Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 02:47 PM EST

PDB ID	:	2OHX
Title	:	REFINED CRYSTAL STRUCTURE OF LIVER ALCOHOL DEHYDROGENASE-NADH COMPLEX AT 1.8 ANGSTROMS RESOLUTION
Authors	:	Al-Karadaghi, S.; Cedergren-Zeppezauer, E.S.
Deposited on	:	1993-08-24
Resolution	:	1.80 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:

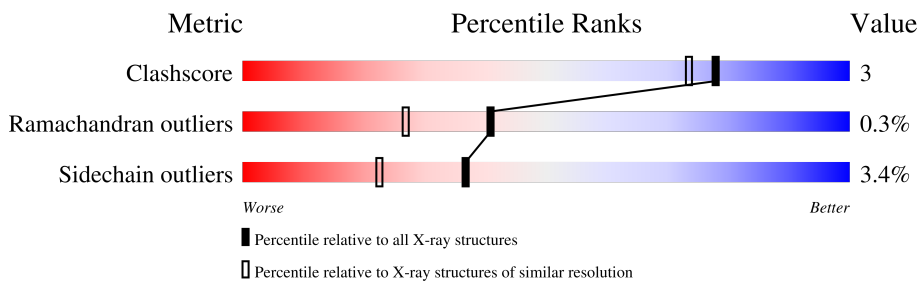|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.3%
Sidechain outliers		3.4%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	92% 6% ·
1	B	374	87% 11% ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6129 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 ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total 2785	C 1769	N 472	O 521	S 23	65	0	0
1	B	374	Total 2785	C 1769	N 472	O 521	S 23	73	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

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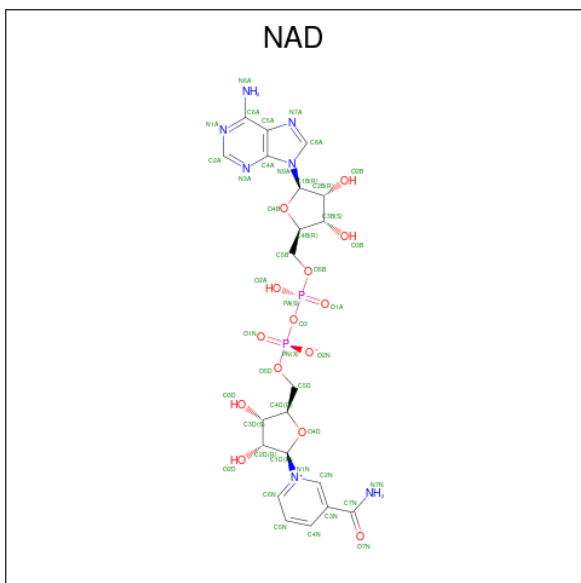
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).
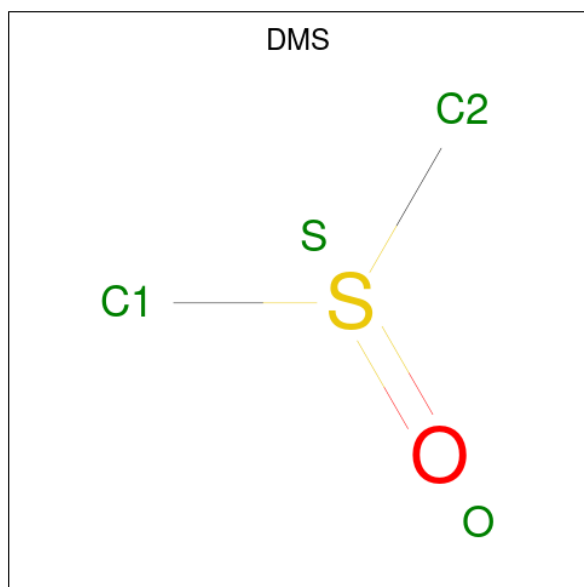
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	241	Total	O	0	0
			241	241		
5	B	218	Total	O	0	0
			218	218		

3 Residue-property plots ⓘ

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. 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. 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.
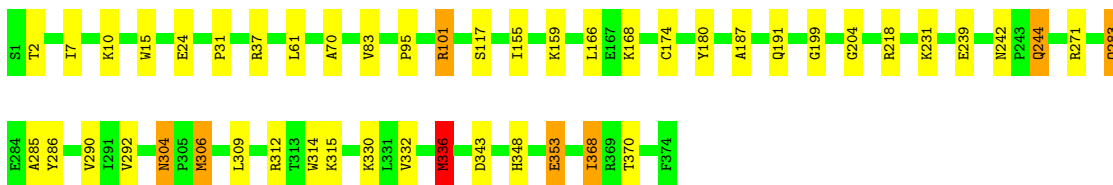
Note EDS was not executed.

• Molecule 1: ALCOHOL DEHYDROGENASE

Chain A:

• Molecule 1: ALCOHOL DEHYDROGENASE

Chain B:

4　Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.76Å　44.54Å　94.61Å 104.80°　102.30°　70.60°	Depositor
Resolution (Å)	10.00　–　1.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.173　,　(Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6129	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	0.80	0/2837	1.37	16/3834 (0.4%)
1	B	0.78	0/2837	1.43	20/3834 (0.5%)
All	All	0.79	0/5674	1.40	36/7668 (0.5%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	ARG	NE-CZ-NH1	24.02	132.31	120.30
1	B	101	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	B	180	TYR	CB-CG-CD1	-8.84	115.69	121.00
1	B	314	TRP	CD1-CG-CD2	8.79	113.34	106.30
1	A	37	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	312	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	A	312	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	271	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	B	101	ARG	NH1-CZ-NH2	-7.64	111.00	119.40
1	B	15	TRP	CD1-CG-CD2	7.43	112.25	106.30
1	B	336	MET	CG-SD-CE	7.42	112.06	100.20
1	B	314	TRP	CE2-CD2-CG	-7.32	101.44	107.30
1	A	15	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	B	15	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	271	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	15	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	A	314	TRP	CD1-CG-CD2	6.94	111.85	106.30
1	A	101	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	15	TRP	CG-CD2-CE3	6.61	139.85	133.90
1	B	306	MET	CG-SD-CE	6.25	110.20	100.20
1	B	271	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	304	ASN	CB-CG-ND2	6.13	131.41	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	VAL	CG1-CB-CG2	-5.96	101.36	110.90
1	B	312	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	314	TRP	CE2-CD2-CG	-5.78	102.67	107.30
1	B	15	TRP	CB-CG-CD1	-5.76	119.50	127.00
1	B	286	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	B	314	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	B	353	GLU	CA-CB-CG	-5.54	101.22	113.40
1	B	368	ILE	N-CA-C	-5.41	96.39	111.00
1	A	129	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	303	MET	CA-CB-CG	5.22	122.18	113.30
1	B	15	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	A	304	ASN	OD1-CG-ND2	-5.02	110.36	121.90
1	A	246	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	B	218	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2785	0	2848	13	0
1	B	2785	0	2848	21	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	241	0	0	2	0
5	B	218	0	0	1	0
All	All	6129	0	5760	32	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 3.

All (32) 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)
5:A:500:HOH:O	1:B:101:ARG:HD3	1.91	0.69
1:B:242:ASN:OD1	1:B:244:GLN:HG2	1.95	0.67
1:B:283:GLN:NE2	1:B:285:ALA:H	1.96	0.63
1:A:336:MET:HA	1:A:336:MET:HE2	1.82	0.59
1:B:283:GLN:HE22	1:B:285:ALA:H	1.52	0.56
1:A:283:GLN:NE2	1:A:285:ALA:H	2.05	0.55
1:A:101:ARG:HE	1:B:283:GLN:HG3	1.72	0.55
1:B:101:ARG:NH2	5:B:407:HOH:O	2.40	0.54
1:B:283:GLN:HE22	1:B:285:ALA:HB3	1.73	0.53
1:B:31:PRO:HD3	1:B:37:ARG:HB2	1.90	0.53
1:A:260:GLY:HA3	5:A:500:HOH:O	2.13	0.48
1:A:283:GLN:HE22	1:A:285:ALA:H	1.62	0.47
1:B:83:VAL:HG12	1:B:159:LYS:HB2	1.95	0.47
1:B:304:ASN:ND2	1:B:306:MET:H	2.13	0.46
1:A:283:GLN:HG3	1:B:101:ARG:NH2	2.31	0.46
1:B:199:GLY:O	1:B:204:GLY:HA3	2.16	0.45
1:A:70:ALA:HB1	1:A:166:LEU:HD22	1.98	0.45
1:B:10:LYS:HA	1:B:24:GLU:O	2.17	0.44
1:B:187:ALA:HB2	1:B:290:VAL:HG21	1.99	0.43
1:A:23:ILE:HD11	1:A:355:ILE:CG2	2.49	0.43
1:B:332:VAL:O	1:B:336:MET:HG2	2.19	0.43
1:B:292:VAL:O	3:B:403:NAD:H2N	2.20	0.42
1:A:231:LYS:HE3	1:A:344:PRO:O	2.20	0.42
1:B:348:HIS:O	1:B:370:THR:HA	2.20	0.41
1:B:70:ALA:HB1	1:B:166:LEU:HD22	2.01	0.41
1:B:168:LYS:HE3	1:B:343:ASP:OD1	2.20	0.41
1:A:174:CYS:SG	3:A:403:NAD:H5N	2.60	0.41
1:B:95:PRO:HB2	1:B:155:ILE:HD12	2.03	0.41
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.20	0.40
1:A:306:MET:SD	1:A:309:LEU:HD12	2.60	0.40
1:B:2:THR:HB	1:B:7:ILE:HD11	2.03	0.40
1:A:304:ASN:ND2	1:A:306:MET:H	2.18	0.40

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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	372/374 (100%)	358 (96%)	14 (4%)	0	100	100
1	B	372/374 (100%)	361 (97%)	9 (2%)	2 (0%)	29	15
All	All	744/748 (100%)	719 (97%)	23 (3%)	2 (0%)	41	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	CYS
1	B	368	ILE

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	308/308 (100%)	300 (97%)	8 (3%)	46	32
1	B	308/308 (100%)	295 (96%)	13 (4%)	30	15
All	All	616/616 (100%)	595 (97%)	21 (3%)	37	22

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	SER
1	A	231	LYS
1	A	239	GLU
1	A	283	GLN

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Mol	Chain	Res	Type
1	A	300	ASN
1	A	304	ASN
1	A	309	LEU
1	A	338	LYS
1	B	61	LEU
1	B	117	SER
1	B	191	GLN
1	B	231	LYS
1	B	239	GLU
1	B	244	GLN
1	B	283	GLN
1	B	304	ASN
1	B	309	LEU
1	B	315	LYS
1	B	330	LYS
1	B	336	MET
1	B	353	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	300	ASN
1	A	304	ASN
1	B	283	GLN
1	B	304	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5　Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	DMS	B	404	2	3,3,3	0.42	0	3,3,3	1.83	2 (66%)
4	DMS	A	404	2	3,3,3	0.32	0	3,3,3	0.90	0
3	NAD	A	403	-	42,48,48	1.17	3 (7%)	50,73,73	1.33	7 (14%)
3	NAD	B	403	-	42,48,48	1.09	2 (4%)	50,73,73	1.37	6 (12%)

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	NAD	A	403	-	-	5/26/62/62	0/5/5/5
3	NAD	B	403	-	-	5/26/62/62	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	NAD	C2N-N1N	4.25	1.40	1.35
3	A	403	NAD	C2N-N1N	3.45	1.39	1.35
3	B	403	NAD	C3N-C7N	2.22	1.53	1.50
3	A	403	NAD	C5A-N7A	-2.22	1.31	1.39
3	A	403	NAD	C2B-C1B	-2.11	1.50	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	NAD	N3A-C2A-N1A	-4.21	122.10	128.68
3	A	403	NAD	C4A-C5A-N7A	4.17	113.75	109.40
3	B	403	NAD	C4A-C5A-N7A	3.43	112.98	109.40
3	B	403	NAD	O4D-C1D-C2D	-3.38	101.98	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	NAD	N3A-C2A-N1A	-3.27	123.57	128.68
3	B	403	NAD	C6N-N1N-C2N	-2.81	119.42	121.97
3	B	403	NAD	C1B-N9A-C4A	-2.61	122.05	126.64
3	A	403	NAD	O4B-C1B-C2B	-2.57	103.17	106.93
3	A	403	NAD	N6A-C6A-N1A	2.57	123.90	118.57
3	A	403	NAD	C5A-C6A-N1A	-2.50	114.68	120.35
3	A	403	NAD	O7N-C7N-C3N	-2.37	116.79	119.63
4	B	404	DMS	C2-S-C1	-2.27	86.76	98.44
4	B	404	DMS	O-S-C2	2.19	117.70	106.54
3	A	403	NAD	O5B-C5B-C4B	-2.18	101.50	108.99
3	B	403	NAD	C5A-C6A-N1A	-2.10	115.60	120.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	NAD	O4D-C1D-N1N-C2N
3	A	403	NAD	O4D-C1D-N1N-C6N
3	A	403	NAD	C2D-C1D-N1N-C2N
3	A	403	NAD	C2D-C1D-N1N-C6N
3	B	403	NAD	O4D-C1D-N1N-C2N
3	B	403	NAD	O4D-C1D-N1N-C6N
3	B	403	NAD	C2D-C1D-N1N-C2N
3	B	403	NAD	C2D-C1D-N1N-C6N
3	B	403	NAD	O4B-C4B-C5B-O5B
3	A	403	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	NAD	1	0
3	B	403	NAD	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 then 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 A 403

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 403

Bond lengths

Bond angles

Torsions

Rings
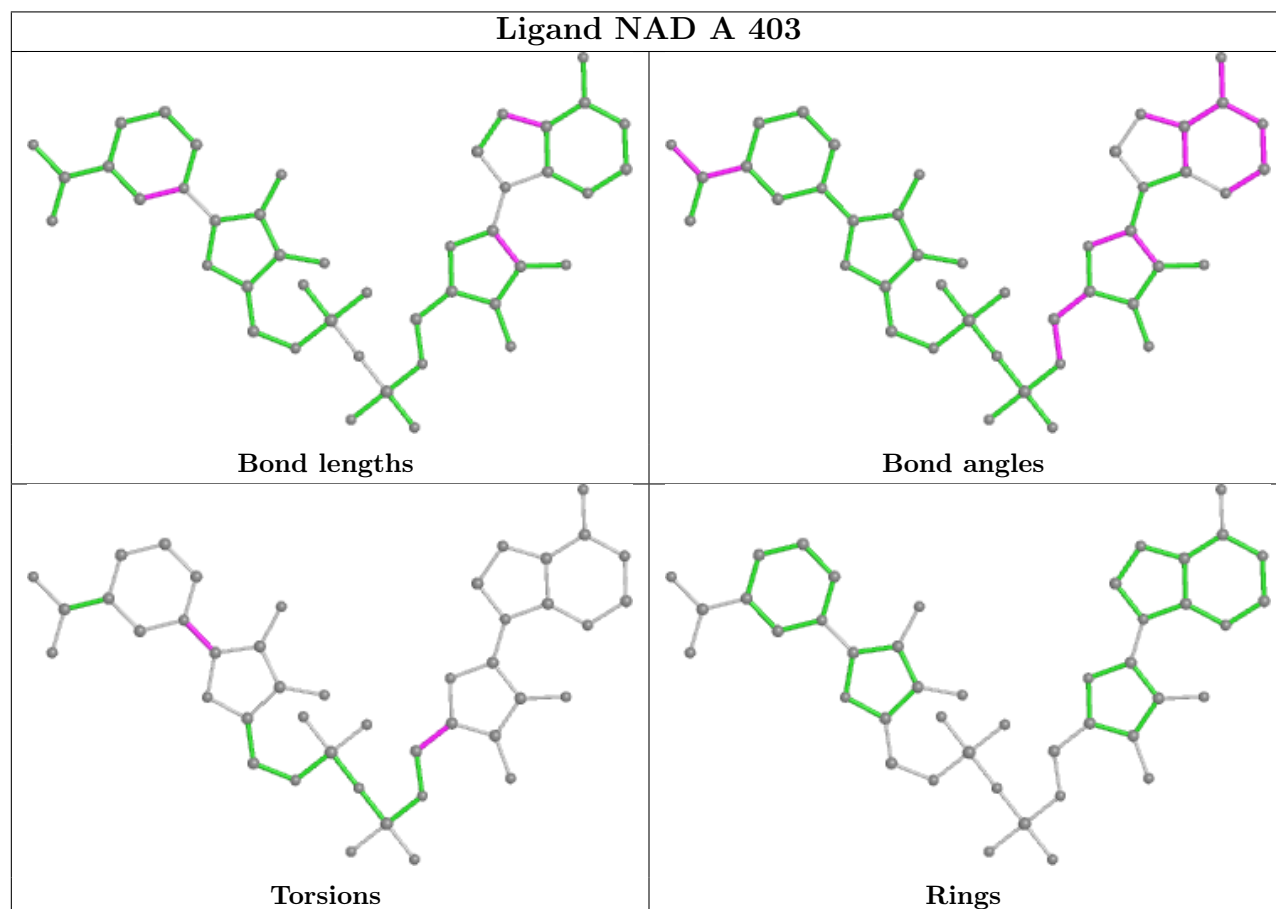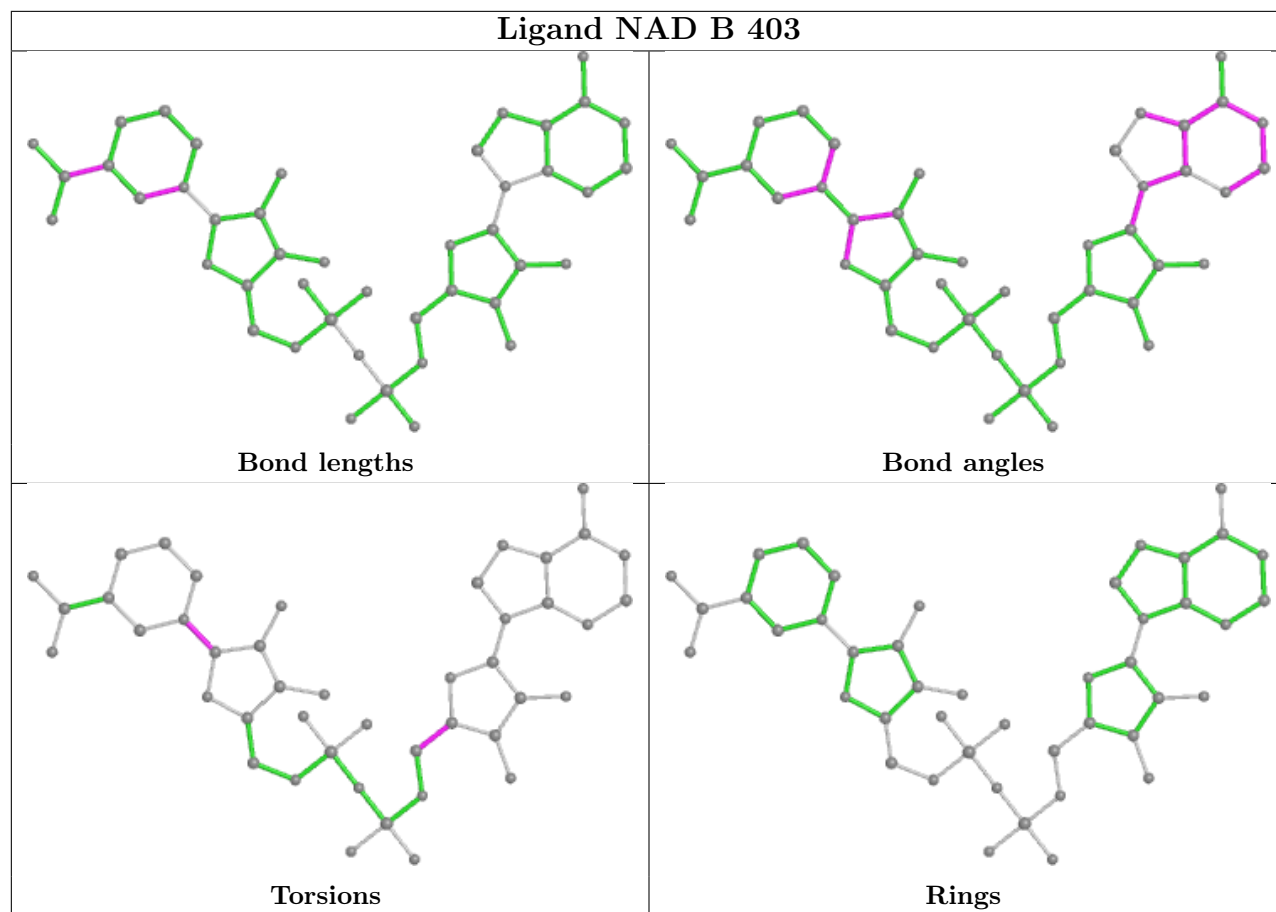
5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.