Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 04:43 PM EDT

PDB ID	:	1U2D
Title	:	Structre of transhydrogenaes (dI.NADH)2(dIII.NADPH)1 asymmetric complex
Authors	:	Mather, O.C.; Singh, A.; van Boxel, G.I.; White, S.A.; Jackson, J.B.
Deposited on	:	2004-07-19
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

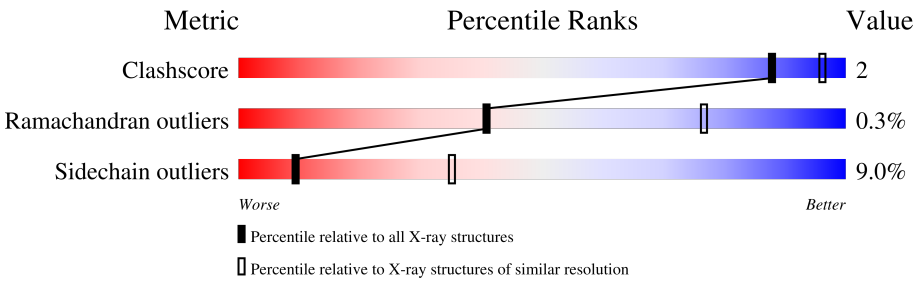
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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	88% 10% •
1	B	384	85% 13% ••
2	C	203	76% 8% • 14%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7060 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.

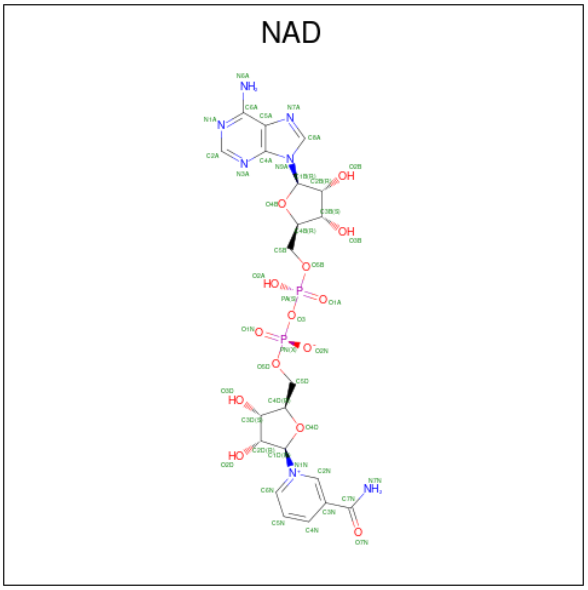
- Molecule 1 is a protein called NAD(P) transhydrogenase subunit alpha part 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	378	2779	1753	479	529	18	0	0	0
1	B	379	2787	1759	480	530	18	0	0	0

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

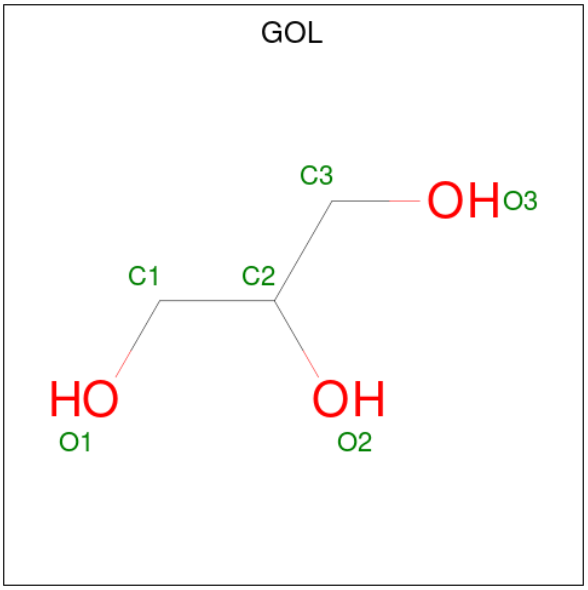
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	174	1311	830	217	253	11	0	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



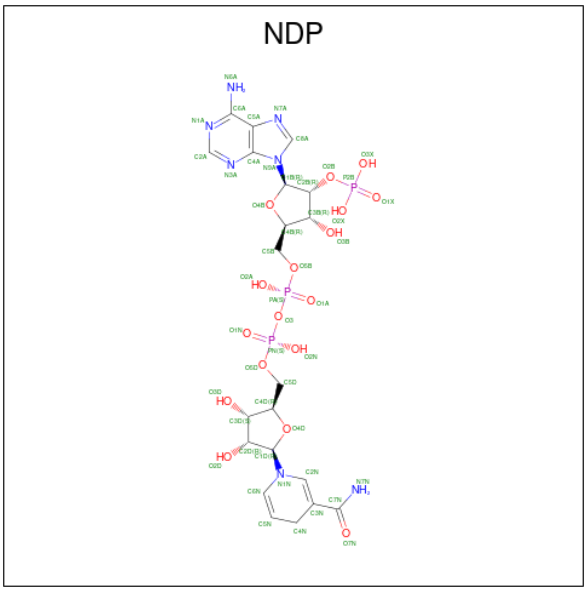
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	B	1	44	21	7	14	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	6	3	3	0	0

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	C	1	48	21	7	17	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	15	15	15	0	0
			Total	O		
6	B	18	18	18	0	0
			Total	O		
6	C	8	8	8	0	0

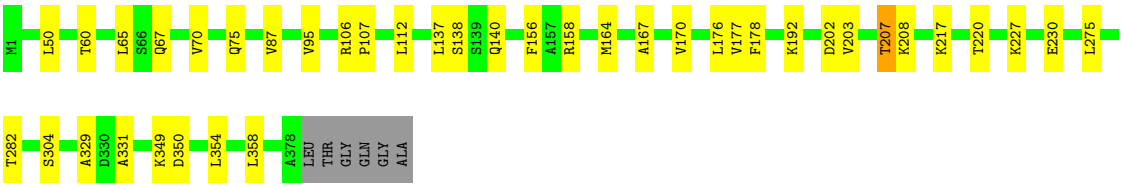
3 Residue-property plots (i)

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.

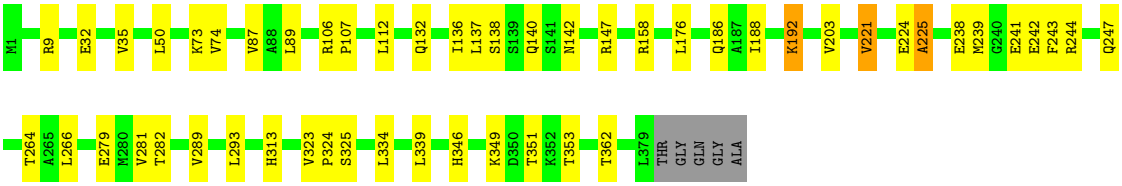
• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

Chain A:



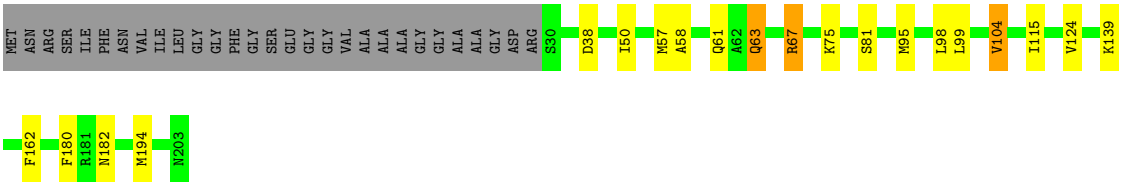
• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

Chain B:



• Molecule 2: NAD(P) transhydrogenase subunit beta

Chain C:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.25Å 74.55Å 204.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.206 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7060	wwPDB-VP
Average B, all atoms (Å^2)	71.0	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: GOL, NDP, 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	0.31	0/2816	0.47	0/3816
1	B	0.31	0/2824	0.49	0/3827
2	C	0.32	0/1334	0.45	0/1803
All	All	0.31	0/6974	0.48	0/9446

There are no bond length outliers.

There are no bond angle outliers.

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	2779	0	2904	10	0
1	B	2787	0	2915	17	0
2	C	1311	0	1303	4	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
4	B	6	0	8	0	0
5	C	48	0	25	0	0
6	A	15	0	0	0	0
6	B	18	0	0	0	0
6	C	8	0	0	0	0
All	All	7060	0	7207	29	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 2.

All (29) 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:B:142:ASN:HD21	1:B:186:GLN:HE21	1.13	0.96
1:A:178:PHE:HB3	1:A:275:LEU:HD13	1.86	0.56
1:B:132:GLN:HE22	1:B:138:SER:CB	2.18	0.55
2:C:63:GLN:HG2	2:C:98:LEU:HB3	1.88	0.55
1:A:329:ALA:HB3	1:B:158:ARG:HG2	1.89	0.53
1:B:87:VAL:HG23	1:B:112:LEU:HD23	1.91	0.52
1:B:264:THR:HG22	1:B:293:LEU:HD12	1.92	0.51
1:A:87:VAL:HG13	1:A:112:LEU:HD23	1.92	0.51
1:A:202:ASP:HB3	1:A:207:THR:HG21	1.94	0.48
1:B:221:VAL:HG11	1:B:247:GLN:HA	1.96	0.47
1:B:136:ILE:O	1:B:140:GLN:HG2	2.14	0.47
1:B:106:ARG:N	1:B:107:PRO:CD	2.78	0.47
1:B:142:ASN:ND2	1:B:186:GLN:HE21	1.95	0.46
1:B:188:ILE:O	1:B:192:LYS:HB2	2.16	0.46
1:B:346:HIS:CD2	1:B:346:HIS:N	2.83	0.46
1:A:70:VAL:HG23	1:A:95:VAL:HG23	1.98	0.45
1:A:106:ARG:N	1:A:107:PRO:CD	2.80	0.45
1:A:167:ALA:HB3	1:B:334:LEU:HD22	1.99	0.44
2:C:99:LEU:HD22	2:C:104:VAL:HG11	1.99	0.44
1:A:140:GLN:OE1	1:A:331:ALA:HB1	2.18	0.43
1:B:203:VAL:HG12	1:B:243:PHE:CE1	2.54	0.43
1:B:282:THR:HG22	1:B:313:HIS:ND1	2.34	0.42
1:A:156:PHE:CZ	1:A:158:ARG:HB2	2.55	0.41
1:B:142:ASN:HD21	1:B:186:GLN:NE2	1.96	0.41
1:B:224:GLU:O	1:B:225:ALA:HB2	2.20	0.41
1:B:323:VAL:N	1:B:324:PRO:CD	2.83	0.40
1:A:202:ASP:OD1	1:A:203:VAL:N	2.55	0.40
2:C:58:ALA:O	2:C:61:GLN:NE2	2.54	0.40
2:C:67:ARG:HG3	2:C:104:VAL:HG12	2.03	0.40

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	376/384 (98%)	353 (94%)	23 (6%)	0	100	100
1	B	377/384 (98%)	352 (93%)	22 (6%)	3 (1%)	19	57
2	C	172/203 (85%)	164 (95%)	8 (5%)	0	100	100
All	All	925/971 (95%)	869 (94%)	53 (6%)	3 (0%)	41	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	225	ALA
1	B	351	THR
1	B	349	LYS

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	293/296 (99%)	269 (92%)	24 (8%)	11	39
1	B	294/296 (99%)	269 (92%)	25 (8%)	10	38
2	C	138/154 (90%)	122 (88%)	16 (12%)	5	23
All	All	725/746 (97%)	660 (91%)	65 (9%)	9	35

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	60	THR
1	A	65	LEU
1	A	67	GLN
1	A	75	GLN
1	A	137	LEU
1	A	138	SER
1	A	164	MET
1	A	170	VAL
1	A	176	LEU
1	A	177	VAL
1	A	192	LYS
1	A	207	THR
1	A	208	LYS
1	A	217	LYS
1	A	220	THR
1	A	227	LYS
1	A	230	GLU
1	A	282	THR
1	A	304	SER
1	A	349	LYS
1	A	350	ASP
1	A	354	LEU
1	A	358	LEU
1	B	9	ARG
1	B	32	GLU
1	B	35	VAL
1	B	50	LEU
1	B	73	LYS
1	B	74	VAL
1	B	89	LEU
1	B	137	LEU
1	B	147	ARG
1	B	176	LEU
1	B	192	LYS
1	B	221	VAL
1	B	238	GLU
1	B	239	MET
1	B	241	GLU
1	B	242	GLU
1	B	244	ARG
1	B	266	LEU
1	B	279	GLU

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Mol	Chain	Res	Type
1	B	281	VAL
1	B	289	VAL
1	B	325	SER
1	B	339	LEU
1	B	353	THR
1	B	362	THR
2	C	38	ASP
2	C	50	ILE
2	C	57	MET
2	C	63	GLN
2	C	67	ARG
2	C	75	LYS
2	C	81	SER
2	C	95	MET
2	C	104	VAL
2	C	115	ILE
2	C	124	VAL
2	C	139	LYS
2	C	162	PHE
2	C	180	PHE
2	C	182	ASN
2	C	194	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	247	GLN
1	B	99	HIS
1	B	132	GLN
1	B	142	ASN
1	B	210	GLN
1	B	247	GLN
1	B	346	HIS
2	C	61	GLN
2	C	63	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 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	$\#\|Z\| > 2$
3	NAD	A	500	-	42,48,48	2.05	6 (14%)	50,73,73	1.72	12 (24%)
3	NAD	B	600	-	42,48,48	2.05	7 (16%)	50,73,73	1.71	11 (22%)
5	NDP	C	400	-	45,52,52	1.35	2 (4%)	53,80,80	1.33	7 (13%)
4	GOL	B	404	-	5,5,5	0.40	0	5,5,5	0.46	0

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
3	NAD	A	500	-	-	1/26/62/62	0/5/5/5
3	NAD	B	600	-	-	2/26/62/62	0/5/5/5
5	NDP	C	400	-	-	15/30/77/77	0/5/5/5
4	GOL	B	404	-	-	0/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	NAD	C4N-C3N	6.71	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	NAD	C4A-N3A	6.54	1.44	1.35
3	B	600	NAD	C4A-N3A	6.51	1.44	1.35
3	B	600	NAD	C4N-C3N	6.48	1.50	1.39
5	C	400	NDP	C4A-N3A	6.41	1.44	1.35
3	B	600	NAD	C5N-C4N	5.13	1.49	1.38
3	A	500	NAD	C5N-C4N	4.98	1.49	1.38
3	B	600	NAD	C2N-N1N	-4.39	1.29	1.35
3	A	500	NAD	C2N-N1N	-4.35	1.29	1.35
5	C	400	NDP	C6N-N1N	-3.71	1.28	1.37
3	A	500	NAD	C6N-N1N	-2.50	1.29	1.35
3	B	600	NAD	C6N-N1N	-2.46	1.29	1.35
3	B	600	NAD	C2N-C3N	-2.23	1.35	1.39
3	B	600	NAD	C6N-C5N	-2.19	1.33	1.38
3	A	500	NAD	C6N-C5N	-2.12	1.33	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	600	NAD	N3A-C2A-N1A	-4.05	122.34	128.68
3	A	500	NAD	N3A-C2A-N1A	-4.01	122.41	128.68
3	B	600	NAD	C2N-C3N-C4N	-4.00	113.72	118.26
3	B	600	NAD	C4A-C5A-N7A	-3.88	105.36	109.40
3	A	500	NAD	C2N-C3N-C4N	-3.88	113.86	118.26
5	C	400	NDP	N3A-C2A-N1A	-3.86	122.65	128.68
3	A	500	NAD	C3N-C7N-N7N	3.84	122.36	117.75
3	B	600	NAD	C6N-N1N-C2N	3.81	125.45	121.97
3	A	500	NAD	C4A-C5A-N7A	-3.79	105.45	109.40
3	A	500	NAD	C3N-C2N-N1N	3.68	124.02	120.43
5	C	400	NDP	C4A-C5A-N7A	-3.48	105.77	109.40
3	B	600	NAD	C3N-C2N-N1N	3.37	123.72	120.43
3	B	600	NAD	PN-O3-PA	-3.32	121.44	132.83
5	C	400	NDP	O4B-C1B-C2B	3.26	112.23	106.59
3	A	500	NAD	C6N-N1N-C2N	3.04	124.74	121.97
3	B	600	NAD	C3N-C7N-N7N	3.00	121.35	117.75
3	A	500	NAD	C2A-N1A-C6A	2.96	123.82	118.75
3	B	600	NAD	C2A-N1A-C6A	2.80	123.54	118.75
3	A	500	NAD	PN-O3-PA	-2.75	123.38	132.83
5	C	400	NDP	O4D-C1D-N1N	2.71	113.36	108.06
3	B	600	NAD	C6N-C5N-C4N	-2.67	115.55	119.44
3	A	500	NAD	O7N-C7N-N7N	-2.65	118.81	122.58
5	C	400	NDP	C2A-N1A-C6A	2.49	123.02	118.75
3	A	500	NAD	C6N-C5N-C4N	-2.49	115.82	119.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	400	NDP	PN-O3-PA	-2.46	124.40	132.83
3	A	500	NAD	O4B-C1B-C2B	-2.40	103.42	106.93
5	C	400	NDP	O4B-C4B-C3B	2.21	109.49	105.11
3	B	600	NAD	O4B-C1B-C2B	-2.15	103.79	106.93
3	A	500	NAD	C5N-C6N-N1N	2.01	123.28	120.40
3	B	600	NAD	O7N-C7N-N7N	-2.00	119.73	122.58

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	NAD	O4D-C1D-N1N-C6N
3	B	600	NAD	C5B-O5B-PA-O1A
5	C	400	NDP	C5B-O5B-PA-O1A
5	C	400	NDP	C5B-O5B-PA-O2A
5	C	400	NDP	C5B-O5B-PA-O3
5	C	400	NDP	O4B-C4B-C5B-O5B
5	C	400	NDP	C2B-O2B-P2B-O2X
5	C	400	NDP	PA-O3-PN-O5D
5	C	400	NDP	C5D-O5D-PN-O1N
5	C	400	NDP	C5D-O5D-PN-O2N
5	C	400	NDP	O4D-C4D-C5D-O5D
5	C	400	NDP	C3D-C4D-C5D-O5D
3	B	600	NAD	C5B-O5B-PA-O3
5	C	400	NDP	C5D-O5D-PN-O3
5	C	400	NDP	O4D-C1D-N1N-C6N
5	C	400	NDP	C2D-C1D-N1N-C6N
5	C	400	NDP	C3B-C4B-C5B-O5B
5	C	400	NDP	PA-O3-PN-O1N

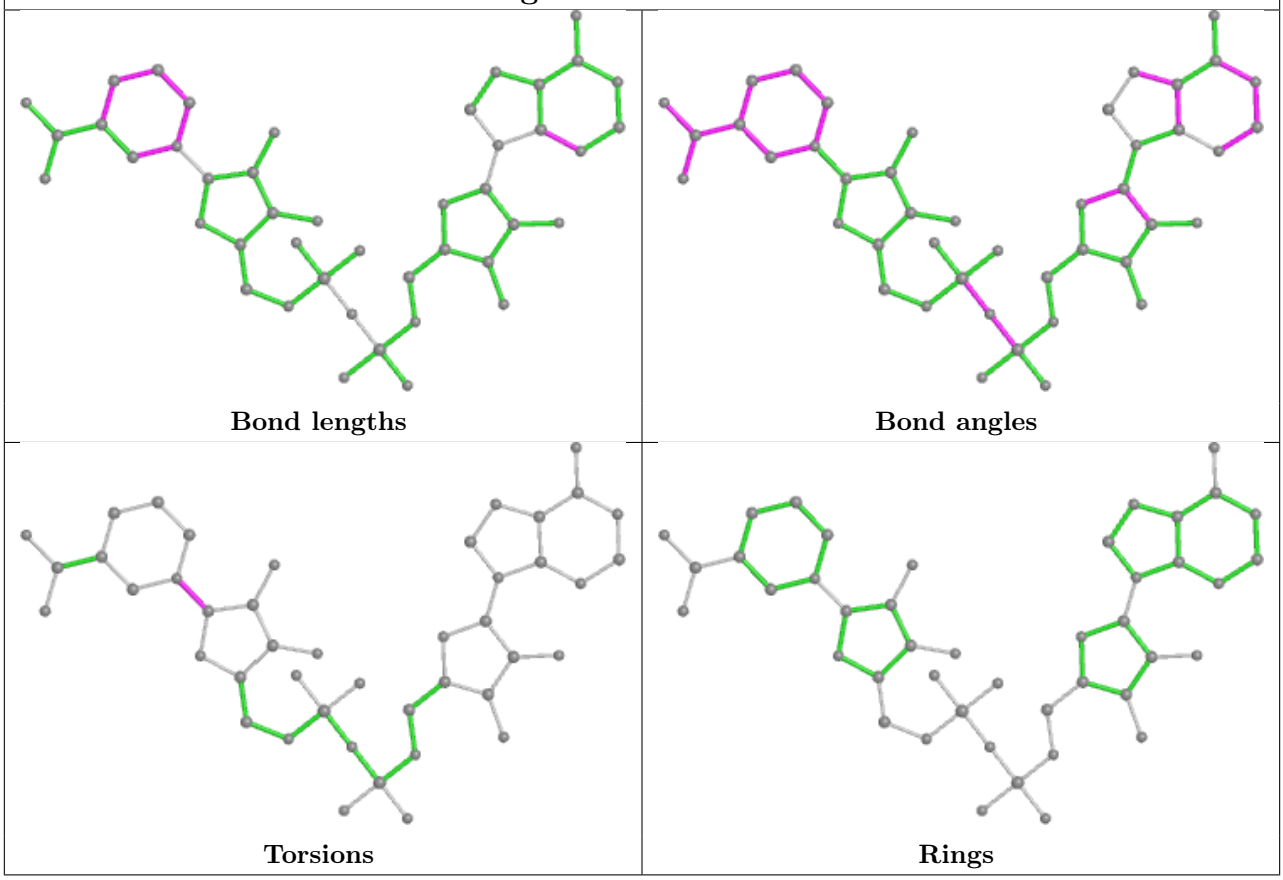
There are no ring outliers.

No monomer is involved in short contacts.

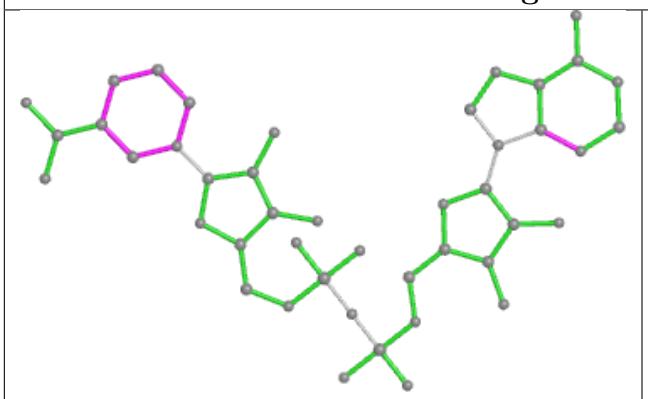
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

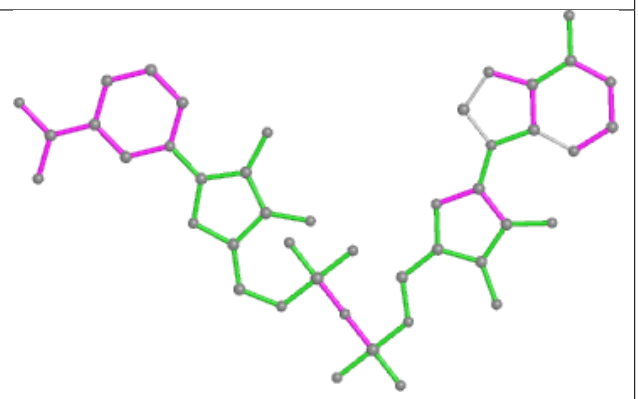
Ligand NAD A 500



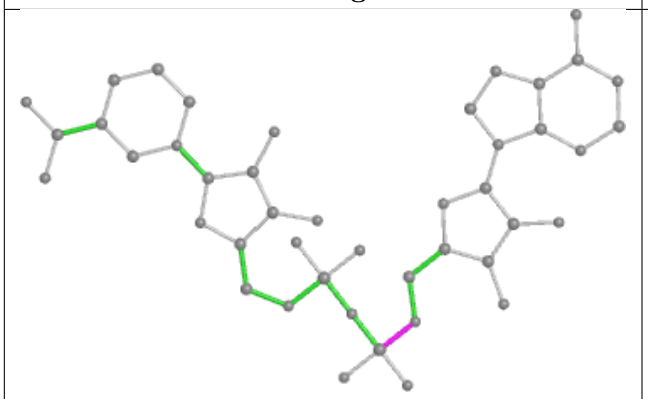
Ligand NAD B 600



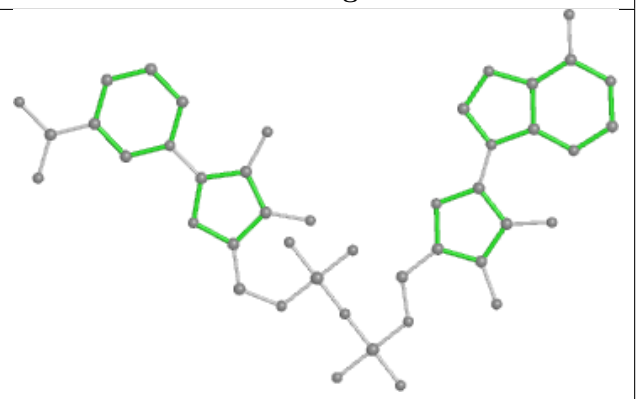
Bond lengths



Bond angles

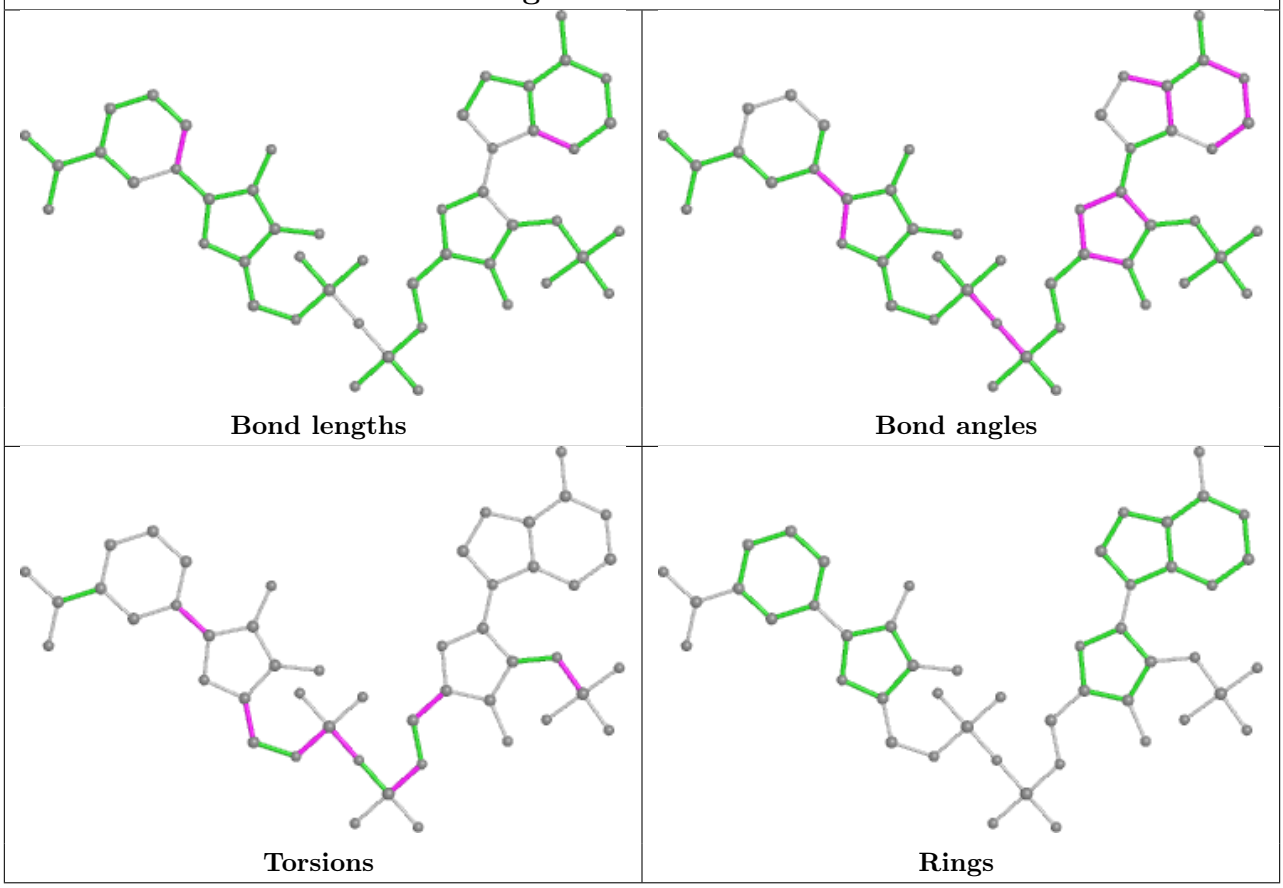


Torsions



Rings

Ligand NDP C 400



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.