



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2017 – 11:42 PM EDT

PDB ID : 1F8G  
Title : THE X-RAY STRUCTURE OF NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE FROM RHODOSPIRILLUM RUBRUM COMPLEXED WITH NAD<sup>+</sup>  
Authors : Buckley, P.A.; Baz Jackson, J.; Schneider, T.; White, S.A.; Rice, D.W.; Baker, P.J.  
Deposited on : unknown  
Resolution : 2.00 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (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)	:	rb-20029824

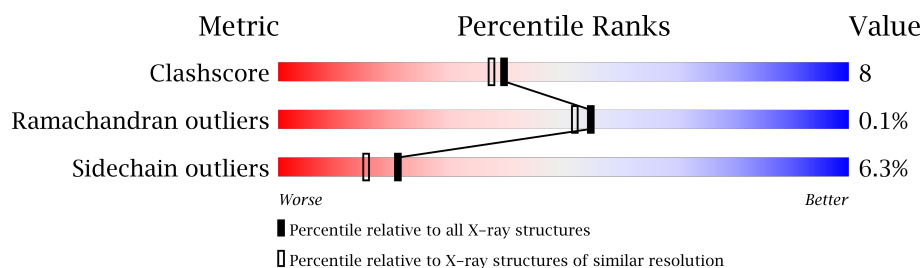
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (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  $\geq 3$ , 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 3 unique types of molecules in this entry. The entry contains 12733 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.

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
C	162	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	163	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	164	MSE	MET	MODIFIED RESIDUE	UNP Q60164
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	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: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 3 is water.

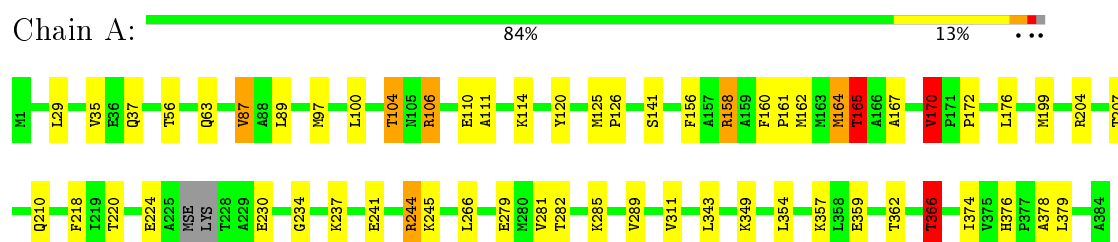
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	406	Total O 406 406	0	0
3	B	398	Total O 398 398	0	0
3	C	389	Total O 389 389	0	0
3	D	266	Total O 266 266	0	0

### 3 Residue-property plots

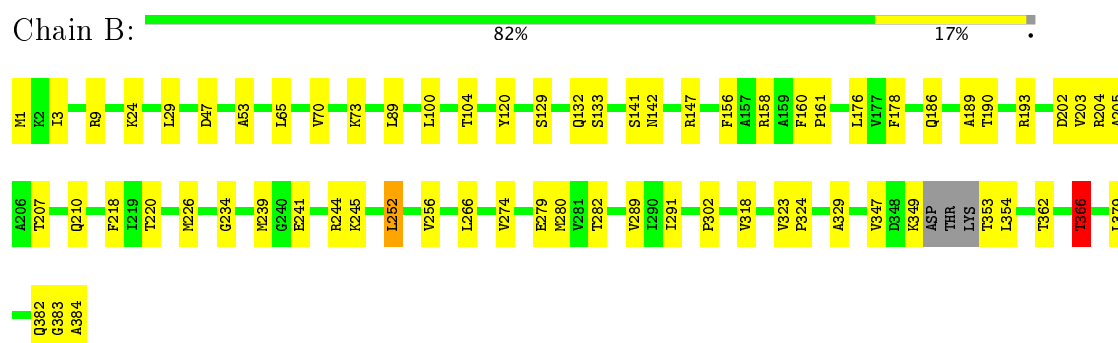
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

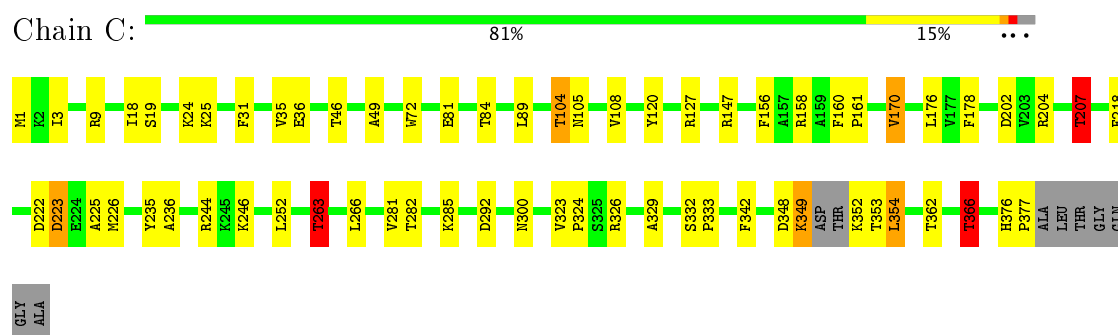
#### • Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE



#### • Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE



#### • Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE



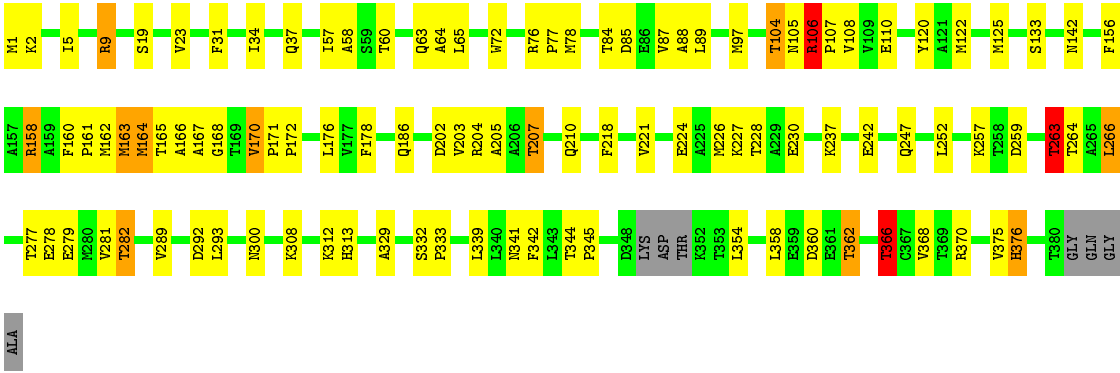
#### • Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain D: 

71%

23%

...



## 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, $\alpha$ , $\beta$ , $\gamma$	65.90 Å 116.60 Å 102.00 Å 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 <sup>2</sup> )	31.0	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

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 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	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

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 8.

The worst 5 of 193 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: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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	377/384 (98%)	367 (97%)	10 (3%)	0	100	100
1	C	371/384 (97%)	357 (96%)	13 (4%)	1 (0%)	44	40
1	D	373/384 (97%)	360 (96%)	12 (3%)	1 (0%)	44	40
All	All	1499/1536 (98%)	1454 (97%)	43 (3%)	2 (0%)	55	52

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%)	15	9
1	B	293/281 (104%)	281 (96%)	12 (4%)	35	31
1	C	291/281 (104%)	272 (94%)	19 (6%)	20	14
1	D	292/281 (104%)	272 (93%)	20 (7%)	18	13
All	All	1169/1124 (104%)	1095 (94%)	74 (6%)	21	15

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
1	D	300	ASN
1	B	247	GLN
1	B	382	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](#)

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	-	41,48,48	1.04	3 (7%)	43,73,73	2.03	7 (16%)
2	NAD	B	2501	-	33,38,48	0.76	0	32,58,73	1.02	1 (3%)
2	NAD	C	2502	-	33,38,48	0.74	1 (3%)	32,58,73	1.25	3 (9%)
2	NAD	D	2503	-	41,48,48	0.96	2 (4%)	43,73,73	2.00	9 (20%)

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	-	-	0/22/62/62	0/5/5/5
2	NAD	B	2501	-	-	0/18/51/62	0/4/4/5
2	NAD	C	2502	-	-	0/18/51/62	0/4/4/5
2	NAD	D	2503	-	-	0/22/62/62	0/5/5/5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2502	NAD	C2A-N1A	2.01	1.37	1.33
2	A	2500	NAD	C2A-N1A	2.19	1.38	1.33
2	D	2503	NAD	C6N-N1N	2.53	1.42	1.35
2	A	2500	NAD	C6N-N1N	2.55	1.42	1.35
2	D	2503	NAD	C3N-C7N	3.77	1.56	1.50

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2500	NAD	C5N-C4N-C3N	-6.25	112.99	120.35
2	D	2503	NAD	C5N-C4N-C3N	-6.00	113.29	120.35
2	D	2503	NAD	C5N-C6N-N1N	-4.57	113.38	120.40
2	A	2500	NAD	C5N-C6N-N1N	-4.40	113.63	120.40
2	C	2502	NAD	C4B-O4B-C1B	-4.35	105.14	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2501	NAD	3	0
2	C	2502	NAD	1	0

## 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.