



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 09:12 PM BST

PDB ID : 4F7I  
Title : Structure of Isopropylmalate dehydrogenase from *Thermus thermophilus* in complex with IPM, Mn and NADH  
Authors : Pallo, A.; Graczer, E.; Zavodszky, P.; Weiss, M.S.; Vas, M.  
Deposited on : 2012-05-16  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 : 2.13.1  
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) : 2.13.1

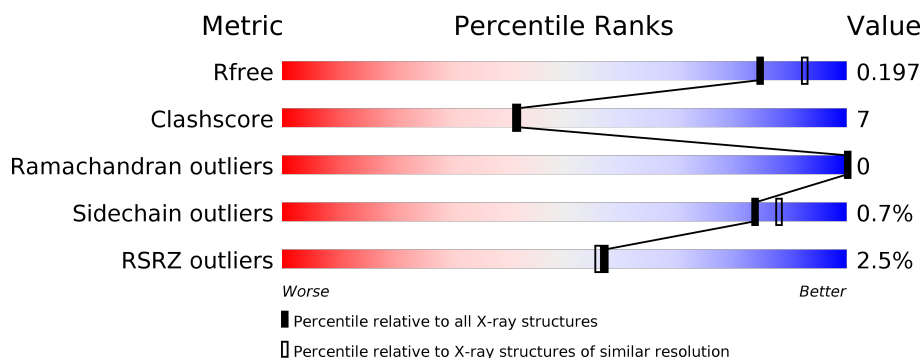
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	359	<div> <div> <div></div> <div>87%</div> <div>10%</div> <div>••</div> </div> </div>
1	B	359	<div> <div> <div></div> <div>88%</div> <div>9%</div> <div>••</div> </div> </div>
1	C	359	<div> <div> <div></div> <div>83%</div> <div>13%</div> <div>•</div> </div> </div>
1	D	359	<div> <div> <div></div> <div>87%</div> <div>11%</div> <div>•</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPO	A	950	-	-	X	-
7	GOL	A	1009	-	-	X	-
7	GOL	B	1010	-	-	X	-
7	GOL	D	1003	-	-	X	-
8	EOH	C	1009	-	-	X	-
8	EOH	C	1010	-	-	X	-
8	EOH	D	1009	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11489 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 3-isopropylmalate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	7	0
			2661	1701	461	492	7			
1	B	350	Total	C	N	O	S	0	5	0
			2656	1696	464	490	6			
1	C	348	Total	C	N	O	S	0	5	0
			2643	1686	463	488	6			
1	D	349	Total	C	N	O	S	0	3	0
			2629	1679	456	487	7			

There are 56 discrepancies between the modelled and reference sequences:

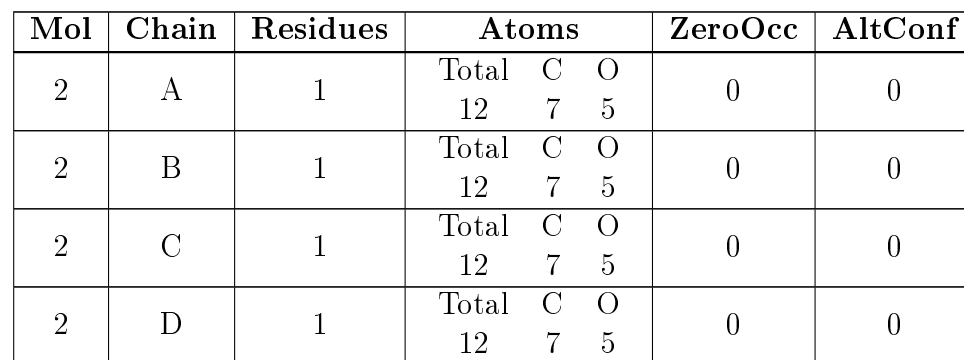
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP Q5SIY4
A	-1	ALA	-	EXPRESSION TAG	UNP Q5SIY4
A	0	SER	-	EXPRESSION TAG	UNP Q5SIY4
A	346	ALA	-	EXPRESSION TAG	UNP Q5SIY4
A	347	ALA	-	EXPRESSION TAG	UNP Q5SIY4
A	348	ALA	-	EXPRESSION TAG	UNP Q5SIY4
A	349	LEU	-	EXPRESSION TAG	UNP Q5SIY4
A	350	GLU	-	EXPRESSION TAG	UNP Q5SIY4
A	351	HIS	-	EXPRESSION TAG	UNP Q5SIY4
A	352	HIS	-	EXPRESSION TAG	UNP Q5SIY4
A	353	HIS	-	EXPRESSION TAG	UNP Q5SIY4
A	354	HIS	-	EXPRESSION TAG	UNP Q5SIY4
A	355	HIS	-	EXPRESSION TAG	UNP Q5SIY4
A	356	HIS	-	EXPRESSION TAG	UNP Q5SIY4
B	-2	MET	-	EXPRESSION TAG	UNP Q5SIY4
B	-1	ALA	-	EXPRESSION TAG	UNP Q5SIY4
B	0	SER	-	EXPRESSION TAG	UNP Q5SIY4
B	346	ALA	-	EXPRESSION TAG	UNP Q5SIY4
B	347	ALA	-	EXPRESSION TAG	UNP Q5SIY4
B	348	ALA	-	EXPRESSION TAG	UNP Q5SIY4
B	349	LEU	-	EXPRESSION TAG	UNP Q5SIY4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	350	GLU	-	EXPRESSION TAG	UNP Q5SIY4
B	351	HIS	-	EXPRESSION TAG	UNP Q5SIY4
B	352	HIS	-	EXPRESSION TAG	UNP Q5SIY4
B	353	HIS	-	EXPRESSION TAG	UNP Q5SIY4
B	354	HIS	-	EXPRESSION TAG	UNP Q5SIY4
B	355	HIS	-	EXPRESSION TAG	UNP Q5SIY4
B	356	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	-2	MET	-	EXPRESSION TAG	UNP Q5SIY4
C	-1	ALA	-	EXPRESSION TAG	UNP Q5SIY4
C	0	SER	-	EXPRESSION TAG	UNP Q5SIY4
C	346	ALA	-	EXPRESSION TAG	UNP Q5SIY4
C	347	ALA	-	EXPRESSION TAG	UNP Q5SIY4
C	348	ALA	-	EXPRESSION TAG	UNP Q5SIY4
C	349	LEU	-	EXPRESSION TAG	UNP Q5SIY4
C	350	GLU	-	EXPRESSION TAG	UNP Q5SIY4
C	351	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	352	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	353	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	354	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	355	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	356	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	-2	MET	-	EXPRESSION TAG	UNP Q5SIY4
D	-1	ALA	-	EXPRESSION TAG	UNP Q5SIY4
D	0	SER	-	EXPRESSION TAG	UNP Q5SIY4
D	346	ALA	-	EXPRESSION TAG	UNP Q5SIY4
D	347	ALA	-	EXPRESSION TAG	UNP Q5SIY4
D	348	ALA	-	EXPRESSION TAG	UNP Q5SIY4
D	349	LEU	-	EXPRESSION TAG	UNP Q5SIY4
D	350	GLU	-	EXPRESSION TAG	UNP Q5SIY4
D	351	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	352	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	353	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	354	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	355	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	356	HIS	-	EXPRESSION TAG	UNP Q5SIY4

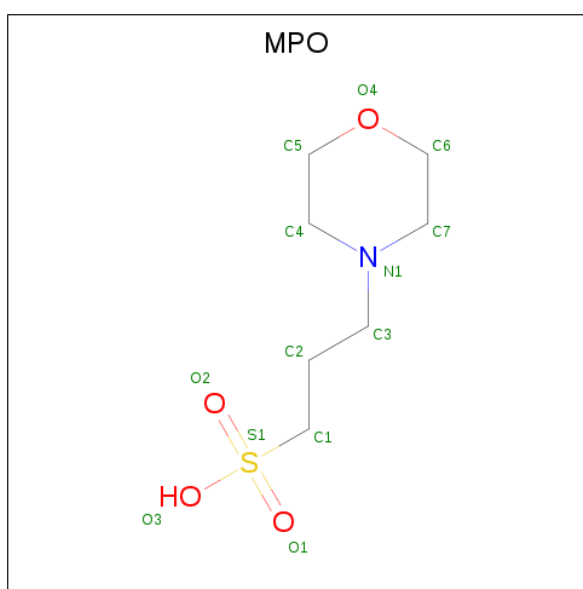
- Molecule 2 is 3-ISOPROPYLMALIC ACID (three-letter code: IPM) (formula: C<sub>7</sub>H<sub>12</sub>O<sub>5</sub>).



- # NAD
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- The image displays the chemical structure of Nicotinamide Adenine Dinucleotide (NAD), a crucial coenzyme. It is composed of two nucleotides linked by a pyrophosphate bridge. The first nucleotide consists of a nicotinamide ring (a pyridine ring with an amide group) attached to a ribose sugar. The second nucleotide consists of an adenine ring (a fused pyrimidine-imidazole system) attached to another ribose sugar. The two ribose sugars are connected via their 5' and 3' phosphate groups, forming a pyrophosphate linkage. The structure is shown in a detailed, ball-and-stick representation with various atoms labeled with their chemical symbols (C, H, N, O, P) and bond types (single, double, triple). The nicotinamide ring is shown in a tautomeric form with a positive charge on the nitrogen atom. The adenine ring is shown in a tautomeric form with a positive charge on the nitrogen atom. The ribose sugars are shown in a chair conformation. The pyrophosphate bridge is shown in a detailed representation with oxygen atoms and phosphorus atoms. The overall structure is a complex, multi-ring system with a high degree of symmetry.

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

- Molecule 4 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	A	1	Total	Mn	0	0
			1	1		

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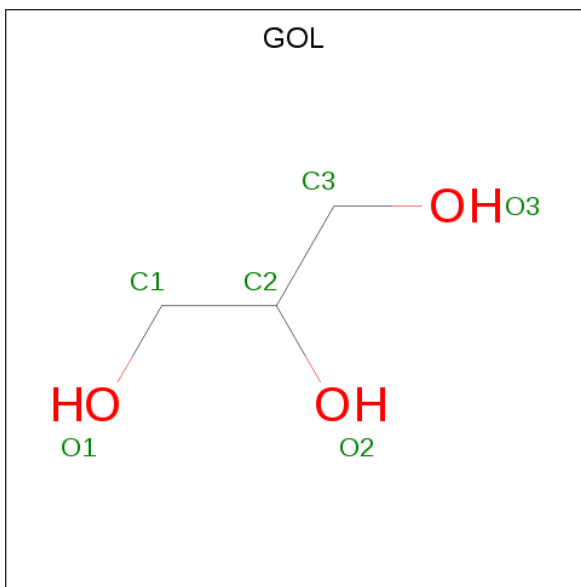
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	K	0	0
			2	2		
6	A	2	Total	K	0	0
			2	2		
6	D	1	Total	K	0	0
			1	1		
6	C	2	Total	K	0	0
			2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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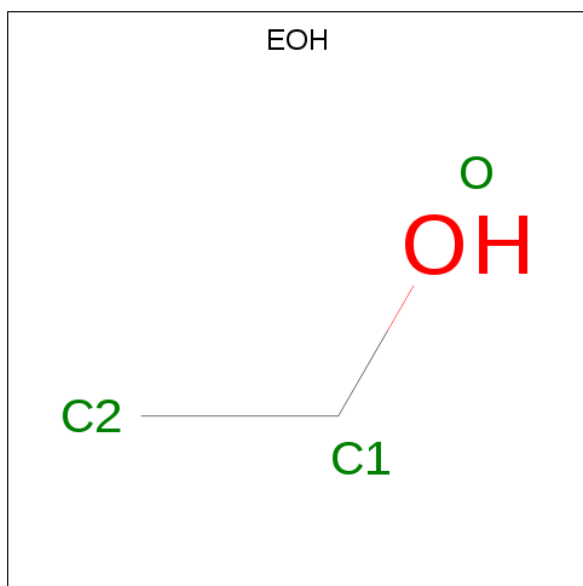
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	C	1	Total 5	C 2	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		

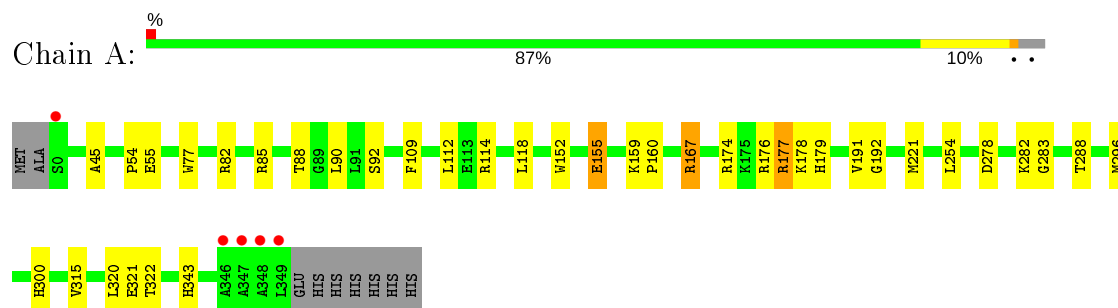
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	112	Total 112	O 112	0	0
9	B	118	Total 118	O 118	0	0
9	C	120	Total 120	O 120	0	0
9	D	90	Total 90	O 90	0	0

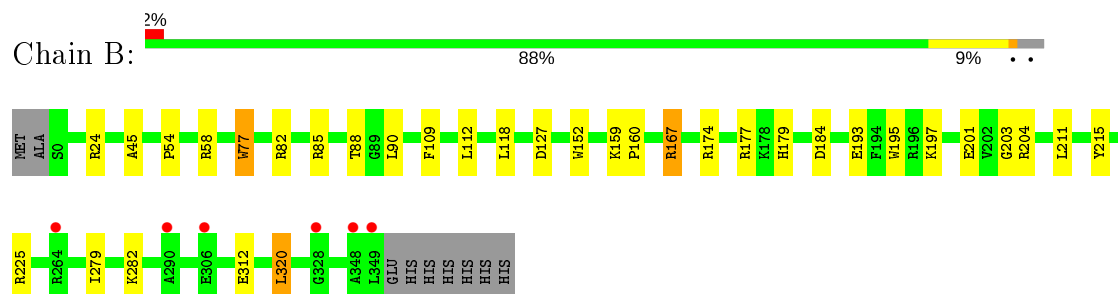
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

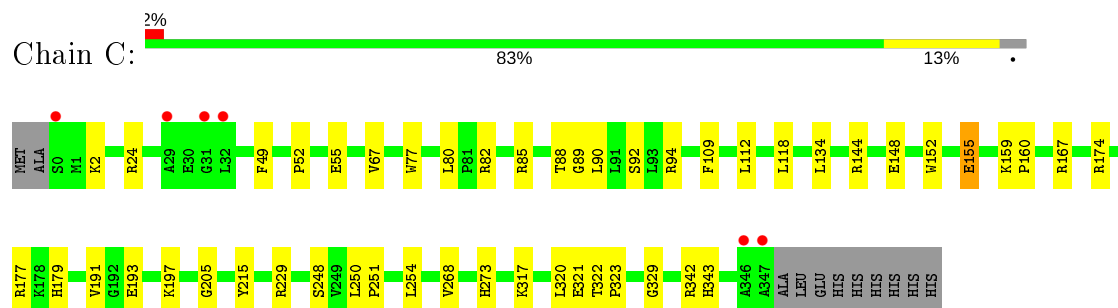
- Molecule 1: 3-isopropylmalate dehydrogenase



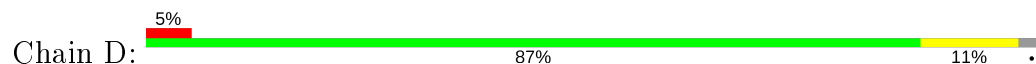
- Molecule 1: 3-isopropylmalate dehydrogenase



- Molecule 1: 3-isopropylmalate dehydrogenase



- Molecule 1: 3-isopropylmalate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.38Å 50.72Å 178.24Å 90.00° 93.09° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 28.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.00) 99.5 (28.06-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.152 , 0.196 0.154 , 0.197	Depositor DCC
$R_{free}$ test set	898 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11489	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: GOL, MN, NAD, MPO, K, EOH, IPM

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	1.03	4/2737 (0.1%)	0.97	8/3714 (0.2%)
1	B	1.02	3/2727 (0.1%)	0.90	7/3700 (0.2%)
1	C	1.03	6/2714 (0.2%)	0.95	6/3683 (0.2%)
1	D	0.95	2/2693 (0.1%)	0.86	3/3656 (0.1%)
All	All	1.01	15/10871 (0.1%)	0.92	24/14753 (0.2%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77	TRP	CD2-CE2	7.11	1.49	1.41
1	C	155	GLU	CD-OE1	-7.01	1.18	1.25
1	C	92	SER	CB-OG	-6.89	1.33	1.42
1	C	152	TRP	CD2-CE2	6.18	1.48	1.41
1	A	77	TRP	CD2-CE2	5.72	1.48	1.41

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	167	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	A	167	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	167	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	A	278[A]	ASP	CB-CG-OD1	7.25	124.82	118.30
1	A	278[B]	ASP	CB-CG-OD1	7.25	124.82	118.30

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	2661	0	2725	39	0
1	B	2656	0	2714	30	0
1	C	2643	0	2694	46	1
1	D	2629	0	2681	30	0
2	A	12	0	9	2	0
2	B	12	0	10	2	0
2	C	12	0	9	2	0
2	D	12	0	9	2	0
3	A	44	0	26	2	0
3	B	44	0	26	1	0
3	C	44	0	26	1	0
3	D	44	0	26	2	0
4	A	13	0	15	6	0
4	C	13	0	15	0	0
4	D	13	0	15	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
7	A	54	0	72	10	0
7	B	42	0	56	12	0
7	C	36	0	43	2	1
7	D	36	0	48	9	0
8	A	3	0	6	1	0
8	B	3	0	6	0	0
8	C	6	0	12	13	0
8	D	6	0	12	5	0
9	A	112	0	0	5	0
9	B	118	0	0	9	0
9	C	120	0	0	12	0
9	D	90	0	0	3	0
All	All	11489	0	11255	156	1



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 7.

The worst 5 of 156 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:C:85:ARG:NH1	9:C:2118:HOH:O	1.62	1.31
1:B:85:ARG:NH1	9:B:2108:HOH:O	1.78	1.11
1:A:296:MET:HG2	7:A:1009:GOL:H12	1.33	1.10
1:C:254:LEU:H	8:D:1009:EOH:H21	1.08	1.09
1:C:85:ARG:HH12	8:C:1010:EOH:H11	1.22	1.01

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:GLY:O	7:C:1008:GOL:O3[1_565]	2.19	0.01

## 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	355/359 (99%)	347 (98%)	8 (2%)	0	100	100
1	B	353/359 (98%)	345 (98%)	8 (2%)	0	100	100
1	C	351/359 (98%)	342 (97%)	9 (3%)	0	100	100
1	D	350/359 (98%)	339 (97%)	11 (3%)	0	100	100
All	All	1409/1436 (98%)	1373 (97%)	36 (3%)	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	275/276 (100%)	274 (100%)	1 (0%)	91	93
1	B	273/276 (99%)	271 (99%)	2 (1%)	84	88
1	C	272/276 (99%)	270 (99%)	2 (1%)	84	88
1	D	270/276 (98%)	267 (99%)	3 (1%)	73	78
All	All	1090/1104 (99%)	1082 (99%)	8 (1%)	84	88

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	LYS
1	D	245	ASP
1	D	2	LYS
1	B	320	LEU
1	C	55	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	HIS
1	B	343	HIS
1	C	343	HIS
1	D	343	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 11 are monoatomic and 1 is modelled with single atom - leaving 45 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	$\# Z  > 2$
8	EOH	A	1012	-	2,2,2	0.75	0	1,1,1	0.51	0
7	GOL	C	1006	-	5,5,5	0.90	0	5,5,5	1.00	0
7	GOL	D	1006	-	5,5,5	0.70	0	5,5,5	1.23	0
7	GOL	B	1006	-	5,5,5	0.51	0	5,5,5	0.35	0
7	GOL	D	1005	-	5,5,5	0.79	0	5,5,5	1.44	1 (20%)
7	GOL	C	1003	-	5,5,5	0.46	0	5,5,5	0.98	0
4	MPO	A	950	-	13,13,13	2.02	1 (7%)	17,17,17	2.74	7 (41%)
7	GOL	C	1004	-	5,5,5	0.69	0	5,5,5	0.38	0
8	EOH	B	1009	-	2,2,2	0.51	0	1,1,1	0.33	0
7	GOL	B	1004	-	5,5,5	0.84	0	5,5,5	0.60	0
7	GOL	D	1007	-	5,5,5	0.65	0	5,5,5	0.94	0
4	MPO	D	950	-	13,13,13	1.85	1 (7%)	17,17,17	2.51	4 (23%)
3	NAD	D	900	-	42,48,48	1.49	3 (7%)	50,73,73	1.67	9 (18%)
7	GOL	A	1011	-	5,5,5	0.17	0	5,5,5	0.92	0
7	GOL	A	1010	-	5,5,5	0.50	0	5,5,5	0.56	0
2	IPM	B	800	5	5,11,11	3.22	1 (20%)	5,15,15	3.20	2 (40%)
7	GOL	C	1008	-	3,3,5	0.79	0	2,2,5	1.09	0
7	GOL	A	1003	-	5,5,5	0.69	0	5,5,5	0.60	0
7	GOL	B	1005	-	5,5,5	0.30	0	5,5,5	1.72	1 (20%)
7	GOL	B	1003	-	5,5,5	0.88	0	5,5,5	1.49	1 (20%)
7	GOL	A	1007	-	5,5,5	0.23	0	5,5,5	0.55	0
8	EOH	D	1010	-	2,2,2	0.59	0	1,1,1	0.22	0
3	NAD	B	900	-	42,48,48	1.58	5 (11%)	50,73,73	1.48	5 (10%)
7	GOL	B	1007	-	5,5,5	0.58	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	A	1005	-	5,5,5	0.33	0	5,5,5	0.51	0
8	EOH	C	1009	-	2,2,2	0.44	0	1,1,1	0.10	0
3	NAD	A	900	-	42,48,48	1.40	7 (16%)	50,73,73	1.84	8 (16%)
7	GOL	B	1008	-	5,5,5	0.39	0	5,5,5	0.46	0
7	GOL	A	1009	-	5,5,5	0.65	0	5,5,5	0.77	0
7	GOL	A	1004	-	5,5,5	0.62	0	5,5,5	0.68	0
3	NAD	C	900	-	42,48,48	1.61	8 (19%)	50,73,73	1.64	9 (18%)
7	GOL	C	1007	-	5,5,5	0.28	0	5,5,5	0.54	0
7	GOL	B	1010	-	5,5,5	0.74	0	5,5,5	1.29	1 (20%)
2	IPM	A	800	5	5,11,11	3.71	2 (40%)	5,15,15	3.99	2 (40%)
7	GOL	D	1003	-	5,5,5	0.61	0	5,5,5	1.75	1 (20%)
7	GOL	D	1008	-	5,5,5	0.55	0	5,5,5	0.45	0
7	GOL	C	1005	-	5,5,5	0.88	0	5,5,5	0.87	0
7	GOL	A	1006	-	5,5,5	0.30	0	5,5,5	1.18	0
7	GOL	A	1008	-	5,5,5	0.45	0	5,5,5	0.47	0
4	MPO	C	950	-	13,13,13	1.89	1 (7%)	17,17,17	2.45	6 (35%)
2	IPM	D	800	5	5,11,11	3.14	2 (40%)	5,15,15	3.19	2 (40%)
8	EOH	C	1010	-	2,2,2	0.46	0	1,1,1	0.07	0
7	GOL	D	1004	-	5,5,5	0.60	0	5,5,5	0.72	0
8	EOH	D	1009	-	2,2,2	0.69	0	1,1,1	0.67	0
2	IPM	C	800	5	5,11,11	2.56	2 (40%)	5,15,15	4.12	2 (40%)

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
7	GOL	C	1006	-	-	2/4/4/4	-
7	GOL	D	1006	-	-	4/4/4/4	-
7	GOL	B	1006	-	-	2/4/4/4	-
7	GOL	D	1005	-	-	1/4/4/4	-
7	GOL	C	1003	-	-	0/4/4/4	-
4	MPO	A	950	-	-	3/7/15/15	0/1/1/1
7	GOL	C	1004	-	-	0/4/4/4	-
7	GOL	B	1003	-	-	4/4/4/4	-
7	GOL	B	1004	-	-	0/4/4/4	-
7	GOL	D	1007	-	-	1/4/4/4	-
4	MPO	D	950	-	-	4/7/15/15	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	D	900	-	-	4/26/62/62	0/5/5/5
7	GOL	A	1011	-	-	4/4/4/4	-
7	GOL	A	1010	-	-	2/4/4/4	-
2	IPM	B	800	5	-	5/8/16/16	-
7	GOL	C	1008	-	-	1/1/1/4	-
7	GOL	A	1003	-	-	0/4/4/4	-
7	GOL	B	1005	-	-	2/4/4/4	-
7	GOL	C	1007	-	-	2/4/4/4	-
7	GOL	A	1007	-	-	2/4/4/4	-
3	NAD	B	900	-	-	5/26/62/62	0/5/5/5
7	GOL	B	1007	-	-	0/4/4/4	-
7	GOL	A	1005	-	-	2/4/4/4	-
3	NAD	A	900	-	-	5/26/62/62	0/5/5/5
7	GOL	B	1008	-	-	3/4/4/4	-
7	GOL	A	1009	-	-	2/4/4/4	-
7	GOL	A	1004	-	-	0/4/4/4	-
3	NAD	C	900	-	-	4/26/62/62	0/5/5/5
7	GOL	B	1010	-	-	4/4/4/4	-
2	IPM	A	800	5	-	4/8/16/16	-
7	GOL	D	1003	-	-	4/4/4/4	-
7	GOL	D	1008	-	-	0/4/4/4	-
7	GOL	C	1005	-	-	2/4/4/4	-
7	GOL	A	1006	-	-	2/4/4/4	-
7	GOL	A	1008	-	-	0/4/4/4	-
4	MPO	C	950	-	-	3/7/15/15	0/1/1/1
2	IPM	D	800	5	-	5/8/16/16	-
7	GOL	D	1004	-	-	2/4/4/4	-
2	IPM	C	800	5	-	5/8/16/16	-

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	IPM	O1-C2	7.43	1.57	1.42
2	B	800	IPM	O1-C2	6.90	1.56	1.42
4	A	950	MPO	C1-S1	-6.71	1.68	1.77
4	C	950	MPO	C1-S1	-6.21	1.68	1.77
4	D	950	MPO	C1-S1	-5.76	1.69	1.77

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	IPM	O1-C2-C3	7.44	127.66	109.09
2	C	800	IPM	O1-C2-C3	7.07	126.72	109.09
4	D	950	MPO	C7-N1-C4	6.30	123.00	108.83
3	A	900	NAD	N3A-C2A-N1A	-6.25	118.91	128.68
3	D	900	NAD	N3A-C2A-N1A	-5.90	119.45	128.68

There are no chirality outliers.

5 of 95 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1009	GOL	C1-C2-C3-O3
7	B	1006	GOL	C1-C2-C3-O3
3	D	900	NAD	O4D-C1D-N1N-C2N
3	D	900	NAD	O4D-C1D-N1N-C6N
3	D	900	NAD	C2D-C1D-N1N-C2N

There are no ring outliers.

31 monomers are involved in 69 short contacts:

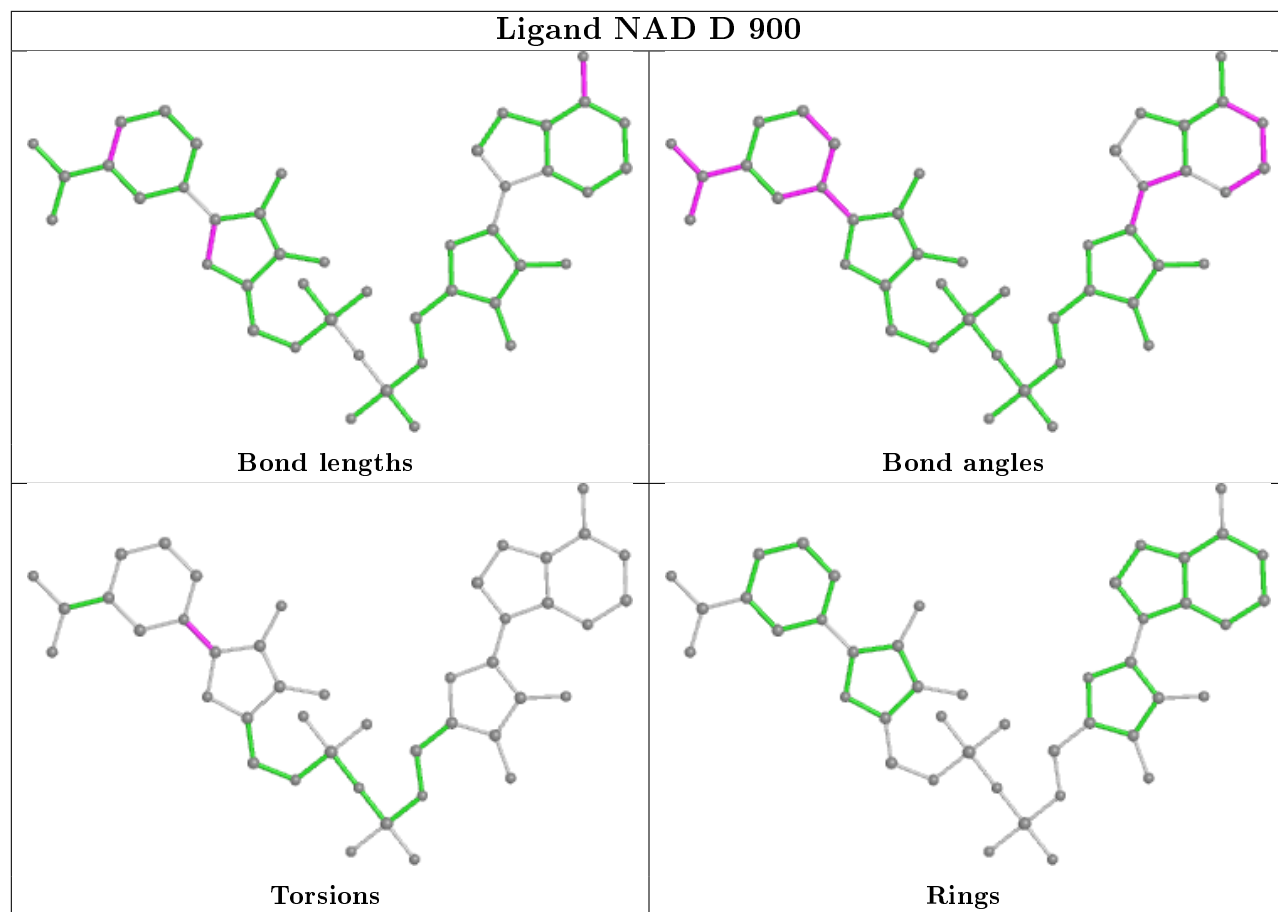
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1012	EOH	1	0
7	D	1006	GOL	1	0
7	B	1006	GOL	1	0
4	A	950	MPO	6	0
7	B	1004	GOL	1	0
7	D	1007	GOL	1	0
4	D	950	MPO	1	0
3	D	900	NAD	2	0
2	B	800	IPM	2	0
7	C	1008	GOL	0	1
7	B	1005	GOL	2	0
7	B	1003	GOL	2	0
7	A	1007	GOL	2	0
8	D	1010	EOH	1	0
3	B	900	NAD	1	0
7	A	1005	GOL	3	0
8	C	1009	EOH	2	0
3	A	900	NAD	2	0
7	A	1009	GOL	4	0
7	A	1004	GOL	1	0
3	C	900	NAD	1	0

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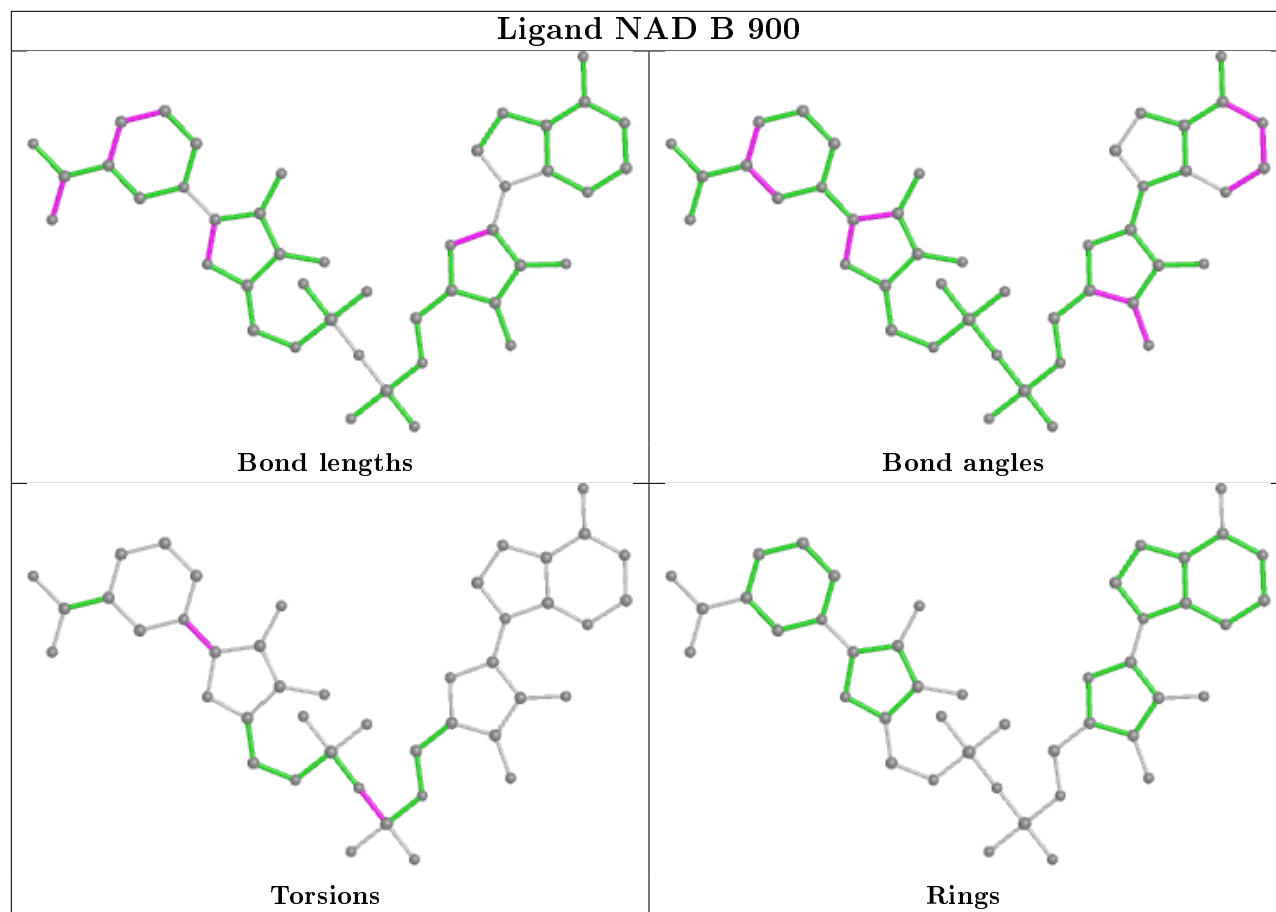
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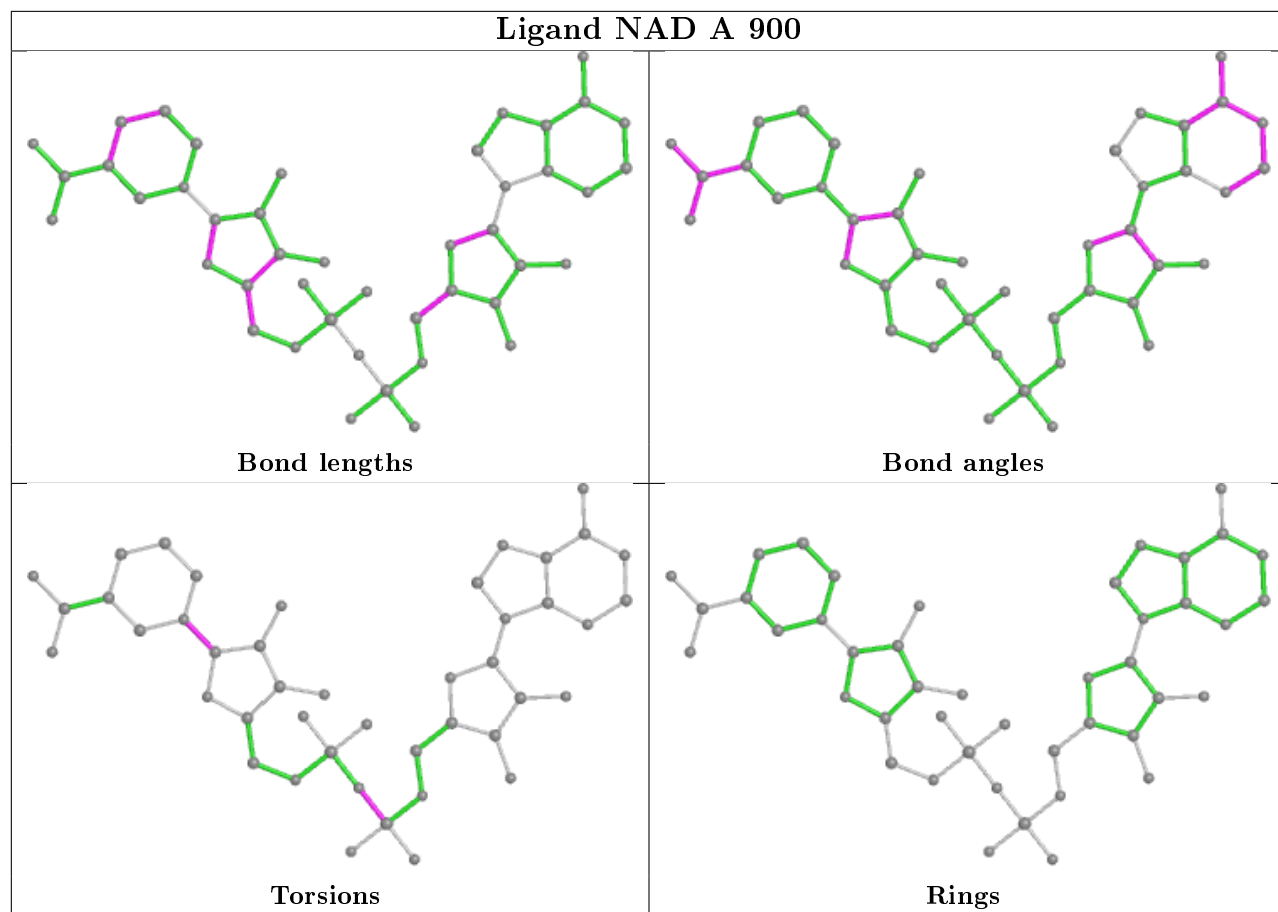
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1007	GOL	2	0
7	B	1010	GOL	6	0
2	A	800	IPM	2	0
7	D	1003	GOL	5	0
7	D	1008	GOL	2	0
2	D	800	IPM	2	0
8	C	1010	EOH	11	0
7	D	1004	GOL	1	0
8	D	1009	EOH	4	0
2	C	800	IPM	2	0

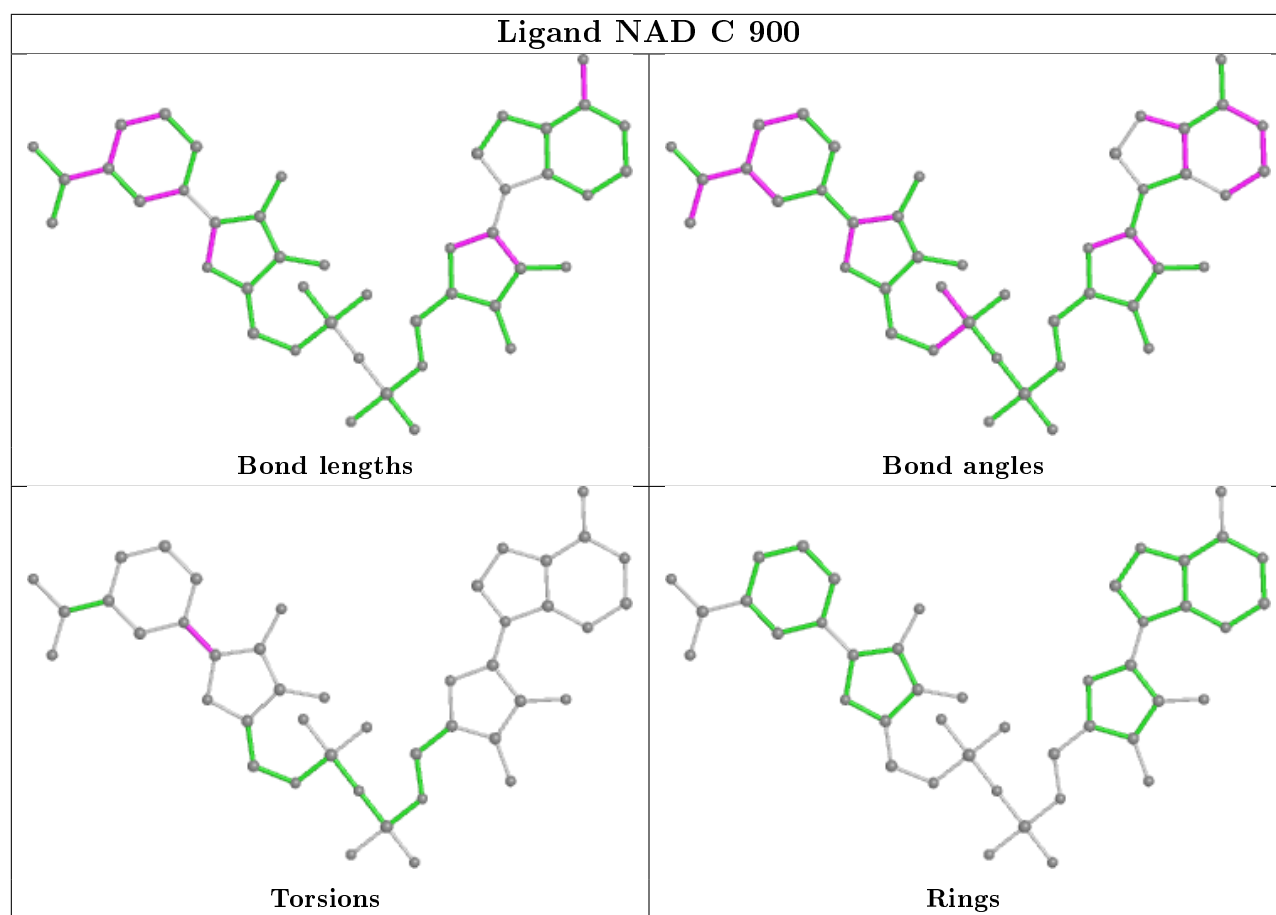
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	350/359 (97%)	-0.27	5 (1%) 75 74	17, 28, 49, 90	2 (0%)
1	B	350/359 (97%)	-0.30	6 (1%) 70 68	19, 29, 49, 64	2 (0%)
1	C	348/359 (96%)	-0.38	6 (1%) 70 68	17, 28, 49, 72	1 (0%)
1	D	349/359 (97%)	-0.14	18 (5%) 27 26	17, 33, 59, 92	3 (0%)
All	All	1397/1436 (97%)	-0.27	35 (2%) 57 56	17, 29, 54, 92	8 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	LEU	12.8
1	A	348	ALA	6.7
1	D	347	ALA	6.5
1	A	347	ALA	4.4
1	D	29	ALA	4.3

### 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( $\text{\AA}^2$ )	Q<0.9
4	MPO	C	950	13/13	0.64	0.32	36,51,80,81	13
4	MPO	A	950	13/13	0.71	0.28	36,49,80,86	13
4	MPO	D	950	13/13	0.72	0.26	38,49,68,69	13
7	GOL	A	1009	6/6	0.74	0.29	40,52,63,66	0
7	GOL	C	1018	1/6	0.79	0.12	44,44,44,44	0
7	GOL	A	1010	6/6	0.80	0.16	52,60,67,67	0
7	GOL	B	1010	6/6	0.81	0.38	40,50,59,62	0
7	GOL	A	1006	6/6	0.85	0.13	43,55,57,58	0
8	EOH	C	1009	3/3	0.85	0.15	43,43,54,60	0
8	EOH	C	1010	3/3	0.86	0.15	46,46,52,59	0
7	GOL	C	1005	6/6	0.87	0.16	47,53,58,60	0
7	GOL	D	1007	6/6	0.88	0.21	51,54,60,61	0
7	GOL	C	1008	5/6	0.88	0.18	36,45,49,49	0
7	GOL	B	1003	6/6	0.89	0.19	35,42,50,53	0
7	GOL	C	1003	6/6	0.92	0.14	33,36,45,52	0
8	EOH	A	1012	3/3	0.92	0.14	30,30,36,38	0
7	GOL	C	1006	6/6	0.92	0.16	29,36,44,47	0
7	GOL	B	1007	6/6	0.92	0.11	33,41,46,48	0
7	GOL	D	1006	6/6	0.92	0.16	36,46,52,61	0
8	EOH	D	1009	3/3	0.93	0.16	19,19,32,45	0
7	GOL	B	1006	6/6	0.94	0.12	29,41,50,79	0
8	EOH	B	1009	3/3	0.94	0.20	38,38,40,48	0
2	IPM	A	800	12/12	0.94	0.15	22,28,34,36	0
7	GOL	D	1003	6/6	0.94	0.15	34,38,41,45	0
8	EOH	D	1010	3/3	0.95	0.14	26,26,34,40	0
7	GOL	A	1008	6/6	0.95	0.16	29,37,39,51	0
7	GOL	A	1011	6/6	0.95	0.19	45,59,62,72	0
7	GOL	D	1008	6/6	0.95	0.13	40,45,50,56	0
7	GOL	D	1004	6/6	0.95	0.10	30,33,34,34	0
7	GOL	B	1008	6/6	0.95	0.11	45,50,51,60	0
2	IPM	D	800	12/12	0.96	0.14	23,29,34,36	0
7	GOL	B	1005	6/6	0.96	0.11	35,38,40,43	0
7	GOL	D	1005	6/6	0.96	0.15	32,35,36,37	0
2	IPM	B	800	12/12	0.96	0.13	25,29,36,39	0
2	IPM	C	800	12/12	0.96	0.13	24,30,35,40	0
7	GOL	A	1005	6/6	0.97	0.17	29,41,53,68	0
7	GOL	A	1003	6/6	0.97	0.09	25,26,31,34	0
7	GOL	A	1007	6/6	0.97	0.08	31,36,39,46	0
7	GOL	A	1004	6/6	0.97	0.12	26,29,39,46	0
6	K	C	1002	1/1	0.98	0.11	49,49,49,49	0
7	GOL	B	1004	6/6	0.98	0.10	24,26,29,31	0
7	GOL	C	1007	6/6	0.98	0.10	24,37,42,54	0
3	NAD	B	900	44/44	0.98	0.07	20,24,29,33	0

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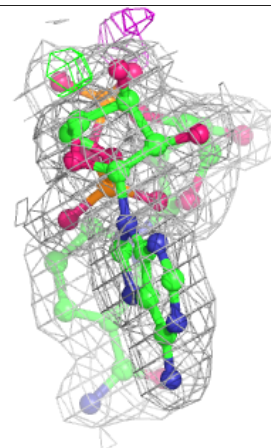
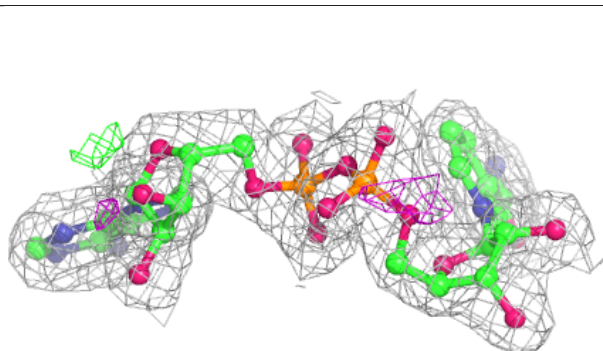
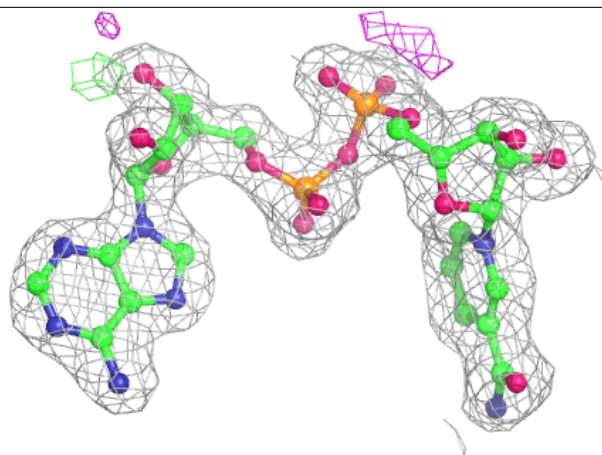
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAD	D	900	44/44	0.98	0.07	19,23,26,32	0
6	K	A	1001	1/1	0.99	0.05	29,29,29,29	0
3	NAD	A	900	44/44	0.99	0.07	16,21,23,25	0
6	K	A	1002	1/1	0.99	0.12	39,39,39,39	0
6	K	B	1002	1/1	0.99	0.10	43,43,43,43	0
6	K	D	1001	1/1	0.99	0.07	25,25,25,25	1
7	GOL	C	1004	6/6	0.99	0.06	25,27,30,33	0
5	MN	B	999	1/1	0.99	0.08	22,22,22,22	0
3	NAD	C	900	44/44	0.99	0.07	19,23,26,31	0
6	K	C	1001	1/1	1.00	0.10	25,25,25,25	0
5	MN	A	999	1/1	1.00	0.10	20,20,20,20	0
6	K	B	1001	1/1	1.00	0.12	22,22,22,22	1
5	MN	C	999	1/1	1.00	0.07	21,21,21,21	0
5	MN	D	999	1/1	1.00	0.09	22,22,22,22	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.

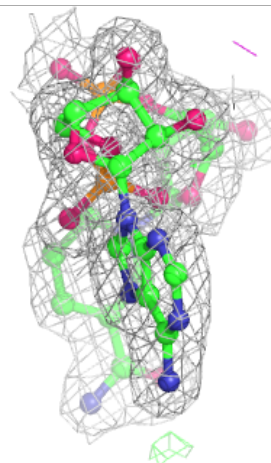
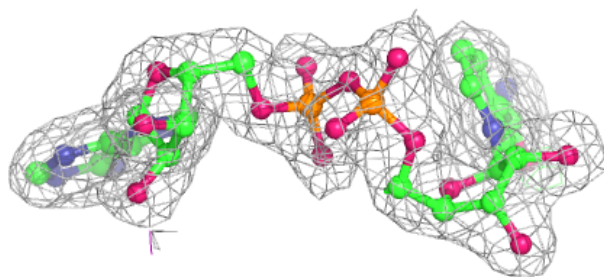
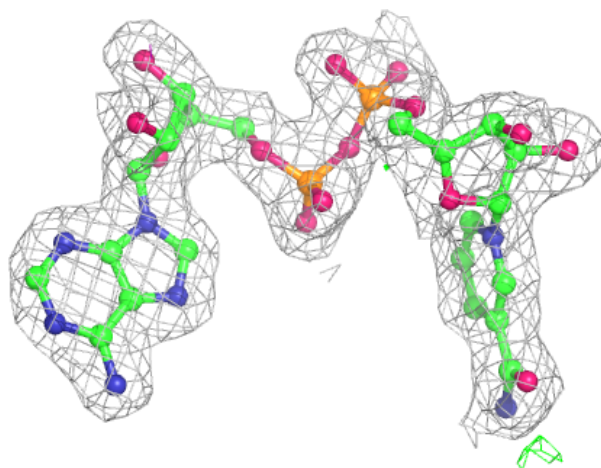
#### Electron density around NAD B 900:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



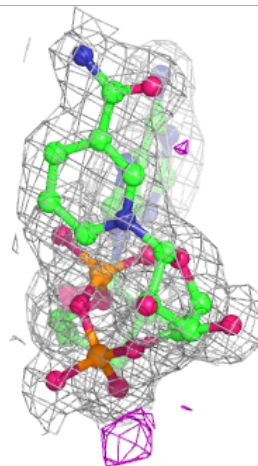
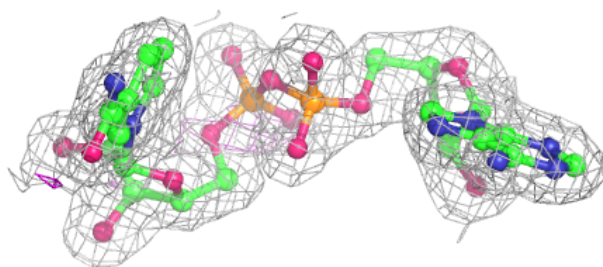
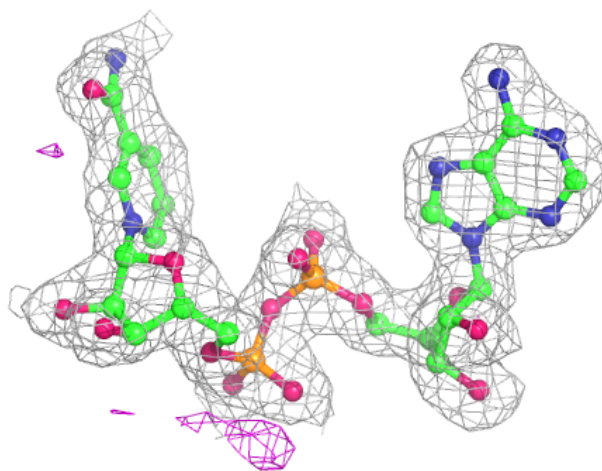
**Electron density around NAD D 900:**

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

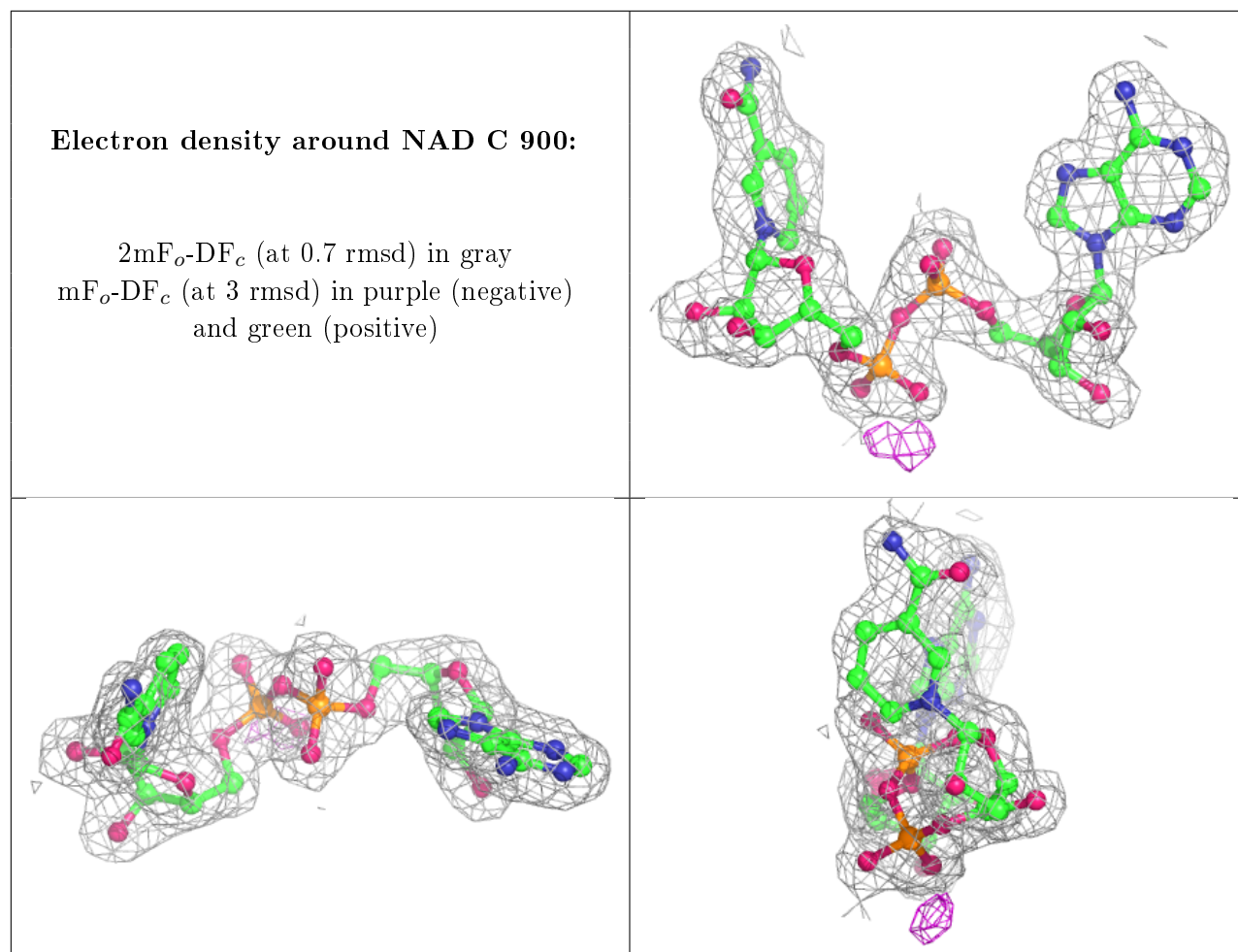


**Electron density around NAD A 900:**

$2mF_o-DF_c$  (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.