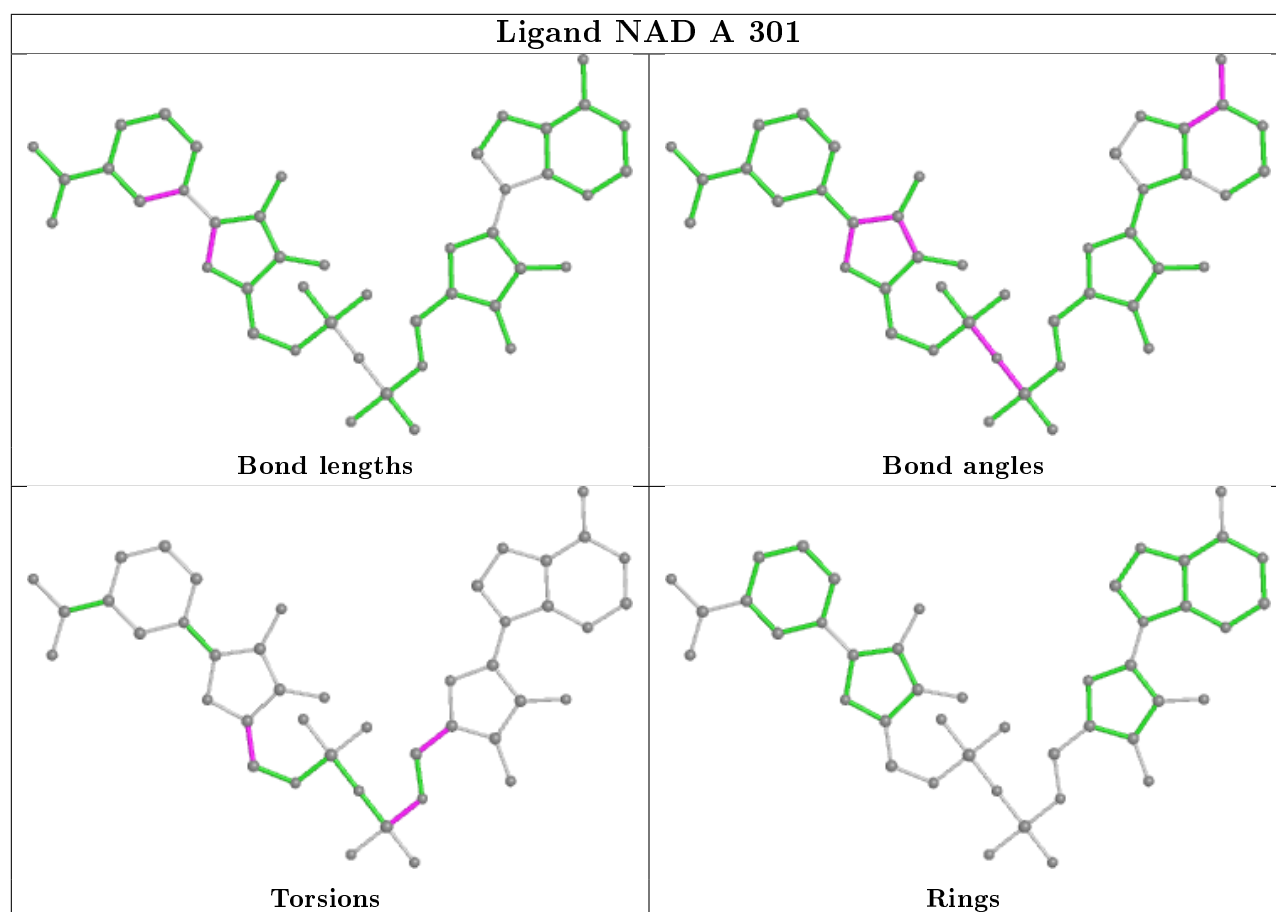


Ligand 68O J 302

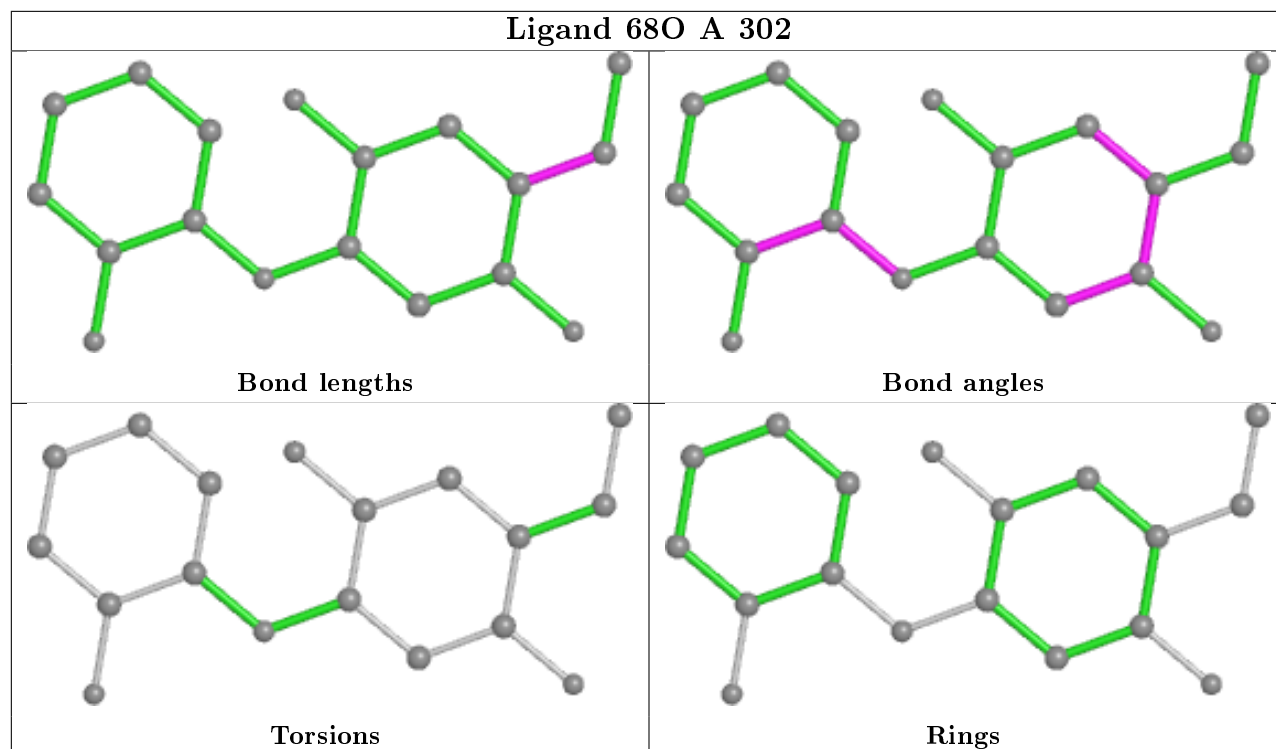


Ligand NAD C 301

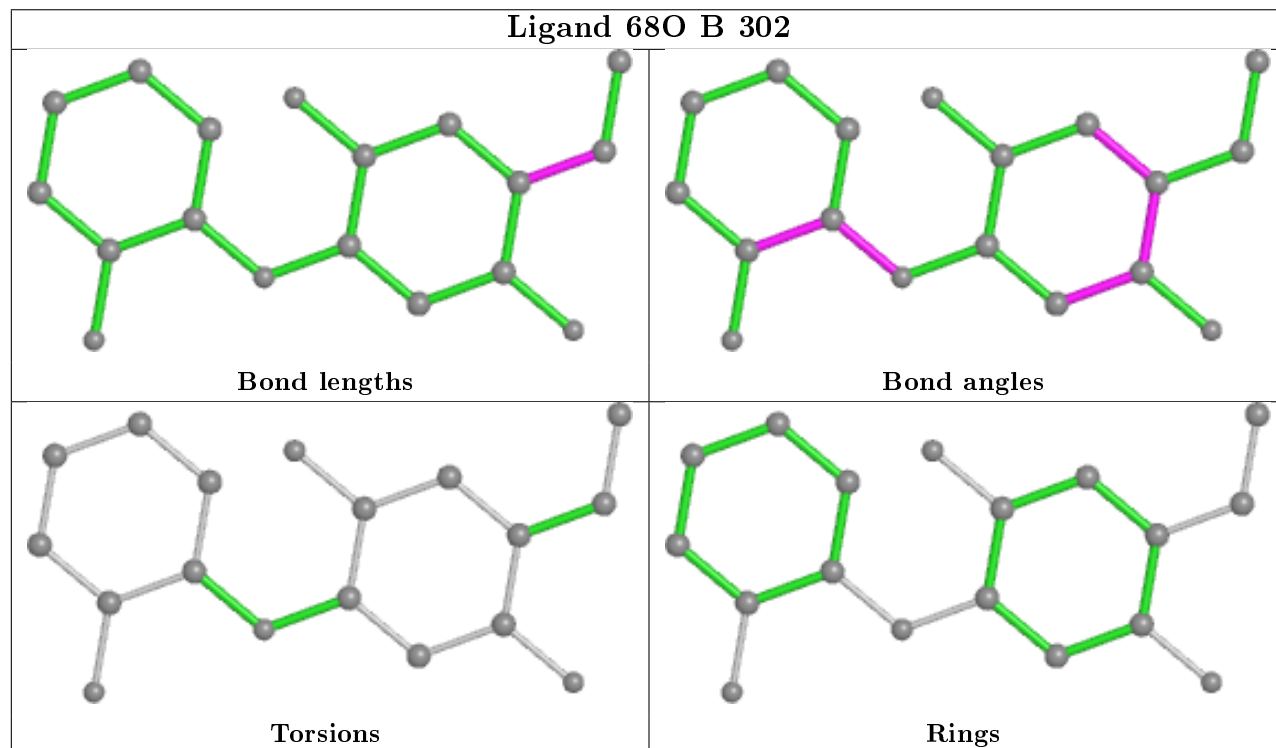




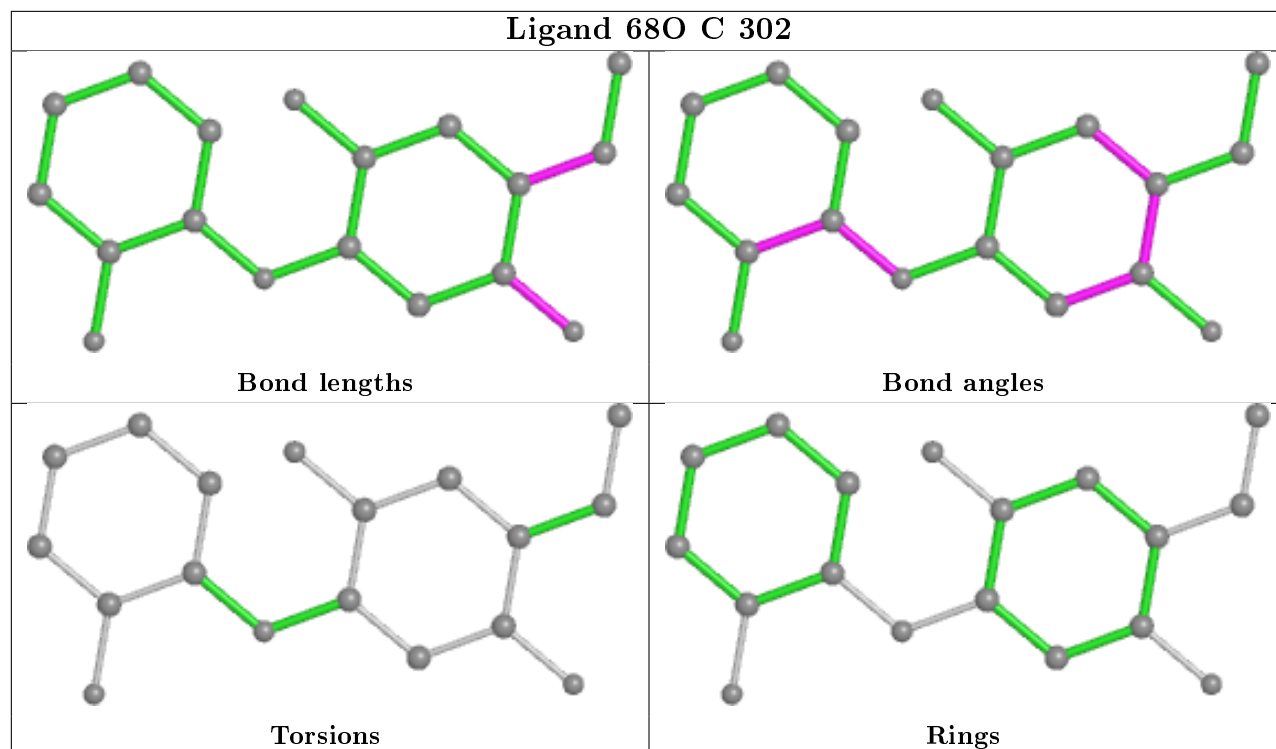
Ligand 68O A 302



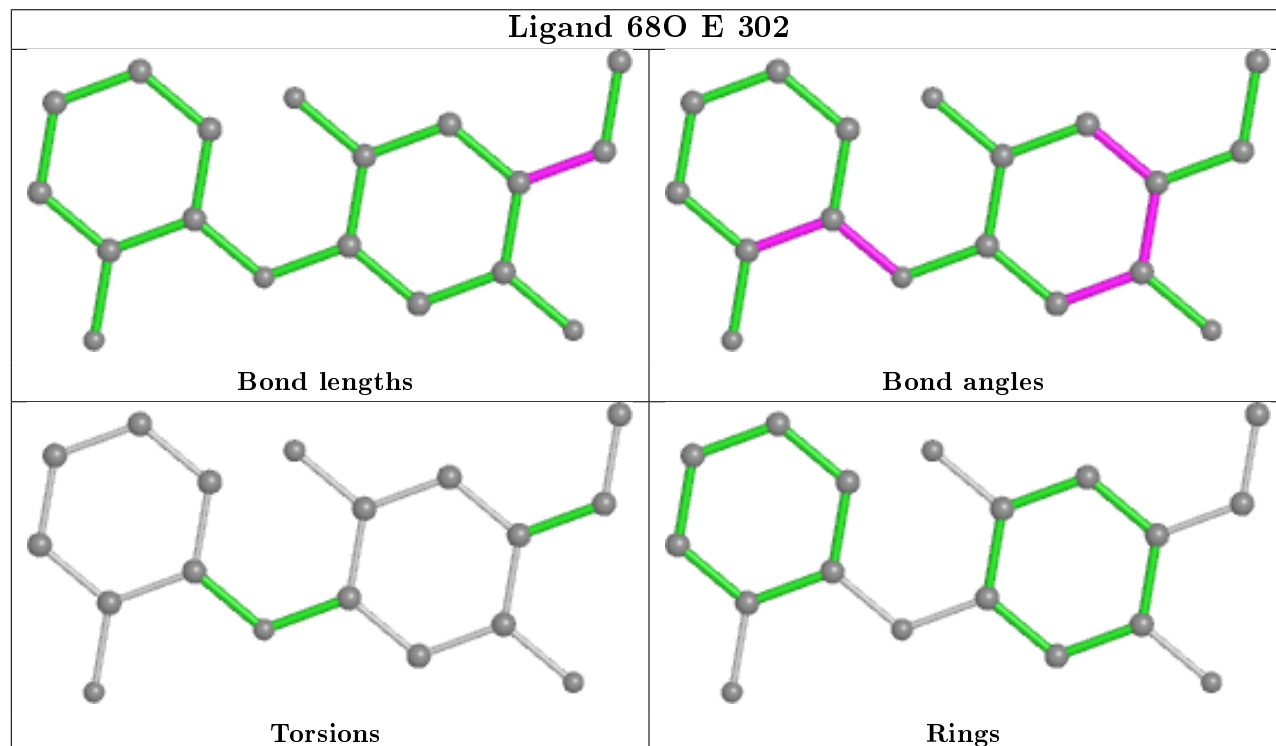
Ligand 68O B 302



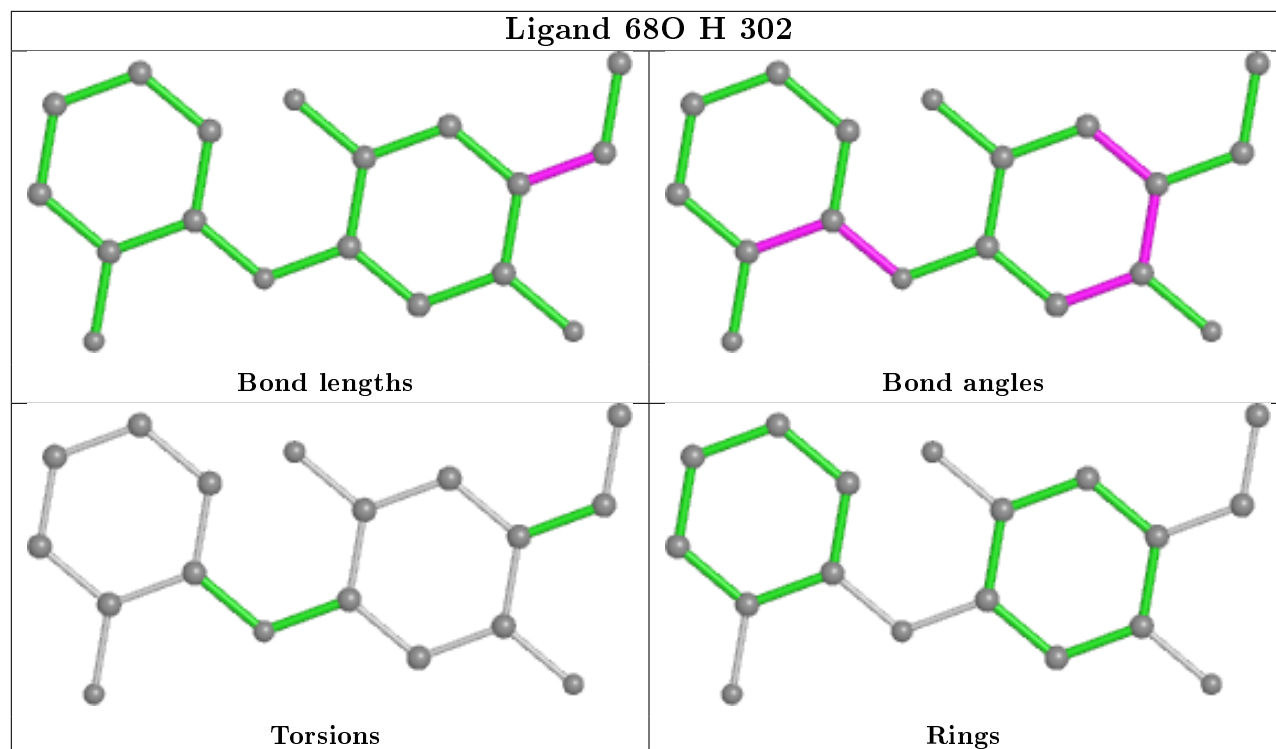
Ligand 68O C 302



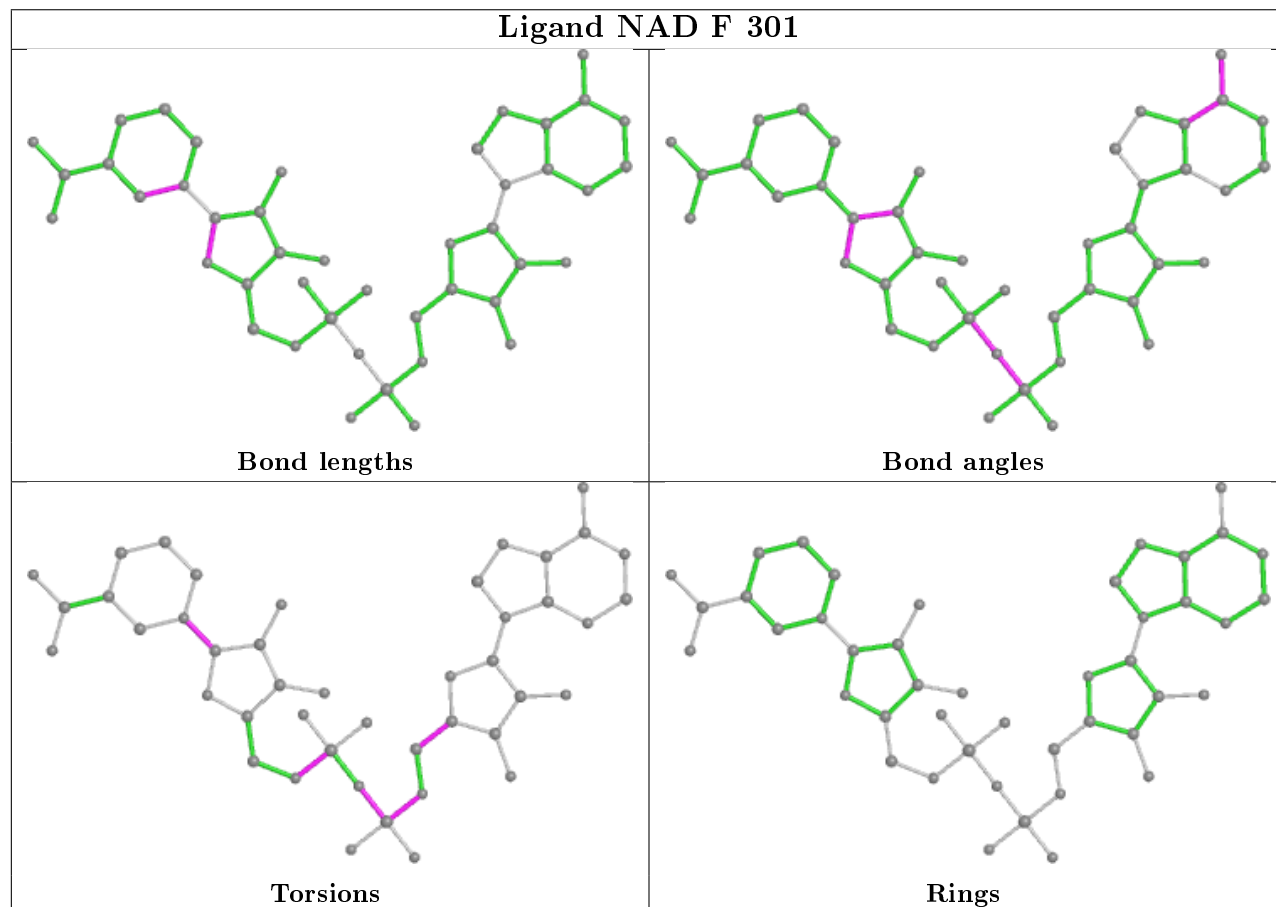
Ligand 68O E 302

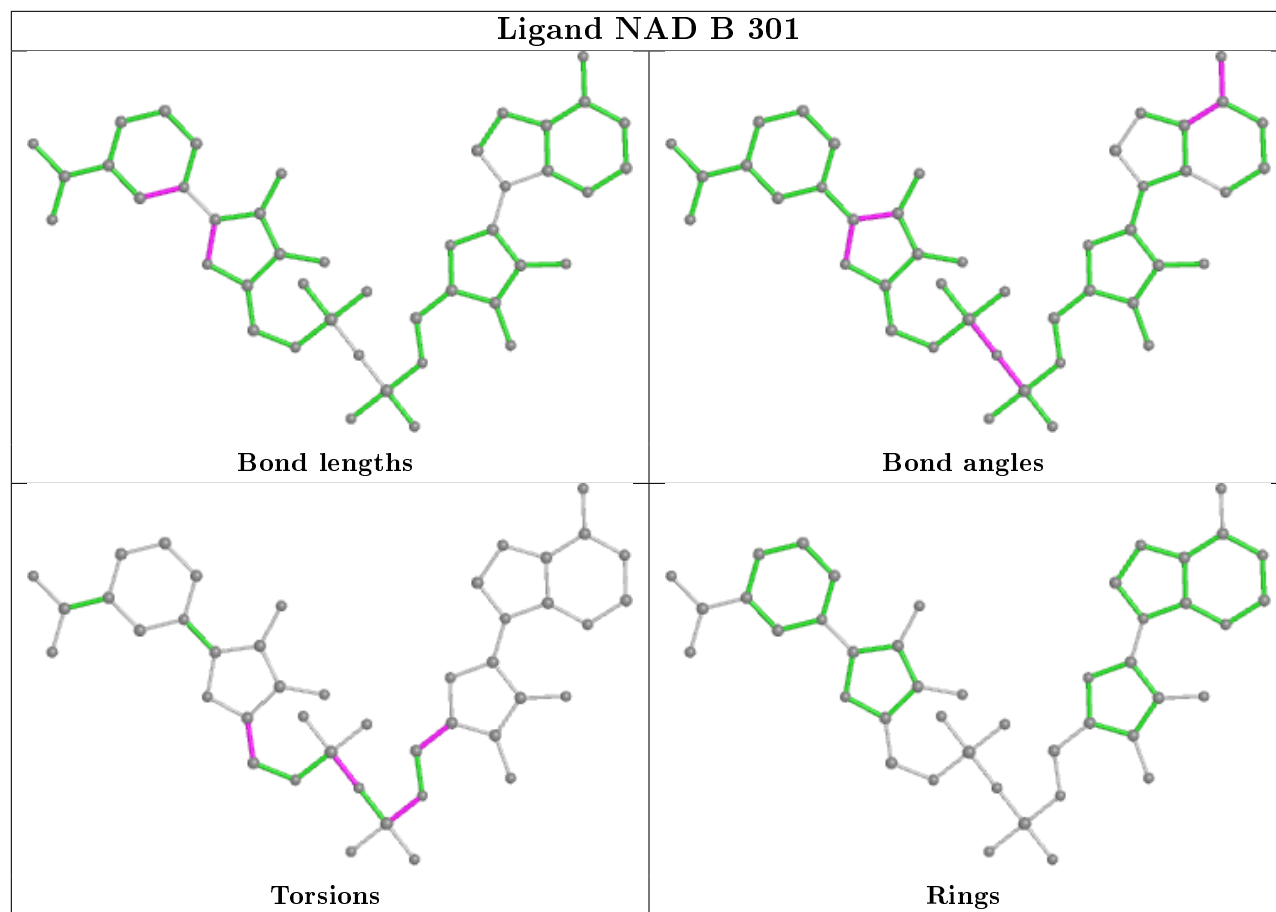


Ligand 68O H 302

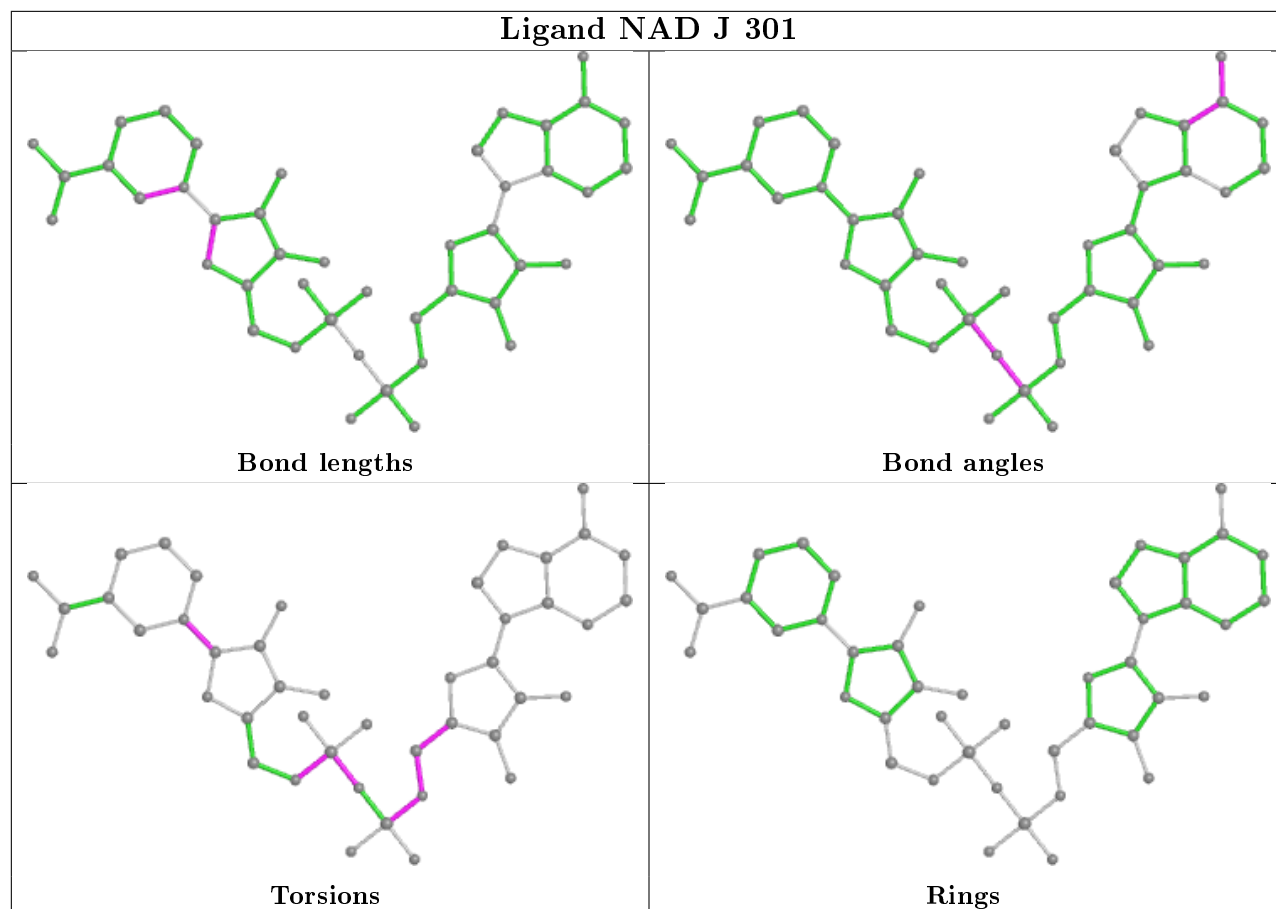


Ligand NAD F 301

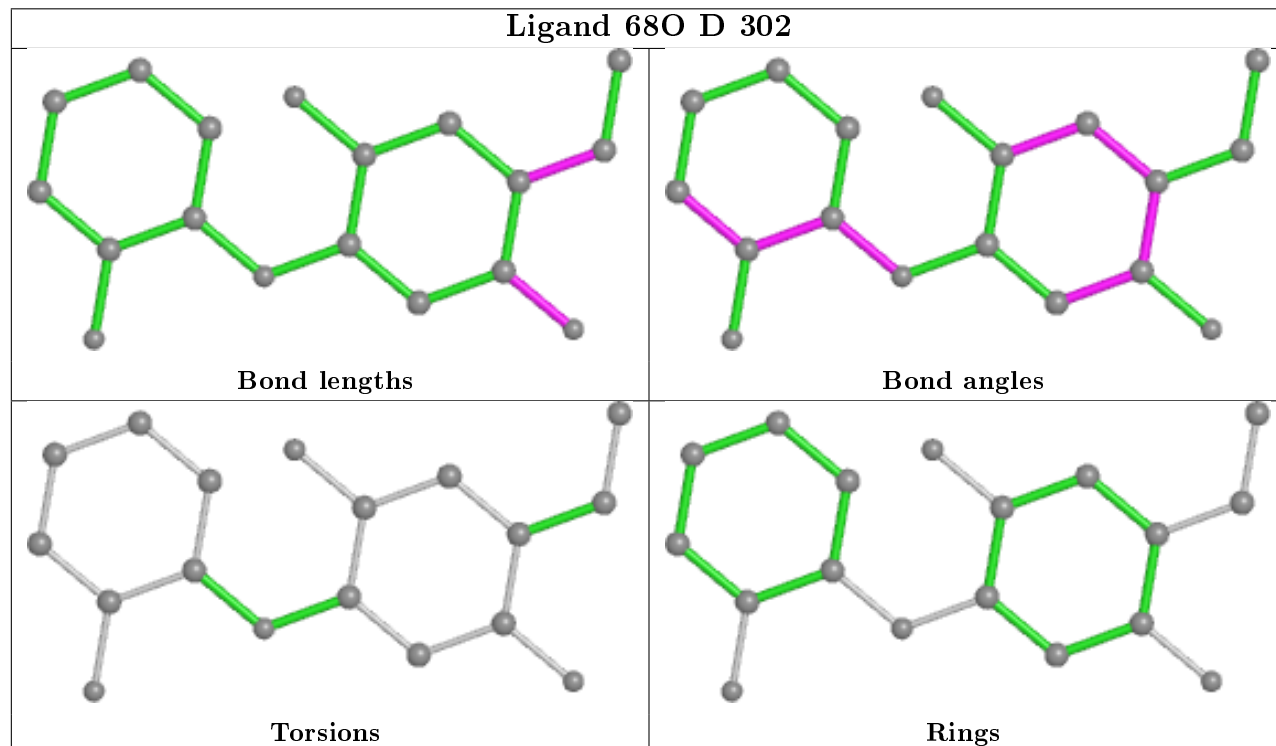


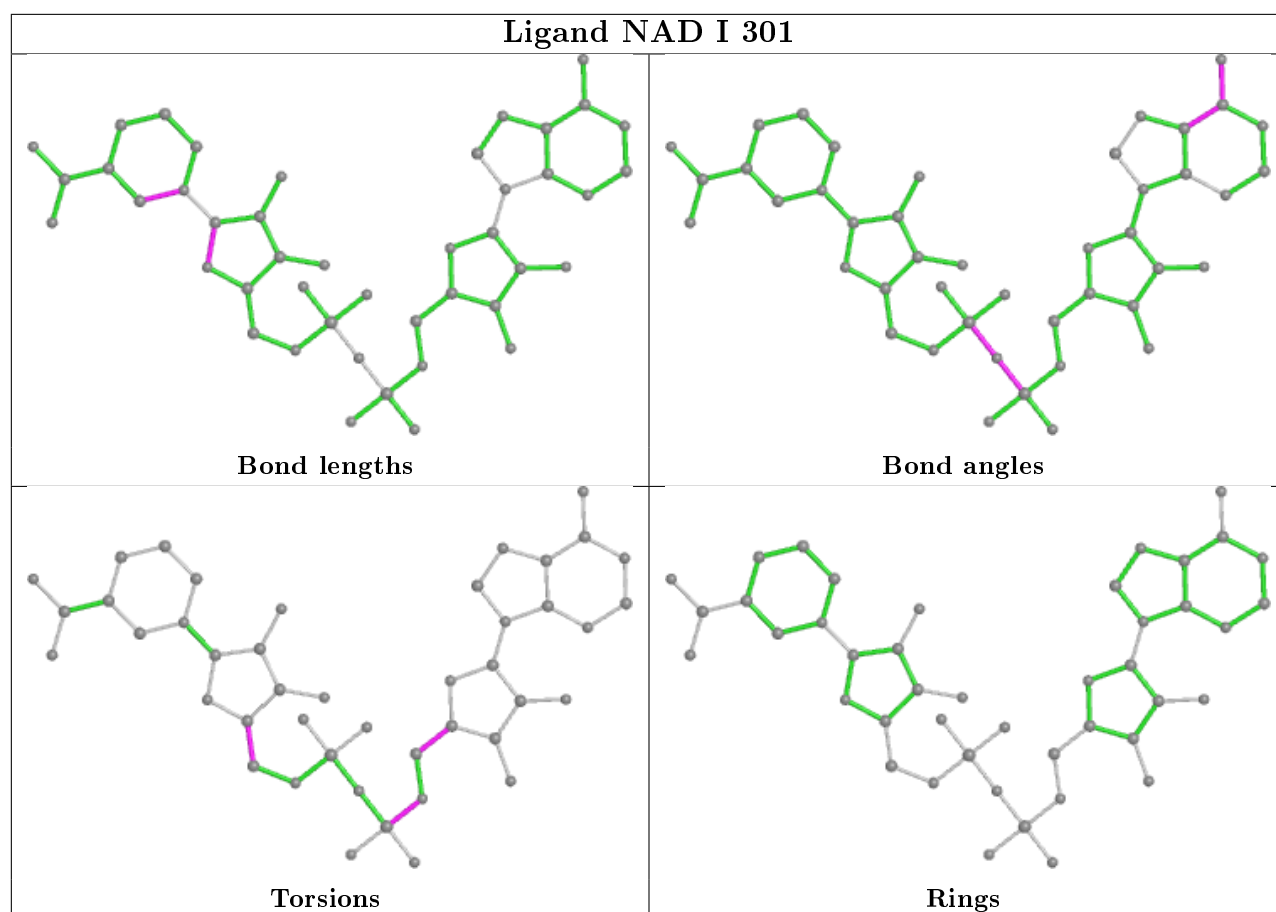


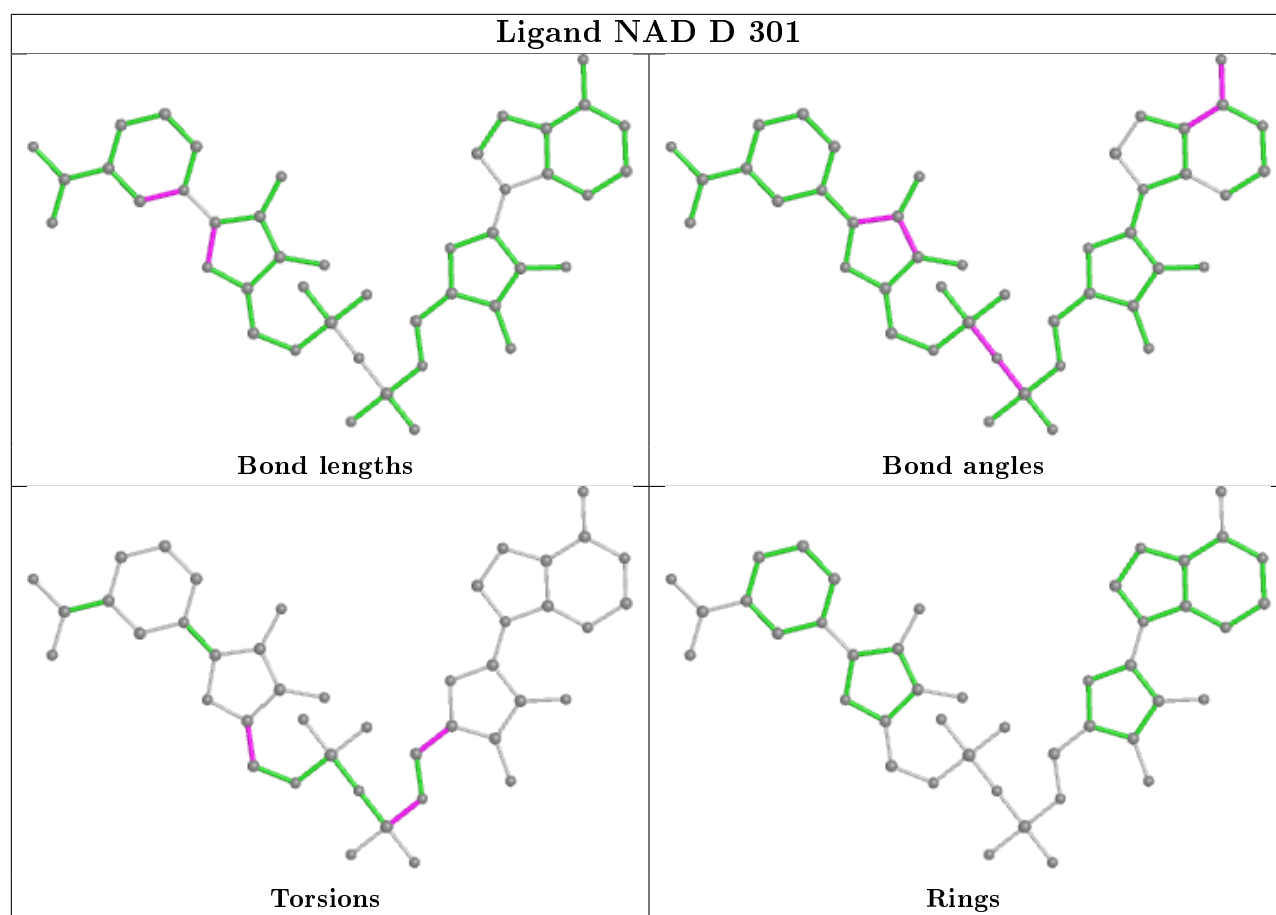
Ligand NAD J 301



Ligand 68O D 302







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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

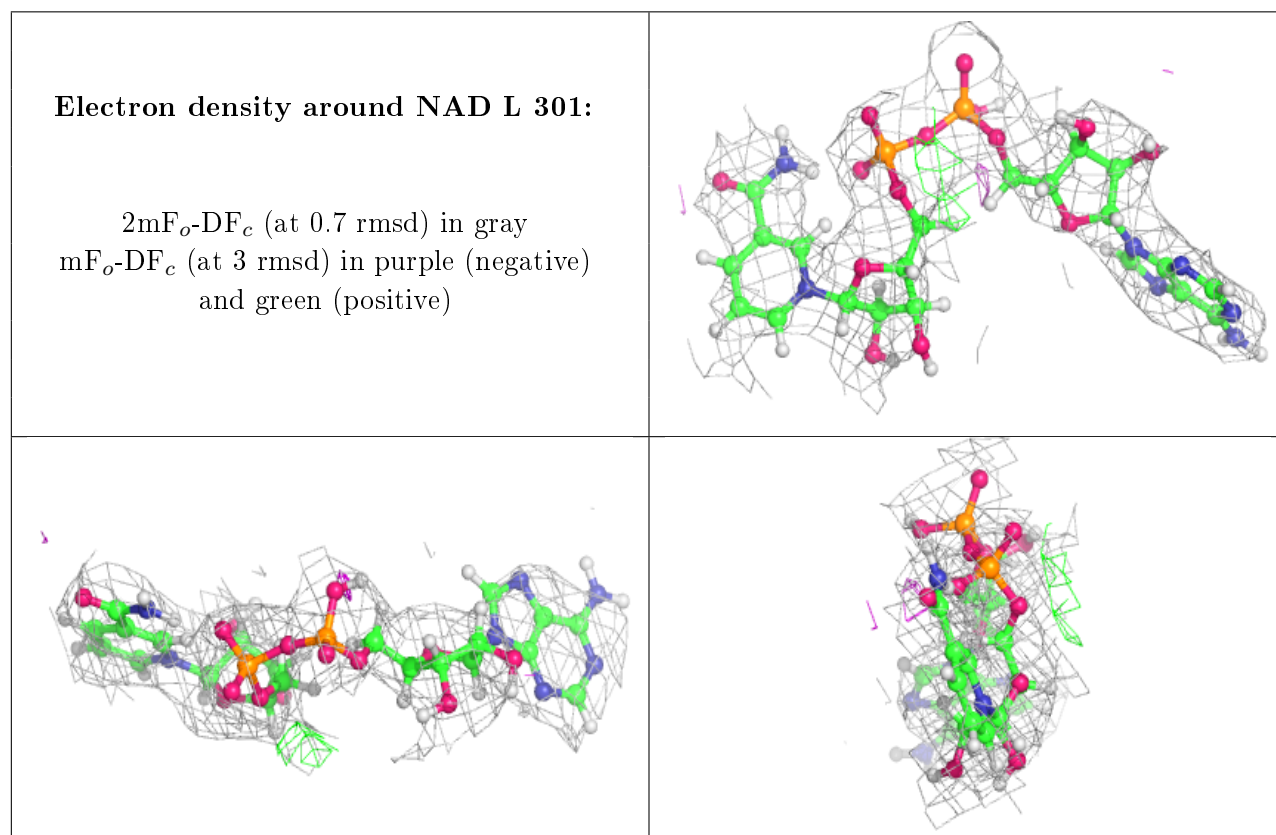
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

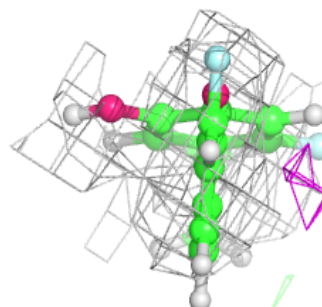
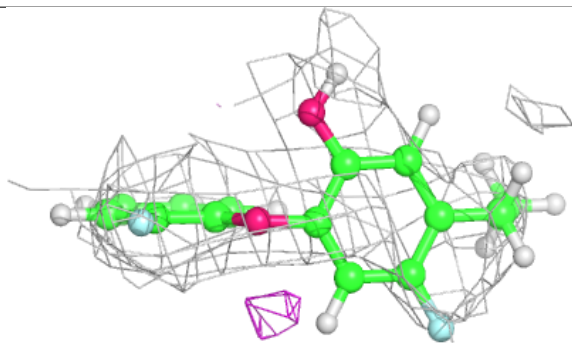
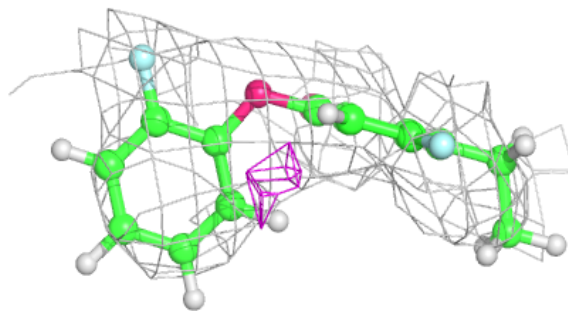
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

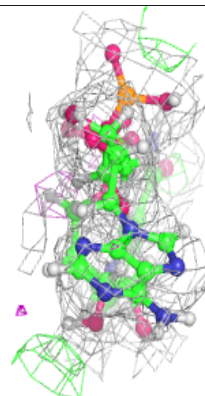
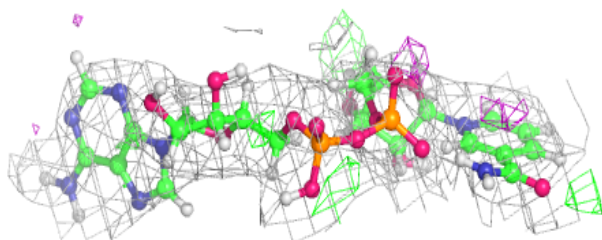
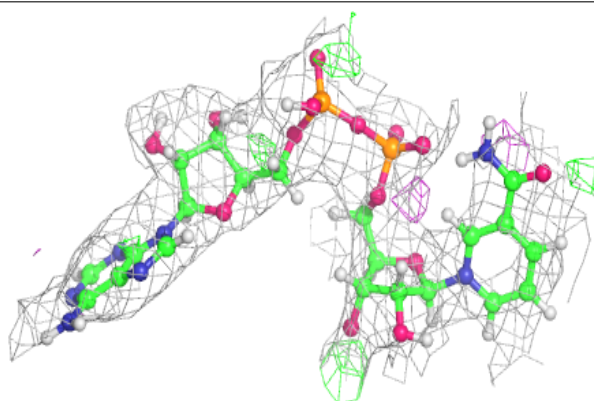


Electron density around 68O F 302:

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

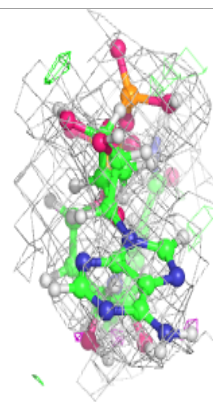
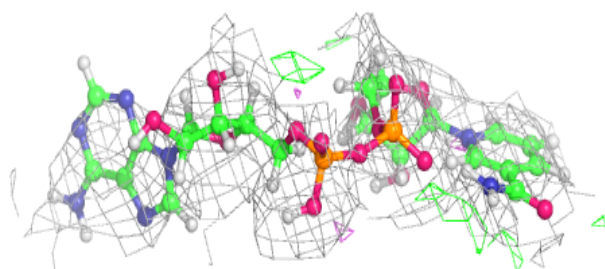
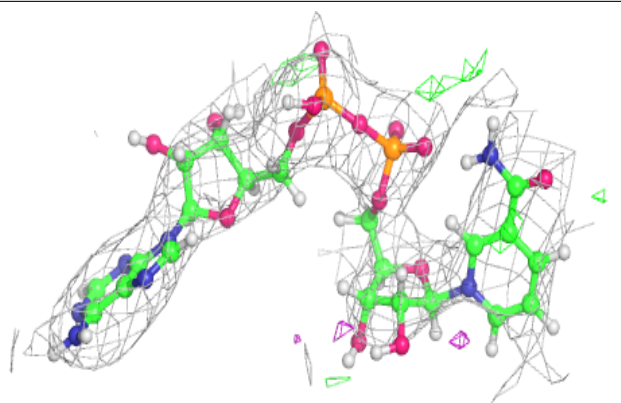
**Electron density around NAD H 301:**

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

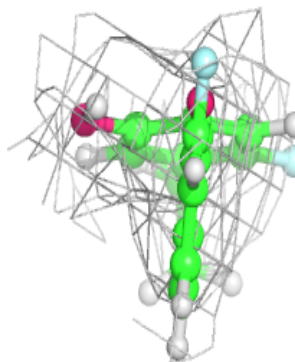
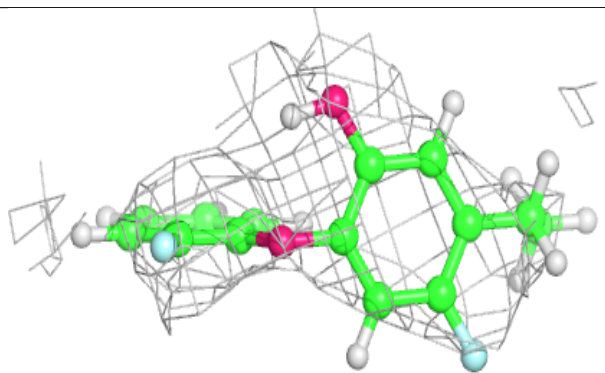
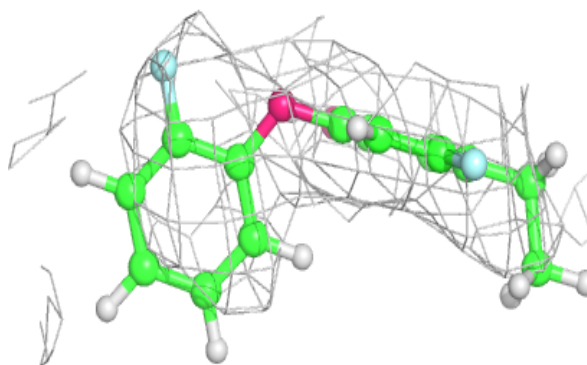


Electron density around NAD E 301:

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

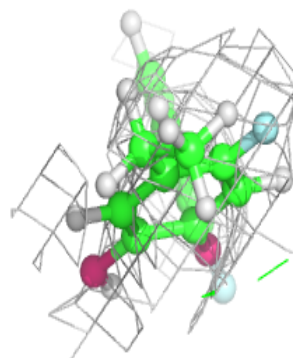
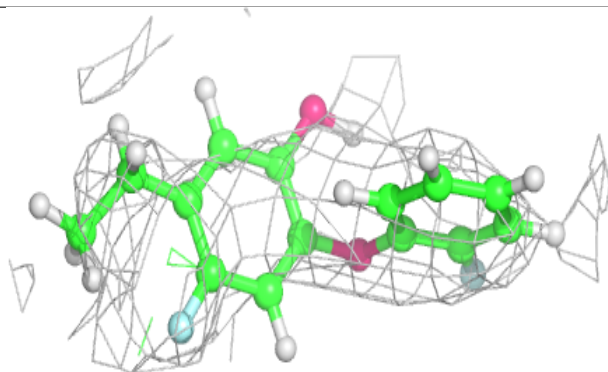
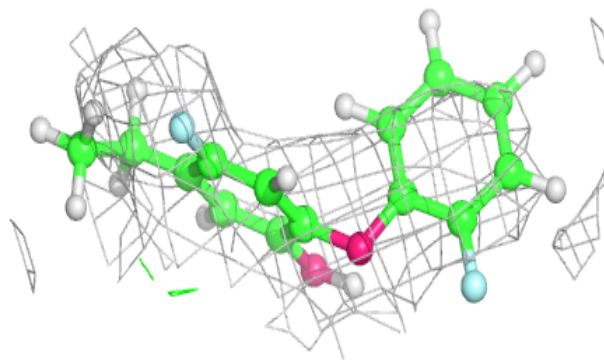
**Electron density around 68O I 302:**

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

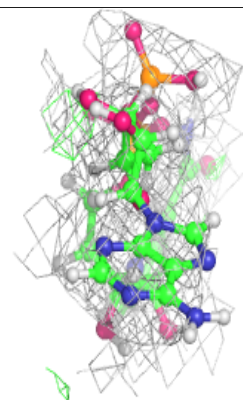
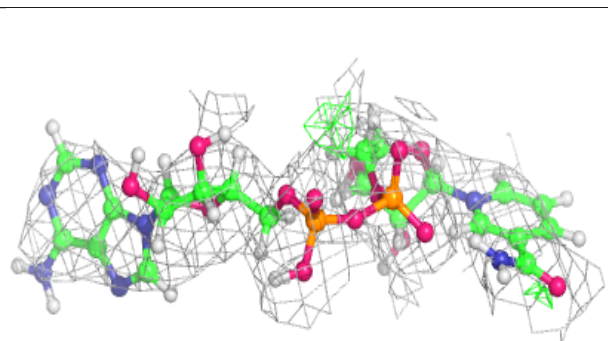
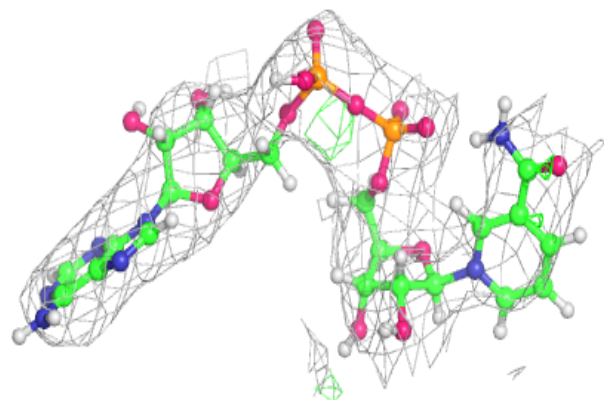


Electron density around 68O K 302:

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

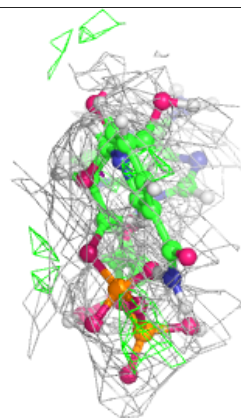
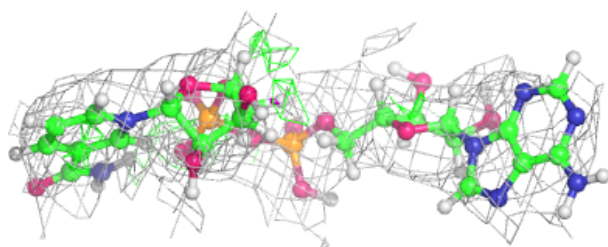
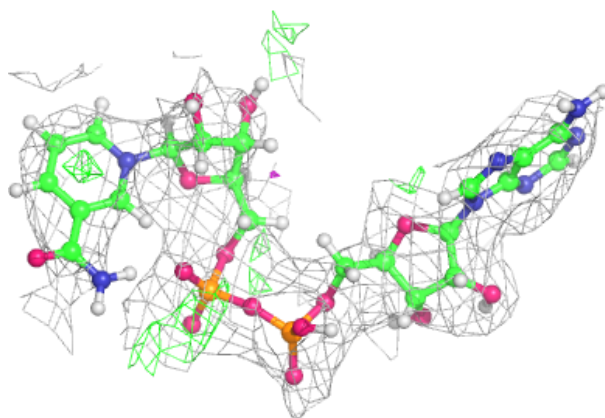
**Electron density around NAD K 301:**

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

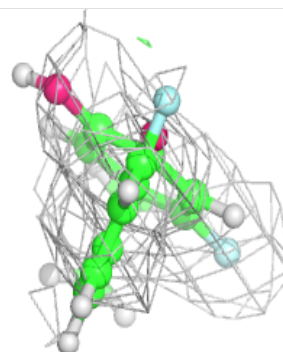
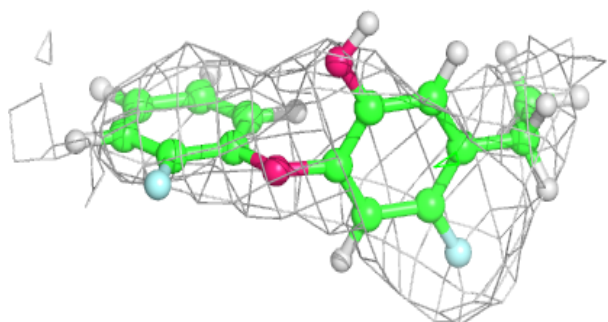
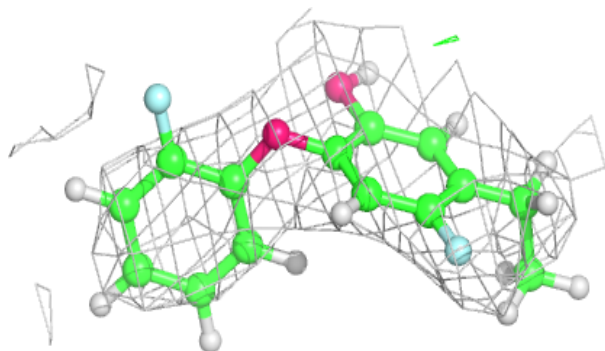


Electron density around NAD G 301:

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

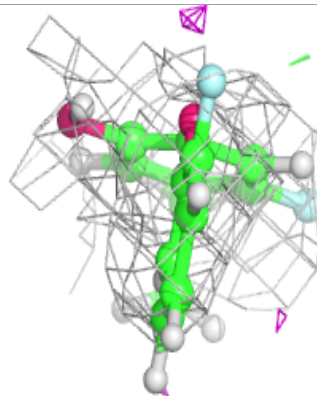
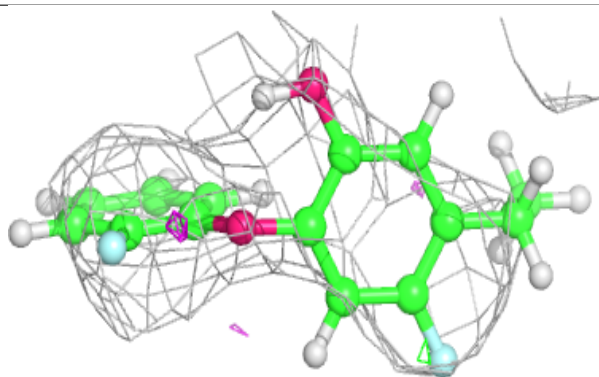
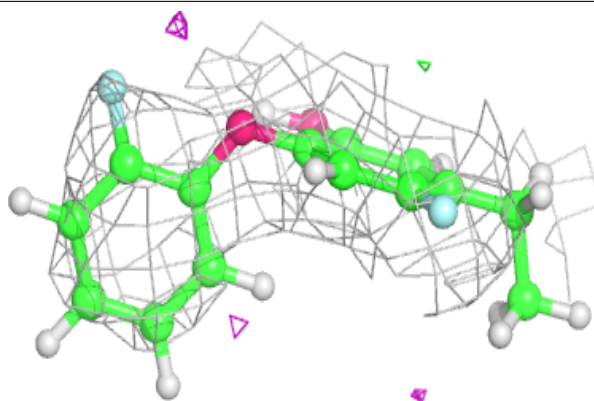
**Electron density around 68O G 302:**

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

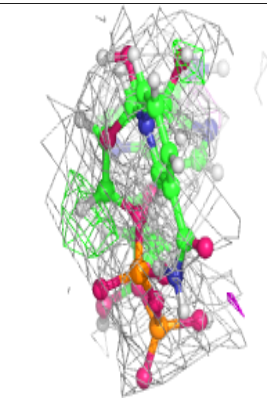
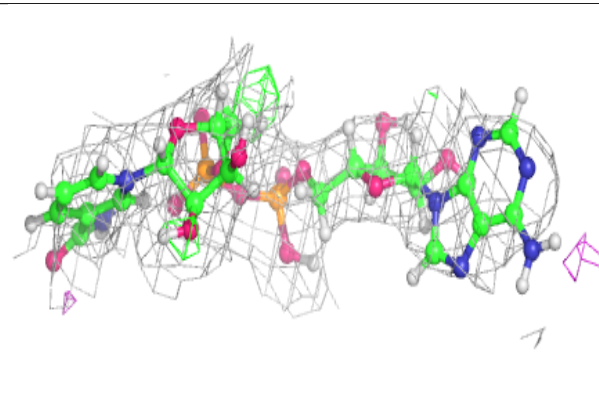
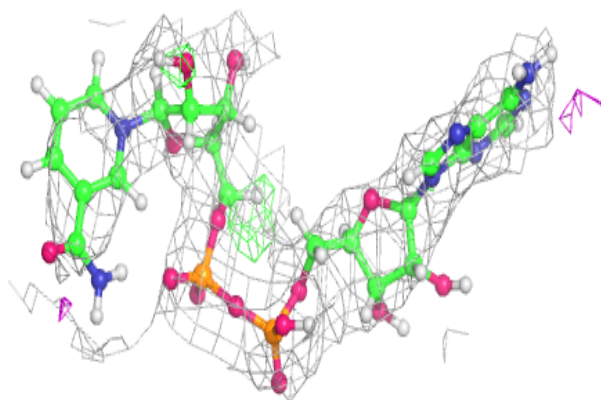


Electron density around 68O J 302:

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

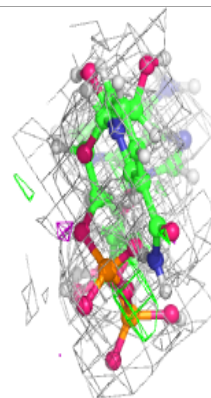
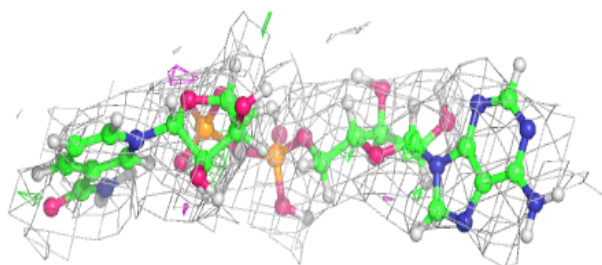
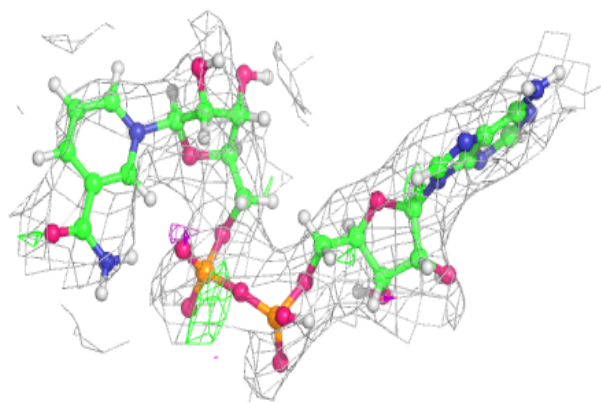
**Electron density around NAD C 301:**

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

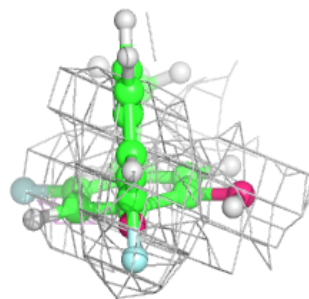
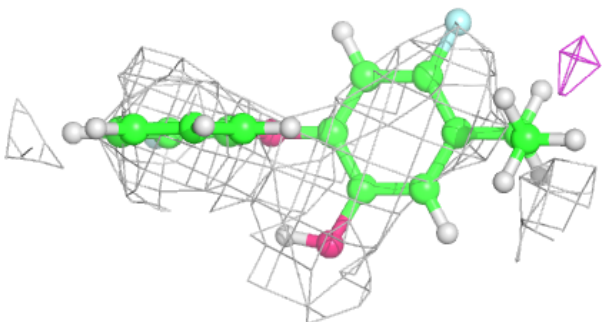
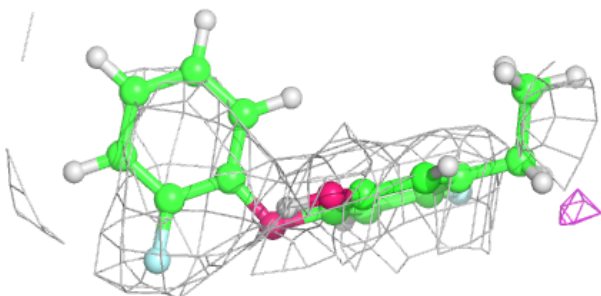


Electron density around NAD A 301:

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

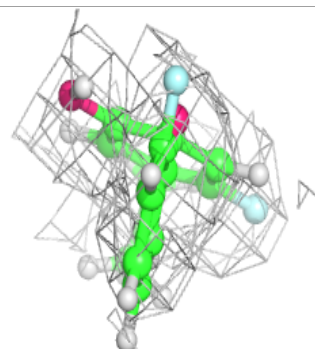
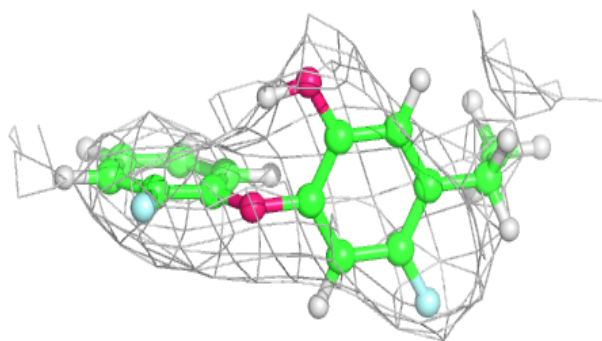
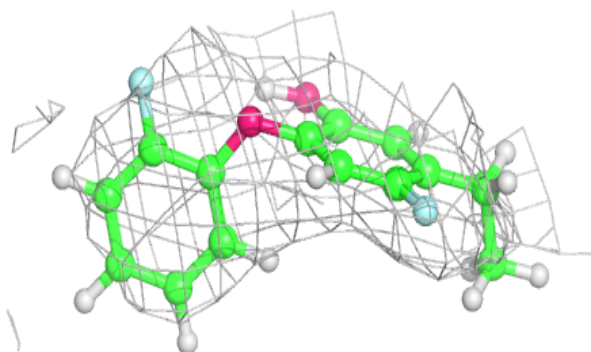
**Electron density around 68O L 302:**

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

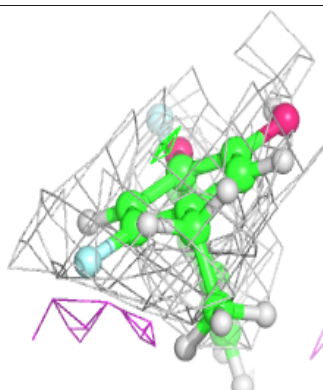
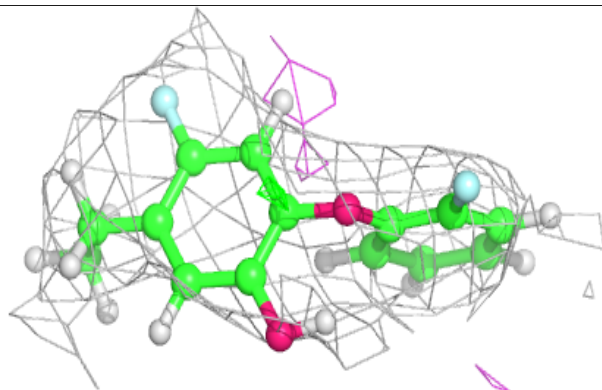
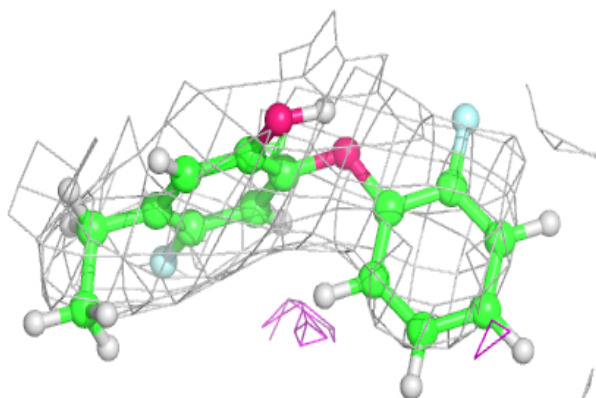


Electron density around 68O A 302:

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

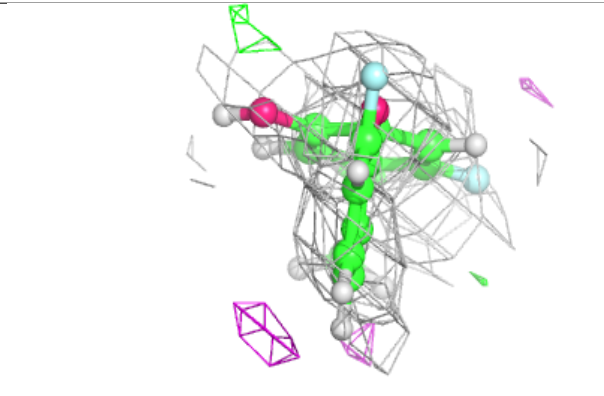
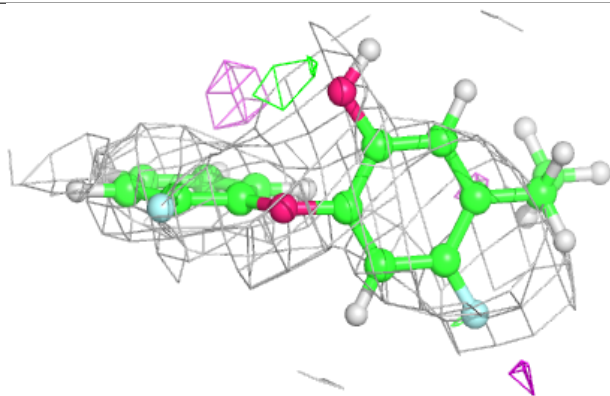
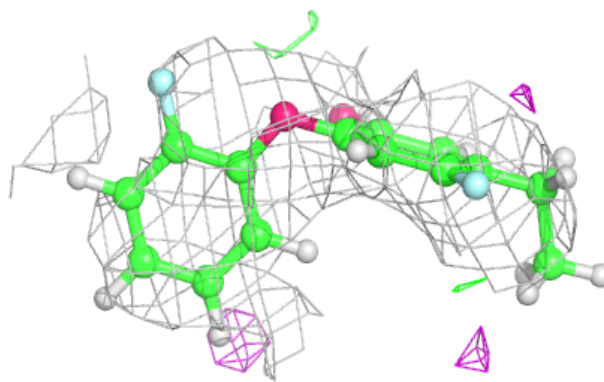
**Electron density around 68O B 302:**

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

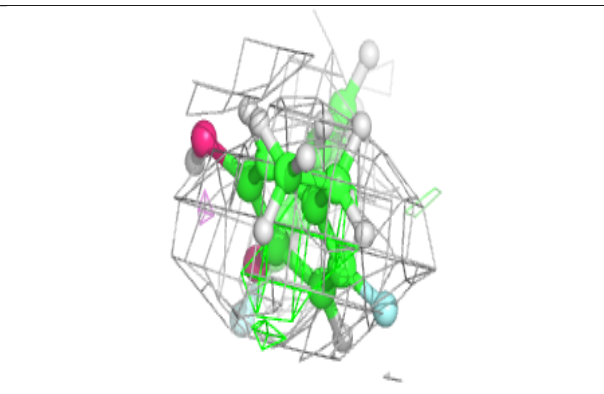
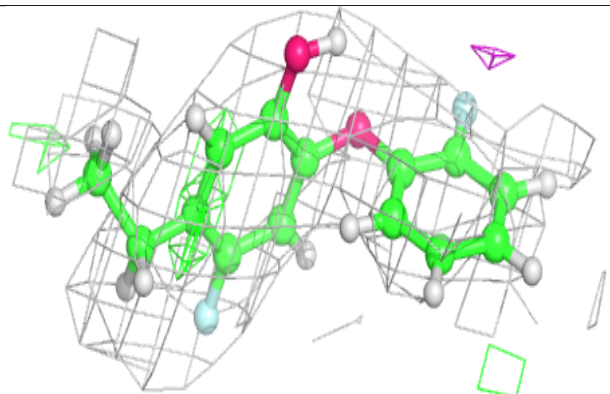
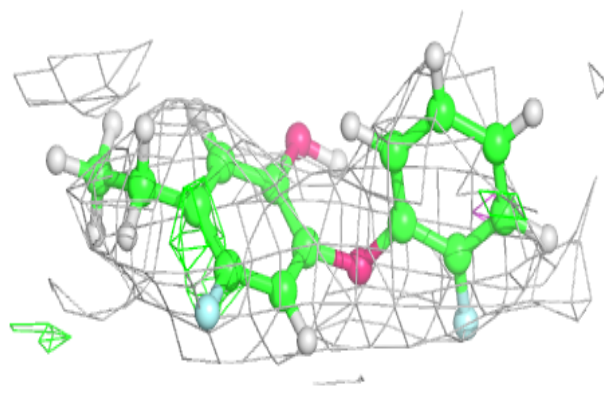


Electron density around 68O C 302:

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

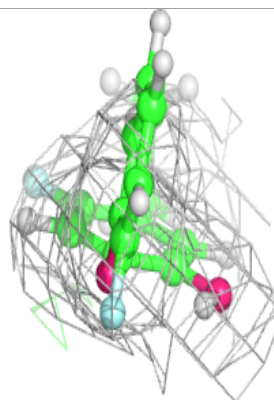
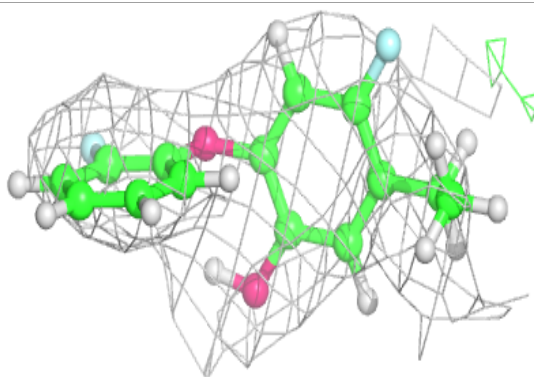
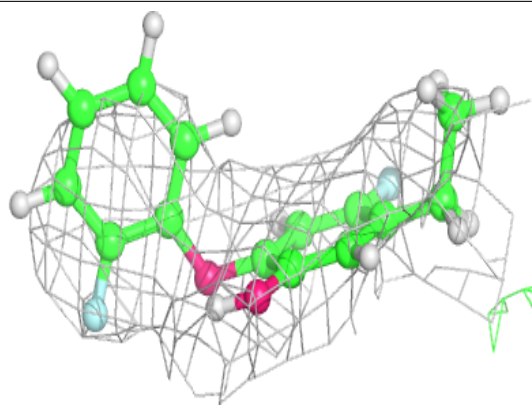
**Electron density around 68O E 302:**

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

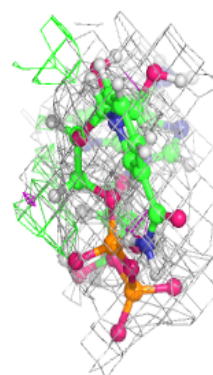
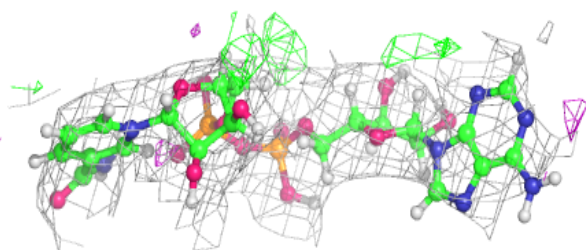
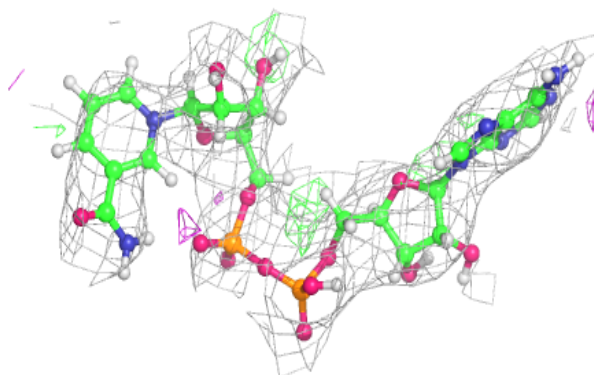


Electron density around 68O H 302:

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

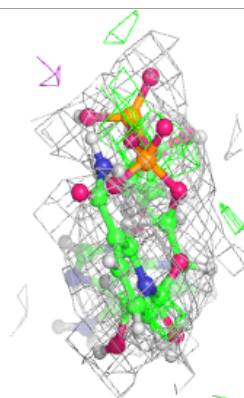
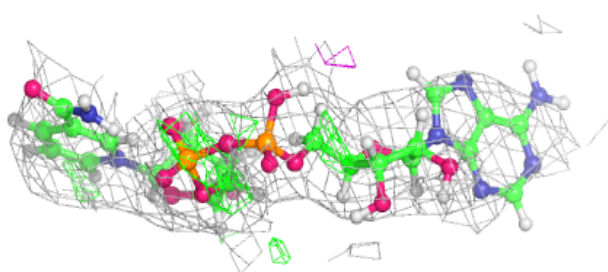
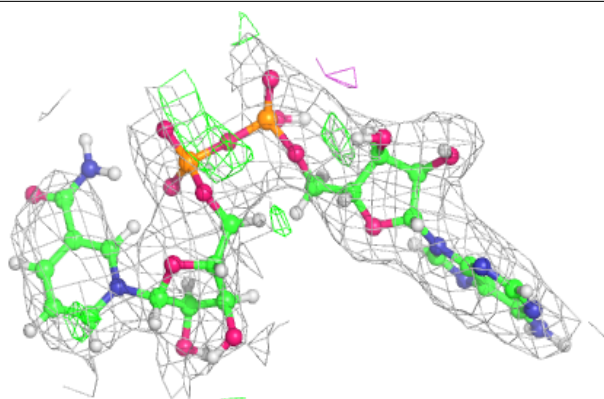
**Electron density around NAD F 301:**

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

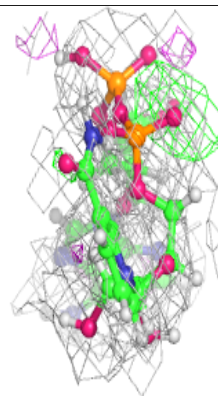
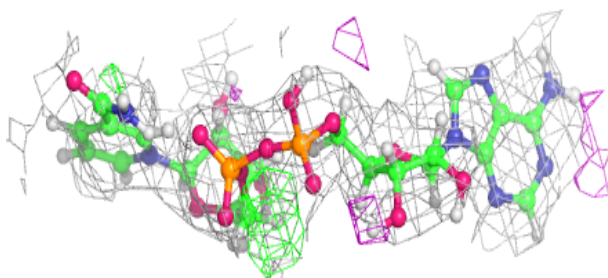
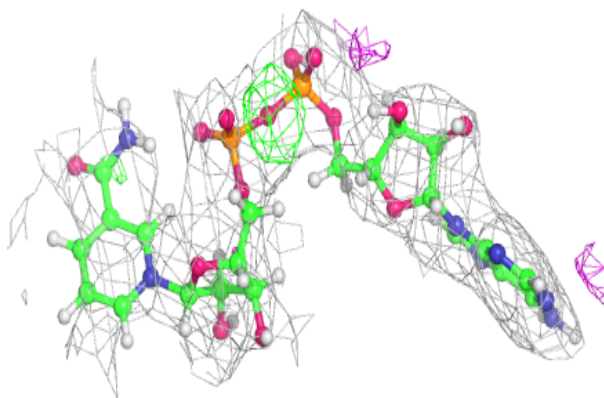


Electron density around NAD B 301:

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

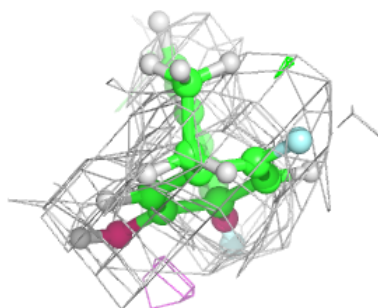
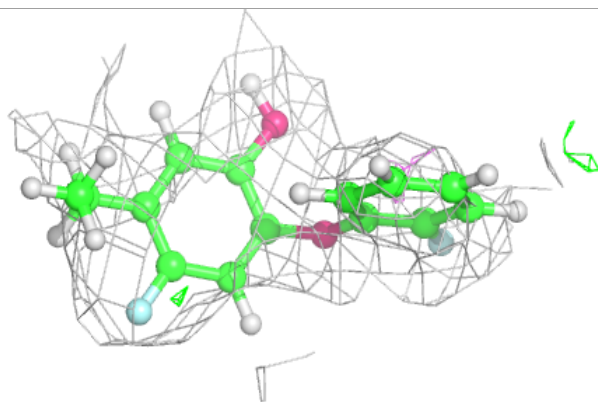
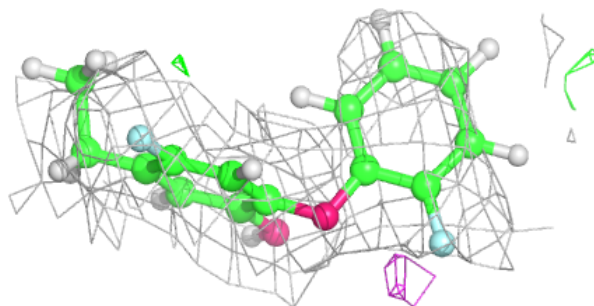
**Electron density around NAD J 301:**

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

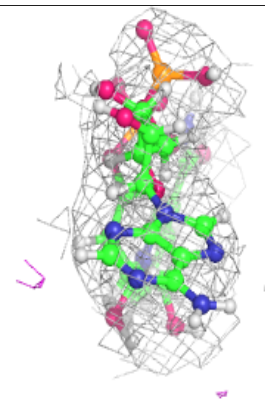
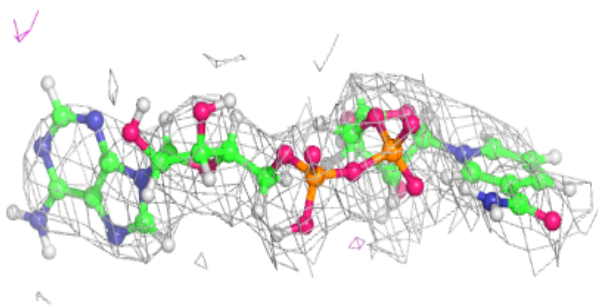
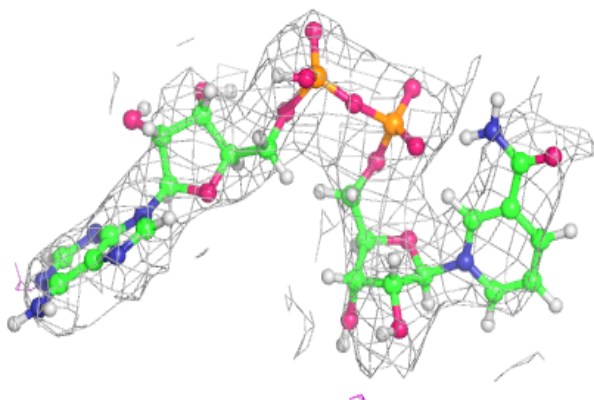


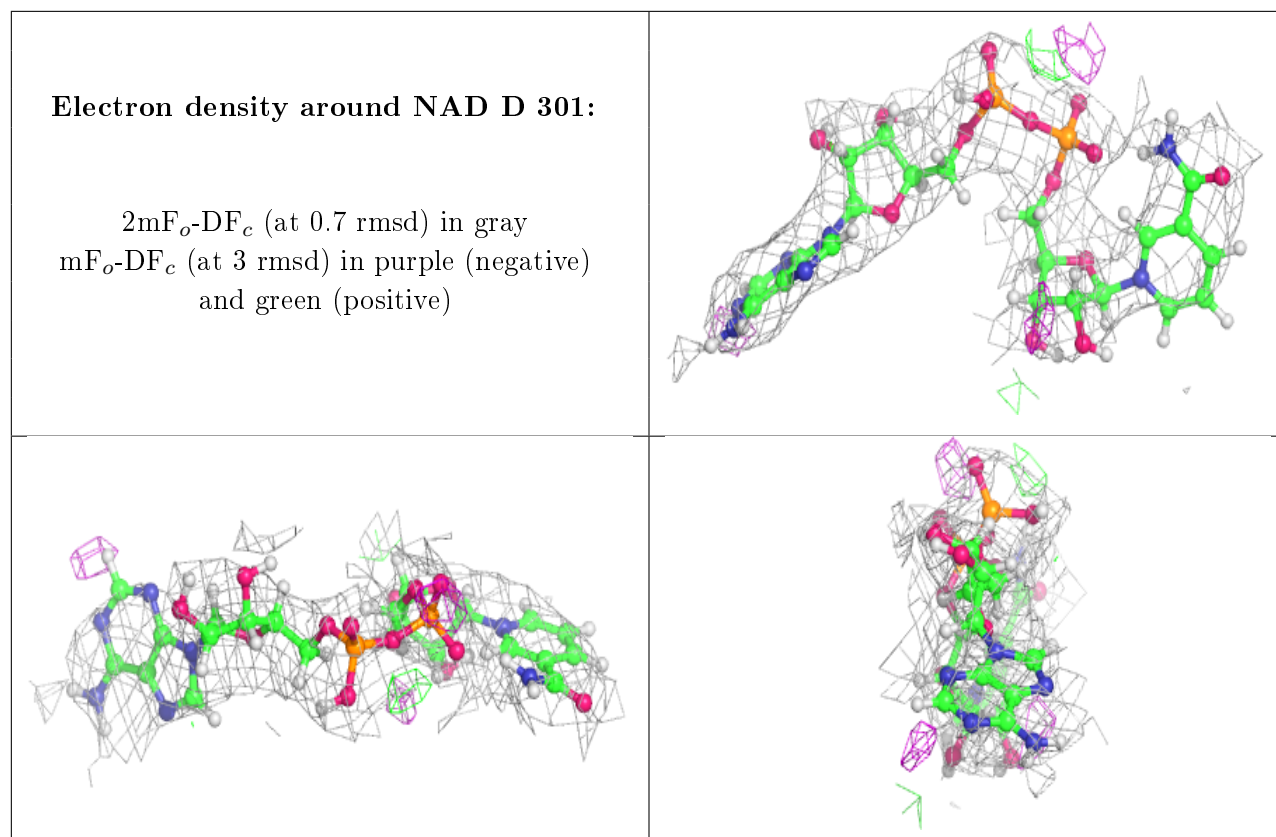
Electron density around 68O D 302:

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

**Electron density around NAD I 301:**

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.