



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2025 – 10:10 PM EST

PDB ID : 9E50
Title : TAD from Carmabin Biosynthetic Pathway in complex with NAD - Crystal Form 2
Authors : Rankin, M.R.; Smith, J.L.
Deposited on : 2024-10-26
Resolution : 1.68 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.3

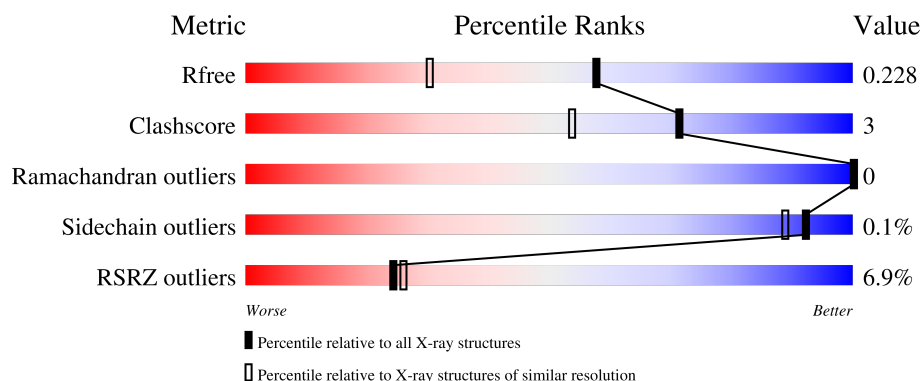
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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))
R_{free}	164625	8422 (1.70-1.66)
Clashscore	180529	1005 (1.68-1.68)
Ramachandran outliers	177936	9065 (1.70-1.66)
Sidechain outliers	177891	9064 (1.70-1.66)
RSRZ outliers	164620	8421 (1.70-1.66)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	399	<div> <div>4%</div> <div>92%</div> <div>6%</div> </div>
1	B	399	<div> <div>9%</div> <div>88%</div> <div>8%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6830 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.

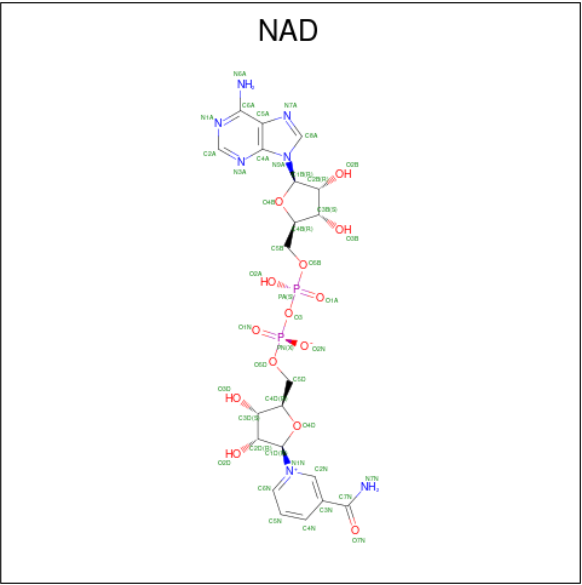
- Molecule 1 is a protein called Amino acid adenylation domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	4	0
			3109	2000	508	583	18			
1	B	383	Total	C	N	O	S	0	1	0
			3001	1931	490	563	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1905	SER	-	expression tag	UNP F4Y2B0
A	1906	ASN	-	expression tag	UNP F4Y2B0
A	1907	ALA	-	expression tag	UNP F4Y2B0
B	1905	SER	-	expression tag	UNP F4Y2B0
B	1906	ASN	-	expression tag	UNP F4Y2B0
B	1907	ALA	-	expression tag	UNP F4Y2B0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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
			44	21	7	14	2		

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	I	0	0
			1	1		
3	B	1	Total	I	0	0
			1	1		

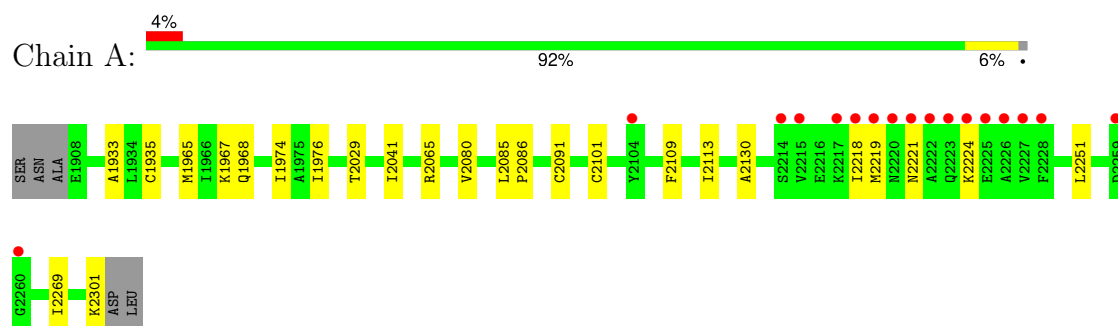
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	447	Total	O	0	0
			447	447		
4	B	183	Total	O	0	0
			183	183		

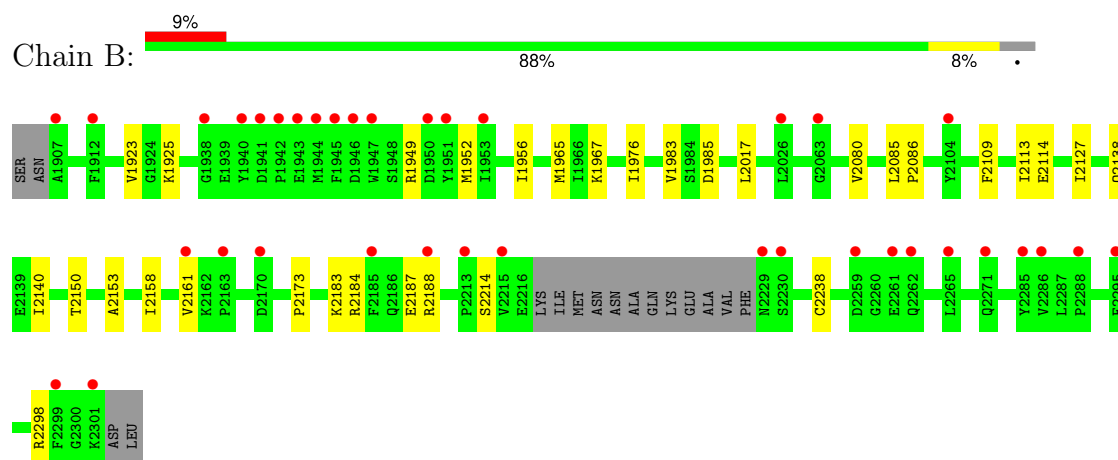
3 Residue-property plots [i](#)

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 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.

- Molecule 1: Amino acid adenylation domain protein



- Molecule 1: Amino acid adenylation domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.43Å 72.81Å 209.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.16 – 1.68 43.16 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.16-1.68) 99.2 (43.16-1.68)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.201 , 0.230 0.201 , 0.228	Depositor DCC
R_{free} test set	95478 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6830	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, IOD

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	0.28	0/3187	0.49	0/4320
1	B	0.25	0/3068	0.45	0/4161
All	All	0.27	0/6255	0.47	0/8481

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

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	3109	0	3124	19	0
1	B	3001	0	3008	21	0
2	A	44	0	25	1	0
2	B	44	0	25	3	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
4	A	447	0	0	3	0
4	B	183	0	0	1	0
All	All	6830	0	6182	40	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 3.

All (40) 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:1935:CYS:SG	4:A:2854:HOH:O	2.50	0.68
1:A:2091:CYS:SG	4:A:2905:HOH:O	2.56	0.60
1:B:2183:LYS:NZ	1:B:2187:GLU:OE2	2.34	0.60
1:A:2251:LEU:HD11	1:A:2269:ILE:HD12	1.83	0.59
1:A:2065:ARG:HD2	1:A:2301:LYS:HE2	1.84	0.59
1:B:1949:ARG:NH1	1:B:1985:ASP:OD1	2.40	0.55
1:A:2029:THR:HG23	1:A:2041:ILE:HD11	1.89	0.54
1:B:1956:ILE:HD12	1:B:2214:SER:HB3	1.90	0.52
1:B:1956:ILE:HG23	1:B:2214:SER:HB2	1.92	0.52
1:B:2188:ARG:O	1:B:2298:ARG:NH1	2.38	0.50
1:A:1967:LYS:HB2	1:A:1974[A]:ILE:HG23	1.94	0.49
1:B:2153:ALA:HB2	1:B:2173:PRO:HG2	1.95	0.48
1:A:1967:LYS:HB2	1:A:1974[A]:ILE:CG2	2.43	0.47
1:A:2101:CYS:HA	1:A:2130:ALA:O	2.14	0.47
1:B:2138:GLN:NE2	4:B:2519:HOH:O	2.48	0.46
1:B:1983:VAL:HG21	1:B:2017:LEU:HD12	1.99	0.45
1:B:2238:CYS:HB2	2:B:2401:NAD:H4N	1.98	0.44
1:B:2080:VAL:HG21	2:B:2401:NAD:H6N	1.99	0.44
1:B:2158:ILE:O	1:B:2161:VAL:HG22	2.18	0.44
1:A:2080:VAL:HG21	2:A:2401:NAD:H6N	2.00	0.43
1:B:2184:ARG:HG3	1:B:2188:ARG:HD3	2.01	0.43
1:B:1923:VAL:HG23	1:B:1925:LYS:HG3	2.01	0.43
1:B:2085:LEU:HB3	1:B:2086:PRO:HD3	2.00	0.43
1:A:1968:GLN:HG3	4:A:2603:HOH:O	2.19	0.43
1:A:2218:ILE:HG13	1:A:2219:MET:N	2.34	0.43
1:A:2218:ILE:HG13	1:A:2219:MET:H	1.84	0.42
1:A:1965:MET:HB2	1:A:1976:ILE:HB	2.01	0.42
1:B:1967:LYS:NZ	3:B:2402:IOD:I	3.21	0.42
1:A:1965:MET:HE1	1:A:1967:LYS:HE2	2.01	0.42
1:A:2085:LEU:HB3	1:A:2086:PRO:HD3	2.01	0.42
1:B:1952:MET:HA	1:B:1956:ILE:HG12	2.01	0.42
1:B:2184:ARG:HA	1:B:2188:ARG:HH11	1.85	0.41
1:B:2114:GLU:HG3	1:B:2127:ILE:HG21	2.02	0.41
1:A:1965:MET:HE3	1:A:1965:MET:HB3	1.92	0.41
1:A:2109:PHE:CE2	1:A:2113:ILE:HD11	2.56	0.41
1:A:2221:ASN:HB2	1:A:2224:LYS:HG3	2.02	0.41
1:B:1965:MET:HB2	1:B:1976:ILE:HB	2.03	0.41
1:B:2109:PHE:CE2	1:B:2113:ILE:HD11	2.55	0.41
1:B:2150:THR:HA	2:B:2401:NAD:O4B	2.21	0.40
1:A:1933:ALA:HB2	1:A:1974[A]:ILE:HD11	2.04	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	396/399 (99%)	387 (98%)	9 (2%)	0	100	100
1	B	380/399 (95%)	373 (98%)	7 (2%)	0	100	100
All	All	776/798 (97%)	760 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	345/345 (100%)	345 (100%)	0	100	100
1	B	332/345 (96%)	331 (100%)	1 (0%)	91	87
All	All	677/690 (98%)	676 (100%)	1 (0%)	92	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2140	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	2401	-	42,48,48	5.57	28 (66%)	50,73,73	1.97	7 (14%)
2	NAD	B	2401	-	42,48,48	5.78	27 (64%)	50,73,73	1.91	5 (10%)

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	2401	-	-	0/26/62/62	0/5/5/5
2	NAD	B	2401	-	-	0/26/62/62	0/5/5/5

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2401	NAD	C2N-N1N	11.94	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2401	NAD	C2N-N1N	11.64	1.47	1.35
2	B	2401	NAD	C4A-N3A	11.27	1.50	1.35
2	B	2401	NAD	C2B-C3B	-10.73	1.24	1.53
2	A	2401	NAD	C4A-N3A	10.39	1.49	1.35
2	A	2401	NAD	C2B-C3B	-10.39	1.25	1.53
2	B	2401	NAD	O4D-C1D	10.28	1.54	1.40
2	A	2401	NAD	O4D-C1D	9.43	1.53	1.40
2	B	2401	NAD	C2A-N3A	8.87	1.45	1.32
2	B	2401	NAD	C2N-C3N	8.81	1.52	1.39
2	A	2401	NAD	C2N-C3N	8.67	1.52	1.39
2	A	2401	NAD	C2A-N3A	8.45	1.45	1.32
2	B	2401	NAD	O4B-C1B	8.28	1.51	1.40
2	A	2401	NAD	C4N-C3N	8.17	1.51	1.39
2	A	2401	NAD	C7N-N7N	8.17	1.48	1.33
2	B	2401	NAD	C4N-C3N	8.08	1.51	1.39
2	B	2401	NAD	C7N-N7N	8.01	1.47	1.33
2	B	2401	NAD	C2D-C3D	-8.00	1.31	1.53
2	A	2401	NAD	C2D-C3D	-7.81	1.32	1.53
2	A	2401	NAD	O4B-C1B	7.44	1.50	1.40
2	B	2401	NAD	C1B-N9A	-7.40	1.31	1.49
2	A	2401	NAD	C6N-C5N	7.29	1.53	1.38
2	B	2401	NAD	C6N-C5N	7.25	1.53	1.38
2	B	2401	NAD	O4B-C4B	-7.14	1.29	1.45
2	A	2401	NAD	C1B-N9A	-6.86	1.33	1.49
2	A	2401	NAD	O4B-C4B	-6.70	1.30	1.45
2	B	2401	NAD	O4D-C4D	-6.70	1.30	1.45
2	B	2401	NAD	C6N-N1N	6.58	1.50	1.35
2	B	2401	NAD	C5N-C4N	6.52	1.50	1.38
2	A	2401	NAD	O4D-C4D	-6.50	1.30	1.45
2	A	2401	NAD	C6N-N1N	6.49	1.50	1.35
2	A	2401	NAD	C3B-C4B	6.44	1.69	1.53
2	B	2401	NAD	C3B-C4B	6.39	1.69	1.53
2	A	2401	NAD	C5N-C4N	6.33	1.49	1.38
2	B	2401	NAD	C2A-N1A	5.94	1.44	1.33
2	A	2401	NAD	C2A-N1A	5.60	1.43	1.33
2	B	2401	NAD	PN-O3	4.81	1.64	1.59
2	A	2401	NAD	PN-O3	4.70	1.64	1.59
2	A	2401	NAD	PA-O3	4.26	1.64	1.59
2	B	2401	NAD	PA-O3	4.15	1.64	1.59
2	B	2401	NAD	C6A-N6A	3.70	1.47	1.34
2	A	2401	NAD	C6A-N6A	3.64	1.47	1.34
2	B	2401	NAD	C3D-C4D	3.59	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2401	NAD	C3D-C4D	3.48	1.61	1.53
2	A	2401	NAD	O2B-C2B	3.31	1.51	1.43
2	B	2401	NAD	O2B-C2B	3.30	1.51	1.43
2	A	2401	NAD	C6A-C5A	2.92	1.54	1.43
2	B	2401	NAD	C3N-C7N	2.84	1.54	1.50
2	B	2401	NAD	C6A-C5A	2.78	1.53	1.43
2	B	2401	NAD	O2D-C2D	2.70	1.49	1.43
2	B	2401	NAD	PA-O5B	2.55	1.69	1.59
2	A	2401	NAD	C3N-C7N	2.50	1.54	1.50
2	A	2401	NAD	O2D-C2D	2.33	1.48	1.43
2	A	2401	NAD	PA-O5B	2.31	1.68	1.59
2	A	2401	NAD	O3B-C3B	2.02	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2401	NAD	C4B-O4B-C1B	-7.40	103.15	109.92
2	A	2401	NAD	C4B-O4B-C1B	-7.23	103.31	109.92
2	A	2401	NAD	N3A-C2A-N1A	-7.23	118.86	128.67
2	B	2401	NAD	N3A-C2A-N1A	-6.83	119.40	128.67
2	B	2401	NAD	C4D-O4D-C1D	-4.97	105.38	109.92
2	A	2401	NAD	C4D-O4D-C1D	-4.68	105.64	109.92
2	A	2401	NAD	O4B-C1B-N9A	4.28	114.42	108.75
2	B	2401	NAD	O4B-C1B-N9A	4.11	114.19	108.75
2	A	2401	NAD	C2N-C3N-C4N	2.19	120.81	118.26
2	A	2401	NAD	C1B-N9A-C4A	-2.17	122.83	126.64
2	B	2401	NAD	C2N-C3N-C4N	2.10	120.70	118.26
2	A	2401	NAD	C5B-C4B-C3B	-2.02	107.94	115.21

There are no chirality outliers.

There are no torsion outliers.

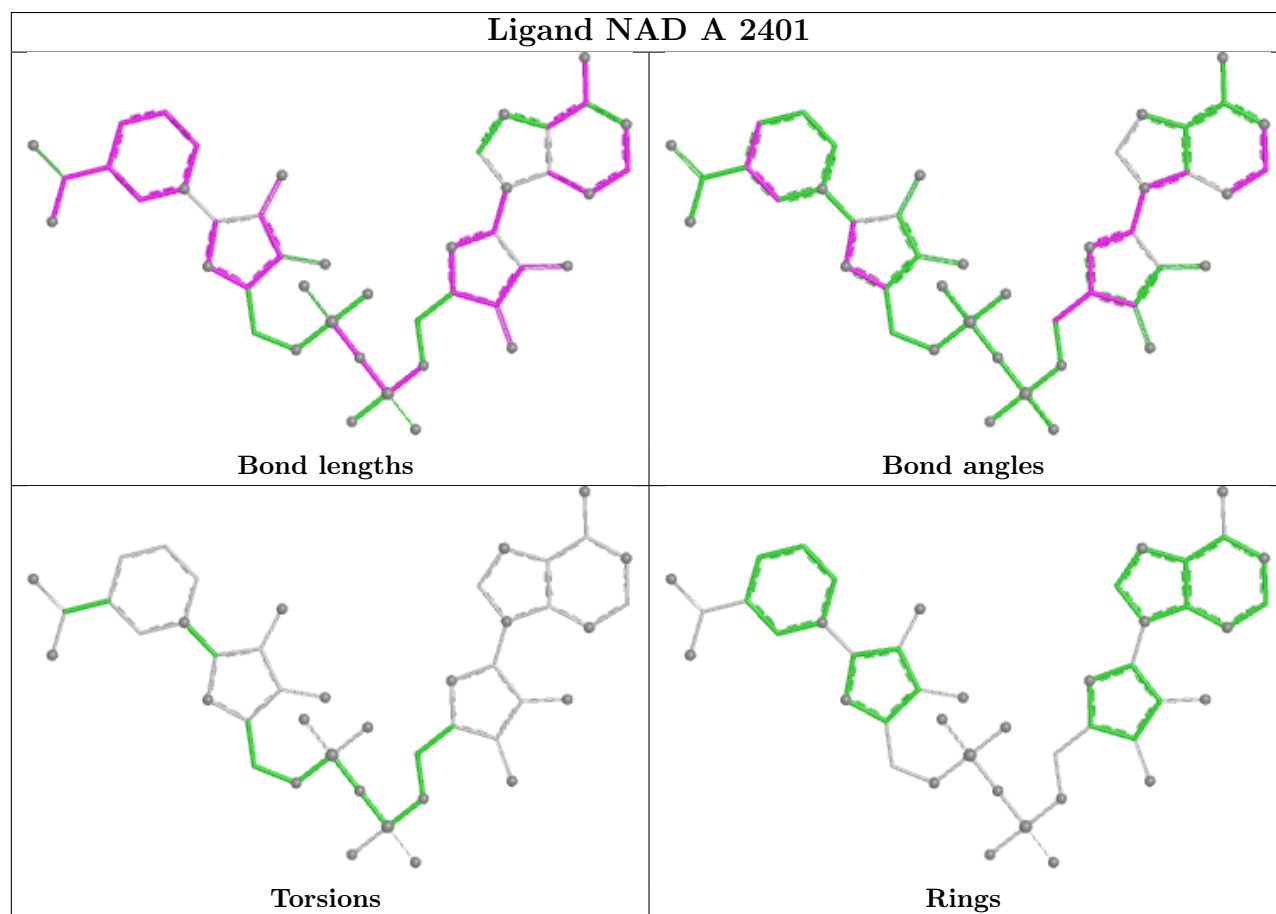
There are no ring outliers.

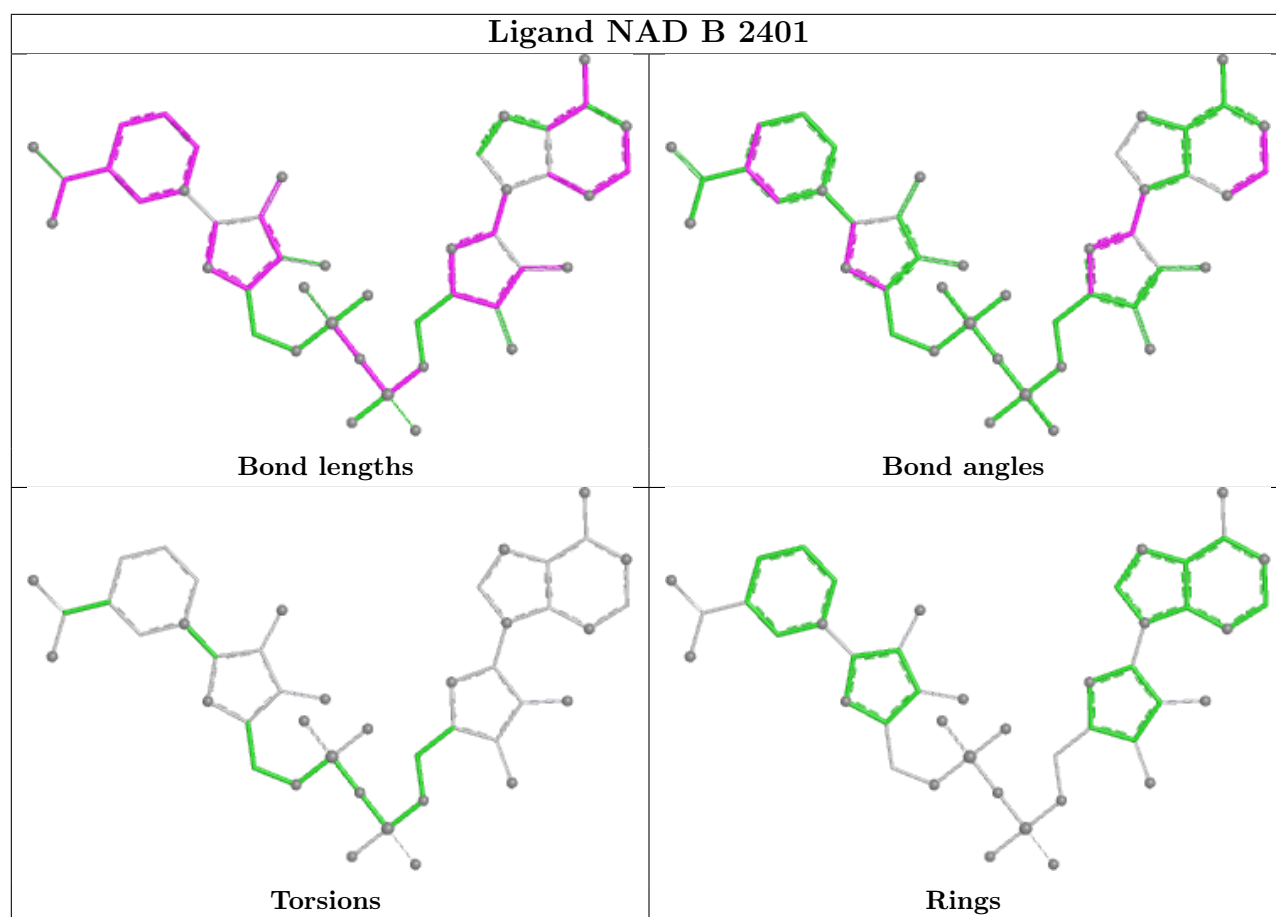
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2401	NAD	1	0
2	B	2401	NAD	3	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 than 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.





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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	394/399 (98%)	0.03	17 (4%) 40 44	11, 24, 55, 99	4 (1%)
1	B	383/399 (95%)	0.73	37 (9%) 15 15	18, 38, 67, 119	1 (0%)
All	All	777/798 (97%)	0.37	54 (6%) 24 26	11, 31, 62, 119	5 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2218	ILE	5.2
1	B	1942	PRO	4.7
1	A	2228	PHE	4.5
1	B	1947	TRP	4.5
1	A	2222	ALA	4.4
1	A	2260	GLY	4.3
1	A	2219	MET	4.2
1	A	2215	VAL	3.9
1	B	1940	TYR	3.6
1	B	1945	PHE	3.4
1	B	2104	TYR	3.3
1	B	1944	MET	3.1
1	A	2226	ALA	3.1
1	A	2225	GLU	2.9
1	B	1951	TYR	2.9
1	B	1907	ALA	2.9
1	B	1941	ASP	2.9
1	A	2227	VAL	2.8
1	A	2217	LYS	2.8
1	B	2215	VAL	2.6
1	B	2299	PHE	2.6
1	B	2259	ASP	2.6
1	B	2295	PHE	2.5
1	A	2221	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	2301	LYS	2.5
1	B	2265	LEU	2.5
1	A	2223	GLN	2.5
1	B	2229	ASN	2.5
1	B	1950	ASP	2.5
1	A	2214	SER	2.5
1	B	2261	GLU	2.5
1	B	1953	ILE	2.3
1	B	2026	LEU	2.3
1	B	1946	ASP	2.3
1	A	2224	LYS	2.3
1	B	1938	GLY	2.3
1	B	2262	GLN	2.3
1	B	2213	PRO	2.2
1	A	2220	ASN	2.2
1	B	1912	PHE	2.2
1	B	2185	PHE	2.2
1	B	1943	GLU	2.2
1	B	2271	GLN	2.2
1	B	2161	VAL	2.2
1	B	2286	VAL	2.2
1	B	2163	PRO	2.1
1	A	2104	TYR	2.1
1	B	2170	ASP	2.1
1	B	2285	TYR	2.1
1	B	2288	PRO	2.1
1	B	2063	GLY	2.0
1	B	2188	ARG	2.0
1	A	2259	ASP	2.0
1	B	2230	SER	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

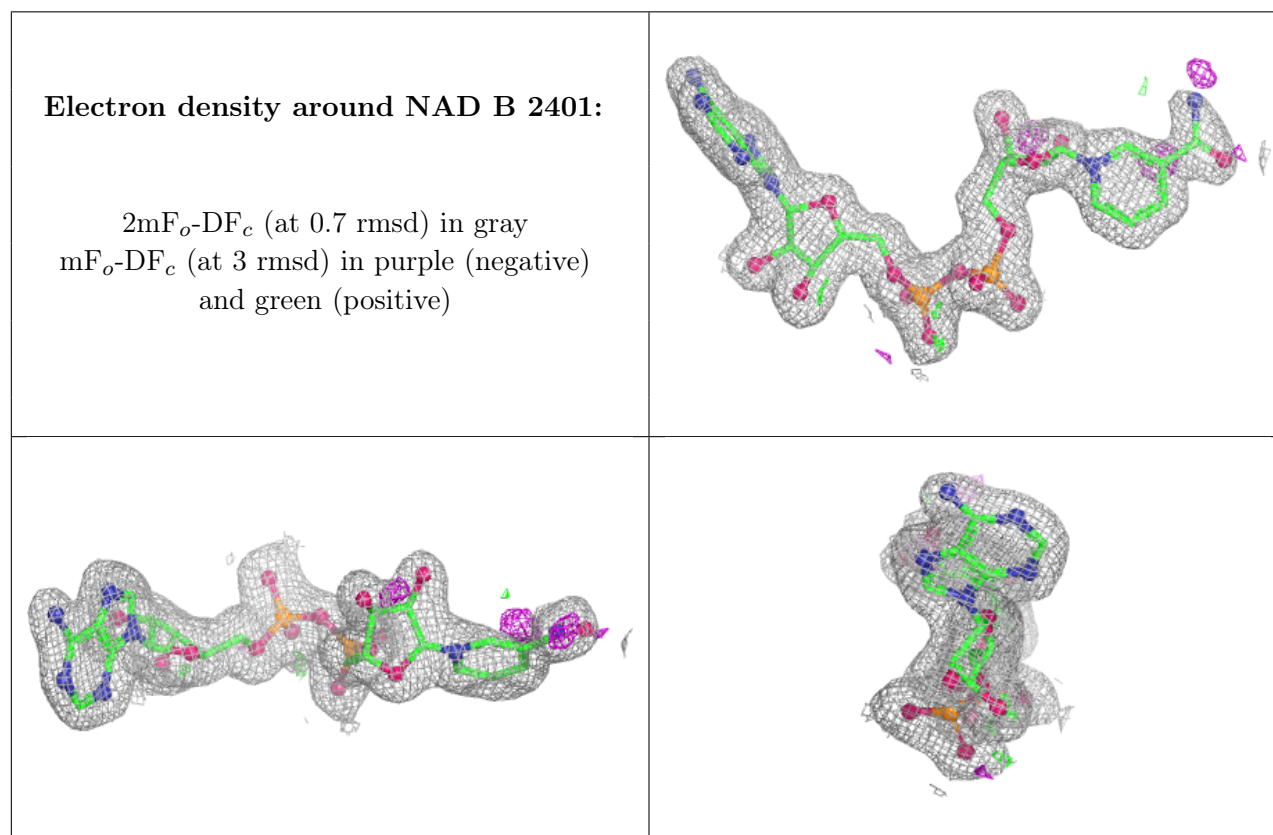
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

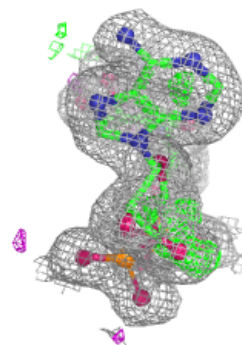
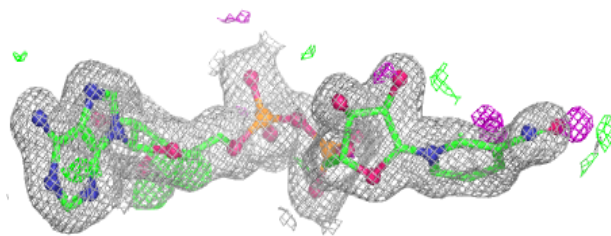
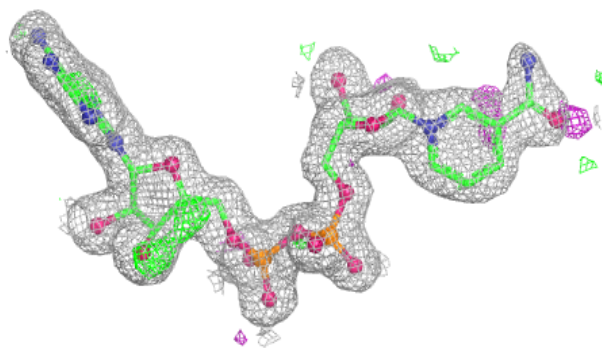
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	B	2401	44/44	0.96	0.08	24,30,38,43	0
2	NAD	A	2401	44/44	0.97	0.07	17,20,33,39	0
3	IOD	B	2402	1/1	0.98	0.05	37,37,37,37	1
3	IOD	A	2402	1/1	0.99	0.02	28,28,28,28	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around NAD A 2401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.