



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 02:23 AM EDT

PDB ID : 6O4L
Title : Structure of ALDH7A1 mutant E399D complexed with NAD
Authors : Tanner, J.J.; Korasick, D.A.; Laciak, A.R.
Deposited on : 2019-02-28
Resolution : 1.85 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16298 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 Alpha-aminoadipic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	508	3853	2445	670	721	17	0	0	0
1	B	507	3838	2438	667	715	18	0	2	0
1	C	508	3832	2434	666	715	17	0	1	0
1	D	509	3824	2428	667	712	17	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49419
A	0	HIS	-	expression tag	UNP P49419
A	399	ASP	GLU	engineered mutation	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
B	399	ASP	GLU	engineered mutation	UNP P49419
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
C	399	ASP	GLU	engineered mutation	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
D	399	ASP	GLU	engineered mutation	UNP P49419

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

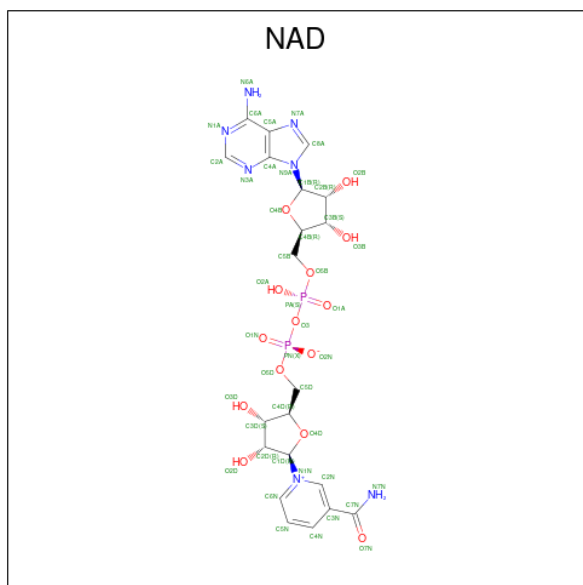


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	212	212	212	0	0
5	B	207	207	207	0	0
5	C	178	178	178	0	0
5	D	160	160	160	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.79Å 127.50Å 88.39Å 90.00° 101.26° 90.00°	Depositor
Resolution (Å)	45.72 – 1.85	Depositor
% Data completeness (in resolution range)	95.4 (45.72-1.85)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.86Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.174 , 0.220	Depositor
Wilson B-factor (Å ²)	27.4	Xtrriage
Anisotropy	0.410	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	16298	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 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
2	EDO	D	601	-	3,3,3	0.48	0	2,2,2	0.39	0
4	NAD	D	602	-	42,48,48	5.21	16 (38%)	50,73,73	1.36	5 (10%)
2	EDO	A	602	-	3,3,3	0.49	0	2,2,2	0.28	0
4	NAD	B	603	-	42,48,48	5.13	16 (38%)	50,73,73	1.30	5 (10%)
4	NAD	C	601	-	42,48,48	5.15	15 (35%)	50,73,73	1.34	5 (10%)
2	EDO	B	601	-	3,3,3	0.45	0	2,2,2	0.56	0
2	EDO	A	601	-	3,3,3	0.48	0	2,2,2	0.38	0
4	NAD	A	604	-	42,48,48	5.00	15 (35%)	50,73,73	1.25	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	601	-	-	0/1/1/1	-
4	NAD	D	602	-	-	2/26/62/62	0/5/5/5
2	EDO	A	602	-	-	0/1/1/1	-
4	NAD	B	603	-	-	1/26/62/62	0/5/5/5
4	NAD	C	601	-	-	4/26/62/62	0/5/5/5
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	A	601	-	-	1/1/1/1	-
4	NAD	A	604	-	-	4/26/62/62	0/5/5/5

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	NAD	C2D-C1D	-15.74	1.29	1.53
4	C	601	NAD	C2D-C1D	-15.71	1.29	1.53
4	D	602	NAD	C2B-C1B	-15.67	1.30	1.53
4	A	604	NAD	C2D-C1D	-15.51	1.30	1.53
4	B	603	NAD	C2B-C1B	-15.42	1.30	1.53
4	D	602	NAD	C2D-C1D	-15.39	1.30	1.53
4	C	601	NAD	O4D-C1D	15.24	1.62	1.41
4	C	601	NAD	C2B-C1B	-15.24	1.30	1.53
4	D	602	NAD	O4D-C1D	15.22	1.62	1.41
4	B	603	NAD	O4D-C1D	14.97	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	NAD	O4D-C1D	14.89	1.61	1.41
4	D	602	NAD	O4B-C1B	14.88	1.61	1.41
4	A	604	NAD	C2B-C1B	-14.81	1.31	1.53
4	C	601	NAD	O4B-C1B	14.22	1.60	1.41
4	B	603	NAD	O4B-C1B	13.75	1.60	1.41
4	A	604	NAD	O4B-C1B	13.01	1.59	1.41
4	B	603	NAD	O4B-C4B	-6.66	1.30	1.45
4	D	602	NAD	C7N-N7N	6.38	1.45	1.33
4	C	601	NAD	O4B-C4B	-6.30	1.30	1.45
4	D	602	NAD	O4B-C4B	-6.28	1.31	1.45
4	A	604	NAD	C7N-N7N	6.25	1.44	1.33
4	A	604	NAD	O4B-C4B	-6.22	1.31	1.45
4	C	601	NAD	C7N-N7N	6.18	1.44	1.33
4	B	603	NAD	C7N-N7N	6.13	1.44	1.33
4	A	604	NAD	O4D-C4D	-5.99	1.31	1.45
4	B	603	NAD	O4D-C4D	-5.96	1.31	1.45
4	C	601	NAD	O4D-C4D	-5.93	1.31	1.45
4	D	602	NAD	O4D-C4D	-5.90	1.31	1.45
4	A	604	NAD	C3N-C7N	3.92	1.56	1.50
4	D	602	NAD	C3N-C7N	3.70	1.56	1.50
4	B	603	NAD	C3N-C7N	3.60	1.56	1.50
4	C	601	NAD	C3N-C7N	3.57	1.55	1.50
4	B	603	NAD	O3D-C3D	-3.24	1.35	1.43
4	A	604	NAD	O3D-C3D	-3.22	1.35	1.43
4	B	603	NAD	C2N-N1N	3.19	1.38	1.35
4	B	603	NAD	O3B-C3B	-3.13	1.35	1.43
4	D	602	NAD	C2A-N3A	3.09	1.37	1.32
4	C	601	NAD	O3D-C3D	-3.08	1.35	1.43
4	D	602	NAD	O3D-C3D	-3.08	1.35	1.43
4	D	602	NAD	O3B-C3B	-3.06	1.35	1.43
4	A	604	NAD	C2A-N3A	3.06	1.37	1.32
4	C	601	NAD	O3B-C3B	-2.99	1.35	1.43
4	B	603	NAD	C2A-N3A	2.89	1.36	1.32
4	C	601	NAD	O2B-C2B	2.83	1.49	1.43
4	D	602	NAD	O2B-C2B	2.79	1.49	1.43
4	D	602	NAD	C6A-N6A	2.78	1.44	1.34
4	A	604	NAD	C2N-N1N	2.75	1.38	1.35
4	A	604	NAD	O3B-C3B	-2.72	1.36	1.43
4	C	601	NAD	C2N-N1N	2.71	1.38	1.35
4	D	602	NAD	C2N-N1N	2.64	1.38	1.35
4	B	603	NAD	O2B-C2B	2.58	1.49	1.43
4	C	601	NAD	C6A-N6A	2.57	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	NAD	C2A-N3A	2.55	1.36	1.32
4	A	604	NAD	C6A-N6A	2.51	1.43	1.34
4	D	602	NAD	O2D-C2D	2.44	1.48	1.43
4	A	604	NAD	O2D-C2D	2.42	1.48	1.43
4	B	603	NAD	C6A-N6A	2.38	1.42	1.34
4	C	601	NAD	O2D-C2D	2.37	1.48	1.43
4	B	603	NAD	O2D-C2D	2.23	1.48	1.43
4	B	603	NAD	C5A-C4A	-2.20	1.35	1.40
4	A	604	NAD	C5A-C4A	-2.13	1.35	1.40
4	D	602	NAD	C5A-C4A	-2.09	1.35	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	NAD	N3A-C2A-N1A	-5.64	119.86	128.68
4	A	604	NAD	N3A-C2A-N1A	-5.27	120.45	128.68
4	C	601	NAD	N3A-C2A-N1A	-5.00	120.86	128.68
4	D	602	NAD	N3A-C2A-N1A	-4.90	121.02	128.68
4	C	601	NAD	C5A-C6A-N6A	3.95	126.36	120.35
4	D	602	NAD	C5A-C6A-N6A	3.91	126.30	120.35
4	D	602	NAD	C6N-N1N-C2N	-3.08	119.16	121.97
4	B	603	NAD	C3D-C2D-C1D	2.87	105.30	100.98
4	A	604	NAD	C5A-C6A-N6A	2.72	124.48	120.35
4	C	601	NAD	O4B-C1B-C2B	-2.63	103.08	106.93
4	C	601	NAD	C6N-N1N-C2N	-2.59	119.61	121.97
4	B	603	NAD	C5A-C6A-N6A	2.53	124.20	120.35
4	D	602	NAD	N6A-C6A-N1A	-2.46	113.48	118.57
4	A	604	NAD	C3D-C2D-C1D	2.45	104.67	100.98
4	D	602	NAD	C3D-C2D-C1D	2.37	104.55	100.98
4	B	603	NAD	C6N-N1N-C2N	-2.30	119.87	121.97
4	A	604	NAD	O4B-C1B-C2B	-2.30	103.56	106.93
4	C	601	NAD	N6A-C6A-N1A	-2.28	113.83	118.57
4	A	604	NAD	C6N-N1N-C2N	-2.24	119.93	121.97
4	B	603	NAD	O7N-C7N-N7N	-2.12	119.56	122.58

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	NAD	C5D-O5D-PN-O1N
4	B	603	NAD	PN-O3-PA-O5B
4	C	601	NAD	C5D-O5D-PN-O1N

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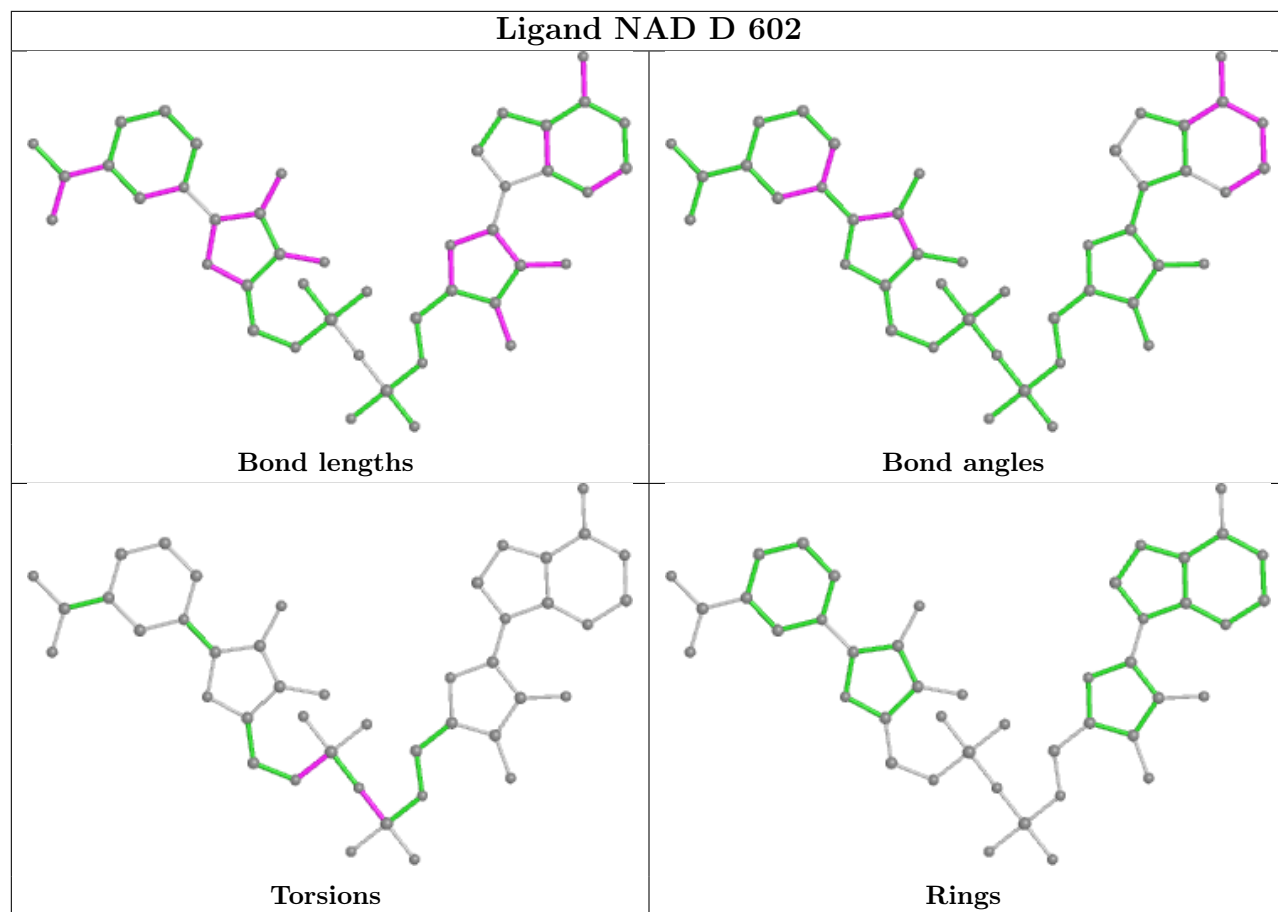
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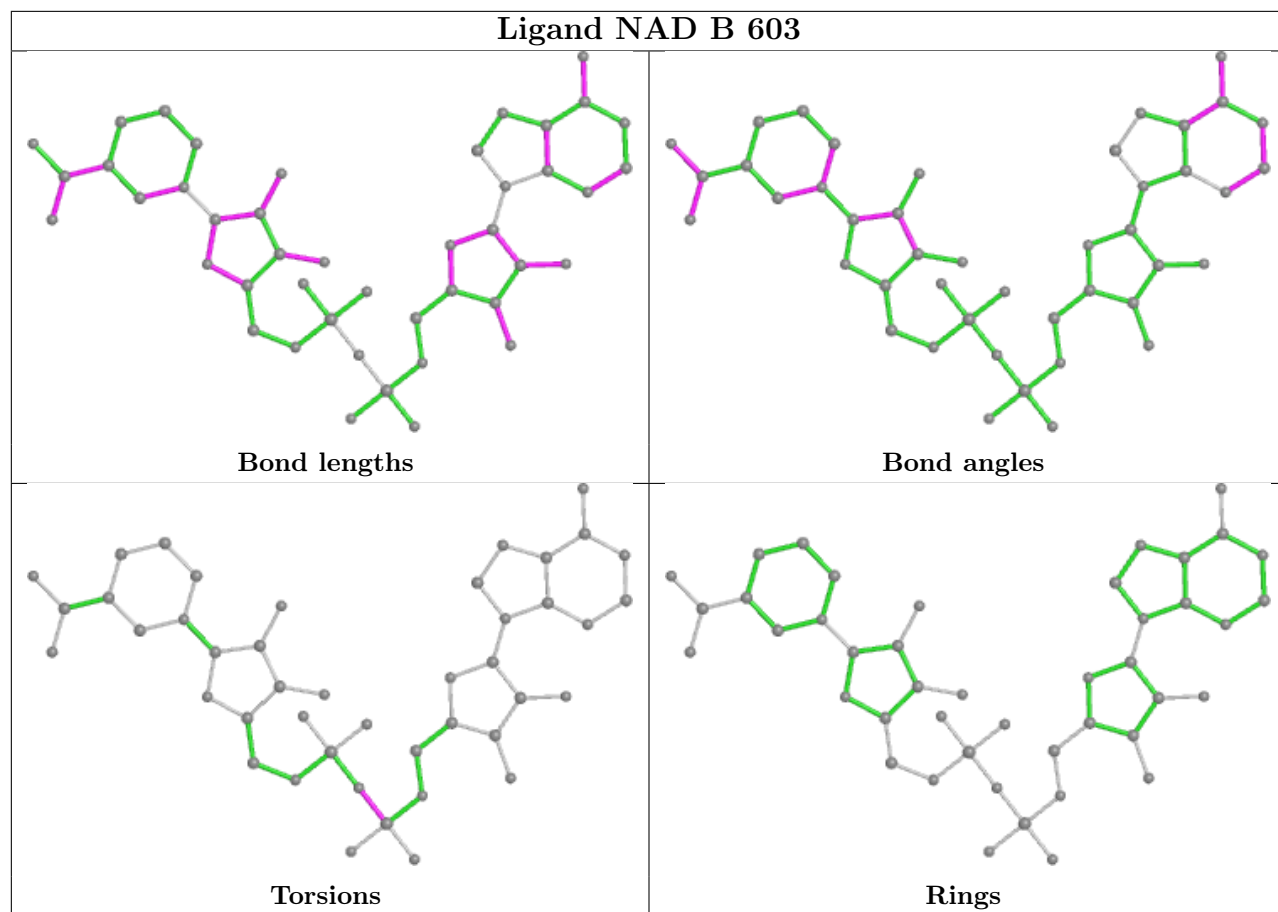
Mol	Chain	Res	Type	Atoms
4	A	604	NAD	PN-O3-PA-O5B
4	C	601	NAD	PN-O3-PA-O5B
4	D	602	NAD	PN-O3-PA-O5B
4	A	604	NAD	C5D-O5D-PN-O3
4	C	601	NAD	C5D-O5D-PN-O3
2	A	601	EDO	O1-C1-C2-O2
4	C	601	NAD	C3D-C4D-C5D-O5D
4	A	604	NAD	C3D-C4D-C5D-O5D
4	D	602	NAD	C5D-O5D-PN-O1N

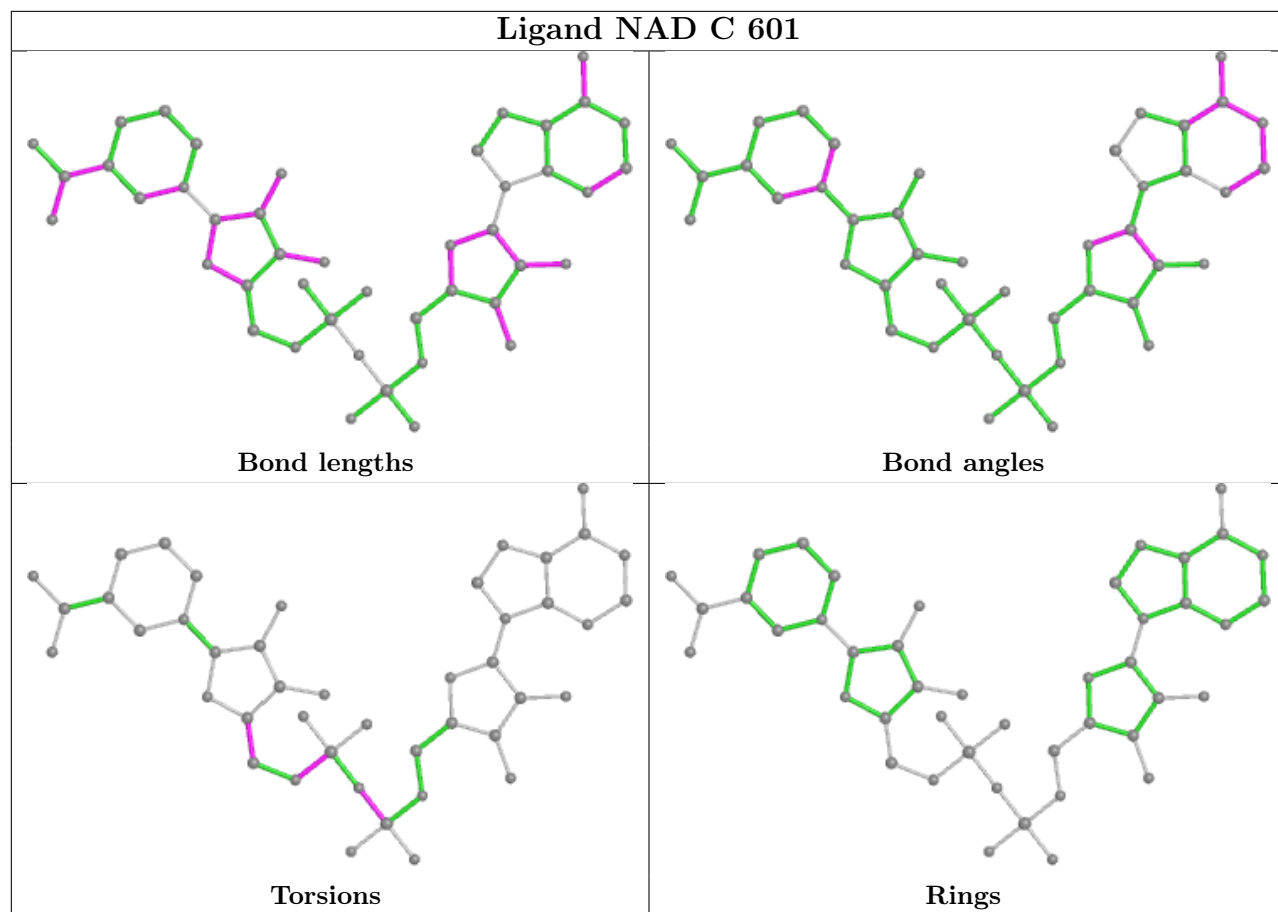
There are no ring outliers.

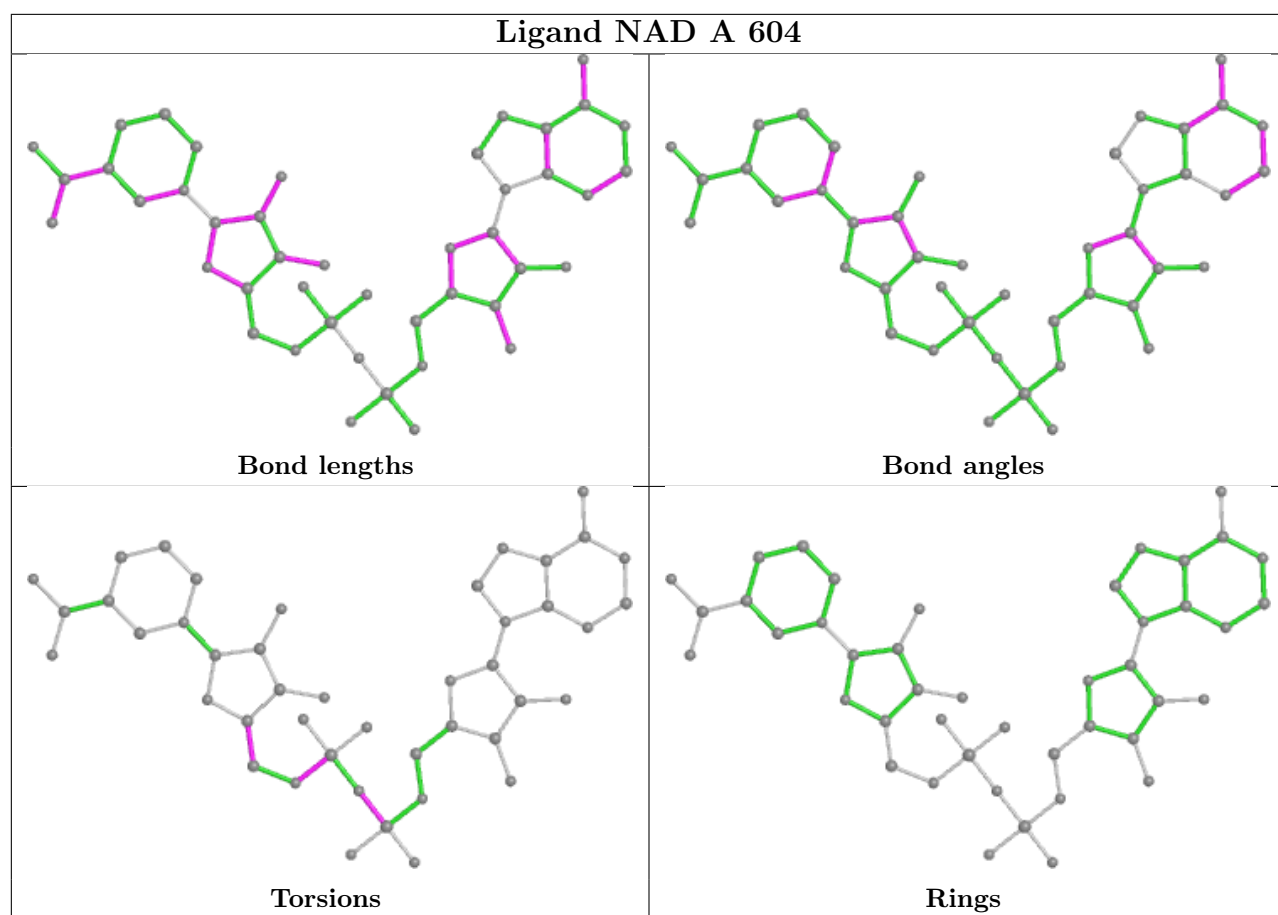
No monomer is involved in short contacts.

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.









4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.