



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 04:49 AM BST

PDB ID : 5MTP  
Title : Crystal structure of M. tuberculosis InhA inhibited by PT514  
Authors : Eltschkner, S.; Pschibul, A.; Spagnuolo, L.A.; Yu, W.; Tonge, P.J.; Kisker, C.  
Deposited on : 2017-01-10  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

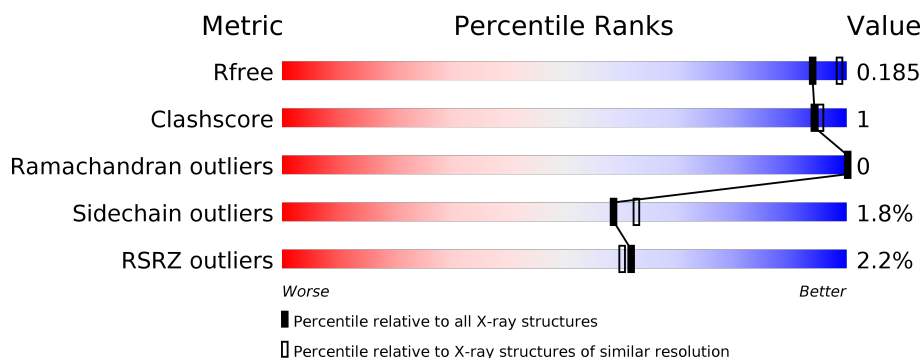
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	289	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>7%</div> </div> </div>
1	B	289	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>7%</div> </div> </div>
1	C	289	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>7%</div> </div> </div>
1	D	289	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>7%</div> </div> </div>
1	E	289	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>7%</div> </div> </div>
1	F	289	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	289	<div><div><div>3%</div><div>84%</div><div>6%</div><div>9%</div></div></div>
1	H	289	<div><div><div>3%</div><div>83%</div><div>7%</div><div>9%</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17867 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	268	Total	C	N	O	S	0	3	0
			2009	1273	348	377	11			
1	B	268	Total	C	N	O	S	0	0	0
			1996	1264	348	374	10			
1	E	268	Total	C	N	O	S	0	1	0
			1999	1266	348	375	10			
1	G	262	Total	C	N	O	S	0	2	0
			1965	1247	342	365	11			
1	C	268	Total	C	N	O	S	0	1	0
			1999	1266	348	375	10			
1	D	268	Total	C	N	O	S	0	0	0
			1996	1264	348	374	10			
1	F	263	Total	C	N	O	S	0	1	0
			1971	1250	343	367	11			
1	H	262	Total	C	N	O	S	0	0	0
			1957	1241	342	364	10			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WGR0
A	-18	GLY	-	expression tag	UNP P9WGR0
A	-17	SER	-	expression tag	UNP P9WGR0
A	-16	SER	-	expression tag	UNP P9WGR0
A	-15	HIS	-	expression tag	UNP P9WGR0
A	-14	HIS	-	expression tag	UNP P9WGR0
A	-13	HIS	-	expression tag	UNP P9WGR0
A	-12	HIS	-	expression tag	UNP P9WGR0
A	-11	HIS	-	expression tag	UNP P9WGR0
A	-10	HIS	-	expression tag	UNP P9WGR0
A	-9	SER	-	expression tag	UNP P9WGR0
A	-8	SER	-	expression tag	UNP P9WGR0
A	-7	GLY	-	expression tag	UNP P9WGR0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP P9WGR0
A	-5	VAL	-	expression tag	UNP P9WGR0
A	-4	PRO	-	expression tag	UNP P9WGR0
A	-3	ARG	-	expression tag	UNP P9WGR0
A	-2	GLY	-	expression tag	UNP P9WGR0
A	-1	SER	-	expression tag	UNP P9WGR0
A	0	HIS	-	expression tag	UNP P9WGR0
B	-19	MET	-	initiating methionine	UNP P9WGR0
B	-18	GLY	-	expression tag	UNP P9WGR0
B	-17	SER	-	expression tag	UNP P9WGR0
B	-16	SER	-	expression tag	UNP P9WGR0
B	-15	HIS	-	expression tag	UNP P9WGR0
B	-14	HIS	-	expression tag	UNP P9WGR0
B	-13	HIS	-	expression tag	UNP P9WGR0
B	-12	HIS	-	expression tag	UNP P9WGR0
B	-11	HIS	-	expression tag	UNP P9WGR0
B	-10	HIS	-	expression tag	UNP P9WGR0
B	-9	SER	-	expression tag	UNP P9WGR0
B	-8	SER	-	expression tag	UNP P9WGR0
B	-7	GLY	-	expression tag	UNP P9WGR0
B	-6	LEU	-	expression tag	UNP P9WGR0
B	-5	VAL	-	expression tag	UNP P9WGR0
B	-4	PRO	-	expression tag	UNP P9WGR0
B	-3	ARG	-	expression tag	UNP P9WGR0
B	-2	GLY	-	expression tag	UNP P9WGR0
B	-1	SER	-	expression tag	UNP P9WGR0
B	0	HIS	-	expression tag	UNP P9WGR0
E	-19	MET	-	initiating methionine	UNP P9WGR0
E	-18	GLY	-	expression tag	UNP P9WGR0
E	-17	SER	-	expression tag	UNP P9WGR0
E	-16	SER	-	expression tag	UNP P9WGR0
E	-15	HIS	-	expression tag	UNP P9WGR0
E	-14	HIS	-	expression tag	UNP P9WGR0
E	-13	HIS	-	expression tag	UNP P9WGR0
E	-12	HIS	-	expression tag	UNP P9WGR0
E	-11	HIS	-	expression tag	UNP P9WGR0
E	-10	HIS	-	expression tag	UNP P9WGR0
E	-9	SER	-	expression tag	UNP P9WGR0
E	-8	SER	-	expression tag	UNP P9WGR0
E	-7	GLY	-	expression tag	UNP P9WGR0
E	-6	LEU	-	expression tag	UNP P9WGR0
E	-5	VAL	-	expression tag	UNP P9WGR0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	PRO	-	expression tag	UNP P9WGR0
E	-3	ARG	-	expression tag	UNP P9WGR0
E	-2	GLY	-	expression tag	UNP P9WGR0
E	-1	SER	-	expression tag	UNP P9WGR0
E	0	HIS	-	expression tag	UNP P9WGR0
G	-19	MET	-	initiating methionine	UNP P9WGR0
G	-18	GLY	-	expression tag	UNP P9WGR0
G	-17	SER	-	expression tag	UNP P9WGR0
G	-16	SER	-	expression tag	UNP P9WGR0
G	-15	HIS	-	expression tag	UNP P9WGR0
G	-14	HIS	-	expression tag	UNP P9WGR0
G	-13	HIS	-	expression tag	UNP P9WGR0
G	-12	HIS	-	expression tag	UNP P9WGR0
G	-11	HIS	-	expression tag	UNP P9WGR0
G	-10	HIS	-	expression tag	UNP P9WGR0
G	-9	SER	-	expression tag	UNP P9WGR0
G	-8	SER	-	expression tag	UNP P9WGR0
G	-7	GLY	-	expression tag	UNP P9WGR0
G	-6	LEU	-	expression tag	UNP P9WGR0
G	-5	VAL	-	expression tag	UNP P9WGR0
G	-4	PRO	-	expression tag	UNP P9WGR0
G	-3	ARG	-	expression tag	UNP P9WGR0
G	-2	GLY	-	expression tag	UNP P9WGR0
G	-1	SER	-	expression tag	UNP P9WGR0
G	0	HIS	-	expression tag	UNP P9WGR0
C	-19	MET	-	initiating methionine	UNP P9WGR0
C	-18	GLY	-	expression tag	UNP P9WGR0
C	-17	SER	-	expression tag	UNP P9WGR0
C	-16	SER	-	expression tag	UNP P9WGR0
C	-15	HIS	-	expression tag	UNP P9WGR0
C	-14	HIS	-	expression tag	UNP P9WGR0
C	-13	HIS	-	expression tag	UNP P9WGR0
C	-12	HIS	-	expression tag	UNP P9WGR0
C	-11	HIS	-	expression tag	UNP P9WGR0
C	-10	HIS	-	expression tag	UNP P9WGR0
C	-9	SER	-	expression tag	UNP P9WGR0
C	-8	SER	-	expression tag	UNP P9WGR0
C	-7	GLY	-	expression tag	UNP P9WGR0
C	-6	LEU	-	expression tag	UNP P9WGR0
C	-5	VAL	-	expression tag	UNP P9WGR0
C	-4	PRO	-	expression tag	UNP P9WGR0
C	-3	ARG	-	expression tag	UNP P9WGR0

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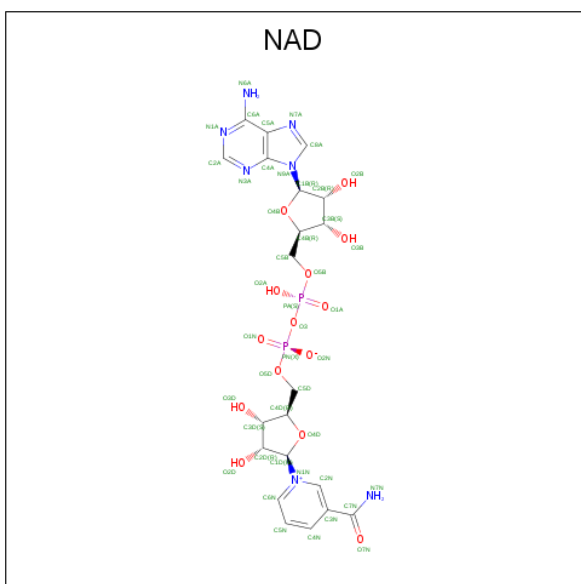
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P9WGR0
C	-1	SER	-	expression tag	UNP P9WGR0
C	0	HIS	-	expression tag	UNP P9WGR0
D	-19	MET	-	initiating methionine	UNP P9WGR0
D	-18	GLY	-	expression tag	UNP P9WGR0
D	-17	SER	-	expression tag	UNP P9WGR0
D	-16	SER	-	expression tag	UNP P9WGR0
D	-15	HIS	-	expression tag	UNP P9WGR0
D	-14	HIS	-	expression tag	UNP P9WGR0
D	-13	HIS	-	expression tag	UNP P9WGR0
D	-12	HIS	-	expression tag	UNP P9WGR0
D	-11	HIS	-	expression tag	UNP P9WGR0
D	-10	HIS	-	expression tag	UNP P9WGR0
D	-9	SER	-	expression tag	UNP P9WGR0
D	-8	SER	-	expression tag	UNP P9WGR0
D	-7	GLY	-	expression tag	UNP P9WGR0
D	-6	LEU	-	expression tag	UNP P9WGR0
D	-5	VAL	-	expression tag	UNP P9WGR0
D	-4	PRO	-	expression tag	UNP P9WGR0
D	-3	ARG	-	expression tag	UNP P9WGR0
D	-2	GLY	-	expression tag	UNP P9WGR0
D	-1	SER	-	expression tag	UNP P9WGR0
D	0	HIS	-	expression tag	UNP P9WGR0
F	-19	MET	-	initiating methionine	UNP P9WGR0
F	-18	GLY	-	expression tag	UNP P9WGR0
F	-17	SER	-	expression tag	UNP P9WGR0
F	-16	SER	-	expression tag	UNP P9WGR0
F	-15	HIS	-	expression tag	UNP P9WGR0
F	-14	HIS	-	expression tag	UNP P9WGR0
F	-13	HIS	-	expression tag	UNP P9WGR0
F	-12	HIS	-	expression tag	UNP P9WGR0
F	-11	HIS	-	expression tag	UNP P9WGR0
F	-10	HIS	-	expression tag	UNP P9WGR0
F	-9	SER	-	expression tag	UNP P9WGR0
F	-8	SER	-	expression tag	UNP P9WGR0
F	-7	GLY	-	expression tag	UNP P9WGR0
F	-6	LEU	-	expression tag	UNP P9WGR0
F	-5	VAL	-	expression tag	UNP P9WGR0
F	-4	PRO	-	expression tag	UNP P9WGR0
F	-3	ARG	-	expression tag	UNP P9WGR0
F	-2	GLY	-	expression tag	UNP P9WGR0
F	-1	SER	-	expression tag	UNP P9WGR0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP P9WGR0
H	-19	MET	-	initiating methionine	UNP P9WGR0
H	-18	GLY	-	expression tag	UNP P9WGR0
H	-17	SER	-	expression tag	UNP P9WGR0
H	-16	SER	-	expression tag	UNP P9WGR0
H	-15	HIS	-	expression tag	UNP P9WGR0
H	-14	HIS	-	expression tag	UNP P9WGR0
H	-13	HIS	-	expression tag	UNP P9WGR0
H	-12	HIS	-	expression tag	UNP P9WGR0
H	-11	HIS	-	expression tag	UNP P9WGR0
H	-10	HIS	-	expression tag	UNP P9WGR0
H	-9	SER	-	expression tag	UNP P9WGR0
H	-8	SER	-	expression tag	UNP P9WGR0
H	-7	GLY	-	expression tag	UNP P9WGR0
H	-6	LEU	-	expression tag	UNP P9WGR0
H	-5	VAL	-	expression tag	UNP P9WGR0
H	-4	PRO	-	expression tag	UNP P9WGR0
H	-3	ARG	-	expression tag	UNP P9WGR0
H	-2	GLY	-	expression tag	UNP P9WGR0
H	-1	SER	-	expression tag	UNP P9WGR0
H	0	HIS	-	expression tag	UNP P9WGR0

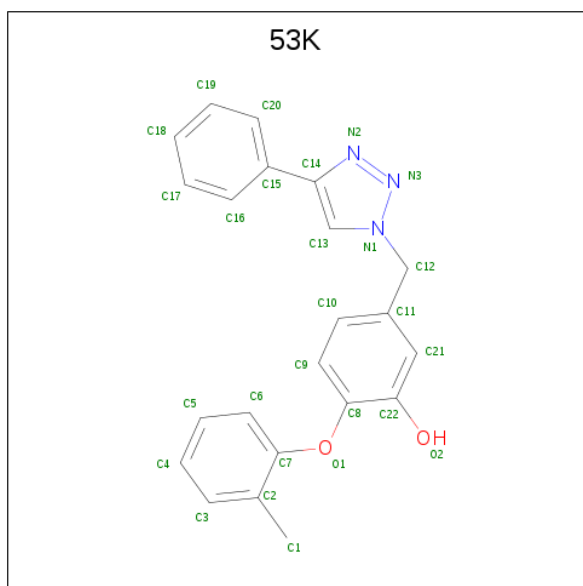
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).





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	E	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	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	F	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		

- Molecule 3 is 2-(2-methylphenoxy)-5-[(4-phenyl-1H-1,2,3-triazol-1-yl)methyl]phenol (three-letter code: 53K) (formula: C<sub>22</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	22	3	2		
3	B	1	Total	C	N	O	0	0
			27	22	3	2		
3	E	1	Total	C	N	O	0	0
			27	22	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			27	22	3	2		
3	C	1	Total	C	N	O	0	0
			27	22	3	2		
3	D	1	Total	C	N	O	0	0
			27	22	3	2		
3	F	1	Total	C	N	O	0	0
			27	22	3	2		
3	H	1	Total	C	N	O	0	0
			27	22	3	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		
5	F	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	198	Total	O	0	0
			198	198		
6	B	148	Total	O	0	0
			148	148		
6	E	153	Total	O	0	1
			154	154		
6	G	176	Total	O	0	0
			176	176		
6	C	195	Total	O	0	0
			195	195		

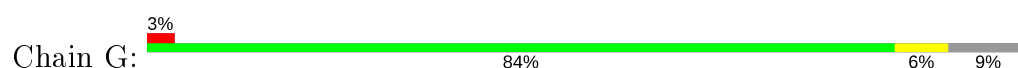
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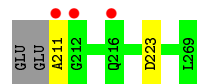
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	183	Total 183	O 183	0	0
6	F	163	Total 163	O 163	0	0
6	H	185	Total 185	O 185	0	0

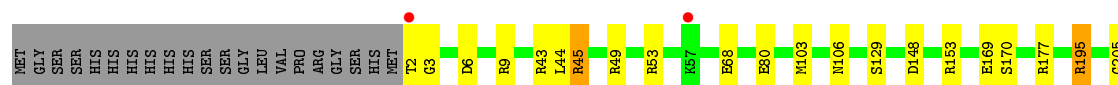
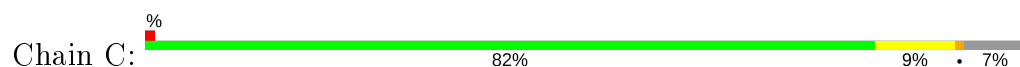


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

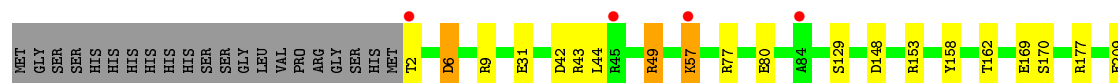
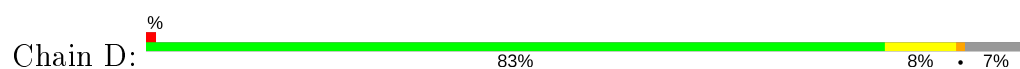




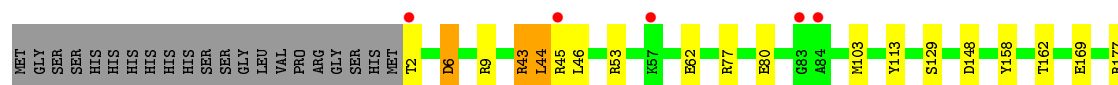
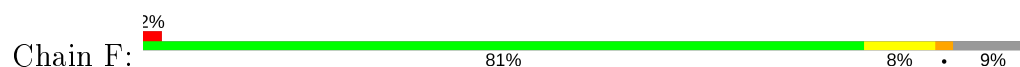
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



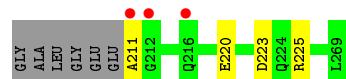
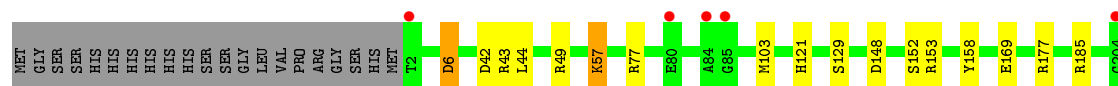
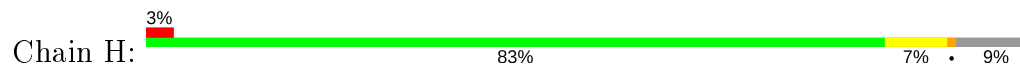
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.04Å 92.31Å 181.16Å 90.00° 96.45° 90.00°	Depositor
Resolution (Å)	47.08 – 2.00 47.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.08-2.00) 99.7 (47.08-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.155 , 0.178 0.165 , 0.185	Depositor DCC
$R_{free}$ test set	9686 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	17867	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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 26.09 % 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 2.8066e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 53K, NAD, CL

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	1.17	6/2056 (0.3%)	1.30	22/2790 (0.8%)
1	B	1.15	7/2034 (0.3%)	1.12	15/2761 (0.5%)
1	C	1.33	19/2040 (0.9%)	1.34	24/2769 (0.9%)
1	D	1.19	9/2034 (0.4%)	1.19	22/2761 (0.8%)
1	E	1.24	11/2040 (0.5%)	1.08	10/2769 (0.4%)
1	F	1.17	8/2011 (0.4%)	1.21	23/2728 (0.8%)
1	G	1.11	4/2008 (0.2%)	1.23	16/2724 (0.6%)
1	H	1.22	8/1994 (0.4%)	1.37	20/2706 (0.7%)
All	All	1.20	72/16217 (0.4%)	1.23	152/22008 (0.7%)

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	129	SER	CB-OG	-16.36	1.21	1.42
1	B	129	SER	CB-OG	-15.15	1.22	1.42
1	D	129	SER	CB-OG	-13.42	1.24	1.42
1	G	204	GLY	N-CA	10.96	1.62	1.46
1	E	223	ASP	CB-CG	10.54	1.73	1.51

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	153	ARG	NE-CZ-NH1	32.89	136.75	120.30
1	G	153	ARG	NE-CZ-NH1	24.78	132.69	120.30
1	C	153	ARG	NE-CZ-NH2	24.24	132.42	120.30
1	H	153	ARG	NE-CZ-NH2	-20.65	109.98	120.30
1	G	153	ARG	NE-CZ-NH2	-17.41	111.59	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	2009	0	2031	15	0
1	B	1996	0	2013	5	1
1	C	1999	0	2018	7	0
1	D	1996	0	2013	4	0
1	E	1999	0	2018	4	0
1	F	1971	0	1993	12	0
1	G	1965	0	1992	1	0
1	H	1957	0	1978	3	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
3	A	27	0	18	0	0
3	B	27	0	19	0	0
3	C	27	0	18	0	0
3	D	27	0	18	1	0
3	E	27	0	18	1	0
3	F	27	0	18	1	0
3	G	27	0	18	0	0
3	H	27	0	19	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	A	198	0	0	1	0
6	B	148	0	0	1	0
6	C	195	0	0	0	0
6	D	183	0	0	2	0
6	E	154	0	0	3	0
6	F	163	0	0	1	0
6	G	176	0	0	0	0
6	H	185	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17867	0	16410	42	1

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 1.

The worst 5 of 42 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:B:2:THR:HG23	6:E:537:HOH:O	1.42	1.20
1:E:223:ASP:HB3	6:E:510:HOH:O	1.74	0.87
1:C:195:ARG:HH22	1:C:215:ILE:HD11	1.47	0.77
1:B:106:ASN:OD1	6:B:401:HOH:O	2.07	0.71
1:A:201:ALA:HB1	1:F:211:ALA:HB2	1.73	0.70

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ARG:NH2	1:B:207:LEU:O[2_556]	2.11	0.09

## 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	269/289 (93%)	259 (96%)	10 (4%)	0	100	100
1	B	266/289 (92%)	254 (96%)	12 (4%)	0	100	100
1	C	267/289 (92%)	256 (96%)	11 (4%)	0	100	100
1	D	266/289 (92%)	253 (95%)	13 (5%)	0	100	100
1	E	267/289 (92%)	256 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	260/289 (90%)	249 (96%)	11 (4%)	0	100	100
1	G	260/289 (90%)	247 (95%)	13 (5%)	0	100	100
1	H	258/289 (89%)	247 (96%)	11 (4%)	0	100	100
All	All	2113/2312 (91%)	2021 (96%)	92 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/222 (93%)	205 (99%)	2 (1%)	76	81
1	B	204/222 (92%)	198 (97%)	6 (3%)	42	43
1	C	205/222 (92%)	203 (99%)	2 (1%)	76	81
1	D	204/222 (92%)	200 (98%)	4 (2%)	55	58
1	E	205/222 (92%)	198 (97%)	7 (3%)	37	36
1	F	203/222 (91%)	199 (98%)	4 (2%)	55	58
1	G	203/222 (91%)	200 (98%)	3 (2%)	65	69
1	H	201/222 (90%)	199 (99%)	2 (1%)	76	81
All	All	1632/1776 (92%)	1602 (98%)	30 (2%)	59	63

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	223	ASP
1	G	6	ASP
1	F	233	LYS
1	G	2	THR
1	G	170	SER

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

Mol	Chain	Res	Type
1	D	224	GLN
1	F	224	GLN
1	H	224	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 5 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	53K	E	302	-	29,30,30	3.44	13 (44%)	37,41,41	2.85	10 (27%)
2	NAD	B	301	-	42,48,48	0.92	1 (2%)	50,73,73	1.25	5 (10%)
3	53K	H	302	-	29,30,30	3.50	12 (41%)	37,41,41	2.70	9 (24%)
3	53K	A	302	-	29,30,30	3.23	13 (44%)	37,41,41	3.50	12 (32%)
3	53K	F	302	-	29,30,30	3.56	11 (37%)	37,41,41	3.04	11 (29%)
2	NAD	D	301	-	42,48,48	0.93	2 (4%)	50,73,73	1.19	5 (10%)
3	53K	D	302	-	29,30,30	3.46	10 (34%)	37,41,41	3.27	9 (24%)
2	NAD	G	301	-	42,48,48	1.03	2 (4%)	50,73,73	1.28	8 (16%)
2	NAD	A	301	-	42,48,48	0.86	2 (4%)	50,73,73	1.18	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	C	301	-	42,48,48	0.88	2 (4%)	50,73,73	1.08	5 (10%)
2	NAD	H	301	-	42,48,48	1.10	2 (4%)	50,73,73	1.28	5 (10%)
3	53K	C	302	-	29,30,30	3.76	11 (37%)	37,41,41	3.12	12 (32%)
3	53K	G	302	-	29,30,30	3.23	9 (31%)	37,41,41	3.03	13 (35%)
2	NAD	E	301	-	42,48,48	0.99	2 (4%)	50,73,73	1.15	5 (10%)
2	NAD	F	301	-	42,48,48	0.90	2 (4%)	50,73,73	1.29	5 (10%)
3	53K	B	302	-	29,30,30	3.41	13 (44%)	37,41,41	3.10	13 (35%)

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
3	53K	E	302	-	-	0/12/12/12	0/4/4/4
2	NAD	B	301	-	-	10/26/62/62	0/5/5/5
3	53K	H	302	-	-	1/12/12/12	0/4/4/4
3	53K	A	302	-	-	2/12/12/12	0/4/4/4
3	53K	F	302	-	-	0/12/12/12	0/4/4/4
2	NAD	D	301	-	-	10/26/62/62	0/5/5/5
3	53K	D	302	-	-	0/12/12/12	0/4/4/4
2	NAD	G	301	-	-	8/26/62/62	0/5/5/5
2	NAD	A	301	-	-	8/26/62/62	0/5/5/5
2	NAD	C	301	-	-	7/26/62/62	0/5/5/5
2	NAD	H	301	-	-	9/26/62/62	0/5/5/5
3	53K	C	302	-	-	0/12/12/12	0/4/4/4
3	53K	G	302	-	-	0/12/12/12	0/4/4/4
2	NAD	E	301	-	-	8/26/62/62	0/5/5/5
2	NAD	F	301	-	-	8/26/62/62	0/5/5/5
3	53K	B	302	-	-	0/12/12/12	0/4/4/4

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	53K	C20-C15	10.52	1.61	1.39
3	F	302	53K	C17-C16	9.91	1.59	1.38
3	E	302	53K	C18-C17	8.38	1.60	1.38
3	D	302	53K	C16-C15	8.38	1.57	1.39
3	H	302	53K	C20-C15	8.30	1.57	1.39

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	53K	C18-C17-C16	-10.45	104.27	120.19
3	A	302	53K	C19-C20-C15	-10.14	107.82	120.56
3	D	302	53K	C18-C17-C16	-8.77	106.83	120.19
3	G	302	53K	C18-C17-C16	-8.42	107.36	120.19
3	B	302	53K	C18-C17-C16	-8.41	107.38	120.19

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAD	C5D-O5D-PN-O1N
2	B	301	NAD	C5D-O5D-PN-O2N
2	B	301	NAD	O4D-C1D-N1N-C2N
2	B	301	NAD	O4D-C1D-N1N-C6N
2	B	301	NAD	C2D-C1D-N1N-C6N

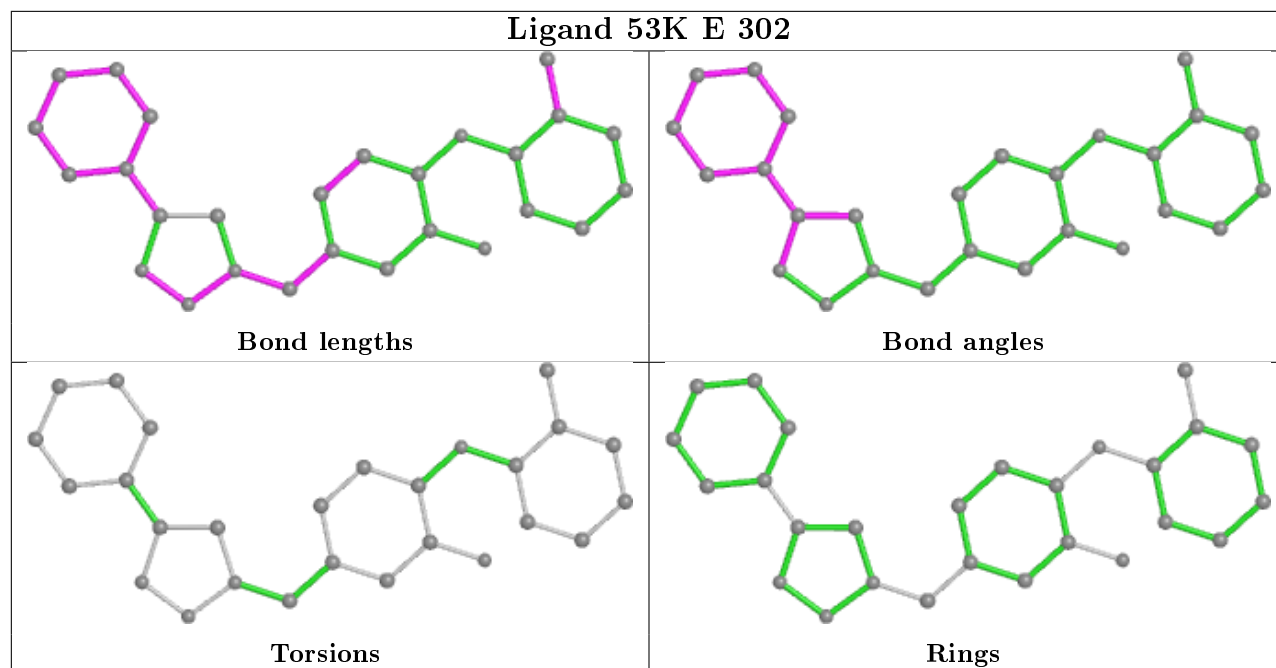
There are no ring outliers.

4 monomers are involved in 4 short contacts:

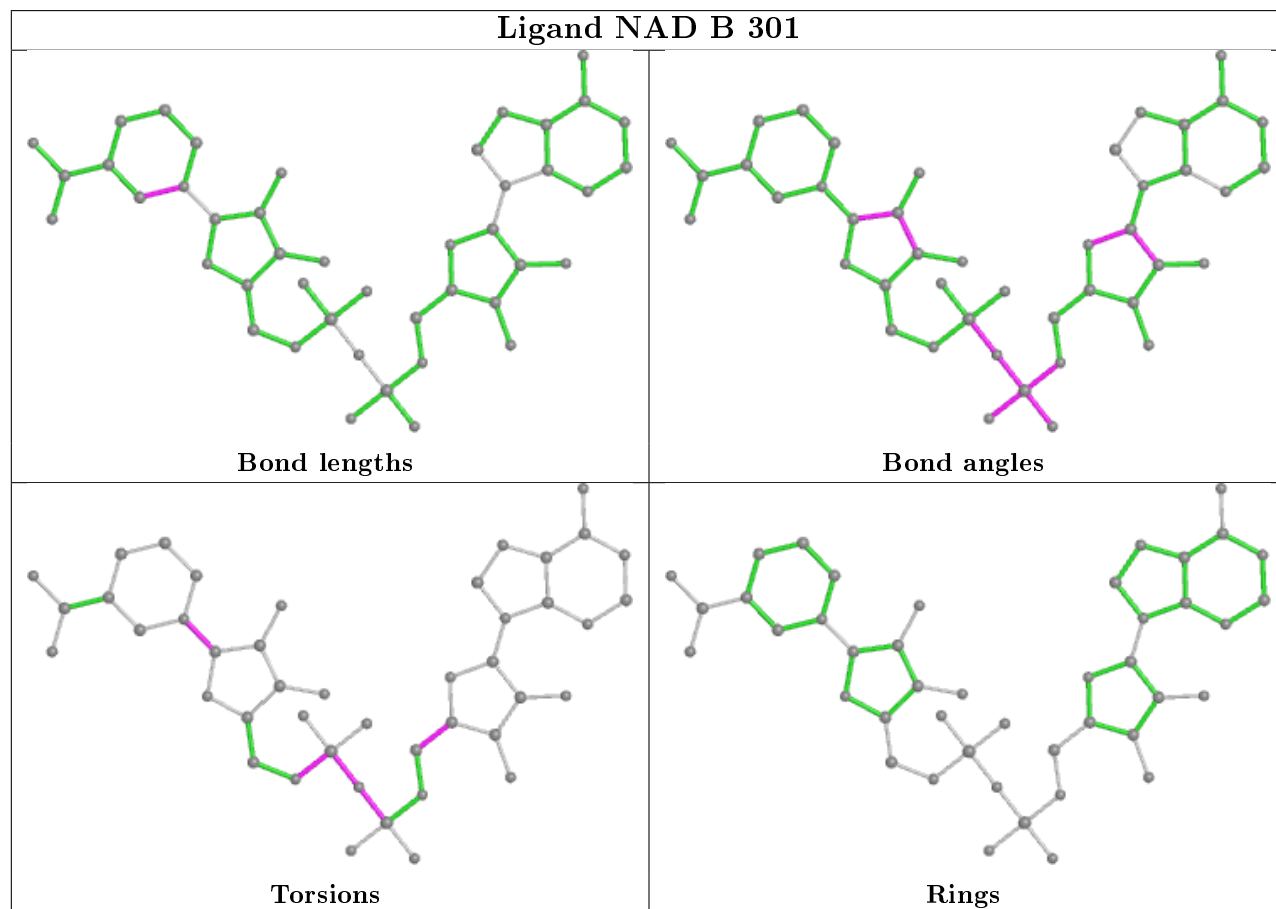
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	53K	1	0
3	H	302	53K	1	0
3	F	302	53K	1	0
3	D	302	53K	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

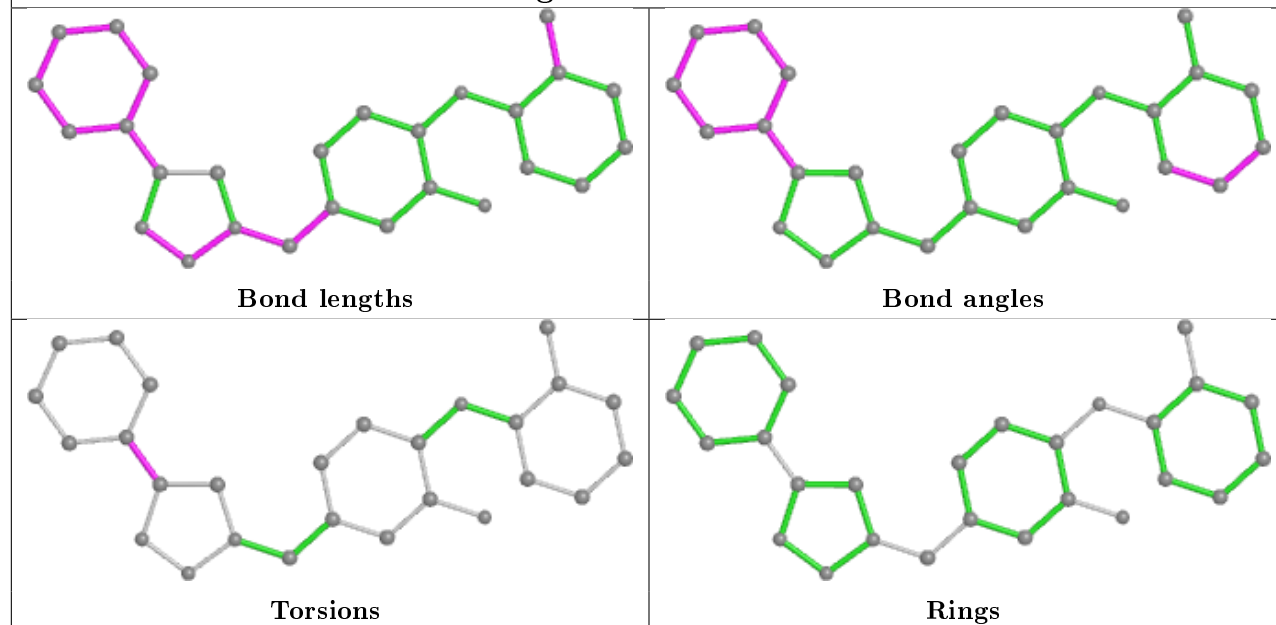
## Ligand 53K E 302



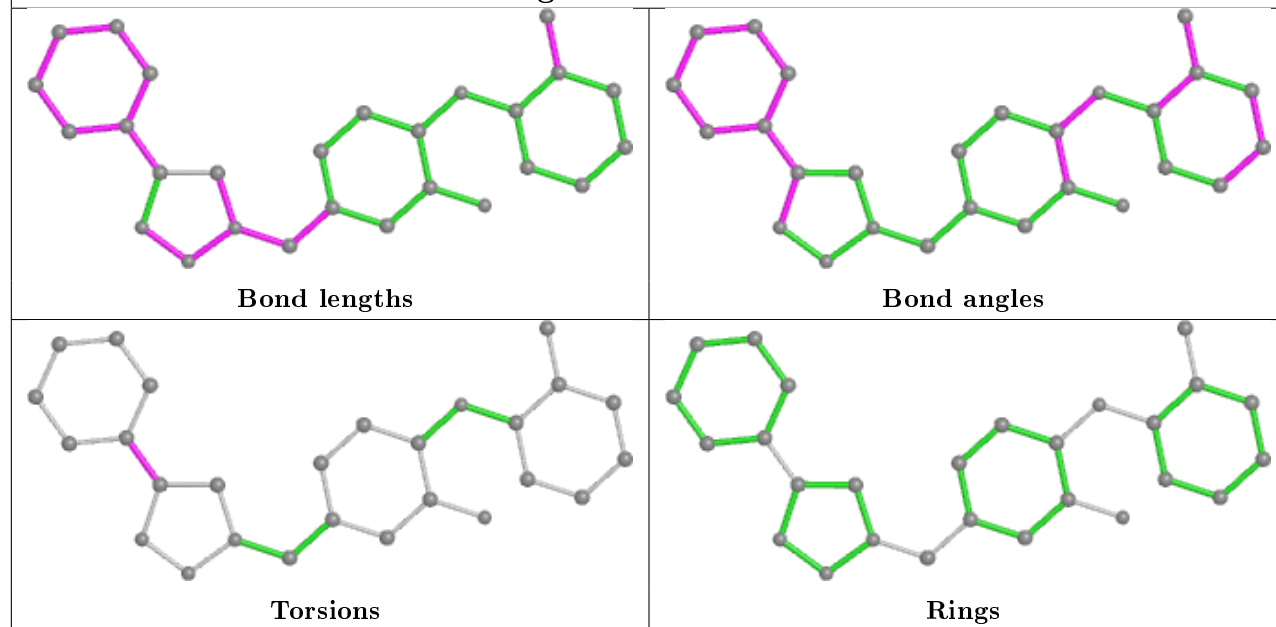
## Ligand NAD B 301



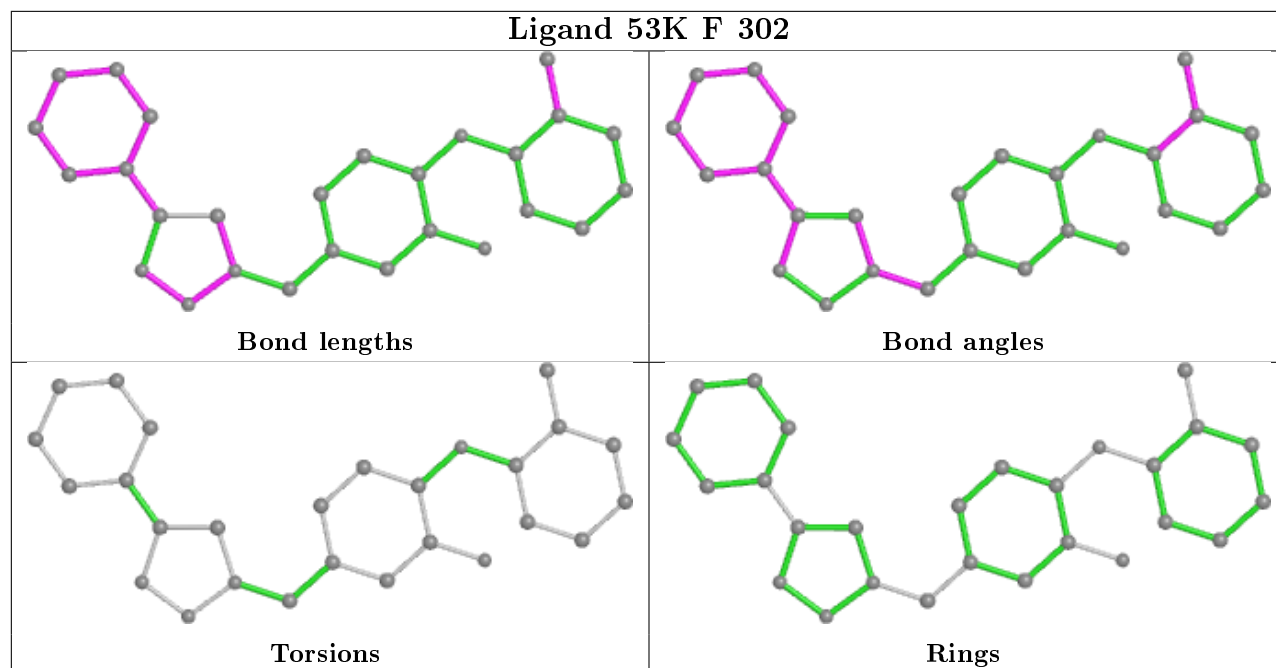
## Ligand 53K H 302



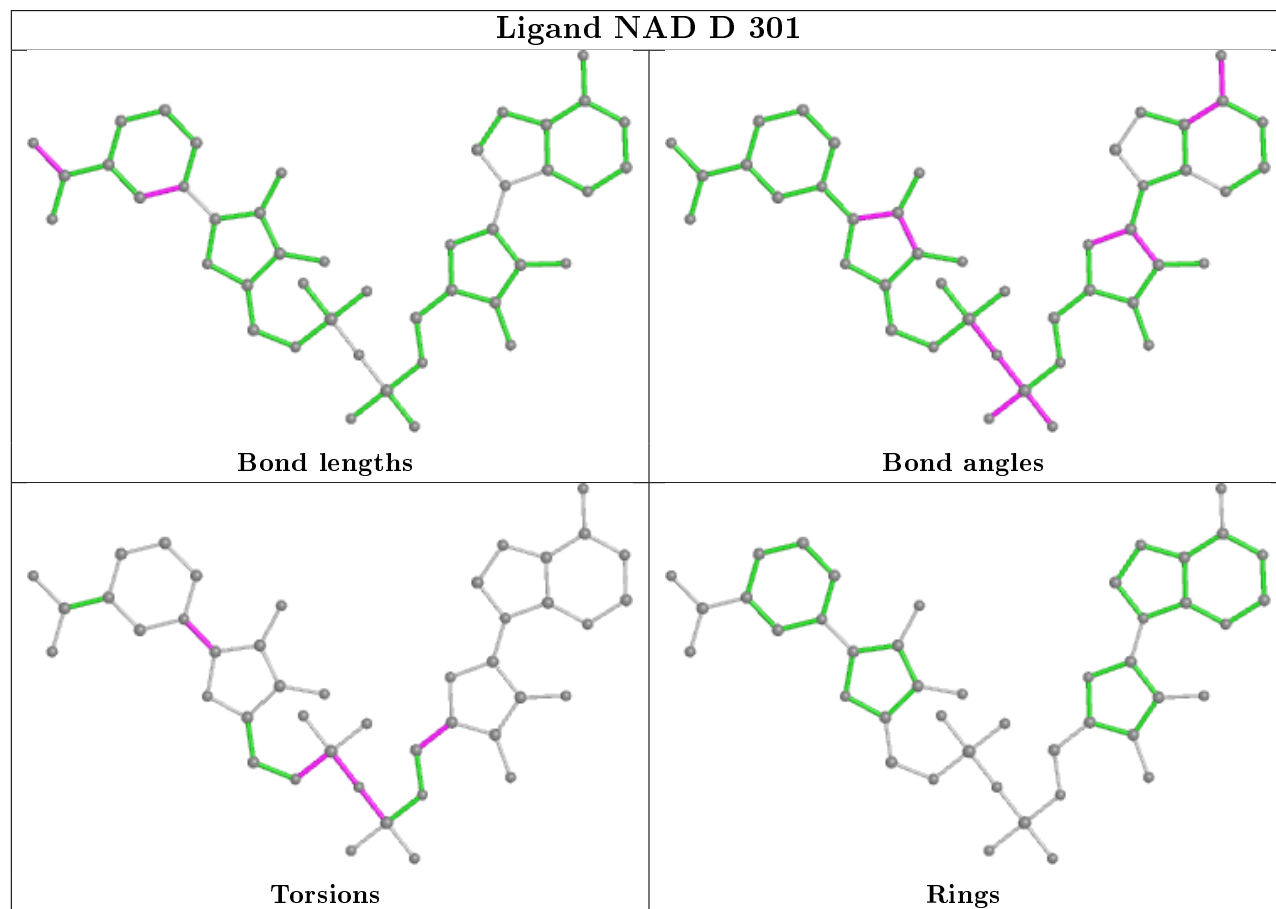
## Ligand 53K A 302



## Ligand 53K F 302

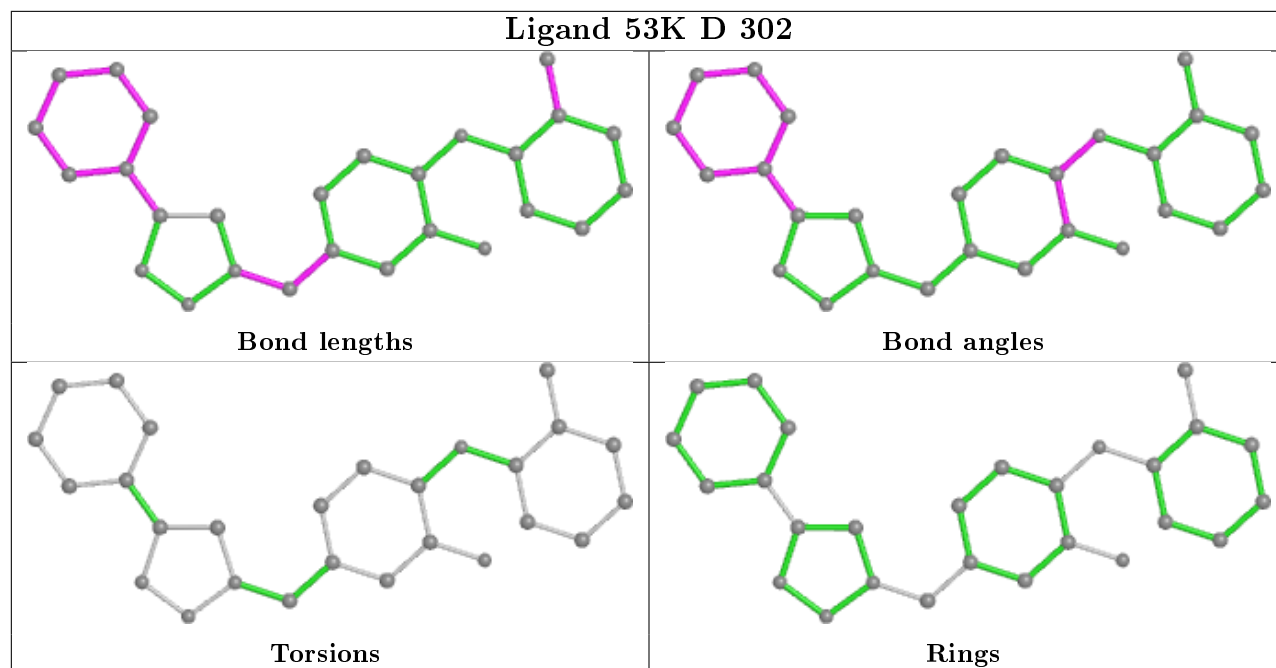


## Ligand NAD D 301

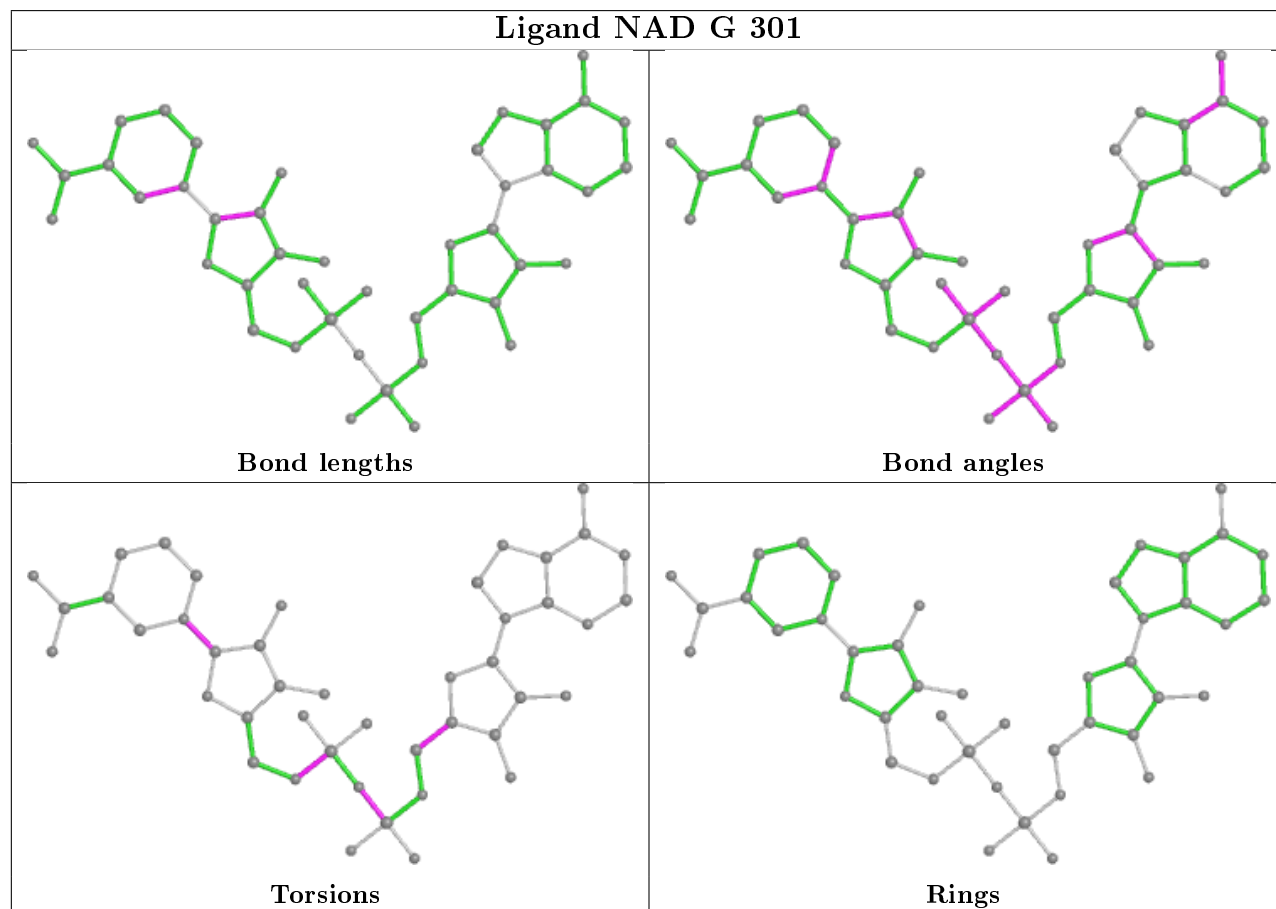


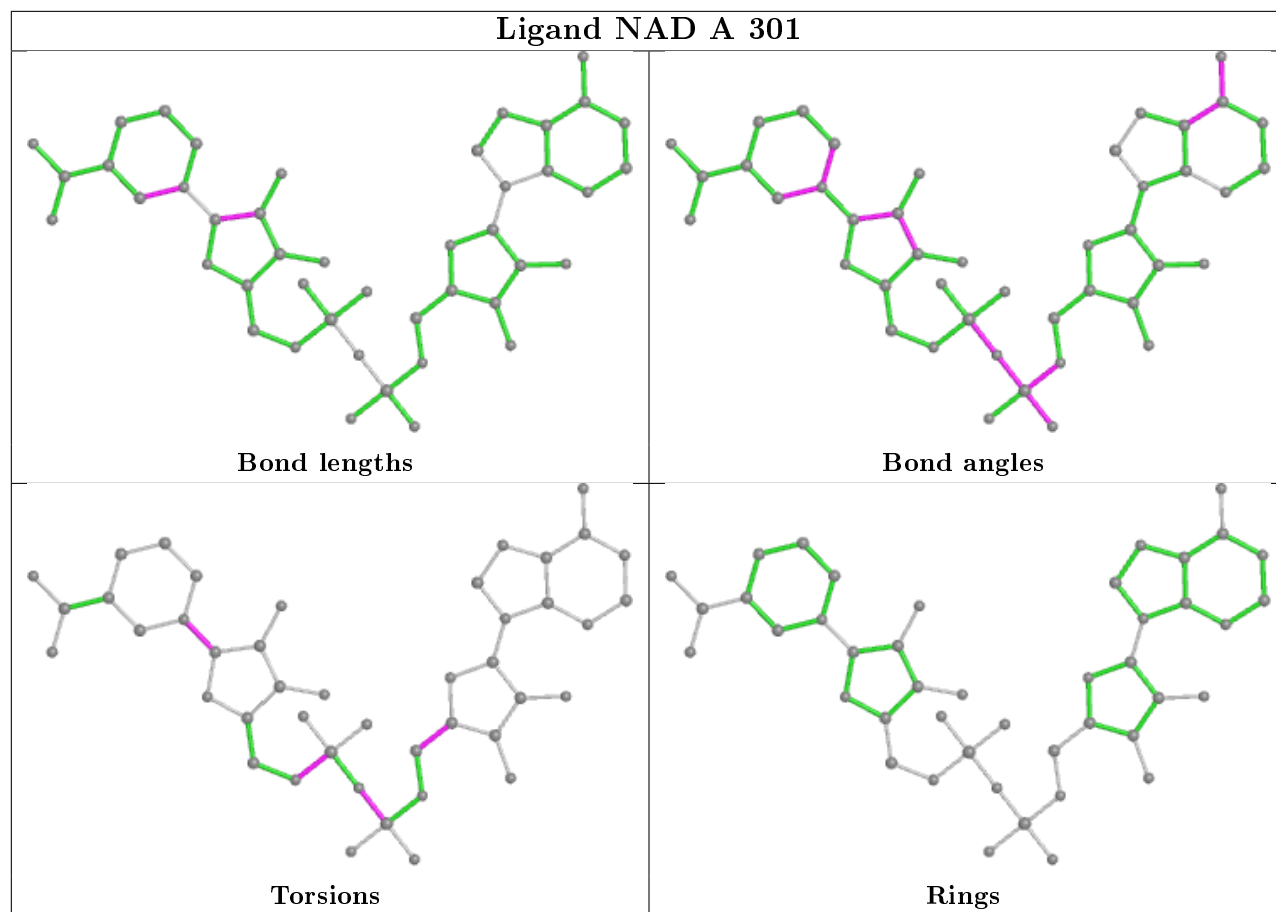


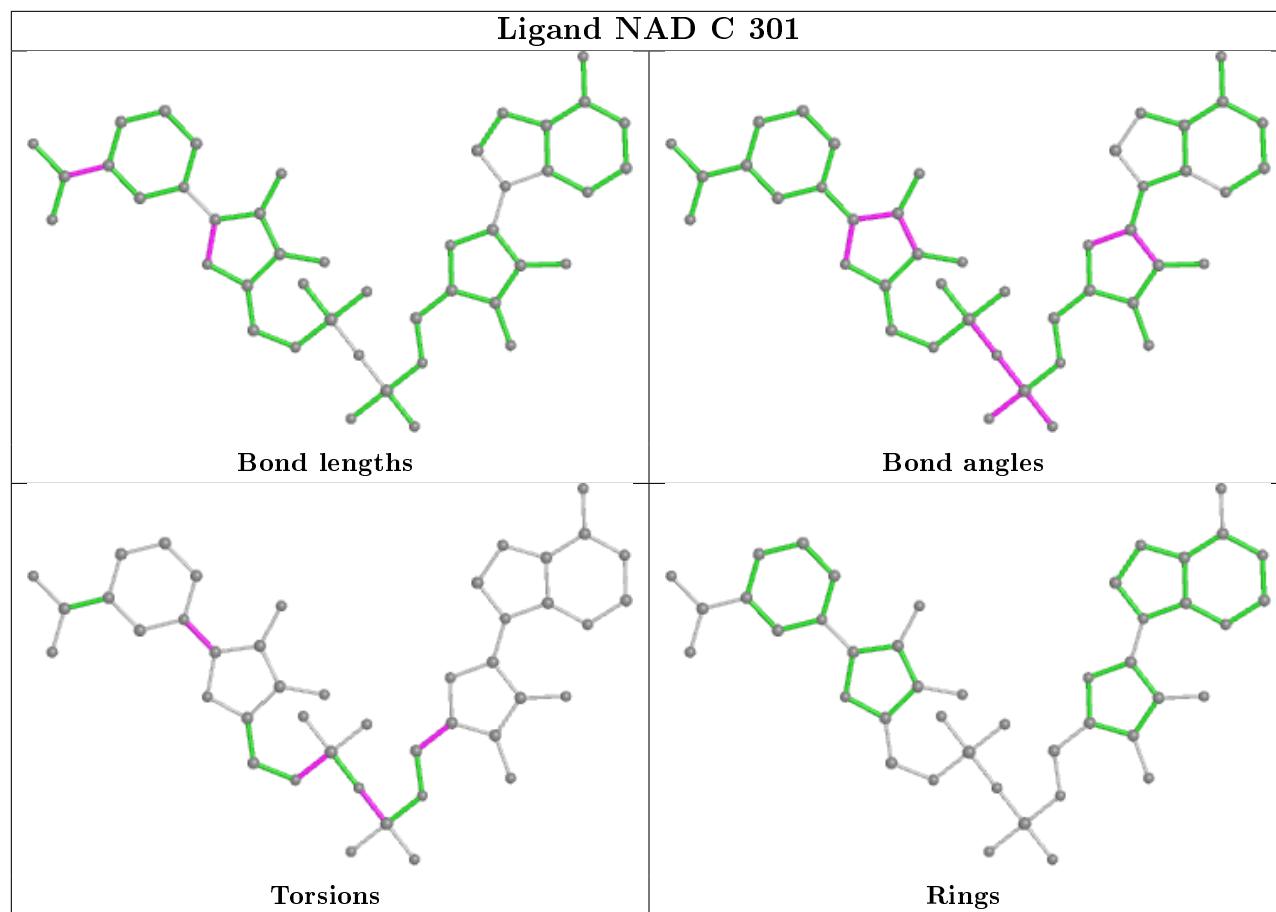
## Ligand 53K D 302

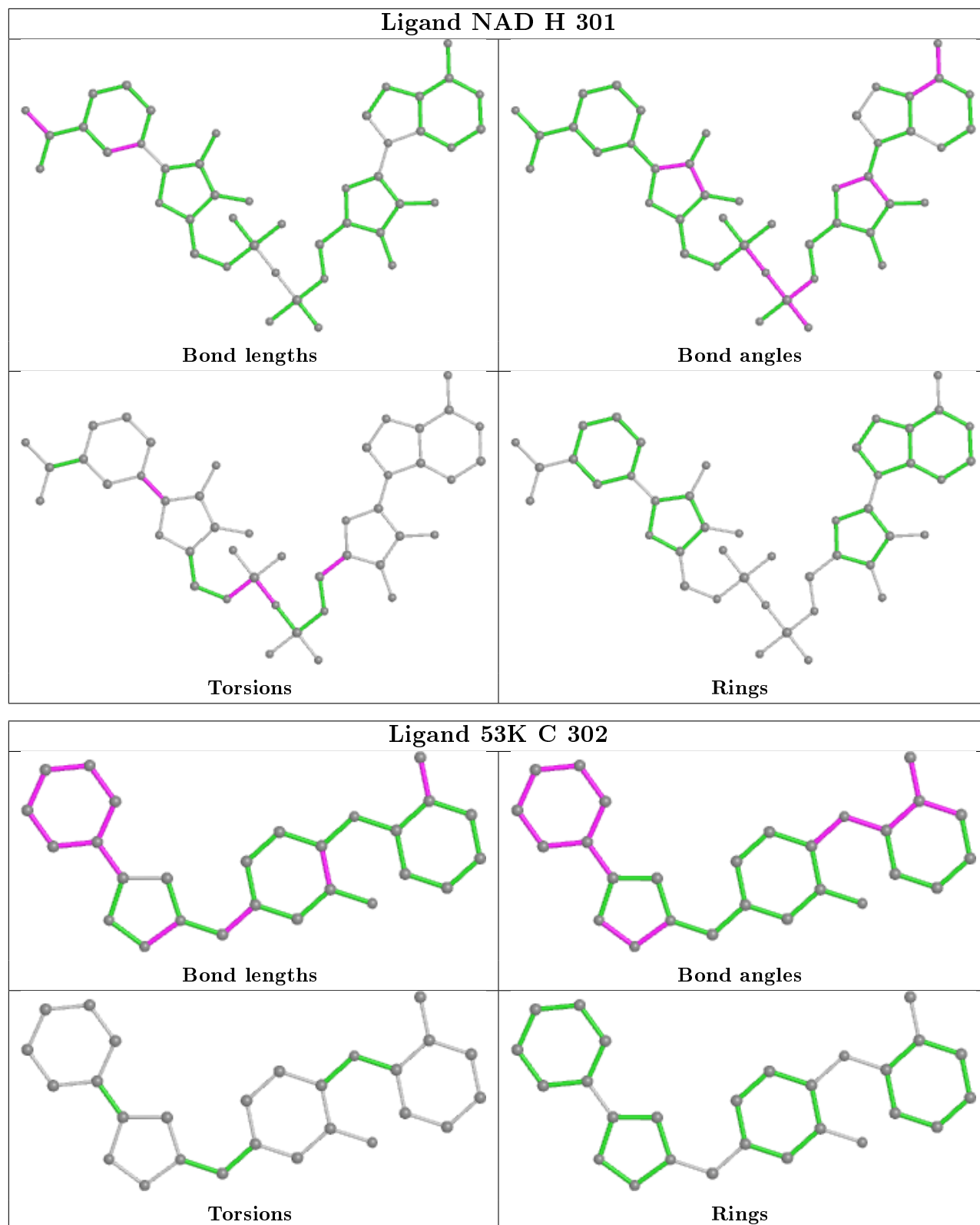


## Ligand NAD G 301

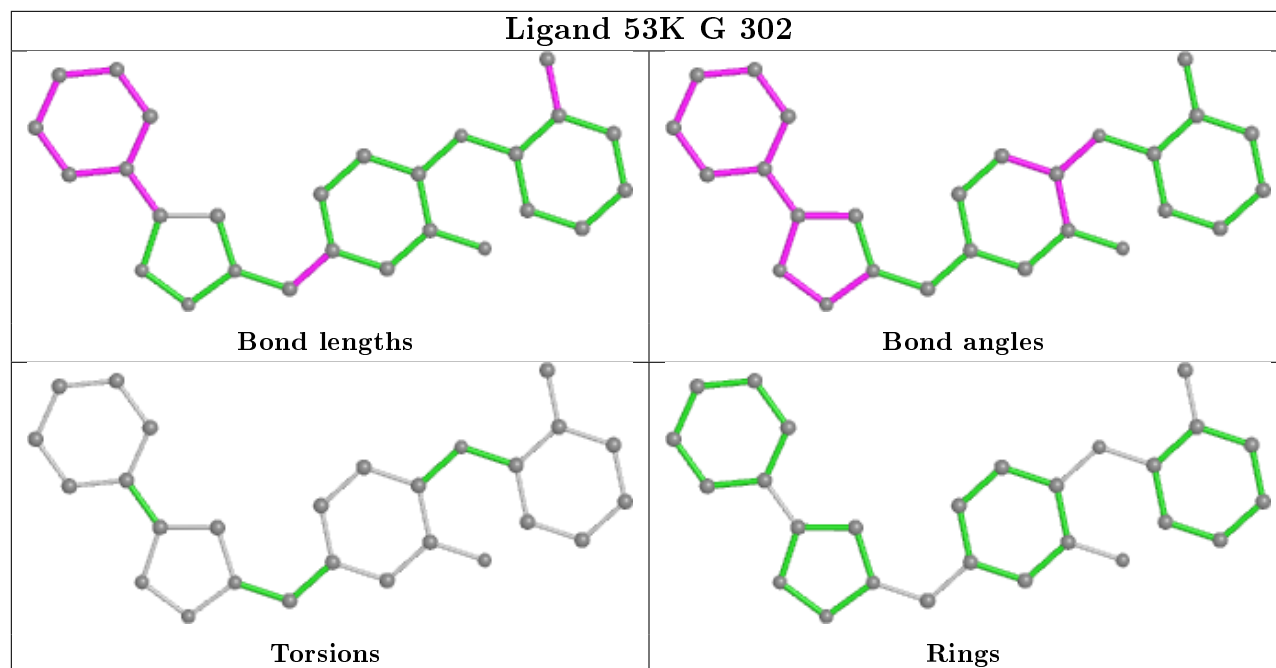




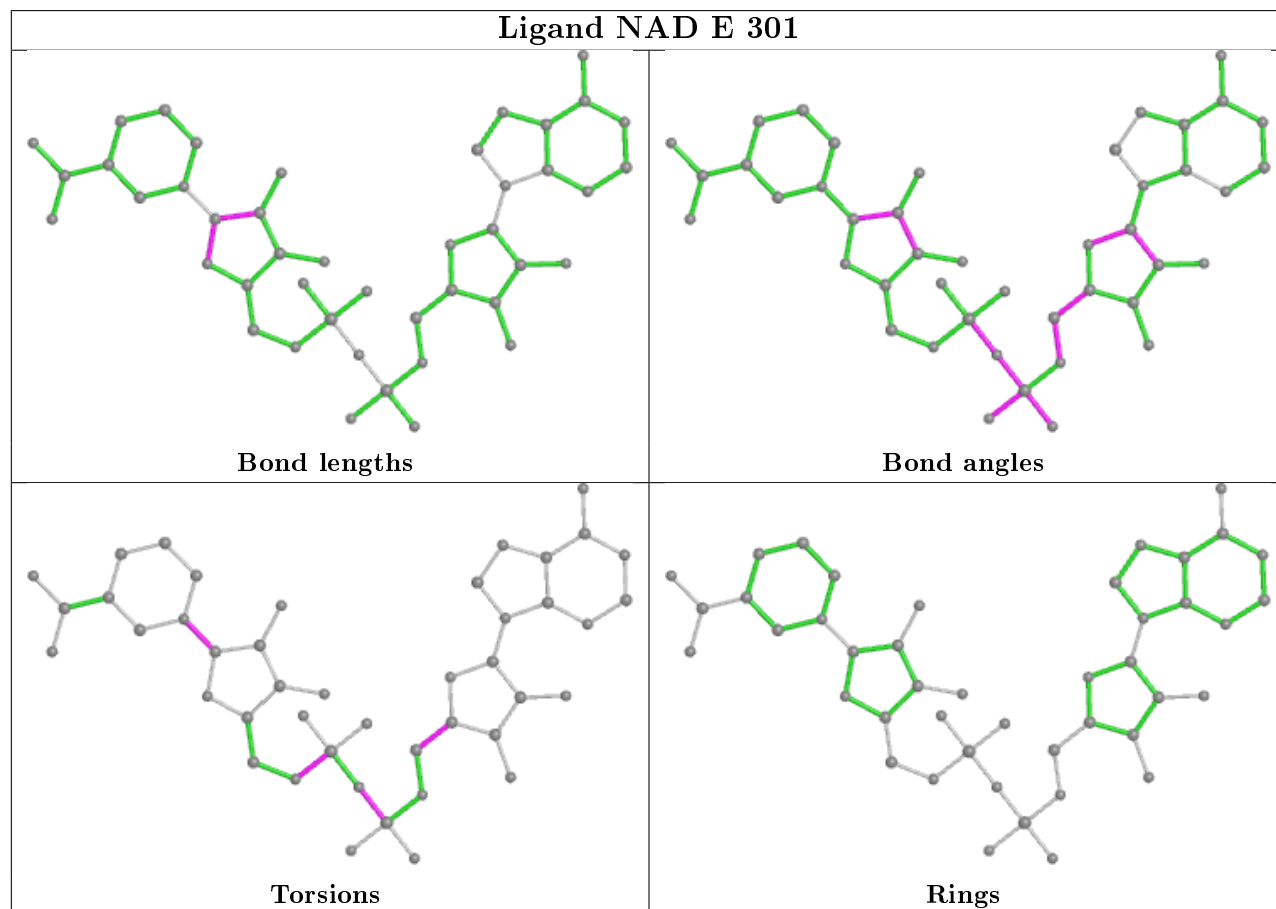


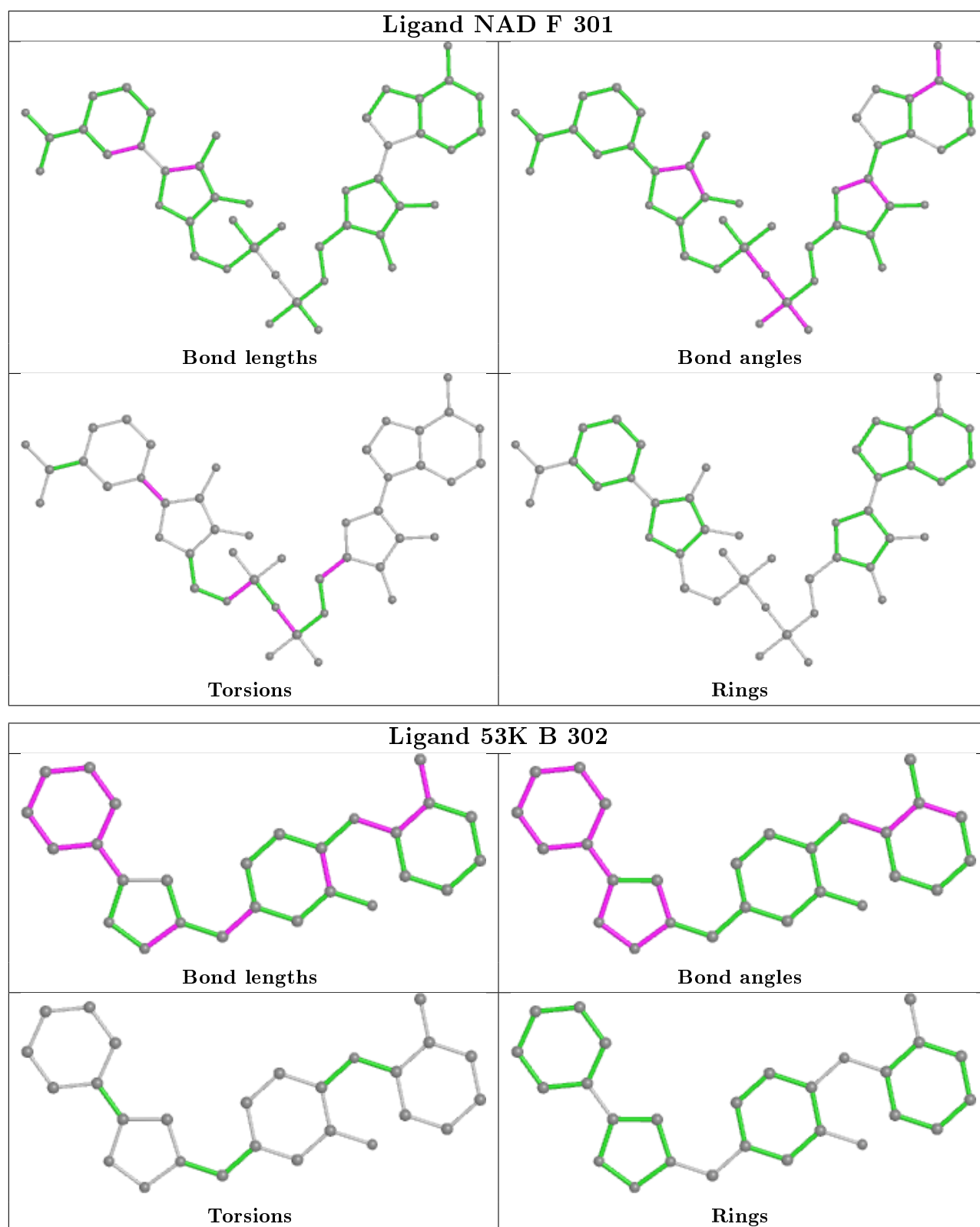


## Ligand 53K G 302



## Ligand NAD E 301





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	268/289 (92%)	-0.50	8 (2%)	50	49	17, 25, 48, 86	0
1	B	268/289 (92%)	-0.22	6 (2%)	62	60	19, 32, 56, 82	0
1	C	268/289 (92%)	-0.59	2 (0%)	87	87	16, 25, 41, 76	0
1	D	268/289 (92%)	-0.34	4 (1%)	73	72	17, 28, 49, 72	0
1	E	268/289 (92%)	-0.42	4 (1%)	73	72	19, 30, 50, 77	0
1	F	263/289 (91%)	-0.41	6 (2%)	60	59	19, 29, 50, 76	0
1	G	262/289 (90%)	-0.43	8 (3%)	49	48	18, 28, 49, 68	0
1	H	262/289 (90%)	-0.37	8 (3%)	49	48	18, 29, 48, 70	0
All	All	2127/2312 (91%)	-0.41	46 (2%)	62	60	16, 28, 50, 86	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	211	ALA	6.2
1	E	2	THR	5.9
1	B	57	LYS	5.2
1	H	204	GLY	5.0
1	B	2	THR	4.8

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

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

### 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 6.4 Ligands ⓘ

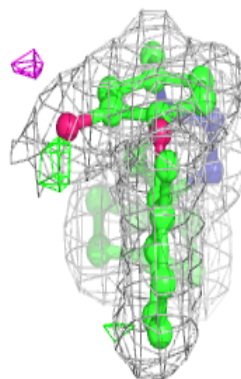
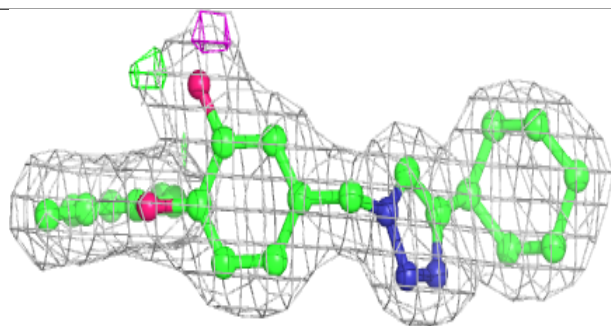
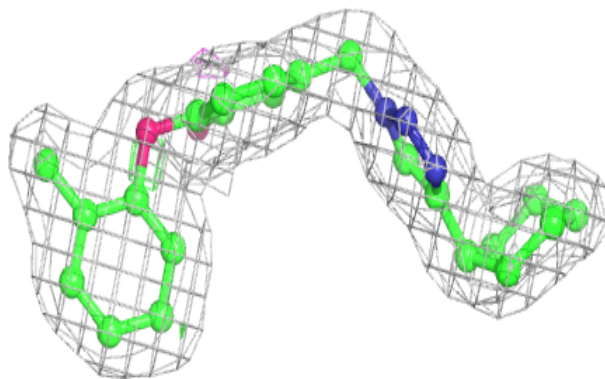
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	53K	H	302	27/27	0.95	0.08	19,23,25,25	0
5	NA	F	303	1/1	0.96	0.27	43,43,43,43	0
4	CL	A	303	1/1	0.96	0.05	35,35,35,35	0
3	53K	A	302	27/27	0.97	0.07	18,21,29,32	0
3	53K	F	302	27/27	0.97	0.07	20,22,24,25	0
2	NAD	B	301	44/44	0.97	0.08	22,26,30,33	0
5	NA	H	303	1/1	0.97	0.14	35,35,35,35	0
3	53K	C	302	27/27	0.97	0.07	19,21,26,29	0
3	53K	G	302	27/27	0.97	0.08	22,24,26,27	0
3	53K	D	302	27/27	0.97	0.08	19,22,26,27	0
3	53K	E	302	27/27	0.97	0.07	20,22,23,25	0
3	53K	B	302	27/27	0.97	0.08	21,25,30,30	0
2	NAD	H	301	44/44	0.98	0.07	20,23,29,31	0
2	NAD	D	301	44/44	0.98	0.07	19,23,27,28	0
2	NAD	E	301	44/44	0.98	0.07	19,23,27,28	0
2	NAD	G	301	44/44	0.98	0.07	20,24,27,29	0
2	NAD	C	301	44/44	0.98	0.06	16,19,21,24	0
4	CL	C	303	1/1	0.98	0.05	35,35,35,35	0
2	NAD	F	301	44/44	0.98	0.07	19,24,27,29	0
5	NA	D	303	1/1	0.98	0.10	32,32,32,32	0
2	NAD	A	301	44/44	0.99	0.06	17,20,22,23	0

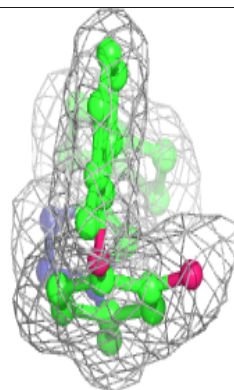
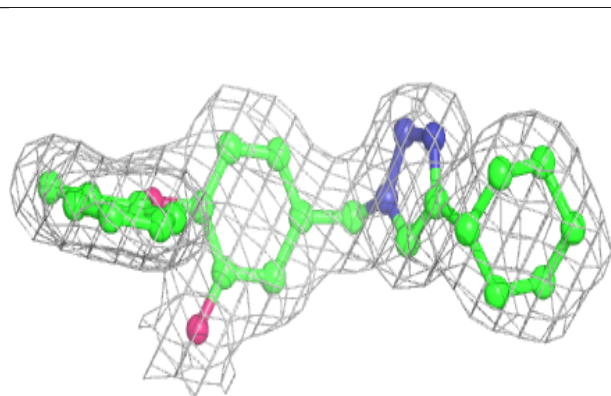
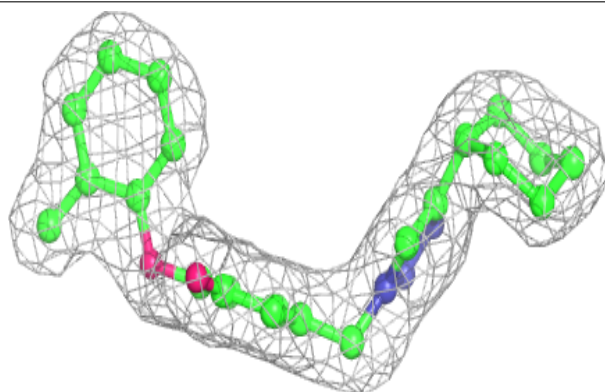
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 53K 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)

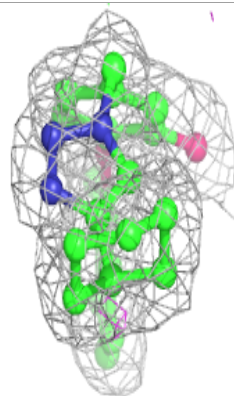
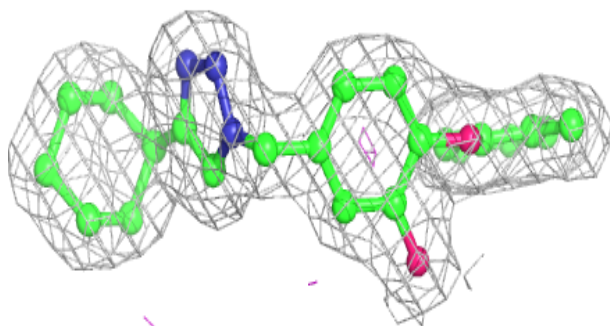
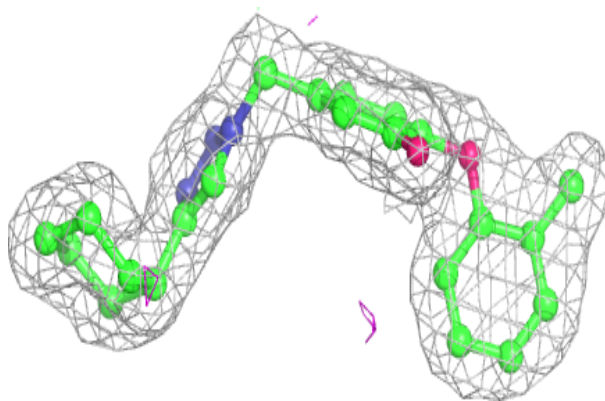
**Electron density around 53K A 302:**

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

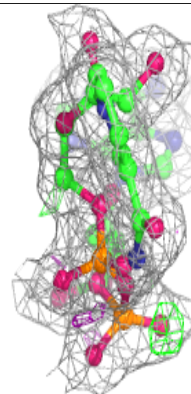
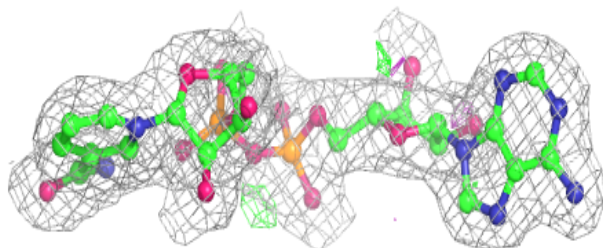
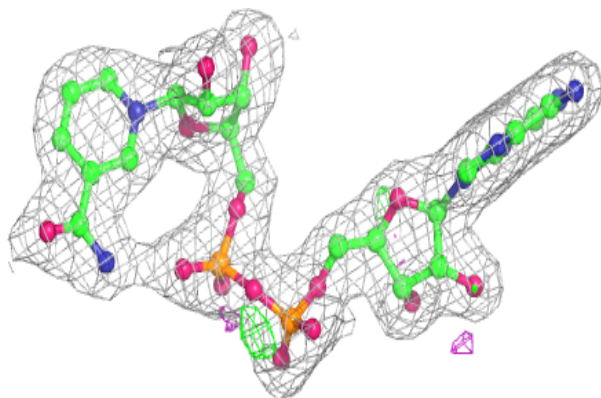


**Electron density around 53K F 302:**

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

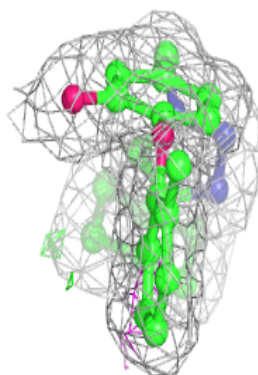
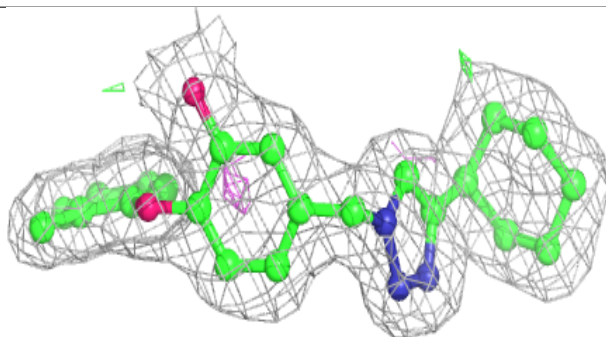
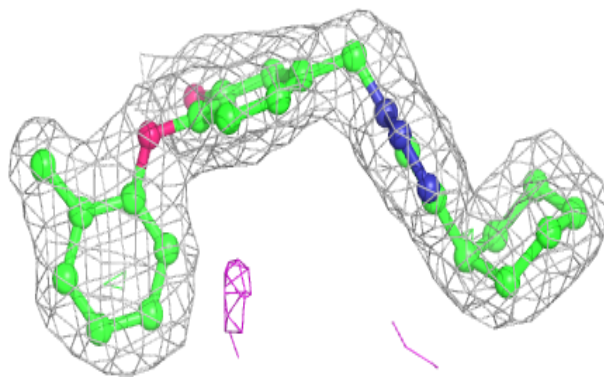
**Electron density around NAD B 301:**

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

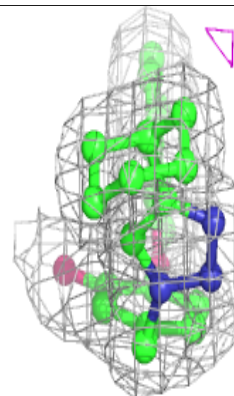
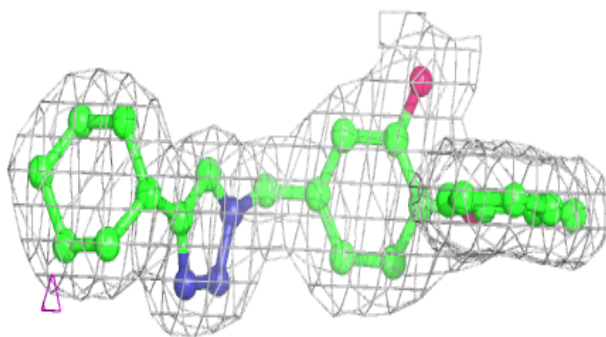
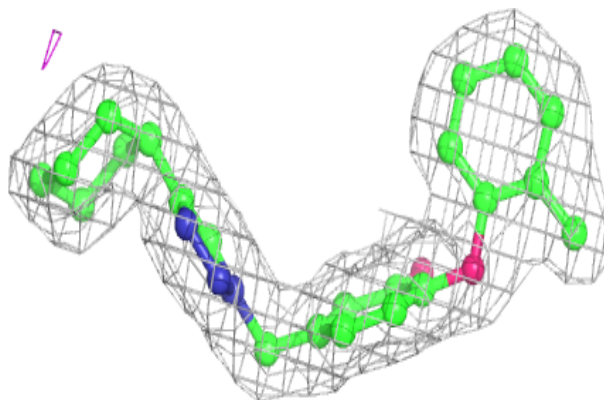


**Electron density around 53K C 302:**

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

**Electron density around 53K G 302:**

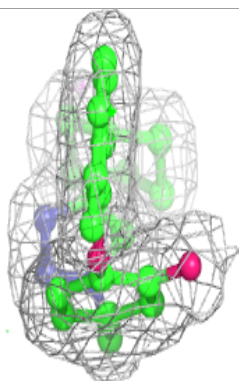
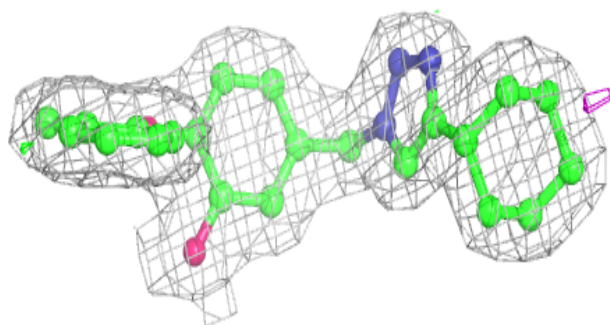
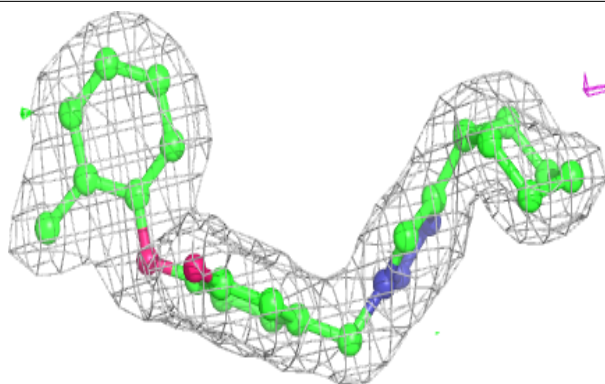
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



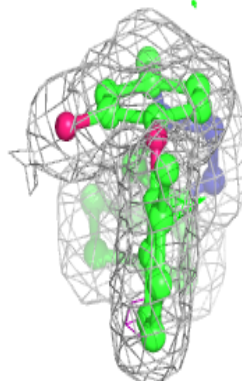
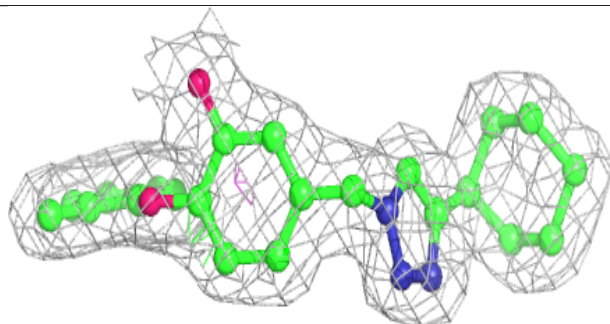
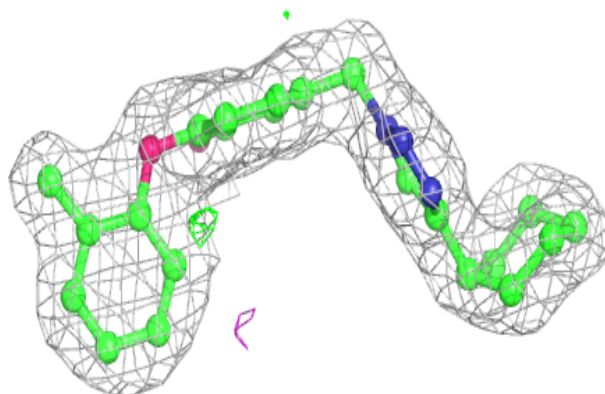


**Electron density around 53K D 302:**

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

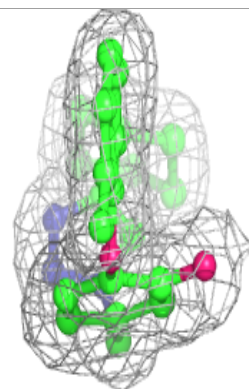
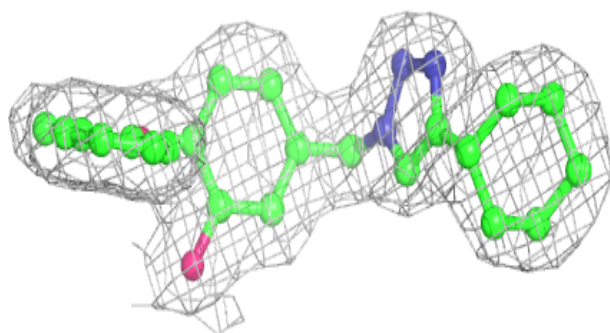
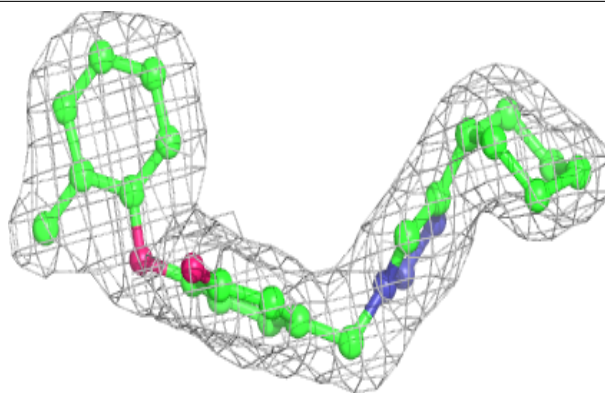
**Electron density around 53K E 302:**

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

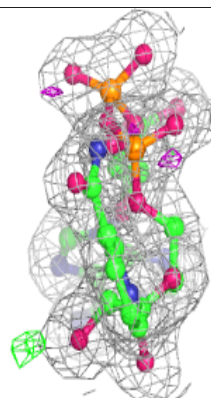
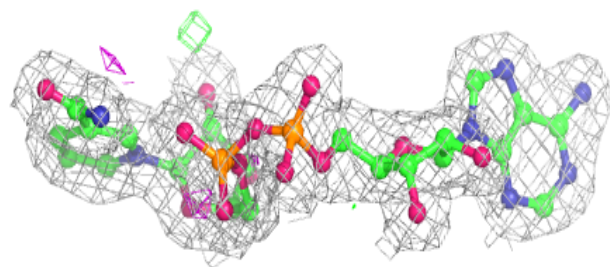
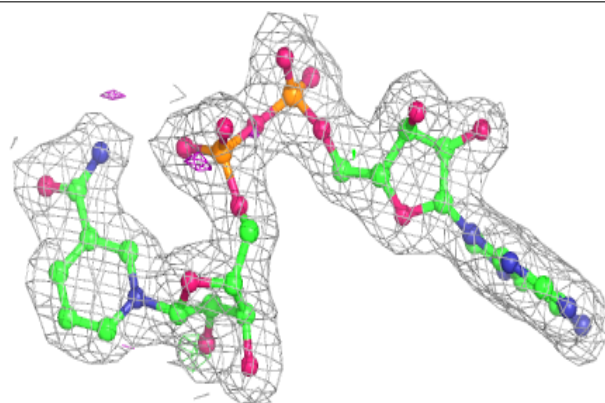


**Electron density around 53K B 302:**

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

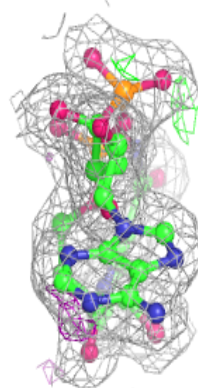
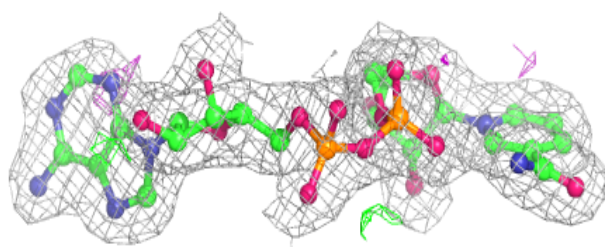
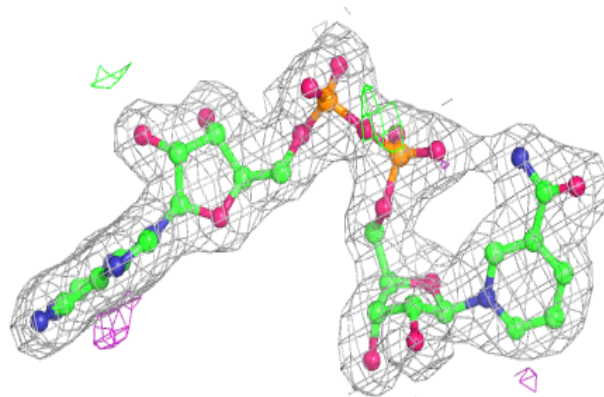
**Electron density around NAD H 301:**

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

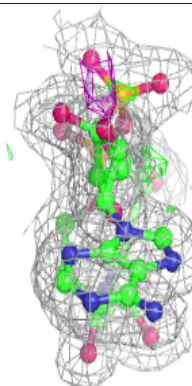
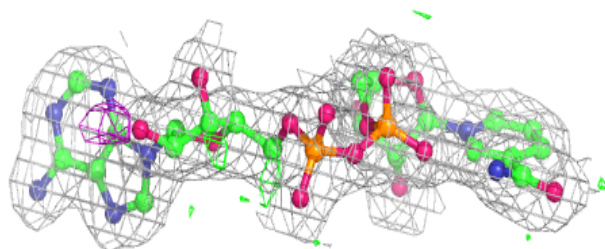
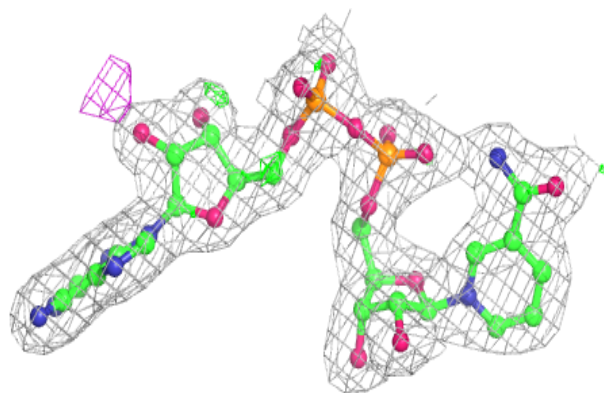


**Electron density around NAD D 301:**

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

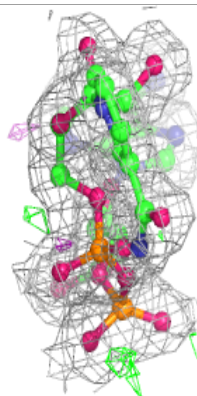
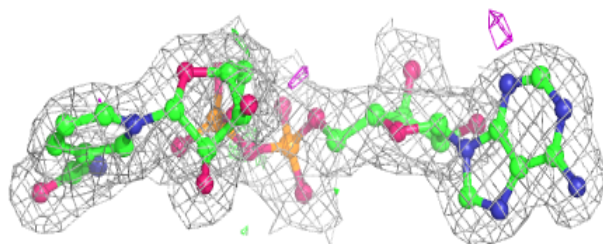
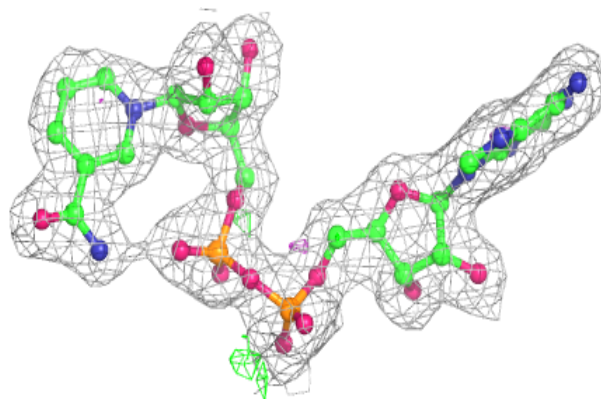
**Electron density around NAD E 301:**

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

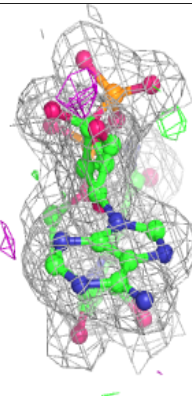
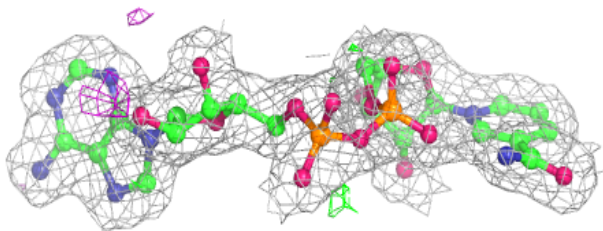
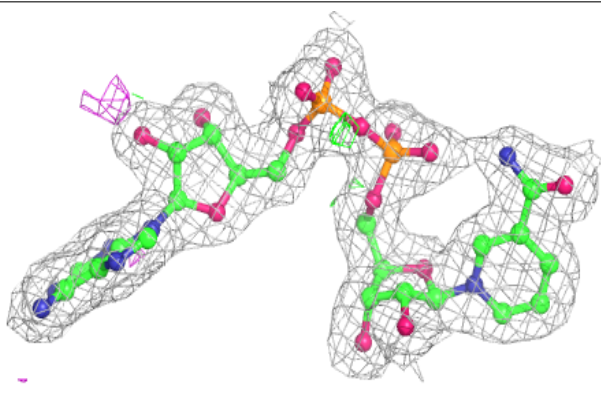


**Electron density around NAD G 301:**

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

**Electron density around NAD C 301:**

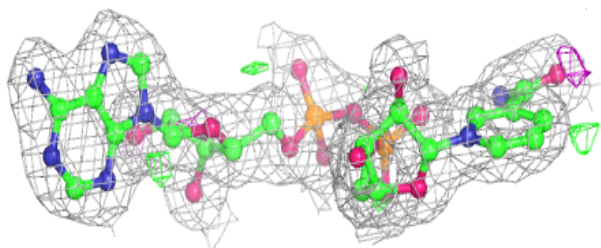
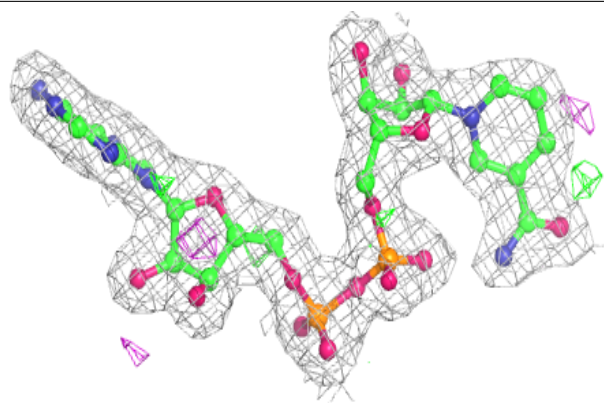
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



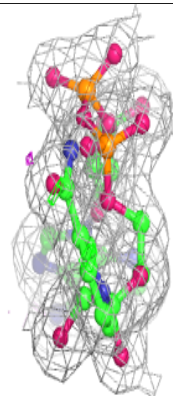
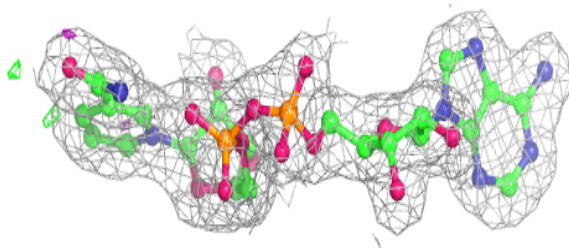
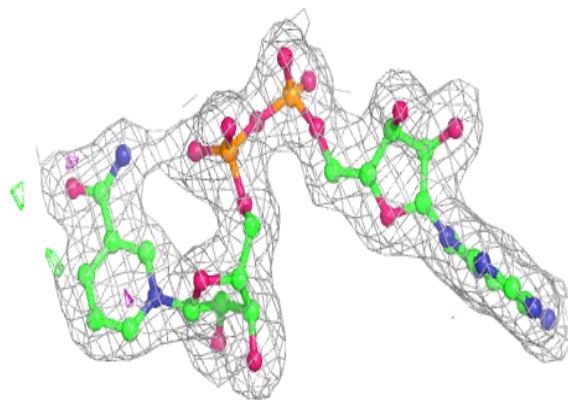


**Electron density around NAD F 301:**

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

**Electron density around NAD 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.