



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 04:14 AM EDT

PDB ID : 9AYI / pdb_00009ayi
Title : Human malic enzyme 2 cofactor complex at 1.89 Angstrom.
Authors : Krinkel, B.A.; Squire, C.J.; Loomes, K.M.
Deposited on : 2024-03-07
Resolution : 1.89 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

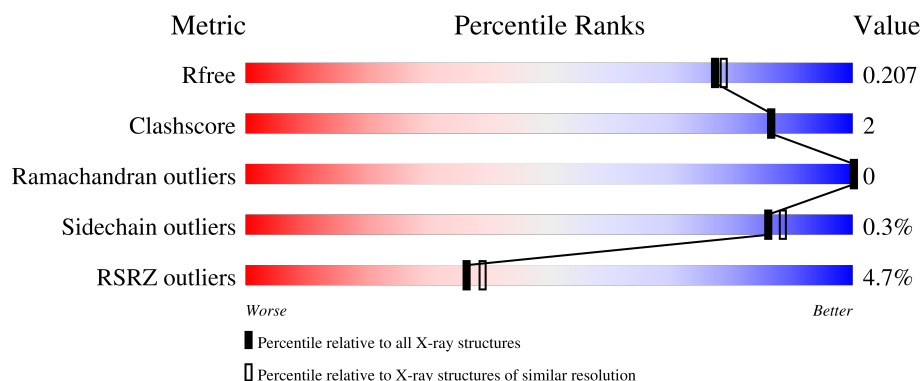
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

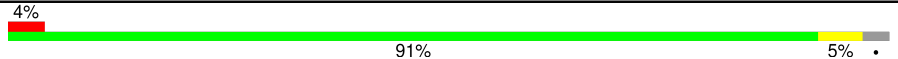
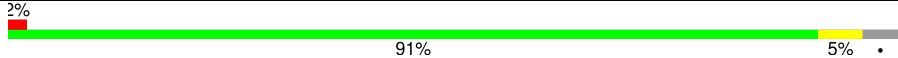
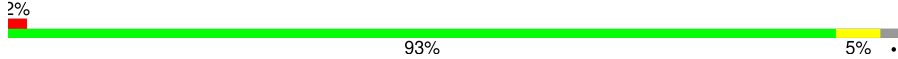
The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	575	
1	B	575	
1	C	575	
1	D	575	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20060 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 NAD-dependent malic enzyme, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	9	0
			4453	2845	759	823	26			
1	B	552	Total	C	N	O	S	0	9	0
			4411	2822	750	815	24			
1	C	558	Total	C	N	O	S	0	8	0
			4451	2846	756	824	25			
1	D	543	Total	C	N	O	S	0	6	0
			4275	2734	732	786	23			

There are 36 discrepancies between the modelled and reference sequences:

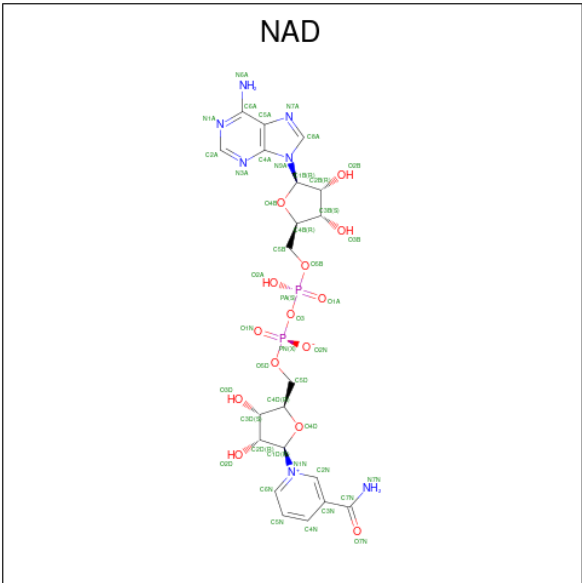
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP P23368
A	585	LEU	-	expression tag	UNP P23368
A	586	GLU	-	expression tag	UNP P23368
A	587	HIS	-	expression tag	UNP P23368
A	588	HIS	-	expression tag	UNP P23368
A	589	HIS	-	expression tag	UNP P23368
A	590	HIS	-	expression tag	UNP P23368
A	591	HIS	-	expression tag	UNP P23368
A	592	HIS	-	expression tag	UNP P23368
B	18	MET	-	initiating methionine	UNP P23368
B	585	LEU	-	expression tag	UNP P23368
B	586	GLU	-	expression tag	UNP P23368
B	587	HIS	-	expression tag	UNP P23368
B	588	HIS	-	expression tag	UNP P23368
B	589	HIS	-	expression tag	UNP P23368
B	590	HIS	-	expression tag	UNP P23368
B	591	HIS	-	expression tag	UNP P23368
B	592	HIS	-	expression tag	UNP P23368
C	18	MET	-	initiating methionine	UNP P23368
C	585	LEU	-	expression tag	UNP P23368
C	586	GLU	-	expression tag	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
C	587	HIS	-	expression tag	UNP P23368
C	588	HIS	-	expression tag	UNP P23368
C	589	HIS	-	expression tag	UNP P23368
C	590	HIS	-	expression tag	UNP P23368
C	591	HIS	-	expression tag	UNP P23368
C	592	HIS	-	expression tag	UNP P23368
D	18	MET	-	initiating methionine	UNP P23368
D	585	LEU	-	expression tag	UNP P23368
D	586	GLU	-	expression tag	UNP P23368
D	587	HIS	-	expression tag	UNP P23368
D	588	HIS	-	expression tag	UNP P23368
D	589	HIS	-	expression tag	UNP P23368
D	590	HIS	-	expression tag	UNP P23368
D	591	HIS	-	expression tag	UNP P23368
D	592	HIS	-	expression tag	UNP P23368

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



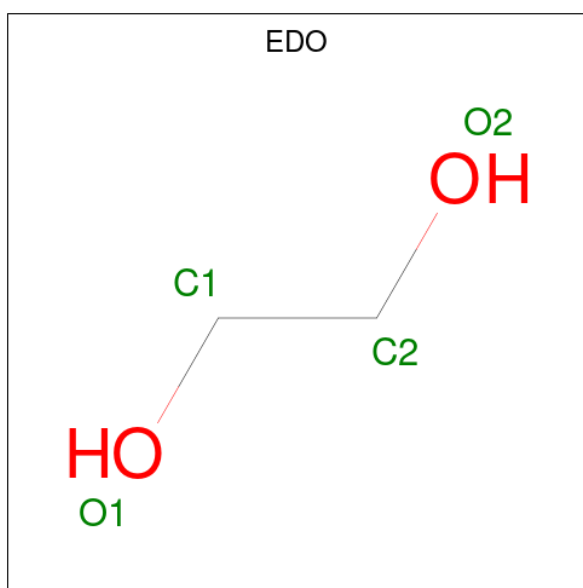
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	1
			88	42	14	28	4		

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	1
			8	4	4		

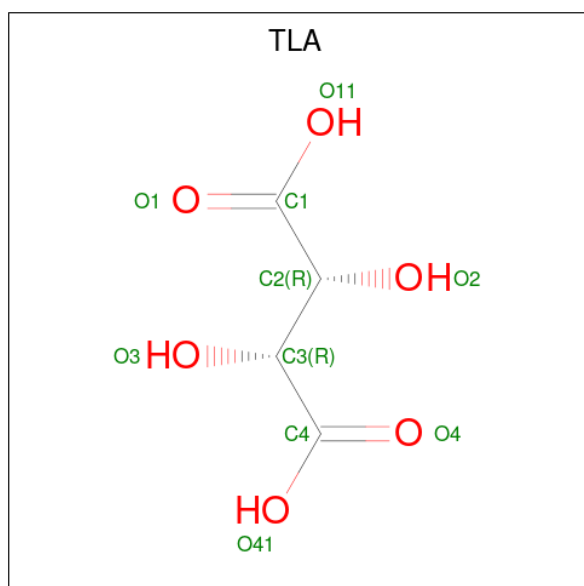
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



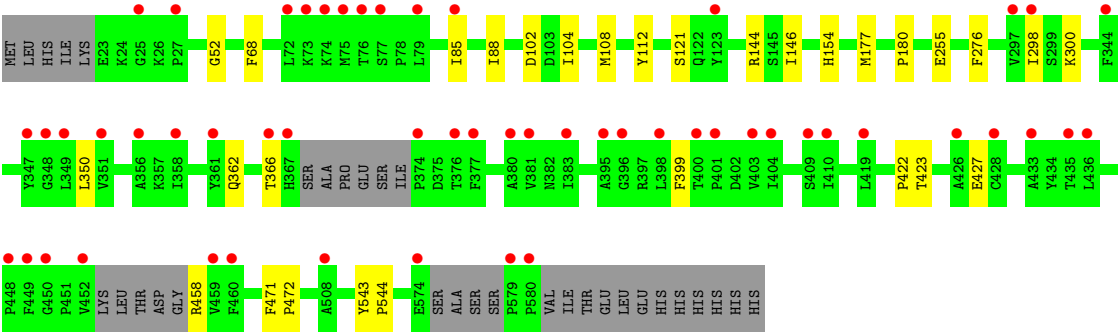
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 4 6	0	0
6	B	1	Total C O 10 4 6	0	0
6	C	1	Total C O 10 4 6	0	0
6	D	1	Total C O 10 4 6	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	544	Total 544	O 544	0	0
7	B	515	Total 515	O 515	0	0
7	C	496	Total 496	O 496	0	0
7	D	405	Total 405	O 405	0	0

- Molecule 1: NAD-dependent malic enzyme, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.33Å 98.17Å 107.74Å 65.32° 70.75° 74.89°	Depositor
Resolution (Å)	47.42 – 1.89 47.42 – 1.89	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.42-1.89) 97.1 (47.42-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.177 , 0.201 0.185 , 0.207	Depositor DCC
R_{free} test set	10256 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20060	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: TLA, CSX, MG, NAD, EDO, 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	0.47	0/4543	0.85	1/6153 (0.0%)
1	B	0.46	0/4503	0.86	2/6097 (0.0%)
1	C	0.46	0/4547	0.85	0/6156
1	D	0.46	0/4367	0.86	2/5915 (0.0%)
All	All	0.47	0/17960	0.85	5/24321 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	471	PHE	CA-CB-CG	5.35	119.15	113.80
1	D	276	PHE	CA-CB-CG	5.17	118.97	113.80
1	D	102	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	102	ASP	CA-CB-CG	5.03	117.63	112.60

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	4453	0	4456	25	0
1	B	4411	0	4431	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4451	0	4471	21	0
1	D	4275	0	4259	18	0
2	A	132	0	78	2	0
2	B	132	0	78	2	0
2	C	88	0	52	4	0
2	D	88	0	52	1	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
3	C	4	0	6	1	0
3	D	8	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	10	0	4	0	0
6	B	10	0	4	1	0
6	C	10	0	4	1	0
6	D	10	0	4	2	0
7	A	544	0	0	0	0
7	B	515	0	0	1	0
7	C	496	0	0	2	0
7	D	405	0	0	0	0
All	All	20060	0	17929	74	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 2.

The worst 5 of 74 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:A:542:ARG:HH22	6:D:601:TLA:H2	1.43	0.82
6:B:603:TLA:H3	1:C:542:ARG:HH22	1.53	0.72
1:B:542:ARG:HH22	6:C:601:TLA:H3	1.56	0.70
2:A:601[B]:NAD:H4N	1:D:154:HIS:HD1	1.56	0.69
1:A:74:LYS:NZ	1:B:122:GLN:O	2.32	0.63

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	564/575 (98%)	552 (98%)	12 (2%)	0	100	100
1	B	558/575 (97%)	549 (98%)	9 (2%)	0	100	100
1	C	564/575 (98%)	554 (98%)	10 (2%)	0	100	100
1	D	540/575 (94%)	531 (98%)	9 (2%)	0	100	100
All	All	2226/2300 (97%)	2186 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	474/489 (97%)	473 (100%)	1 (0%)	87	90
1	B	471/489 (96%)	470 (100%)	1 (0%)	87	90
1	C	477/489 (98%)	476 (100%)	1 (0%)	87	90
1	D	451/489 (92%)	449 (100%)	2 (0%)	84	87
All	All	1873/1956 (96%)	1868 (100%)	5 (0%)	86	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
1	B	357	LYS

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Mol	Chain	Res	Type
1	C	114	PRO
1	D	121	SER
1	D	458	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	223	GLN
1	C	330	ASN
1	D	43	GLN
1	C	425	GLN
1	B	425	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSX	C	120	1	3,6,7	0.65	0	1,6,8	0.08	0
1	CSX	B	120	1	3,6,7	0.65	0	1,6,8	0.63	0
1	CSX	A	120	1	3,6,7	0.70	0	1,6,8	0.42	0
1	CSX	D	120	1	3,6,7	0.64	0	1,6,8	0.13	0

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
1	CSX	C	120	1	-	0/2/5/7	-
1	CSX	B	120	1	-	0/2/5/7	-
1	CSX	A	120	1	-	0/2/5/7	-
1	CSX	D	120	1	-	0/2/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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	EDO	C	602	-	3,3,3	0.08	0	2,2,2	0.14	0
3	EDO	A	603	-	3,3,3	0.12	0	2,2,2	0.18	0
3	EDO	A	602	-	3,3,3	0.11	0	2,2,2	0.21	0
3	EDO	D	604[A]	-	3,3,3	0.13	0	2,2,2	0.12	0
2	NAD	B	602[A]	-	46,48,48	0.50	0	64,73,73	0.52	0
2	NAD	A	601[B]	-	46,48,48	0.49	0	64,73,73	0.58	0
2	NAD	C	604	-	46,48,48	0.52	0	64,73,73	0.61	0
6	TLA	C	601	-	9,9,9	1.02	0	12,12,12	0.93	0
3	EDO	B	604	-	3,3,3	0.09	0	2,2,2	0.22	0
2	NAD	D	605	-	46,48,48	0.49	0	64,73,73	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	A	605	-	46,48,48	0.48	0	64,73,73	0.65	1 (1%)
2	NAD	D	603	-	46,48,48	0.45	0	64,73,73	0.53	0
2	NAD	C	605	-	46,48,48	0.45	0	64,73,73	0.60	0
6	TLA	A	607	-	9,9,9	1.08	0	12,12,12	0.93	0
2	NAD	A	601[A]	-	46,48,48	0.49	0	64,73,73	0.53	0
3	EDO	D	604[B]	-	3,3,3	0.09	0	2,2,2	0.09	0
2	NAD	B	602[B]	-	46,48,48	0.52	0	64,73,73	0.54	0
6	TLA	D	601	-	9,9,9	1.04	0	12,12,12	0.94	0
2	NAD	B	605	-	46,48,48	0.51	0	64,73,73	0.53	0
6	TLA	B	603	-	9,9,9	1.05	0	12,12,12	0.97	0

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	EDO	C	602	-	-	0/1/1/1	-
3	EDO	A	603	-	-	1/1/1/1	-
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	D	604[A]	-	-	1/1/1/1	-
2	NAD	B	602[A]	-	-	6/30/62/62	0/5/5/5
2	NAD	A	601[B]	-	-	7/30/62/62	0/5/5/5
2	NAD	C	604	-	-	4/30/62/62	0/5/5/5
6	TLA	C	601	-	-	8/12/12/12	-
3	EDO	B	604	-	-	1/1/1/1	-
2	NAD	D	605	-	-	7/30/62/62	0/5/5/5
2	NAD	A	605	-	-	4/30/62/62	0/5/5/5
2	NAD	D	603	-	-	5/30/62/62	0/5/5/5
2	NAD	C	605	-	-	3/30/62/62	0/5/5/5
6	TLA	A	607	-	-	8/12/12/12	-
2	NAD	A	601[A]	-	-	9/30/62/62	0/5/5/5
3	EDO	D	604[B]	-	-	1/1/1/1	-
2	NAD	B	602[B]	-	-	4/30/62/62	0/5/5/5
6	TLA	D	601	-	-	4/12/12/12	-
2	NAD	B	605	-	-	6/30/62/62	0/5/5/5
6	TLA	B	603	-	-	6/12/12/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	605	NAD	C4D-O4D-C1D	-2.65	107.50	109.92

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601[A]	NAD	C5B-O5B-PA-O2A
2	A	601[A]	NAD	C5B-O5B-PA-O3
2	A	601[A]	NAD	C2D-C1D-N1N-C6N
2	A	601[B]	NAD	C5B-O5B-PA-O1A
2	A	601[B]	NAD	C5B-O5B-PA-O2A

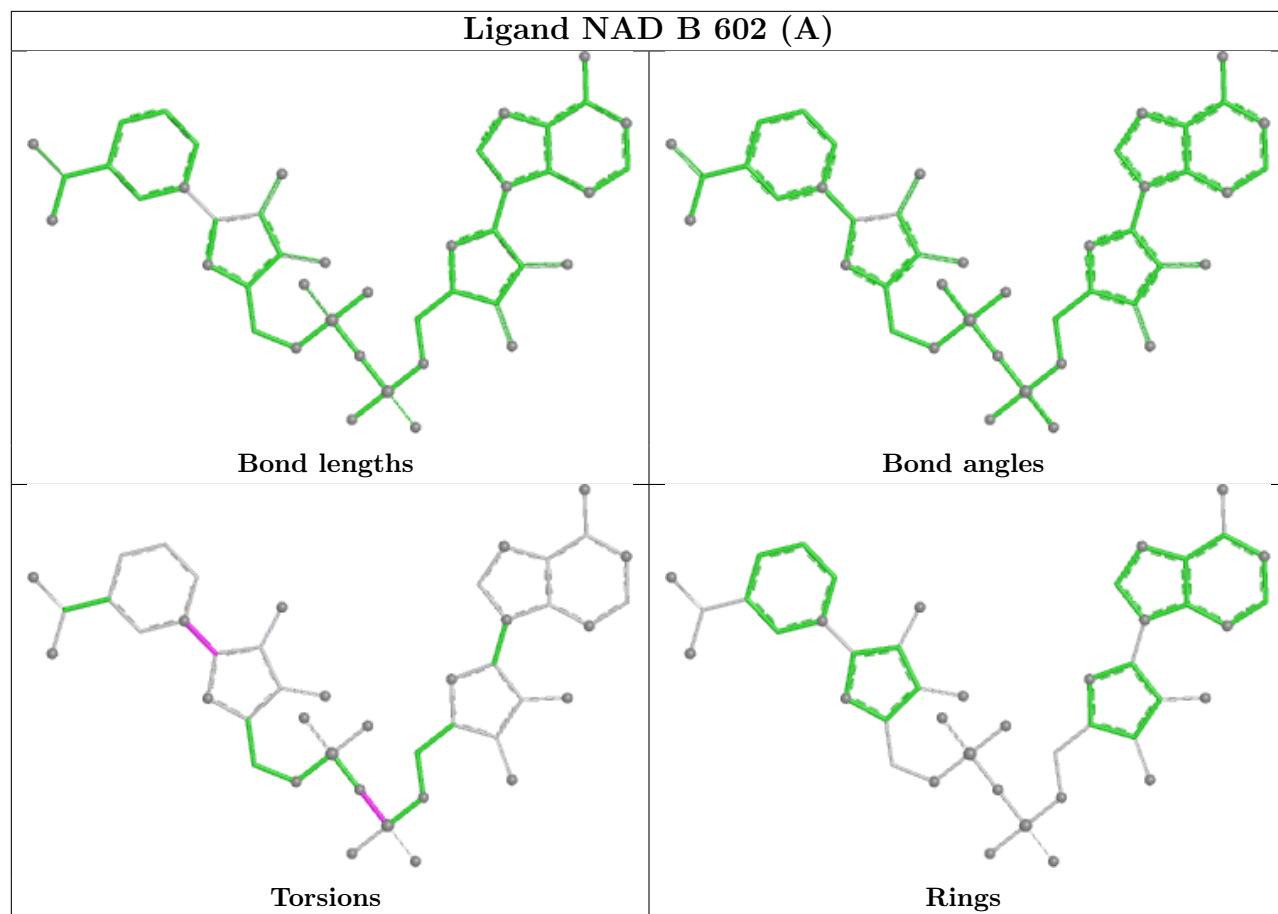
There are no ring outliers.

10 monomers are involved in 14 short contacts:

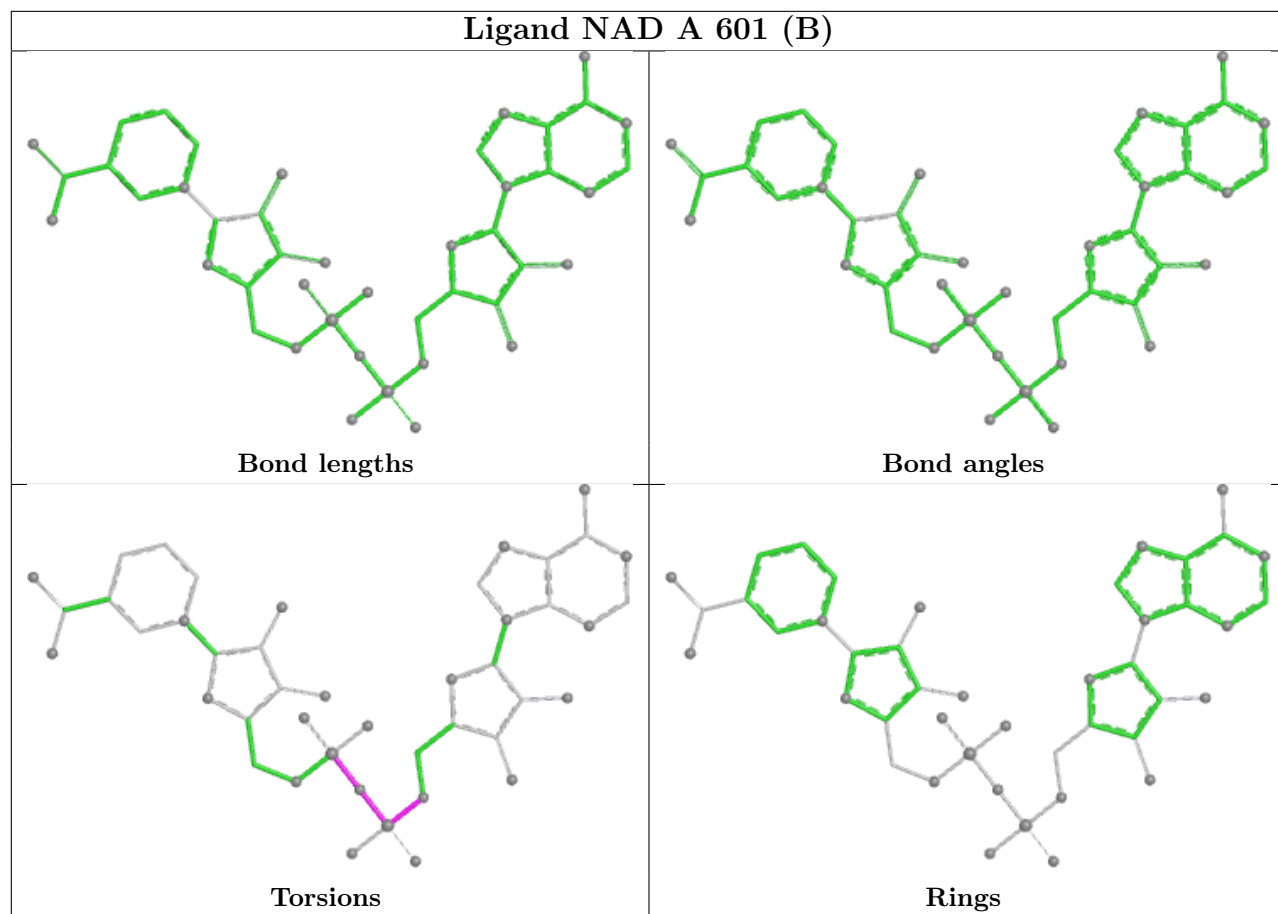
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	EDO	1	0
2	A	601[B]	NAD	1	0
2	C	604	NAD	3	0
6	C	601	TLA	1	0
2	D	605	NAD	1	0
2	C	605	NAD	1	0
2	A	601[A]	NAD	1	0
6	D	601	TLA	2	0
2	B	605	NAD	2	0
6	B	603	TLA	1	0

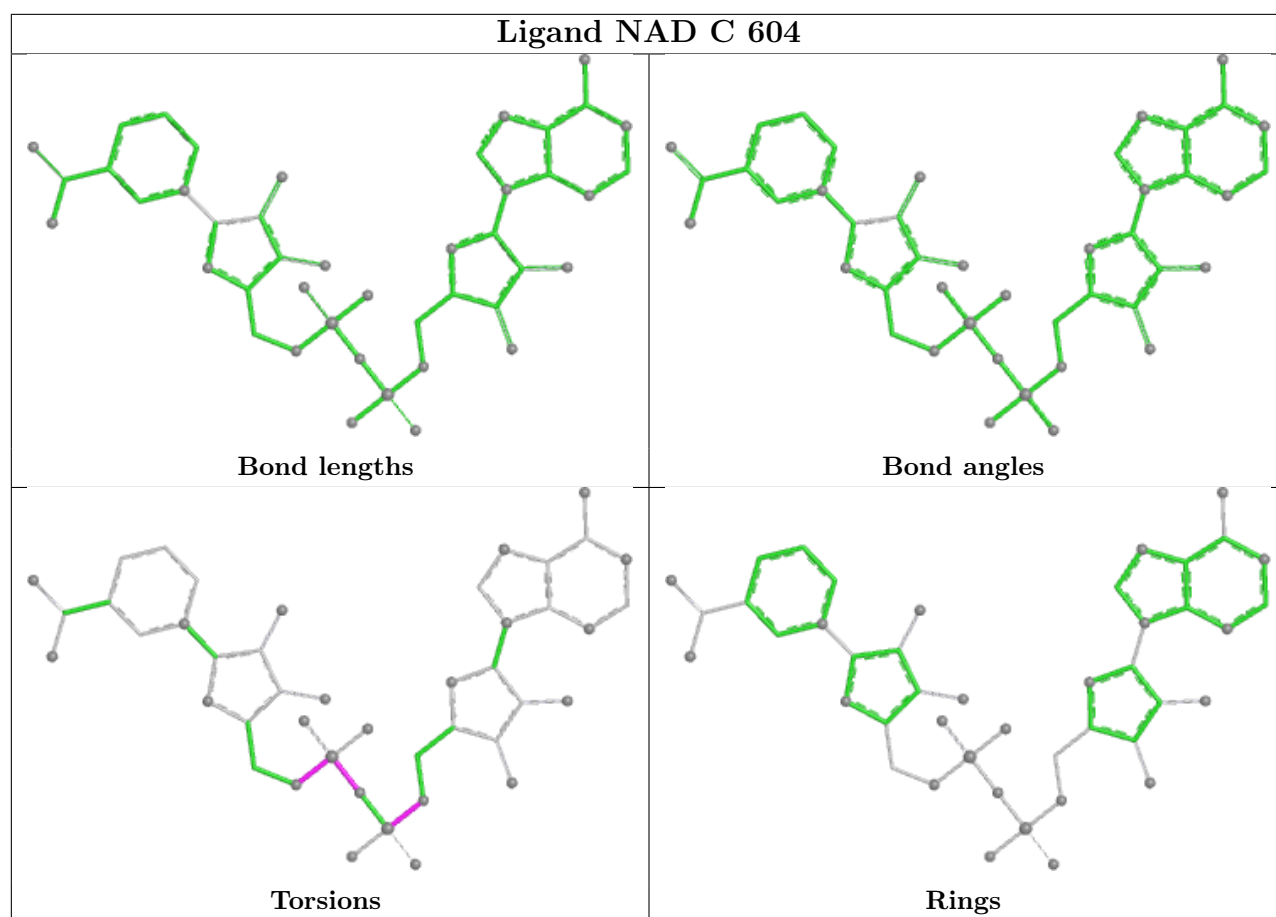
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

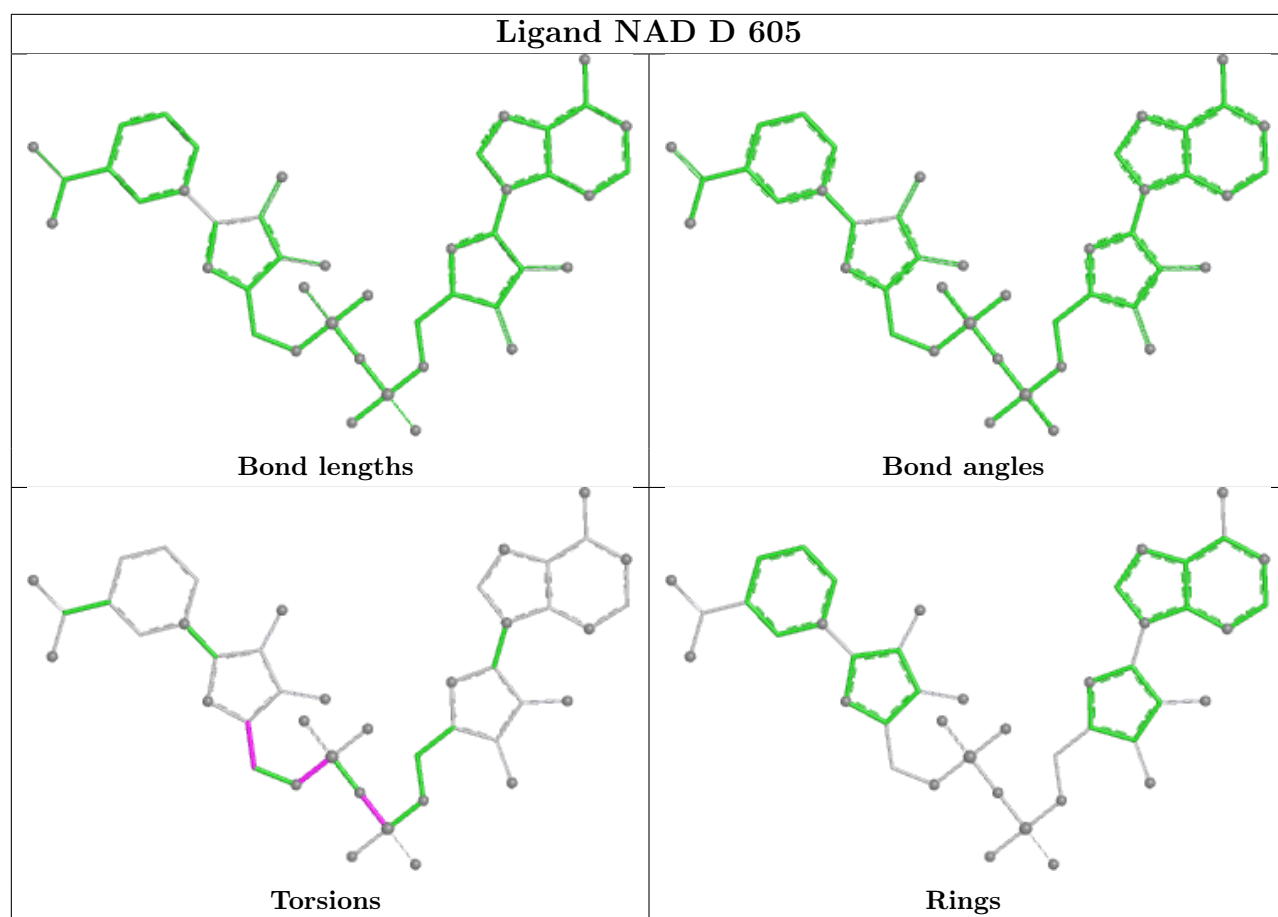
Ligand NAD B 602 (A)

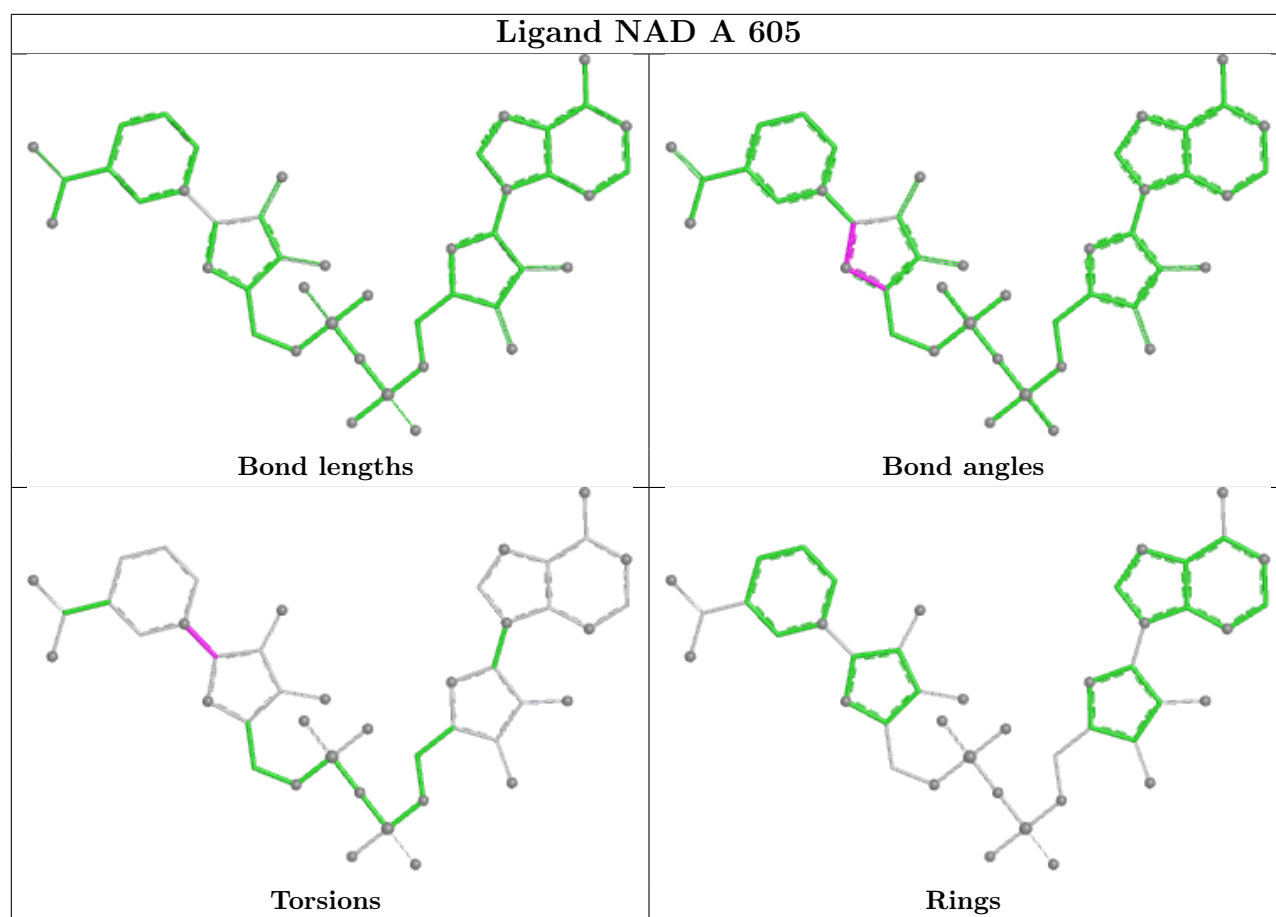


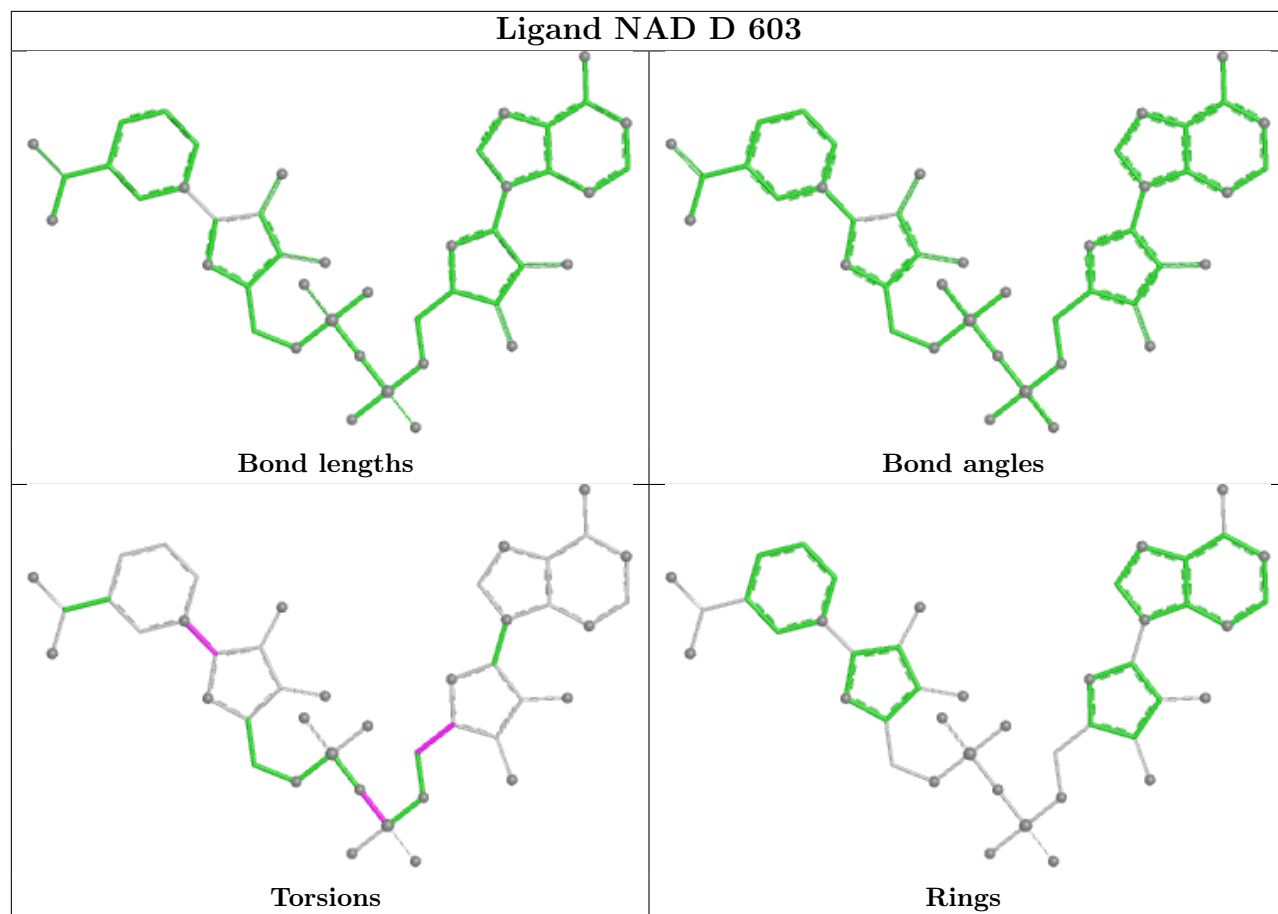
Ligand NAD A 601 (B)

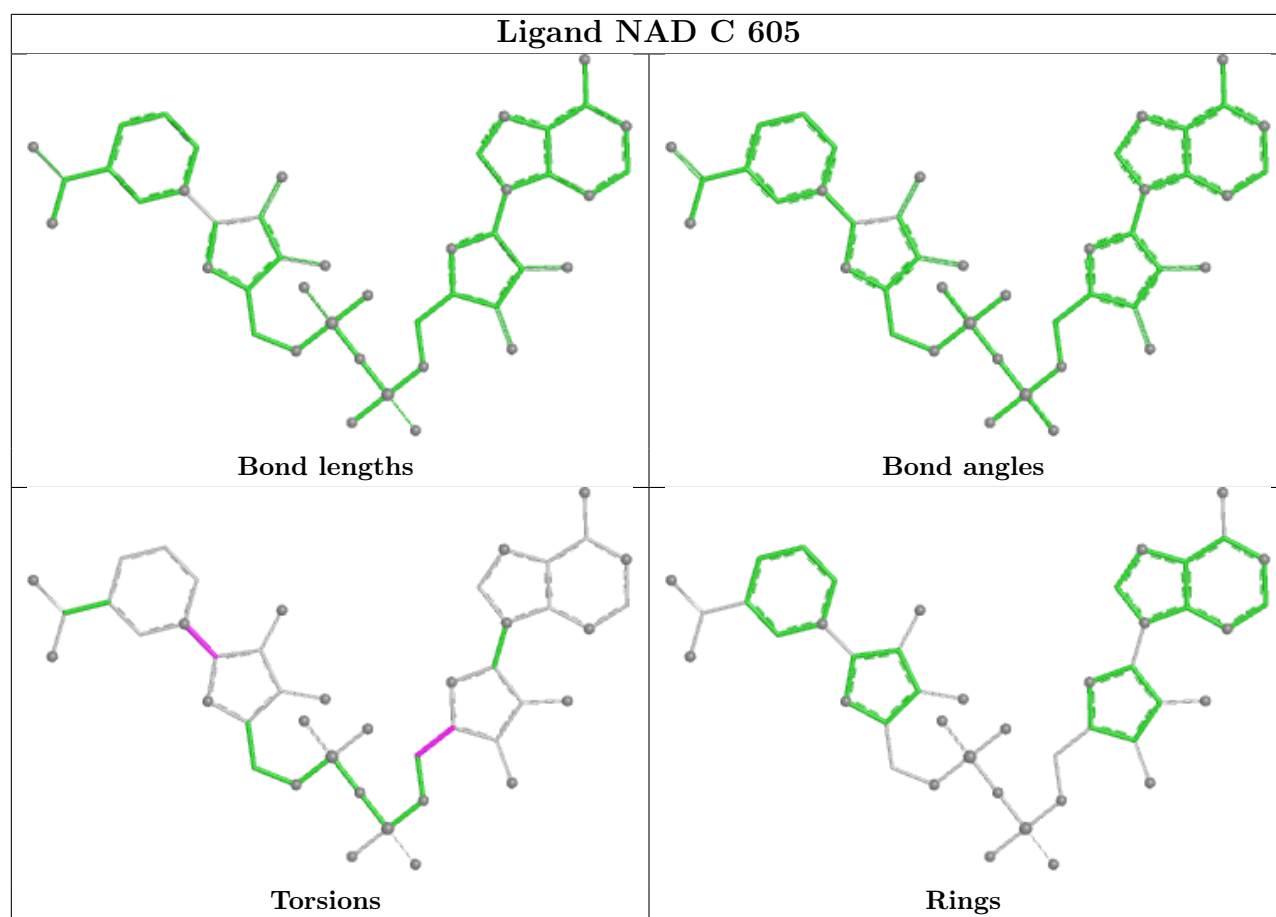


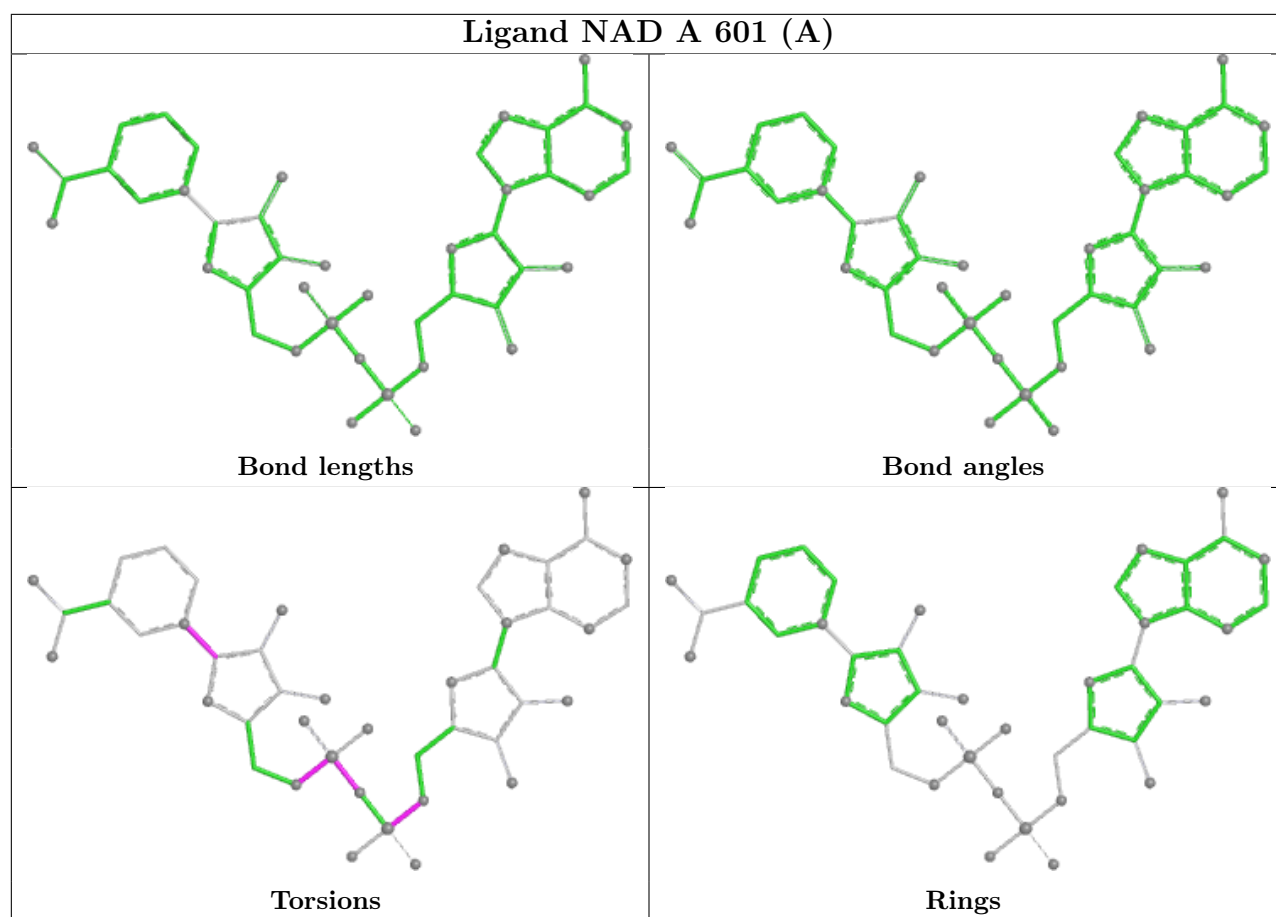




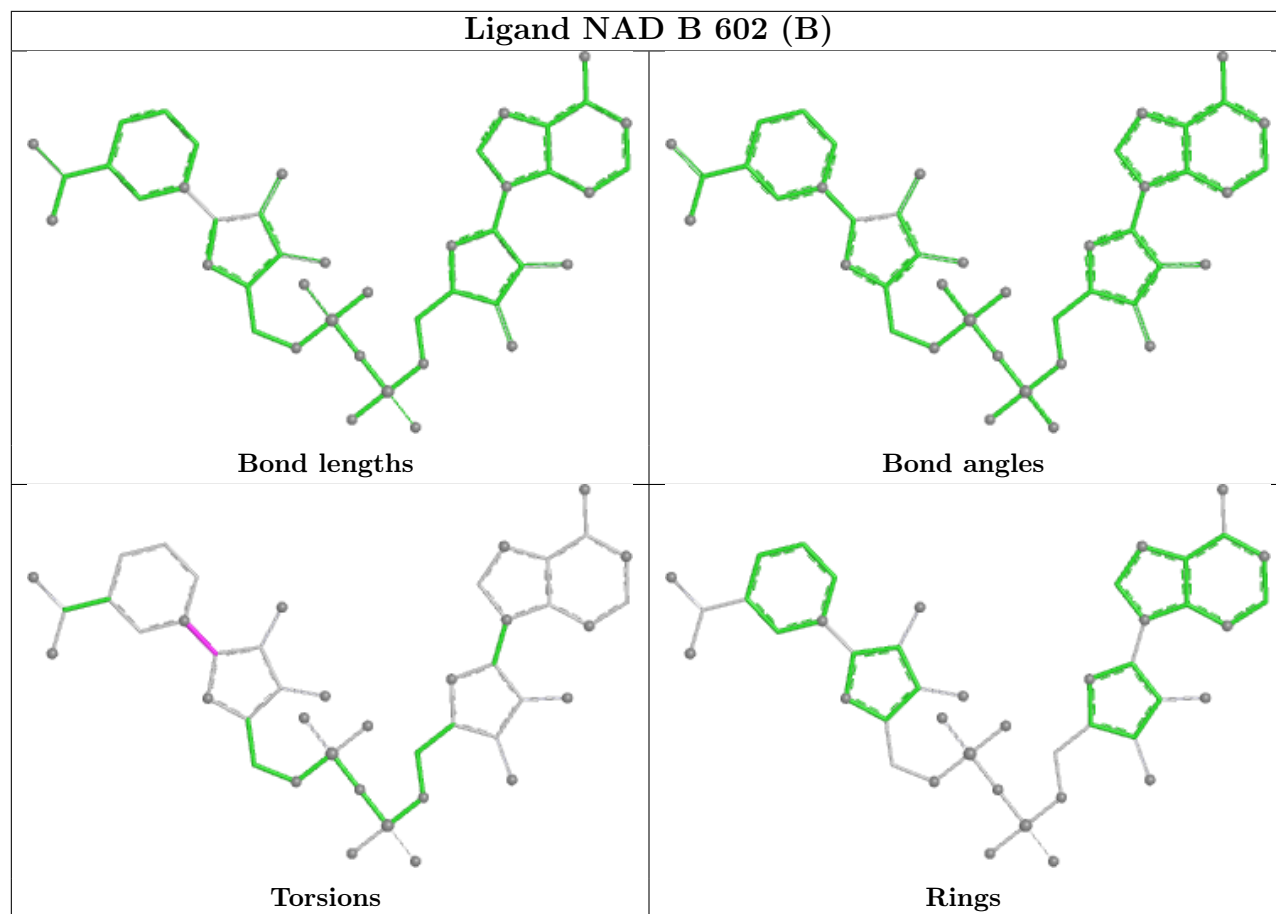


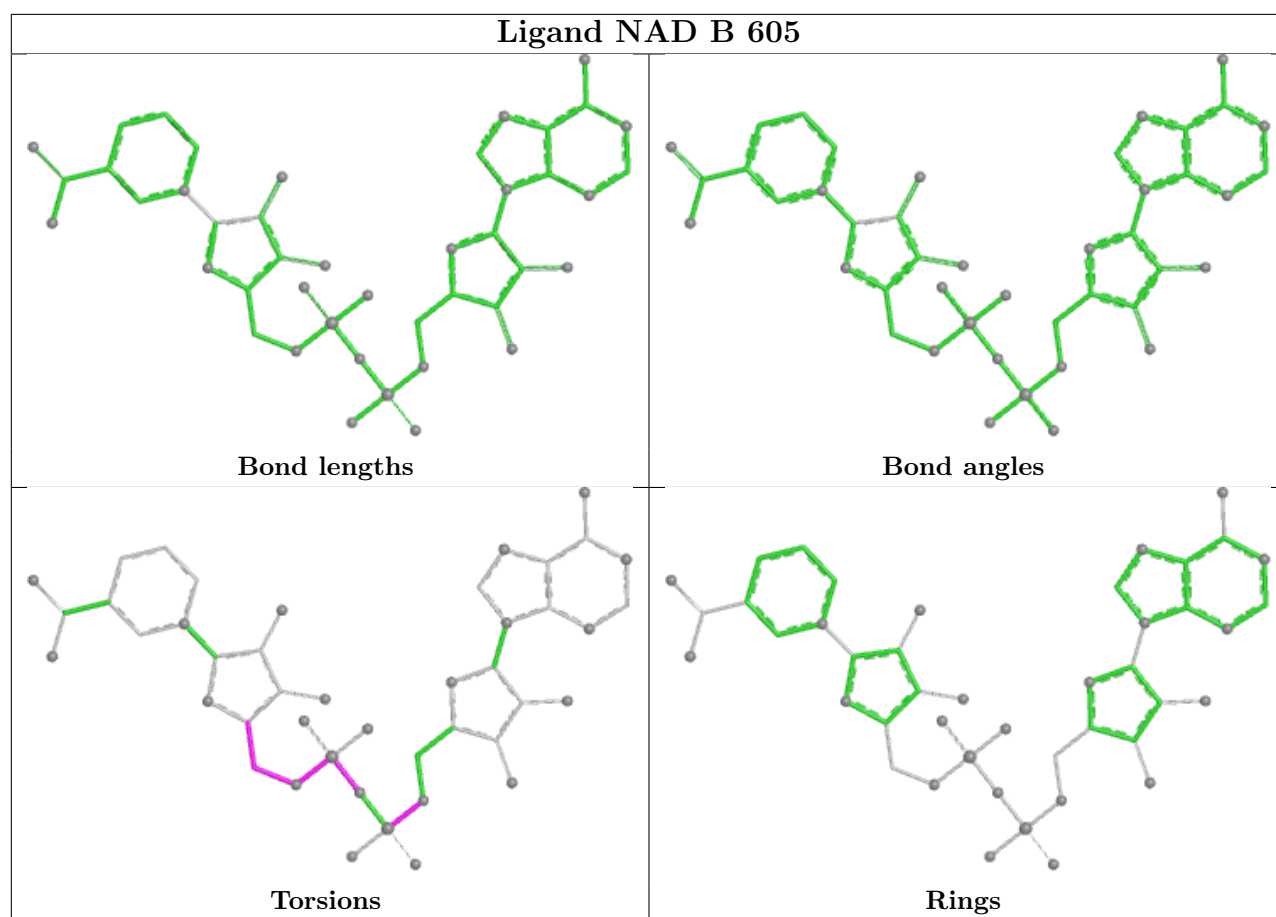






Ligand NAD B 602 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	555/575 (96%)	0.06	23 (4%) 41 44	7, 27, 50, 72	9 (1%)
1	B	551/575 (95%)	0.07	13 (2%) 59 63	12, 27, 49, 78	9 (1%)
1	C	557/575 (96%)	0.18	14 (2%) 58 62	8, 29, 52, 72	8 (1%)
1	D	542/575 (94%)	0.48	54 (9%) 12 13	13, 31, 63, 83	6 (1%)
All	All	2205/2300 (95%)	0.20	104 (4%) 36 39	7, 29, 55, 83	32 (1%)

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	75	MET	5.1
1	D	374	PRO	4.6
1	C	177[A]	MET	4.5
1	C	573	PRO	4.0
1	A	177[A]	MET	4.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSX	C	120	7/8	0.78	0.18	49,52,57,59	0
1	CSX	A	120	7/8	0.79	0.21	41,45,48,50	0
1	CSX	D	120	7/8	0.87	0.14	44,47,50,50	0
1	CSX	B	120	7/8	0.89	0.13	45,46,53,54	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

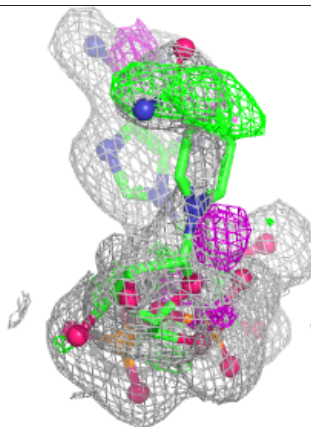
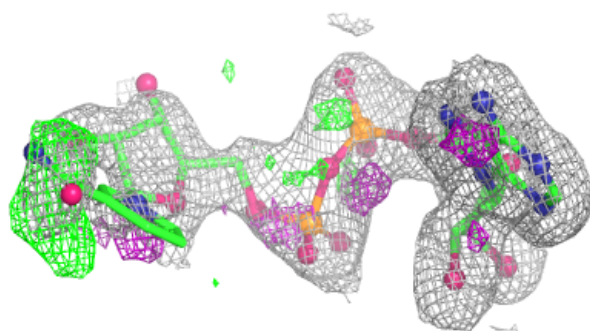
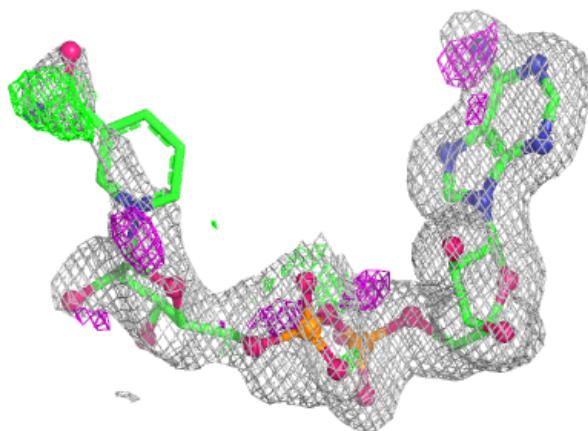
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	602	4/4	0.67	0.20	52,54,56,59	0
6	TLA	A	607	10/10	0.71	0.16	50,59,64,64	0
6	TLA	C	601	10/10	0.80	0.14	49,60,61,68	0
2	NAD	A	601[A]	44/44	0.81	0.17	22,32,39,40	44
2	NAD	A	601[B]	44/44	0.81	0.17	21,38,61,65	44
2	NAD	D	603	44/44	0.81	0.15	47,52,66,67	0
3	EDO	B	604	4/4	0.82	0.15	43,45,46,47	0
3	EDO	D	604[B]	4/4	0.83	0.24	35,35,35,35	4
3	EDO	A	603	4/4	0.83	0.14	46,46,47,48	0
3	EDO	D	604[A]	4/4	0.83	0.24	29,30,30,30	4
6	TLA	B	603	10/10	0.84	0.14	50,61,69,72	0
6	TLA	D	601	10/10	0.85	0.12	46,55,62,64	0
3	EDO	C	602	4/4	0.87	0.13	49,49,51,51	0
2	NAD	C	605	44/44	0.92	0.09	33,37,41,41	0
2	NAD	B	602[A]	44/44	0.92	0.09	23,27,40,40	44
2	NAD	B	602[B]	44/44	0.92	0.09	22,27,39,40	44
2	NAD	B	605	44/44	0.94	0.11	19,39,62,65	0
2	NAD	C	604	44/44	0.94	0.11	22,41,66,69	0
2	NAD	D	605	44/44	0.95	0.10	21,38,61,64	0
5	MG	B	606	1/1	0.96	0.09	30,30,30,30	0
5	MG	A	606	1/1	0.97	0.07	34,34,34,34	0
2	NAD	A	605	44/44	0.97	0.06	22,25,34,35	0
4	CL	B	601	1/1	0.99	0.04	24,24,24,24	0
4	CL	A	604	1/1	1.00	0.03	25,25,25,25	0
4	CL	C	603	1/1	1.00	0.03	22,22,22,22	0
4	CL	D	602	1/1	1.00	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.

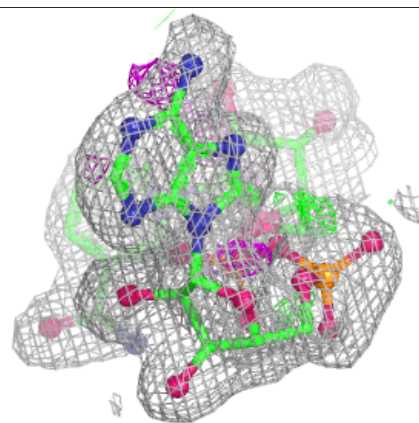
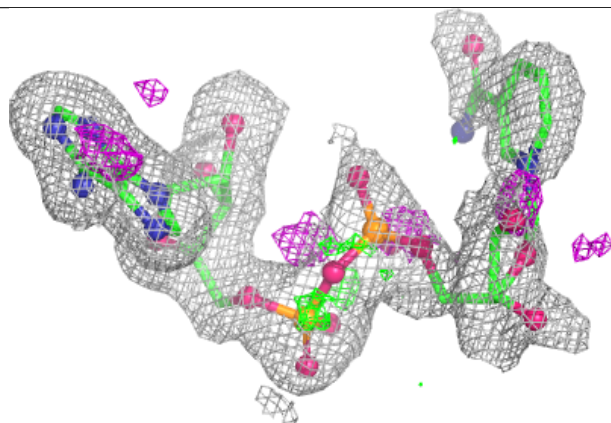
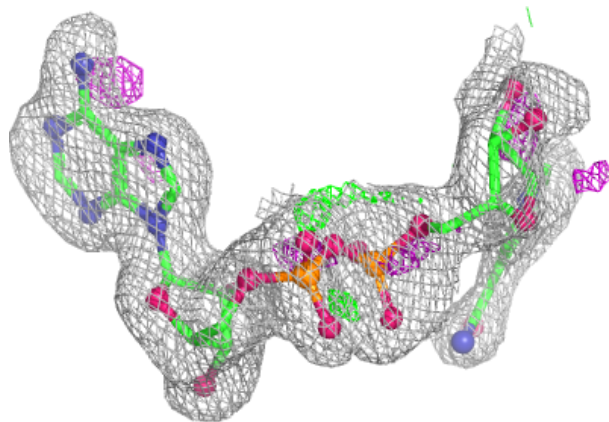
Electron density around NAD A 601 (A):

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

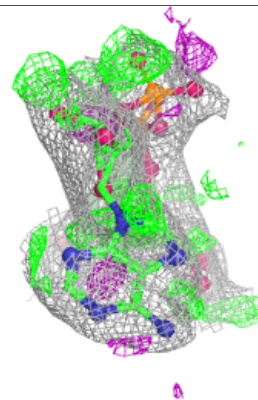
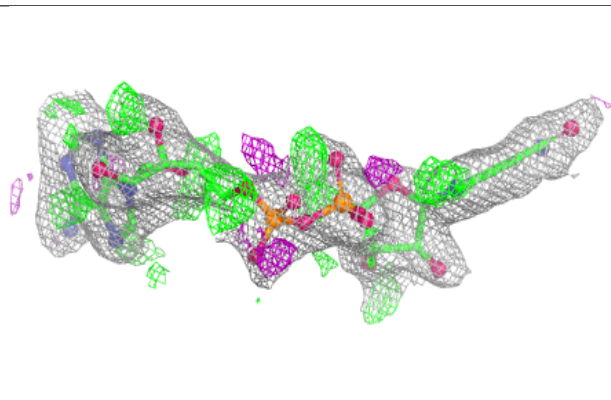
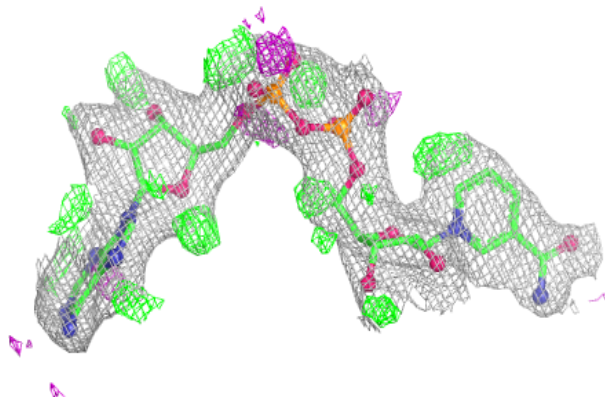


Electron density around NAD A 601 (B):

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

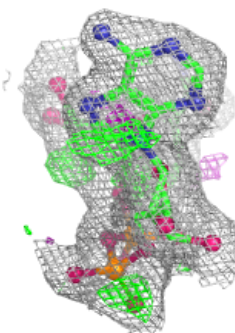
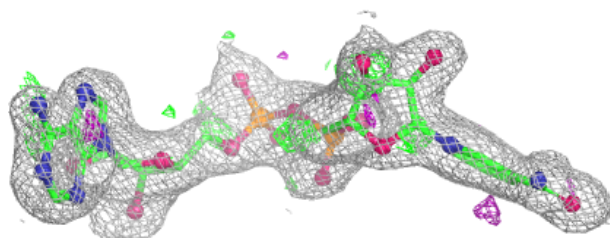
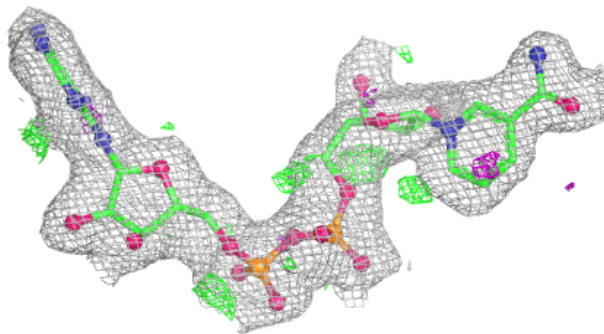
**Electron density around NAD D 603:**

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

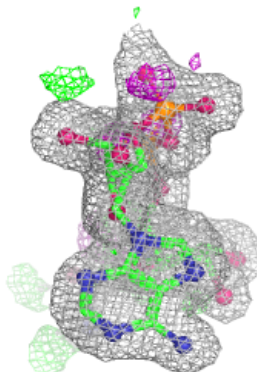
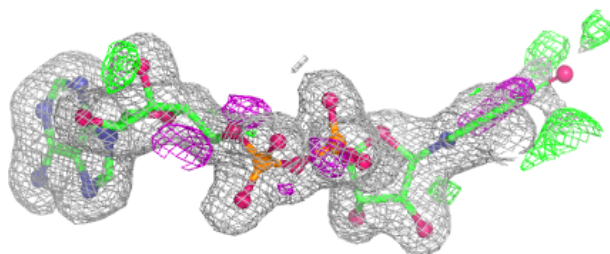
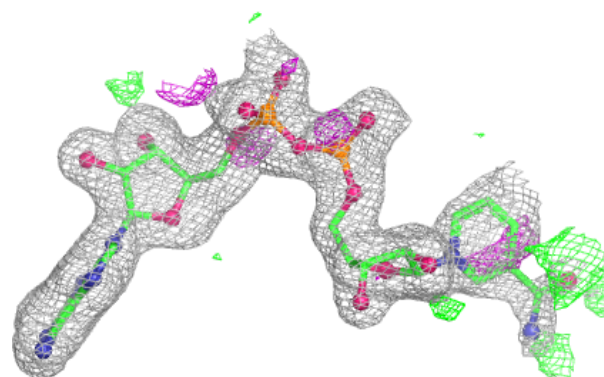


Electron density around NAD C 605:

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

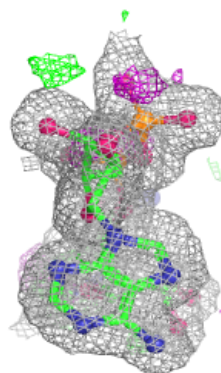
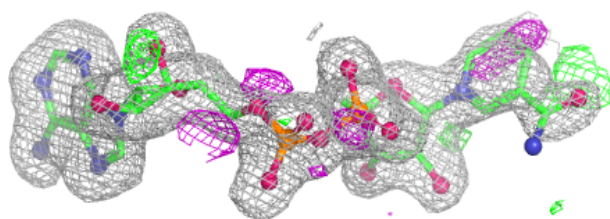
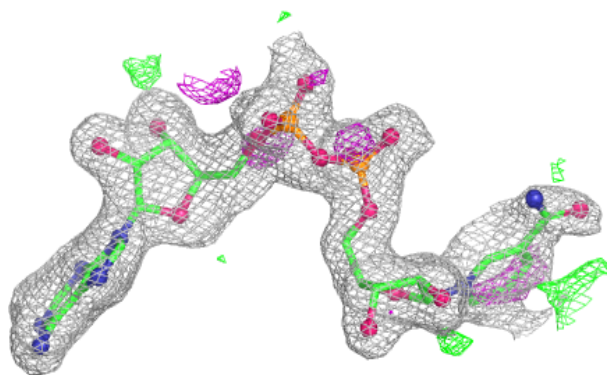
**Electron density around NAD B 602 (A):**

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

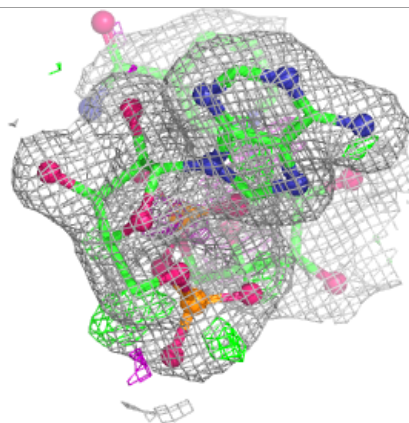
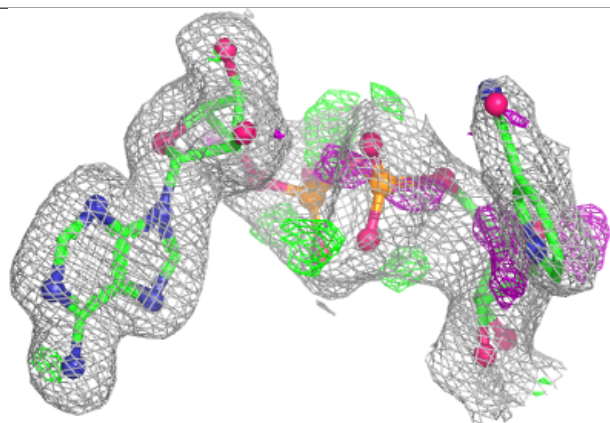
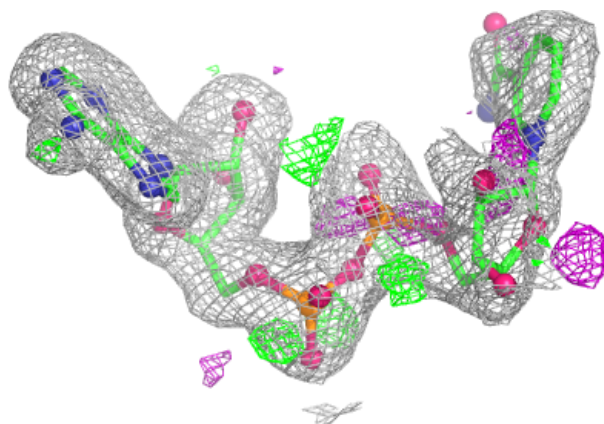


Electron density around NAD B 602 (B):

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

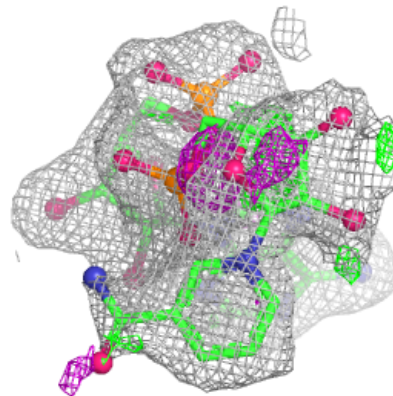
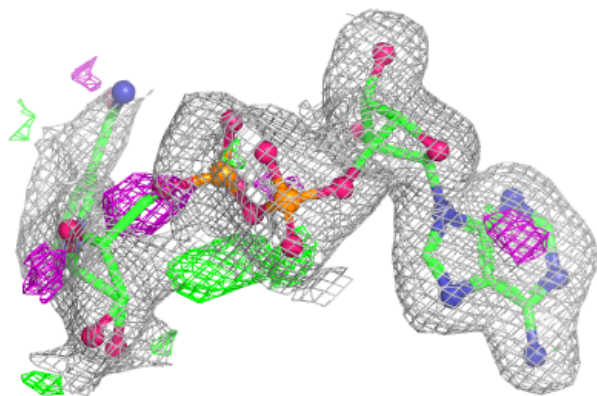
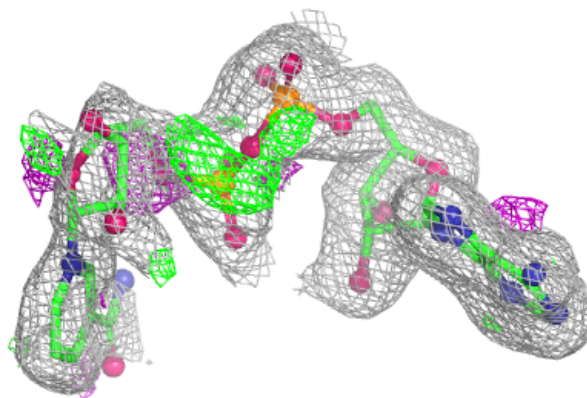
**Electron density around NAD B 605:**

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and green (positive)



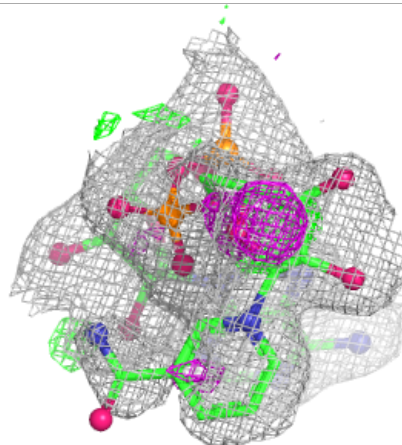
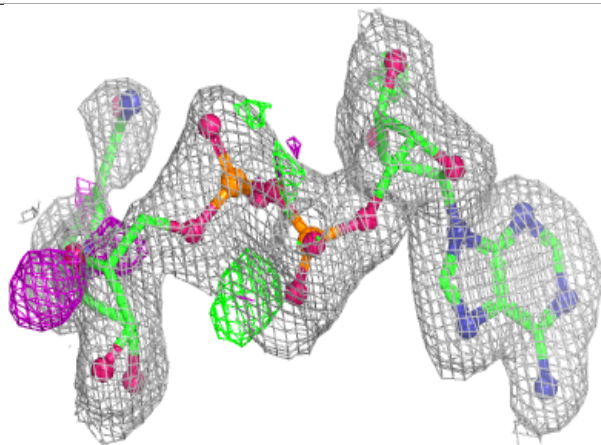
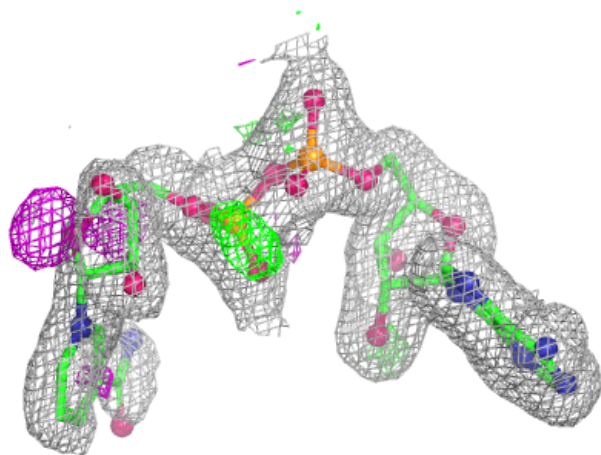
Electron density around NAD C 604:

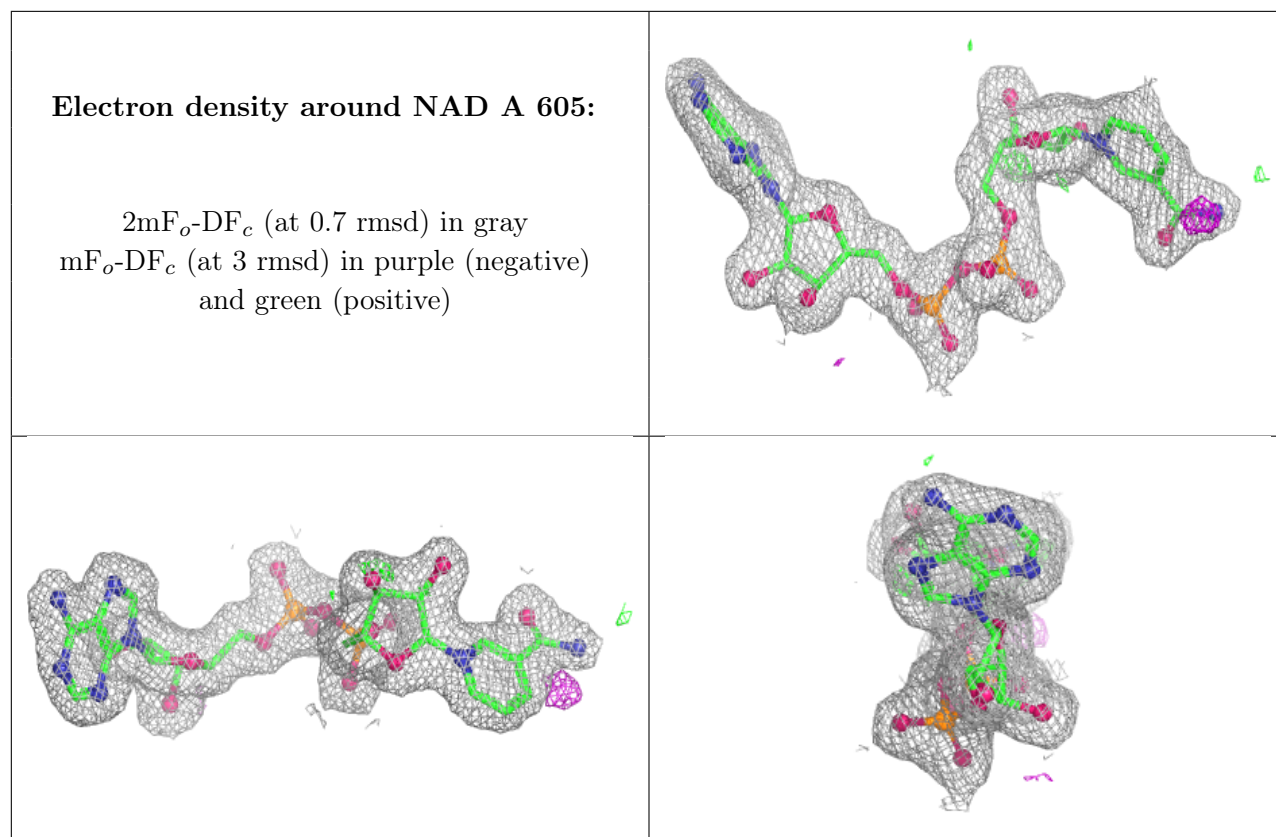
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAD D 605:

$2mF_o-DF_c$ (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.