



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2024 – 08:14 AM EDT

PDB ID : 6ADH
Title : STRUCTURE OF TRICLINIC TERNARY COMPLEX OF HORSE LIVER
ALCOHOL DEHYDROGENASE AT 2.9 ANGSTROMS RESOLUTION
Authors : Eklund, H.
Deposited on : 1984-01-16
Resolution : 2.90 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

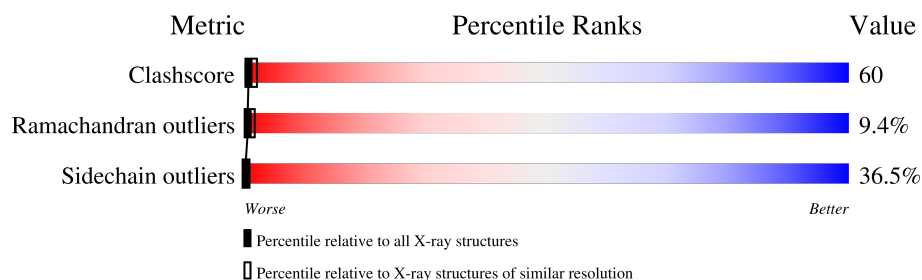
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	
1	B	374	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5669 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.

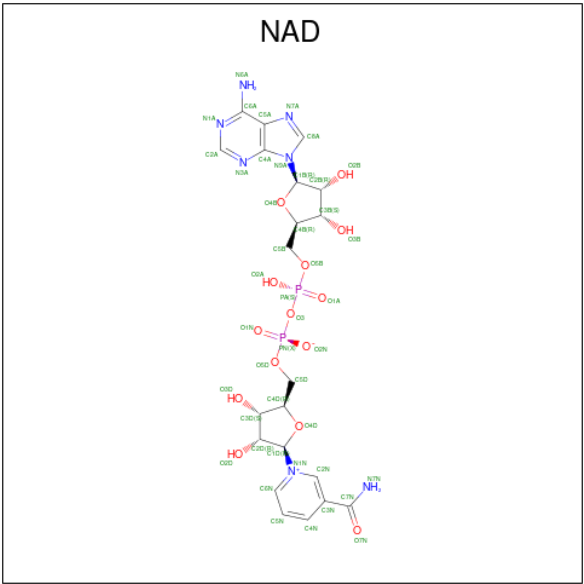
- Molecule 1 is a protein called HOLO-LIVER ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	154	0	0
			2784	1769	472	520	23			
1	B	374	Total	C	N	O	S	151	0	0
			2785	1769	472	521	23			

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

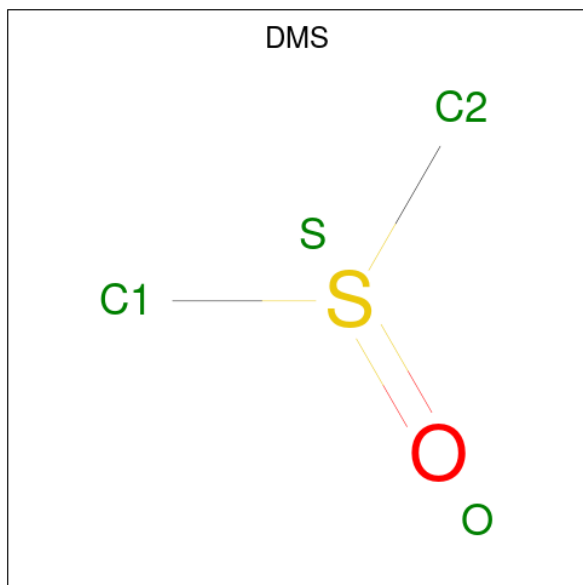
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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).



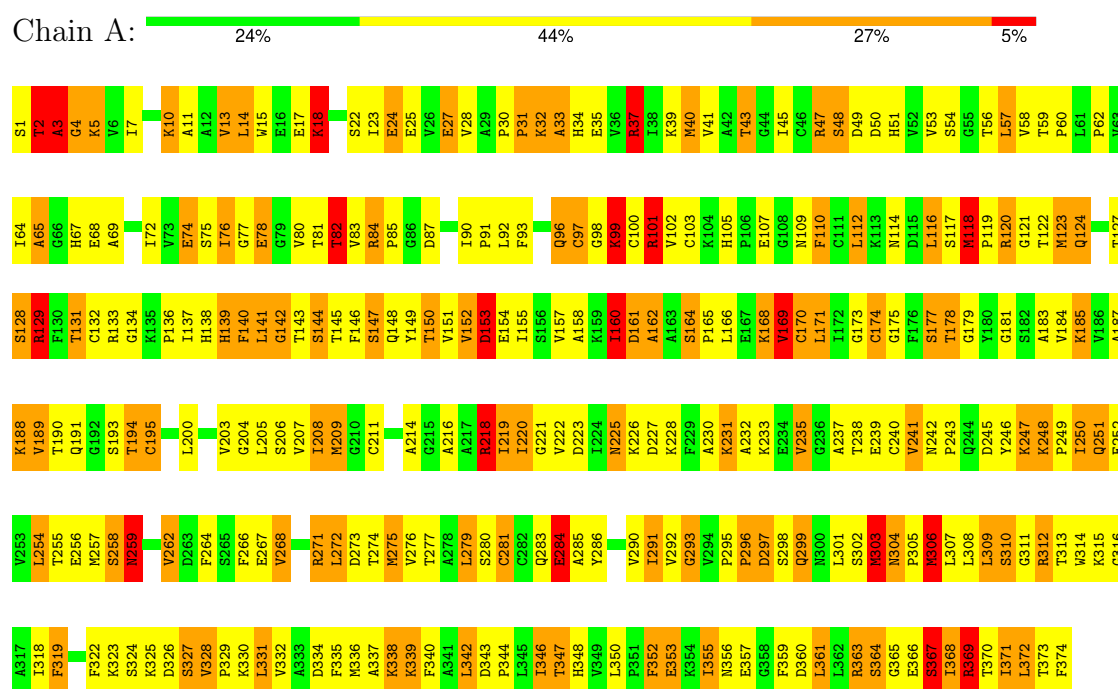
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

3 Residue-property plots

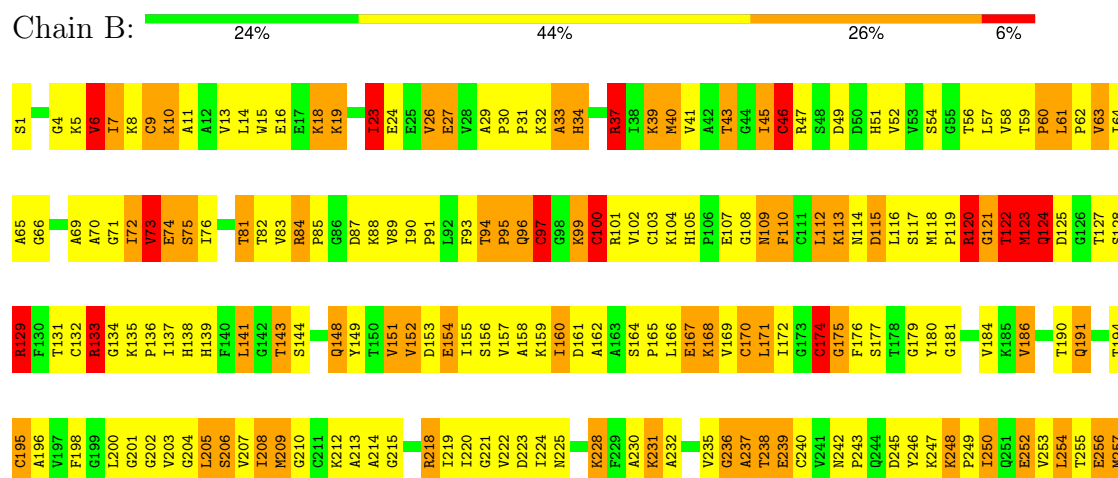
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: HOLO-LIVER ALCOHOL DEHYDROGENASE



• Molecule 1: HOLO-LIVER ALCOHOL DEHYDROGENASE



S258	K259	V262	D263	F264	S265	F266	E267	V268	I269	G270	R271	L272	D273	T274	R275	A278	L279	S280	C281	C282	Q283	E284	A285	Y286	G287	V288	S289	V290	I291	V292	G293	V294	P295	P296	D297	L301	S302	R303	N304	P305	R306	L307	L308	L309	S310	G311	R312	T313	W314	K315	L318	F319	F322	R323
S324	K325	S326	S327	V328	P329	K330	L331	V332	A333	D334	F335	M336	K339	F340	A341	L342	D343	P344	L345	I346	T347	H348	V349	L350	P351	F352	E353	K354	I355	N356	E357	L361	L362	R363	S364	G365	E366	S367	I368	R369	T370	I371	L372	T373	F374									

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	52.00Å 44.60Å 94.40Å 104.40° 101.90° 70.70°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5669	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: NAD, ZN, DMS

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	1.03	1/2836 (0.0%)	1.51	43/3834 (1.1%)
1	B	1.15	6/2837 (0.2%)	1.65	54/3834 (1.4%)
All	All	1.09	7/5673 (0.1%)	1.58	97/7668 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	CYS	CA-CB	8.44	1.72	1.53
1	B	282	CYS	CA-CB	7.60	1.70	1.53
1	A	240	CYS	CB-SG	7.06	1.94	1.82
1	B	170	CYS	CB-SG	7.06	1.94	1.82
1	B	9	CYS	CB-SG	6.70	1.93	1.82

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	CYS	N-CA-CB	23.70	153.26	110.60
1	B	122	THR	O-C-N	11.07	140.41	122.70
1	A	195	CYS	CA-CB-SG	9.37	130.87	114.00
1	A	1	SER	O-C-N	9.19	137.40	122.70
1	B	73	VAL	O-C-N	9.15	137.34	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	46	CYS	CA

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	2784	0	2848	324	55
1	B	2785	0	2849	358	59
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	25	4	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
All	All	5669	0	5760	655	63

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 60.

The worst 5 of 655 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:132:CYS:HB2	1:A:137:ILE:CD1	1.61	1.29
1:A:255:THR:O	1:A:259:ASN:HA	1.42	1.18
1:B:24:GLU:HG2	1:B:132:CYS:SG	1.86	1.15
1:A:23:ILE:CD1	1:A:353:GLU:HA	1.77	1.13
1:A:132:CYS:HB2	1:A:137:ILE:HD11	1.22	1.12

The worst 5 of 63 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:NZ	1:B:245:ASP:OD1[1_655]	0.31	1.89
1:B:16:GLU:OE2	1:B:81:THR:CG2[1_545]	0.68	1.52
1:A:245:ASP:O	1:B:248:LYS:CB[1_655]	0.71	1.49
1:A:247:LYS:N	1:B:247:LYS:N[1_655]	0.72	1.48
1:A:248:LYS:CD	1:B:245:ASP:CB[1_655]	0.75	1.45

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	372/374 (100%)	281 (76%)	53 (14%)	38 (10%)	0	1
1	B	372/374 (100%)	282 (76%)	58 (16%)	32 (9%)	0	1
All	All	744/748 (100%)	563 (76%)	111 (15%)	70 (9%)	0	1

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	33	ALA
1	A	65	ALA
1	A	99	LYS
1	A	109	ASN

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	308/308 (100%)	196 (64%)	112 (36%)	0	0
1	B	308/308 (100%)	195 (63%)	113 (37%)	0	0
All	All	616/616 (100%)	391 (64%)	225 (36%)	0	0

5 of 225 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	19	LYS
1	B	369	ARG
1	B	112	LEU
1	B	357	GLU
1	B	306	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	109	ASN
1	B	124	GLN
1	B	300	ASN
1	B	225	ASN
1	B	242	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 oligosaccharides 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	$\# Z > 2$
3	NAD	B	377	-	42,48,48	1.98	7 (16%)	50,73,73	2.08	9 (18%)
4	DMS	B	378	2	3,3,3	0.61	0	3,3,3	0.18	0
4	DMS	A	378	2	3,3,3	0.57	0	3,3,3	0.16	0
3	NAD	A	377	-	42,48,48	1.51	6 (14%)	50,73,73	1.85	8 (16%)

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	B	377	-	-	9/26/62/62	0/5/5/5
3	NAD	A	377	-	-	8/26/62/62	0/5/5/5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	377	NAD	C5B-C4B	-8.00	1.27	1.51
3	A	377	NAD	PN-O3	5.80	1.65	1.59
3	B	377	NAD	PN-O3	4.94	1.64	1.59
3	A	377	NAD	C3N-C7N	4.53	1.57	1.50
3	B	377	NAD	C3N-C7N	3.89	1.56	1.50

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	377	NAD	C5N-C4N-C3N	-7.98	112.52	120.36
3	A	377	NAD	C5N-C4N-C3N	-7.46	113.03	120.36
3	B	377	NAD	C6N-C5N-C4N	5.88	127.92	119.45
3	A	377	NAD	C6N-C5N-C4N	5.75	127.74	119.45
3	B	377	NAD	O4B-C4B-C5B	5.19	125.96	109.33

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

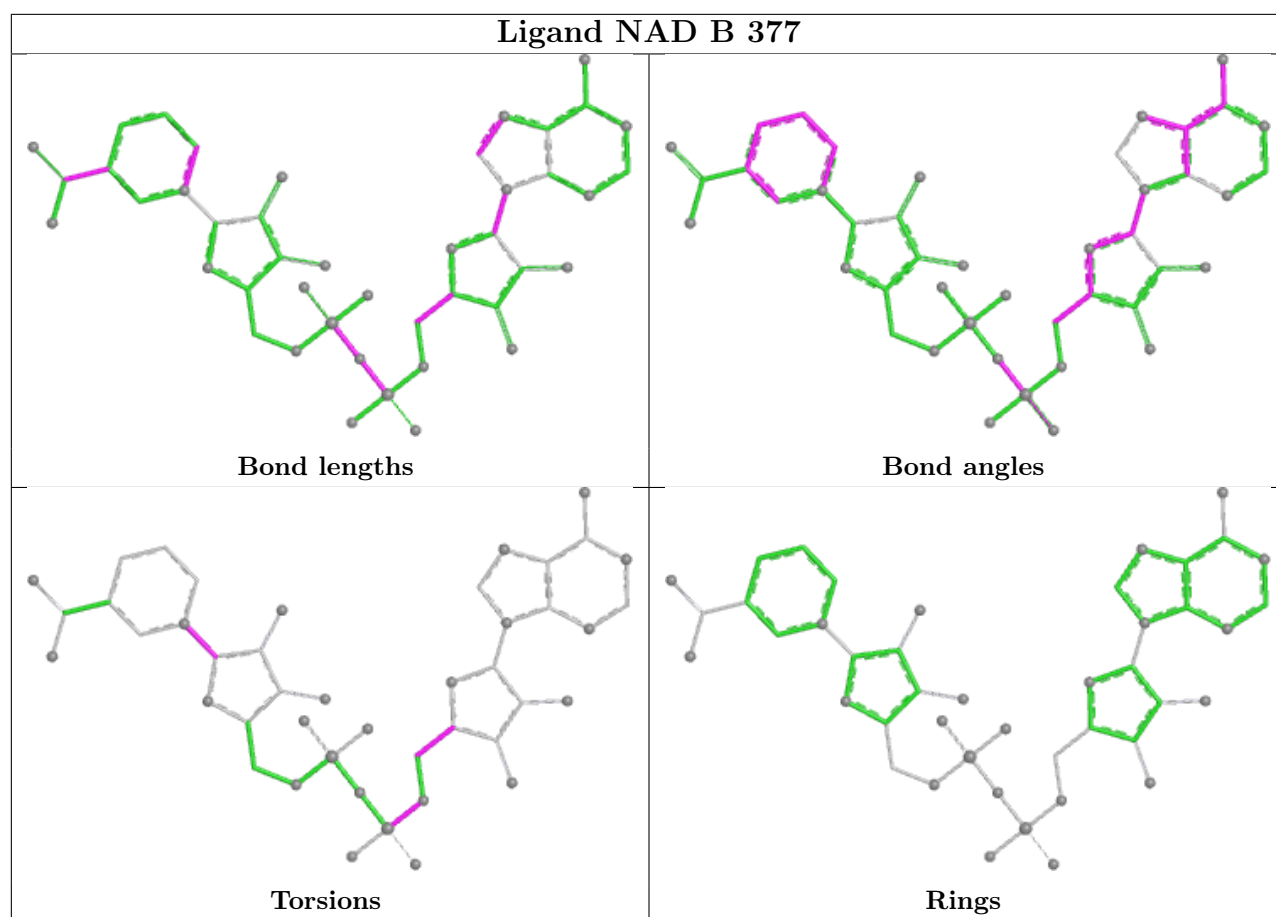
Mol	Chain	Res	Type	Atoms
3	A	377	NAD	C5B-O5B-PA-O1A
3	A	377	NAD	C5B-O5B-PA-O3
3	A	377	NAD	O4D-C1D-N1N-C2N
3	A	377	NAD	O4D-C1D-N1N-C6N
3	A	377	NAD	C2D-C1D-N1N-C2N

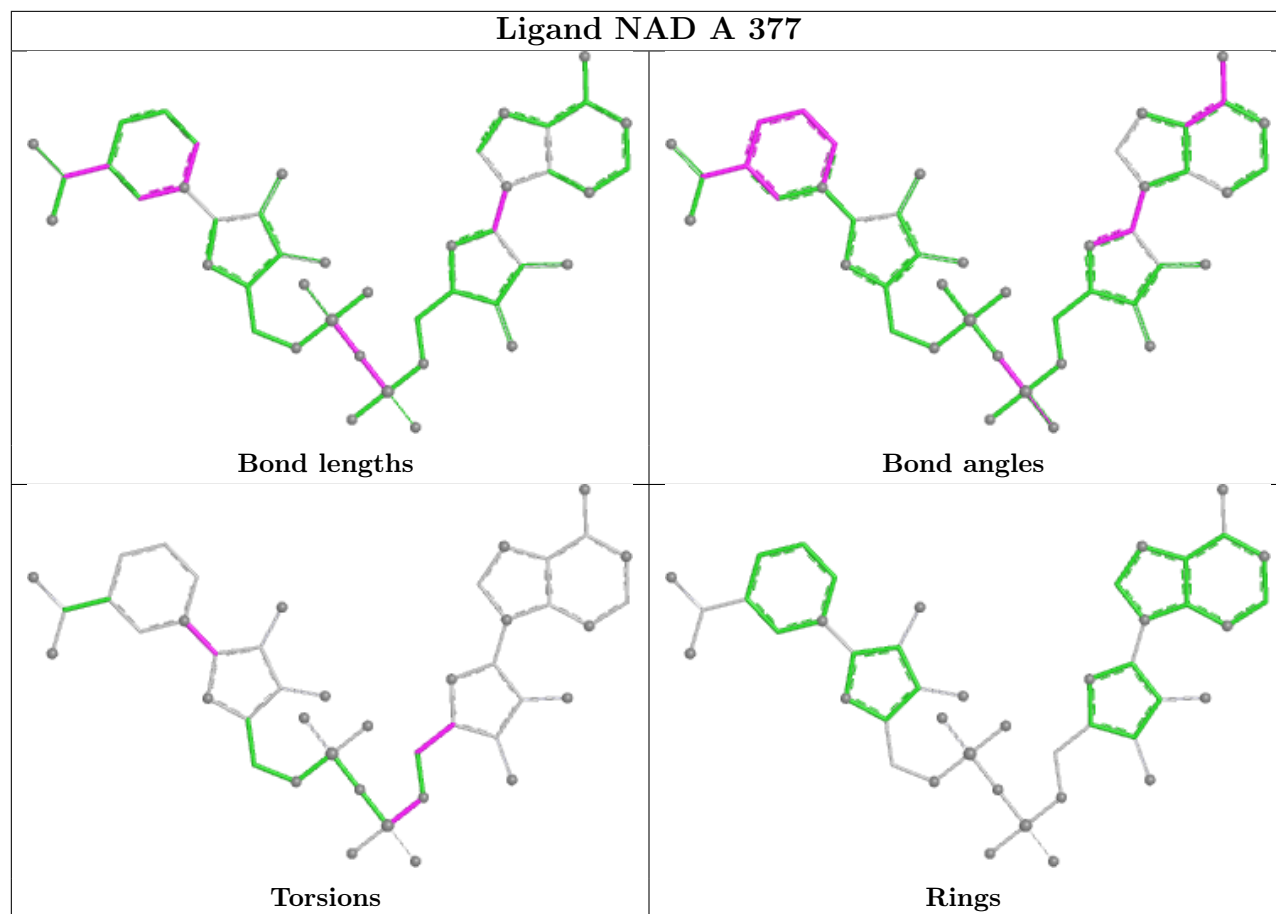
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	377	NAD	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.