



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:34 PM UTC

PDB ID : 3WMX / pdb_00003wmx
Title : GalE-like L-Threonine dehydrogenase from Cupriavidus necator (holo form)
Authors : Nakano, S.; Okazaki, S.; Tokiwa, H.; Asano, Y.
Deposited on : 2013-11-29
Resolution : 2.50 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

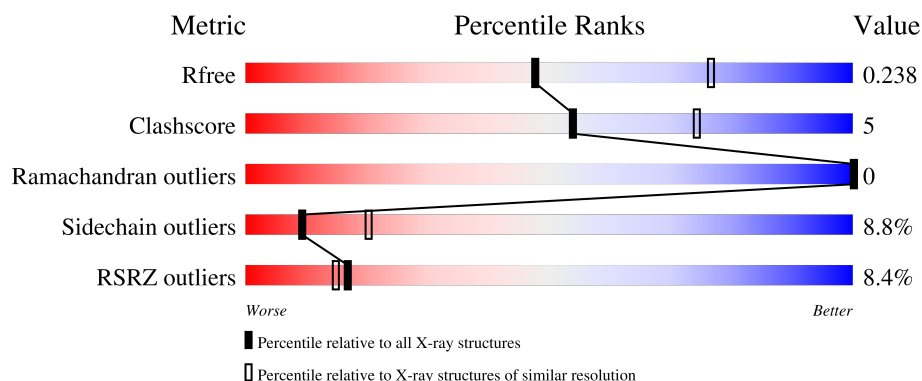
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	358	0% 75% 9% • 13%
1	B	358	3% 75% 8% • 14%
1	C	358	2% 75% 9% • 14%
1	D	358	23% 68% 15% • 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9738 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 dependent epimerase/dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2385	1511	415	447	12			
1	B	308	Total	C	N	O	S	0	0	0
			2371	1502	412	445	12			
1	C	308	Total	C	N	O	S	0	0	0
			2372	1503	412	445	12			
1	D	304	Total	C	N	O	S	0	0	0
			2351	1491	407	441	12			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q0K312
A	-18	GLY	-	expression tag	UNP Q0K312
A	-17	SER	-	expression tag	UNP Q0K312
A	-16	SER	-	expression tag	UNP Q0K312
A	-15	HIS	-	expression tag	UNP Q0K312
A	-14	HIS	-	expression tag	UNP Q0K312
A	-13	HIS	-	expression tag	UNP Q0K312
A	-12	HIS	-	expression tag	UNP Q0K312
A	-11	HIS	-	expression tag	UNP Q0K312
A	-10	HIS	-	expression tag	UNP Q0K312
A	-9	SER	-	expression tag	UNP Q0K312
A	-8	SER	-	expression tag	UNP Q0K312
A	-7	GLY	-	expression tag	UNP Q0K312
A	-6	LEU	-	expression tag	UNP Q0K312
A	-5	VAL	-	expression tag	UNP Q0K312
A	-4	PRO	-	expression tag	UNP Q0K312
A	-3	ARG	-	expression tag	UNP Q0K312
A	-2	GLY	-	expression tag	UNP Q0K312
A	-1	SER	-	expression tag	UNP Q0K312
A	0	HIS	-	expression tag	UNP Q0K312
A	319	ASP	-	expression tag	UNP Q0K312

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Chain	Residue	Modelled	Actual	Comment	Reference
A	320	PRO	-	expression tag	UNP Q0K312
A	321	ALA	-	expression tag	UNP Q0K312
A	322	ALA	-	expression tag	UNP Q0K312
A	323	ASN	-	expression tag	UNP Q0K312
A	324	LYS	-	expression tag	UNP Q0K312
A	325	ALA	-	expression tag	UNP Q0K312
A	326	ARG	-	expression tag	UNP Q0K312
A	327	LYS	-	expression tag	UNP Q0K312
A	328	GLU	-	expression tag	UNP Q0K312
A	329	ALA	-	expression tag	UNP Q0K312
A	330	GLU	-	expression tag	UNP Q0K312
A	331	LEU	-	expression tag	UNP Q0K312
A	332	ALA	-	expression tag	UNP Q0K312
A	333	ALA	-	expression tag	UNP Q0K312
A	334	ALA	-	expression tag	UNP Q0K312
A	335	THR	-	expression tag	UNP Q0K312
A	336	ALA	-	expression tag	UNP Q0K312
A	337	GLU	-	expression tag	UNP Q0K312
A	338	GLN	-	expression tag	UNP Q0K312
B	-19	MET	-	expression tag	UNP Q0K312
B	-18	GLY	-	expression tag	UNP Q0K312
B	-17	SER	-	expression tag	UNP Q0K312
B	-16	SER	-	expression tag	UNP Q0K312
B	-15	HIS	-	expression tag	UNP Q0K312
B	-14	HIS	-	expression tag	UNP Q0K312
B	-13	HIS	-	expression tag	UNP Q0K312
B	-12	HIS	-	expression tag	UNP Q0K312
B	-11	HIS	-	expression tag	UNP Q0K312
B	-10	HIS	-	expression tag	UNP Q0K312
B	-9	SER	-	expression tag	UNP Q0K312
B	-8	SER	-	expression tag	UNP Q0K312
B	-7	GLY	-	expression tag	UNP Q0K312
B	-6	LEU	-	expression tag	UNP Q0K312
B	-5	VAL	-	expression tag	UNP Q0K312
B	-4	PRO	-	expression tag	UNP Q0K312
B	-3	ARG	-	expression tag	UNP Q0K312
B	-2	GLY	-	expression tag	UNP Q0K312
B	-1	SER	-	expression tag	UNP Q0K312
B	0	HIS	-	expression tag	UNP Q0K312
B	319	ASP	-	expression tag	UNP Q0K312
B	320	PRO	-	expression tag	UNP Q0K312
B	321	ALA	-	expression tag	UNP Q0K312

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Chain	Residue	Modelled	Actual	Comment	Reference
B	322	ALA	-	expression tag	UNP Q0K312
B	323	ASN	-	expression tag	UNP Q0K312
B	324	LYS	-	expression tag	UNP Q0K312
B	325	ALA	-	expression tag	UNP Q0K312
B	326	ARG	-	expression tag	UNP Q0K312
B	327	LYS	-	expression tag	UNP Q0K312
B	328	GLU	-	expression tag	UNP Q0K312
B	329	ALA	-	expression tag	UNP Q0K312
B	330	GLU	-	expression tag	UNP Q0K312
B	331	LEU	-	expression tag	UNP Q0K312
B	332	ALA	-	expression tag	UNP Q0K312
B	333	ALA	-	expression tag	UNP Q0K312
B	334	ALA	-	expression tag	UNP Q0K312
B	335	THR	-	expression tag	UNP Q0K312
B	336	ALA	-	expression tag	UNP Q0K312
B	337	GLU	-	expression tag	UNP Q0K312
B	338	GLN	-	expression tag	UNP Q0K312
C	-19	MET	-	expression tag	UNP Q0K312
C	-18	GLY	-	expression tag	UNP Q0K312
C	-17	SER	-	expression tag	UNP Q0K312
C	-16	SER	-	expression tag	UNP Q0K312
C	-15	HIS	-	expression tag	UNP Q0K312
C	-14	HIS	-	expression tag	UNP Q0K312
C	-13	HIS	-	expression tag	UNP Q0K312
C	-12	HIS	-	expression tag	UNP Q0K312
C	-11	HIS	-	expression tag	UNP Q0K312
C	-10	HIS	-	expression tag	UNP Q0K312
C	-9	SER	-	expression tag	UNP Q0K312
C	-8	SER	-	expression tag	UNP Q0K312
C	-7	GLY	-	expression tag	UNP Q0K312
C	-6	LEU	-	expression tag	UNP Q0K312
C	-5	VAL	-	expression tag	UNP Q0K312
C	-4	PRO	-	expression tag	UNP Q0K312
C	-3	ARG	-	expression tag	UNP Q0K312
C	-2	GLY	-	expression tag	UNP Q0K312
C	-1	SER	-	expression tag	UNP Q0K312
C	0	HIS	-	expression tag	UNP Q0K312
C	319	ASP	-	expression tag	UNP Q0K312
C	320	PRO	-	expression tag	UNP Q0K312
C	321	ALA	-	expression tag	UNP Q0K312
C	322	ALA	-	expression tag	UNP Q0K312
C	323	ASN	-	expression tag	UNP Q0K312

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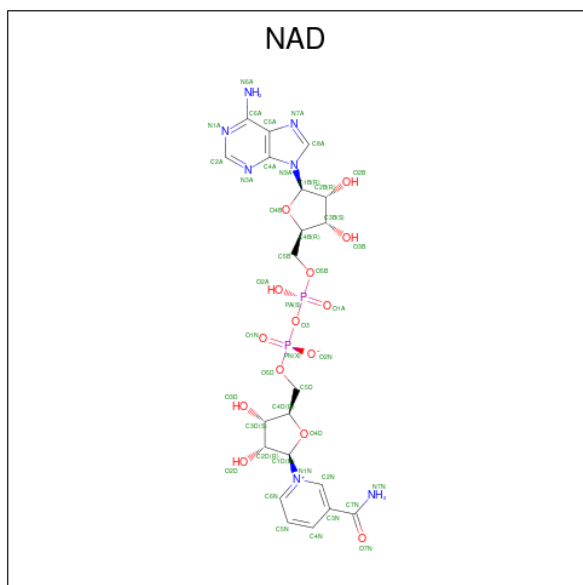
Chain	Residue	Modelled	Actual	Comment	Reference
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C	325	ALA	-	expression tag	UNP Q0K312
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C	327	LYS	-	expression tag	UNP Q0K312
C	328	GLU	-	expression tag	UNP Q0K312
C	329	ALA	-	expression tag	UNP Q0K312
C	330	GLU	-	expression tag	UNP Q0K312
C	331	LEU	-	expression tag	UNP Q0K312
C	332	ALA	-	expression tag	UNP Q0K312
C	333	ALA	-	expression tag	UNP Q0K312
C	334	ALA	-	expression tag	UNP Q0K312
C	335	THR	-	expression tag	UNP Q0K312
C	336	ALA	-	expression tag	UNP Q0K312
C	337	GLU	-	expression tag	UNP Q0K312
C	338	GLN	-	expression tag	UNP Q0K312
D	-19	MET	-	expression tag	UNP Q0K312
D	-18	GLY	-	expression tag	UNP Q0K312
D	-17	SER	-	expression tag	UNP Q0K312
D	-16	SER	-	expression tag	UNP Q0K312
D	-15	HIS	-	expression tag	UNP Q0K312
D	-14	HIS	-	expression tag	UNP Q0K312
D	-13	HIS	-	expression tag	UNP Q0K312
D	-12	HIS	-	expression tag	UNP Q0K312
D	-11	HIS	-	expression tag	UNP Q0K312
D	-10	HIS	-	expression tag	UNP Q0K312
D	-9	SER	-	expression tag	UNP Q0K312
D	-8	SER	-	expression tag	UNP Q0K312
D	-7	GLY	-	expression tag	UNP Q0K312
D	-6	LEU	-	expression tag	UNP Q0K312
D	-5	VAL	-	expression tag	UNP Q0K312
D	-4	PRO	-	expression tag	UNP Q0K312
D	-3	ARG	-	expression tag	UNP Q0K312
D	-2	GLY	-	expression tag	UNP Q0K312
D	-1	SER	-	expression tag	UNP Q0K312
D	0	HIS	-	expression tag	UNP Q0K312
D	319	ASP	-	expression tag	UNP Q0K312
D	320	PRO	-	expression tag	UNP Q0K312
D	321	ALA	-	expression tag	UNP Q0K312
D	322	ALA	-	expression tag	UNP Q0K312
D	323	ASN	-	expression tag	UNP Q0K312
D	324	LYS	-	expression tag	UNP Q0K312
D	325	ALA	-	expression tag	UNP Q0K312

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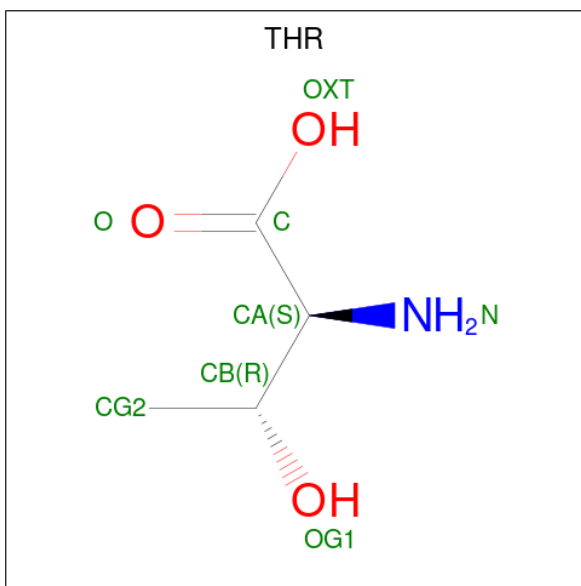
Chain	Residue	Modelled	Actual	Comment	Reference
D	326	ARG	-	expression tag	UNP Q0K312
D	327	LYS	-	expression tag	UNP Q0K312
D	328	GLU	-	expression tag	UNP Q0K312
D	329	ALA	-	expression tag	UNP Q0K312
D	330	GLU	-	expression tag	UNP Q0K312
D	331	LEU	-	expression tag	UNP Q0K312
D	332	ALA	-	expression tag	UNP Q0K312
D	333	ALA	-	expression tag	UNP Q0K312
D	334	ALA	-	expression tag	UNP Q0K312
D	335	THR	-	expression tag	UNP Q0K312
D	336	ALA	-	expression tag	UNP Q0K312
D	337	GLU	-	expression tag	UNP Q0K312
D	338	GLN	-	expression tag	UNP Q0K312

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is THREONINE (CCD ID: THR) (formula: $C_4H_9NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

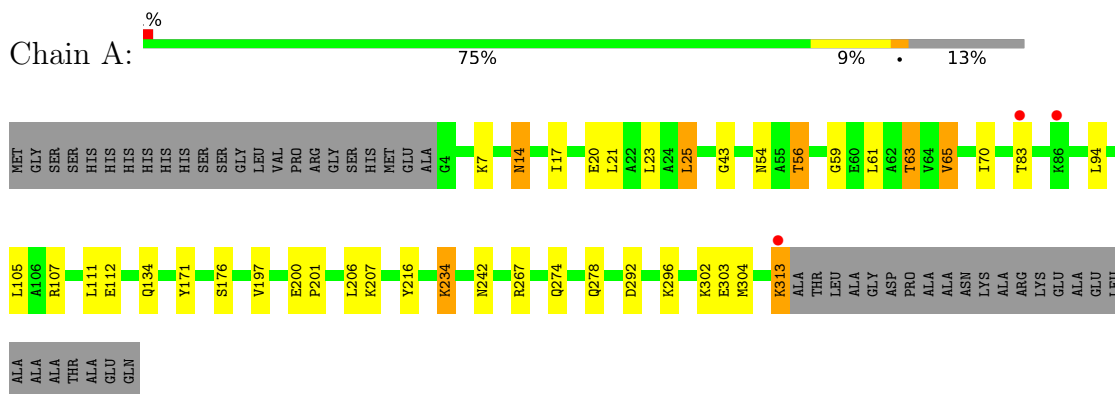
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	17	Total	O	0	0
			17	17		
4	C	14	Total	O	0	0
			14	14		
4	D	1	Total	O	0	0
			1	1		

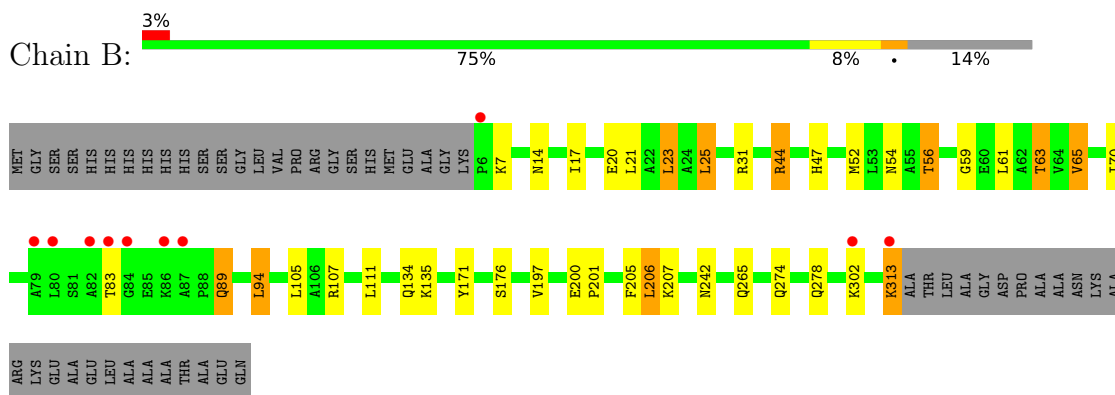
3 Residue-property plots [i](#)

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.

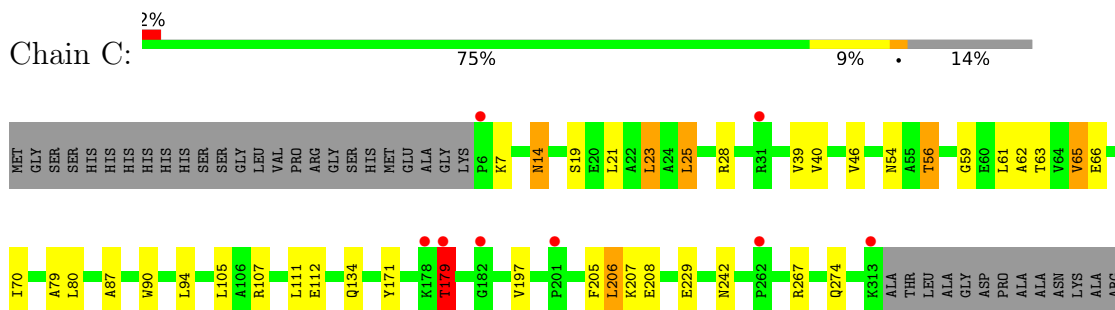
- Molecule 1: NAD dependent epimerase/dehydratase



- Molecule 1: NAD dependent epimerase/dehydratase

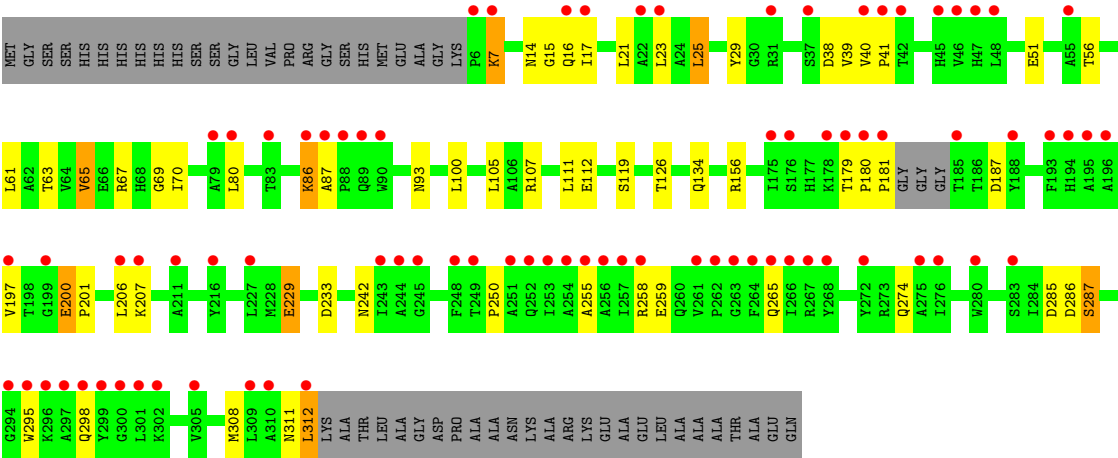


- Molecule 1: NAD dependent epimerase/dehydratase



LYS
GLU
ALA
GLU
LEU
ALA
ALA
ALA
THR
ALA
GLU
GLN

● Molecule 1: NAD dependent epimerase/dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.60Å 88.11Å 113.60Å 90.00° 105.47° 90.00°	Depositor
Resolution (Å)	40.87 – 2.50 40.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.87-2.50) 99.9 (40.87-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.78 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.204 , 0.239 0.209 , 0.238	Depositor DCC
R_{free} test set	2997 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9738	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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 [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	0.68	0/2445	0.82	0/3333
1	B	0.60	0/2431	0.81	0/3314
1	C	0.61	0/2432	0.85	4/3316 (0.1%)
1	D	0.52	0/2410	0.83	0/3287
All	All	0.60	0/9718	0.83	4/13250 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	THR	CA-C-N	-7.41	114.32	119.66
1	C	179	THR	C-N-CA	-7.41	114.32	119.66
1	C	87	ALA	CA-C-N	5.03	124.47	119.24
1	C	87	ALA	C-N-CA	5.03	124.47	119.24

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	2385	0	2342	23	0
1	B	2371	0	2323	27	0
1	C	2372	0	2327	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2351	0	2304	30	0
2	A	44	0	26	3	0
2	B	44	0	26	2	0
2	C	44	0	26	1	0
2	D	44	0	26	4	0
3	A	8	0	6	1	0
3	B	8	0	6	0	0
4	A	35	0	0	3	0
4	B	17	0	0	1	0
4	C	14	0	0	0	0
4	D	1	0	0	0	0
All	All	9738	0	9412	93	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 5.

All (93) 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:313:LYS:HA	4:A:512:HOH:O	1.55	1.03
1:A:43:GLY:O	1:B:44:ARG:NH2	2.07	0.88
1:D:255:ALA:O	1:D:258:ARG:HG2	1.80	0.82
1:A:313:LYS:O	1:A:313:LYS:HG2	1.78	0.81
1:C:19:SER:OG	1:C:179:THR:HG21	1.83	0.76
1:B:313:LYS:O	1:B:313:LYS:CG	2.33	0.76
1:D:285:ASP:OD2	1:D:287:SER:OG	2.02	0.75
1:B:134:GLN:HE22	1:B:242:ASN:H	1.32	0.75
1:A:134:GLN:HE22	1:A:242:ASN:H	1.33	0.75
1:D:134:GLN:HE22	1:D:242:ASN:H	1.35	0.74
1:A:313:LYS:CA	4:A:512:HOH:O	2.23	0.74
1:C:134:GLN:HE22	1:C:242:ASN:H	1.37	0.73
1:B:313:LYS:O	1:B:313:LYS:HG2	1.89	0.71
1:B:59:GLY:O	1:B:63:THR:HG23	1.93	0.69
1:A:59:GLY:O	1:A:63:THR:HG23	1.94	0.68
1:D:179:THR:HB	1:D:180:PRO:HD2	1.76	0.67
1:C:59:GLY:O	1:C:63:THR:HG23	1.95	0.66
1:A:313:LYS:O	1:A:313:LYS:CG	2.41	0.66
1:B:89:GLN:HE21	1:B:89:GLN:HA	1.61	0.64
1:B:200:GLU:HG3	1:B:201:PRO:HD2	1.80	0.64
1:D:200:GLU:HG3	1:D:201:PRO:HD2	1.80	0.64
1:D:181:PRO:O	1:D:187:ASP:OD1	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ILE:HD12	2:D:401:NAD:H51N	1.81	0.61
1:A:54:ASN:OD1	1:A:56:THR:HB	2.03	0.59
1:B:54:ASN:OD1	1:B:56:THR:HB	2.04	0.58
1:B:89:GLN:HE22	1:D:100:LEU:HD13	1.69	0.57
1:D:255:ALA:HA	1:D:258:ARG:CD	2.34	0.57
1:B:31:ARG:HG2	1:B:47:HIS:HD2	1.69	0.56
1:C:61:LEU:O	1:C:65:VAL:HG13	2.06	0.55
1:B:20:GLU:OE1	1:B:176:SER:OG	2.16	0.55
1:C:65:VAL:HB	1:C:70:ILE:HB	1.87	0.55
1:A:200:GLU:HG3	1:A:201:PRO:HD2	1.88	0.55
1:A:207:LYS:H	1:A:274:GLN:NE2	2.04	0.55
1:D:15:GLY:HA3	2:D:401:NAD:O2A	2.07	0.55
1:D:61:LEU:O	1:D:65:VAL:HG13	2.07	0.55
1:B:61:LEU:O	1:B:65:VAL:HG13	2.07	0.55
1:D:207:LYS:H	1:D:274:GLN:NE2	2.05	0.54
1:C:207:LYS:H	1:C:274:GLN:NE2	2.06	0.54
1:B:65:VAL:HB	1:B:70:ILE:HB	1.90	0.54
1:D:259:GLU:O	1:D:259:GLU:HG2	2.08	0.54
1:A:61:LEU:O	1:A:65:VAL:HG13	2.08	0.53
1:B:207:LYS:H	1:B:274:GLN:NE2	2.07	0.53
1:A:65:VAL:HB	1:A:70:ILE:HB	1.91	0.53
1:D:65:VAL:HB	1:D:70:ILE:HB	1.91	0.52
1:A:94:LEU:HD23	1:A:94:LEU:C	2.33	0.52
1:A:17:ILE:HD12	2:A:401:NAD:H51N	1.91	0.52
1:C:171:TYR:HB2	2:C:401:NAD:C5N	2.40	0.52
1:B:135:LYS:HE3	1:D:126:THR:HG21	1.93	0.51
1:C:54:ASN:OD1	1:C:56:THR:HB	2.10	0.50
1:D:29:TYR:OH	1:D:229:GLU:OE2	2.18	0.49
1:A:20:GLU:OE1	1:A:176:SER:OG	2.23	0.49
1:D:255:ALA:HA	1:D:258:ARG:HD3	1.95	0.49
1:A:171:TYR:HB2	2:A:401:NAD:C5N	2.42	0.48
1:A:216:TYR:CG	1:A:304:MET:HG3	2.49	0.47
2:A:401:NAD:C4N	3:A:402:THR:HB	2.45	0.47
1:A:313:LYS:N	4:A:512:HOH:O	2.43	0.47
1:B:17:ILE:HD12	2:B:401:NAD:H51N	1.97	0.46
1:B:21:LEU:HG	1:B:25:LEU:HD22	1.98	0.46
1:A:21:LEU:HG	1:A:25:LEU:HD22	1.98	0.46
1:C:21:LEU:HG	1:C:25:LEU:HD22	1.98	0.46
1:D:7:LYS:HG3	1:D:70:ILE:HA	1.98	0.45
1:B:14:ASN:ND2	4:B:502:HOH:O	2.50	0.45
1:D:286:ASP:OD1	1:D:295:TRP:HD1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:ASP:OD1	2:D:401:NAD:H1B	2.17	0.45
1:C:14:ASN:HD22	1:C:14:ASN:N	2.16	0.44
1:B:205:PHE:CD1	1:B:206:LEU:HD13	2.53	0.43
1:D:86:LYS:HA	1:D:87:ALA:HA	1.69	0.43
1:D:14:ASN:OD1	1:D:40:VAL:CG2	2.67	0.43
1:D:308:MET:O	1:D:312:LEU:HB3	2.18	0.43
1:B:94:LEU:CD2	1:B:94:LEU:C	2.92	0.42
1:D:16:GLN:HA	1:D:179:THR:HG21	2.00	0.42
1:D:119:SER:HB2	2:D:401:NAD:H6N	2.01	0.42
1:C:23:LEU:HD12	1:C:23:LEU:HA	1.93	0.42
1:B:59:GLY:O	1:B:63:THR:CG2	2.66	0.42
1:A:216:TYR:CD2	1:A:304:MET:HG3	2.55	0.42
1:B:94:LEU:HD23	1:B:94:LEU:O	2.20	0.42
1:B:23:LEU:HD12	1:B:23:LEU:HA	1.93	0.42
1:C:205:PHE:CD1	1:C:206:LEU:HD13	2.55	0.42
1:D:21:LEU:HG	1:D:25:LEU:HD22	2.00	0.42
1:B:31:ARG:HD2	1:B:47:HIS:HB2	2.02	0.41
1:D:51:GLU:OE2	1:D:67:ARG:NH2	2.47	0.41
1:C:28:ARG:NE	1:C:229:GLU:OE2	2.49	0.41
1:A:14:ASN:HD22	1:A:14:ASN:N	2.19	0.41
1:B:171:TYR:HB2	2:B:401:NAD:C5N	2.51	0.41
1:C:79:ALA:HB1	1:C:90:TRP:CZ3	2.56	0.41
1:D:207:LYS:O	1:D:250:PRO:HG2	2.20	0.41
1:B:14:ASN:N	1:B:14:ASN:HD22	2.19	0.41
1:B:94:LEU:C	1:B:94:LEU:HD23	2.46	0.41
1:A:234:LYS:HE2	1:A:292:ASP:O	2.21	0.41
1:C:62:ALA:O	1:C:66:GLU:HB2	2.22	0.40
1:D:40:VAL:HA	1:D:41:PRO:HD3	1.84	0.40
1:A:296:LYS:HB2	1:A:296:LYS:HE3	1.84	0.40
1:D:7:LYS:HG2	1:D:69:GLY:O	2.21	0.40

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	308/358 (86%)	303 (98%)	5 (2%)	0	100	100
1	B	306/358 (86%)	300 (98%)	6 (2%)	0	100	100
1	C	306/358 (86%)	299 (98%)	7 (2%)	0	100	100
1	D	300/358 (84%)	291 (97%)	9 (3%)	0	100	100
All	All	1220/1432 (85%)	1193 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	245/278 (88%)	225 (92%)	20 (8%)	10	23
1	B	244/278 (88%)	224 (92%)	20 (8%)	10	23
1	C	244/278 (88%)	224 (92%)	20 (8%)	10	23
1	D	243/278 (87%)	218 (90%)	25 (10%)	7	14
All	All	976/1112 (88%)	891 (91%)	85 (9%)	9	21

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	14	ASN
1	A	23	LEU
1	A	25	LEU
1	A	56	THR
1	A	63	THR
1	A	65	VAL
1	A	83	THR
1	A	105	LEU
1	A	107	ARG

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Mol	Chain	Res	Type
1	A	111	LEU
1	A	112	GLU
1	A	197	VAL
1	A	206	LEU
1	A	234	LYS
1	A	267	ARG
1	A	278	GLN
1	A	302	LYS
1	A	303	GLU
1	A	313	LYS
1	B	7	LYS
1	B	23	LEU
1	B	25	LEU
1	B	44	ARG
1	B	52	MET
1	B	56	THR
1	B	63	THR
1	B	65	VAL
1	B	83	THR
1	B	89	GLN
1	B	94	LEU
1	B	105	LEU
1	B	107	ARG
1	B	111	LEU
1	B	197	VAL
1	B	206	LEU
1	B	265	GLN
1	B	278	GLN
1	B	302	LYS
1	B	313	LYS
1	C	7	LYS
1	C	14	ASN
1	C	23	LEU
1	C	25	LEU
1	C	39	VAL
1	C	40	VAL
1	C	46	VAL
1	C	56	THR
1	C	65	VAL
1	C	80	LEU
1	C	94	LEU
1	C	105	LEU

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Mol	Chain	Res	Type
1	C	107	ARG
1	C	111	LEU
1	C	112	GLU
1	C	179	THR
1	C	197	VAL
1	C	206	LEU
1	C	208	GLU
1	C	267	ARG
1	D	7	LYS
1	D	23	LEU
1	D	25	LEU
1	D	39	VAL
1	D	56	THR
1	D	63	THR
1	D	65	VAL
1	D	80	LEU
1	D	86	LYS
1	D	93	ASN
1	D	105	LEU
1	D	107	ARG
1	D	111	LEU
1	D	112	GLU
1	D	156	ARG
1	D	197	VAL
1	D	200	GLU
1	D	206	LEU
1	D	229	GLU
1	D	233	ASP
1	D	265	GLN
1	D	287	SER
1	D	298	GLN
1	D	311	ASN
1	D	312	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	47	HIS
1	A	89	GLN
1	A	93	ASN
1	A	108	GLN

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Mol	Chain	Res	Type
1	A	134	GLN
1	A	161	ASN
1	A	162	HIS
1	A	274	GLN
1	B	14	ASN
1	B	33	ASN
1	B	89	GLN
1	B	108	GLN
1	B	134	GLN
1	B	265	GLN
1	B	274	GLN
1	C	33	ASN
1	C	108	GLN
1	C	134	GLN
1	C	161	ASN
1	C	274	GLN
1	D	33	ASN
1	D	89	GLN
1	D	134	GLN
1	D	161	ASN
1	D	162	HIS
1	D	177	HIS
1	D	260	GLN
1	D	265	GLN
1	D	274	GLN
1	D	311	ASN

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

6 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	401	-	46,48,48	1.22	7 (15%)	64,73,73	1.67	13 (20%)
3	THR	A	402	-	7,7,7	0.85	0	8,9,9	0.94	0
3	THR	B	402	-	7,7,7	1.00	1 (14%)	8,9,9	1.77	2 (25%)
2	NAD	D	401	-	46,48,48	1.15	4 (8%)	64,73,73	1.67	14 (21%)
2	NAD	C	401	-	46,48,48	1.09	5 (10%)	64,73,73	1.60	13 (20%)
2	NAD	A	401	-	46,48,48	1.21	4 (8%)	64,73,73	1.75	11 (17%)

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	401	-	-	3/30/62/62	0/5/5/5
3	THR	A	402	-	-	8/8/8/8	-
3	THR	B	402	-	-	3/8/8/8	-
2	NAD	D	401	-	-	10/30/62/62	0/5/5/5
2	NAD	C	401	-	-	3/30/62/62	0/5/5/5
2	NAD	A	401	-	-	4/30/62/62	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAD	C5A-C4A	4.43	1.47	1.39
2	C	401	NAD	C5A-C4A	4.08	1.46	1.39
2	B	401	NAD	C5A-C4A	3.99	1.46	1.39
2	A	401	NAD	C5A-C4A	3.81	1.45	1.39
2	B	401	NAD	PN-O3	3.06	1.62	1.59
2	A	401	NAD	PN-O3	3.00	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C5A-C6A	2.89	1.49	1.41
2	B	401	NAD	C5A-N7A	-2.67	1.34	1.39
2	D	401	NAD	C5A-C6A	2.60	1.48	1.41
2	B	401	NAD	PA-O3	2.56	1.62	1.59
2	C	401	NAD	C8A-N7A	2.45	1.36	1.31
2	D	401	NAD	C4A-N9A	-2.41	1.32	1.37
2	D	401	NAD	C8A-N7A	2.31	1.36	1.31
2	B	401	NAD	C4A-N9A	-2.31	1.32	1.37
2	C	401	NAD	C5A-N7A	-2.27	1.34	1.39
3	B	402	THR	OXT-C	-2.24	1.23	1.30
2	C	401	NAD	C5A-C6A	2.20	1.47	1.41
2	A	401	NAD	C4A-N9A	-2.20	1.33	1.37
2	B	401	NAD	C8A-N7A	2.14	1.35	1.31
2	C	401	NAD	C4A-N9A	-2.12	1.33	1.37
2	B	401	NAD	C5A-C6A	2.05	1.46	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAD	C5A-C4A-N3A	-5.51	119.14	126.72
2	C	401	NAD	C5A-C4A-N3A	-5.33	119.38	126.72
2	A	401	NAD	C5A-C4A-N3A	-5.23	119.52	126.72
2	B	401	NAD	N3A-C4A-N9A	4.78	135.29	127.17
2	D	401	NAD	C5A-C4A-N3A	-4.41	120.64	126.72
2	A	401	NAD	N3A-C4A-N9A	4.32	134.51	127.17
2	C	401	NAD	N3A-C4A-N9A	4.28	134.44	127.17
2	A	401	NAD	C4A-N9A-C8A	4.22	110.17	105.74
2	B	401	NAD	N3A-C2A-N1A	-4.19	122.24	128.58
2	A	401	NAD	C4A-C5A-N7A	-4.01	105.99	110.58
2	D	401	NAD	N3A-C2A-N1A	-3.89	122.69	128.58
2	D	401	NAD	C4A-N9A-C8A	3.87	109.81	105.74
2	B	401	NAD	C2A-N3A-C4A	3.87	121.28	111.83
2	C	401	NAD	C2A-N3A-C4A	3.80	121.11	111.83
2	D	401	NAD	N3A-C4A-N9A	3.79	133.62	127.17
2	A	401	NAD	C2A-N3A-C4A	3.74	120.96	111.83
2	A	401	NAD	N3A-C2A-N1A	-3.60	123.13	128.58
2	D	401	NAD	O4B-C1B-N9A	3.56	114.94	108.09
2	B	401	NAD	C4A-N9A-C8A	3.51	109.43	105.74
2	C	401	NAD	N3A-C2A-N1A	-3.51	123.27	128.58
2	D	401	NAD	C2A-N3A-C4A	3.48	120.33	111.83
2	A	401	NAD	N9A-C8A-N7A	-3.27	109.30	113.94
2	A	401	NAD	C5A-N7A-C8A	3.26	108.58	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	THR	OXT-C-O	-3.25	116.70	124.08
3	B	402	THR	OXT-C-CA	3.18	125.11	114.15
2	D	401	NAD	C4A-C5A-N7A	-3.14	107.00	110.58
2	C	401	NAD	C4A-N9A-C8A	3.11	109.00	105.74
2	A	401	NAD	C6A-C5A-N7A	3.08	138.03	132.09
2	C	401	NAD	C4A-C5A-N7A	-2.96	107.20	110.58
2	C	401	NAD	C3N-C7N-N7N	2.85	121.25	117.74
2	B	401	NAD	C4A-C5A-N7A	-2.80	107.38	110.58
2	A	401	NAD	C3N-C7N-N7N	2.80	121.19	117.74
2	D	401	NAD	N9A-C8A-N7A	-2.71	110.09	113.94
2	B	401	NAD	O4B-C1B-N9A	2.69	113.25	108.09
2	C	401	NAD	O4B-C1B-N9A	2.66	113.20	108.09
2	C	401	NAD	N9A-C8A-N7A	-2.61	110.23	113.94
2	D	401	NAD	C6A-C5A-N7A	2.61	137.12	132.09
2	C	401	NAD	C5A-N7A-C8A	2.51	107.39	103.45
2	D	401	NAD	C5A-N7A-C8A	2.49	107.37	103.45
2	B	401	NAD	N9A-C8A-N7A	-2.43	110.49	113.94
2	D	401	NAD	C4A-N9A-C1B	-2.39	121.05	126.63
2	B	401	NAD	C5A-N7A-C8A	2.35	107.15	103.45
2	D	401	NAD	O2A-PA-O1A	2.30	123.16	112.44
2	B	401	NAD	O2A-PA-O1A	2.21	122.71	112.44
2	D	401	NAD	O2N-PN-O1N	2.19	122.61	112.44
2	C	401	NAD	C6A-C5A-N7A	2.17	136.26	132.09
2	C	401	NAD	O2N-PN-O1N	2.16	122.49	112.44
2	A	401	NAD	O7N-C7N-N7N	-2.11	119.56	122.62
2	B	401	NAD	C2A-N1A-C6A	2.11	122.20	118.73
2	C	401	NAD	O2A-PA-O1A	2.09	122.17	112.44
2	D	401	NAD	C2A-N1A-C6A	2.08	122.15	118.73
2	B	401	NAD	N6A-C6A-N1A	2.04	122.91	118.38
2	B	401	NAD	C3N-C7N-N7N	2.01	120.22	117.74

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5D-O5D-PN-O3
2	A	401	NAD	C5D-O5D-PN-O1N
2	B	401	NAD	C5D-O5D-PN-O2N
2	D	401	NAD	C5B-O5B-PA-O2A
2	D	401	NAD	C5B-O5B-PA-O3
2	D	401	NAD	C3B-C4B-C5B-O5B
2	D	401	NAD	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	D	401	NAD	C5D-O5D-PN-O1N
2	D	401	NAD	C5D-O5D-PN-O2N
3	A	402	THR	OXT-C-CA-N
3	A	402	THR	O-C-CA-CB
3	A	402	THR	OXT-C-CA-CB
3	A	402	THR	N-CA-CB-CG2
3	A	402	THR	C-CA-CB-OG1
3	A	402	THR	C-CA-CB-CG2
3	B	402	THR	O-C-CA-CB
3	B	402	THR	OXT-C-CA-CB
2	D	401	NAD	O4B-C4B-C5B-O5B
3	B	402	THR	OXT-C-CA-N
2	D	401	NAD	C2B-C1B-N9A-C8A
3	A	402	THR	O-C-CA-N
3	A	402	THR	N-CA-CB-OG1
2	C	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	C5D-O5D-PN-O2N
2	B	401	NAD	C5D-O5D-PN-O3
2	D	401	NAD	O4B-C1B-N9A-C8A
2	C	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	C2B-C1B-N9A-C8A
2	D	401	NAD	PA-O3-PN-O1N
2	A	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	O4B-C4B-C5B-O5B

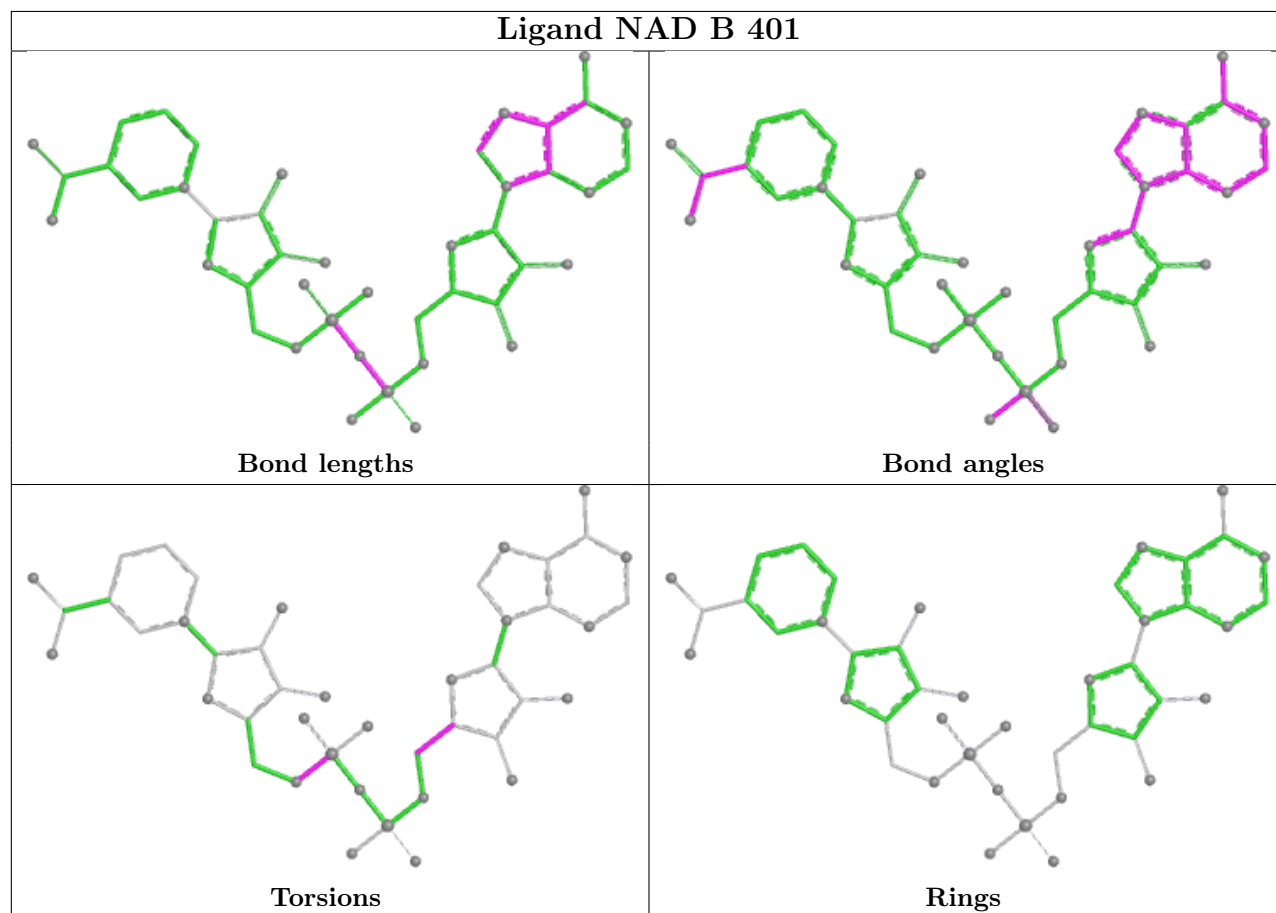
There are no ring outliers.

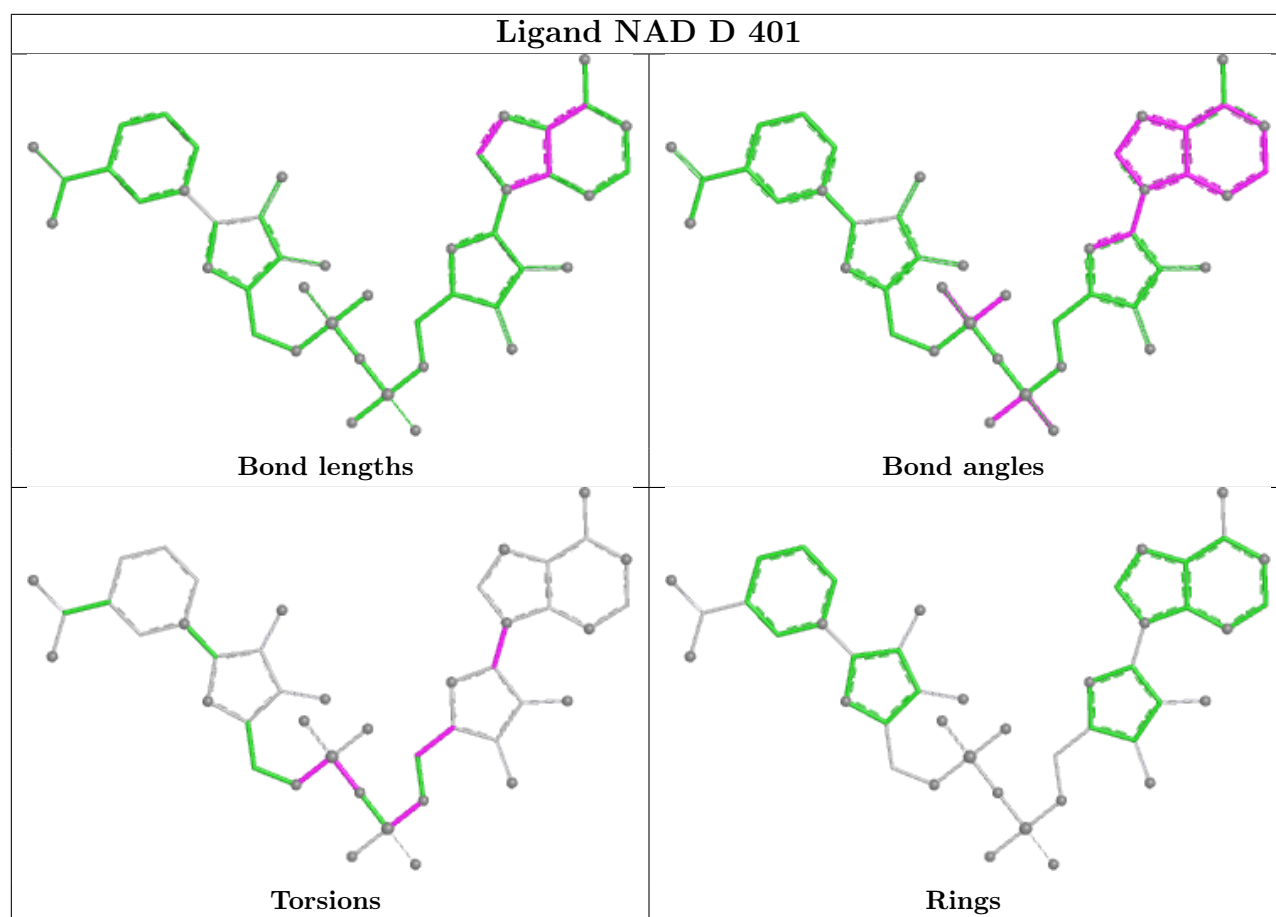
5 monomers are involved in 10 short contacts:

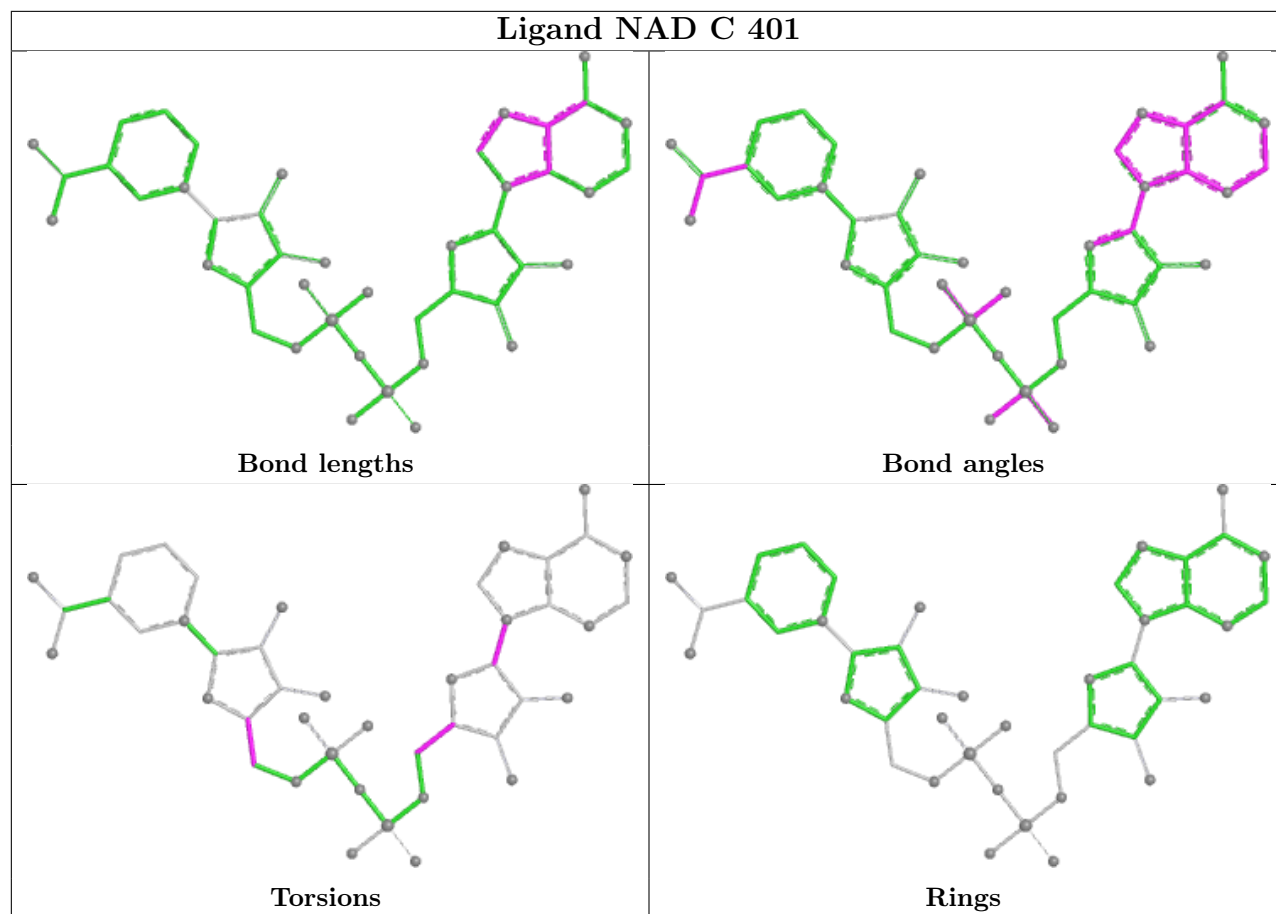
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAD	2	0
3	A	402	THR	1	0
2	D	401	NAD	4	0
2	C	401	NAD	1	0
2	A	401	NAD	3	0

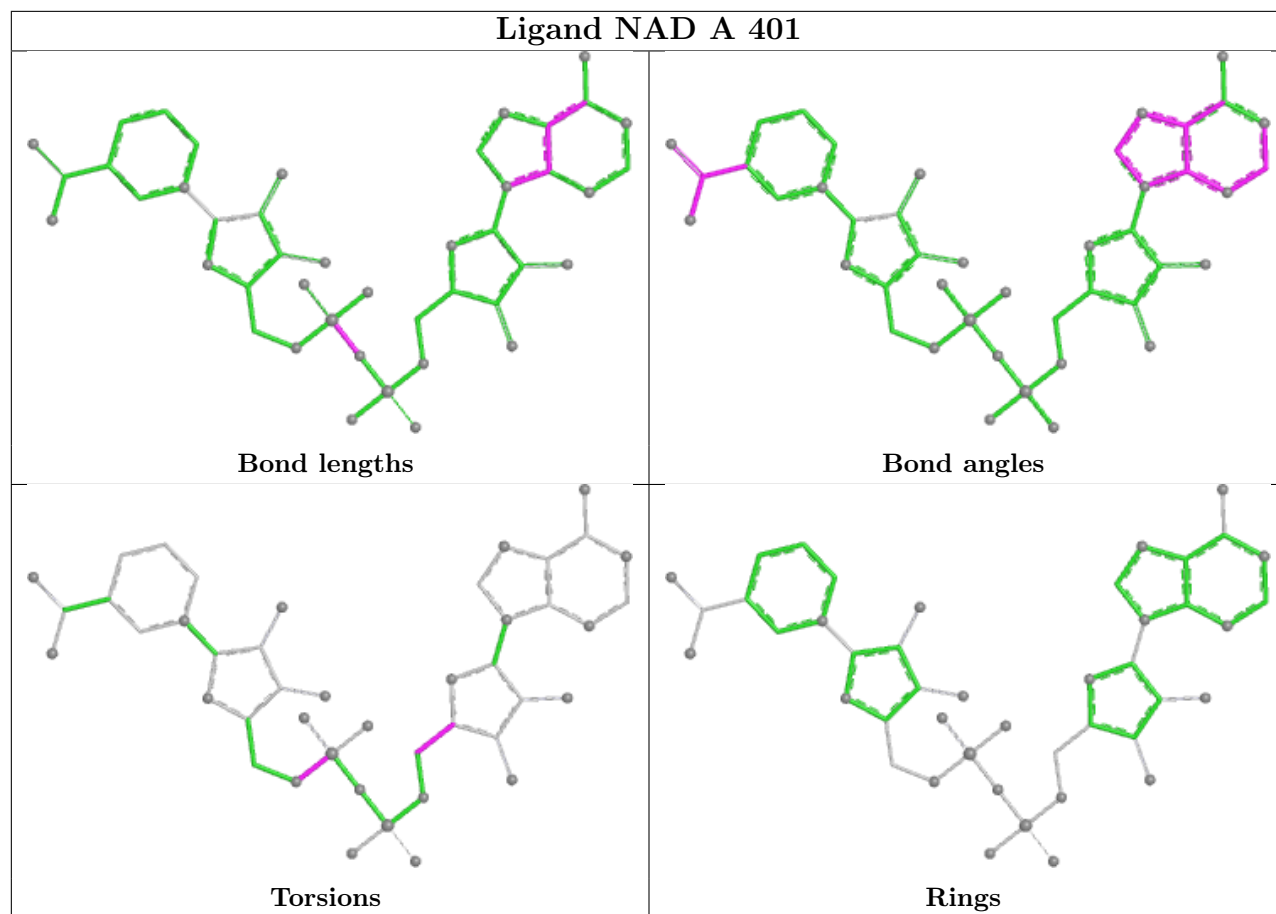
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

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	310/358 (86%)	-0.37	3 (0%) 79 76	19, 28, 50, 81	0
1	B	308/358 (86%)	0.03	10 (3%) 50 46	25, 39, 65, 94	0
1	C	308/358 (86%)	-0.08	8 (2%) 57 52	22, 36, 62, 90	0
1	D	304/358 (84%)	1.47	82 (26%) 1 1	30, 71, 99, 123	0
All	All	1230/1432 (85%)	0.25	103 (8%) 17 15	19, 39, 86, 123	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	181	PRO	6.1
1	D	309	LEU	5.7
1	D	254	ALA	5.6
1	D	6	PRO	5.5
1	D	264	PHE	5.4
1	D	258	ARG	4.8
1	D	16	GLN	4.8
1	D	305	VAL	4.7
1	D	257	ILE	4.6
1	D	301	LEU	4.6
1	D	256	ALA	4.5
1	D	194	HIS	4.4
1	C	182	GLY	4.3
1	D	266	ILE	4.3
1	D	263	GLY	4.1
1	D	299	TYR	3.8
1	D	89	GLN	3.7
1	D	188	TYR	3.7
1	D	46	VAL	3.5
1	D	185	THR	3.5
1	D	251	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	6	PRO	3.4
1	B	87	ALA	3.4
1	D	47	HIS	3.3
1	D	262	PRO	3.3
1	B	83	THR	3.3
1	D	265	GLN	3.3
1	D	90	TRP	3.2
1	B	313	LYS	3.2
1	D	197	VAL	3.2
1	D	87	ALA	3.1
1	D	267	ARG	3.1
1	A	83	THR	3.1
1	D	275	ALA	3.1
1	D	248	PHE	3.1
1	C	313	LYS	3.0
1	D	312	LEU	3.0
1	D	245	GLY	3.0
1	D	55	ALA	3.0
1	D	272	TYR	3.0
1	D	17	ILE	3.0
1	C	201	PRO	3.0
1	D	216	TYR	3.0
1	B	80	LEU	3.0
1	D	42	THR	2.9
1	D	253	ILE	2.9
1	B	82	ALA	2.9
1	D	211	ALA	2.9
1	D	261	VAL	2.8
1	D	297	ALA	2.8
1	D	48	LEU	2.8
1	D	244	ALA	2.8
1	D	249	THR	2.8
1	D	180	PRO	2.8
1	D	88	PRO	2.7
1	D	175	ILE	2.7
1	D	296	LYS	2.7
1	C	179	THR	2.7
1	D	310	ALA	2.7
1	B	302	LYS	2.6
1	C	31	ARG	2.6
1	B	86	LYS	2.5
1	D	268	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	276	ILE	2.5
1	B	79	ALA	2.5
1	D	252	GLN	2.5
1	D	193	PHE	2.4
1	D	283	SER	2.4
1	D	86	LYS	2.4
1	D	295	TRP	2.4
1	D	227	LEU	2.3
1	D	255	ALA	2.3
1	D	302	LYS	2.3
1	D	23	LEU	2.3
1	A	86	LYS	2.3
1	C	6	PRO	2.3
1	D	199	GLY	2.3
1	D	176	SER	2.3
1	D	83	THR	2.2
1	D	206	LEU	2.2
1	D	243	ILE	2.2
1	D	179	THR	2.2
1	D	22	ALA	2.2
1	D	195	ALA	2.2
1	D	7	LYS	2.2
1	D	40	VAL	2.2
1	D	196	ALA	2.2
1	D	207	LYS	2.2
1	B	84	GLY	2.2
1	D	298	GLN	2.1
1	D	294	GLY	2.1
1	D	37	SER	2.1
1	D	79	ALA	2.1
1	D	80	LEU	2.1
1	D	300	GLY	2.1
1	D	31	ARG	2.1
1	D	280	TRP	2.1
1	D	178	LYS	2.1
1	D	41	PRO	2.1
1	D	45	HIS	2.1
1	A	313	LYS	2.0
1	C	178	LYS	2.0
1	C	262	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

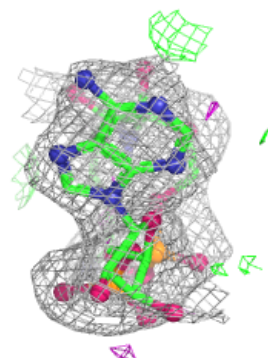
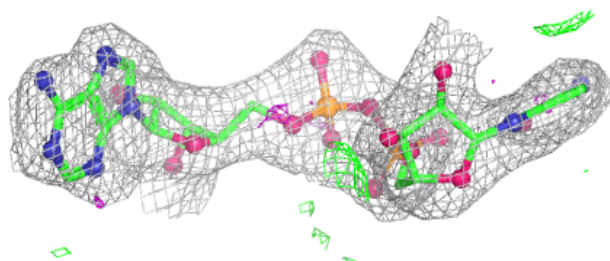
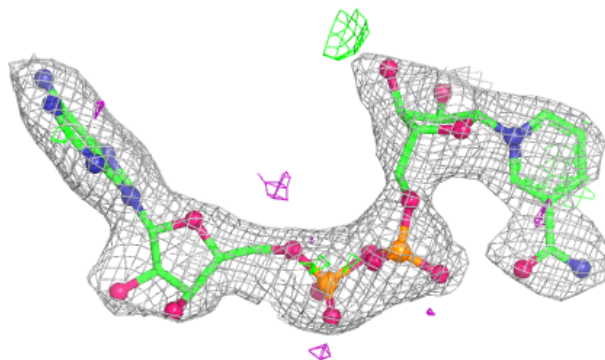
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	THR	A	402	8/8	0.85	0.16	37,50,52,58	0
2	NAD	D	401	44/44	0.89	0.12	47,66,75,88	0
3	THR	B	402	8/8	0.89	0.18	45,67,71,74	0
2	NAD	A	401	44/44	0.98	0.05	18,22,27,29	0
2	NAD	B	401	44/44	0.98	0.05	20,26,35,37	0
2	NAD	C	401	44/44	0.98	0.06	23,29,33,35	0

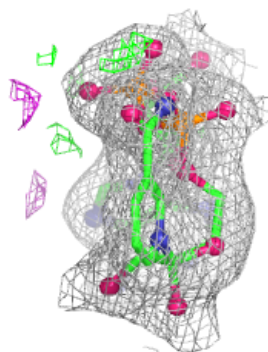
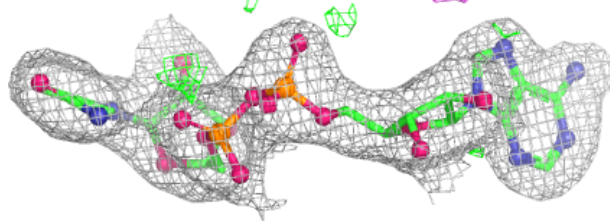
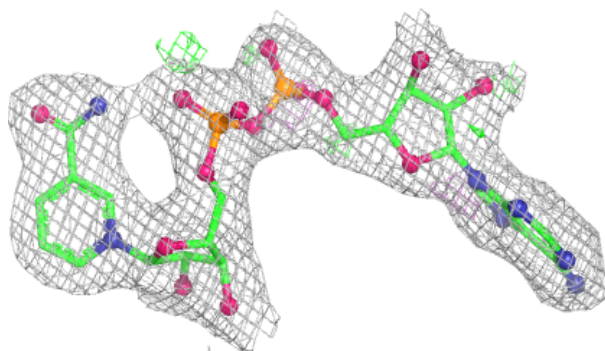
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 401:

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

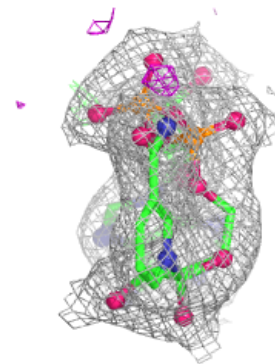
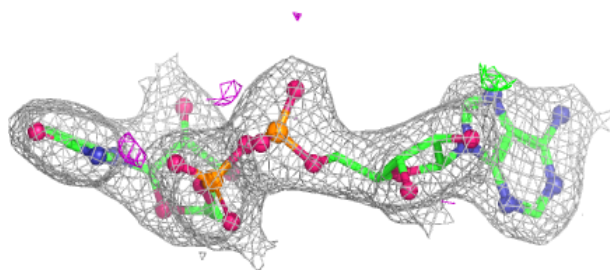
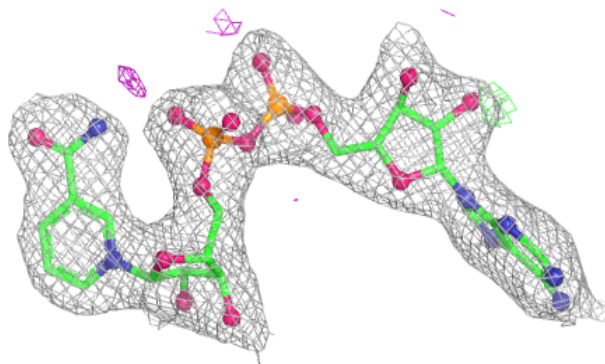
**Electron density around NAD A 401:**

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

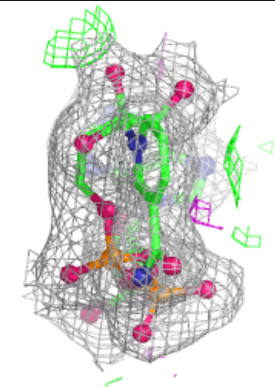
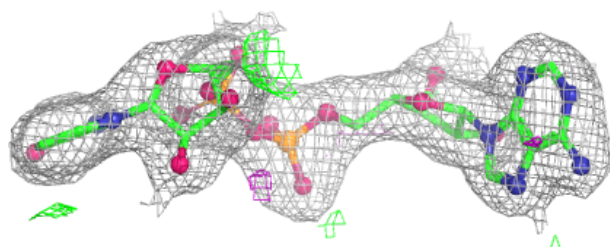
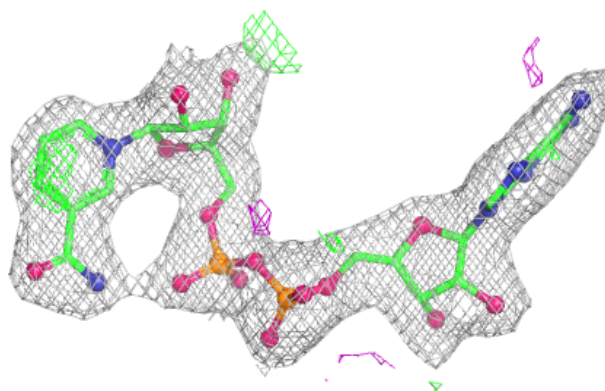


Electron density around NAD B 401:

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

**Electron density around NAD C 401:**

$2mF_o-DF_c$ (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.