



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 08:00 pm BST

PDB ID : 1L7E
Title : Crystal Structure of R. rubrum Transhydrogenase Domain I with Bound NADH
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Deposited on : 2002-03-14
Resolution : 1.90 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 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) : 2.11

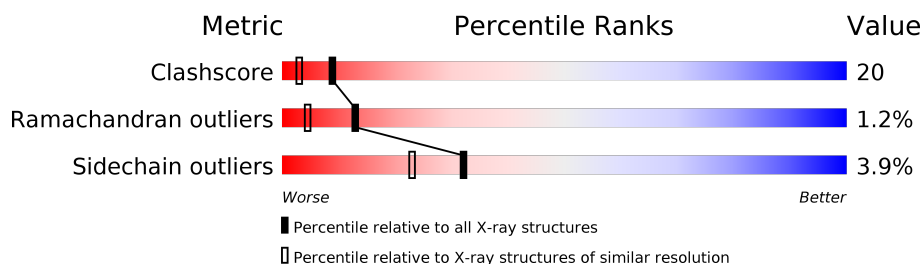
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 on 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	384	
1	B	384	
1	C	384	
1	D	384	

2 Entry composition [i](#)

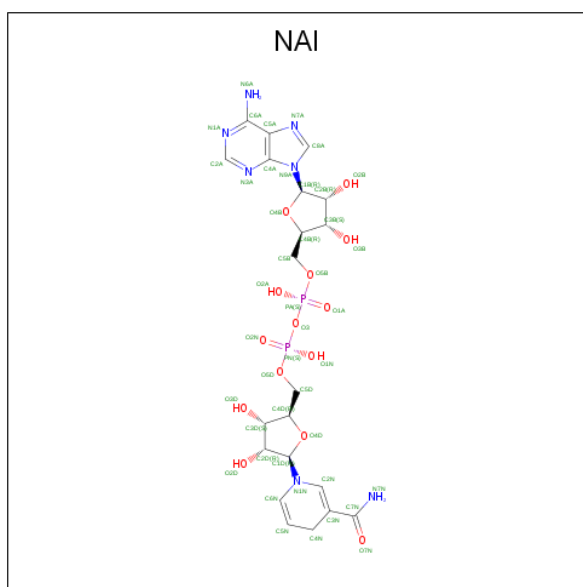
There are 3 unique types of molecules in this entry. The entry contains 11327 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 nicotinamide nucleotide Transhydrogenase, subunit alpha 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2736	1727	472	520	17			
1	B	357	Total	C	N	O	S	0	0	0
			2618	1655	456	491	16			
1	C	353	Total	C	N	O	S	0	0	0
			2586	1636	448	486	16			
1	D	367	Total	C	N	O	S	0	0	0
			2692	1701	467	507	17			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total 136	O 136	0	0
3	B	136	Total 136	O 136	0	0
3	C	158	Total 158	O 158	0	0
3	D	177	Total 177	O 177	0	0

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.14Å 116.68Å 92.60Å 90.00° 106.28° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11327	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: NAI

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	0.40	0/2772	0.74	7/3756 (0.2%)
1	B	0.34	0/2652	0.63	1/3596 (0.0%)
1	C	0.36	0/2620	0.64	0/3554
1	D	0.36	0/2727	0.63	0/3694
All	All	0.37	0/10771	0.66	8/14600 (0.1%)

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	A	1	2

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	GLY	C-N-CA	9.19	141.61	122.30
1	A	234	GLY	C-N-CA	7.52	140.50	121.70
1	A	241	GLU	OE1-CD-OE2	-7.38	114.44	123.30
1	A	231	THR	N-CA-CB	5.92	121.56	110.30
1	A	235	TYR	CB-CG-CD1	-5.60	117.64	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	231	THR	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	GLY	Mainchain
1	A	241	GLU	Mainchain

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	2736	0	2857	121	0
1	B	2618	0	2752	115	0
1	C	2586	0	2717	118	0
1	D	2692	0	2819	100	0
2	A	44	0	27	1	0
2	D	44	0	27	1	0
3	A	136	0	0	2	0
3	B	136	0	0	6	0
3	C	158	0	0	1	0
3	D	177	0	0	6	0
All	All	11327	0	11199	444	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 20.

The worst 5 of 444 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:C:1077:THR:H	1:C:1080:MET:HE3	0.98	1.08
1:D:1557:LYS:HD2	1:D:1557:LYS:H	1.30	0.97
1:C:906:ARG:H	1:C:907:PRO:HD2	1.30	0.96
1:B:748:ASP:O	1:B:749:LYS:HG2	1.66	0.95
1:A:163:MET:HB2	1:A:170:VAL:HG12	1.49	0.94

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	368/384 (96%)	344 (94%)	21 (6%)	3 (1%)	19	9
1	B	353/384 (92%)	327 (93%)	21 (6%)	5 (1%)	11	3
1	C	349/384 (91%)	324 (93%)	18 (5%)	7 (2%)	7	1
1	D	363/384 (94%)	344 (95%)	17 (5%)	2 (1%)	25	15
All	All	1433/1536 (93%)	1339 (93%)	77 (5%)	17 (1%)	13	4

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	A	376	HIS
1	B	502	ALA
1	C	866	SER
1	C	906	ARG

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	289/296 (98%)	279 (96%)	10 (4%)	36	27
1	B	277/296 (94%)	272 (98%)	5 (2%)	59	55
1	C	274/296 (93%)	260 (95%)	14 (5%)	24	14
1	D	284/296 (96%)	269 (95%)	15 (5%)	22	13
All	All	1124/1184 (95%)	1080 (96%)	44 (4%)	32	23

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	943	LEU
1	C	1052	LEU
1	D	1550	ASP
1	C	963	MET
1	C	976	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	586	GLN
1	B	720	HIS
1	D	1410	GLN
1	B	647	GLN
1	C	867	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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
2	NAI	A	701	-	42,48,48	2.53	14 (33%)	47,73,73	1.90	9 (19%)
2	NAI	D	702	-	42,48,48	2.48	15 (35%)	47,73,73	1.96	10 (21%)

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	NAI	A	701	-	-	10/25/72/72	0/5/5/5
2	NAI	D	702	-	-	12/25/72/72	0/5/5/5

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NAI	C2A-N3A	7.33	1.43	1.32
2	D	702	NAI	C2A-N3A	7.25	1.43	1.32
2	A	701	NAI	C4A-N3A	6.93	1.45	1.35
2	D	702	NAI	C7N-C3N	6.60	1.62	1.48
2	D	702	NAI	C4A-N3A	6.50	1.44	1.35

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	702	NAI	C3N-C2N-N1N	-6.35	114.03	123.10
2	A	701	NAI	C3N-C2N-N1N	-6.33	114.06	123.10
2	D	702	NAI	C2A-N1A-C6A	4.60	126.62	118.75
2	A	701	NAI	N3A-C2A-N1A	-4.59	121.51	128.68
2	A	701	NAI	C2A-N1A-C6A	4.52	126.49	118.75

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

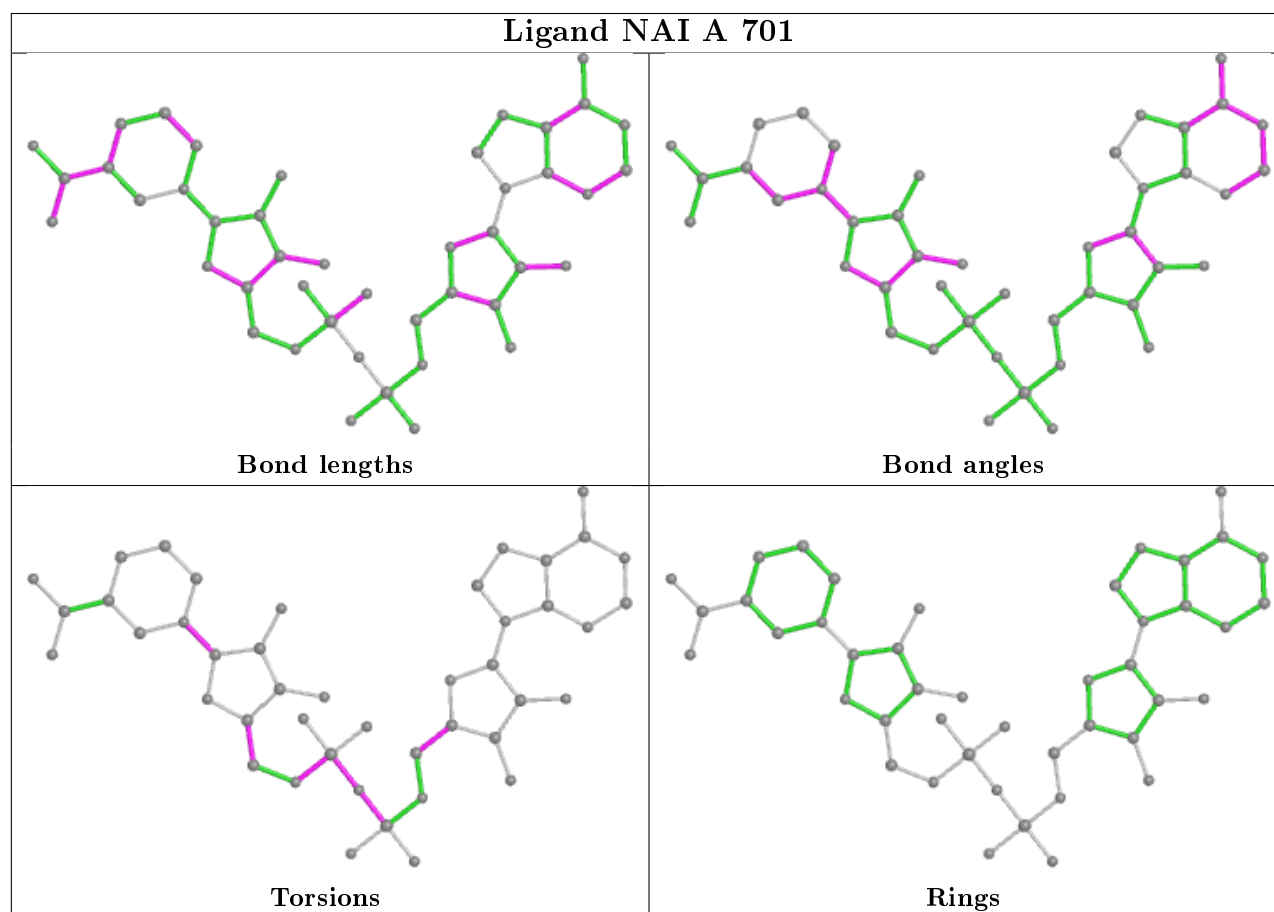
Mol	Chain	Res	Type	Atoms
2	A	701	NAI	C5D-O5D-PN-O1N
2	A	701	NAI	O4D-C4D-C5D-O5D
2	A	701	NAI	C3D-C4D-C5D-O5D
2	D	702	NAI	O4B-C4B-C5B-O5B
2	D	702	NAI	C5D-O5D-PN-O1N

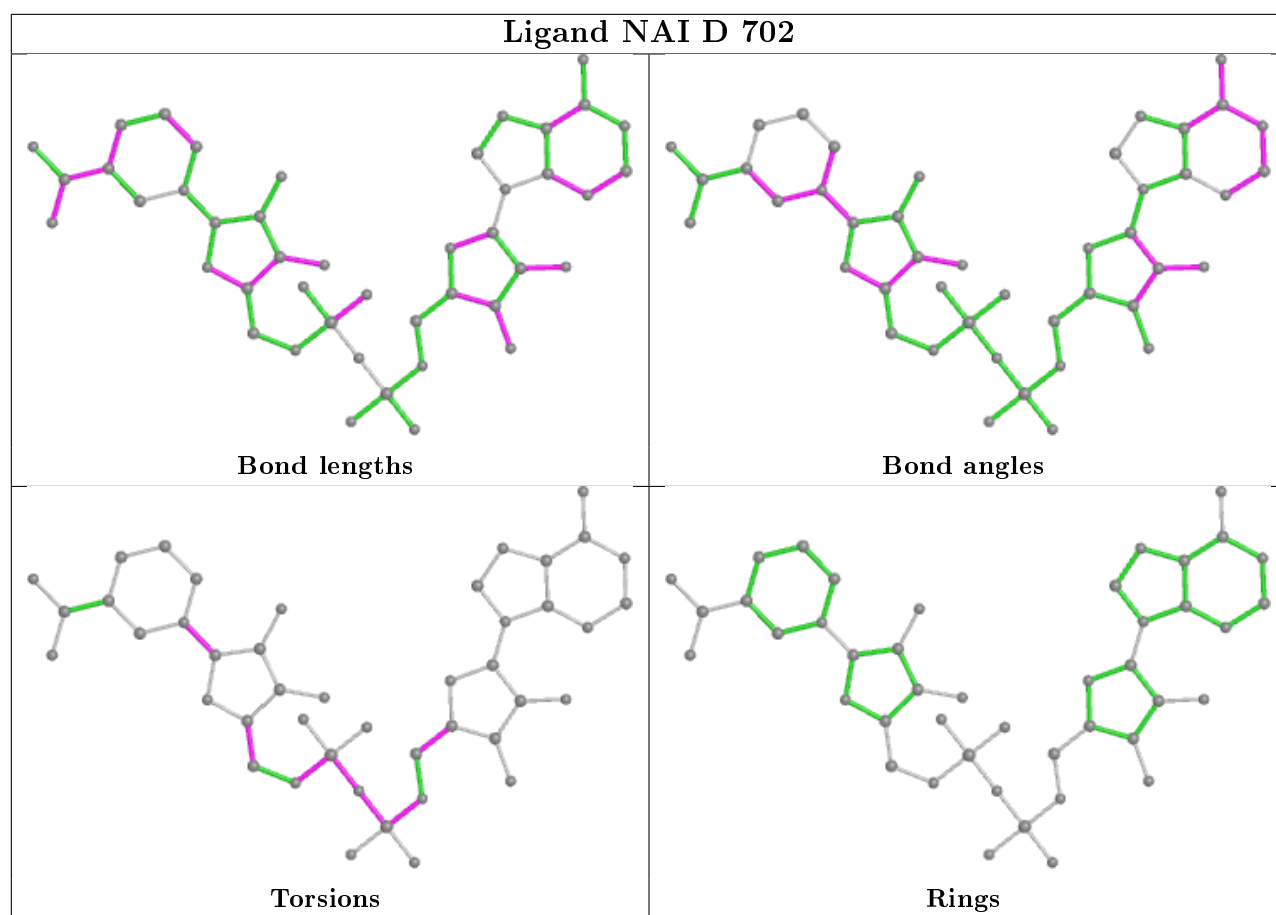
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NAI	1	0
2	D	702	NAI	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.





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.