



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 04:18 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 Full wwPDB X-ray Structure Validation 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

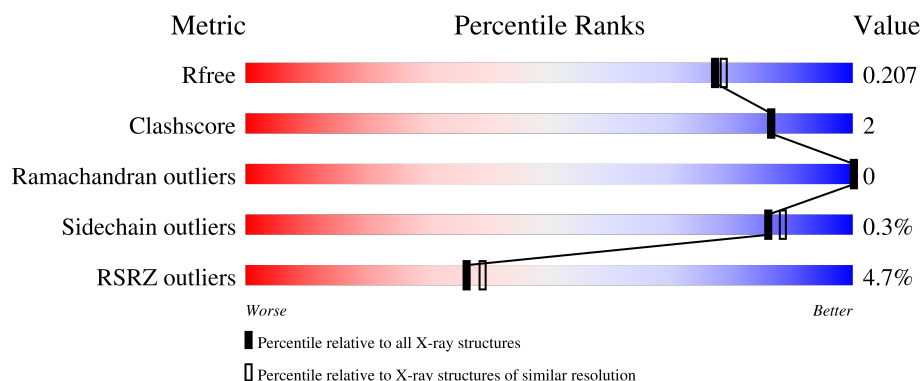
1 Overall quality at a glance

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	4% 91% 5% .
1	B	575	2% 91% 5% .
1	C	575	2% 93% 5% .
1	D	575	9% 89% 5% 6%

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:

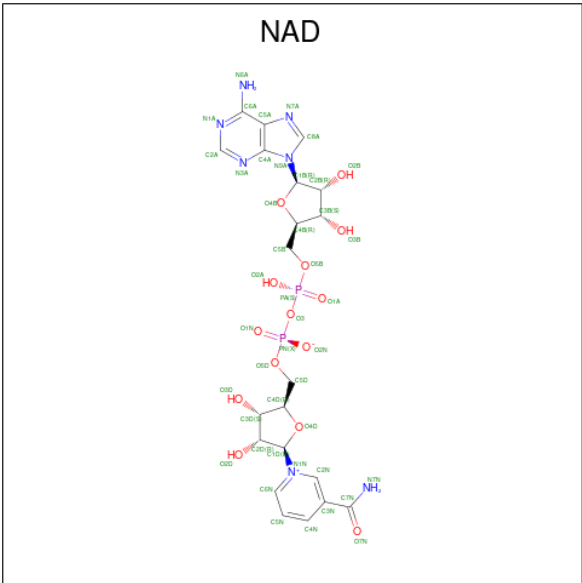
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP P23368
A	585	LEU	-	expression tag	UNP P23368
A	586	GLU	-	expression tag	UNP P23368
A	587	HIS	-	expression tag	UNP P23368
A	588	HIS	-	expression tag	UNP P23368
A	589	HIS	-	expression tag	UNP P23368
A	590	HIS	-	expression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



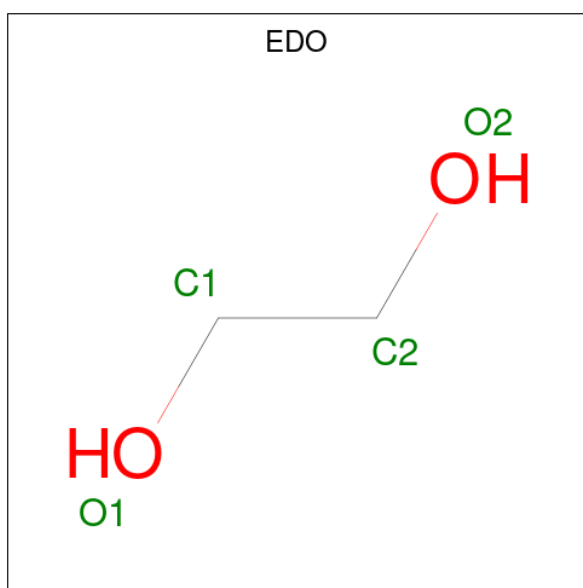
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	1
			88	42	14	28	4		

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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		

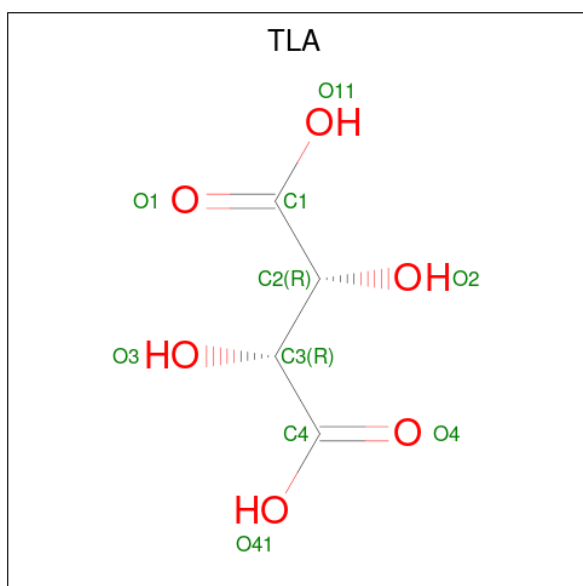
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

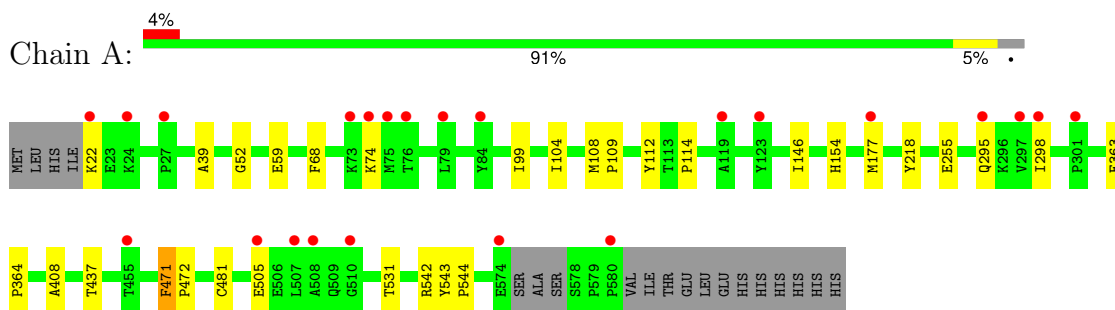
- Molecule 7 is water.

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

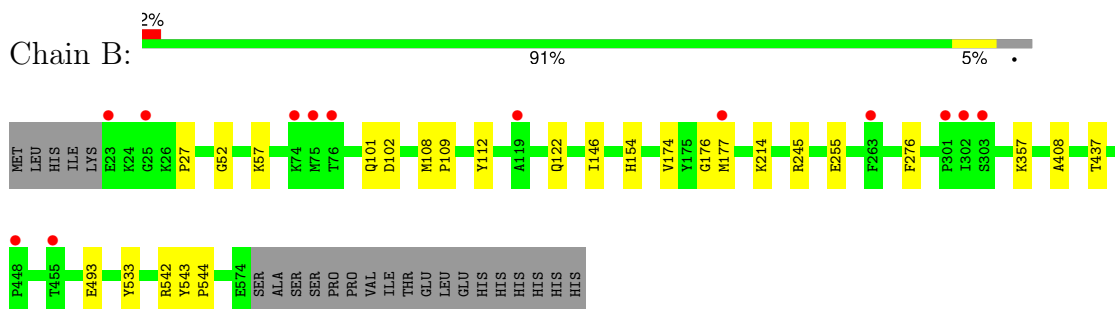
3 Residue-property plots [i](#)

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.

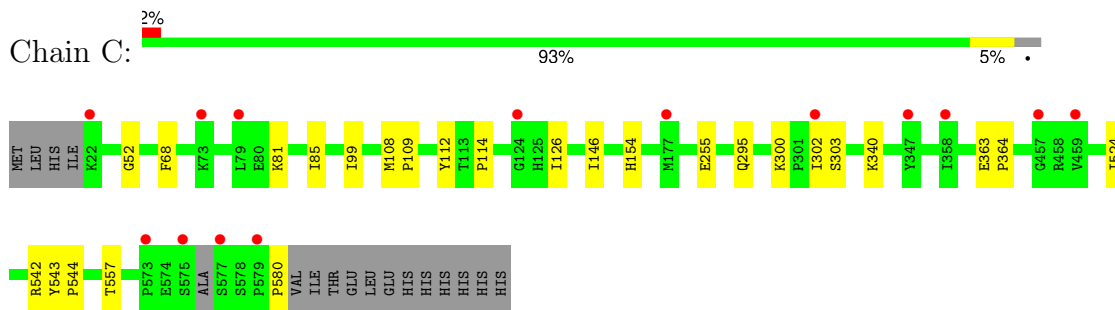
- Molecule 1: NAD-dependent malic enzyme, mitochondrial



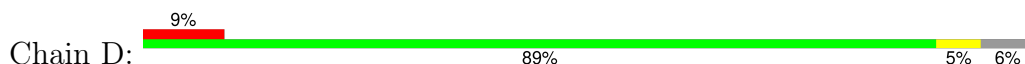
- Molecule 1: NAD-dependent malic enzyme, mitochondrial

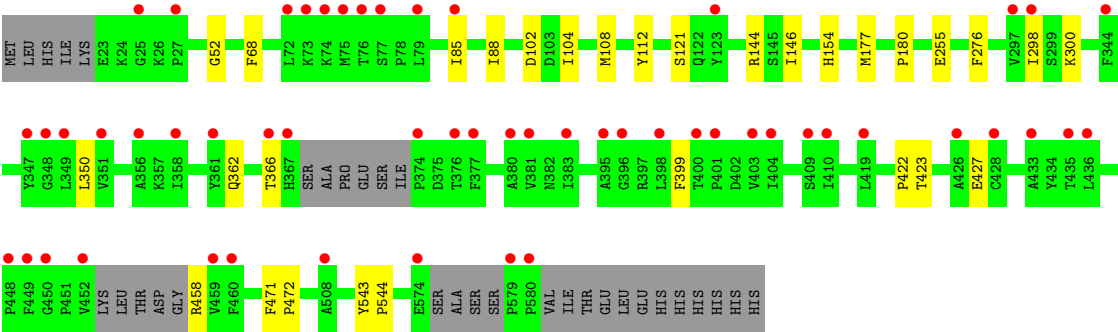


- Molecule 1: NAD-dependent malic enzyme, mitochondrial



- 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

5.1 Standard geometry

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

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.

All (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
1:A:295[B]:GLN:HE21	1:A:295[B]:GLN:HA	1.63	0.63
2:B:605:NAD:H4N	1:C:154:HIS:HD1	1.67	0.60
2:C:605:NAD:PA	7:C:715:HOH:O	2.61	0.57
1:B:154:HIS:HD1	2:C:604:NAD:H4N	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:TYR:HA	1:C:544:PRO:C	2.32	0.53
1:A:218:TYR:O	1:B:57:LYS:HD2	2.08	0.53
1:A:543:TYR:HA	1:A:544:PRO:C	2.33	0.53
1:D:543:TYR:HA	1:D:544:PRO:C	2.33	0.53
1:A:177[B]:MET:O	1:A:177[B]:MET:HE2	2.08	0.53
1:C:303:SER:HA	1:C:340:LYS:HE3	1.91	0.53
1:B:214:LYS:C	1:C:580:PRO:HG3	2.34	0.52
1:C:81:LYS:O	1:C:85[B]:ILE:HG13	2.10	0.51
1:D:68:PHE:HZ	1:D:85:ILE:HG12	1.74	0.51
1:A:22:LYS:HA	1:B:27:PRO:HB3	1.93	0.51
1:B:493[B]:GLU:HG3	1:B:533:TYR:CD1	2.46	0.51
1:B:543:TYR:HA	1:B:544:PRO:C	2.36	0.50
1:A:542:ARG:NH2	6:D:601:TLA:H2	2.22	0.50
1:A:408:ALA:HB2	1:A:437:THR:HG22	1.95	0.49
1:C:68:PHE:CE2	1:C:99[A]:ILE:CG2	2.96	0.49
1:A:68:PHE:CE2	1:A:99:ILE:HG23	2.47	0.49
1:B:112:TYR:OH	1:B:255:GLU:OE1	2.31	0.48
1:C:524:ILE:HD12	1:C:557[A]:THR:HG21	1.96	0.48
1:A:154:HIS:HD1	2:D:605:NAD:H4N	1.78	0.48
1:B:245:ARG:O	2:C:604:NAD:H6N	2.15	0.47
1:D:104:ILE:O	1:D:108:MET:HG3	2.14	0.47
2:B:605:NAD:H4N	1:C:154:HIS:ND1	2.28	0.47
1:C:52:GLY:HA3	1:D:146:ILE:HG23	1.97	0.46
1:B:177[B]:MET:O	1:B:177[B]:MET:HG3	2.14	0.46
1:A:177[B]:MET:HE3	1:A:177[B]:MET:HA	1.98	0.46
1:C:300:LYS:NZ	7:C:710:HOH:O	2.49	0.46
1:C:146:ILE:HG23	1:D:52:GLY:HA3	1.98	0.45
1:A:177[B]:MET:O	1:A:177[B]:MET:CE	2.64	0.45
1:B:101:GLN:NE2	7:B:715:HOH:O	2.49	0.45
1:D:112:TYR:OH	1:D:255:GLU:OE2	2.34	0.45
1:D:350:LEU:HB3	1:D:366:THR:HG22	1.99	0.45
1:C:68:PHE:CE2	1:C:99[A]:ILE:HG23	2.52	0.45
1:A:481:CYS:SG	1:A:531:THR:HG23	2.57	0.45
1:A:295[B]:GLN:NE2	1:A:298:ILE:O	2.50	0.44
1:A:104:ILE:O	1:A:108:MET:HG3	2.17	0.44
1:A:505[A]:GLU:H	1:A:505[A]:GLU:CD	2.25	0.44
1:D:68:PHE:CD1	1:D:68:PHE:C	2.95	0.44
1:C:112:TYR:OH	1:C:255:GLU:OE2	2.35	0.44
1:B:154:HIS:ND1	2:C:604:NAD:H4N	2.32	0.43
1:A:363:GLU:N	1:A:364:PRO:CD	2.81	0.43
1:D:68:PHE:CZ	1:D:85:ILE:HG12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:GLU:N	1:C:364:PRO:CD	2.82	0.43
1:C:295[A]:GLN:NE2	3:C:602:EDO:O1	2.51	0.43
1:A:108:MET:N	1:A:109:PRO:CD	2.82	0.43
1:C:108:MET:N	1:C:109:PRO:HD2	2.33	0.43
1:D:298:ILE:HG22	1:D:300:LYS:HB2	2.01	0.43
1:C:126:ILE:HD12	1:D:88:ILE:HD12	2.01	0.42
1:D:362:GLN:O	1:D:366:THR:HG23	2.19	0.42
1:C:295[A]:GLN:OE1	1:C:302:ILE:HD11	2.20	0.42
1:B:174:VAL:C	1:B:176[B]:GLY:H	2.26	0.42
1:A:471:PHE:CG	1:A:472:PRO:HD3	2.55	0.42
1:C:68:PHE:CE2	1:C:99[A]:ILE:HG21	2.54	0.42
1:B:108:MET:N	1:B:109:PRO:CD	2.83	0.42
1:A:112:TYR:OH	1:A:255:GLU:OE2	2.39	0.41
1:A:146:ILE:HG23	1:B:52:GLY:HA3	2.02	0.41
1:A:295[B]:GLN:HE21	1:A:295[B]:GLN:CA	2.24	0.41
1:D:471:PHE:CG	1:D:472:PRO:HD3	2.56	0.41
2:A:601[A]:NAD:H72N	1:D:144:ARG:HH22	1.68	0.41
1:A:52:GLY:HA3	1:B:146:ILE:HG23	2.03	0.41
1:D:177[A]:MET:O	1:D:180:PRO:HD2	2.20	0.41
1:C:68:PHE:HZ	1:C:85[B]:ILE:HG12	1.85	0.41
1:D:422:PRO:O	1:D:423:THR:C	2.64	0.41
1:A:39:ALA:HA	1:A:59:GLU:O	2.21	0.40
1:B:408:ALA:HB2	1:B:437:THR:HG22	2.04	0.40
1:D:399:PHE:CG	1:D:427:GLU:HB3	2.56	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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
1	C	114	PRO
1	D	121	SER
1	D	458	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	B	43	GLN
1	B	89	GLN

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Mol	Chain	Res	Type
1	B	421	ASN
1	B	425	GLN
1	C	43	GLN
1	C	122	GLN
1	C	223	GLN
1	C	330	ASN
1	C	425	GLN
1	D	43	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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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(°)	Ideal(°)
2	A	605	NAD	C4D-O4D-C1D	-2.65	107.50	109.92

There are no chirality outliers.

All (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
2	A	601[B]	NAD	C5B-O5B-PA-O3
2	A	605	NAD	O4D-C1D-N1N-C6N
2	A	605	NAD	C2D-C1D-N1N-C6N
2	B	602[A]	NAD	O4D-C1D-N1N-C2N
2	B	602[A]	NAD	O4D-C1D-N1N-C6N
2	B	602[A]	NAD	C2D-C1D-N1N-C2N
2	B	602[A]	NAD	C2D-C1D-N1N-C6N
2	B	602[B]	NAD	O4D-C1D-N1N-C6N
2	B	602[B]	NAD	C2D-C1D-N1N-C6N
2	C	604	NAD	C5B-O5B-PA-O2A
2	C	604	NAD	C5B-O5B-PA-O3
2	C	604	NAD	C5D-O5D-PN-O1N
2	C	605	NAD	O4D-C1D-N1N-C6N
2	D	603	NAD	O4D-C1D-N1N-C6N
2	D	605	NAD	C5D-O5D-PN-O3
2	D	605	NAD	C5D-O5D-PN-O2N
6	A	607	TLA	C2-C3-C4-O41
6	B	603	TLA	O1-C1-C2-C3
6	B	603	TLA	O11-C1-C2-C3
6	C	601	TLA	C2-C3-C4-O4
6	C	601	TLA	C2-C3-C4-O41
6	D	601	TLA	O3-C3-C4-O4
6	D	601	TLA	O3-C3-C4-O41
6	B	603	TLA	O1-C1-C2-O2
6	B	603	TLA	O11-C1-C2-O2
6	C	601	TLA	O1-C1-C2-O2
6	C	601	TLA	O11-C1-C2-O2
6	C	601	TLA	O3-C3-C4-O4
6	C	601	TLA	O3-C3-C4-O41
6	A	607	TLA	O11-C1-C2-C3
6	A	607	TLA	C2-C3-C4-O4
6	C	601	TLA	O1-C1-C2-C3
6	C	601	TLA	O11-C1-C2-C3
6	D	601	TLA	C2-C3-C4-O4
6	D	601	TLA	C2-C3-C4-O41
6	A	607	TLA	O3-C3-C4-O4
6	A	607	TLA	O3-C3-C4-O41

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Mol	Chain	Res	Type	Atoms
6	A	607	TLA	O1-C1-C2-C3
6	B	603	TLA	O3-C3-C4-O4
6	B	603	TLA	O3-C3-C4-O41
6	A	607	TLA	O1-C1-C2-O2
6	A	607	TLA	O11-C1-C2-O2
2	D	605	NAD	O4D-C4D-C5D-O5D
2	D	605	NAD	C3D-C4D-C5D-O5D
3	D	604[B]	EDO	O1-C1-C2-O2
2	D	603	NAD	PN-O3-PA-O1A
2	D	605	NAD	PN-O3-PA-O1A
2	A	601[A]	NAD	PA-O3-PN-O1N
2	A	601[B]	NAD	PA-O3-PN-O2N
2	C	604	NAD	PA-O3-PN-O1N
2	A	601[A]	NAD	C5D-O5D-PN-O3
2	A	601[A]	NAD	C5D-O5D-PN-O1N
2	A	601[A]	NAD	C5D-O5D-PN-O2N
2	B	605	NAD	C5B-O5B-PA-O1A
2	B	605	NAD	C5D-O5D-PN-O1N
2	D	605	NAD	C5D-O5D-PN-O1N
2	A	601[B]	NAD	PN-O3-PA-O1A
2	A	601[A]	NAD	C2D-C1D-N1N-C2N
2	A	605	NAD	C2D-C1D-N1N-C2N
2	B	602[B]	NAD	C2D-C1D-N1N-C2N
2	A	605	NAD	O4D-C1D-N1N-C2N
2	B	602[B]	NAD	O4D-C1D-N1N-C2N
2	C	605	NAD	O4B-C4B-C5B-O5B
2	C	605	NAD	O4D-C1D-N1N-C2N
2	D	603	NAD	O4D-C1D-N1N-C2N
2	A	601[A]	NAD	PA-O3-PN-O2N
2	B	602[A]	NAD	PN-O3-PA-O1A
2	D	603	NAD	PN-O3-PA-O2A
2	B	605	NAD	O4D-C4D-C5D-O5D
2	D	603	NAD	O4B-C4B-C5B-O5B
3	B	604	EDO	O1-C1-C2-O2
3	A	602	EDO	O1-C1-C2-O2
3	A	603	EDO	O1-C1-C2-O2
3	D	604[A]	EDO	O1-C1-C2-O2
2	B	605	NAD	C4D-C5D-O5D-PN
2	A	601[B]	NAD	PN-O3-PA-O2A
2	A	601[B]	NAD	PA-O3-PN-O1N
2	B	602[A]	NAD	PN-O3-PA-O2A
2	B	605	NAD	PA-O3-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	D	605	NAD	PN-O3-PA-O2A
2	B	605	NAD	PA-O3-PN-O2N

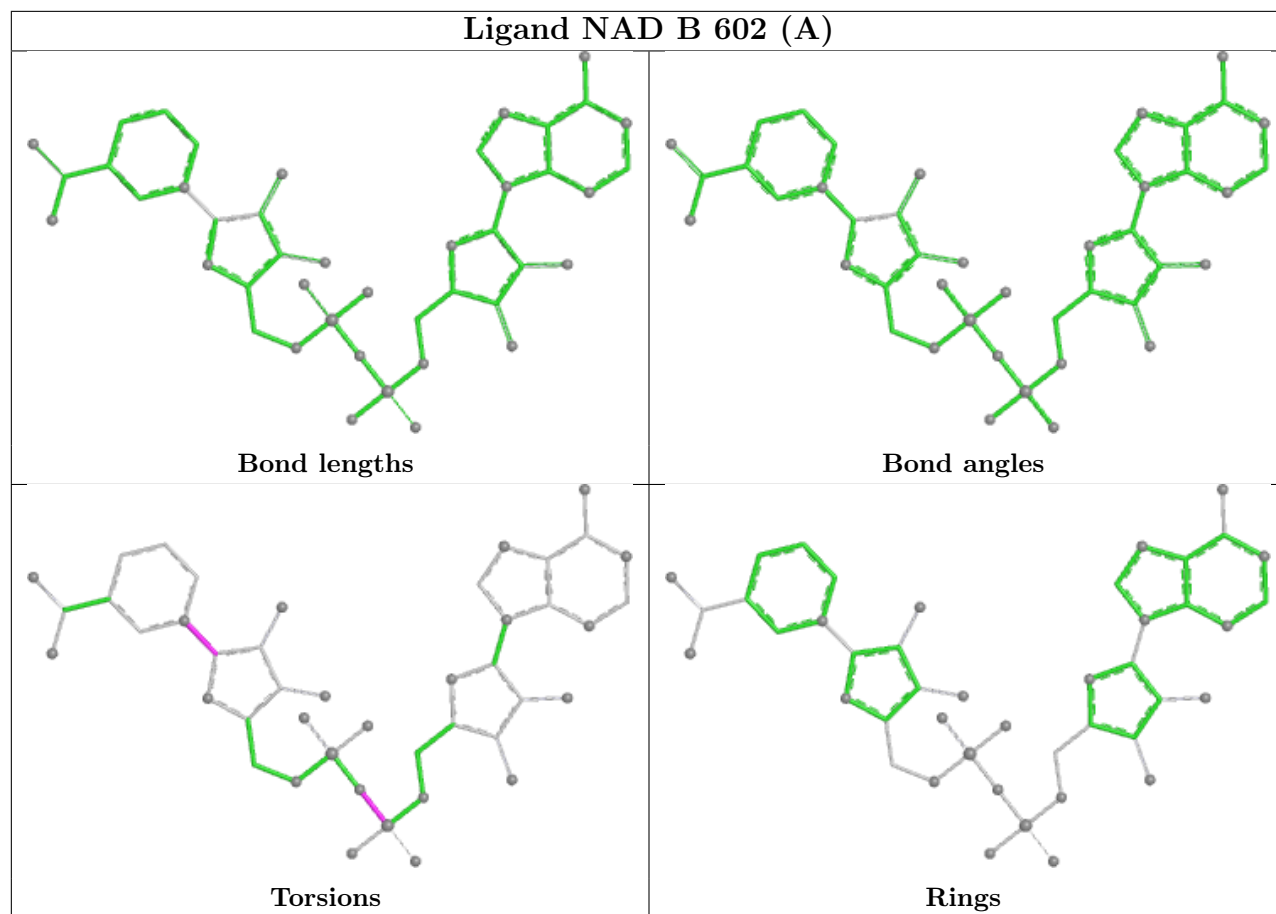
There are no ring outliers.

10 monomers are involved in 14 short contacts:

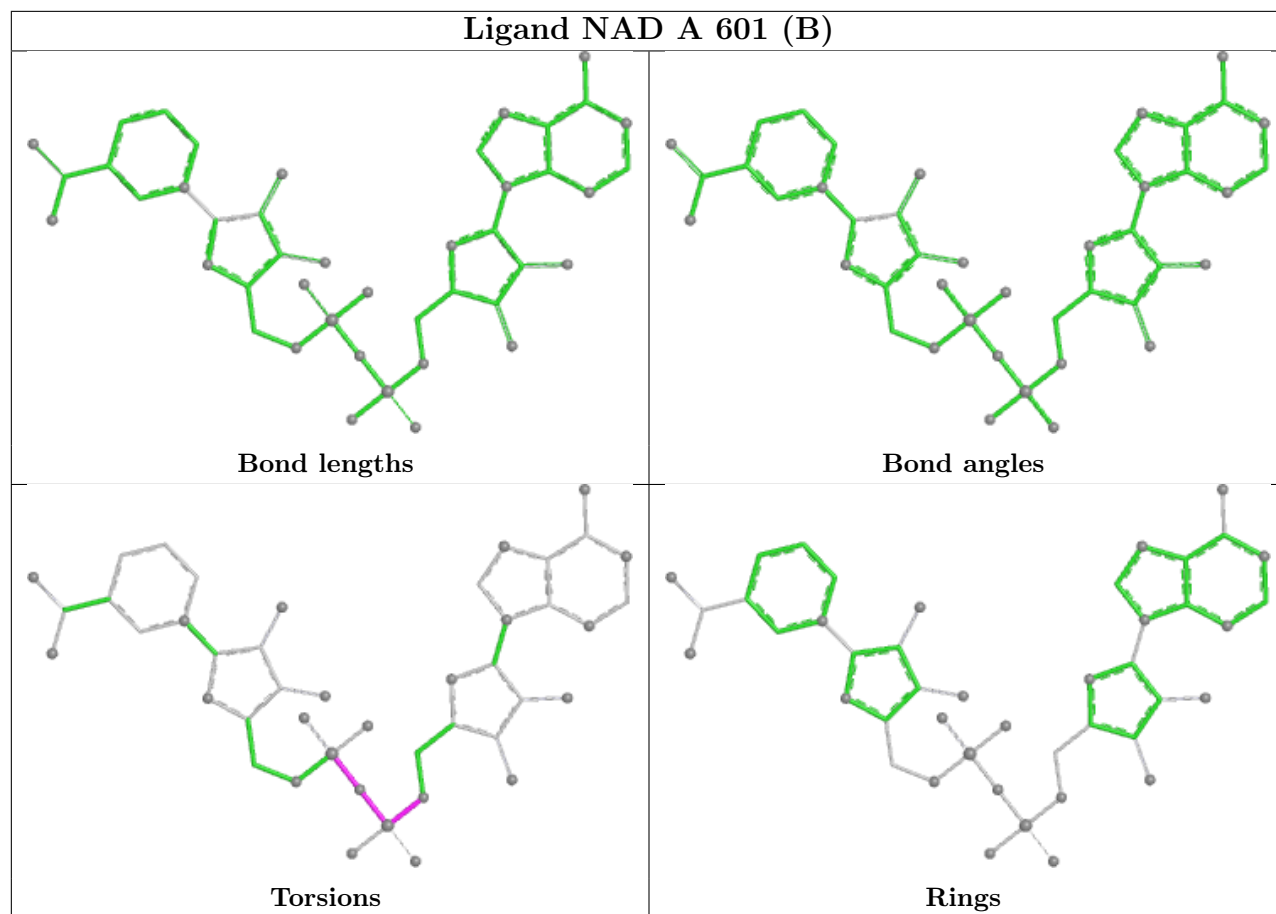
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	EDO	1	0
2	A	601[B]	NAD	1	0
2	C	604	NAD	3	0
6	C	601	TLA	1	0
2	D	605	NAD	1	0
2	C	605	NAD	1	0
2	A	601[A]	NAD	1	0
6	D	601	TLA	2	0
2	B	605	NAD	2	0
6	B	603	TLA	1	0

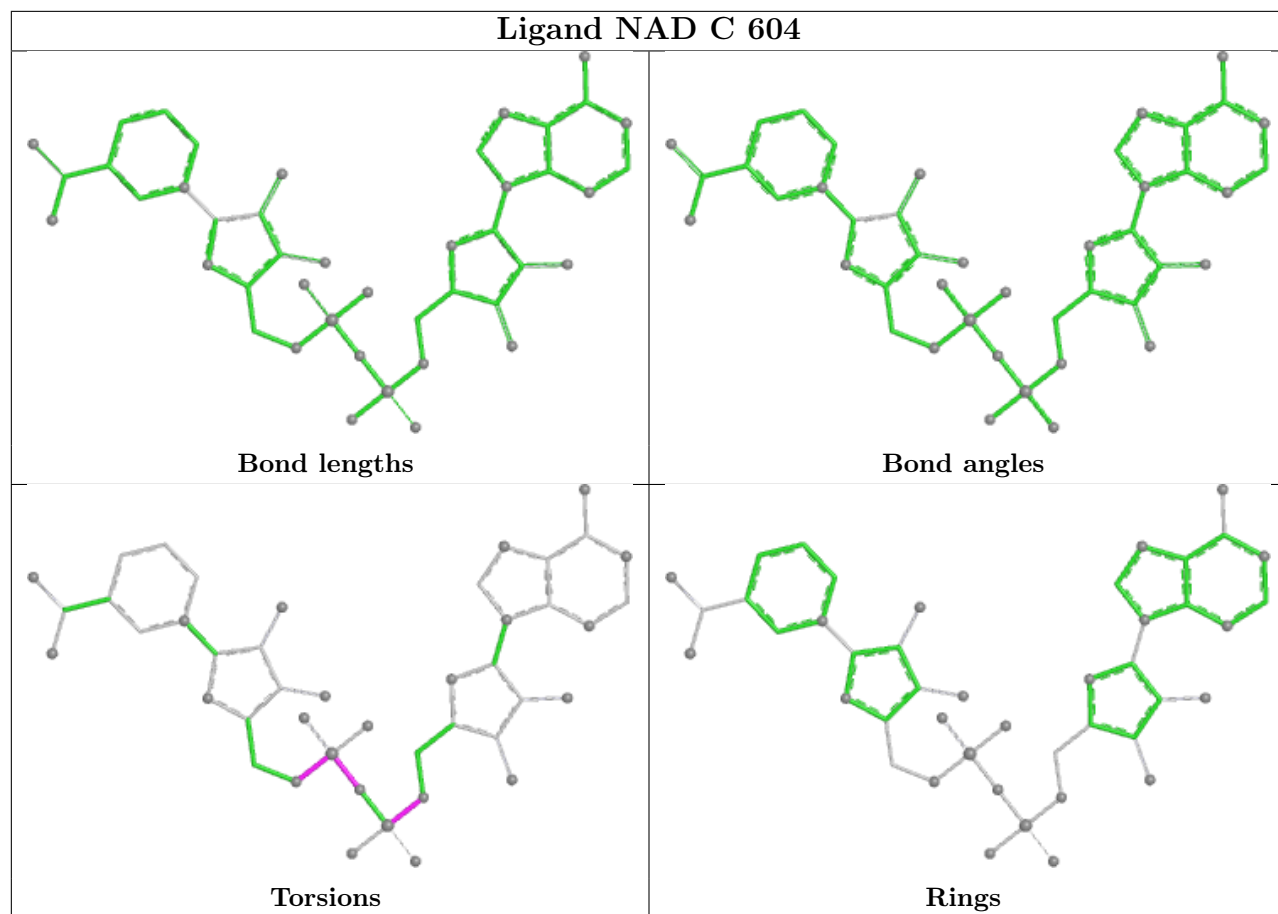
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

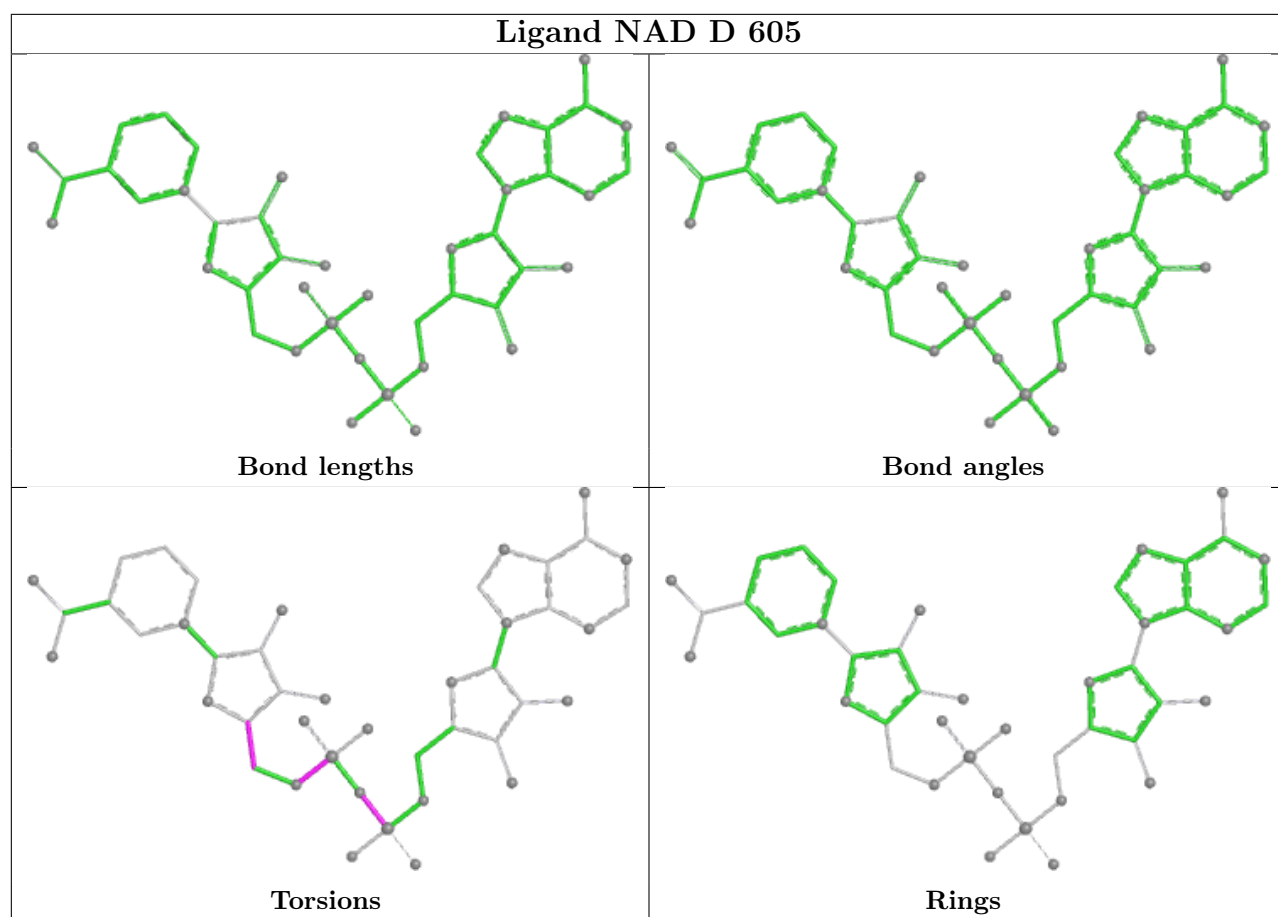
Ligand NAD B 602 (A)

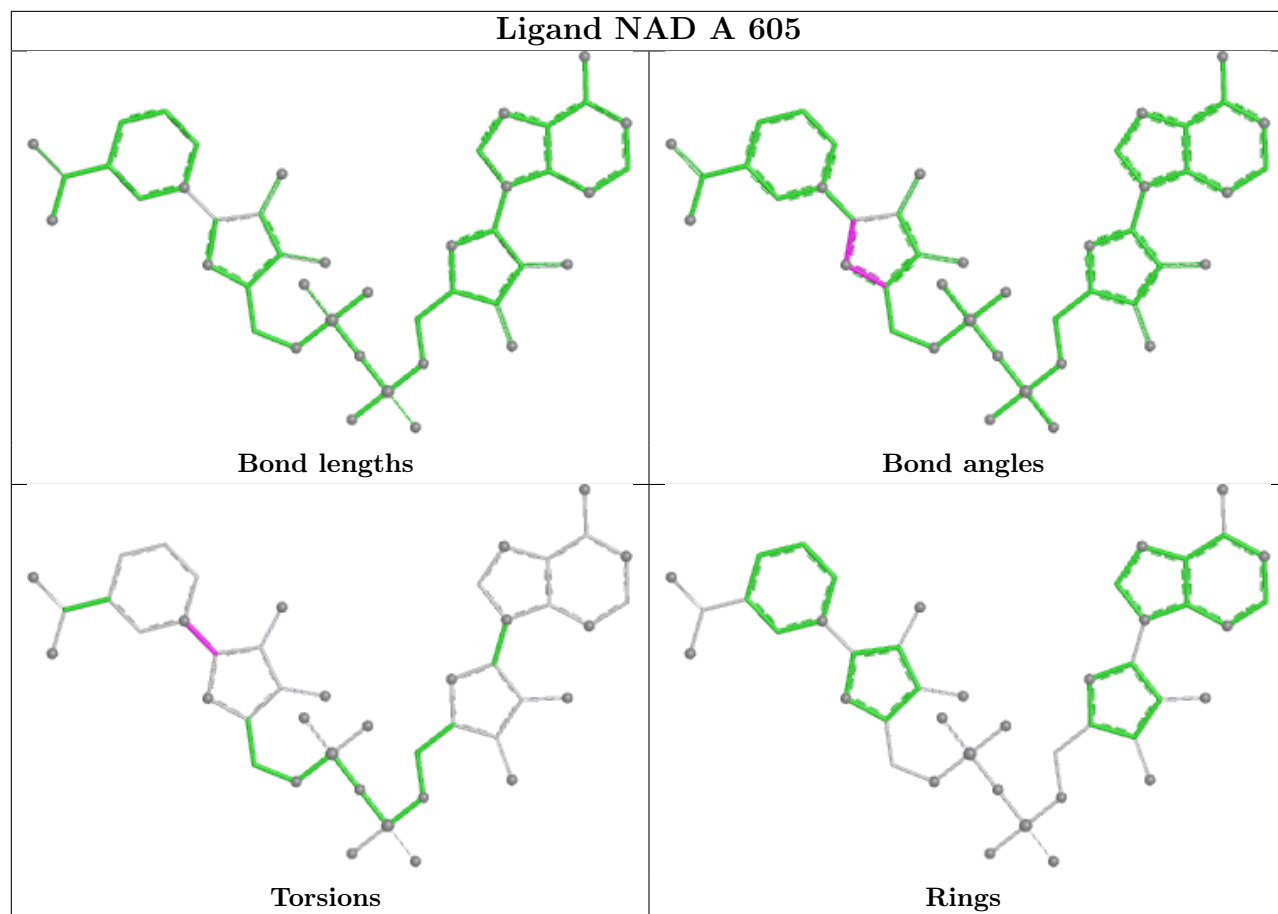


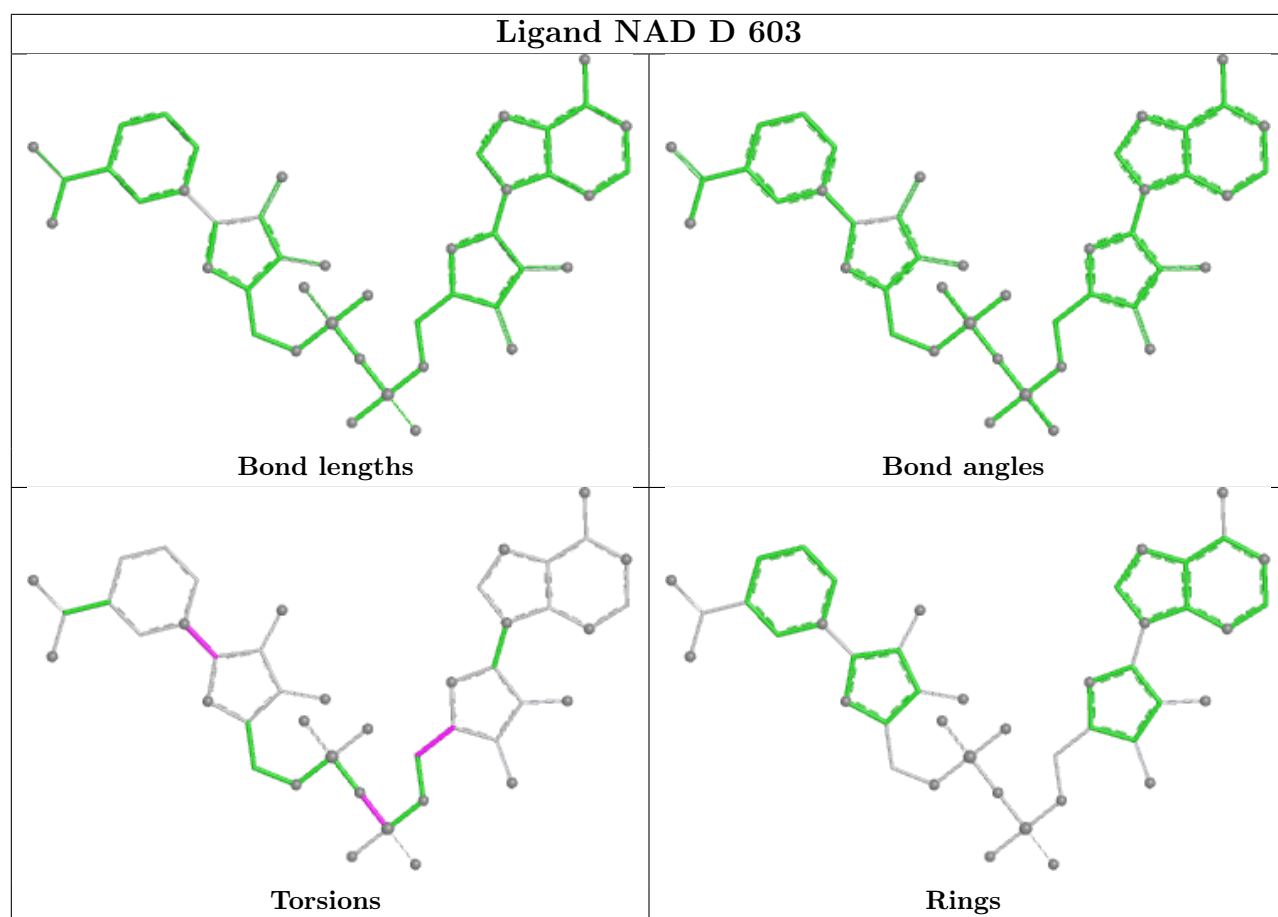
Ligand NAD A 601 (B)

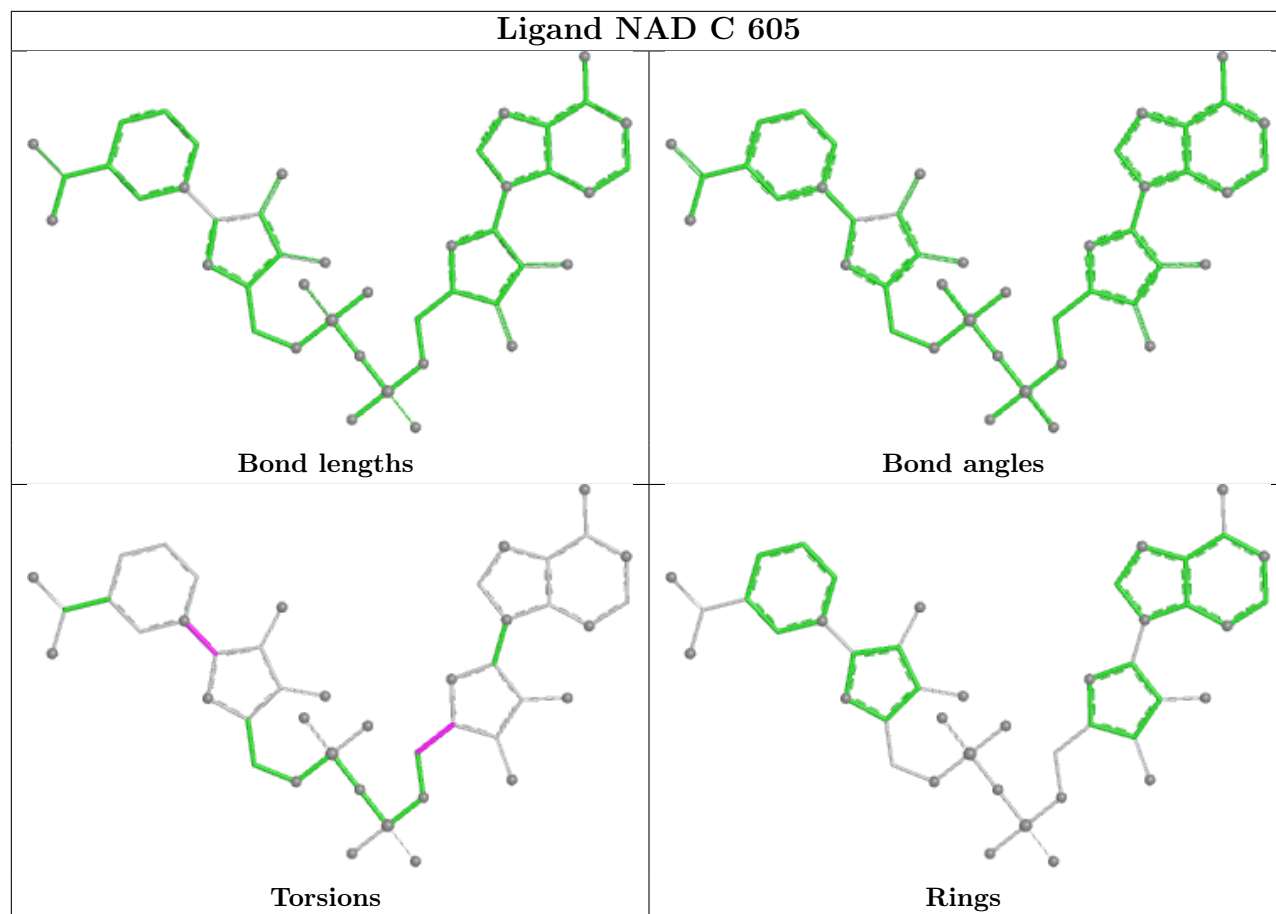


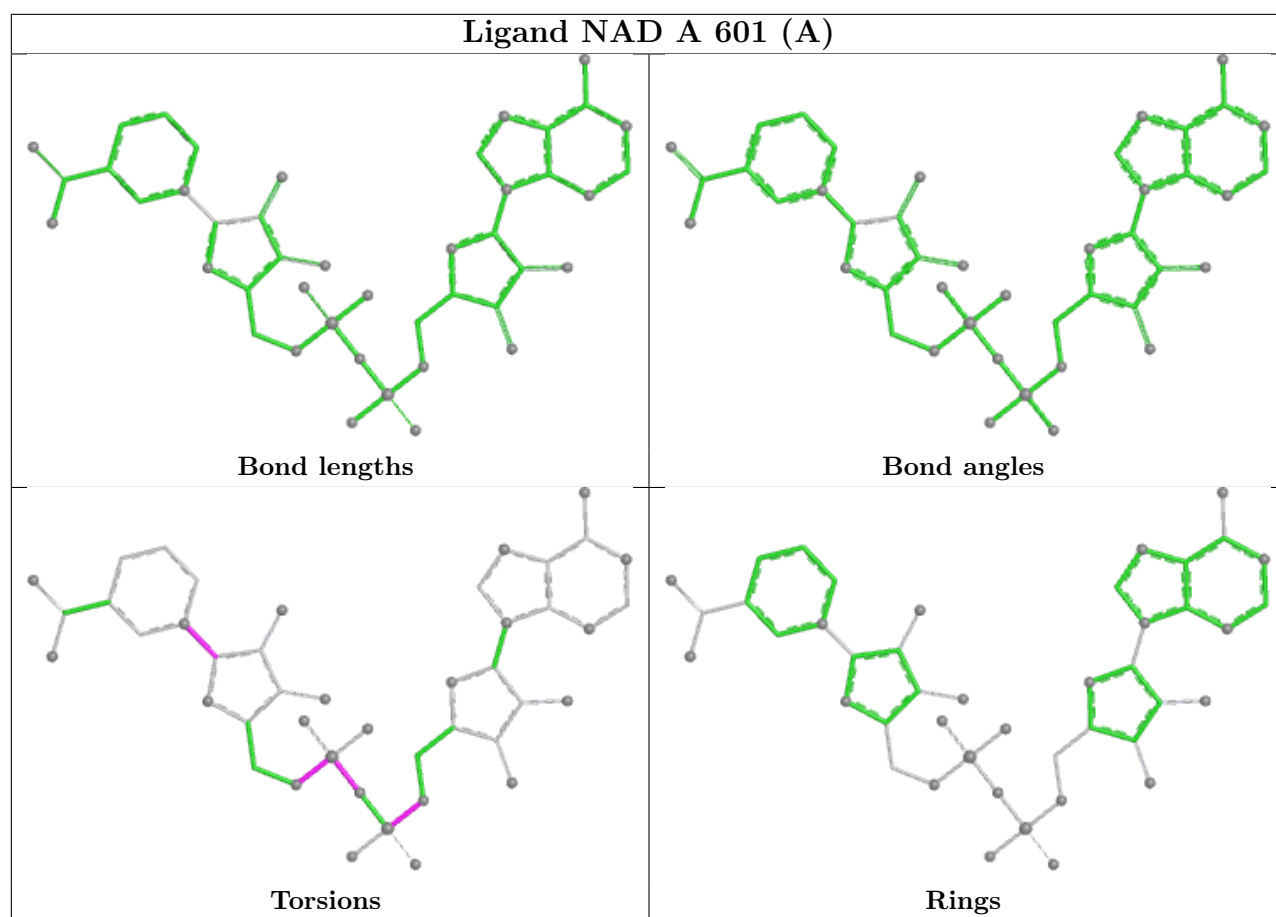


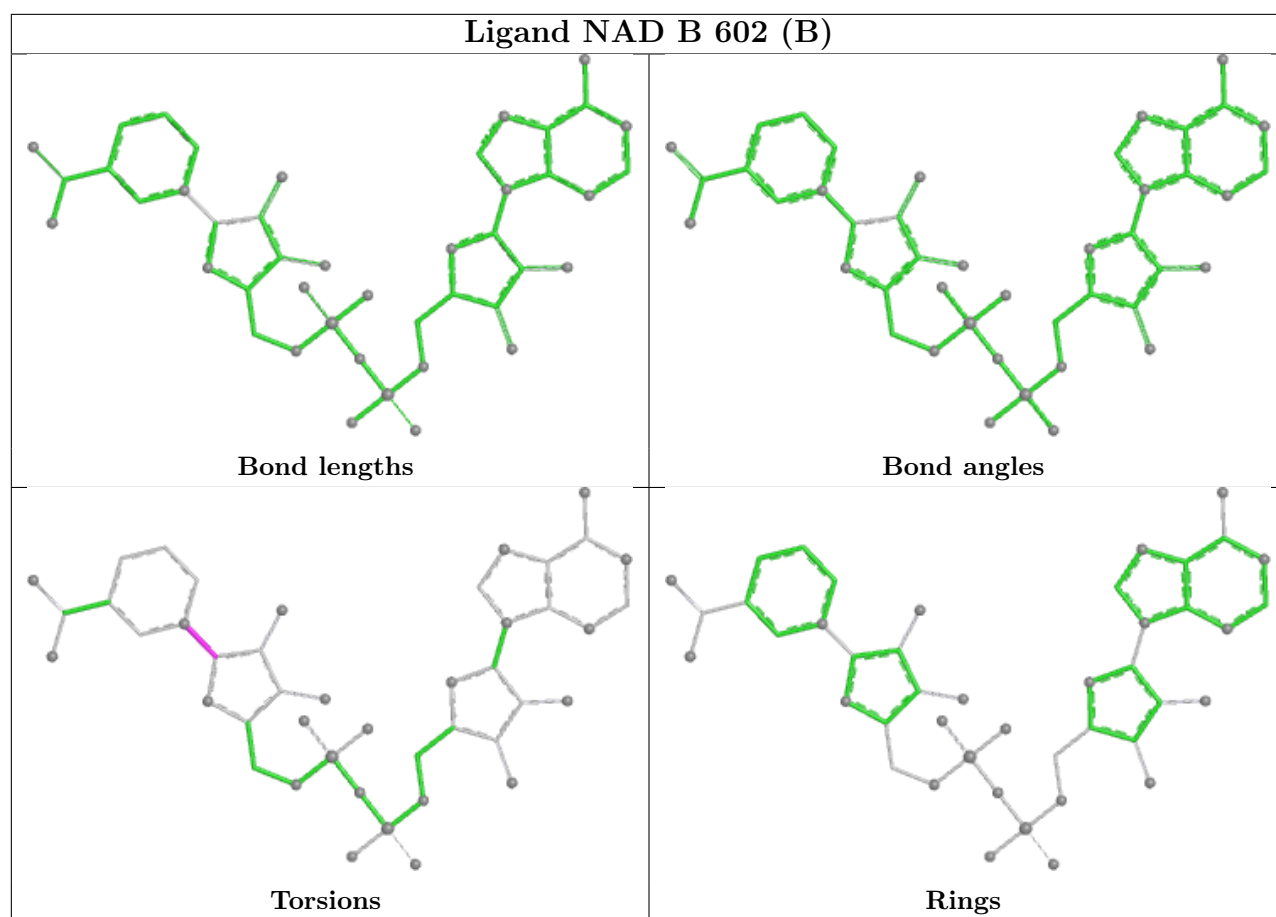


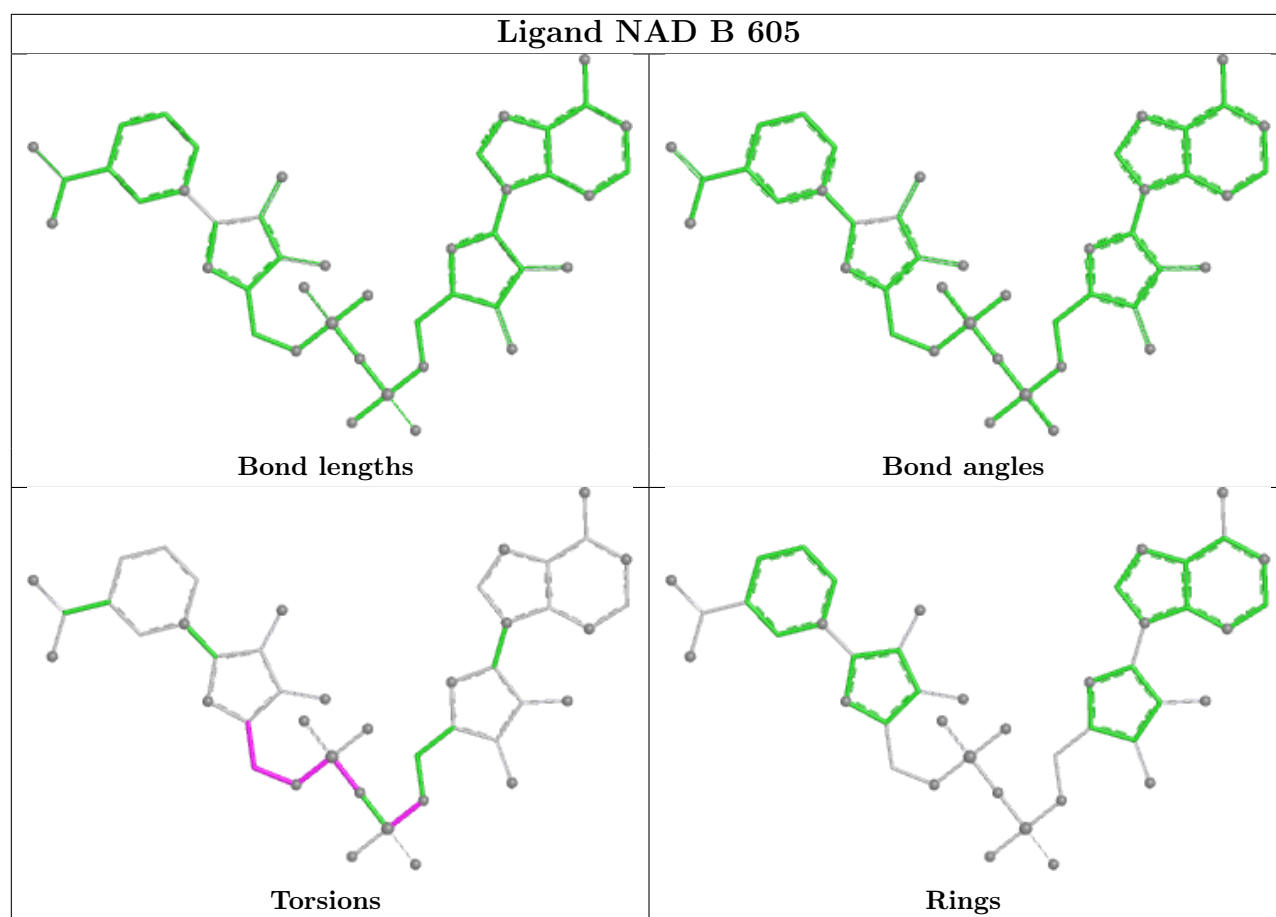












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)

All (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
1	B	75	MET	4.0
1	A	297	VAL	4.0
1	A	580	PRO	4.0
1	D	395	ALA	3.7
1	C	22	LYS	3.7
1	D	452	VAL	3.6
1	A	22	LYS	3.6
1	A	510	GLY	3.6
1	D	76	THR	3.5
1	C	577	SER	3.5
1	B	119	ALA	3.4
1	D	426	ALA	3.3
1	A	298	ILE	3.2
1	B	76	THR	3.2
1	A	76	THR	3.2
1	A	508	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	302	ILE	3.0
1	D	383	ILE	3.0
1	D	396	GLY	2.9
1	A	74	LYS	2.9
1	D	347	TYR	2.9
1	D	358	ILE	2.8
1	B	263[A]	PHE	2.8
1	A	119	ALA	2.8
1	D	380	ALA	2.7
1	D	433	ALA	2.7
1	D	459	VAL	2.7
1	D	74	LYS	2.7
1	A	123	TYR	2.7
1	A	75	MET	2.7
1	D	72	LEU	2.6
1	D	436	LEU	2.6
1	B	302	ILE	2.6
1	D	381	VAL	2.6
1	D	361	TYR	2.6
1	D	435	THR	2.6
1	D	448	PRO	2.6
1	A	507	LEU	2.6
1	C	358	ILE	2.6
1	D	450	GLY	2.6
1	D	297	VAL	2.6
1	C	579	PRO	2.5
1	A	79	LEU	2.5
1	A	73	LYS	2.5
1	D	377	PHE	2.5
1	D	410	ILE	2.5
1	C	459	VAL	2.5
1	D	298	ILE	2.5
1	C	79	LEU	2.4
1	B	23	GLU	2.4
1	B	177[A]	MET	2.4
1	D	579	PRO	2.4
1	B	25	GLY	2.4
1	D	348	GLY	2.4
1	D	428	CYS	2.4
1	D	376	THR	2.3
1	A	295[A]	GLN	2.3
1	D	419	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	508	ALA	2.3
1	C	575	SER	2.3
1	D	351	VAL	2.3
1	D	79	LEU	2.3
1	D	367	HIS	2.3
1	D	344	PHE	2.3
1	C	124	GLY	2.3
1	D	77	SER	2.3
1	C	73	LYS	2.3
1	A	574	GLU	2.2
1	D	401	PRO	2.2
1	B	74	LYS	2.2
1	D	460	PHE	2.2
1	D	409	SER	2.2
1	D	574	GLU	2.2
1	B	455	THR	2.2
1	D	366	THR	2.2
1	B	303	SER	2.2
1	D	398	LEU	2.2
1	A	301	PRO	2.2
1	D	27	PRO	2.2
1	A	24	LYS	2.2
1	D	449	PHE	2.1
1	D	403	VAL	2.1
1	D	25	GLY	2.1
1	A	27	PRO	2.1
1	D	349	LEU	2.1
1	D	73	LYS	2.1
1	A	84	TYR	2.1
1	C	347	TYR	2.1
1	D	123	TYR	2.1
1	D	404	ILE	2.1
1	D	356	ALA	2.1
1	A	505[A]	GLU	2.0
1	D	400	THR	2.0
1	B	301	PRO	2.0
1	B	448	PRO	2.0
1	D	85	ILE	2.0
1	A	455	THR	2.0
1	C	457	GLY	2.0
1	D	580	PRO	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
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

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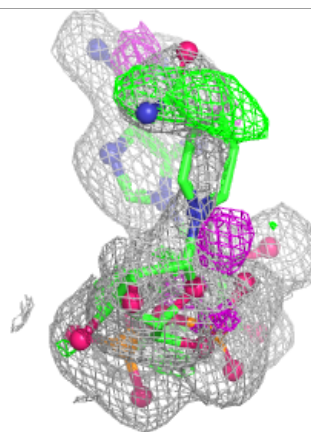
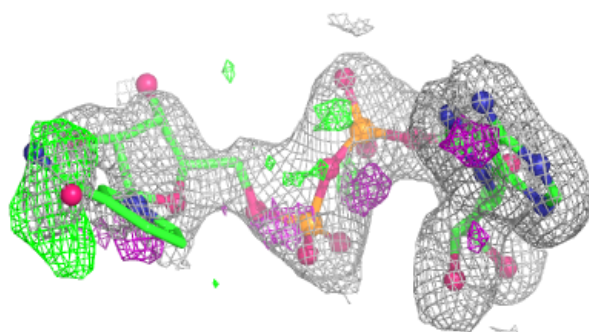
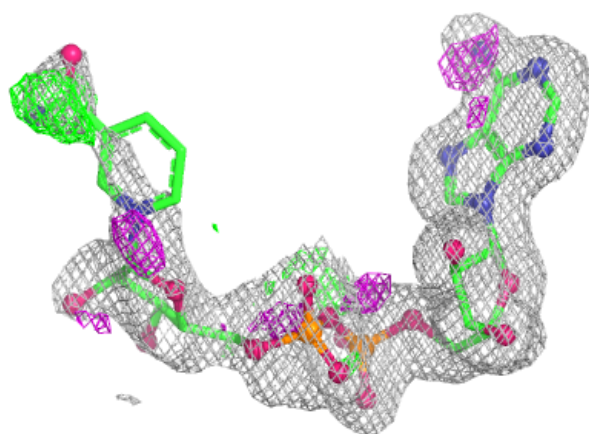
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	D	605	44/44	0.95	0.10	21,38,61,64	0
5	MG	B	606	1/1	0.96	0.09	30,30,30,30	0
5	MG	A	606	1/1	0.97	0.07	34,34,34,34	0
2	NAD	A	605	44/44	0.97	0.06	22,25,34,35	0
4	CL	B	601	1/1	0.99	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.

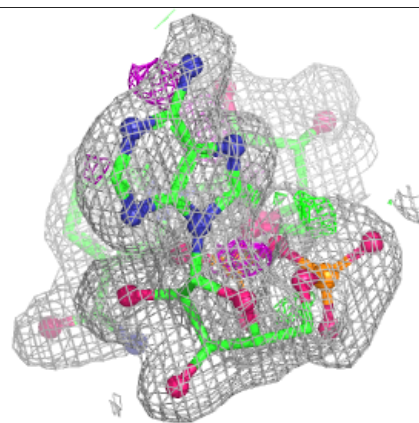
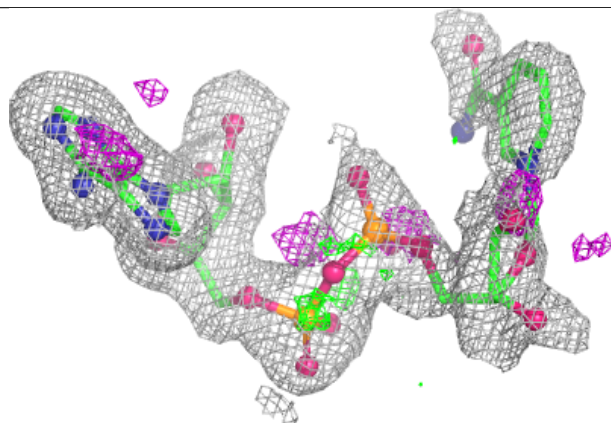
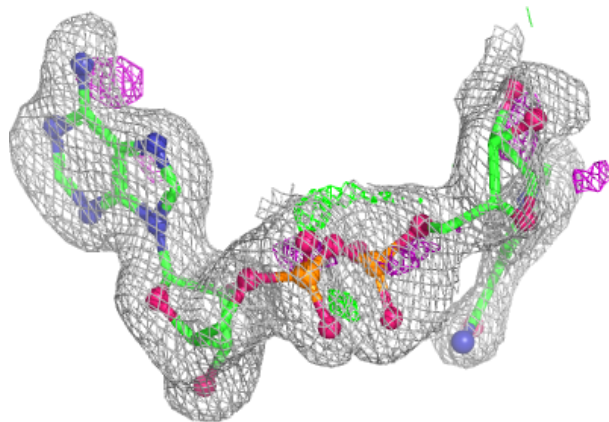
Electron density around NAD A 601 (A):

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

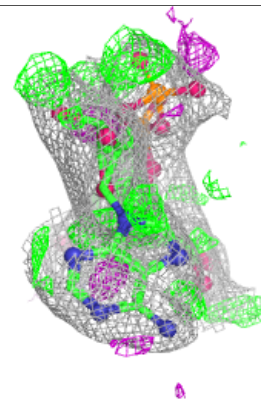
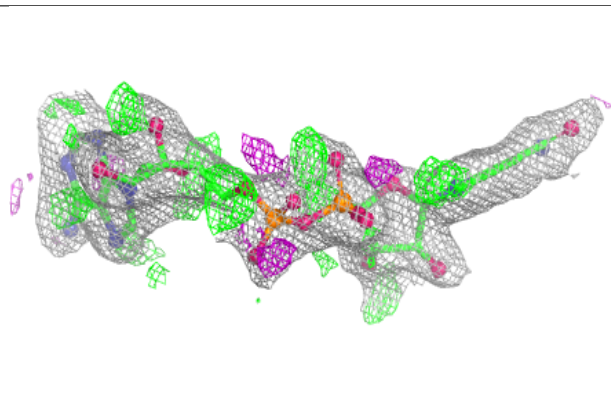
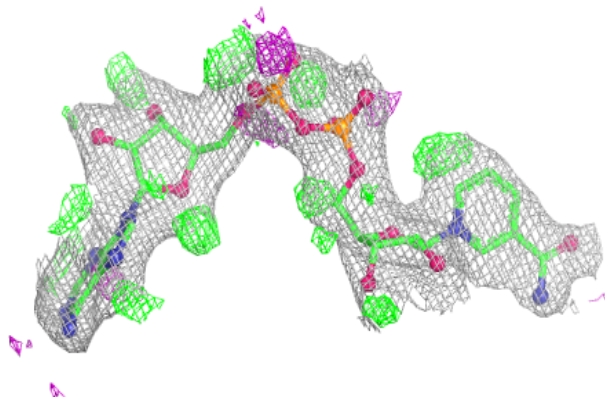


Electron density around NAD A 601 (B):

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and green (positive)

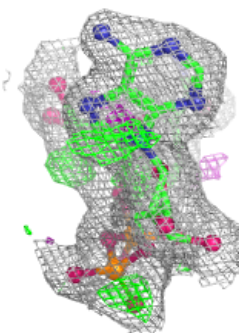
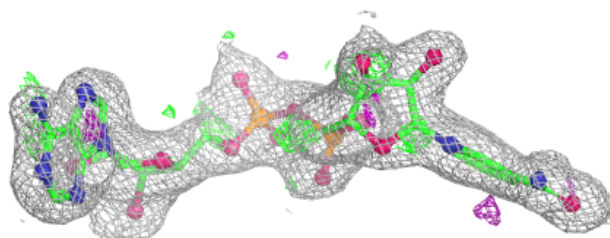
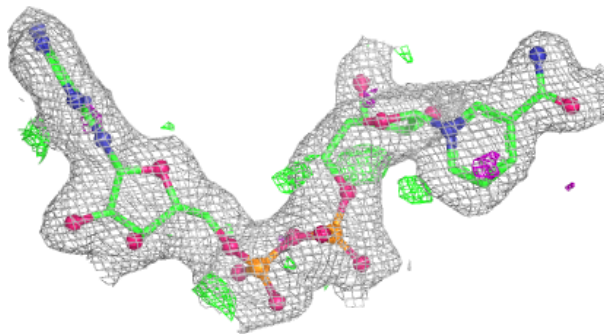
**Electron density around NAD D 603:**

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and green (positive)

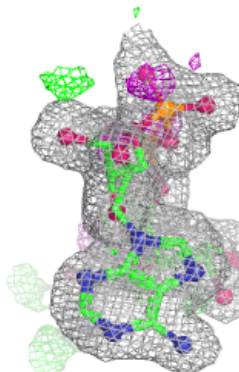
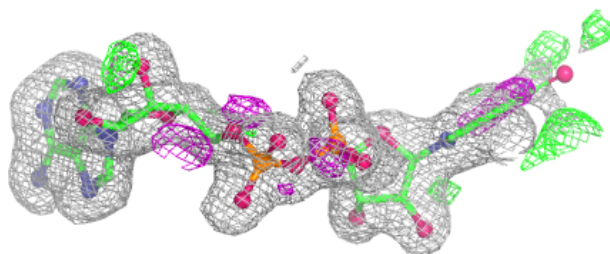
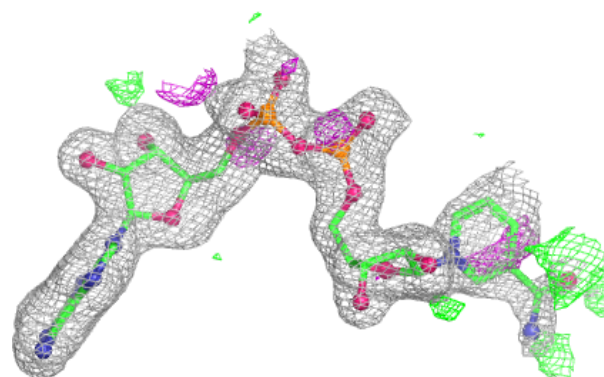


Electron density around NAD C 605:

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and green (positive)

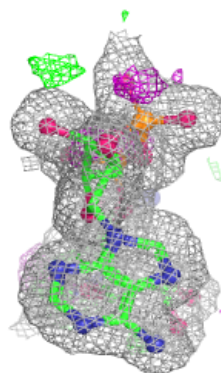
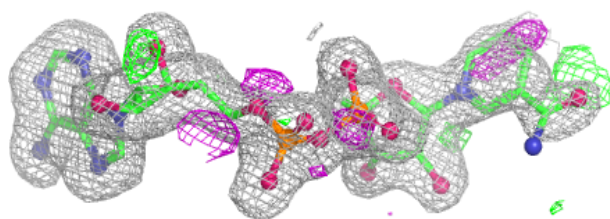
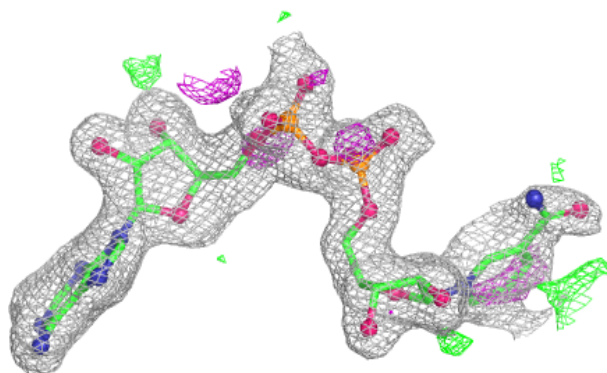
**Electron density around NAD B 602 (A):**

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

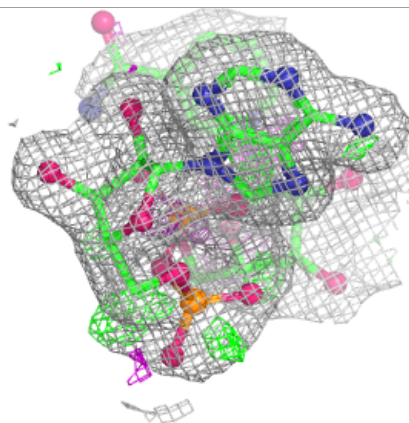
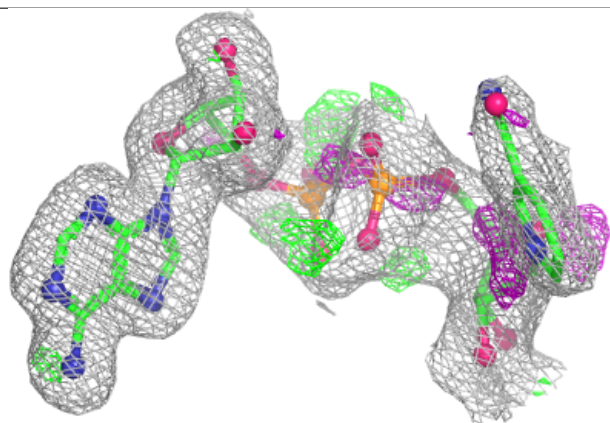
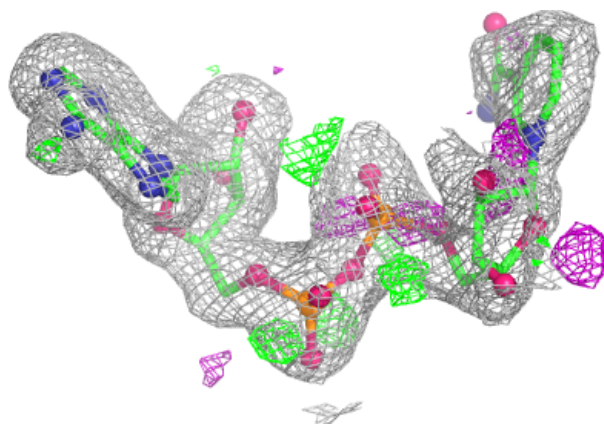


Electron density around NAD B 602 (B):

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and green (positive)

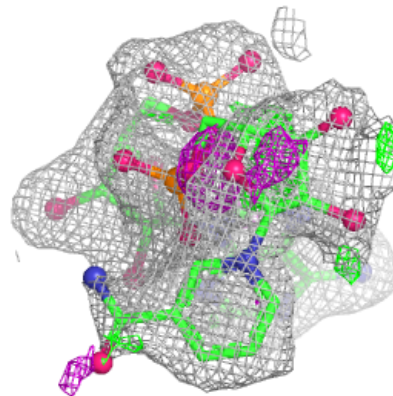
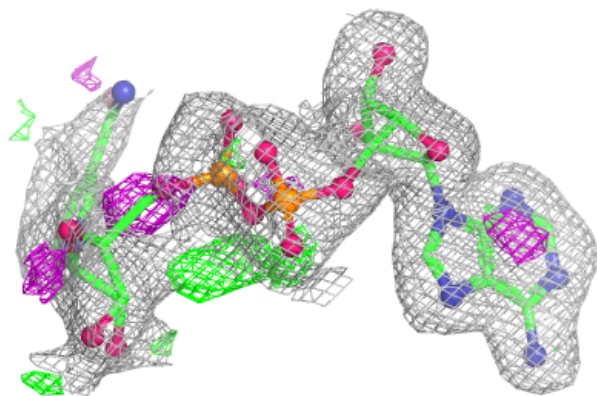
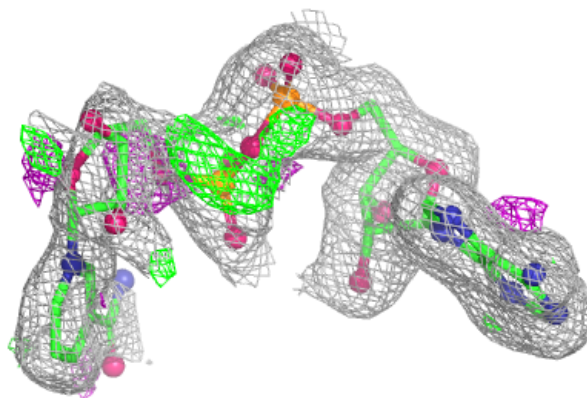
**Electron density around NAD B 605:**

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and green (positive)



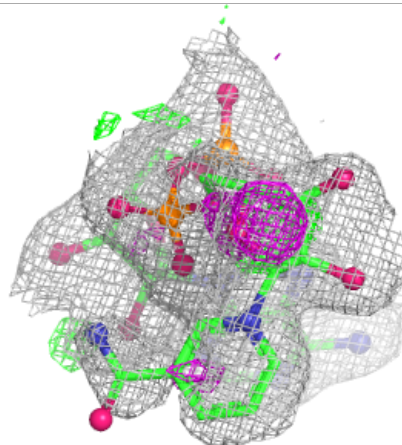
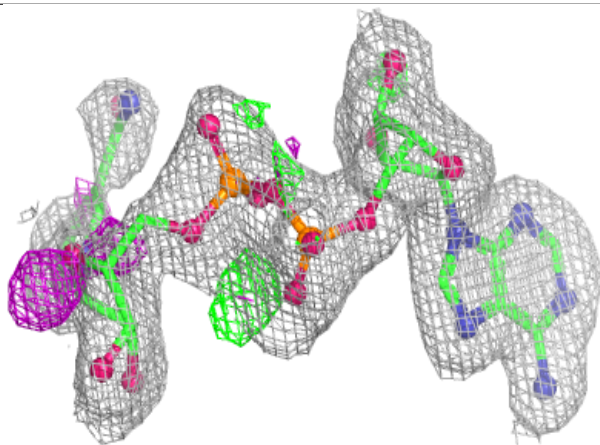
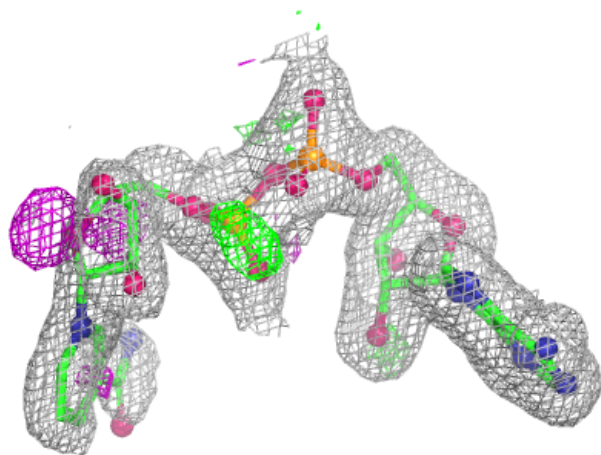
Electron density around NAD C 604:

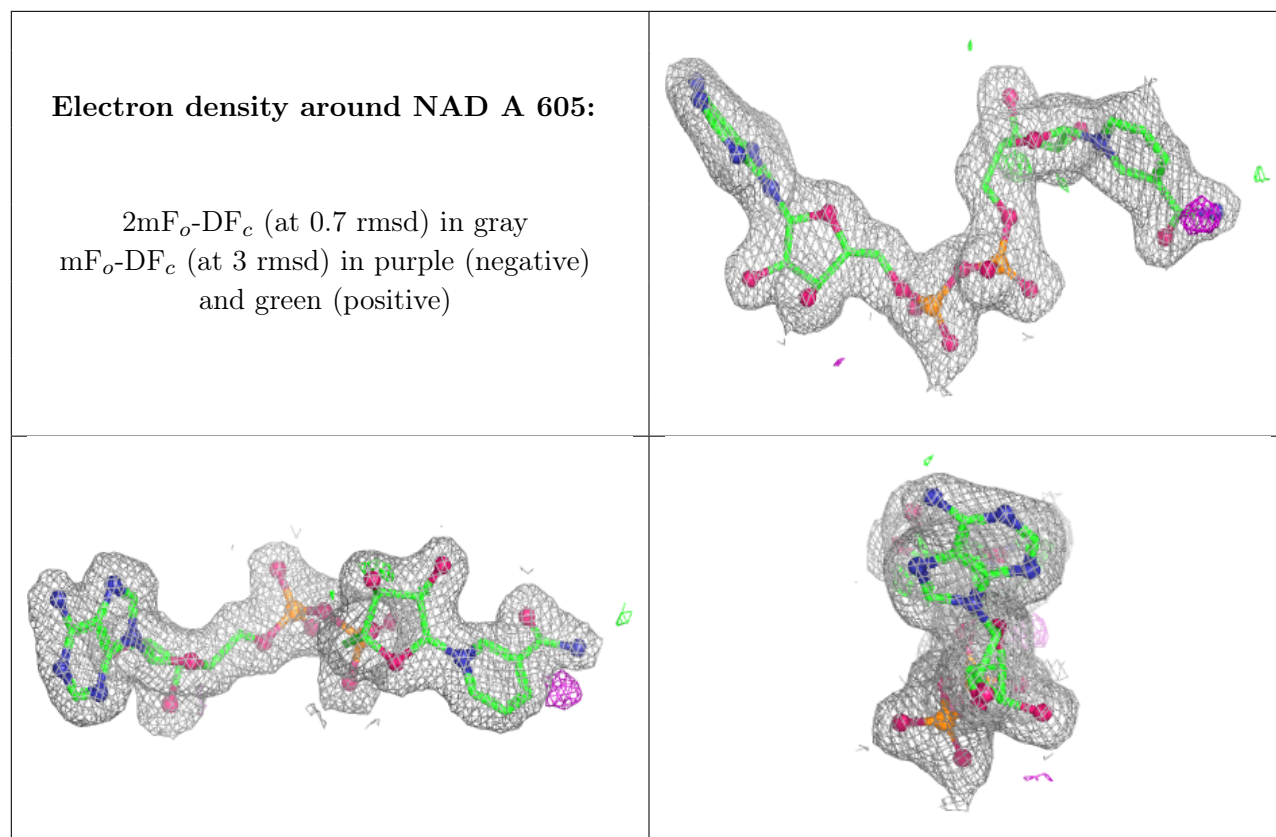
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and green (positive)



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.