



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:58 am GMT

PDB ID : 1L7D
Title : Crystal Structure of *R. rubrum* Transhydrogenase Domain I without Bound NAD(H)
Authors : Prasad, G.S.; Wahlberg, M.; Sridhar, V.; Yamaguchi, M.; Hatefi, Y.; Stout, C.D.
Deposited on : 2002-03-14
Resolution : 1.81 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

<http://wwpdb.org/validation/2016/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
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

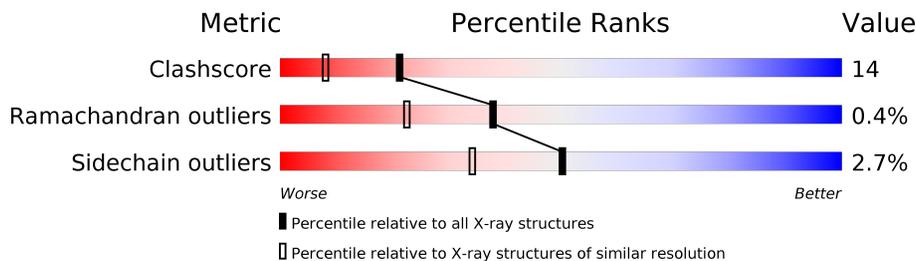
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	112137	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

There are 2 unique types of molecules in this entry. The entry contains 11344 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
			Total	C	N	O	S			
1	A	354	Total 2589	C 1638	N 448	O 487	S 16	0	0	0
1	B	358	Total 2620	C 1656	N 454	O 494	S 16	0	0	0
1	C	355	Total 2604	C 1648	N 451	O 489	S 16	0	0	0
1	D	353	Total 2592	C 1640	N 449	O 487	S 16	0	0	0

- Molecule 2 is water.

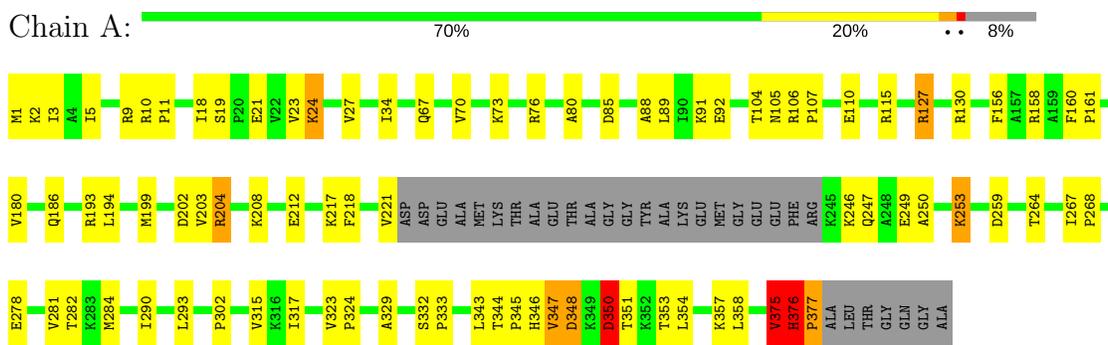
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	184	Total 184	O 184	0	0
2	B	243	Total 243	O 243	0	0
2	C	291	Total 291	O 291	0	0
2	D	221	Total 221	O 221	0	0

3 Residue-property plots [i](#)

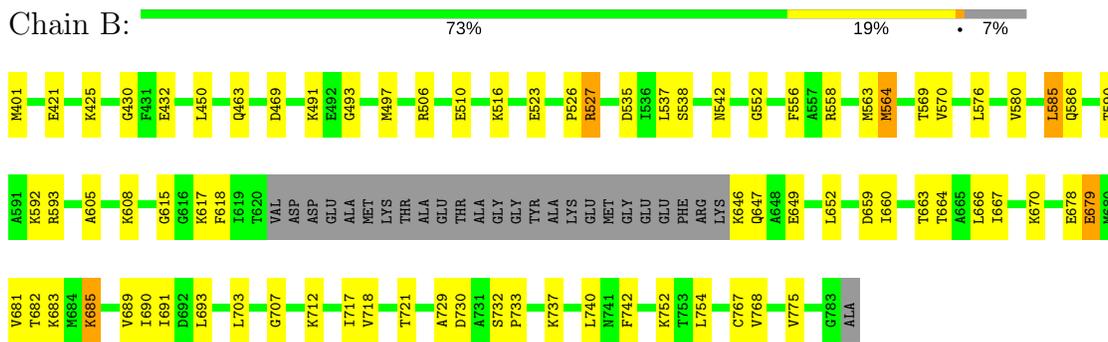
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

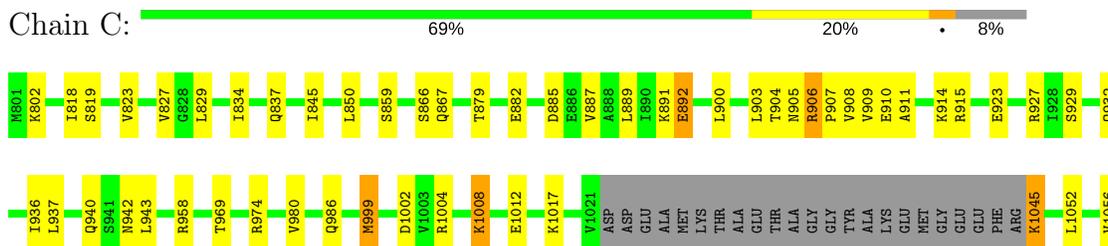
- Molecule 1: nicotinamide nucleotide Transhydrogenase, subunit alpha 1



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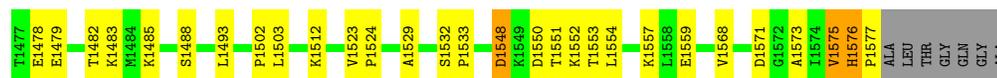
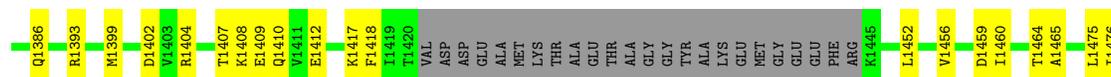
- Molecule 1: nicotinamide nucleotide Transhydrogenase, subunit alpha 1





- Molecule 1: nicotinamide nucleotide Transhydrogenase, subunit alpha 1

Chain D: 70% 21% 8%



4 Data and refinement statistics

Xtrriage (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	66.96Å 117.13Å 94.23Å 90.00° 108.26° 90.00°	Depositor
Resolution (Å)	50.00 – 1.81	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.81)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.220 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	11344	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	0.49	4/2623 (0.2%)	0.76	8/3560 (0.2%)
1	B	0.32	0/2654	0.62	1/3600 (0.0%)
1	C	0.37	2/2638 (0.1%)	0.69	5/3578 (0.1%)
1	D	0.35	1/2626 (0.0%)	0.66	4/3561 (0.1%)
All	All	0.38	7/10541 (0.1%)	0.69	18/14299 (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	3	6
1	B	1	0
All	All	4	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	ASP	CA-C	-10.05	1.26	1.52
1	A	348	ASP	C-N	8.76	1.54	1.34
1	A	377	PRO	N-CD	6.40	1.56	1.47
1	C	1150	ASP	C-N	5.68	1.47	1.34
1	A	347	VAL	C-N	-5.62	1.21	1.34

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASP	CA-C-N	-10.66	93.76	117.20
1	A	348	ASP	O-C-N	9.64	138.13	122.70
1	D	1576	HIS	C-N-CD	9.34	148.01	128.40
1	A	377	PRO	CA-N-CD	-8.41	99.72	111.50
1	C	1150	ASP	O-C-N	7.55	134.78	122.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	374	ILE	CB
1	A	375	VAL	CA
1	A	376	HIS	CA
1	B	401	MET	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	VAL	Mainchain
1	A	350	ASP	Mainchain
1	A	375	VAL	Mainchain,Peptide
1	A	376	HIS	Mainchain,Peptide

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	2589	0	2714	85	1
1	B	2620	0	2754	67	0
1	C	2604	0	2744	80	0
1	D	2592	0	2730	68	0
2	A	184	0	0	3	0
2	B	243	0	0	5	1
2	C	291	0	0	7	0
2	D	221	0	0	1	0
All	All	11344	0	10942	291	1

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 14.

The worst 5 of 291 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:127:ARG:HH21	1:A:127:ARG:H	1.11	0.94
1:B:401:MET:N	1:B:469:ASP:OD2	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:837:GLN:HE21	1:C:859:SER:HA	1.41	0.84
1:D:1286:GLU:HA	1:D:1289:LEU:HD23	1.60	0.83
1:D:1308:VAL:O	1:D:1312:LEU:HD23	1.79	0.82

All (1) 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:377:PRO:O	2:B:2379:HOH:O[2_545]	1.71	0.49

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	350/384 (91%)	329 (94%)	20 (6%)	1 (0%)	44	28
1	B	354/384 (92%)	340 (96%)	14 (4%)	0	100	100
1	C	351/384 (91%)	332 (95%)	14 (4%)	5 (1%)	13	3
1	D	349/384 (91%)	337 (97%)	12 (3%)	0	100	100
All	All	1404/1536 (91%)	1338 (95%)	60 (4%)	6 (0%)	38	22

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	HIS
1	C	1150	ASP
1	C	866	SER
1	C	892	GLU
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	274/296 (93%)	266 (97%)	8 (3%)	48 31
1	B	278/296 (94%)	271 (98%)	7 (2%)	53 37
1	C	277/296 (94%)	267 (96%)	10 (4%)	40 23
1	D	276/296 (93%)	271 (98%)	5 (2%)	64 52
All	All	1105/1184 (93%)	1075 (97%)	30 (3%)	50 34

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	679	GLU
1	C	969	THR
1	D	1337	LEU
1	C	943	LEU
1	C	999	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	720	HIS
1	C	867	GLN
1	D	1410	GLN
1	B	741	ASN
1	B	782	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.