



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:40 PM UTC

PDB ID : 1BI9 / pdb_00001bi9
Title : RETINAL DEHYDROGENASE TYPE TWO WITH NAD BOUND
Authors : Newcomer, M.E.; Lamb, A.L.
Deposited on : 1998-06-23
Resolution : 2.70 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

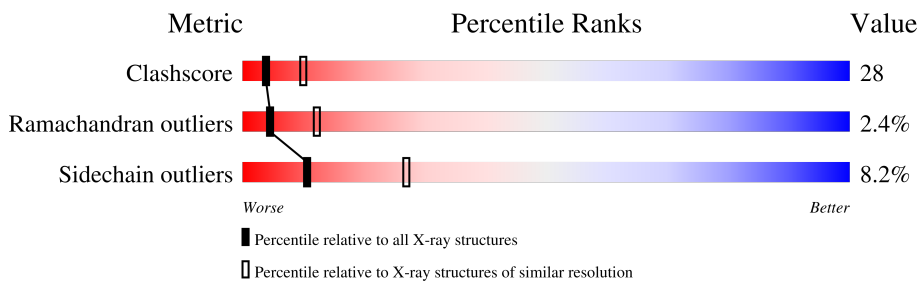
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	499	47% 43% 6% .
1	B	499	48% 42% 6% .
1	C	499	47% 41% 7% .
1	D	499	49% 40% 7% .

2 Entry composition [i](#)

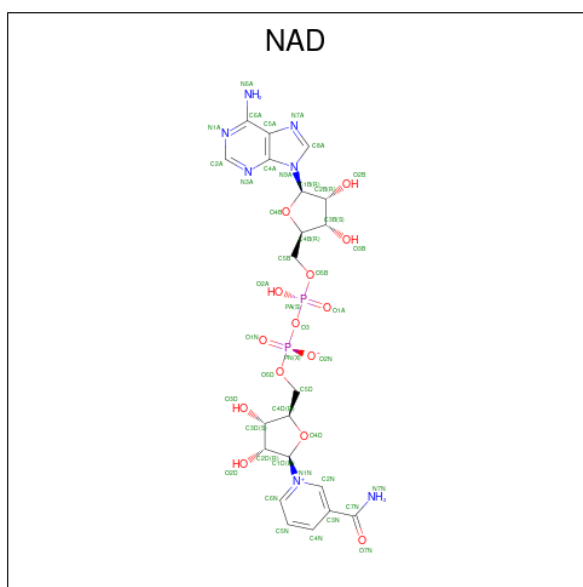
There are 4 unique types of molecules in this entry. The entry contains 15156 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RETINAL DEHYDROGENASE TYPE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3697	2356	628	694	19			
1	B	477	Total	C	N	O	S	0	0	0
			3689	2351	627	693	18			
1	C	480	Total	C	N	O	S	0	0	0
			3710	2363	631	697	19			
1	D	482	Total	C	N	O	S	0	0	0
			3726	2373	634	700	19			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Cl	0	0
			2	2		

- Molecule 4 is water.

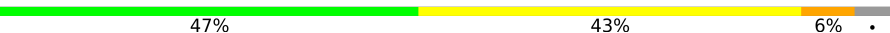
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	53	Total	O	0	0
			53	53		
4	C	68	Total	O	0	0
			68	68		
4	D	66	Total	O	0	0
			66	66		

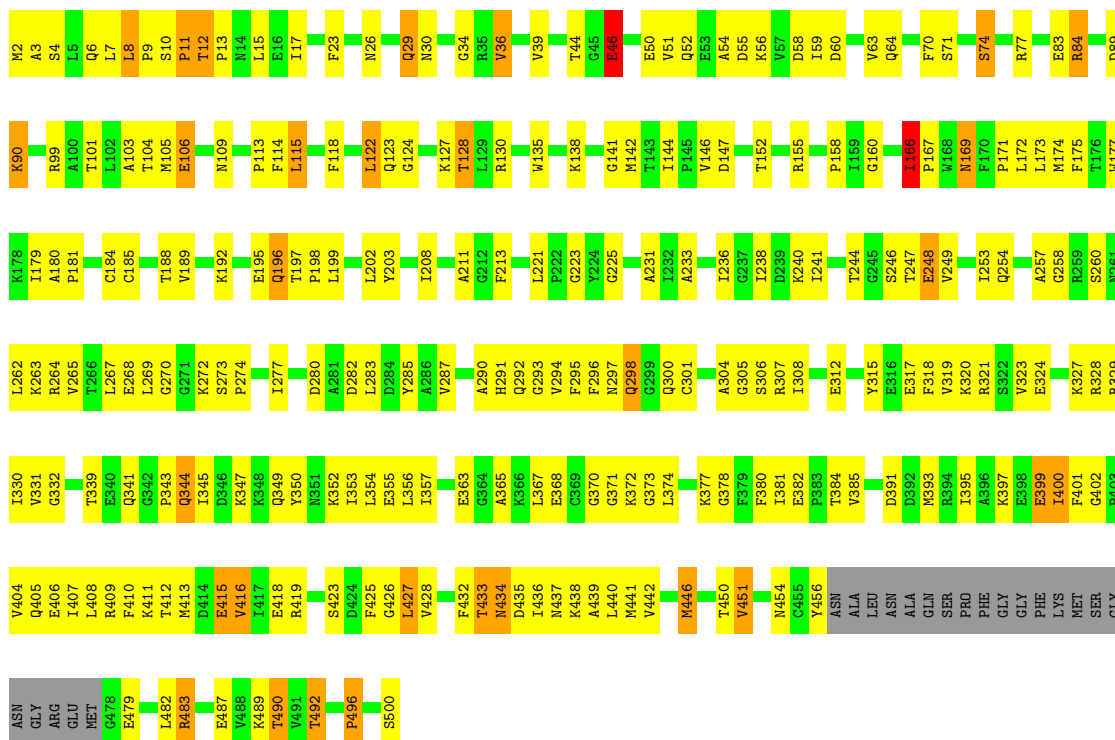
3 Residue-property plots

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.

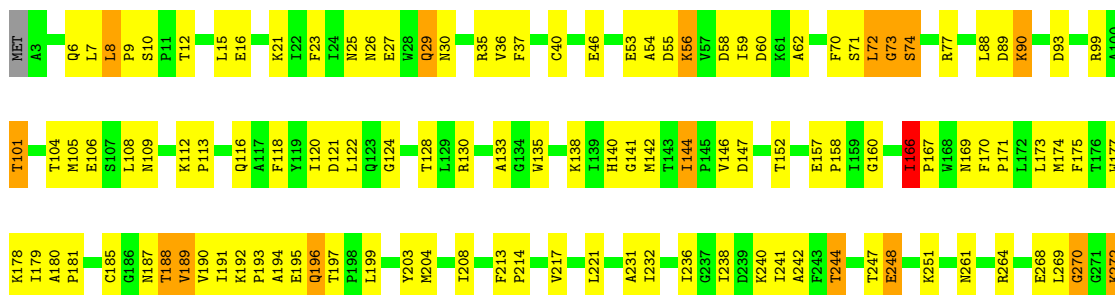
• Molecule 1: RETINAL DEHYDROGENASE TYPE II

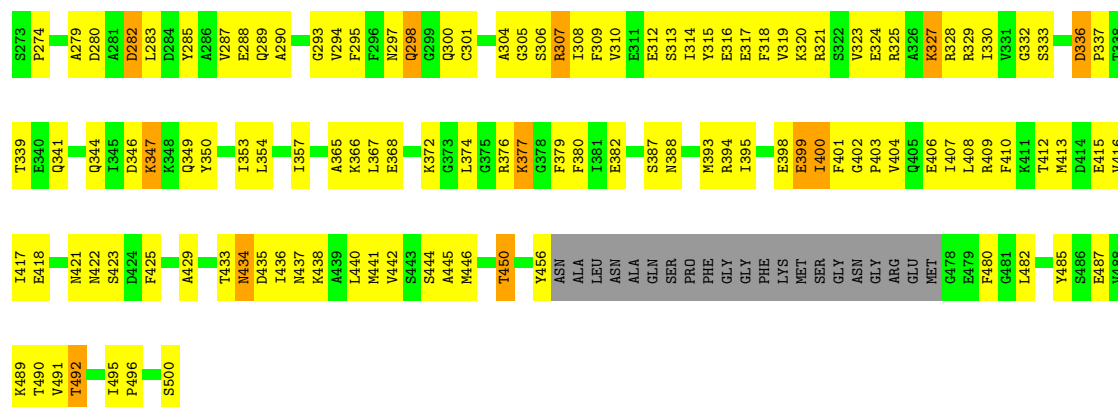
Chain A: 



• Molecule 1: RETINAL DEHYDROGENASE TYPE II

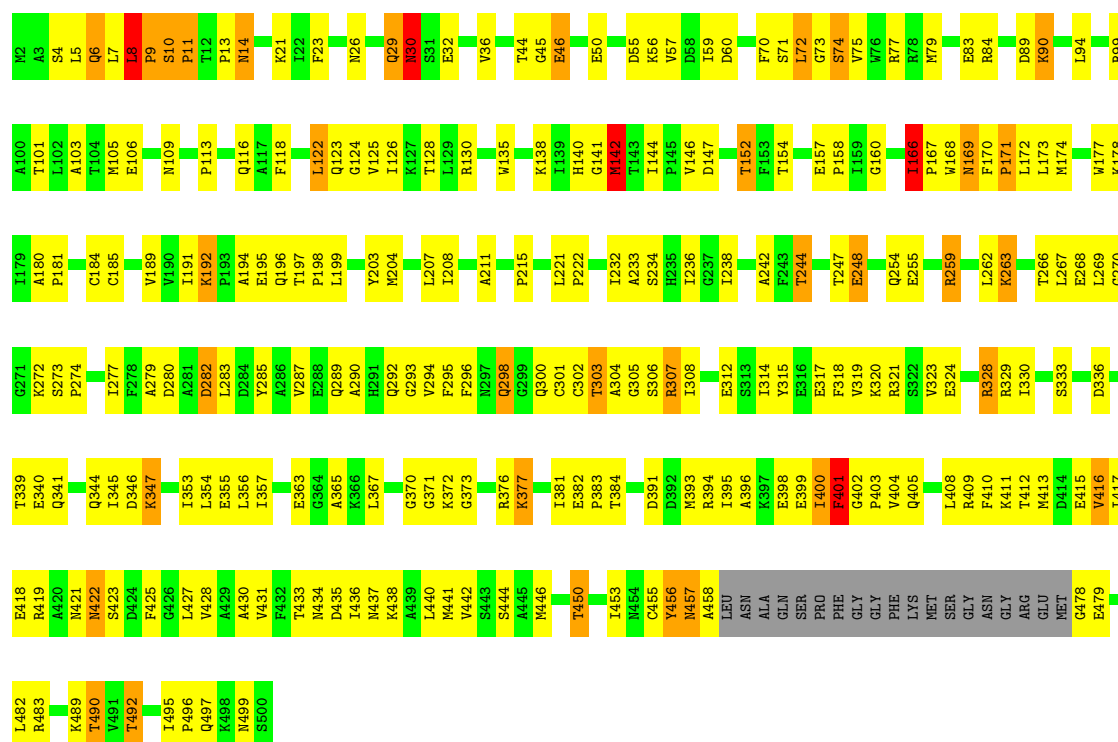
Chain B: 





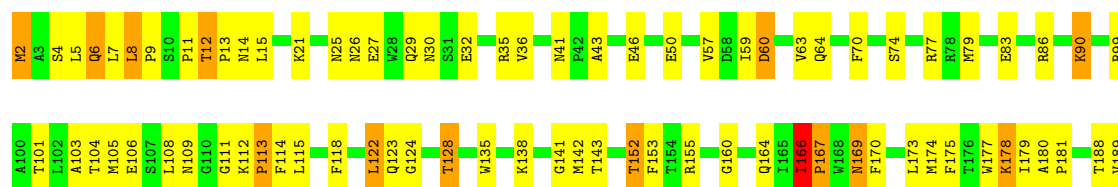
• Molecule 1: RETINAL DEHYDROGENASE TYPE II

Chain C: 47% 41% 7% . .



• Molecule 1: RETINAL DEHYDROGENASE TYPE II

Chain D: 49% 40% 7% .



K494	I495	P496	S500	A429	A430	V431	F432	T433	N434	D435	I436	N437	K438	A439	L440	M441	V442	M446	Q447	A448	G449	T450	V451	W452	I453	N454	C455	Y456	N457	A458	L459	N460	ALA	GLN	SER	PRO	PHE	GLY	GLY	PHE	LYS	MET	SER	GLY	ASN	GLY	ARG	GLU	MET	G478	E479	F480	G481	L482	R483	E487	T490	V491	T492	V493																																						
K494	I495	P496	S500	I357	K358	S359	E363	G364	A365	K366	L367	G370	G371	K372	G373	R376	K377	G378	F379	F380	I381	E382	S387	N388	D392	M393	R394	I395	A396	K397	E398	E399	I400	F401	G402	P403	V404	Q405	E406	I407	L408	R409	F410	M413	V416	I417	E418	N421	R422	S423	T424	F425	G426	L427	V428	D282	L283	V287	Q288	Q289	Q300	C301	C302	T303	A304	G305	S306	R307	I314	Y315	E316	E317	F318	I319	K320	R321	S322	V323	E324	R325	R328	R329	I330	V331	G332	P337	T338	T339	G342	P343	Q344	I345	D346	K347	K348	Q349	I353	L356
K494	I495	P496	S500	I190	I191	E195	Q196	T197	P198	L199	L202	Y203	L208	A211	G212	F213	P214	P215	G216	V217	I220	L221	P222	I236	F243	T244	G245	S246	T247	E248	V249	I253	Q254	E255	R259	L262	K263	R264	E268	L269	G270	G271	K272	S273	P274	N275	I276	L277	F278	A279	D280	A281																																														

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.80Å 167.30Å 107.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	95.1 (30.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.234 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15156	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

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: NAD, 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	0/3772	0.96	17/5104 (0.3%)
1	B	0.47	0/3764	0.95	15/5094 (0.3%)
1	C	0.52	0/3785	0.99	16/5122 (0.3%)
1	D	0.49	0/3801	0.99	18/5144 (0.3%)
All	All	0.49	0/15122	0.97	66/20464 (0.3%)

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	LYS	N-CA-C	-11.05	99.32	111.36
1	C	123	GLN	N-CA-C	-8.48	102.12	111.36
1	D	345	ILE	N-CA-C	8.02	118.80	110.62
1	B	141	GLY	N-CA-C	-7.92	101.72	112.57
1	D	199	LEU	N-CA-C	7.81	119.49	110.97

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	3697	0	3699	224	0
1	B	3689	0	3690	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3710	0	3710	224	2
1	D	3726	0	3727	230	2
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	C	2	0	0	0	0
4	A	37	0	0	1	0
4	B	53	0	0	3	0
4	C	68	0	0	5	0
4	D	66	0	0	2	0
All	All	15156	0	14874	847	2

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 28.

The worst 5 of 847 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:D:152:THR:HG22	1:D:492:THR:HB	1.33	1.10
1:B:495:ILE:HG22	1:D:440:LEU:HD13	1.36	1.05
1:A:152:THR:HG22	1:A:492:THR:HB	1.38	1.04
1:C:329:ARG:NH1	1:C:341:GLN:HB2	1.74	1.01
1:C:272:LYS:HD3	1:C:423:SER:HB2	1.41	0.99

All (2) 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:C:255:GLU:OE2	1:D:259:ARG:NH2[2_565]	2.05	0.15
1:C:259:ARG:NH2	1:D:255:GLU:OE2[2_565]	2.07	0.13

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	474/499 (95%)	416 (88%)	48 (10%)	10 (2%)	5	15
1	B	473/499 (95%)	423 (89%)	37 (8%)	13 (3%)	4	10
1	C	476/499 (95%)	419 (88%)	42 (9%)	15 (3%)	3	7
1	D	478/499 (96%)	423 (88%)	48 (10%)	7 (2%)	8	22
All	All	1901/1996 (95%)	1681 (88%)	175 (9%)	45 (2%)	4	12

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	74	SER
1	A	260	SER
1	A	270	GLY
1	B	72	LEU

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	394/409 (96%)	364 (92%)	30 (8%)	12	30
1	B	393/409 (96%)	366 (93%)	27 (7%)	14	34
1	C	395/409 (97%)	358 (91%)	37 (9%)	8	21
1	D	397/409 (97%)	361 (91%)	36 (9%)	9	22
All	All	1579/1636 (96%)	1449 (92%)	130 (8%)	10	27

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	259	ARG
1	D	307	ARG
1	B	327	LYS

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Mol	Chain	Res	Type
1	B	307	ARG
1	D	400	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	6	GLN
1	D	275	ASN
1	C	196	GLN
1	D	254	GLN
1	D	457	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 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	$\# Z > 2$
2	NAD	B	702	-	28,29,48	1.86	7 (25%)	43,45,73	2.17	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	C	703	-	28,29,48	2.03	14 (50%)	43,45,73	2.16	10 (23%)
2	NAD	A	701	-	28,29,48	1.96	8 (28%)	43,45,73	2.22	12 (27%)
2	NAD	D	704	-	28,29,48	1.79	7 (25%)	43,45,73	2.17	10 (23%)

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	NAD	B	702	-	-	0/16/32/62	0/3/3/5
2	NAD	C	703	-	-	4/16/32/62	0/3/3/5
2	NAD	A	701	-	-	4/16/32/62	0/3/3/5
2	NAD	D	704	-	-	1/16/32/62	0/3/3/5

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NAD	C4A-N3A	4.85	1.43	1.34
2	B	702	NAD	C4A-N3A	4.27	1.42	1.34
2	D	704	NAD	C4A-N3A	4.15	1.42	1.34
2	A	701	NAD	C5A-N7A	-3.90	1.32	1.39
2	D	704	NAD	C5A-N7A	-3.89	1.32	1.39

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NAD	N3A-C4A-N9A	6.93	138.95	127.17
2	D	704	NAD	C5A-C4A-N3A	-6.83	117.31	126.72
2	C	703	NAD	C5A-C4A-N3A	-6.78	117.38	126.72
2	C	703	NAD	N3A-C4A-N9A	6.72	138.59	127.17
2	A	701	NAD	C5A-C4A-N3A	-6.65	117.56	126.72

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	NAD	PA-O3-PN-O2N
2	C	703	NAD	C5B-O5B-PA-O1A
2	C	703	NAD	C5B-O5B-PA-O2A

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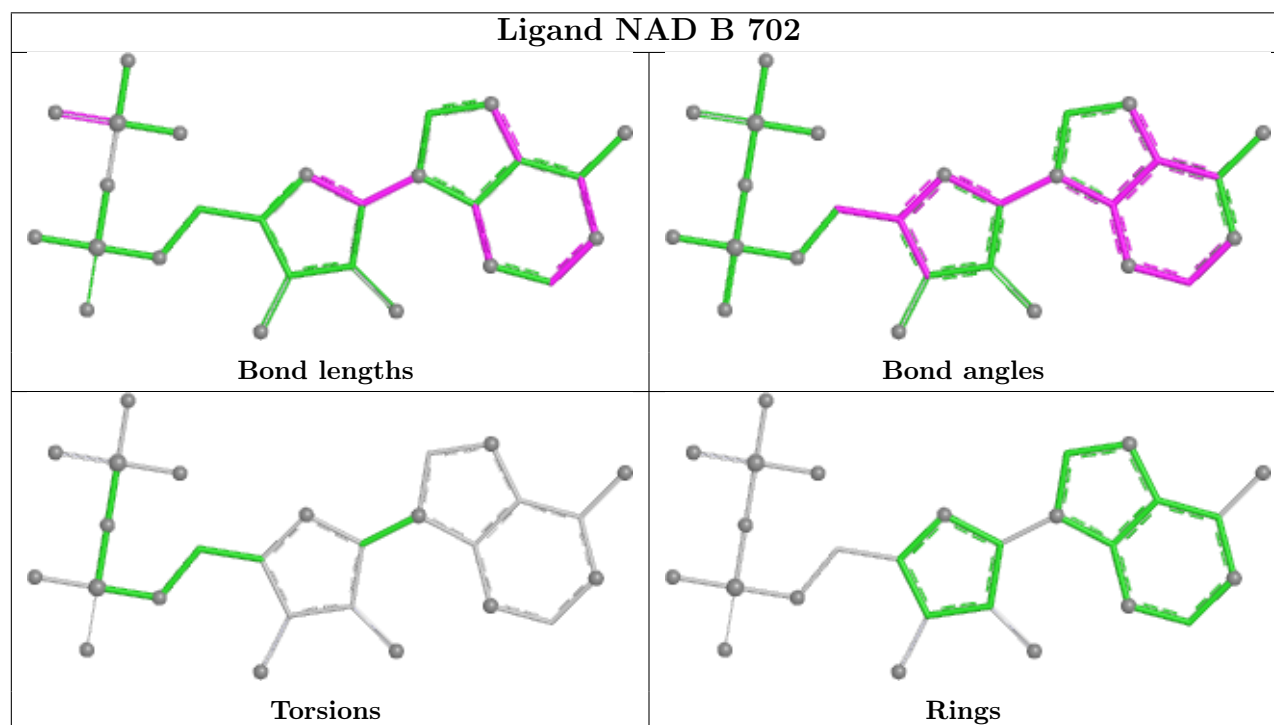
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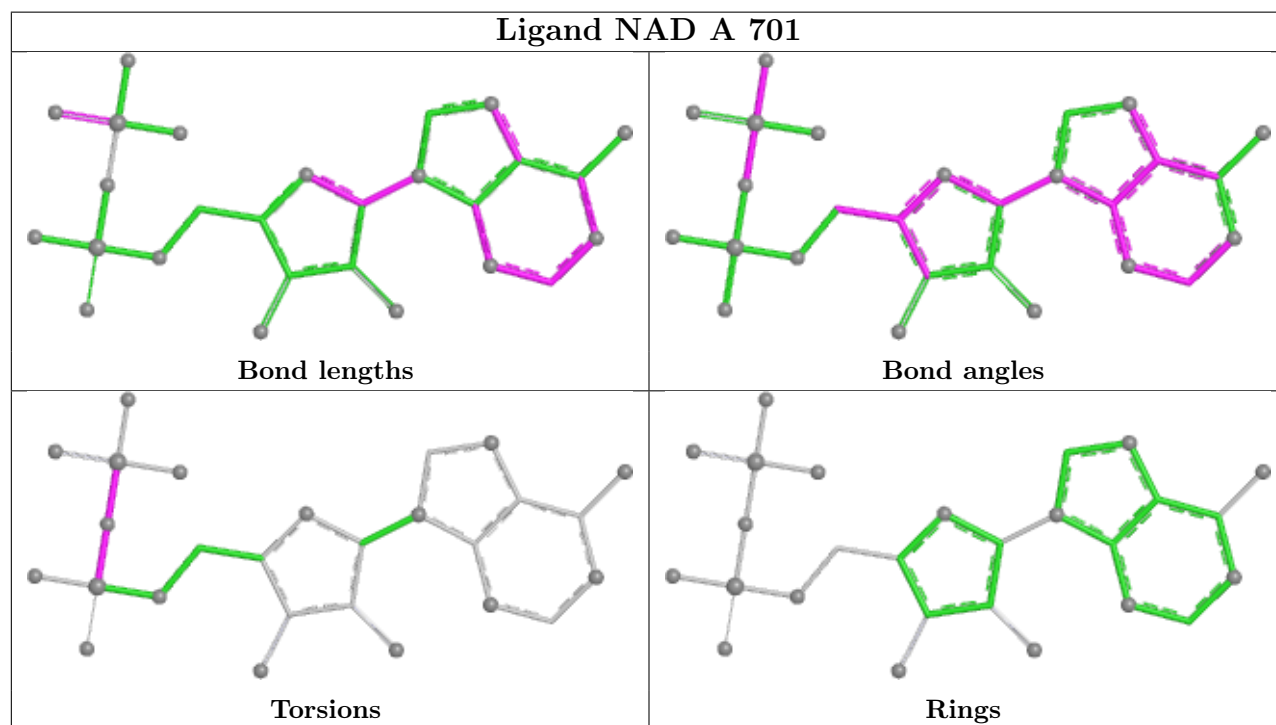
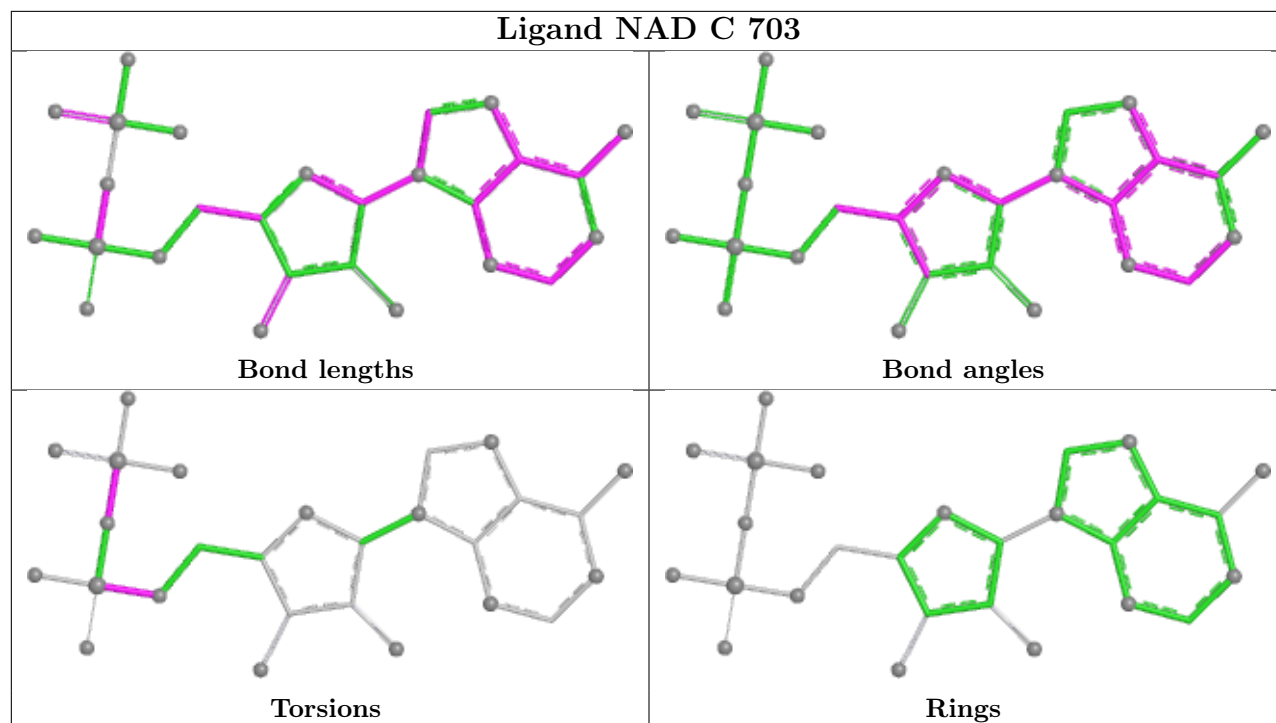
Mol	Chain	Res	Type	Atoms
2	C	703	NAD	PA-O3-PN-O5D
2	A	701	NAD	PN-O3-PA-O1A

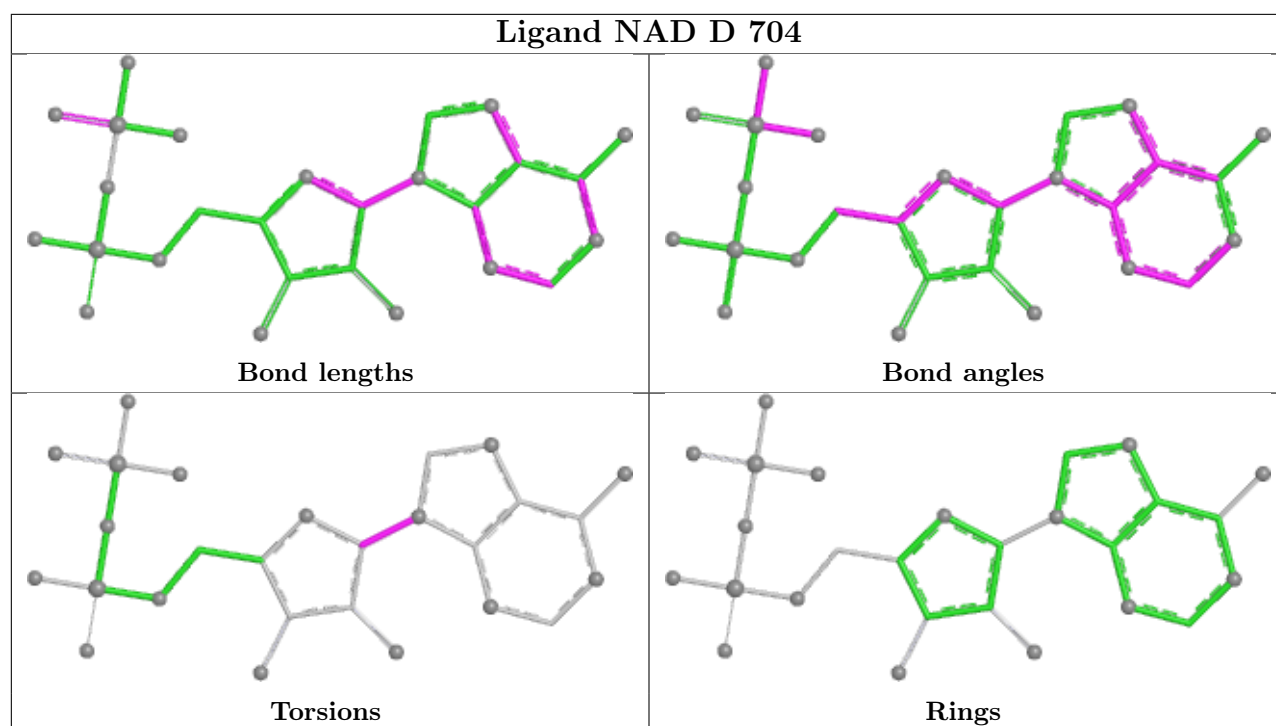
There are no ring outliers.

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.







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

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.