



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 01:38 PM BST

PDB ID : 3WMX  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

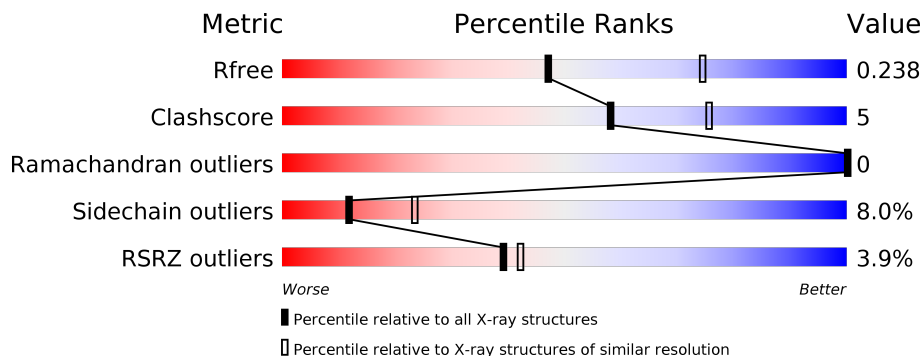
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	358	
1	C	358	
1	D	358	

## 2 Entry composition [i](#)

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

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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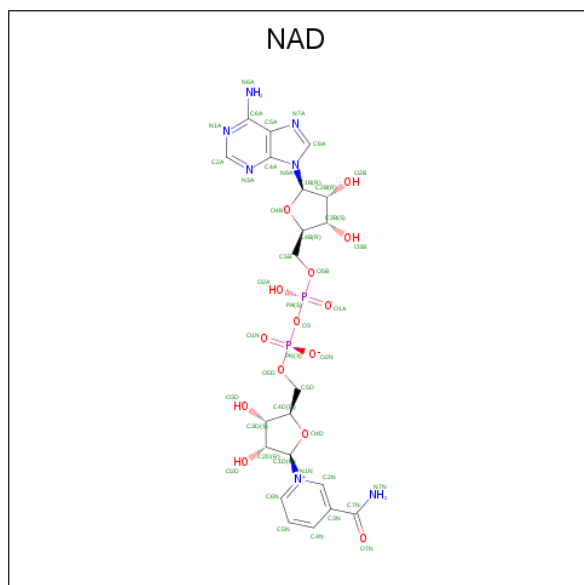
Chain	Residue	Modelled	Actual	Comment	Reference
C	324	LYS	-	EXPRESSION TAG	UNP Q0K312
C	325	ALA	-	EXPRESSION TAG	UNP Q0K312
C	326	ARG	-	EXPRESSION TAG	UNP Q0K312
C	327	LYS	-	EXPRESSION TAG	UNP Q0K312
C	328	GLU	-	EXPRESSION TAG	UNP Q0K312
C	329	ALA	-	EXPRESSION TAG	UNP Q0K312
C	330	GLU	-	EXPRESSION TAG	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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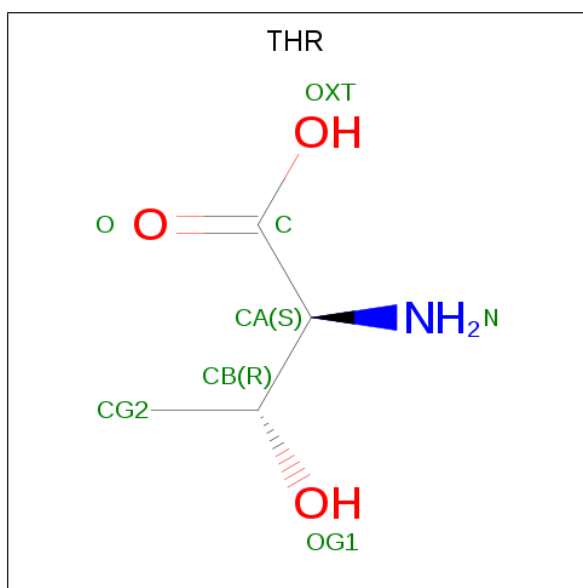
Chain	Residue	Modelled	Actual	Comment	Reference
D	326	ARG	-	EXPRESSION TAG	UNP Q0K312
D	327	LYS	-	EXPRESSION TAG	UNP Q0K312
D	328	GLU	-	EXPRESSION TAG	UNP Q0K312
D	329	ALA	-	EXPRESSION TAG	UNP Q0K312
D	330	GLU	-	EXPRESSION TAG	UNP Q0K312
D	331	LEU	-	EXPRESSION TAG	UNP Q0K312
D	332	ALA	-	EXPRESSION TAG	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 (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		
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		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is THREONINE (three-letter code: THR) (formula:  $C_4H_9NO_3$ ).



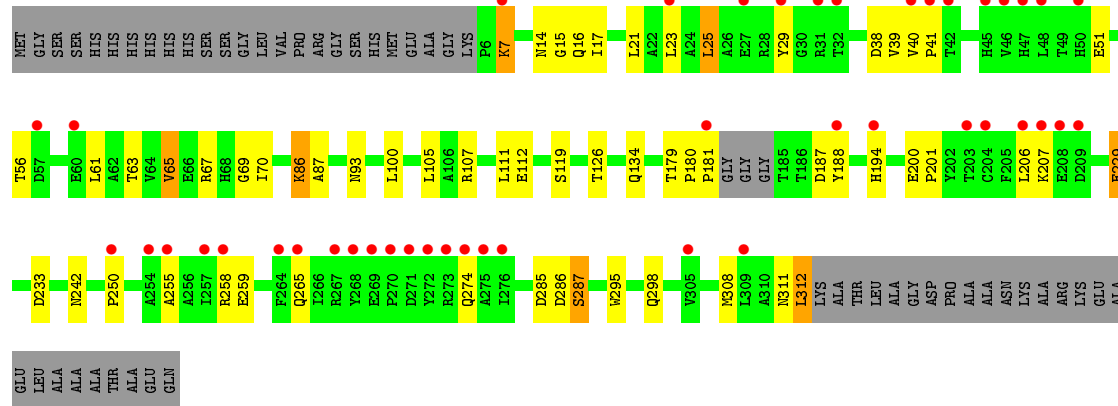
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- 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		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 100.0 (40.87-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.78 (at 2.51Å)	Xtrriage
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 (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtrriage
Anisotropy	0.108	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9738	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.49	0/2445	0.63	0/3333
1	B	0.43	0/2431	0.60	0/3314
1	C	0.43	0/2432	0.60	0/3316
1	D	0.37	0/2410	0.59	0/3287
All	All	0.43	0/9718	0.60	0/13250

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	2385	0	2342	23	0
1	B	2371	0	2323	25	0
1	C	2372	0	2327	15	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	91	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 (91) 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:HG2	1:A:313:LYS:O	1.78	0.81
1:C:19:SER:OG	1:C:179:THR:HG21	1.83	0.76
1:B:313:LYS:CG	1:B:313:LYS:O	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:HG2	1:B:313:LYS:O	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:CG	1:A:313:LYS:O	2.41	0.66
1:B:89:GLN:HA	1:B:89:GLN:HE21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:D:259:GLU:O	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: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: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:94:LEU:HD23	1:A:94:LEU:C	2.33	0.47
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
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:A:20:GLU:OE1	1:A:176:SER:OG	2.23	0.43
1:D:308:MET:O	1:D:312:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:C:23:LEU:HD12	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:HA	1:B:23:LEU:HD12	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:HD22	1:B:14:ASN:N	2.19	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:HE3	1:A:296:LYS:HB2	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 [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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [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	245/278 (88%)	228 (93%)	17 (7%)	15	30
1	B	244/278 (88%)	226 (93%)	18 (7%)	13	27
1	C	244/278 (88%)	225 (92%)	19 (8%)	12	24
1	D	243/278 (87%)	220 (90%)	23 (10%)	8	17
All	All	976/1112 (88%)	899 (92%)	77 (8%)	12	24

All (77) 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
1	A	111	LEU
1	A	112	GLU
1	A	188	TYR
1	A	206	LEU
1	A	267	ARG
1	A	303	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	313	LYS
1	B	7	LYS
1	B	14	ASN
1	B	23	LEU
1	B	25	LEU
1	B	44	ARG
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	188	TYR
1	B	206	LEU
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	46	VAL
1	C	56	THR
1	C	65	VAL
1	C	94	LEU
1	C	105	LEU
1	C	107	ARG
1	C	111	LEU
1	C	112	GLU
1	C	178	LYS
1	C	179	THR
1	C	188	TYR
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	56	THR
1	D	63	THR
1	D	65	VAL
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	188	TYR
1	D	194	HIS
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	14	ASN
1	A	33	ASN
1	A	89	GLN
1	A	108	GLN
1	A	134	GLN
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	274	GLN
1	C	14	ASN
1	C	33	ASN
1	C	108	GLN
1	C	134	GLN
1	C	177	HIS
1	C	274	GLN
1	D	33	ASN

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Mol	Chain	Res	Type
1	D	134	GLN
1	D	177	HIS
1	D	265	GLN
1	D	274	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](#)

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	A	401	-	42,48,48	0.91	1 (2%)	50,73,73	1.33	6 (12%)
2	NAD	C	401	-	42,48,48	0.83	1 (2%)	50,73,73	1.19	6 (12%)
2	NAD	D	401	-	42,48,48	0.84	2 (4%)	50,73,73	1.28	6 (12%)
2	NAD	B	401	-	42,48,48	0.78	0	50,73,73	1.19	6 (12%)
3	THR	B	402	-	4,7,7	0.63	0	4,9,9	0.59	0
3	THR	A	402	-	4,7,7	0.62	0	4,9,9	0.45	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
2	NAD	A	401	-	-	4/26/62/62	0/5/5/5
2	NAD	C	401	-	-	3/26/62/62	0/5/5/5
2	NAD	D	401	-	-	8/26/62/62	0/5/5/5
2	NAD	B	401	-	-	4/26/62/62	0/5/5/5
3	THR	B	402	-	-	0/4/8/8	-
3	THR	A	402	-	-	4/4/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C2D-C1D	-2.41	1.50	1.53
2	D	401	NAD	C5A-C4A	2.29	1.47	1.40
2	C	401	NAD	C5A-C4A	2.05	1.46	1.40
2	D	401	NAD	C2A-N3A	2.01	1.35	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAD	N3A-C2A-N1A	-4.12	122.24	128.68
2	D	401	NAD	N3A-C2A-N1A	-3.83	122.69	128.68
2	A	401	NAD	N3A-C2A-N1A	-3.55	123.13	128.68
2	A	401	NAD	PN-O3-PA	-3.50	120.82	132.83
2	C	401	NAD	N3A-C2A-N1A	-3.46	123.27	128.68
2	A	401	NAD	C4A-C5A-N7A	-3.27	105.99	109.40
2	D	401	NAD	C1B-N9A-C4A	-3.18	121.05	126.64
2	D	401	NAD	PN-O3-PA	-3.09	122.23	132.83
2	C	401	NAD	C3N-C7N-N7N	2.91	121.25	117.75
2	A	401	NAD	C3N-C7N-N7N	2.86	121.19	117.75
2	B	401	NAD	PN-O3-PA	-2.83	123.13	132.83
2	C	401	NAD	PN-O3-PA	-2.41	124.54	132.83
2	A	401	NAD	C1B-N9A-C4A	-2.41	122.40	126.64
2	D	401	NAD	C4A-C5A-N7A	-2.31	107.00	109.40
2	D	401	NAD	O2A-PA-O1A	2.21	123.16	112.24
2	A	401	NAD	O7N-C7N-N7N	-2.12	119.56	122.58
2	B	401	NAD	O2A-PA-O1A	2.12	122.71	112.24
2	C	401	NAD	C4A-C5A-N7A	-2.11	107.20	109.40
2	D	401	NAD	O2N-PN-O1N	2.10	122.61	112.24
2	B	401	NAD	N6A-C6A-N1A	2.09	122.91	118.57
2	C	401	NAD	O2N-PN-O1N	2.07	122.49	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAD	C3N-C7N-N7N	2.05	120.22	117.75
2	B	401	NAD	C2A-N1A-C6A	2.01	122.20	118.75
2	C	401	NAD	O2A-PA-O1A	2.01	122.17	112.24

There are no chirality outliers.

All (23) torsion outliers are listed below:

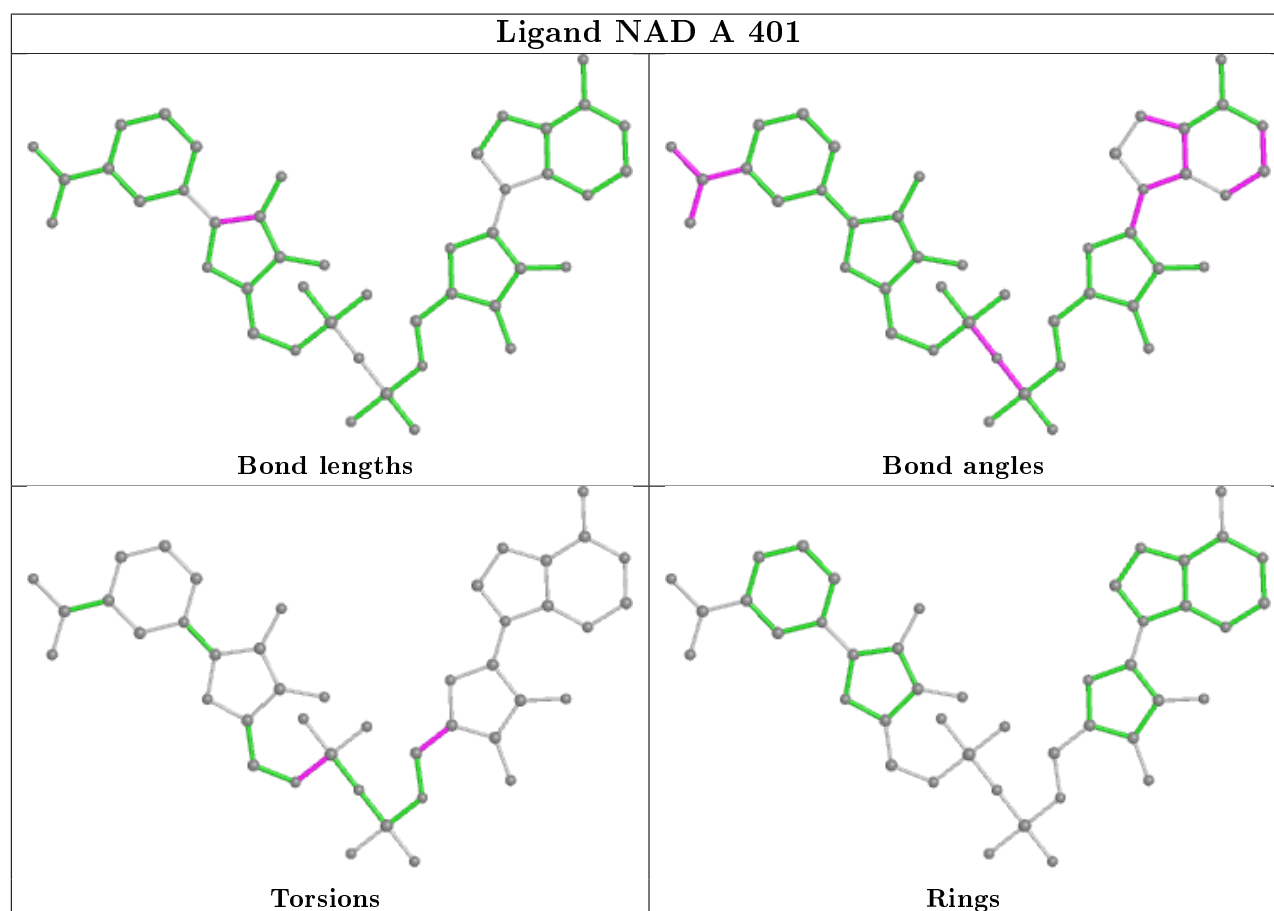
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5D-O5D-PN-O1N
2	D	401	NAD	C5B-O5B-PA-O2A
2	D	401	NAD	C5B-O5B-PA-O3
2	D	401	NAD	C3B-C4B-C5B-O5B
2	D	401	NAD	C5D-O5D-PN-O1N
2	D	401	NAD	C5D-O5D-PN-O2N
2	B	401	NAD	C5D-O5D-PN-O2N
3	A	402	THR	N-CA-CB-CG2
3	A	402	THR	C-CA-CB-OG1
2	D	401	NAD	O4B-C4B-C5B-O5B
3	A	402	THR	N-CA-CB-OG1
2	A	401	NAD	C5D-O5D-PN-O3
2	B	401	NAD	C5D-O5D-PN-O3
2	A	401	NAD	C5D-O5D-PN-O2N
2	C	401	NAD	O4D-C4D-C5D-O5D
2	C	401	NAD	O4B-C4B-C5B-O5B
3	A	402	THR	C-CA-CB-CG2
2	A	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	C5D-O5D-PN-O3
2	C	401	NAD	C3D-C4D-C5D-O5D
2	D	401	NAD	PA-O3-PN-O1N
2	B	401	NAD	C5D-O5D-PN-O1N

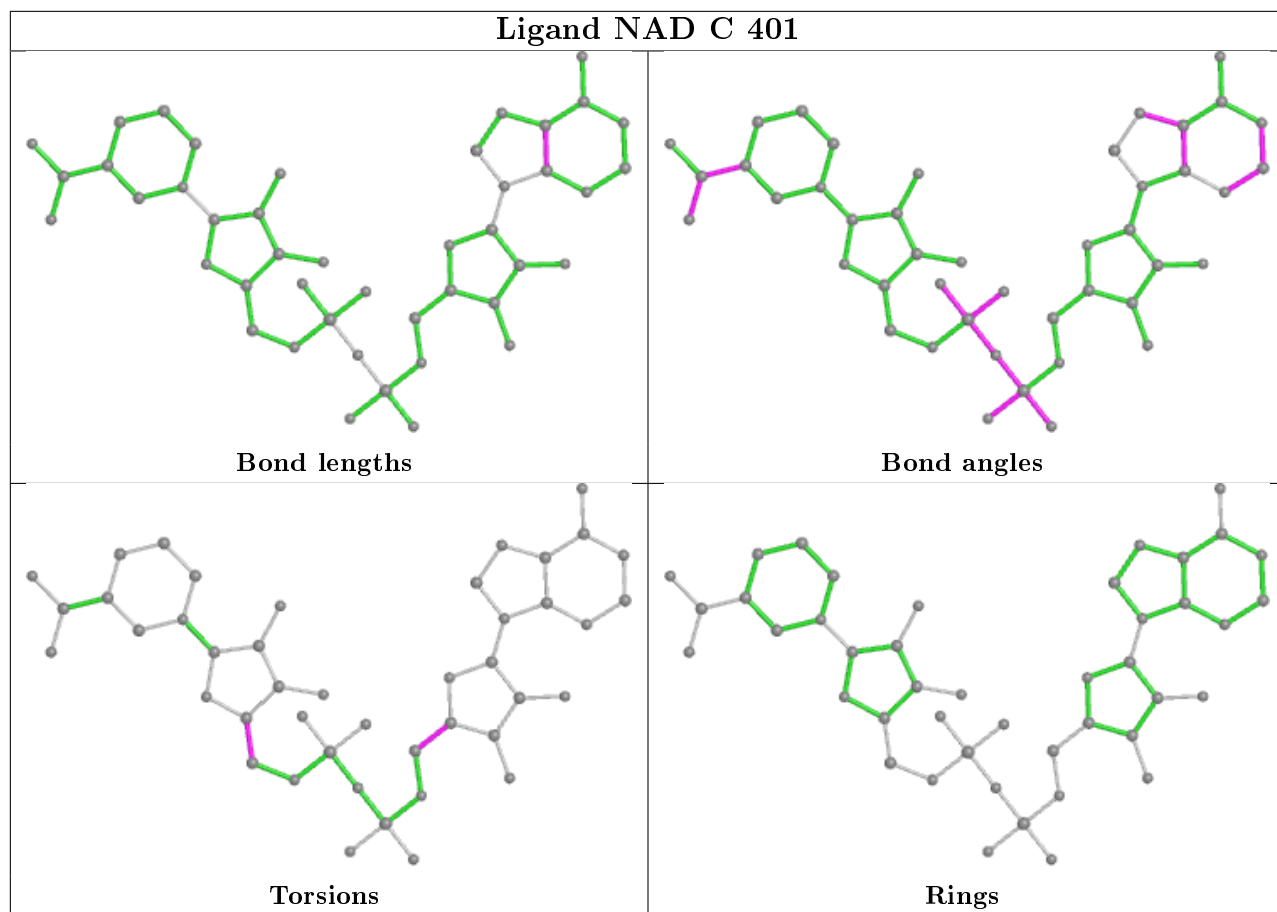
There are no ring outliers.

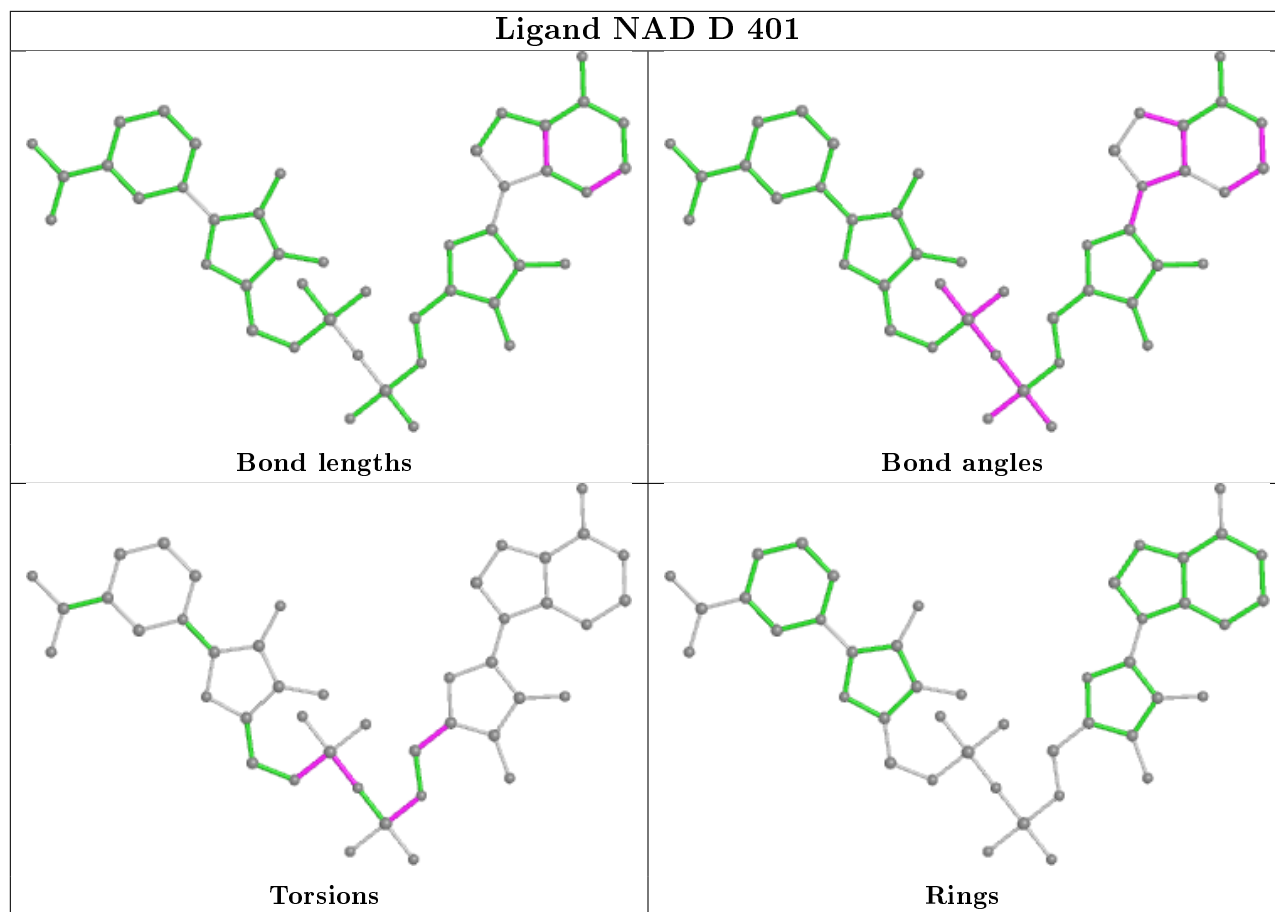
5 monomers are involved in 10 short contacts:

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

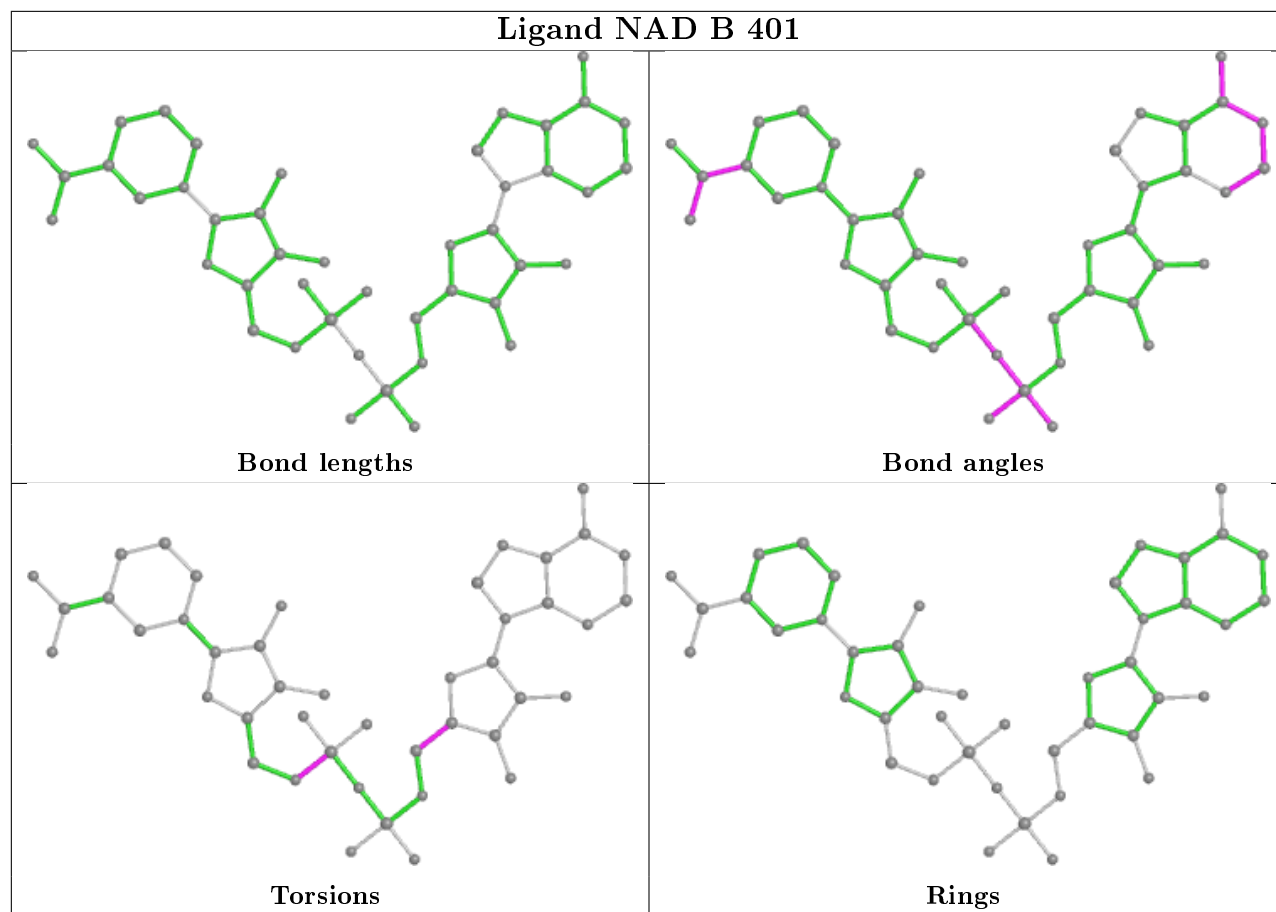
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	310/358 (86%)	-0.34	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	19, 28, 50, 81	0
1	B	308/358 (86%)	-0.10	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	25, 39, 65, 94	0
1	C	308/358 (86%)	-0.04	4 (1%) <span style="border: 1px solid blue; padding: 2px;">77</span> <span style="border: 1px solid blue; padding: 2px;">79</span>	22, 36, 62, 90	0
1	D	304/358 (84%)	0.86	44 (14%) <span style="border: 1px solid red; padding: 2px;">2</span> <span style="border: 1px solid red; padding: 2px;">2</span>	30, 71, 99, 123	0
All	All	1230/1432 (85%)	0.09	48 (3%) <span style="border: 1px solid red; padding: 2px;">39</span> <span style="border: 1px solid red; padding: 2px;">42</span>	19, 39, 86, 123	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	258	ARG	5.4
1	D	254	ALA	4.9
1	D	23	LEU	4.4
1	D	47	HIS	4.4
1	D	272	TYR	4.2
1	D	45	HIS	4.0
1	D	46	VAL	4.0
1	D	309	LEU	3.9
1	D	42	THR	3.2
1	D	60	GLU	3.2
1	D	275	ALA	3.2
1	D	41	PRO	3.2
1	D	194	HIS	3.1
1	D	269	GLU	3.1
1	D	255	ALA	3.0
1	D	29	TYR	3.0
1	D	264	PHE	2.9
1	D	31	ARG	2.9
1	D	305	VAL	2.9
1	D	206	LEU	2.8
1	D	270	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	203	THR	2.7
1	D	32	THR	2.6
1	D	181	PRO	2.6
1	D	27	GLU	2.6
1	D	257	ILE	2.5
1	D	267	ARG	2.5
1	D	271	ASP	2.5
1	C	199	GLY	2.4
1	D	207	LYS	2.4
1	D	209	ASP	2.4
1	C	310	ALA	2.4
1	D	48	LEU	2.4
1	D	40	VAL	2.3
1	D	265	GLN	2.2
1	C	66	GLU	2.2
1	D	250	PRO	2.2
1	D	50	HIS	2.2
1	D	208	GLU	2.2
1	D	204	CYS	2.1
1	D	276	ILE	2.1
1	D	7	LYS	2.1
1	D	268	TYR	2.1
1	D	274	GLN	2.1
1	D	273	ARG	2.1
1	D	188	TYR	2.0
1	D	57	ASP	2.0
1	C	182	GLY	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 monosaccharides in this entry.

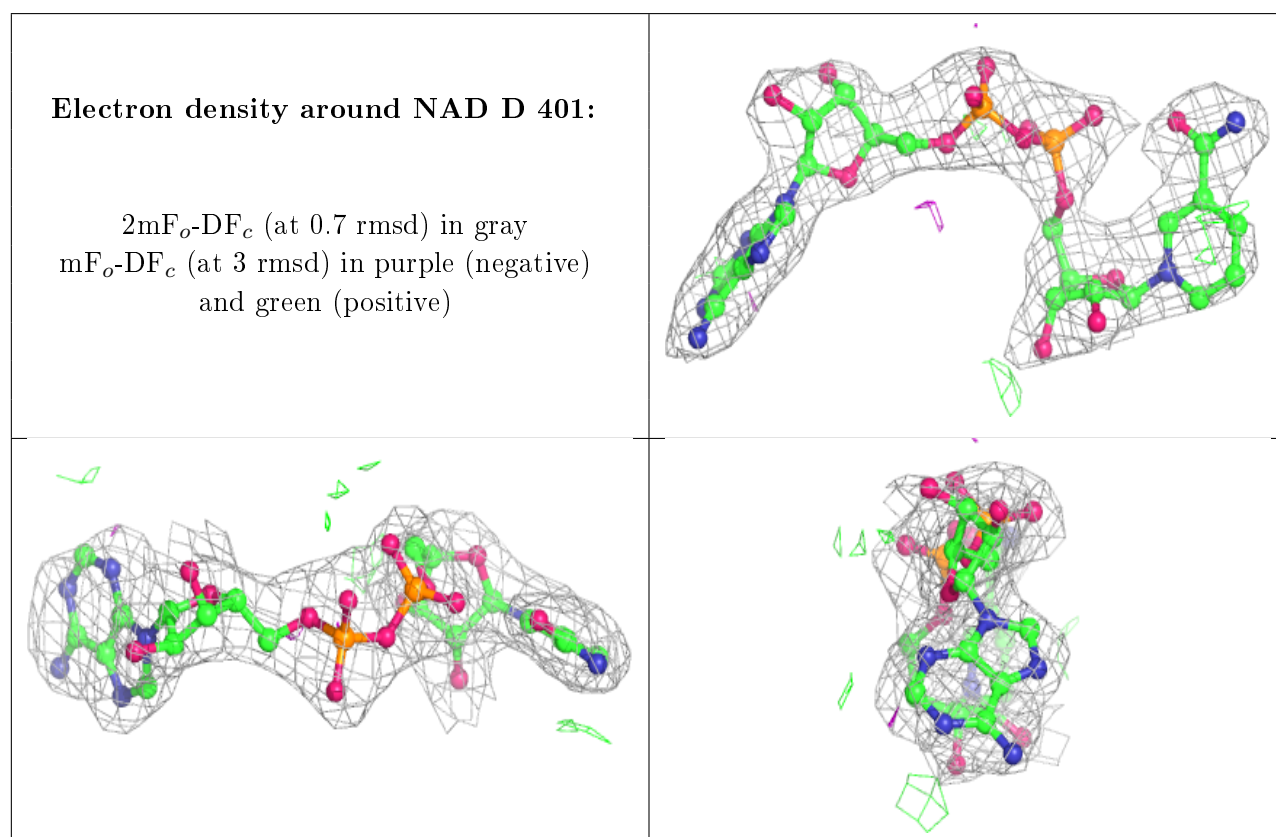
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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.

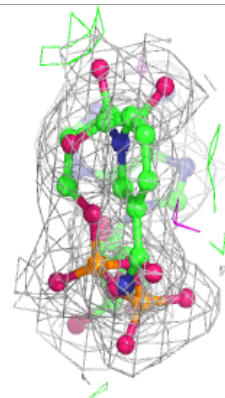
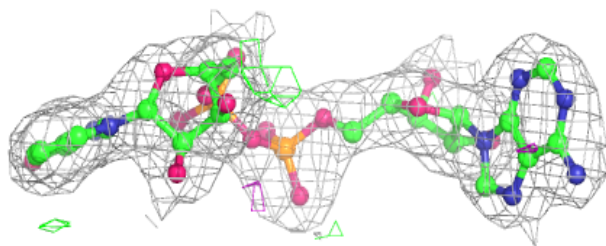
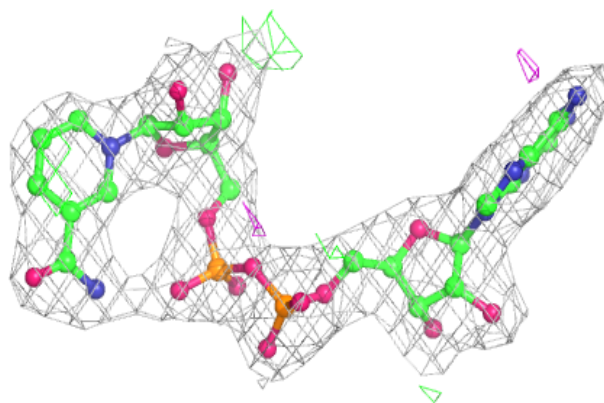
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	THR	A	402	8/8	0.88	0.25	37,50,52,58	0
3	THR	B	402	8/8	0.90	0.22	45,67,71,74	0
2	NAD	D	401	44/44	0.92	0.16	47,66,75,88	0
2	NAD	C	401	44/44	0.97	0.13	23,29,33,35	0
2	NAD	A	401	44/44	0.98	0.13	18,22,27,29	0
2	NAD	B	401	44/44	0.98	0.13	20,26,35,37	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.

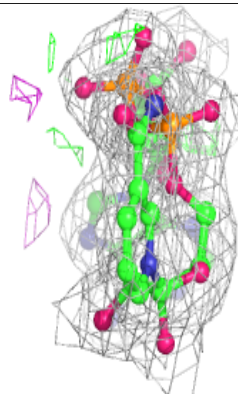
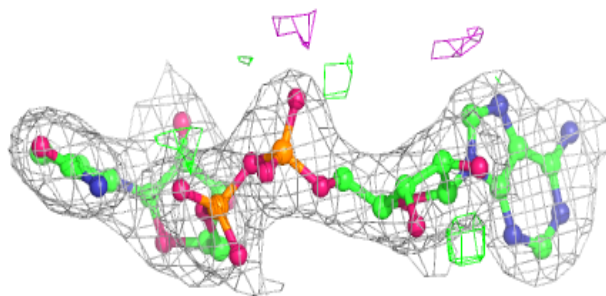
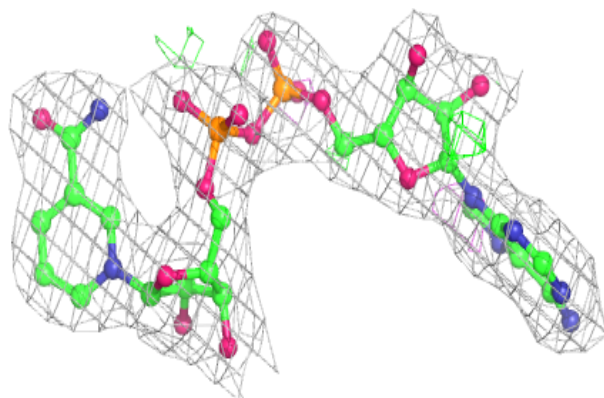


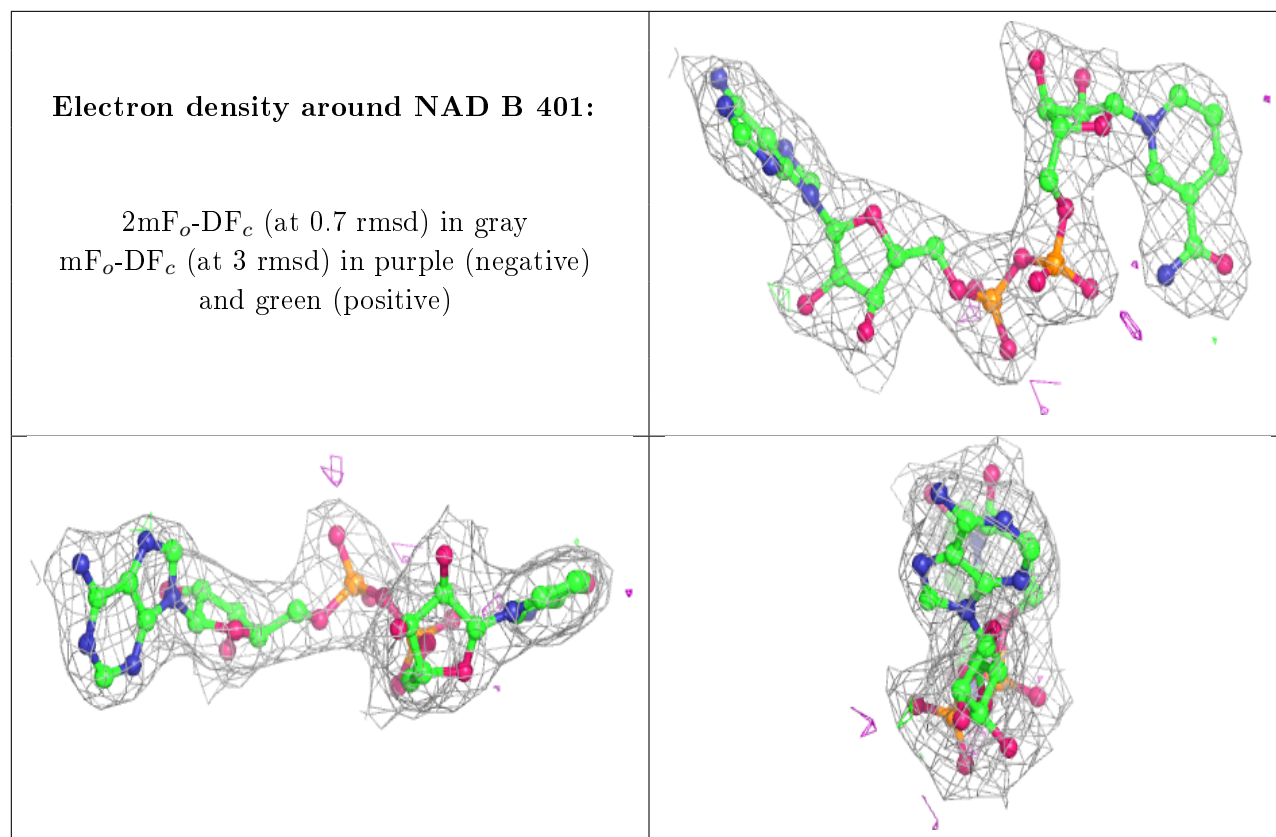
**Electron density around NAD C 401:**

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

**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.