wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 06:49 PM EDT

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 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 (i) 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 (1)) were used in the production of this report:

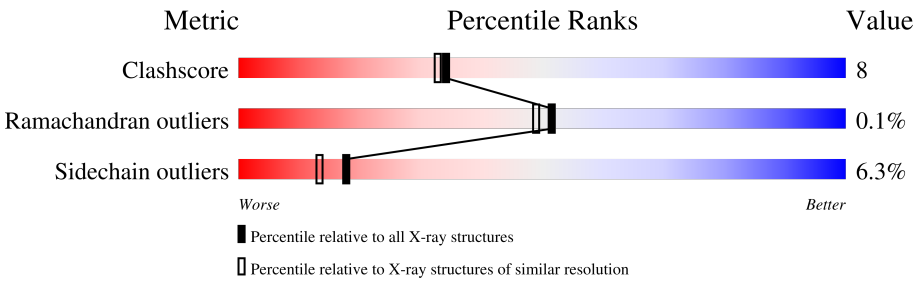
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	384	84% 13% • ••
1	B	384	82% 17% •
1	C	384	81% 15% •• •
1	D	384	71% 23% • • •

2 Entry composition (i)

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

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
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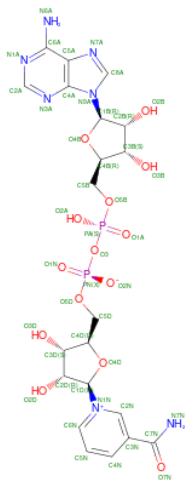
C	164	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	199	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	226	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	239	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	280	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	284	MSE	MET	MODIFIED RESIDUE	UNP Q60164
C	356	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	1	MSE	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
D	162	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	163	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	164	MSE	MET	MODIFIED RESIDUE	UNP Q60164
D	199	MSE	MET	MODIFIED RESIDUE	UNP Q60164
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: $C_{21}H_{27}N_7O_{14}P_2$).

NAD



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

- Molecule 3 is water.

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

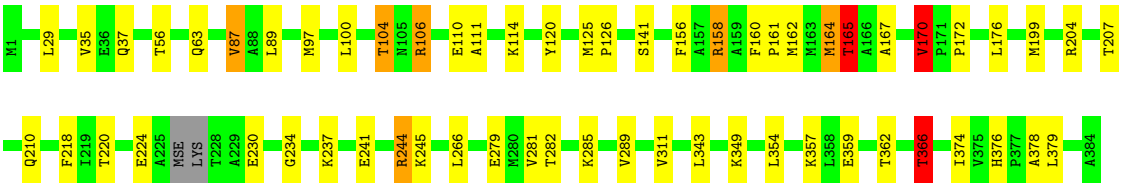
3 Residue-property plots (i)

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.

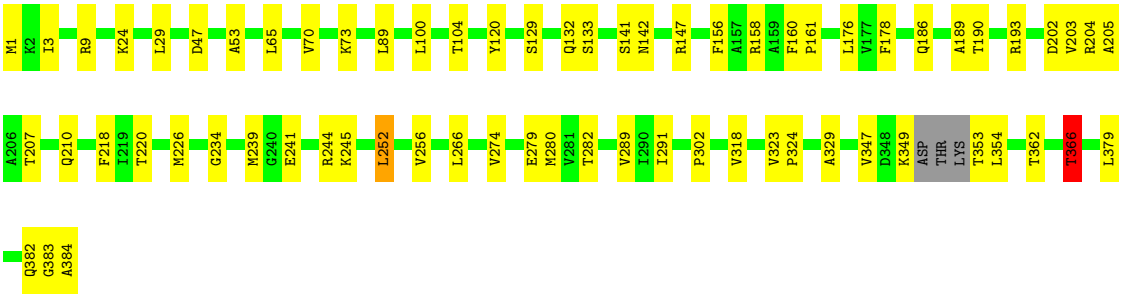
• Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain A:



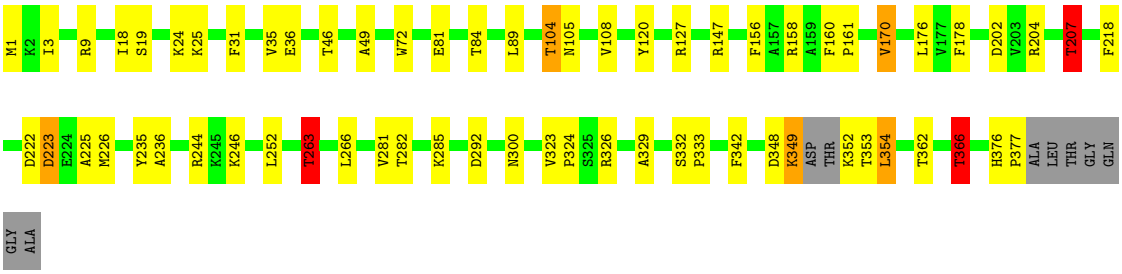
• Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain B:



• Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain C:



• Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain D:

71%
23%
• • •

M1 K2 I5 R9 S19 V23 F31 I34 Q37 I57 A58 S59 T60 Q63 A64 L65 W72 R76 P77 N78 T84 D85 E86 V87 A88 L89 M97 T104 N105 R106 P107 V108 V109 E110 Y120 A121 M122 M125 S133 N142 F156
A157 R158 A159 F160 P161 M162 M163 M164 T165 A166 A167 G168 T169 V170 P171 P172 L176 V177 F178 Q186 D202 V203 R204 A205 A206 T207 Q210 F218 V221 E224 A225 M226 K227 T228 A229 E230 K237 E242 Q247 L252 K257 T258 D259 T263 T264 A265 L266
T277 E278 E279 M280 V281 T282 V289 D292 L293 N300 K308 K312 H313 A329 S332 P333 L339 L340 N341 F342 L343 T344 P345 D348 LYS ASP THR K352 T353 L354 L358 E359 D360 E361 T362 T366 C367 V368 T369 R370 V375 H376 T380 GLY GLN GLY
ALA

4 Data and refinement statistics (i)

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	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 (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(^{o})	Ideal(^{o})
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 (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	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%)	41	37
1	D	373/384 (97%)	360 (96%)	12 (3%)	1 (0%)	41	37
All	All	1499/1536 (98%)	1454 (97%)	43 (3%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

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

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	293/281 (104%)	270 (92%)	23 (8%)	12	8
1	B	293/281 (104%)	281 (96%)	12 (4%)	30	28
1	C	291/281 (104%)	272 (94%)	19 (6%)	17	12
1	D	292/281 (104%)	272 (93%)	20 (7%)	16	11
All	All	1169/1124 (104%)	1095 (94%)	74 (6%)	18	13

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

Mol	Chain	Res	Type
1	D	104	THR
1	D	362	THR
1	D	163	MSE
1	D	257	LYS
1	B	73	LYS

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

Mol	Chain	Res	Type
1	C	105	ASN
1	D	142	ASN
1	D	132	GLN
1	D	186	GLN
1	A	376	HIS

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 monosaccharides 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	B	2501	-	33,38,48	0.79	0	37,58,73	1.01	3 (8%)
2	NAD	C	2502	-	33,38,48	0.77	1 (3%)	37,58,73	1.08	4 (10%)
2	NAD	A	2500	-	42,48,48	1.08	3 (7%)	50,73,73	1.91	7 (14%)
2	NAD	D	2503	-	42,48,48	0.99	2 (4%)	50,73,73	1.91	8 (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	B	2501	-	-	4/18/51/62	0/4/4/5
2	NAD	C	2502	-	-	2/18/51/62	0/4/4/5
2	NAD	A	2500	-	-	2/26/62/62	0/5/5/5
2	NAD	D	2503	-	-	1/26/62/62	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	A	2500	NAD	C3N-C7N	3.87	1.56	1.50
2	D	2503	NAD	C3N-C7N	3.86	1.56	1.50
2	A	2500	NAD	C6N-N1N	2.72	1.42	1.35
2	D	2503	NAD	C6N-N1N	2.69	1.42	1.35
2	A	2500	NAD	C2A-N1A	2.21	1.38	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2500	NAD	C5N-C4N-C3N	-6.21	112.99	120.34
2	D	2503	NAD	C5N-C4N-C3N	-5.96	113.29	120.34
2	A	2500	NAD	C6N-C5N-C4N	5.90	128.01	119.44
2	D	2503	NAD	C6N-C5N-C4N	5.77	127.82	119.44
2	D	2503	NAD	C5N-C6N-N1N	-4.89	113.38	120.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2501	NAD	C5D-O5D-PN-O3
2	B	2501	NAD	C5D-O5D-PN-O1N
2	B	2501	NAD	O4D-C4D-C5D-O5D
2	B	2501	NAD	C3D-C4D-C5D-O5D
2	C	2502	NAD	O4D-C4D-C5D-O5D

There are no ring outliers.

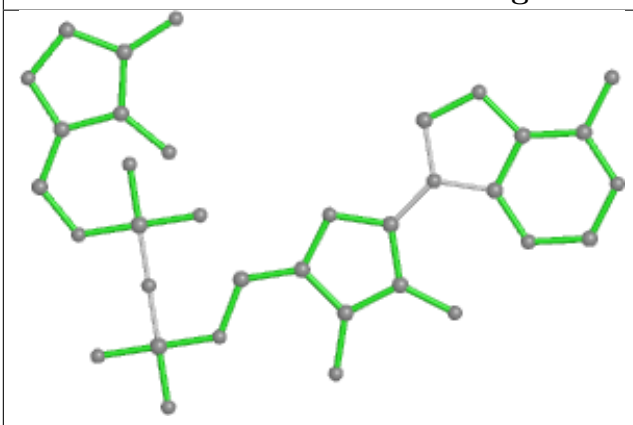
2 monomers are involved in 4 short contacts:

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

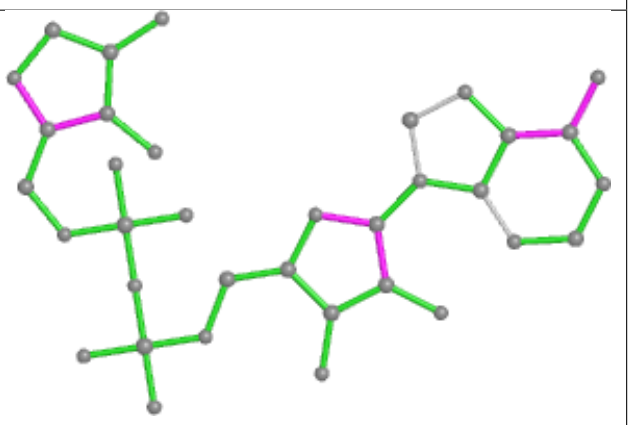
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

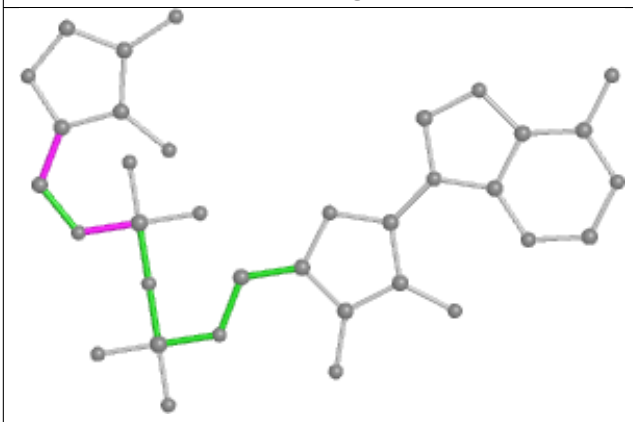
Ligand NAD B 2501



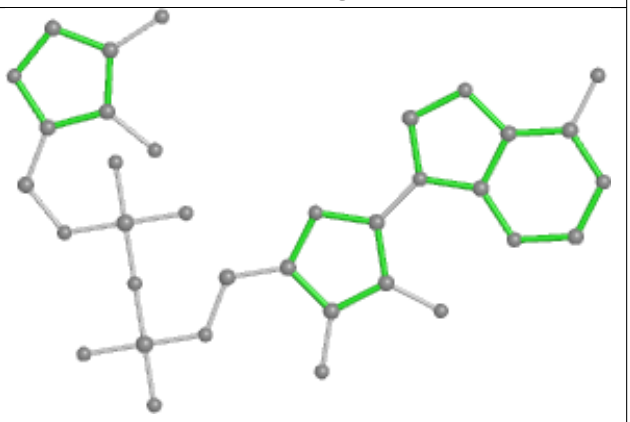
Bond lengths



Bond angles

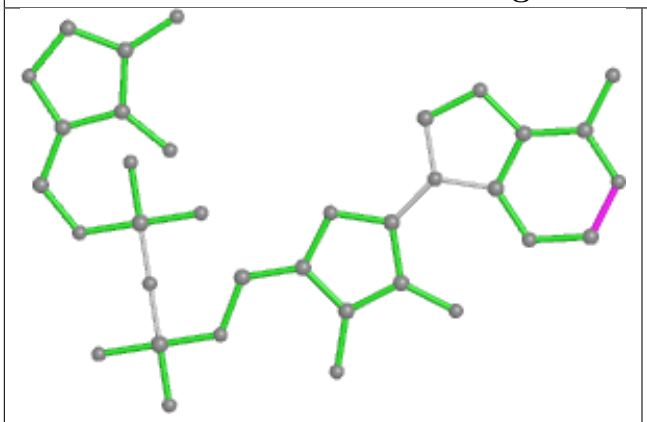


Torsions

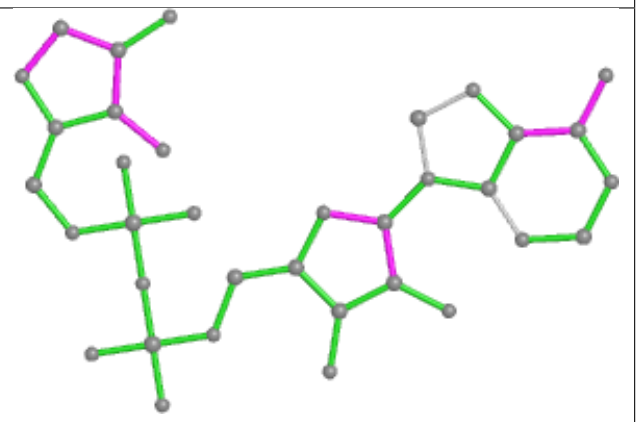


Rings

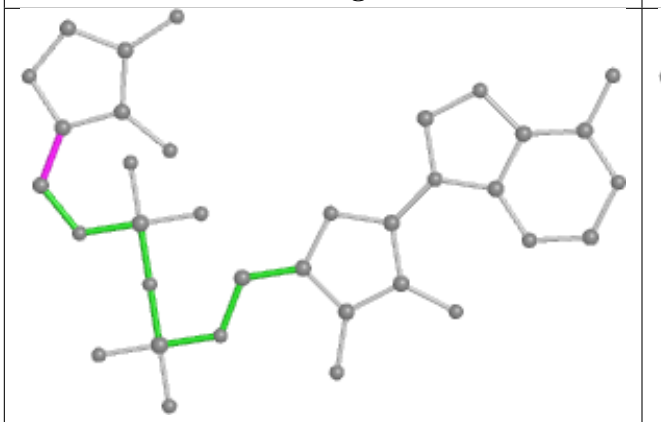
Ligand NAD C 2502



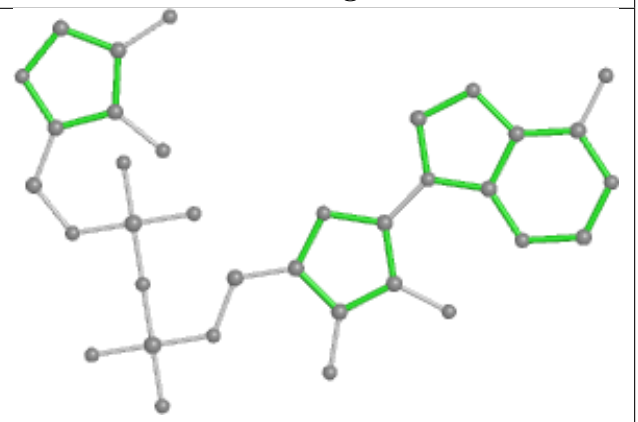
Bond lengths



Bond angles

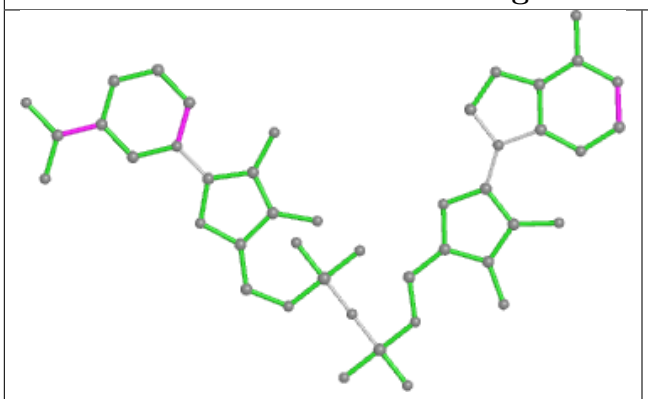


Torsions

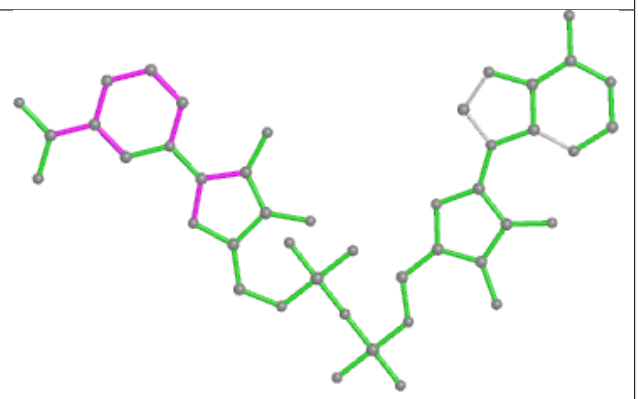


Rings

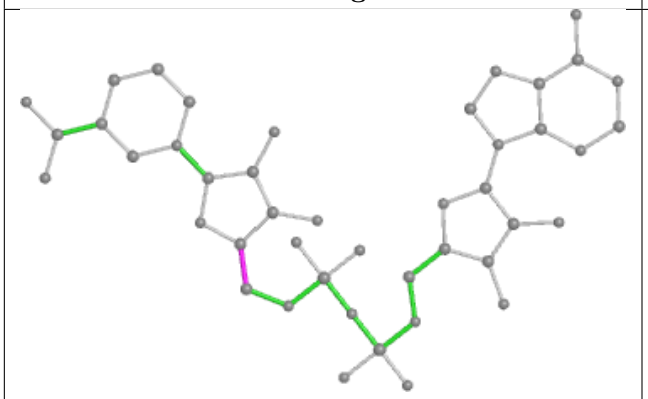
Ligand NAD A 2500



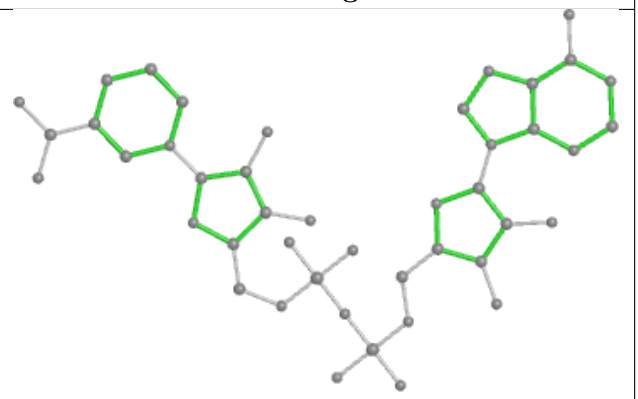
Bond lengths



Bond angles

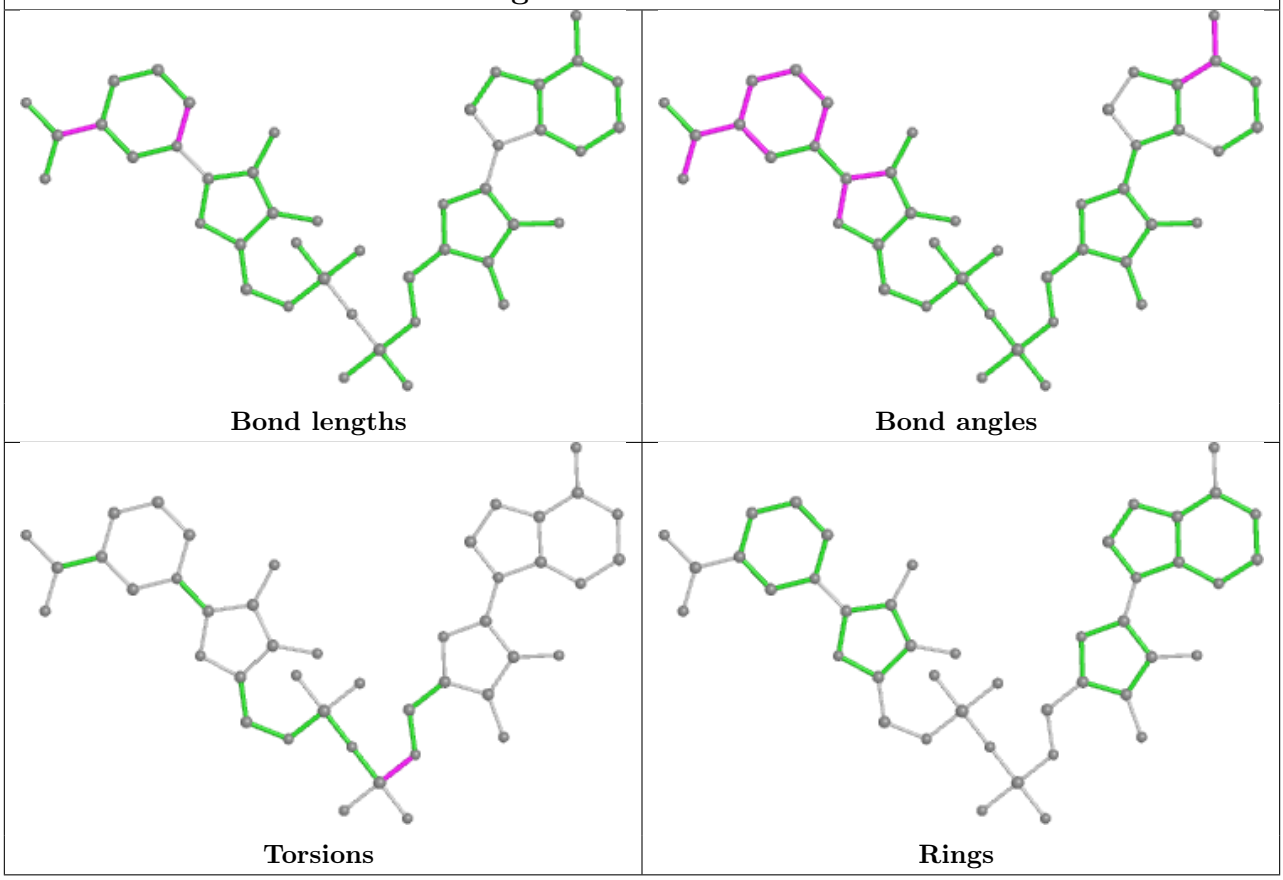


Torsions



Rings

Ligand NAD D 2503



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.