



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 27, 2024 – 06:53 PM EST

PDB ID : 1CW3  
Title : HUMAN MITOCHONDRIAL ALDEHYDE DEHYDROGENASE COM-  
PLEXED WITH NAD<sup>+</sup> AND MN<sup>2+</sup>  
Authors : Ni, L.; Zhou, J.; Hurley, T.D.; Weiner, H.  
Deposited on : 1999-08-25  
Resolution : 2.58 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) 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 : 2.36  
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) : 2.36

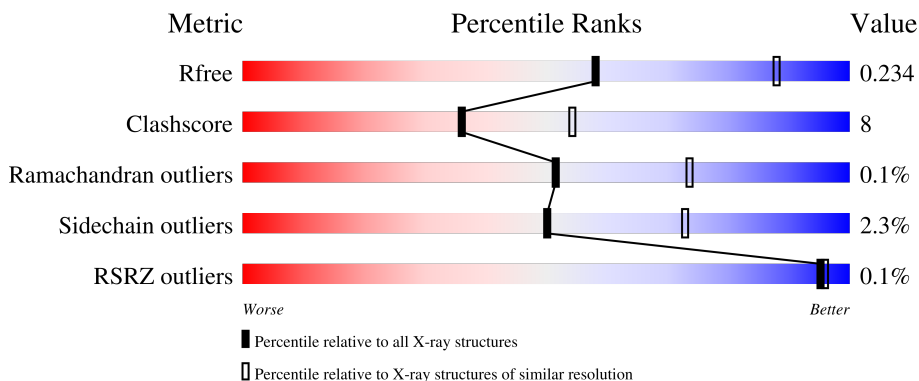
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	494	 82% 18%
1	B	494	 79% 20%
1	C	494	 82% 17%
1	D	494	 81% 18%
1	E	494	 78% 22%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain	
1	F	494	 82%	18%
1	G	494	 83%	16%
1	H	494	 81%	18%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 31839 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 MITOCHONDRIAL ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	494	3798	2415	648	717	18	0	0	0
1	B	494	3798	2415	648	717	18	0	0	0
1	C	494	3798	2415	648	717	18	0	0	0
1	D	494	3798	2415	648	717	18	0	0	0
1	E	494	3798	2415	648	717	18	0	0	0
1	F	494	3798	2415	648	717	18	0	0	0
1	G	494	3798	2415	648	717	18	0	0	0
1	H	494	3798	2415	648	717	18	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

*Continued on next page...*

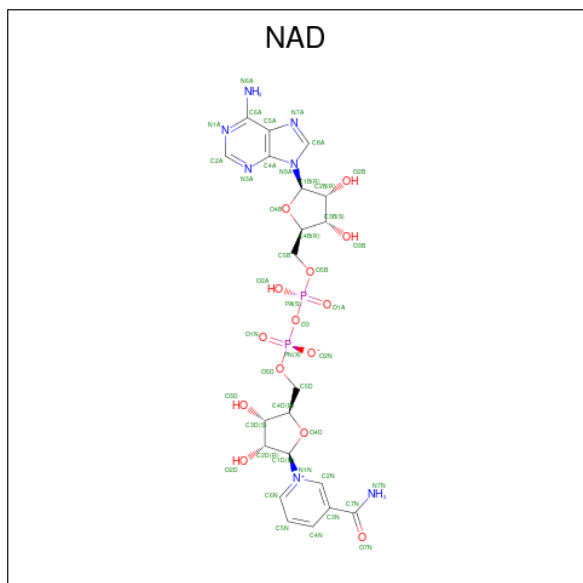
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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


- Molecule 5 is water.

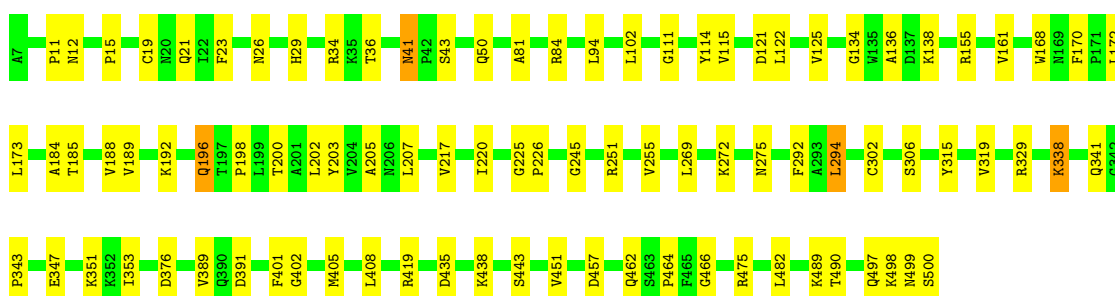
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total	O	0	0
			127	127		
5	B	118	Total	O	0	0
			118	118		
5	C	127	Total	O	0	0
			127	127		
5	D	147	Total	O	0	0
			147	147		
5	E	132	Total	O	0	0
			132	132		
5	F	140	Total	O	0	0
			140	140		
5	G	148	Total	O	0	0
			148	148		
5	H	148	Total	O	0	0
			148	148		

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

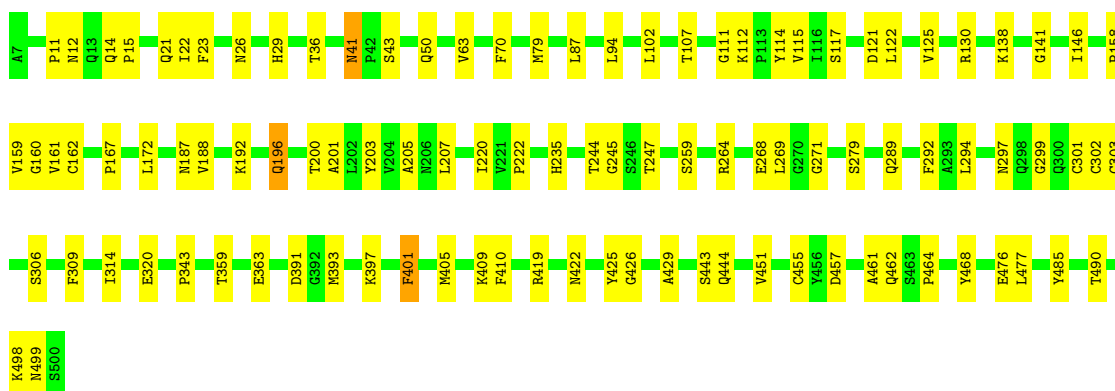
#### • Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain A:  82% 18%




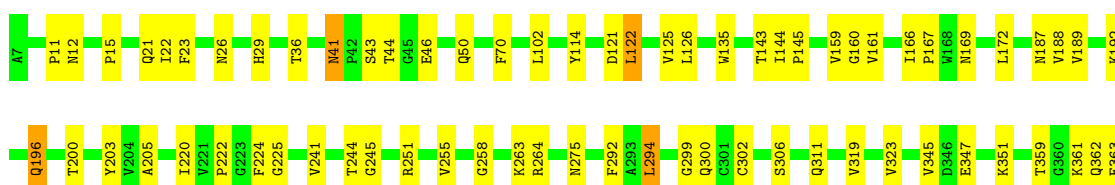
#### • Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain B:  79% 20%



#### • Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

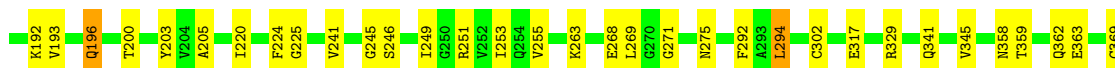
Chain C:  82% 17%





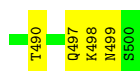
- Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain D: 81% 18%



- Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain E: 78% 22%



- Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

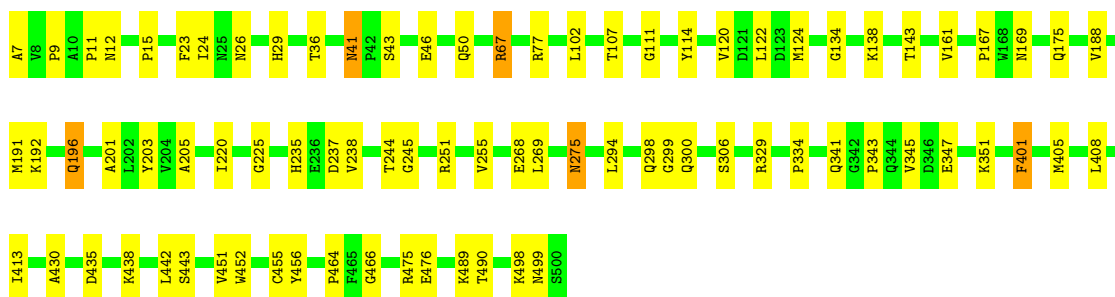
Chain F: 82% 18%



- Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

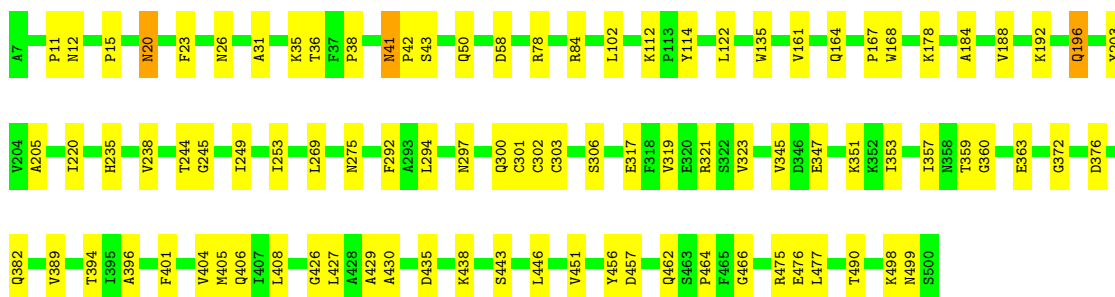
Chain G: 83% 16%





- Molecule 1: MITOCHONDRIAL ALDEHYDE DEHYDROGENASE

Chain H: 81% 18%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.40Å 176.30Å 102.00Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	45.00 – 2.58 44.03 – 2.58	Depositor EDS
% Data completeness (in resolution range)	91.6 (45.00-2.58) 91.4 (44.03-2.58)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.76 (at 2.58Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.175 , 0.242 0.172 , 0.234	Depositor DCC
$R_{free}$ test set	7234 reflections (7.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtrriage
Anisotropy	0.303	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 3.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.149 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	31839	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0/3882	0.61	0/5267
1	B	0.37	0/3882	0.61	0/5267
1	C	0.37	0/3882	0.61	0/5267
1	D	0.38	0/3882	0.63	0/5267
1	E	0.36	0/3882	0.60	0/5267
1	F	0.37	0/3882	0.60	0/5267
1	G	0.37	0/3882	0.61	0/5267
1	H	0.38	0/3882	0.61	0/5267
All	All	0.37	0/31056	0.61	0/42136

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	0	3745	63	0
1	B	3798	0	3745	72	0
1	C	3798	0	3745	61	0
1	D	3798	0	3745	61	0
1	E	3798	0	3745	69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3798	0	3745	65	0
1	G	3798	0	3745	57	0
1	H	3798	0	3745	66	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	44	0	26	3	0
4	B	44	0	26	2	0
4	C	44	0	26	7	0
4	D	44	0	26	5	0
4	E	44	0	26	3	0
4	F	44	0	26	4	0
4	G	44	0	26	4	0
4	H	44	0	26	6	0
5	A	127	0	0	5	0
5	B	118	0	0	5	0
5	C	127	0	0	2	0
5	D	147	0	0	7	0
5	E	132	0	0	5	0
5	F	140	0	0	5	0
5	G	148	0	0	2	0
5	H	148	0	0	3	0
All	All	31839	0	30168	488	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 488 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:GLU:HG2	1:C:351:LYS:HE2	1.53	0.89
1:A:196:GLN:H	1:A:196:GLN:HE21	1.28	0.81
1:F:196:GLN:H	1:F:196:GLN:HE21	1.28	0.81
1:G:196:GLN:H	1:G:196:GLN:HE21	1.29	0.80
1:A:347:GLU:HG2	1:A:351:LYS:HE2	1.64	0.79

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	492/494 (100%)	470 (96%)	22 (4%)	0	100	100
1	B	492/494 (100%)	475 (96%)	16 (3%)	1 (0%)	47	69
1	C	492/494 (100%)	469 (95%)	23 (5%)	0	100	100
1	D	492/494 (100%)	468 (95%)	23 (5%)	1 (0%)	47	69
1	E	492/494 (100%)	473 (96%)	19 (4%)	0	100	100
1	F	492/494 (100%)	473 (96%)	19 (4%)	0	100	100
1	G	492/494 (100%)	470 (96%)	22 (4%)	0	100	100
1	H	492/494 (100%)	472 (96%)	19 (4%)	1 (0%)	47	69
All	All	3936/3952 (100%)	3770 (96%)	163 (4%)	3 (0%)	51	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	426	GLY
1	D	426	GLY
1	H	426	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/399 (100%)	388 (97%)	11 (3%)	43	67
1	B	399/399 (100%)	391 (98%)	8 (2%)	55	76
1	C	399/399 (100%)	390 (98%)	9 (2%)	50	73
1	D	399/399 (100%)	390 (98%)	9 (2%)	50	73
1	E	399/399 (100%)	390 (98%)	9 (2%)	50	73
1	F	399/399 (100%)	389 (98%)	10 (2%)	47	70
1	G	399/399 (100%)	391 (98%)	8 (2%)	55	76
1	H	399/399 (100%)	390 (98%)	9 (2%)	50	73
All	All	3192/3192 (100%)	3119 (98%)	73 (2%)	50	73

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	46	GLU
1	H	401	PHE
1	G	122	LEU
1	H	41	ASN
1	C	196	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	275	ASN
1	H	20	ASN
1	F	406	GLN
1	G	196	GLN
1	H	89	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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
4	NAD	F	6502	2	42,48,48	1.52	4 (9%)	50,73,73	2.01	17 (34%)
4	NAD	A	1502	2	42,48,48	1.48	4 (9%)	50,73,73	1.90	14 (28%)
4	NAD	B	2502	2	42,48,48	1.38	5 (11%)	50,73,73	1.33	5 (10%)
4	NAD	E	5502	2	42,48,48	1.48	4 (9%)	50,73,73	1.88	16 (32%)
4	NAD	C	3502	2	42,48,48	1.34	4 (9%)	50,73,73	1.26	3 (6%)
4	NAD	G	7502	2	42,48,48	1.44	5 (11%)	50,73,73	1.43	8 (16%)
4	NAD	D	4502	2	42,48,48	1.55	5 (11%)	50,73,73	1.63	10 (20%)
4	NAD	H	8502	2	42,48,48	1.58	3 (7%)	50,73,73	1.95	14 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	F	6502	2	-	6/26/62/62	0/5/5/5
4	NAD	A	1502	2	-	7/26/62/62	0/5/5/5
4	NAD	B	2502	2	-	2/26/62/62	0/5/5/5
4	NAD	E	5502	2	-	4/26/62/62	0/5/5/5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	C	3502	2	-	2/26/62/62	0/5/5/5
4	NAD	G	7502	2	-	7/26/62/62	0/5/5/5
4	NAD	D	4502	2	-	6/26/62/62	0/5/5/5
4	NAD	H	8502	2	-	11/26/62/62	0/5/5/5

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	8502	NAD	C2N-N1N	6.69	1.43	1.35
4	F	6502	NAD	C2N-N1N	6.33	1.42	1.35
4	A	1502	NAD	C2N-N1N	6.19	1.42	1.35
4	E	5502	NAD	C2N-N1N	6.12	1.42	1.35
4	D	4502	NAD	C2N-N1N	6.11	1.42	1.35

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	6502	NAD	C6N-N1N-C2N	-6.13	116.38	121.97
4	A	1502	NAD	C6N-N1N-C2N	-5.81	116.67	121.97
4	H	8502	NAD	C2N-N1N-C1D	5.24	130.81	119.14
4	G	7502	NAD	O4D-C1D-C2D	-4.93	99.72	106.93
4	E	5502	NAD	O5D-C5D-C4D	4.59	124.79	108.99

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1502	NAD	C5D-O5D-PN-O1N
4	A	1502	NAD	C5D-O5D-PN-O2N
4	B	2502	NAD	PN-O3-PA-O5B
4	D	4502	NAD	C5D-O5D-PN-O1N
4	D	4502	NAD	C5D-O5D-PN-O2N

There are no ring outliers.

8 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	6502	NAD	4	0
4	A	1502	NAD	3	0
4	B	2502	NAD	2	0

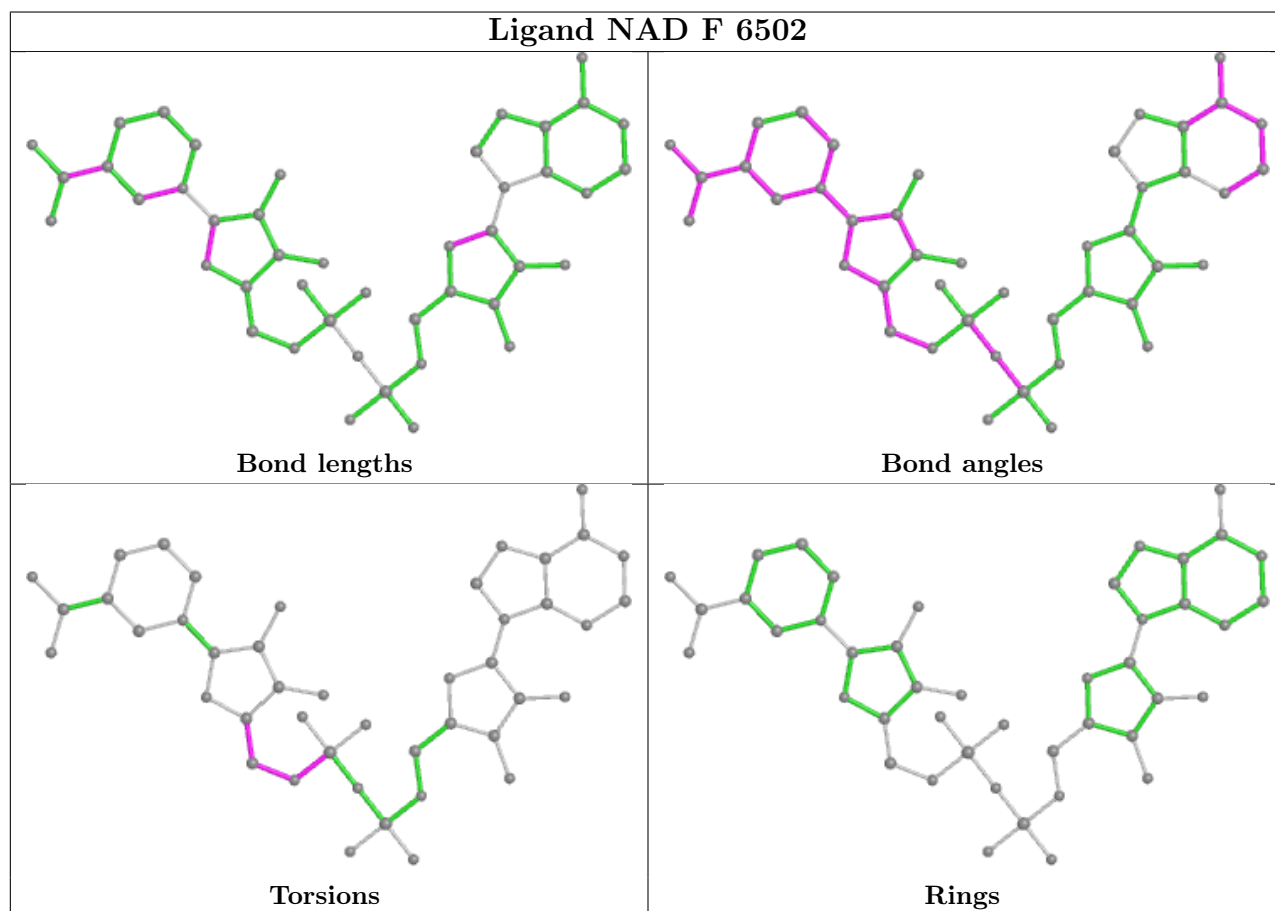
*Continued on next page...*

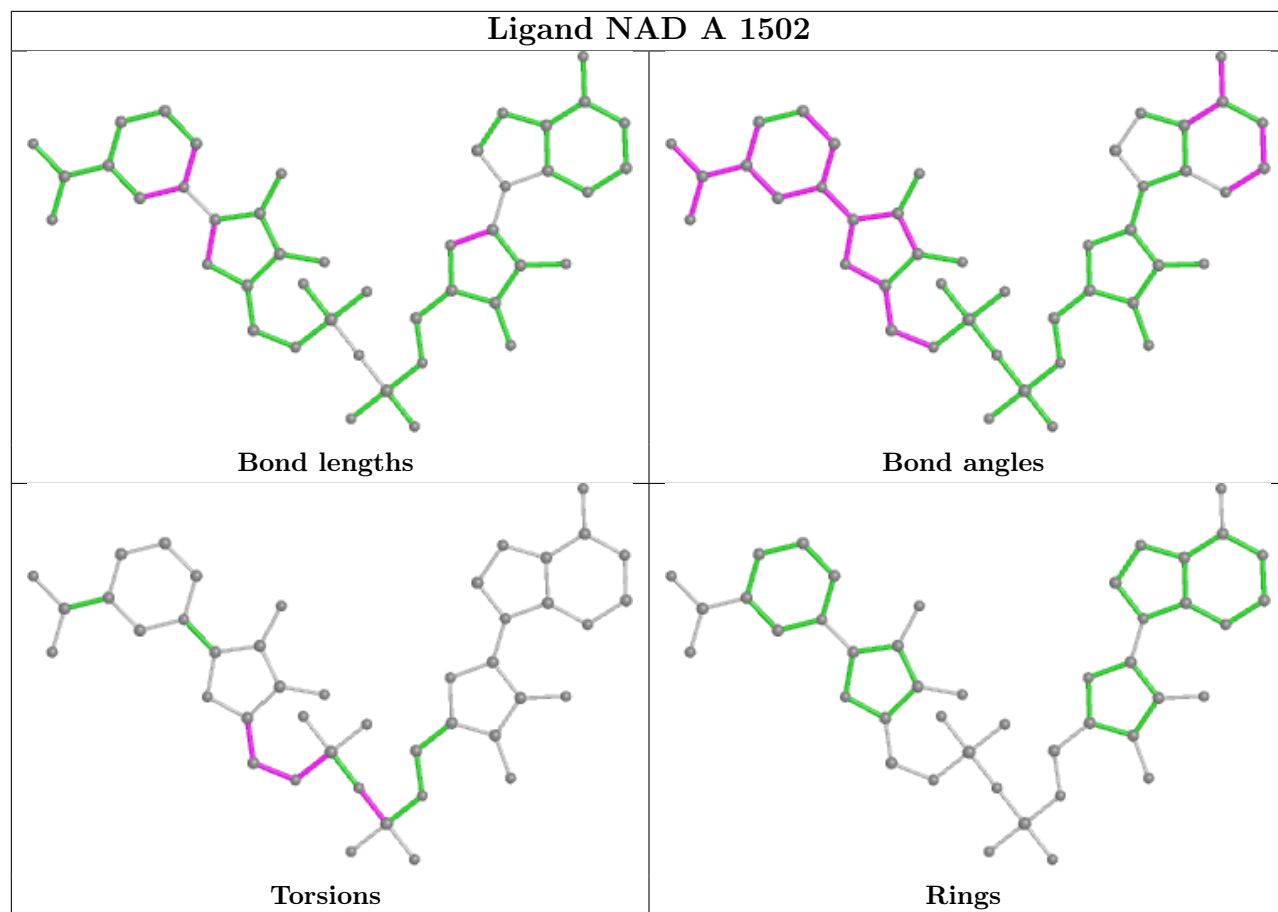


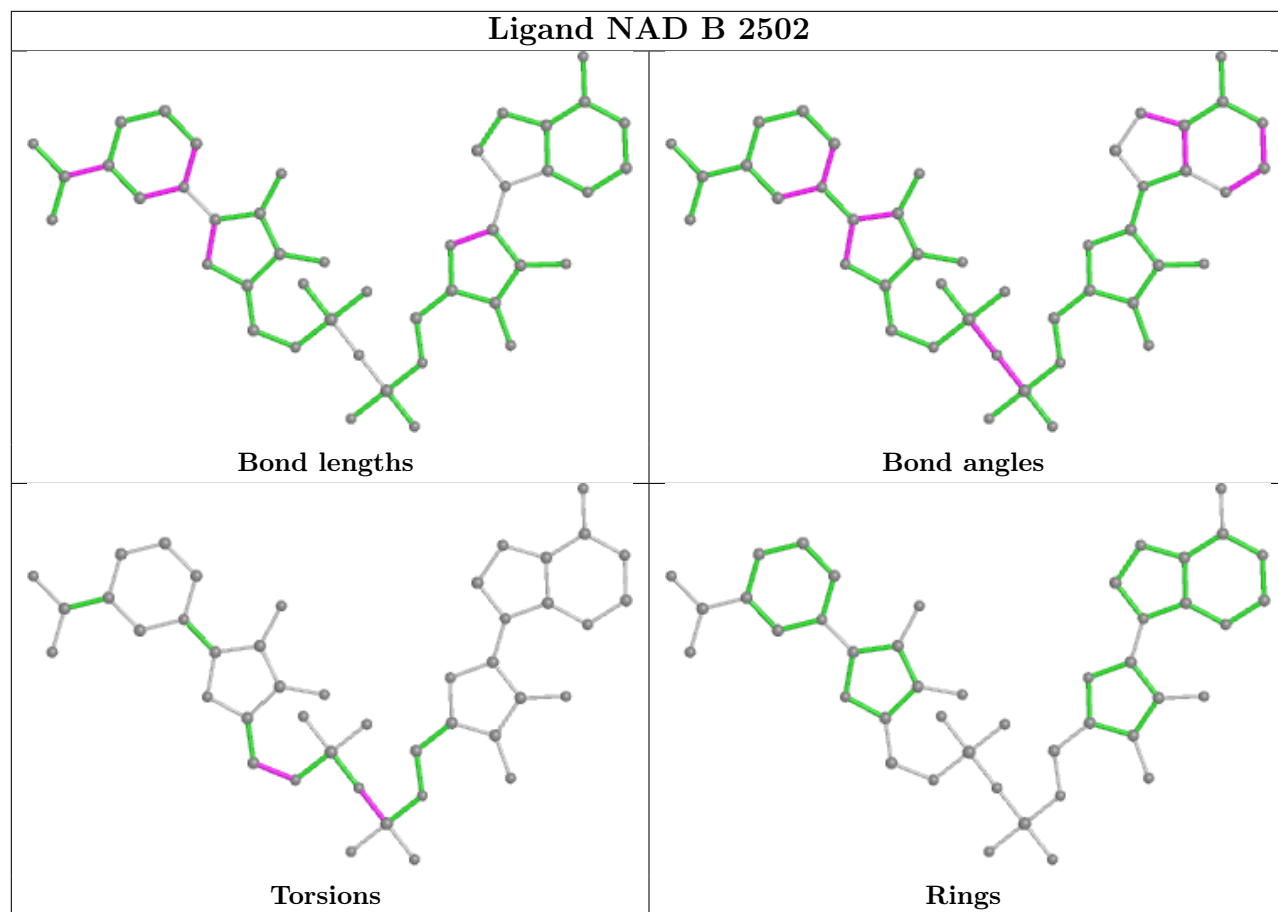
*Continued from previous page...*

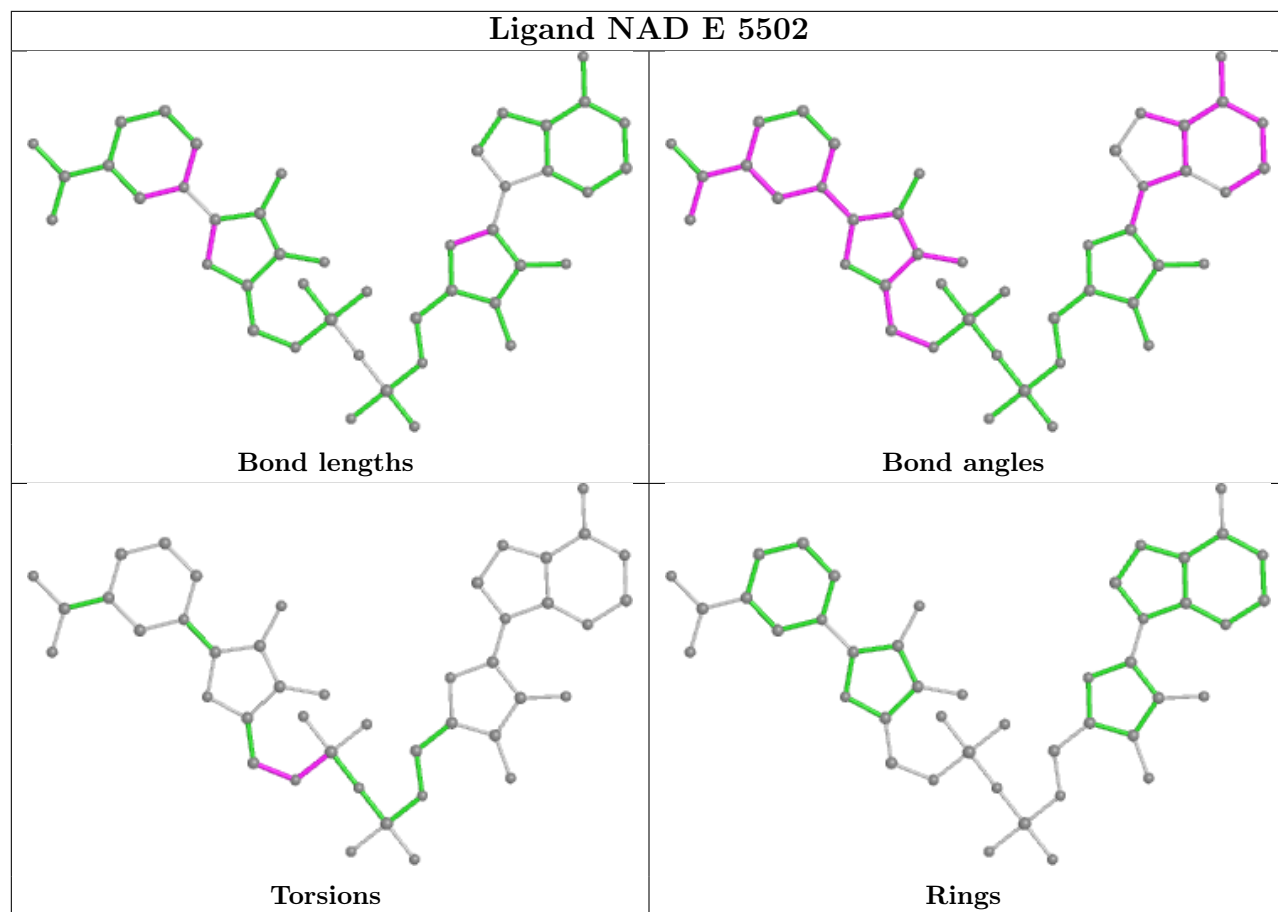
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	5502	NAD	3	0
4	C	3502	NAD	7	0
4	G	7502	NAD	4	0
4	D	4502	NAD	5	0
4	H	8502	NAD	6	0

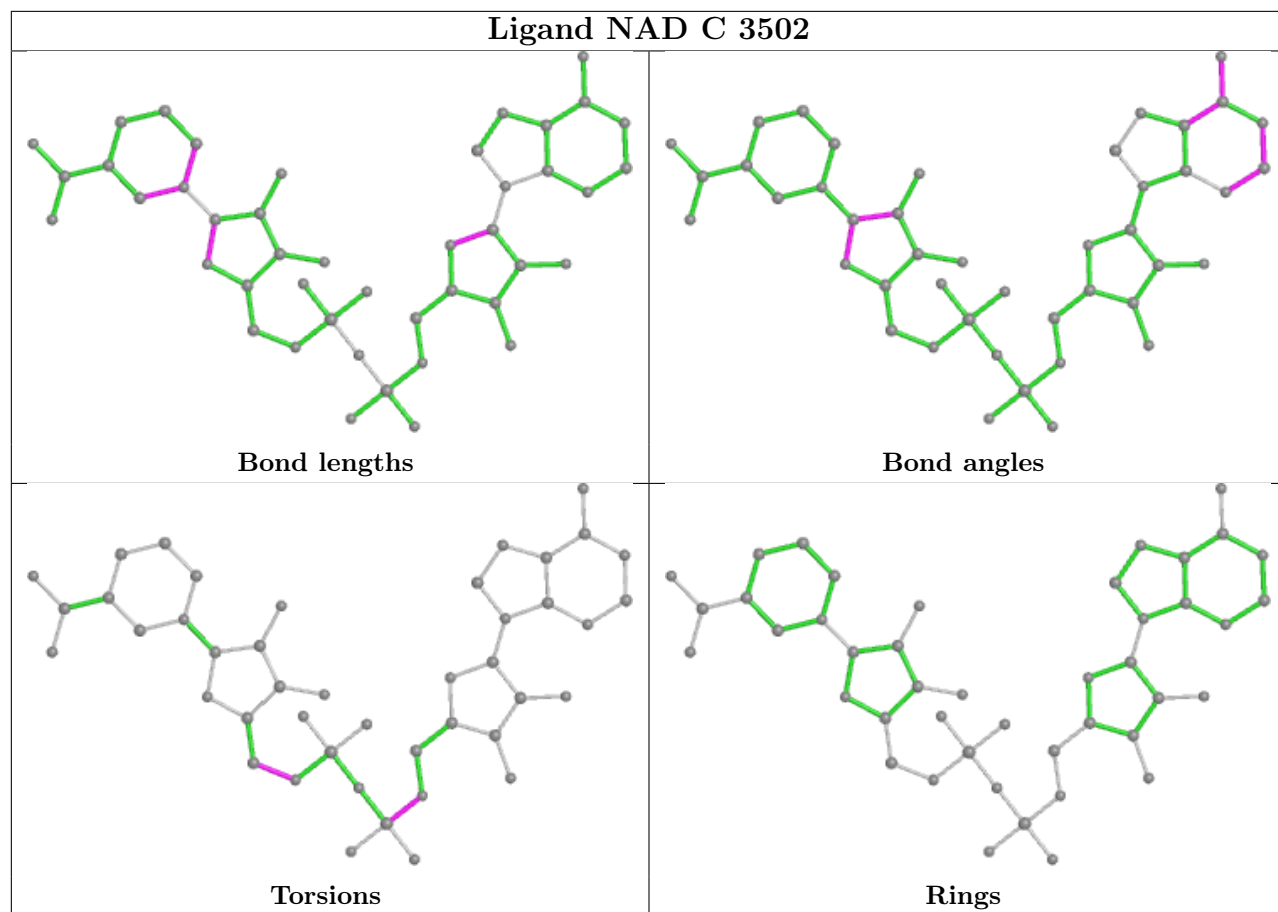
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

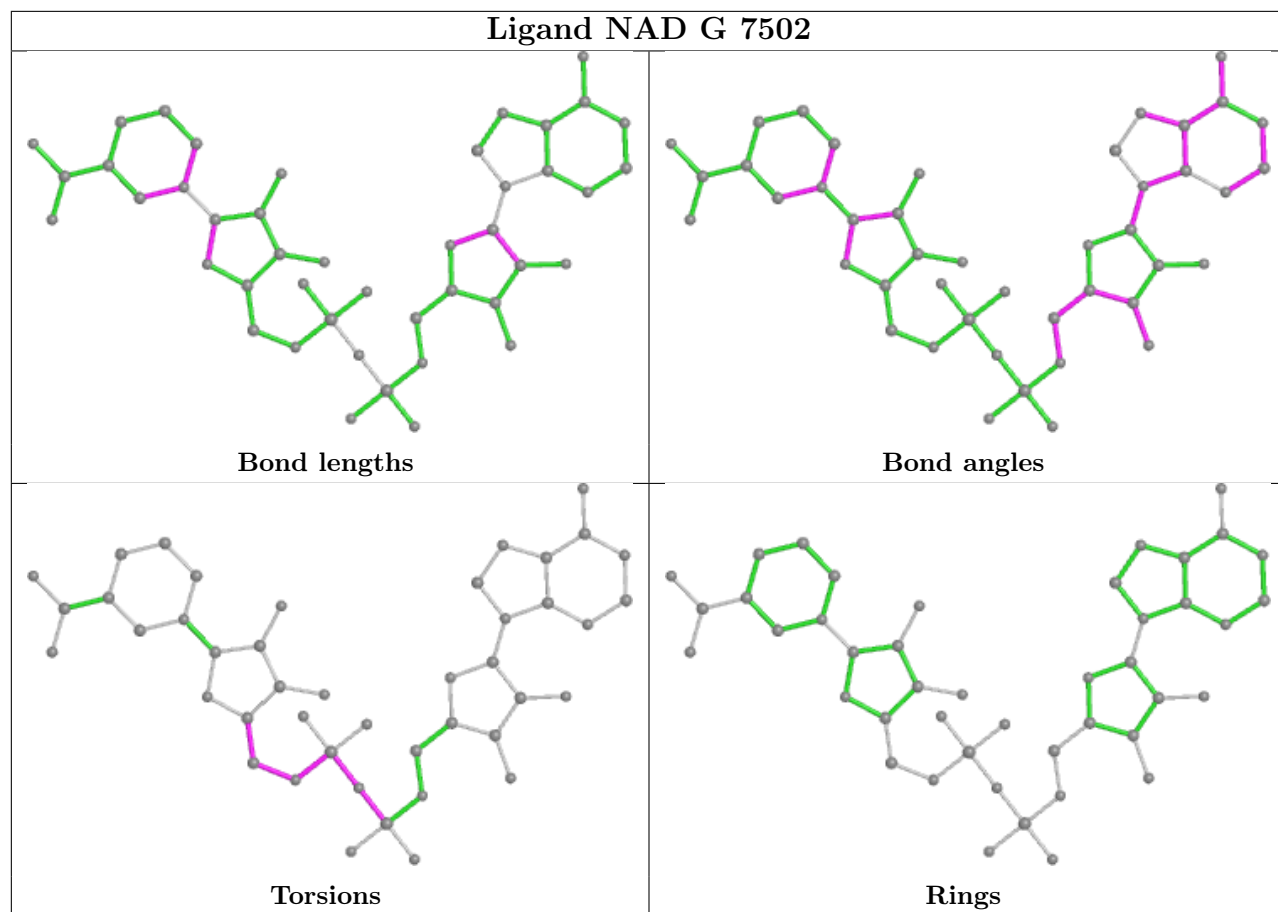


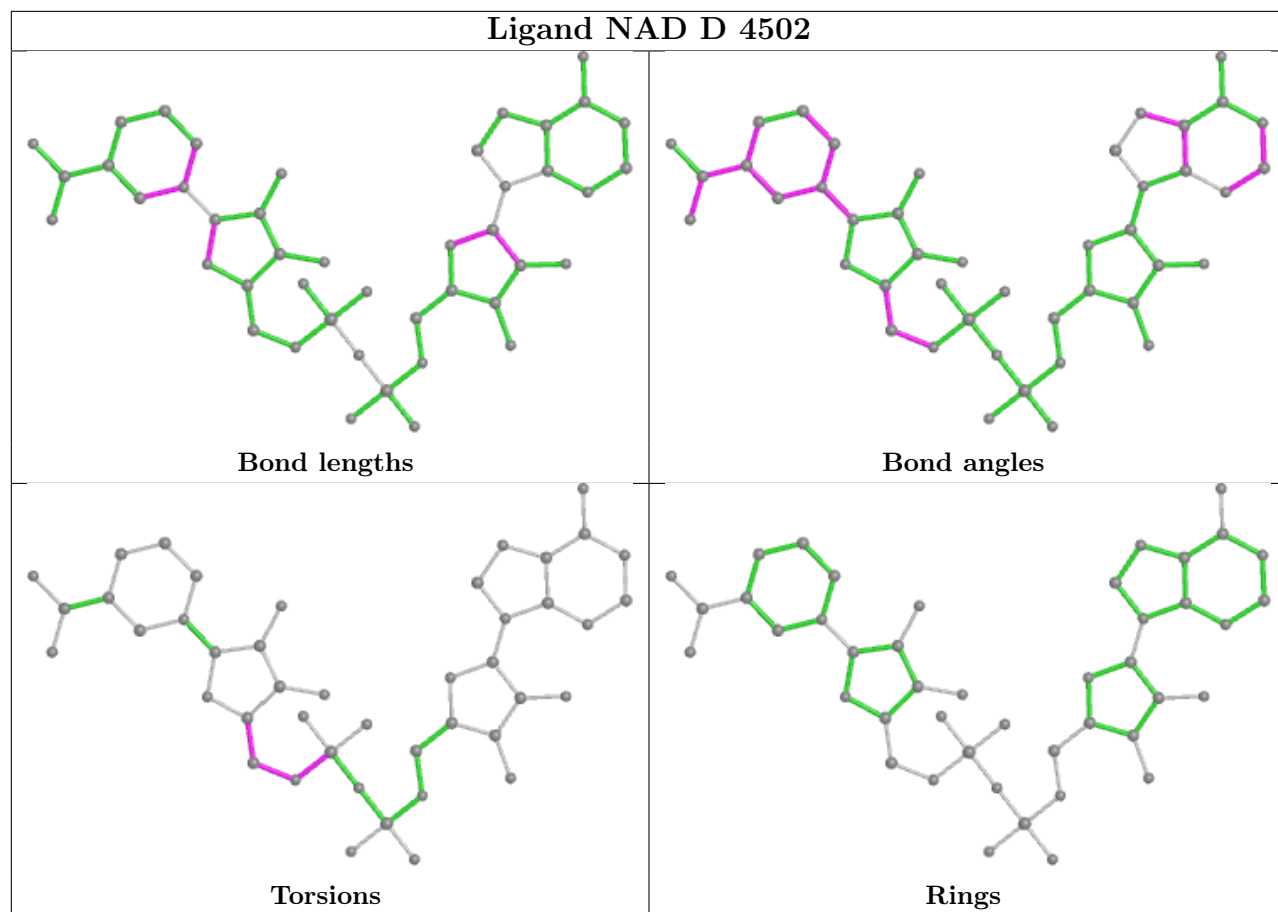


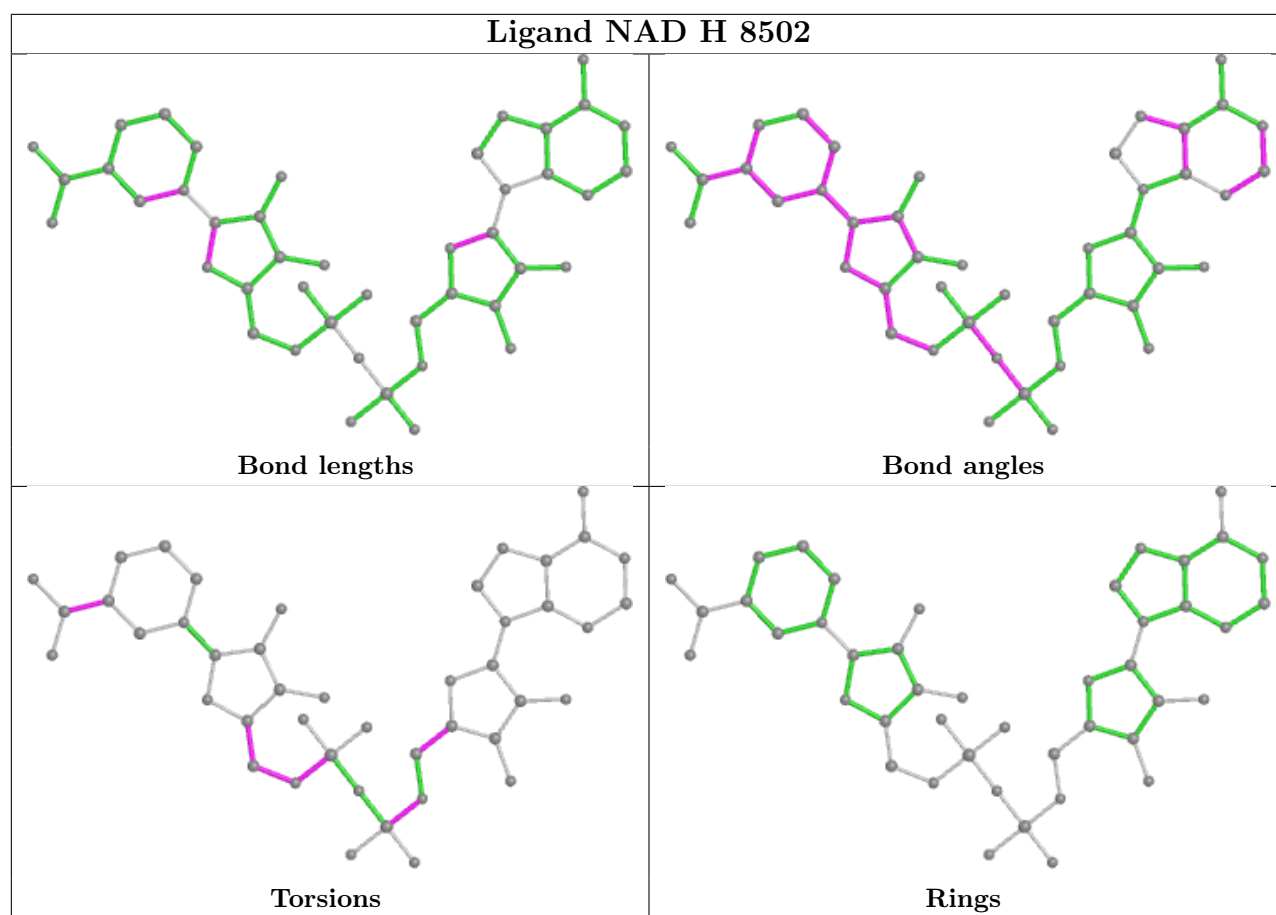












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	494/494 (100%)	-0.60	0 100 100	11, 28, 42, 61	0
1	B	494/494 (100%)	-0.55	0 100 100	8, 30, 48, 70	0
1	C	494/494 (100%)	-0.55	0 100 100	8, 29, 48, 70	0
1	D	494/494 (100%)	-0.64	0 100 100	9, 25, 41, 68	0
1	E	494/494 (100%)	-0.59	1 (0%) 95 95	13, 30, 47, 72	0
1	F	494/494 (100%)	-0.48	2 (0%) 92 92	13, 33, 53, 73	0
1	G	494/494 (100%)	-0.63	0 100 100	11, 29, 45, 59	0
1	H	494/494 (100%)	-0.67	0 100 100	11, 26, 40, 70	0
All	All	3952/3952 (100%)	-0.59	3 (0%) 95 96	8, 29, 47, 73	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	365	ALA	3.2
1	E	7	ALA	3.1
1	F	376	ASP	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

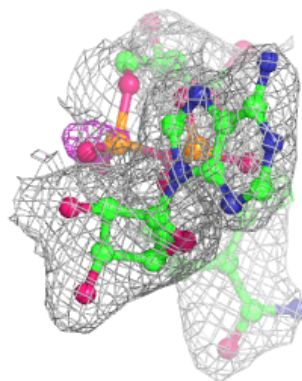
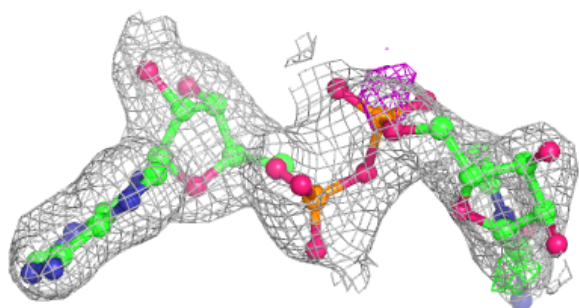
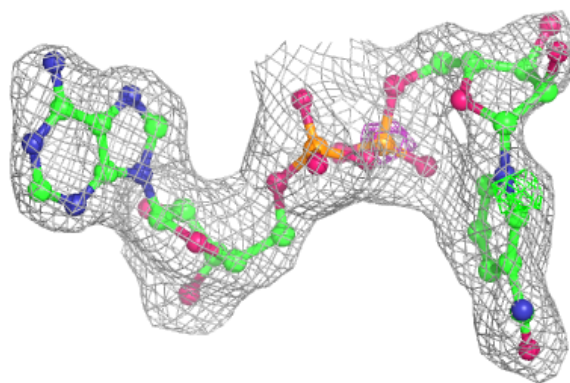
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MN	A	1503	1/1	0.70	0.18	42,42,42,42	1
3	MG	C	3501	1/1	0.72	0.09	37,37,37,37	0
2	MN	F	6503	1/1	0.84	0.14	59,59,59,59	1
3	MG	E	5501	1/1	0.87	0.07	38,38,38,38	0
2	MN	G	7503	1/1	0.92	0.12	36,36,36,36	1
4	NAD	F	6502	44/44	0.92	0.15	23,53,71,74	0
3	MG	G	7501	1/1	0.93	0.08	32,32,32,32	0
4	NAD	E	5502	44/44	0.93	0.14	29,47,71,73	0
2	MN	C	3503	1/1	0.93	0.10	33,33,33,33	1
3	MG	H	8501	1/1	0.94	0.11	31,31,31,31	0
4	NAD	A	1502	44/44	0.94	0.15	25,47,70,74	0
4	NAD	B	2502	44/44	0.94	0.16	20,48,74,75	0
4	NAD	C	3502	44/44	0.94	0.14	17,35,61,65	0
3	MG	F	6501	1/1	0.94	0.07	33,33,33,33	0
2	MN	B	2503	1/1	0.94	0.12	43,43,43,43	1
4	NAD	D	4502	44/44	0.95	0.13	9,28,60,62	0
3	MG	D	4501	1/1	0.95	0.08	24,24,24,24	0
2	MN	D	4503	1/1	0.95	0.17	28,28,28,28	1
4	NAD	G	7502	44/44	0.95	0.13	22,37,61,62	0
4	NAD	H	8502	44/44	0.95	0.14	11,45,69,72	0
2	MN	E	5503	1/1	0.97	0.06	40,40,40,40	1
3	MG	A	1501	1/1	0.97	0.07	27,27,27,27	0
2	MN	H	8503	1/1	0.98	0.03	35,35,35,35	1
3	MG	B	2501	1/1	0.98	0.04	23,23,23,23	0

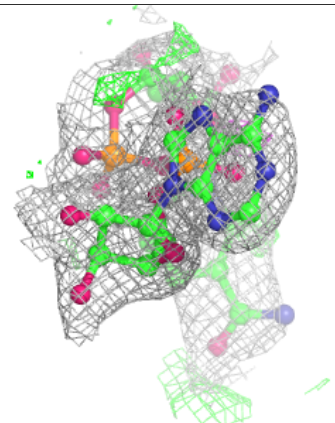
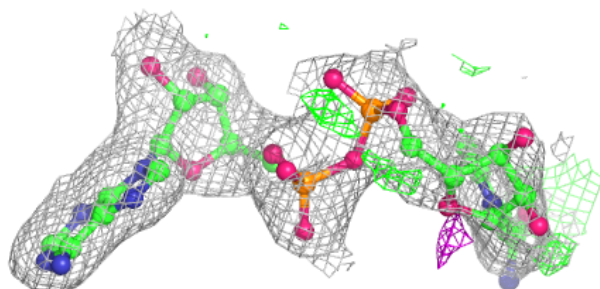
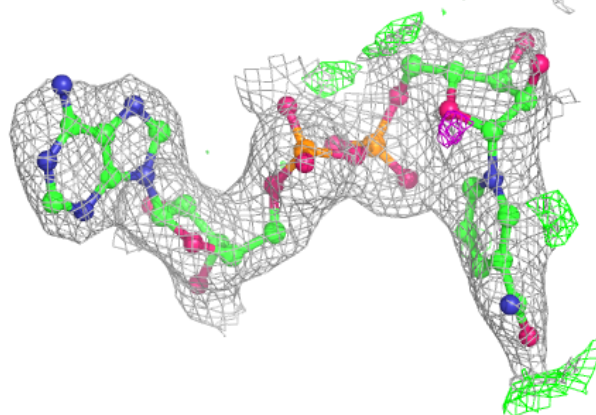
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD F 6502:**

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

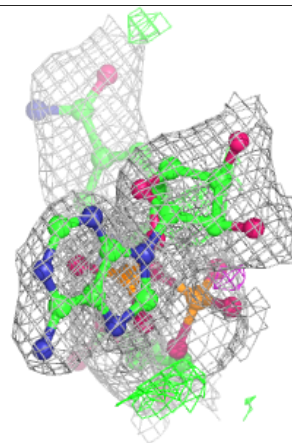
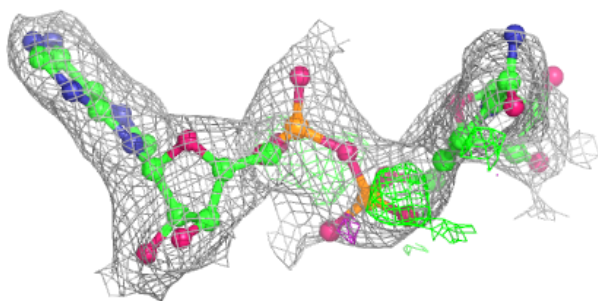
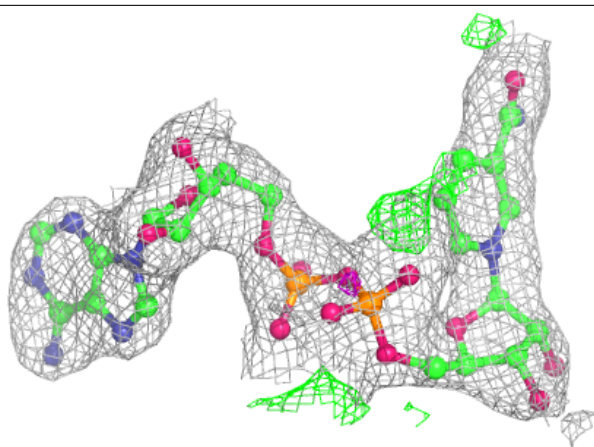
**Electron density around NAD E 5502:**

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

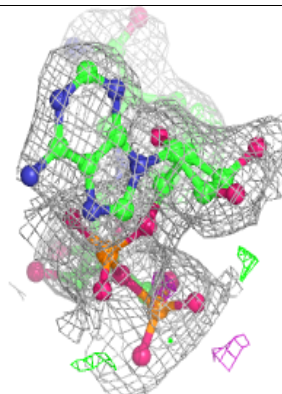
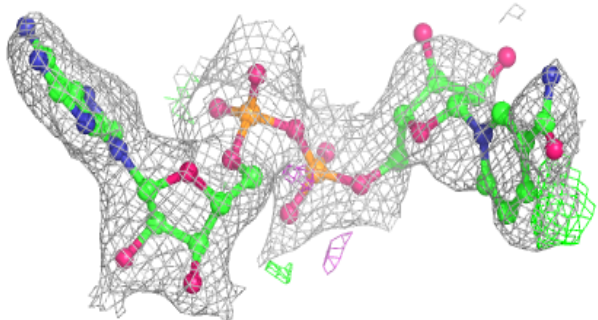
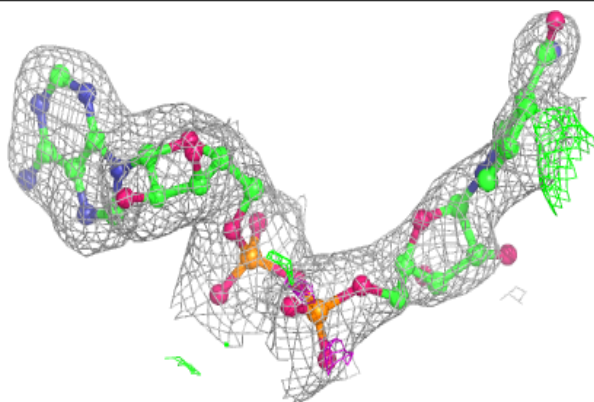


**Electron density around NAD A 1502:**

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

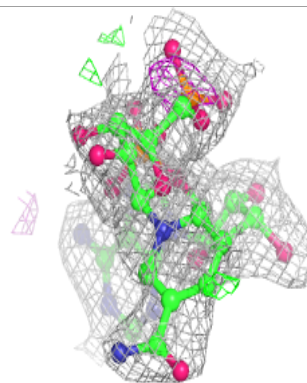
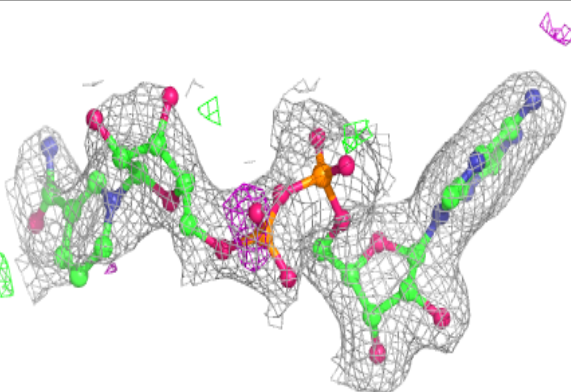
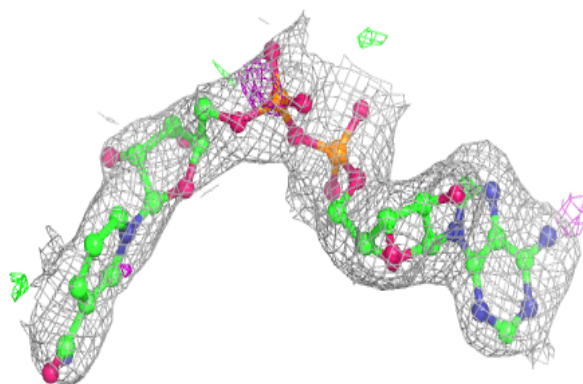
**Electron density around NAD B 2502:**

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



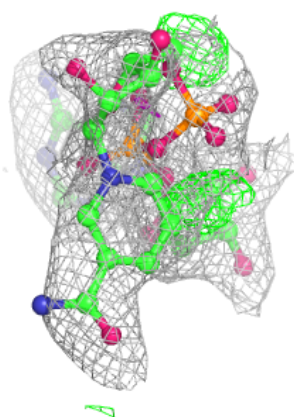
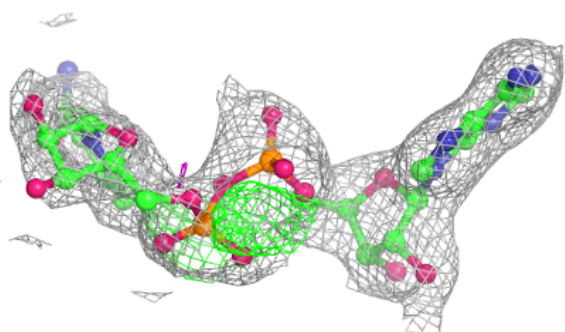
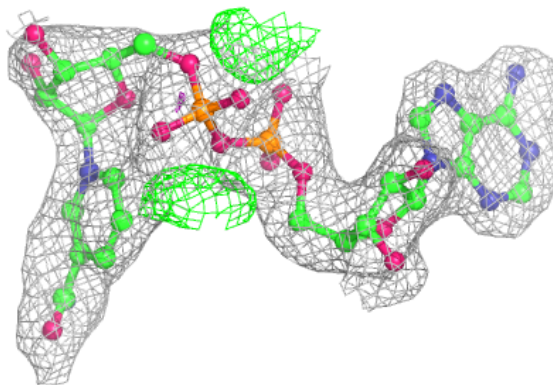
**Electron density around NAD C 3502:**

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



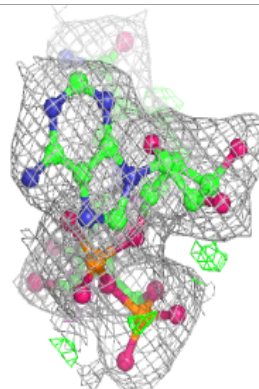
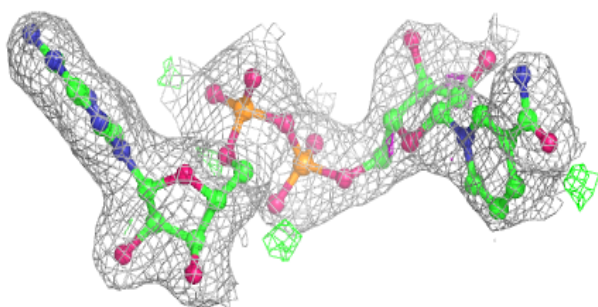
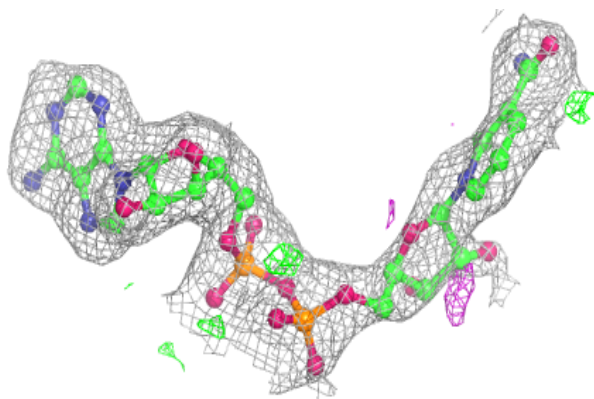
**Electron density around NAD D 4502:**

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

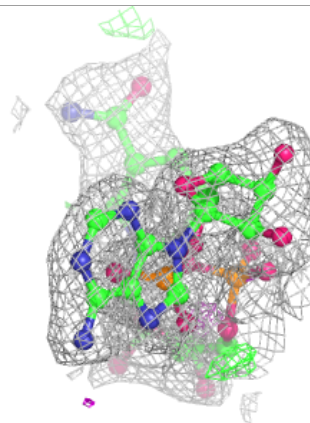
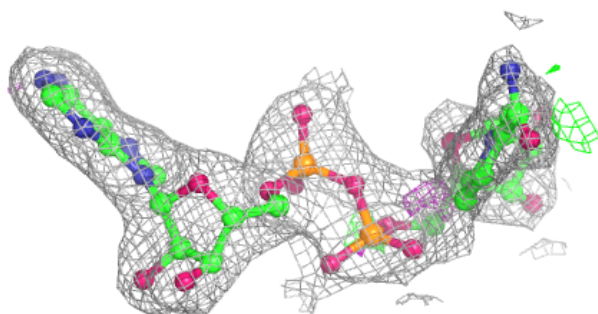
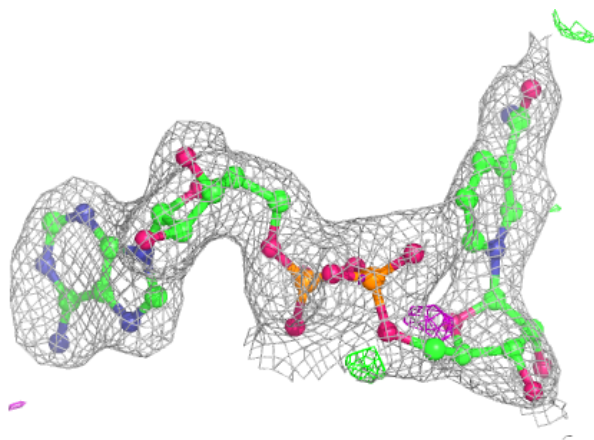


**Electron density around NAD G 7502:**

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

**Electron density around NAD H 8502:**

$2mF_o-DF_c$  (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.