



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 10:10 PM GMT

PDB ID : 1F8G
Title : THE X-RAY STRUCTURE OF NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE FROM RHODOSPIRILLUM RUBRUM COMPLEXED WITH NAD⁺
Authors : Buckley, P.A.; Baz Jackson, J.; Schneider, T.; White, S.A.; Rice, D.W.; Baker, P.J.
Deposited on : 2000-06-30
Resolution : 2.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

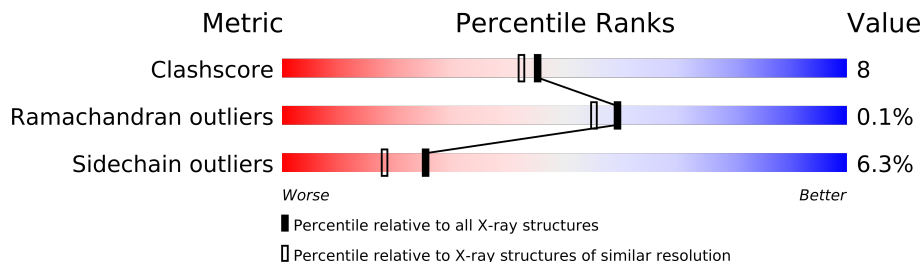
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 3 unique types of molecules in this entry. The entry contains 12733 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	Se	0	0	0
			2795	1763	480	535	3	14			
1	B	381	Total	C	N	O	S	Se	0	0	0
			2792	1761	482	531	3	15			
1	C	375	Total	C	N	O	S	Se	0	0	0
			2759	1742	476	523	3	15			
1	D	377	Total	C	N	O	S	Se	0	0	0
			2770	1749	477	526	3	15			

There are 60 discrepancies between the modelled and reference sequences:

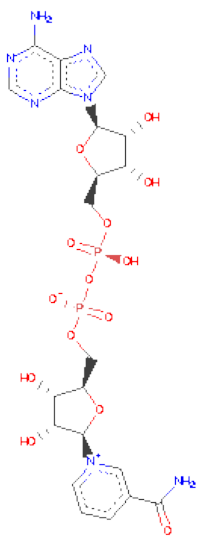
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	78	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	97	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	122	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	125	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	134	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	162	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	163	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	164	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	199	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	226	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	239	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	280	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	284	MSE	MET	MODIFIED RESIDUE	UNP Q60164
A	356	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	78	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	97	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	122	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	125	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	134	MSE	MET	MODIFIED RESIDUE	UNP Q60164

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Chain	Residue	Modelled	Actual	Comment	Reference
B	162	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	163	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	164	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	199	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	226	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	239	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	280	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	284	MSE	MET	MODIFIED RESIDUE	UNP Q60164
B	356	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	78	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	97	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	122	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	125	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	134	MSE	MET	MODIFIED RESIDUE	UNP Q60164
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C	199	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	226	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	239	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	280	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	284	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	356	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	78	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	97	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	122	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	125	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	134	MSE	MET	MODIFIED RESIDUE	UNP Q60164
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D	226	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	239	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	280	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	284	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	356	MSE	MET	MODIFIED RESIDUE	UNP Q60164

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	C	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	406	Total	O	0	0
			406	406		
3	B	398	Total	O	0	0
			398	398		
3	C	389	Total	O	0	0
			389	389		
3	D	266	Total	O	0	0
			266	266		

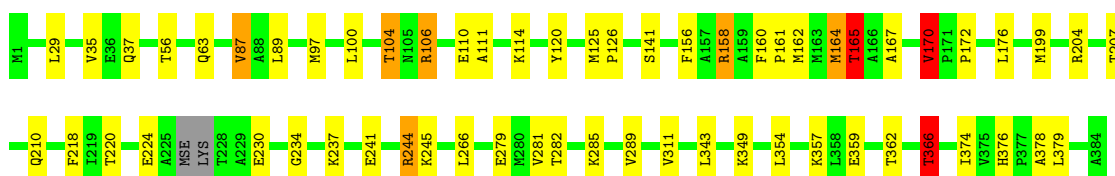
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

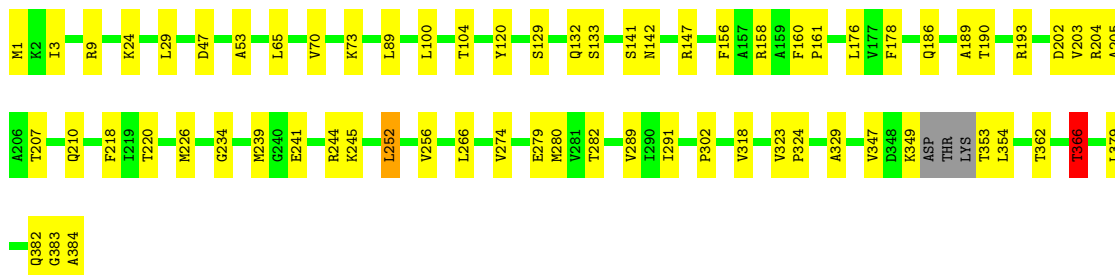
• Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain A: 



• Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain B: 



• Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain C: 



• Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain D: 

ALA	T277	A157	M1
	E278	R158	K2
	E279	A159	I5
	V280	P160	R9
	T281	M162	S19
	T282	M163	V23
	V289	M164	F31
	D292	A166	I34
	L293	A167	Q37
	N300	T169	I57
	K308	P171	A88
	K312	P172	S59
	H313	L176	T60
	A329	F178	Q63
	S332	Q186	A64
	P333	D202	L65
	L339	V203	W72
	L340	R204	R76
	N341	A205	P77
	F342	A206	M78
	L343	T207	T84
	T344	Q210	D85
	P345	F218	F86
	D348	V221	V87
	L35	E224	A88
	ASP	A225	L89
	THR	M226	M97
	L352	K227	T104
	L354	T228	N105
	L358	A229	R106
	S359	E230	P107
	P360	K237	V108
	E361	E242	V109
	L362	E247	E110
	T366	Q247	Y120
	C367	L252	A121
	V368	K257	M122
	L369	T258	M125
	R370	D259	S133
	V375	T263	N142
	H376	A265	F145
	L380	L268	
	GLY	GLN	
	GLY	GLY	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.90Å 116.60Å 102.00Å 90.00° 104.22° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12733	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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

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	0.43	0/2818	1.01	11/3798 (0.3%)
1	B	0.42	0/2814	1.01	4/3789 (0.1%)
1	C	0.44	1/2781 (0.0%)	1.02	8/3743 (0.2%)
1	D	0.39	0/2792	0.98	11/3760 (0.3%)
All	All	0.42	1/11205 (0.0%)	1.00	34/15090 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	377	PRO	N-CD	5.34	1.55	1.47

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	B	366	THR	N-CA-CB	-7.40	96.23	110.30
1	C	263	THR	N-CA-CB	-7.20	96.63	110.30
1	A	237	LYS	CA-C-O	6.98	134.77	120.10
1	D	263	THR	N-CA-CB	-6.94	97.12	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2795	0	2911	36	0
1	B	2792	0	2916	47	0
1	C	2759	0	2887	39	0
1	D	2770	0	2897	75	0
2	A	44	0	26	0	0
2	B	35	0	19	3	0
2	C	35	0	19	1	0
2	D	44	0	26	0	0
3	A	406	0	0	4	0
3	B	398	0	0	3	0
3	C	389	0	0	5	0
3	D	266	0	0	5	0
All	All	12733	0	11701	193	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 193 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:263:THR:HG23	1:D:300:ASN:HD22	1.26	0.99
1:C:202:ASP:HB3	1:C:207:THR:HG21	1.48	0.94
1:D:263:THR:HG22	1:D:292:ASP:HA	1.53	0.90
1:A:97:MSE:HE1	1:A:343:LEU:HD13	1.52	0.90
1:A:162:MSE:SE	1:A:164:MSE:HE3	2.23	0.88

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	378/384 (98%)	370 (98%)	8 (2%)	0	100	100
1	B	377/384 (98%)	367 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	371/384 (97%)	357 (96%)	13 (4%)	1 (0%)	50	44
1	D	373/384 (97%)	360 (96%)	12 (3%)	1 (0%)	50	44
All	All	1499/1536 (98%)	1454 (97%)	43 (3%)	2 (0%)	59	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	223	ASP
1	D	376	HIS

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	293/281 (104%)	270 (92%)	23 (8%)	18	11
1	B	293/281 (104%)	281 (96%)	12 (4%)	41	35
1	C	291/281 (104%)	272 (94%)	19 (6%)	24	17
1	D	292/281 (104%)	272 (93%)	20 (7%)	22	15
All	All	1169/1124 (104%)	1095 (94%)	74 (6%)	25	18

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	366	THR
1	C	207	THR
1	D	281	VAL
1	B	382	GLN
1	C	84	THR

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	210	GLN
1	B	313	HIS

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Mol	Chain	Res	Type
1	D	300	ASN
1	B	247	GLN
1	B	382	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	NAD	A	2500	-	48,48,48	0.92	3 (6%)	73,73,73	1.72	13 (17%)
2	NAD	B	2501	-	36,38,48	0.70	0	54,58,73	1.15	4 (7%)
2	NAD	C	2502	-	36,38,48	0.66	0	54,58,73	1.20	6 (11%)
2	NAD	D	2503	-	48,48,48	0.85	2 (4%)	73,73,73	1.68	12 (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
2	NAD	A	2500	-	-	0/30/62/62	0/3/5/5
2	NAD	B	2501	-	-	0/22/51/62	0/2/4/5
2	NAD	C	2502	-	-	0/22/51/62	0/2/4/5
2	NAD	D	2503	-	-	0/30/62/62	0/3/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2500	NAD	C3N-C7N	3.41	1.56	1.50
2	D	2503	NAD	C3N-C7N	3.41	1.56	1.50
2	A	2500	NAD	C6N-N1N	2.31	1.42	1.35
2	D	2503	NAD	C6N-N1N	2.29	1.42	1.35
2	A	2500	NAD	C2A-N1A	2.08	1.38	1.33

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2500	NAD	C5N-C4N-C3N	-5.64	112.99	120.32
2	D	2503	NAD	C5N-C4N-C3N	-5.41	113.29	120.32
2	A	2500	NAD	C6N-C5N-C4N	5.40	128.01	119.44
2	D	2503	NAD	C6N-C5N-C4N	5.28	127.82	119.44
2	A	2500	NAD	C2N-C3N-C4N	4.25	123.12	118.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.