



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 12:42 am BST

PDB ID : 4ZZ7
Title : Crystal structure of methylmalonate-semialdehyde dehydrogenase (DddC) from *Oceanimonas doudoroffii*
Authors : Do, H.; Lee, C.W.; Lee, S.G.; Kang, H.; Park, C.M.; Kim, H.J.; Park, H.; Park, H.; Lee, J.H.
Deposited on : 2015-05-22
Resolution : 2.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
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) : 2.11

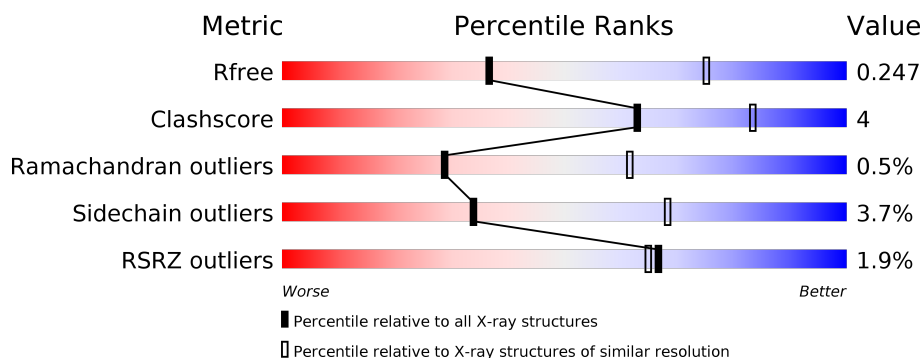
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 ≥ 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	501	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 0% 86% 10% .. </div> </div>
1	B	501	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 2% 85% 11% .. </div> </div>
1	C	501	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 2% 84% 12% .. </div> </div>
1	D	501	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 86% 10% .. </div> </div>
1	E	501	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 2% 86% 10% .. </div> </div>
1	F	501	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 5% 83% 14% . </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	501	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>87%</div><div>9%</div><div>• •</div></div></div>
1	H	501	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>86%</div><div>10%</div><div>•</div></div></div>
1	I	501	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>85%</div><div>11%</div><div>• •</div></div></div>
1	J	501	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>85%</div><div>11%</div><div>• •</div></div></div>
1	K	501	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>86%</div><div>10%</div><div>• •</div></div></div>
1	L	501	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>85%</div><div>12%</div><div>• •</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 45549 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 Methylmalonate-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3722	2338	656	704	24			
1	B	488	Total	C	N	O	S	0	0	0
			3718	2336	655	703	24			
1	C	487	Total	C	N	O	S	0	0	0
			3709	2331	654	700	24			
1	D	488	Total	C	N	O	S	0	0	0
			3718	2336	655	703	24			
1	E	488	Total	C	N	O	S	0	0	0
			3718	2336	655	703	24			
1	F	488	Total	C	N	O	S	0	0	0
			3718	2336	655	703	24			
1	G	487	Total	C	N	O	S	0	0	0
			3709	2331	654	700	24			
1	H	486	Total	C	N	O	S	0	0	0
			3698	2325	650	699	24			
1	I	488	Total	C	N	O	S	0	0	0
			3718	2336	655	703	24			
1	J	487	Total	C	N	O	S	0	1	0
			3721	2337	658	703	23			
1	K	487	Total	C	N	O	S	0	0	0
			3709	2331	654	700	24			
1	L	488	Total	C	N	O	S	0	0	0
			3718	2336	655	703	24			

There are 36 discrepancies between the modelled and reference sequences:

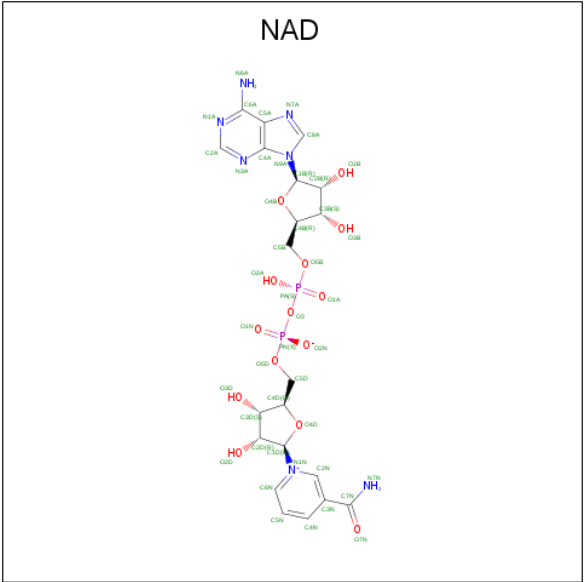
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP G5CZI2
A	-1	SER	-	expression tag	UNP G5CZI2
A	0	HIS	-	expression tag	UNP G5CZI2
B	-2	GLY	-	expression tag	UNP G5CZI2
B	-1	SER	-	expression tag	UNP G5CZI2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP G5CZI2
C	-2	GLY	-	expression tag	UNP G5CZI2
C	-1	SER	-	expression tag	UNP G5CZI2
C	0	HIS	-	expression tag	UNP G5CZI2
D	-2	GLY	-	expression tag	UNP G5CZI2
D	-1	SER	-	expression tag	UNP G5CZI2
D	0	HIS	-	expression tag	UNP G5CZI2
E	-2	GLY	-	expression tag	UNP G5CZI2
E	-1	SER	-	expression tag	UNP G5CZI2
E	0	HIS	-	expression tag	UNP G5CZI2
F	-2	GLY	-	expression tag	UNP G5CZI2
F	-1	SER	-	expression tag	UNP G5CZI2
F	0	HIS	-	expression tag	UNP G5CZI2
G	-2	GLY	-	expression tag	UNP G5CZI2
G	-1	SER	-	expression tag	UNP G5CZI2
G	0	HIS	-	expression tag	UNP G5CZI2
H	-2	GLY	-	expression tag	UNP G5CZI2
H	-1	SER	-	expression tag	UNP G5CZI2
H	0	HIS	-	expression tag	UNP G5CZI2
I	-2	GLY	-	expression tag	UNP G5CZI2
I	-1	SER	-	expression tag	UNP G5CZI2
I	0	HIS	-	expression tag	UNP G5CZI2
J	-2	GLY	-	expression tag	UNP G5CZI2
J	-1	SER	-	expression tag	UNP G5CZI2
J	0	HIS	-	expression tag	UNP G5CZI2
K	-2	GLY	-	expression tag	UNP G5CZI2
K	-1	SER	-	expression tag	UNP G5CZI2
K	0	HIS	-	expression tag	UNP G5CZI2
L	-2	GLY	-	expression tag	UNP G5CZI2
L	-1	SER	-	expression tag	UNP G5CZI2
L	0	HIS	-	expression tag	UNP G5CZI2

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	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		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total	O	0	0
			76	76		
3	B	91	Total	O	0	0
			91	91		
3	C	98	Total	O	0	0
			98	98		
3	D	104	Total	O	0	0
			104	104		
3	E	45	Total	O	0	0
			45	45		
3	F	21	Total	O	0	0
			21	21		

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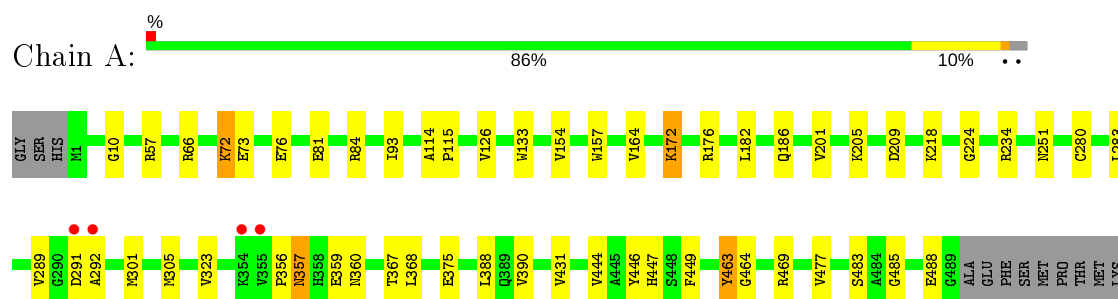
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	37	Total 37	O 37	0	0
3	H	44	Total 44	O 44	0	0
3	I	60	Total 60	O 60	0	0
3	J	31	Total 31	O 31	0	0
3	K	54	Total 54	O 54	0	0
3	L	48	Total 48	O 48	0	0

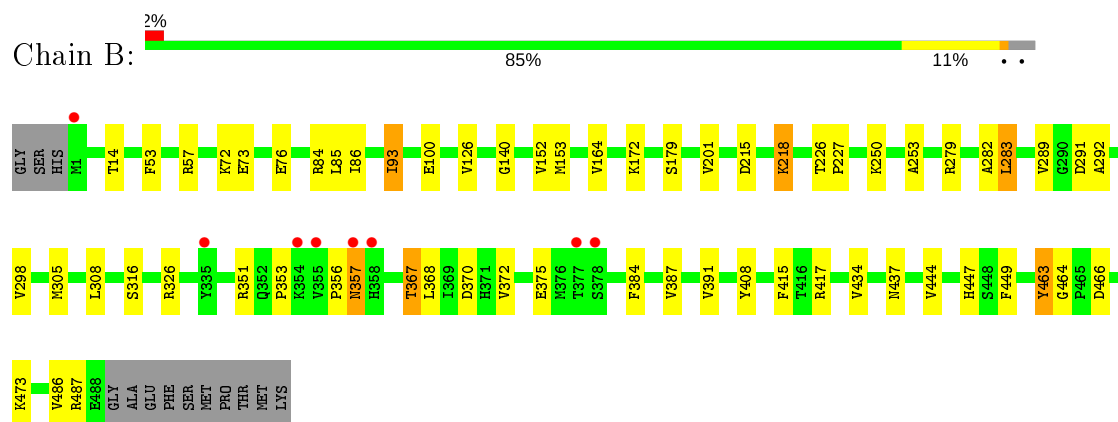
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

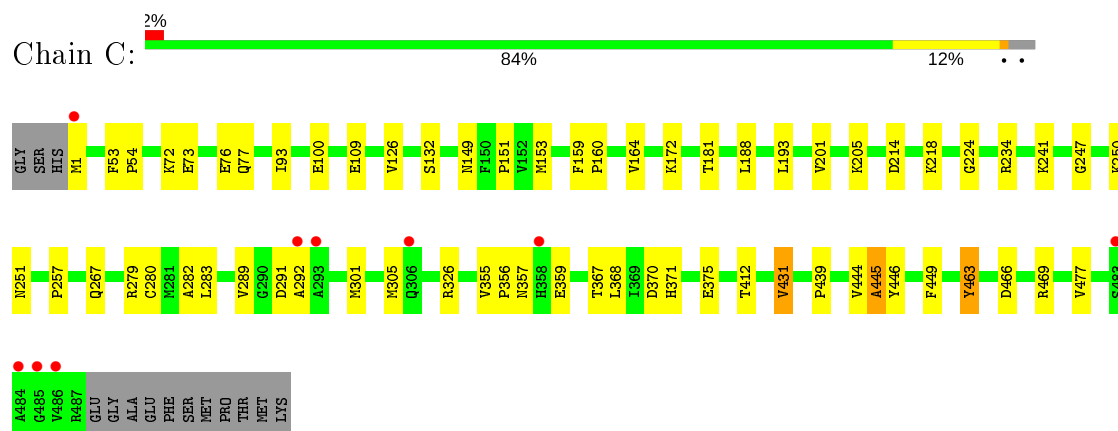
- Molecule 1: Methylmalonate-semialdehyde dehydrogenase



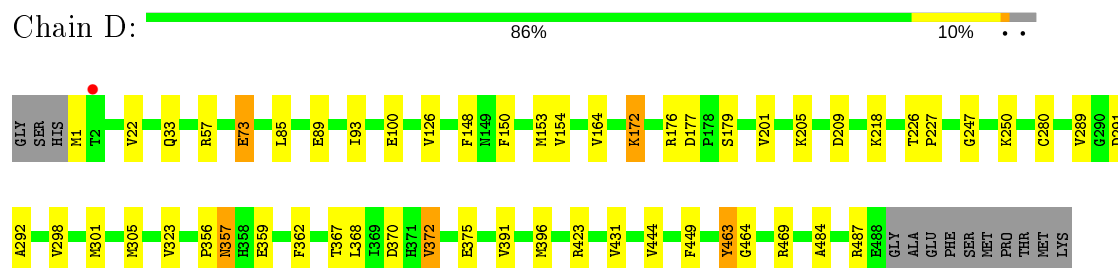
- Molecule 1: Methylmalonate-semialdehyde dehydrogenase



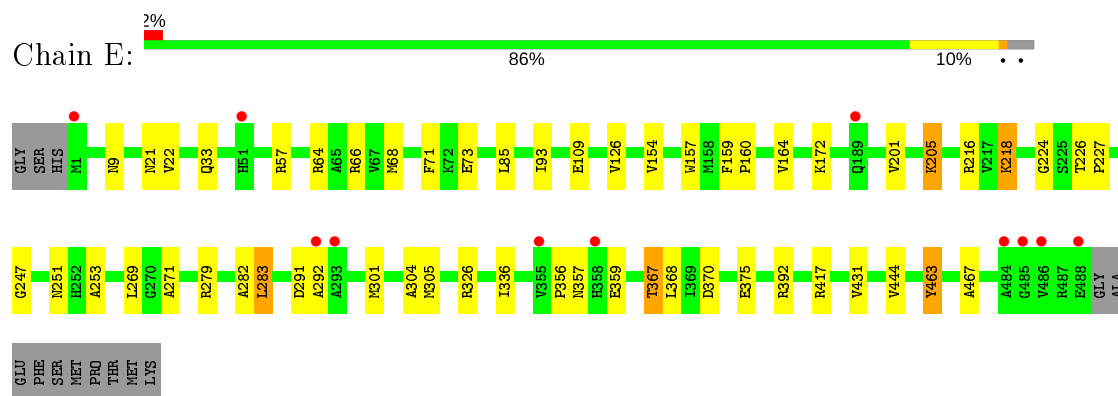
- Molecule 1: Methylmalonate-semialdehyde dehydrogenase



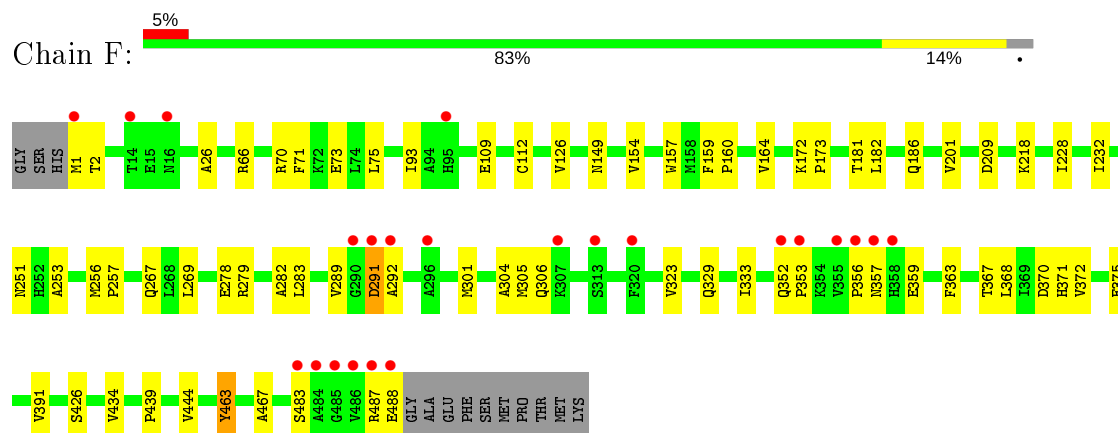
- Molecule 1: Methylmalonate-semialdehyde dehydrogenase



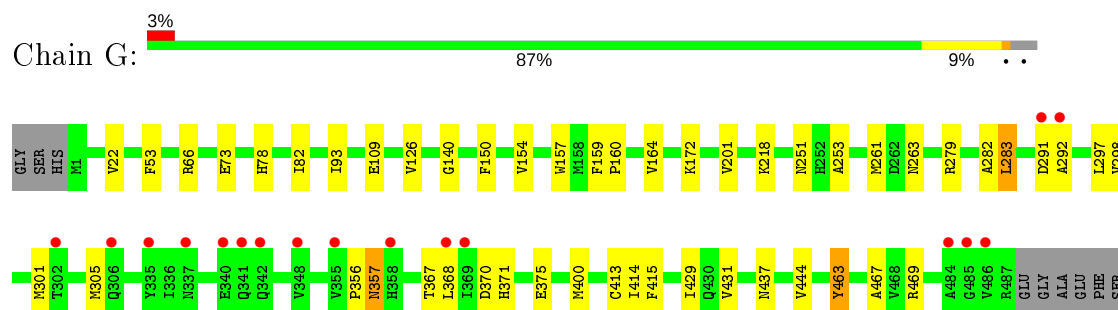
- Molecule 1: Methylmalonate-semialdehyde dehydrogenase



- Molecule 1: Methylmalonate-semialdehyde dehydrogenase




- Molecule 1: Methylmalonate-semialdehyde dehydrogenase



MET
PRO
THR
MET
LYS


• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain H:  86% 10%

GLY SER HIS M1 R13 K72 E76 R84 I93 E100 E109 A114 P115 V126 P151 V152 M153 F159 P160 V164 K172 T181 Q189 V201 K218 K250 N251 H252 A253 R279 C280 H281 L283 V289 G290 D291 A292 V298

MET
LYS


• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain I:  85% 11%

GLY SER HIS M1 T2 R13 A26 F53 R57 L85 I93 A114 P115 V126 L368 G140 M149 V154 W157 V164 K172 E175 L188 L193 V201 E206 K218 G224 S225 T226 P227 L246 K250 N251 H252 A253 Q267

E488 GLY ALA GLU PHE SER MET PRO MET LYS

• Molecule 1: Methylmalonate-semialdehyde dehydrogenase


Chain J:  85% 11%

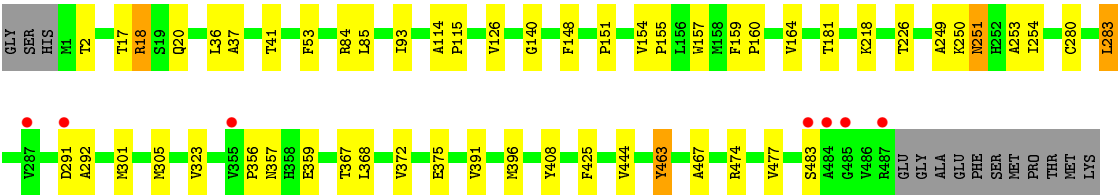
GLY SER HIS MET T2 N9 A26 R64 F71 K72 E73 L74 L75 E81 R84 L85 E89 I93 E100 V126 M153 F159 P160 K172 S179 S180 T181 L182 Q186 L187 L188 L193 V201 D215 K218 K250 N251 H252 A253

P257 Q267 R279 A282 L283 V289 G290 D291 A292 M301 E73 L74 L75 V323 R326 Q352 V355 P356 M357 H358 G361 T367 L368 T369 D370 H371 V372 E375 Y379 V391 S426 V431 V434 P439 V444 A445 Y446 F449 H461 A462

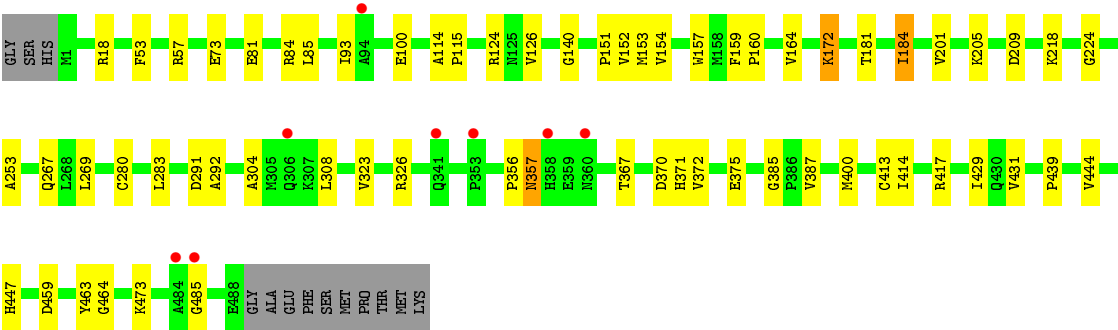
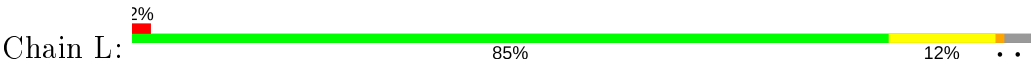
Y463 A467 A484 Q485 Y486 R487 E488 GLY ALA GLU PHE SER MET PRO MET LYS

• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain K:  86% 10%



● Molecule 1: Methylmalonate-semialdehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	156.70Å 160.30Å 238.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.90 49.66 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.01-2.90) 99.3 (49.66-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.185 , 0.246 0.188 , 0.247	Depositor DCC
R_{free} test set	6657 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	45549	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.79% 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	0.56	0/3803	0.75	1/5161 (0.0%)
1	B	0.59	0/3799	0.77	2/5156 (0.0%)
1	C	0.58	0/3790	0.75	2/5144 (0.0%)
1	D	0.58	0/3799	0.76	2/5156 (0.0%)
1	E	0.53	0/3799	0.72	2/5156 (0.0%)
1	F	0.51	0/3799	0.70	0/5156
1	G	0.52	0/3790	0.69	0/5144
1	H	0.54	0/3779	0.72	2/5130 (0.0%)
1	I	0.55	0/3799	0.75	3/5156 (0.1%)
1	J	0.54	0/3802	0.70	3/5160 (0.1%)
1	K	0.53	0/3790	0.71	0/5144
1	L	0.53	0/3799	0.72	1/5156 (0.0%)
All	All	0.55	0/45548	0.73	18/61819 (0.0%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	H	469	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	L	57	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	57	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	J	64	ARG	NE-CZ-NH1	5.82	123.21	120.30

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	3722	0	3652	38	0
1	B	3718	0	3649	32	0
1	C	3709	0	3643	44	0
1	D	3718	0	3649	31	0
1	E	3718	0	3649	30	0
1	F	3718	0	3649	35	0
1	G	3709	0	3643	27	0
1	H	3698	0	3630	28	0
1	I	3718	0	3649	45	0
1	J	3721	0	3649	32	0
1	K	3709	0	3643	34	0
1	L	3718	0	3649	38	0
2	A	44	0	26	10	0
2	C	44	0	26	10	0
2	D	44	0	26	4	0
2	E	44	0	26	2	0
2	I	44	0	26	18	0
2	L	44	0	26	6	0
3	A	76	0	0	4	0
3	B	91	0	0	2	0
3	C	98	0	0	2	0
3	D	104	0	0	1	0
3	E	45	0	0	1	0
3	F	21	0	0	0	0
3	G	37	0	0	3	0
3	H	44	0	0	1	0
3	I	60	0	0	0	0
3	J	31	0	0	1	0
3	K	54	0	0	3	0
3	L	48	0	0	2	0
All	All	45549	0	43910	380	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 4.

The worst 5 of 380 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:I:280:CYS:SG	2:I:501:NAD:C4N	2.35	1.14
1:I:280:CYS:SG	2:I:501:NAD:C5N	2.39	1.10
1:I:224:GLY:O	2:I:501:NAD:O2D	1.75	1.04
1:A:280:CYS:SG	2:A:501:NAD:C4N	2.53	0.96
1:D:356:PRO:HA	1:D:357:ASN:HB2	1.55	0.86

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	487/501 (97%)	463 (95%)	22 (4%)	2 (0%)	34	66
1	B	486/501 (97%)	463 (95%)	21 (4%)	2 (0%)	34	66
1	C	485/501 (97%)	463 (96%)	20 (4%)	2 (0%)	34	66
1	D	486/501 (97%)	463 (95%)	20 (4%)	3 (1%)	25	58
1	E	486/501 (97%)	462 (95%)	23 (5%)	1 (0%)	47	78
1	F	486/501 (97%)	457 (94%)	25 (5%)	4 (1%)	19	51
1	G	485/501 (97%)	465 (96%)	18 (4%)	2 (0%)	34	66
1	H	484/501 (97%)	461 (95%)	21 (4%)	2 (0%)	34	66
1	I	486/501 (97%)	465 (96%)	19 (4%)	2 (0%)	34	66
1	J	486/501 (97%)	459 (94%)	25 (5%)	2 (0%)	34	66
1	K	485/501 (97%)	458 (94%)	24 (5%)	3 (1%)	25	58
1	L	486/501 (97%)	463 (95%)	20 (4%)	3 (1%)	25	58
All	All	5828/6012 (97%)	5542 (95%)	258 (4%)	28 (0%)	29	61

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	463	TYR

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Mol	Chain	Res	Type
1	H	463	TYR
1	I	463	TYR
1	K	483	SER
1	D	357	ASN

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	394/404 (98%)	378 (96%)	16 (4%)	30	64
1	B	394/404 (98%)	378 (96%)	16 (4%)	30	64
1	C	393/404 (97%)	381 (97%)	12 (3%)	40	74
1	D	394/404 (98%)	377 (96%)	17 (4%)	29	62
1	E	394/404 (98%)	379 (96%)	15 (4%)	33	67
1	F	394/404 (98%)	380 (96%)	14 (4%)	35	69
1	G	393/404 (97%)	380 (97%)	13 (3%)	38	72
1	H	392/404 (97%)	377 (96%)	15 (4%)	33	67
1	I	394/404 (98%)	378 (96%)	16 (4%)	30	64
1	J	394/404 (98%)	378 (96%)	16 (4%)	30	64
1	K	393/404 (97%)	380 (97%)	13 (3%)	38	72
1	L	394/404 (98%)	382 (97%)	12 (3%)	41	75
All	All	4723/4848 (97%)	4548 (96%)	175 (4%)	34	68

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	172	LYS
1	G	263	ASN
1	K	368	LEU
1	F	209	ASP
1	F	368	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	389	GLN
1	G	16	ASN
1	H	479	GLN
1	C	318	ASN
1	I	189	GLN

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 carbohydrates 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	L	501	-	42,48,48	0.90	2 (4%)	50,73,73	1.46	6 (12%)
2	NAD	E	501	-	42,48,48	1.05	5 (11%)	50,73,73	1.46	9 (18%)
2	NAD	C	501	-	42,48,48	1.02	3 (7%)	50,73,73	1.30	6 (12%)
2	NAD	A	501	-	42,48,48	0.99	3 (7%)	50,73,73	1.25	3 (6%)
2	NAD	I	501	-	42,48,48	0.99	3 (7%)	50,73,73	1.58	11 (22%)
2	NAD	D	501	-	42,48,48	0.87	2 (4%)	50,73,73	1.34	7 (14%)

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	L	501	-	-	12/26/62/62	0/5/5/5
2	NAD	E	501	-	-	5/26/62/62	0/5/5/5
2	NAD	C	501	-	-	8/26/62/62	0/5/5/5
2	NAD	A	501	-	-	10/26/62/62	0/5/5/5
2	NAD	I	501	-	-	14/26/62/62	0/5/5/5
2	NAD	D	501	-	-	4/26/62/62	0/5/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAD	C5A-C4A	3.06	1.49	1.40
2	C	501	NAD	C5A-C4A	2.75	1.48	1.40
2	D	501	NAD	C5A-C4A	2.73	1.48	1.40
2	L	501	NAD	O4D-C1D	2.66	1.44	1.41
2	I	501	NAD	C5A-C4A	2.63	1.47	1.40

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	NAD	O7N-C7N-C3N	4.39	124.89	119.63
2	I	501	NAD	O7N-C7N-C3N	4.14	124.59	119.63
2	L	501	NAD	C3N-C7N-N7N	4.01	122.56	117.75
2	I	501	NAD	N3A-C2A-N1A	-3.94	122.52	128.68
2	L	501	NAD	O7N-C7N-C3N	-3.85	115.02	119.63

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

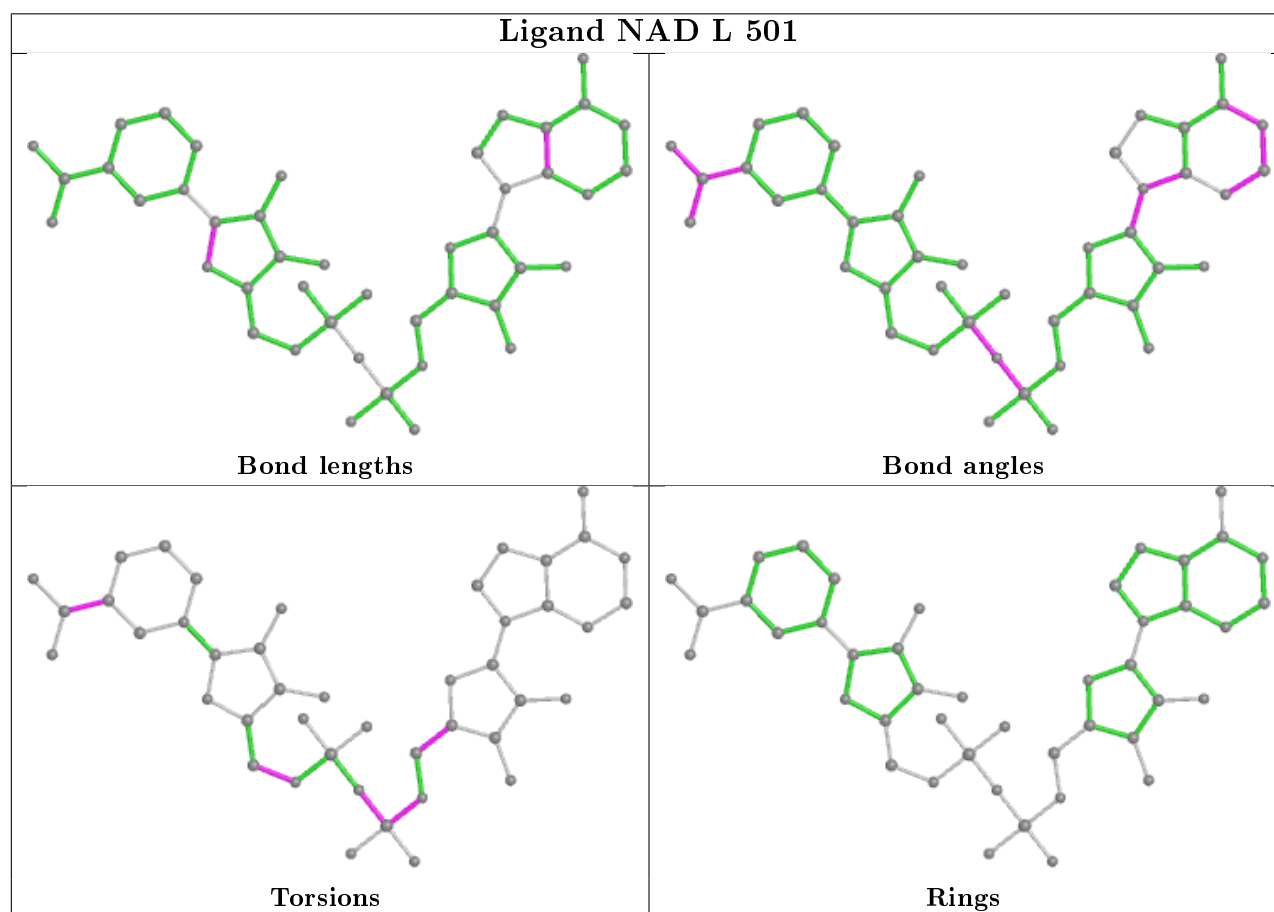
Mol	Chain	Res	Type	Atoms
2	L	501	NAD	C5B-O5B-PA-O3
2	C	501	NAD	C5B-O5B-PA-O1A
2	C	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	C3B-C4B-C5B-O5B
2	A	501	NAD	C5B-O5B-PA-O1A

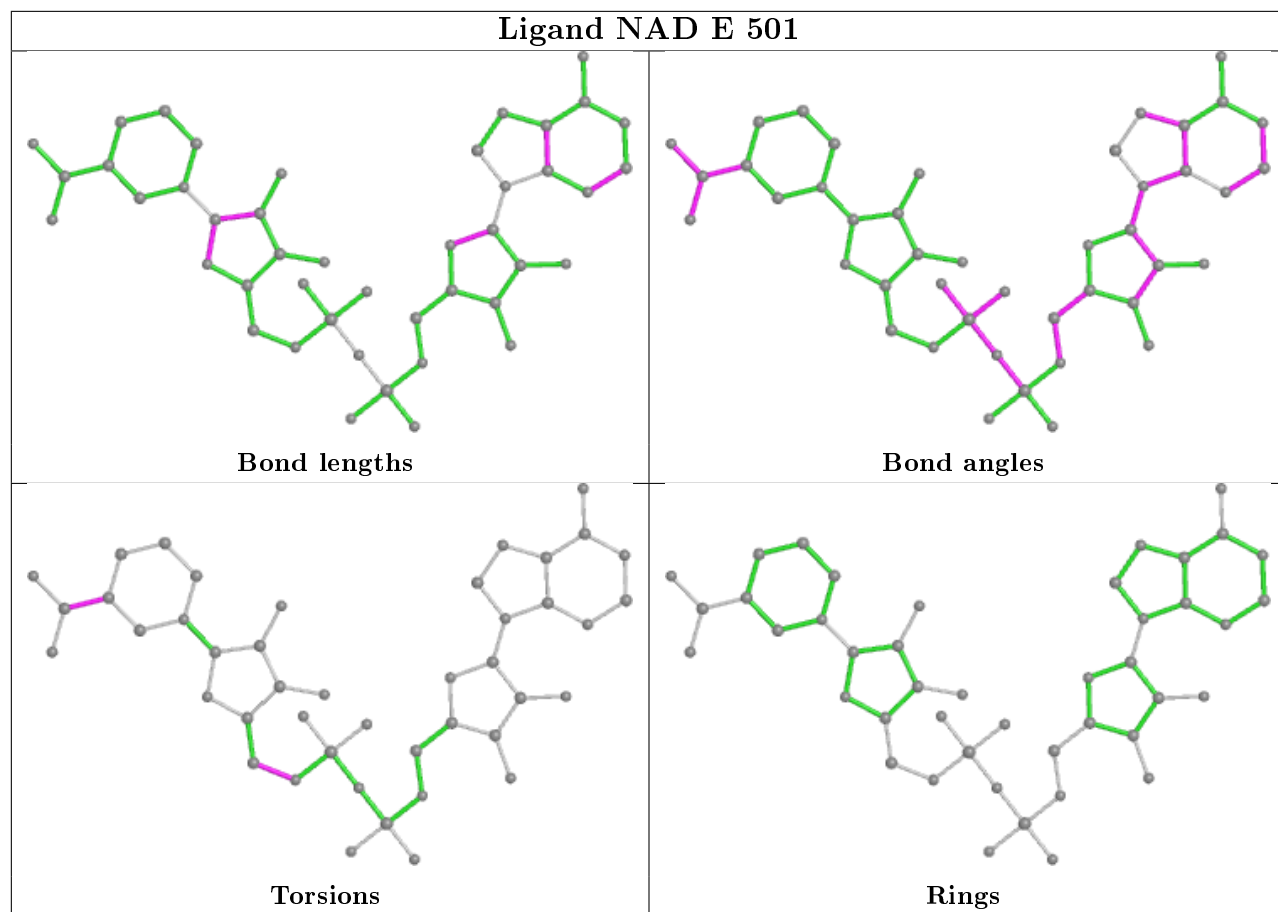
There are no ring outliers.

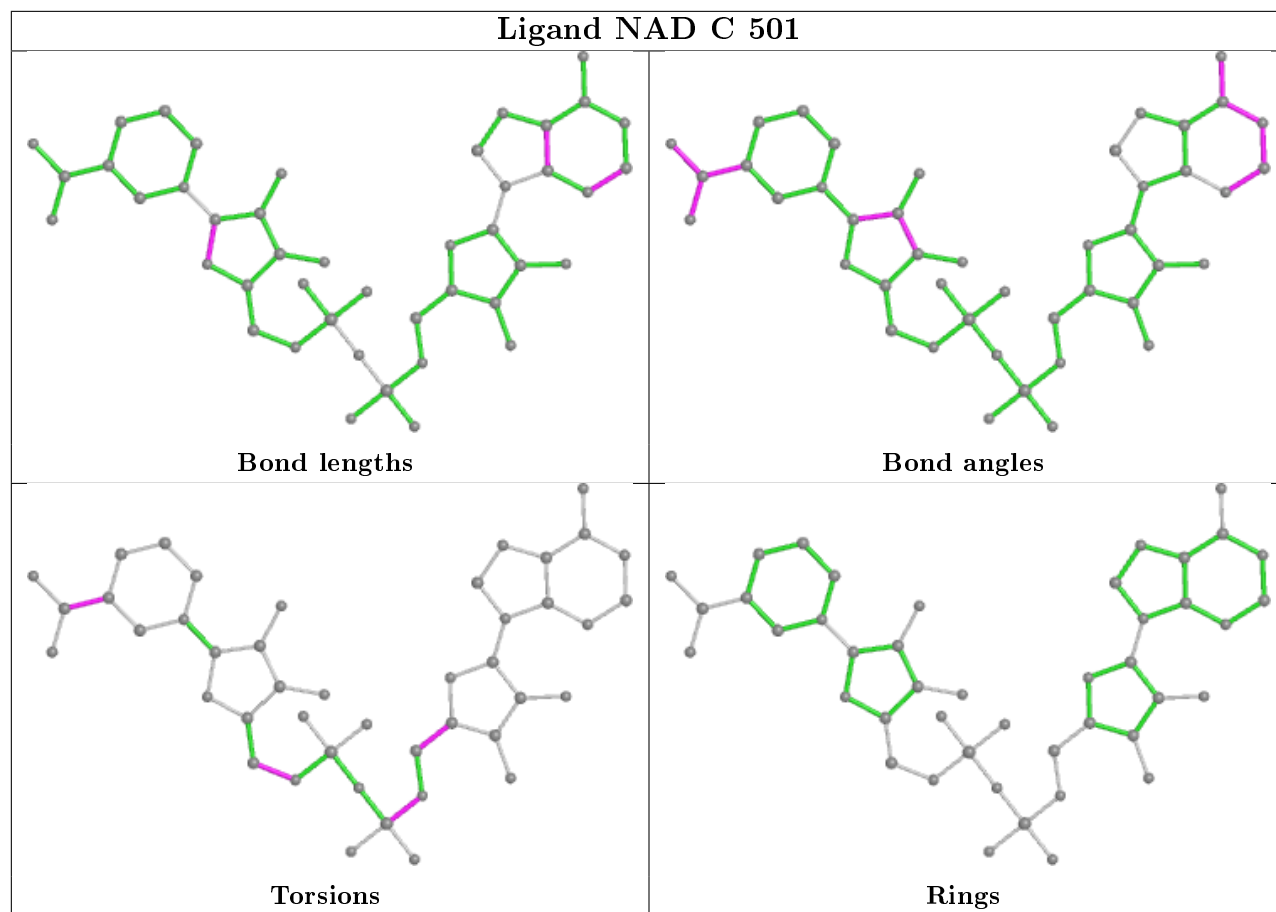
6 monomers are involved in 50 short contacts:

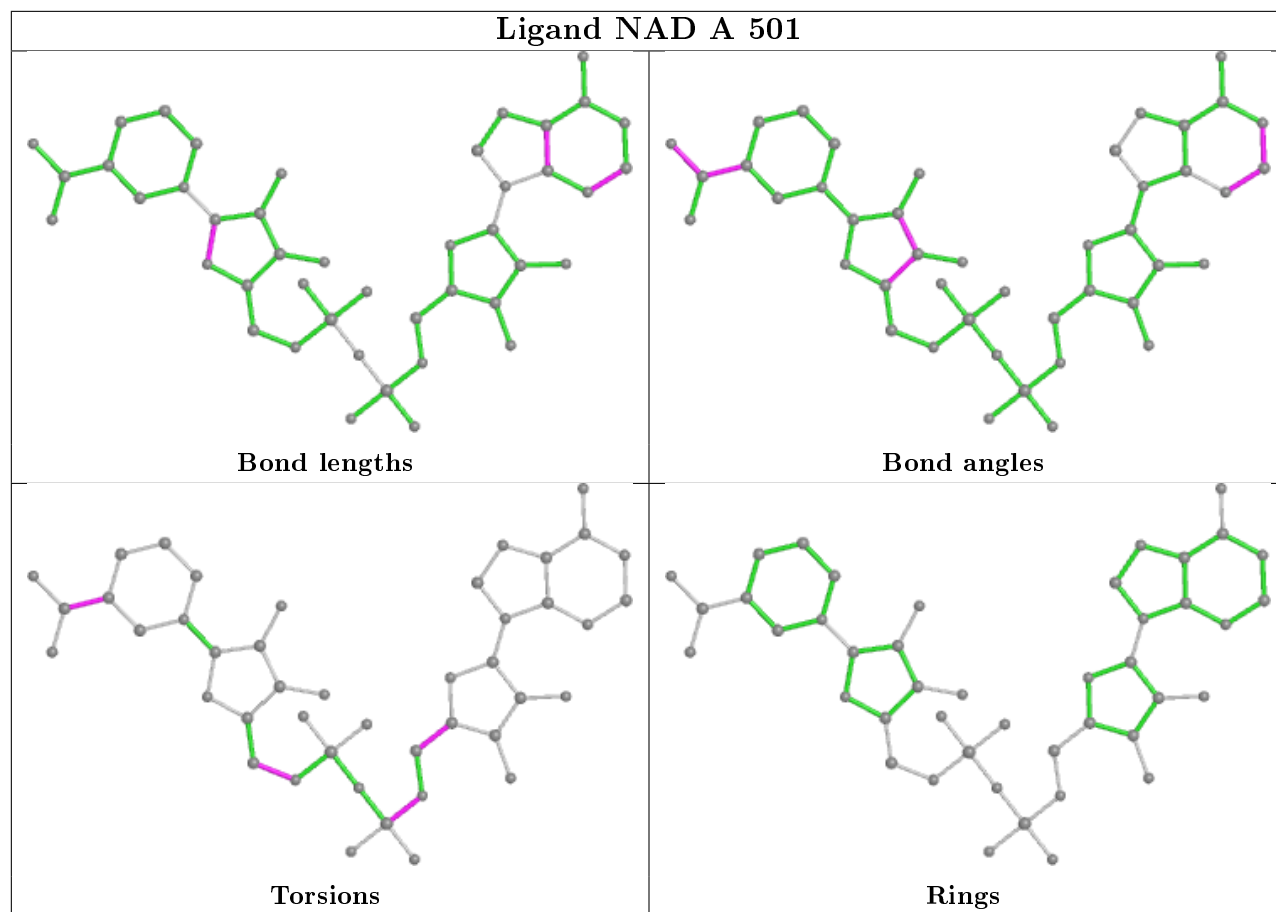
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	501	NAD	6	0
2	E	501	NAD	2	0
2	C	501	NAD	10	0
2	A	501	NAD	10	0
2	I	501	NAD	18	0
2	D	501	NAD	4	0

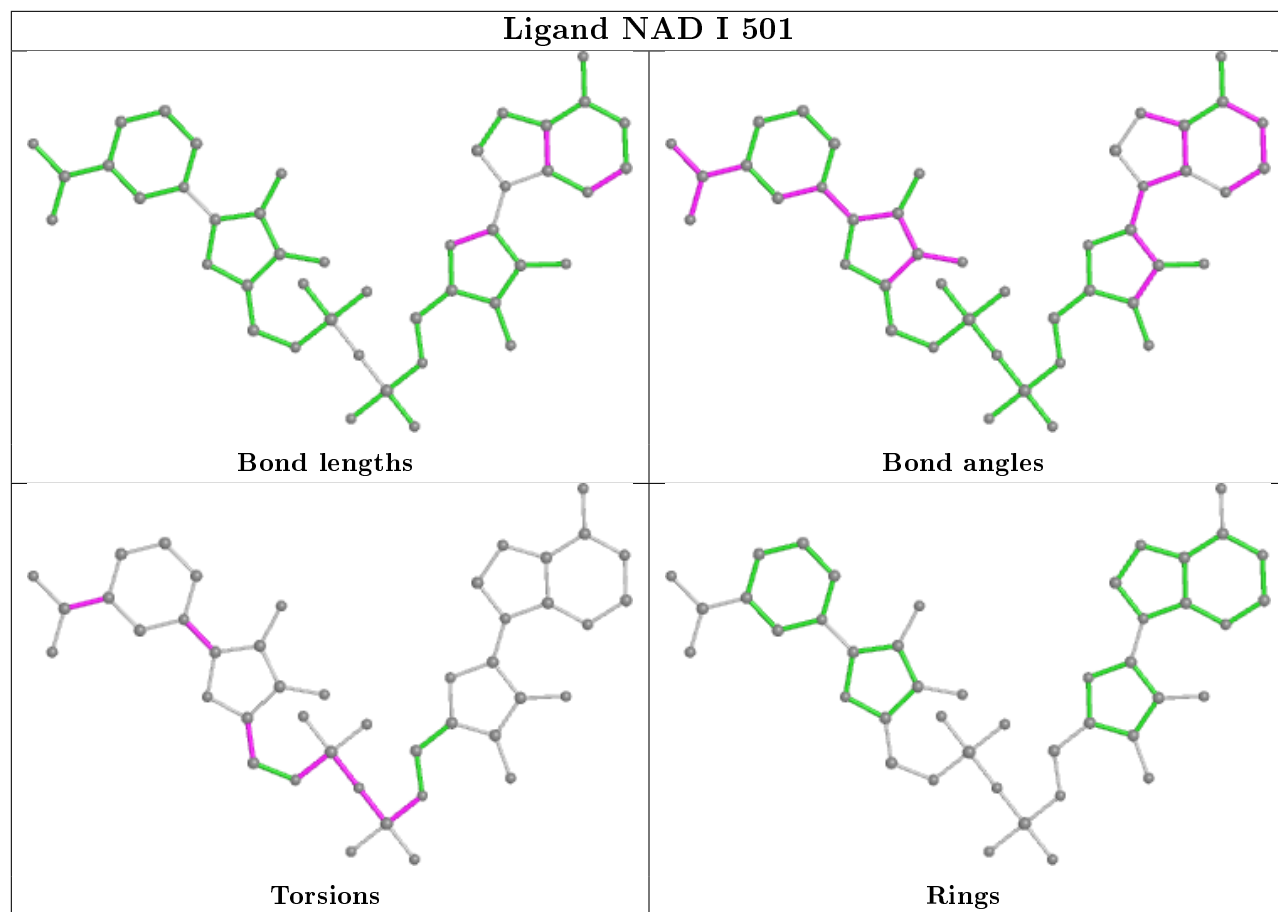
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

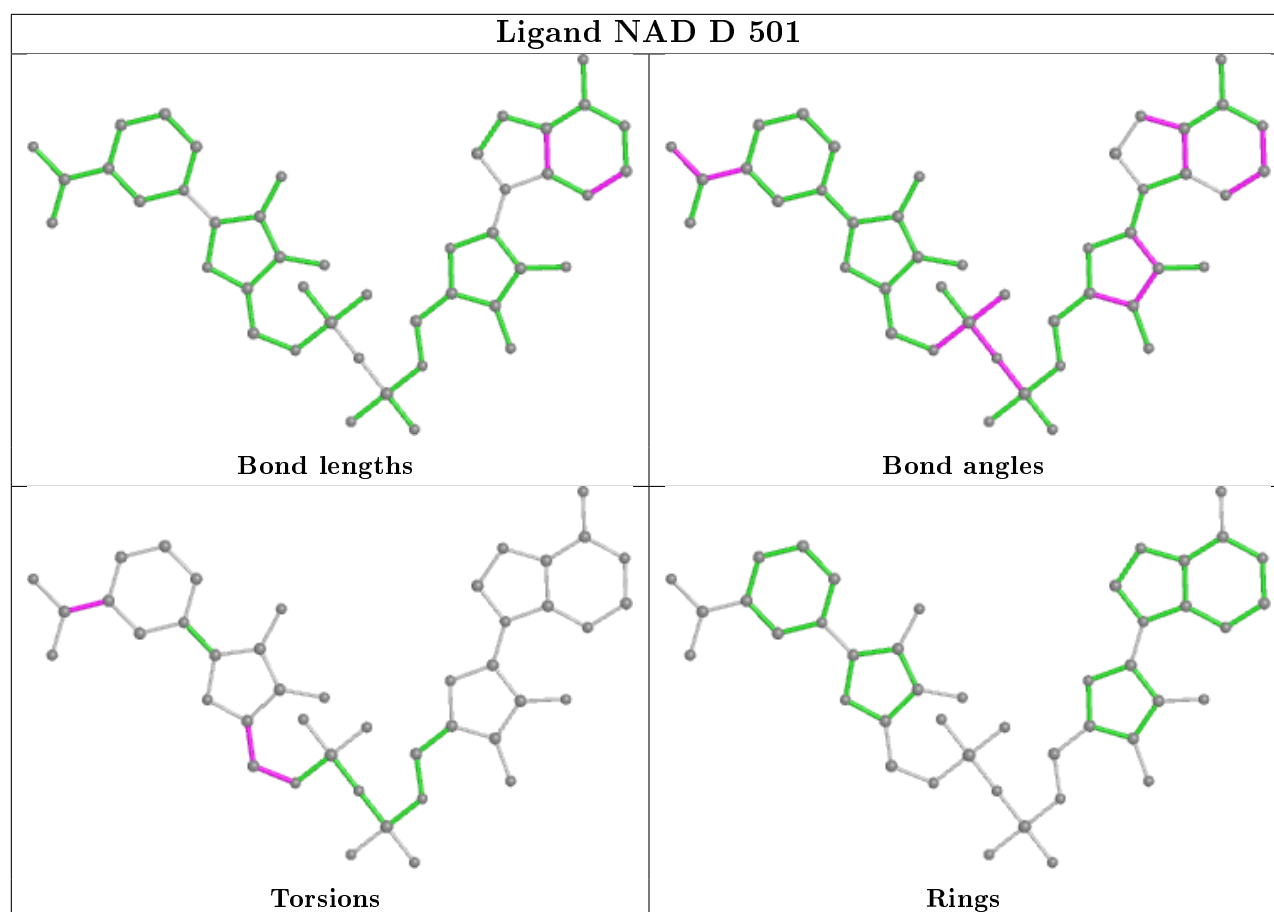












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	489/501 (97%)	-0.31	4 (0%) 86 86	11, 25, 46, 92	0
1	B	488/501 (97%)	-0.33	8 (1%) 72 71	10, 24, 50, 101	0
1	C	487/501 (97%)	-0.35	9 (1%) 68 67	11, 23, 49, 87	0
1	D	488/501 (97%)	-0.33	1 (0%) 95 95	11, 23, 44, 73	0
1	E	488/501 (97%)	-0.15	11 (2%) 60 58	14, 34, 68, 106	0
1	F	488/501 (97%)	0.17	23 (4%) 31 28	18, 45, 78, 142	0
1	G	487/501 (97%)	0.04	17 (3%) 44 38	16, 37, 76, 118	0
1	H	486/501 (97%)	-0.08	7 (1%) 75 75	17, 34, 64, 107	0
1	I	488/501 (97%)	-0.11	6 (1%) 79 79	12, 27, 61, 98	0
1	J	487/501 (97%)	-0.08	10 (2%) 63 61	16, 34, 74, 123	0
1	K	487/501 (97%)	-0.24	7 (1%) 75 75	13, 30, 62, 119	0
1	L	488/501 (97%)	-0.06	8 (1%) 72 71	14, 34, 65, 97	0
All	All	5851/6012 (97%)	-0.15	111 (1%) 66 65	10, 30, 65, 142	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	484	ALA	6.6
1	J	355	VAL	6.1
1	G	355	VAL	5.8
1	F	486	VAL	5.7
1	J	488	GLU	5.4

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

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

6.3 Carbohydrates ⓘ

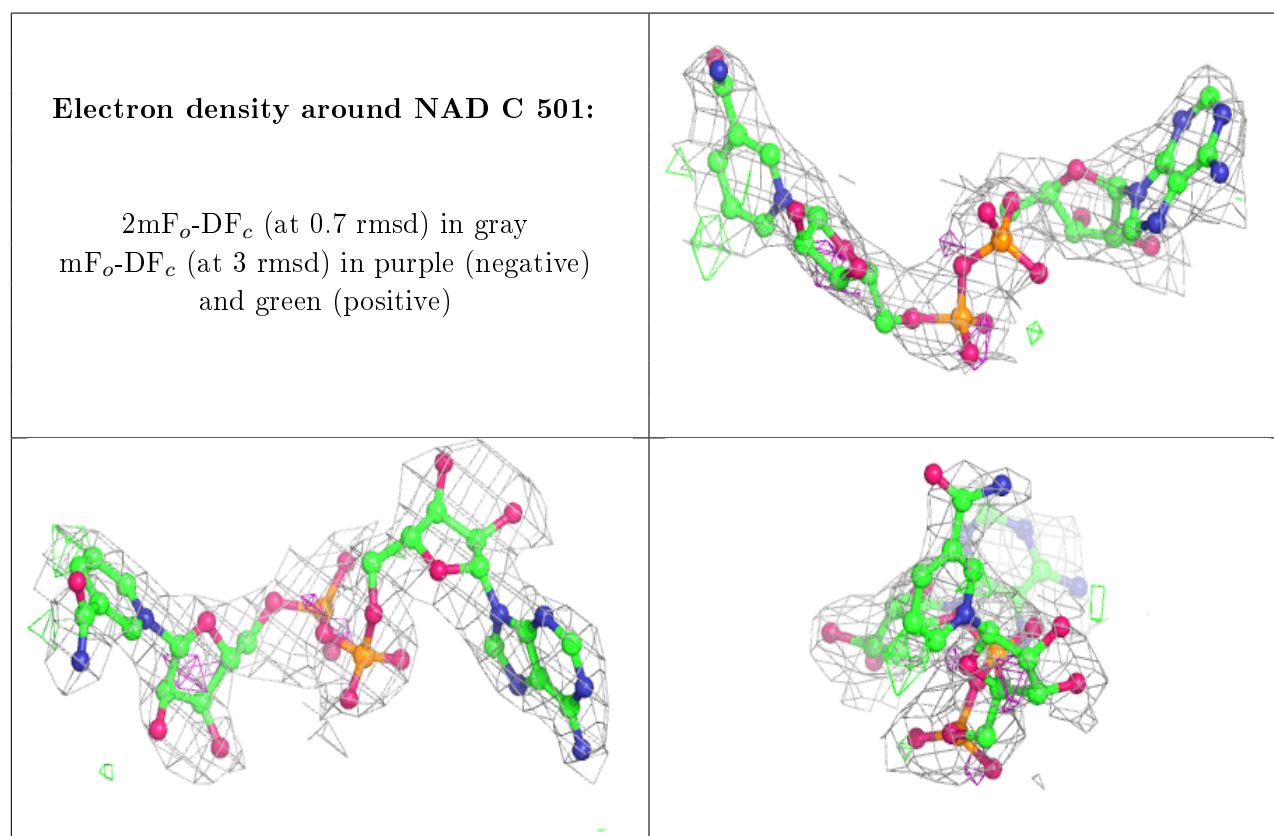
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

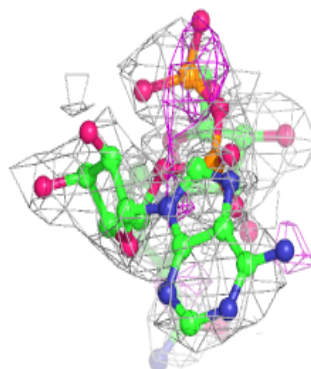
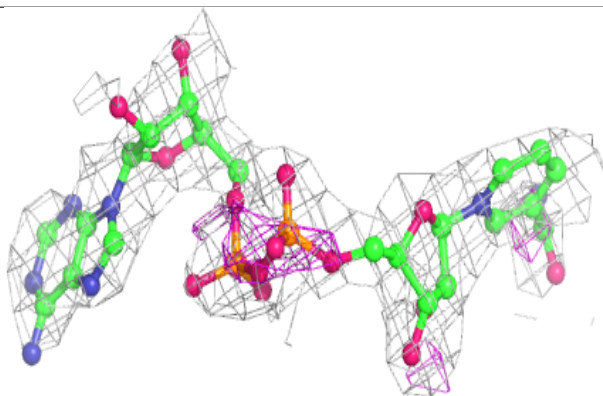
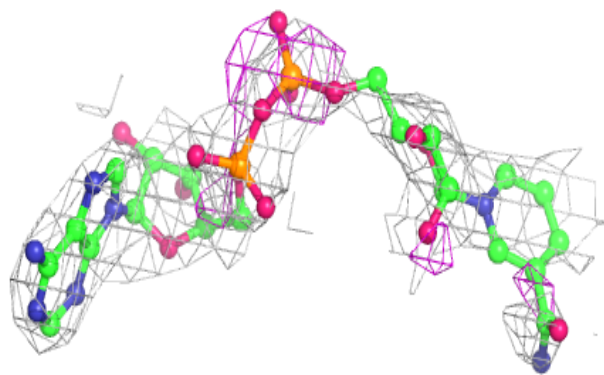
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	C	501	44/44	0.89	0.25	39,48,54,59	0
2	NAD	I	501	44/44	0.91	0.23	42,52,63,66	0
2	NAD	A	501	44/44	0.92	0.21	32,46,73,79	0
2	NAD	L	501	44/44	0.95	0.20	38,43,65,72	0
2	NAD	D	501	44/44	0.95	0.16	24,29,34,36	0
2	NAD	E	501	44/44	0.96	0.16	34,40,47,48	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.

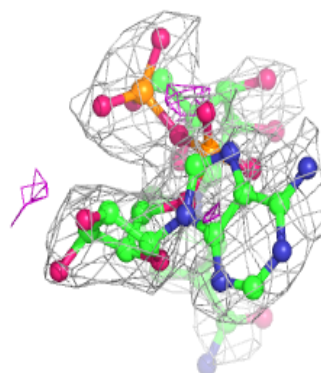
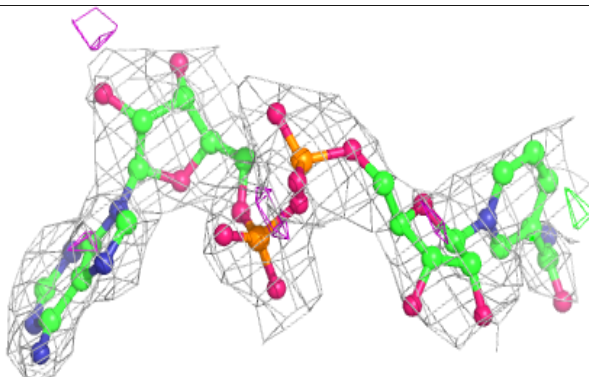
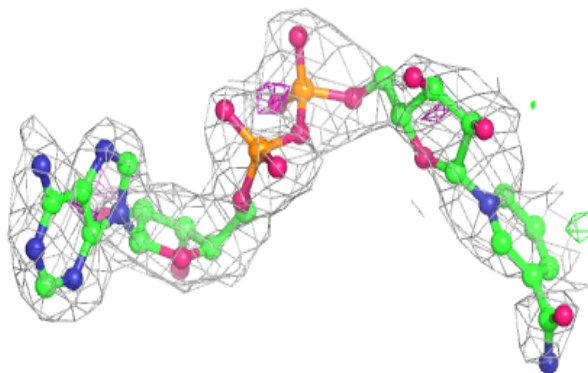


Electron density around NAD I 501:

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

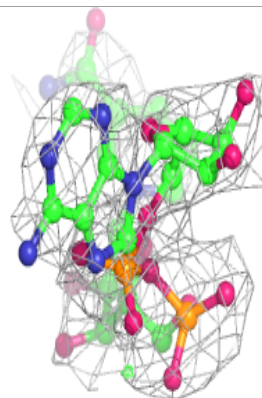
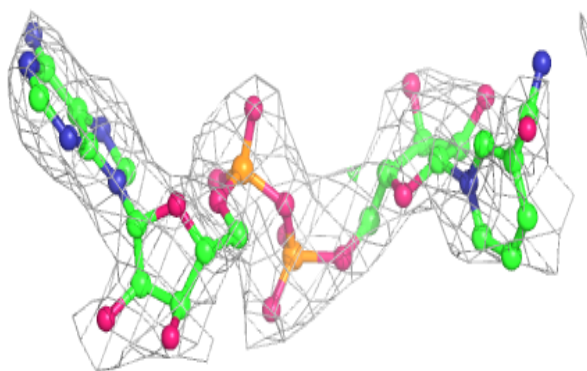
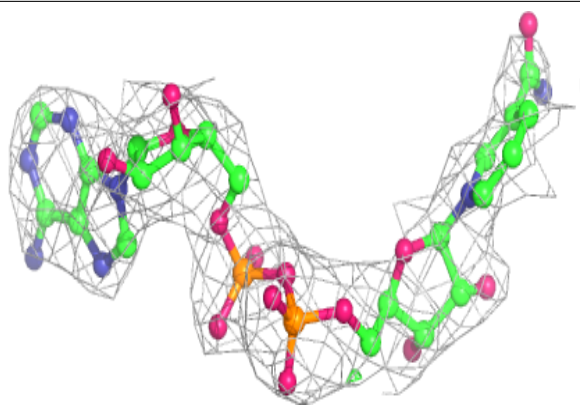
**Electron density around NAD A 501:**

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

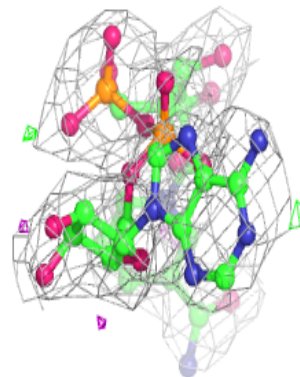
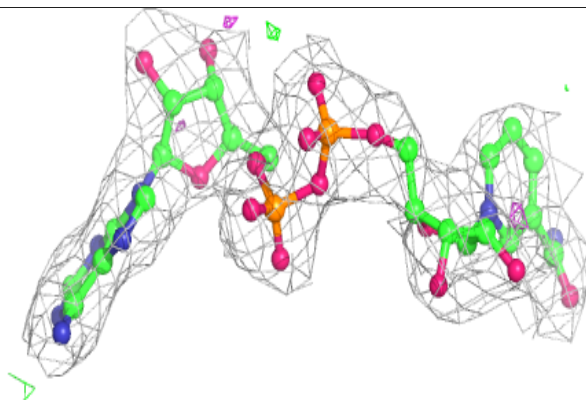
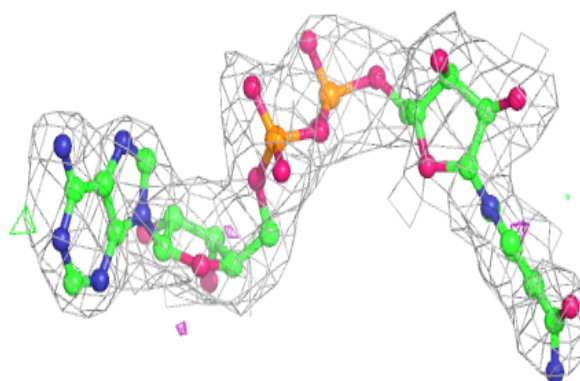


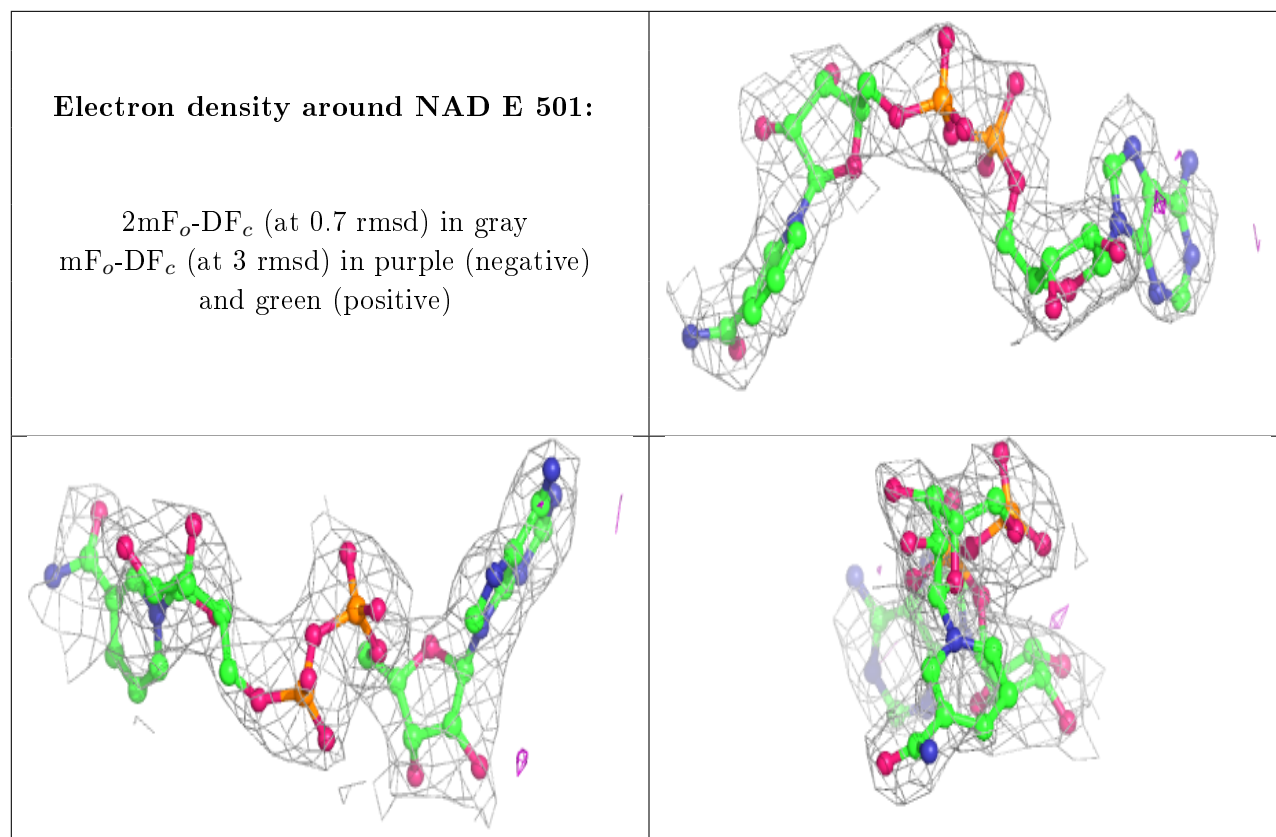
Electron density around NAD L 501:

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

**Electron density around NAD D 501:**

$2mF_o-DF_c$ (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.