wwPDB X-ray Structure Validation Summary Report (i)

May 18, 2020 – 12:16 am BST

PDB ID	:	1PJL
Title	:	Crystal structure of human m-NAD-ME in ternary complex with NAD and Lu3+
Authors	:	Yang, Z.; Batra, R.; Floyd, D.L.; Hung, H.-C.; Chang, G.-G.; Tong, L.
Deposited on	:	2003-06-03
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

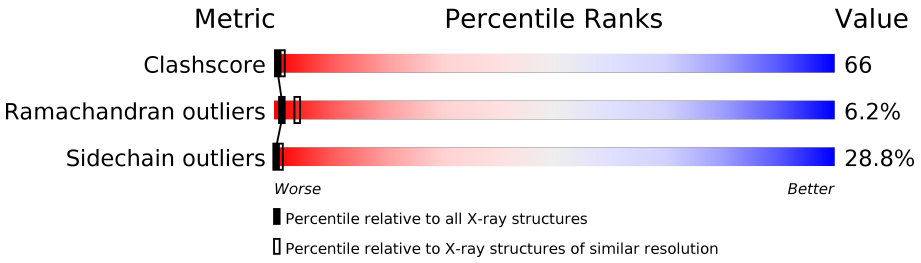
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	584	21% 52% 21% • 6%
1	B	584	20% 49% 25% • 6%
1	C	584	23% 47% 23% • 6%
1	D	584	20% 49% 24% • 6%
1	E	584	22% 53% 19% • 6%
1	F	584	24% 50% 19% • 6%
1	G	584	17% 54% 22% • 6%
1	H	584	23% 50% 20% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 35527 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 malic enzyme, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	B	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	C	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	D	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	E	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	F	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	G	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	H	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	343	MSE	MET	MODIFIED RESIDUE	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
A	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1001	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1029	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1038	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1047	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1075	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1086	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1108	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1177	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1219	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1239	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1325	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1327	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1343	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1407	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1539	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2001	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2029	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2038	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2047	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2075	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2086	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2108	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2177	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2219	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2239	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2325	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2327	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2343	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2407	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2539	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3001	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3029	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3038	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3047	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3075	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3086	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3108	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3177	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3219	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3239	MSE	MET	MODIFIED RESIDUE	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
D	3325	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3327	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3343	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3407	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3539	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4001	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4029	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4038	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4047	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4075	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4086	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4108	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4177	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4219	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4239	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4325	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4327	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4343	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4407	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4539	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5001	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5029	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5038	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5047	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5075	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5086	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5108	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5177	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5219	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5239	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5325	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5327	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5343	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5407	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5539	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6001	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6029	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6038	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6047	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6075	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6086	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6108	MSE	MET	MODIFIED RESIDUE	UNP P23368

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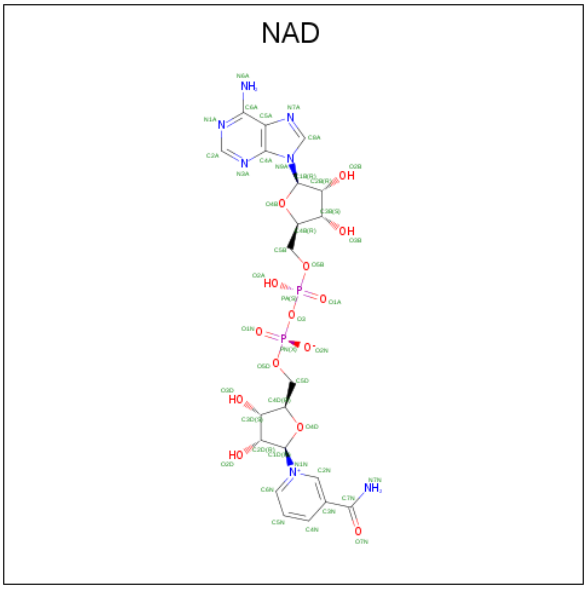
Chain	Residue	Modelled	Actual	Comment	Reference
G	6177	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6219	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6239	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6325	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6327	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6343	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6407	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6539	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7001	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7029	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7038	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7047	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7075	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7086	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7108	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7177	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7219	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7239	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7325	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7327	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7343	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7407	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7539	MSE	MET	MODIFIED RESIDUE	UNP P23368

- Molecule 2 is LUTETIUM (III) ION (three-letter code: LU) (formula: Lu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Lu 1 1	0	0
2	D	1	Total Lu 1 1	0	0
2	E	1	Total Lu 1 1	0	0
2	H	1	Total Lu 1 1	0	0
2	B	1	Total Lu 1 1	0	0
2	C	1	Total Lu 1 1	0	0
2	A	1	Total Lu 1 1	0	0
2	F	1	Total Lu 1 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	A	1	Total	C	N	O	P	17	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	18	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	18	0
			44	21	7	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	6	Total	O	0	0
			6	6		
4	C	11	Total	O	0	0
			11	11		
4	D	6	Total	O	0	0
			6	6		
4	E	6	Total	O	0	0
			6	6		
4	F	10	Total	O	0	0
			10	10		
4	G	5	Total	O	0	0
			5	5		
4	H	10	Total	O	0	0
			10	10		

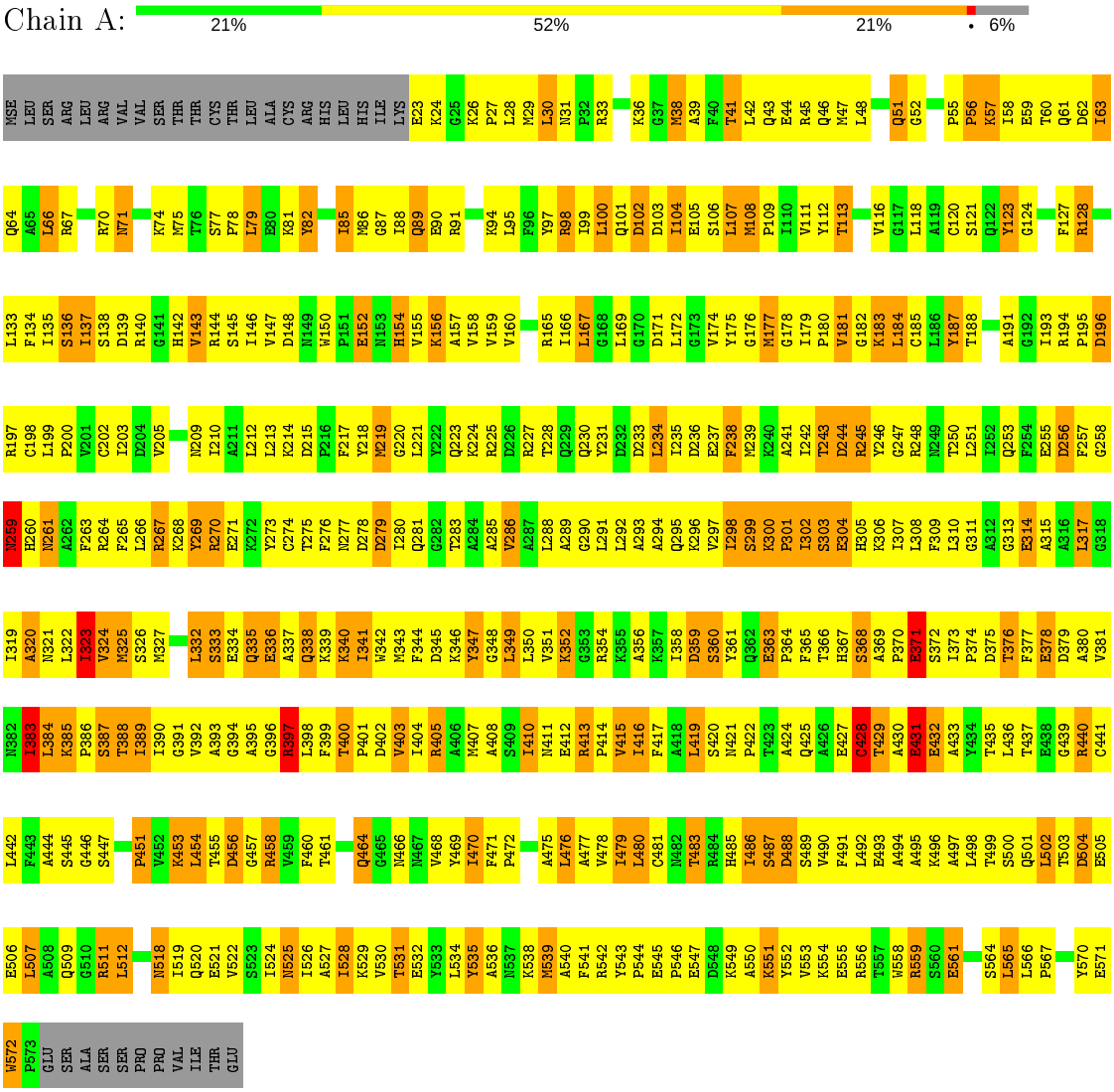
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

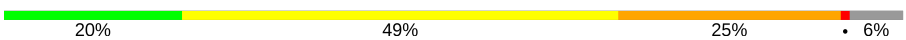
- Molecule 1: NAD-dependent malic enzyme, mitochondrial

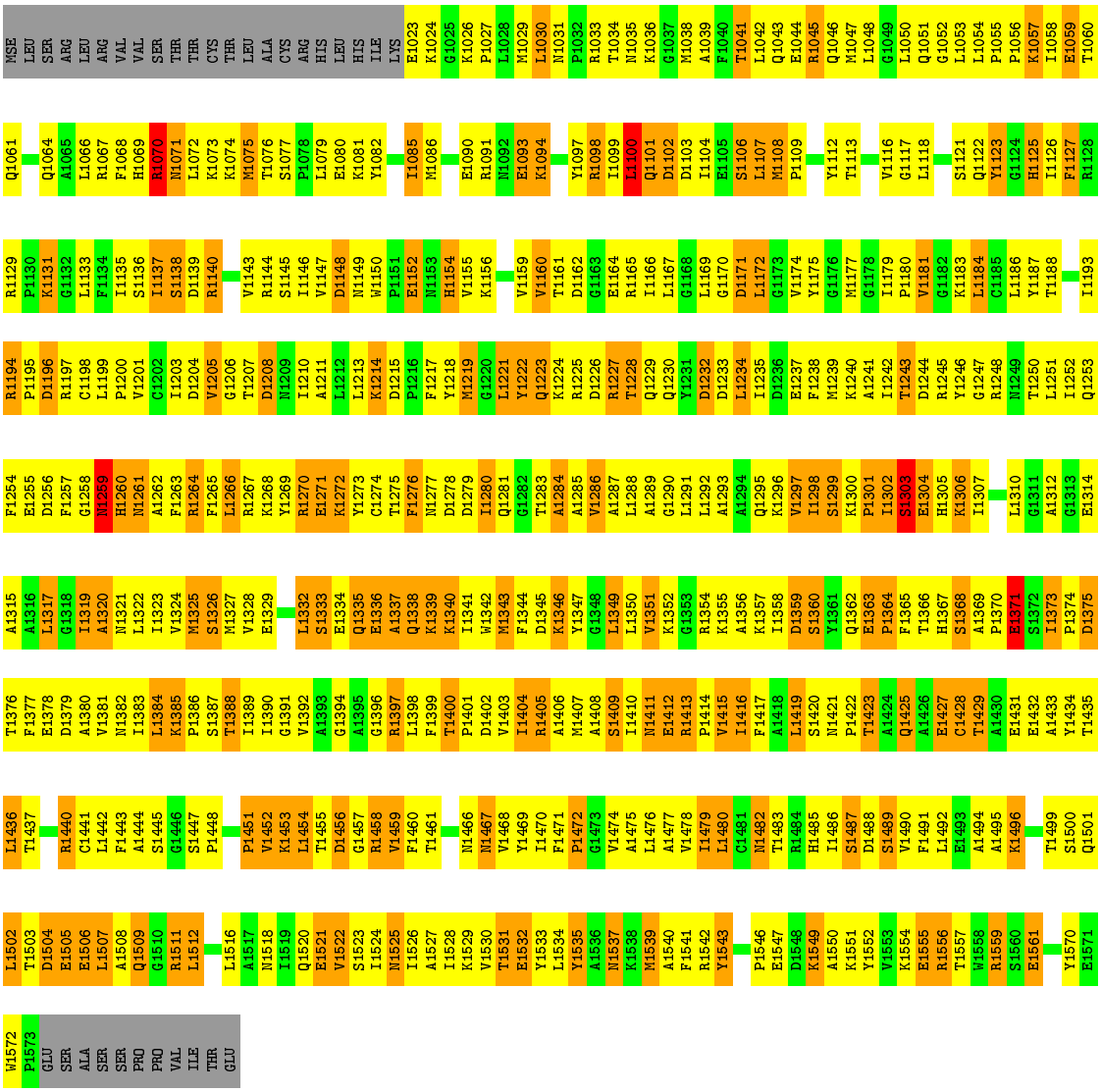
Chain A:



- Molecule 1: NAD-dependent malic enzyme, mitochondrial

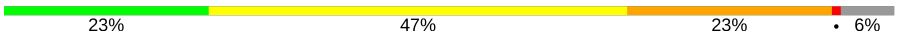
Chain B:

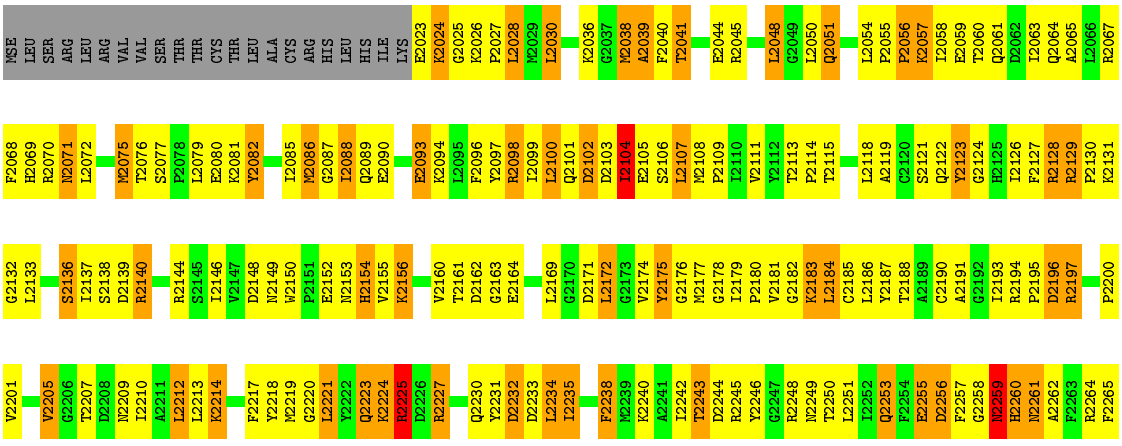


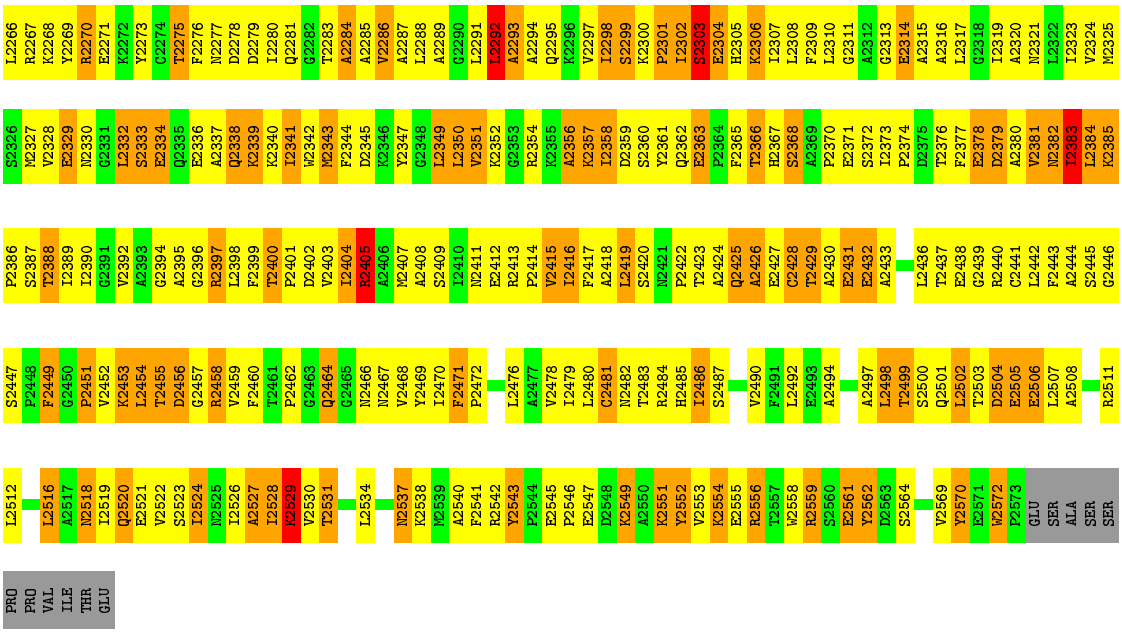


• Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain C:

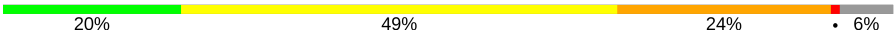


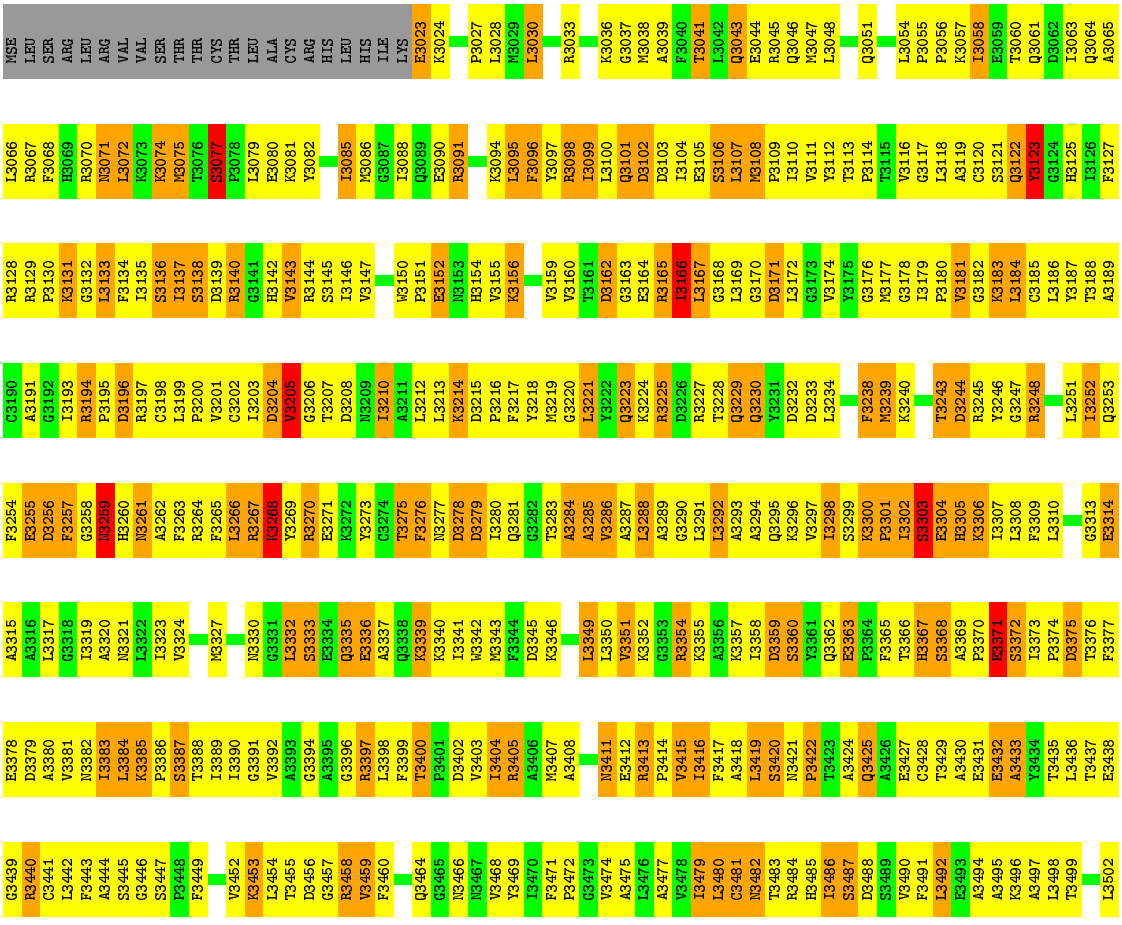




- Molecule 1: NAD-dependent malic enzyme, mitochondrial

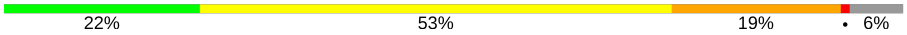
Chain D:

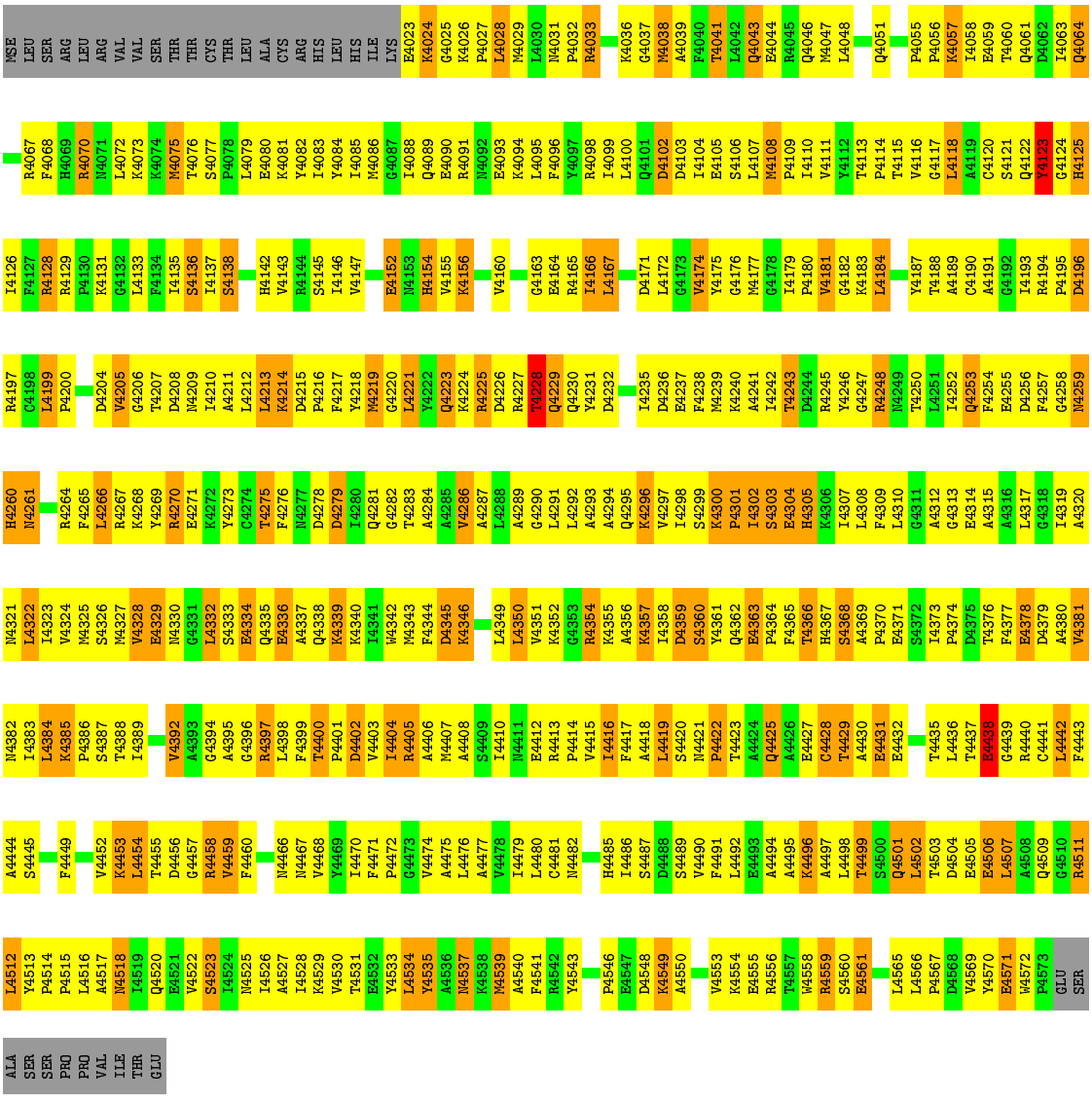




• Molecule 1: NAD-dependent malic enzyme, mitochondrial

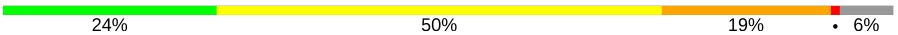
Chain E:

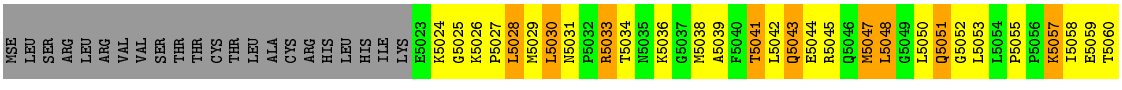


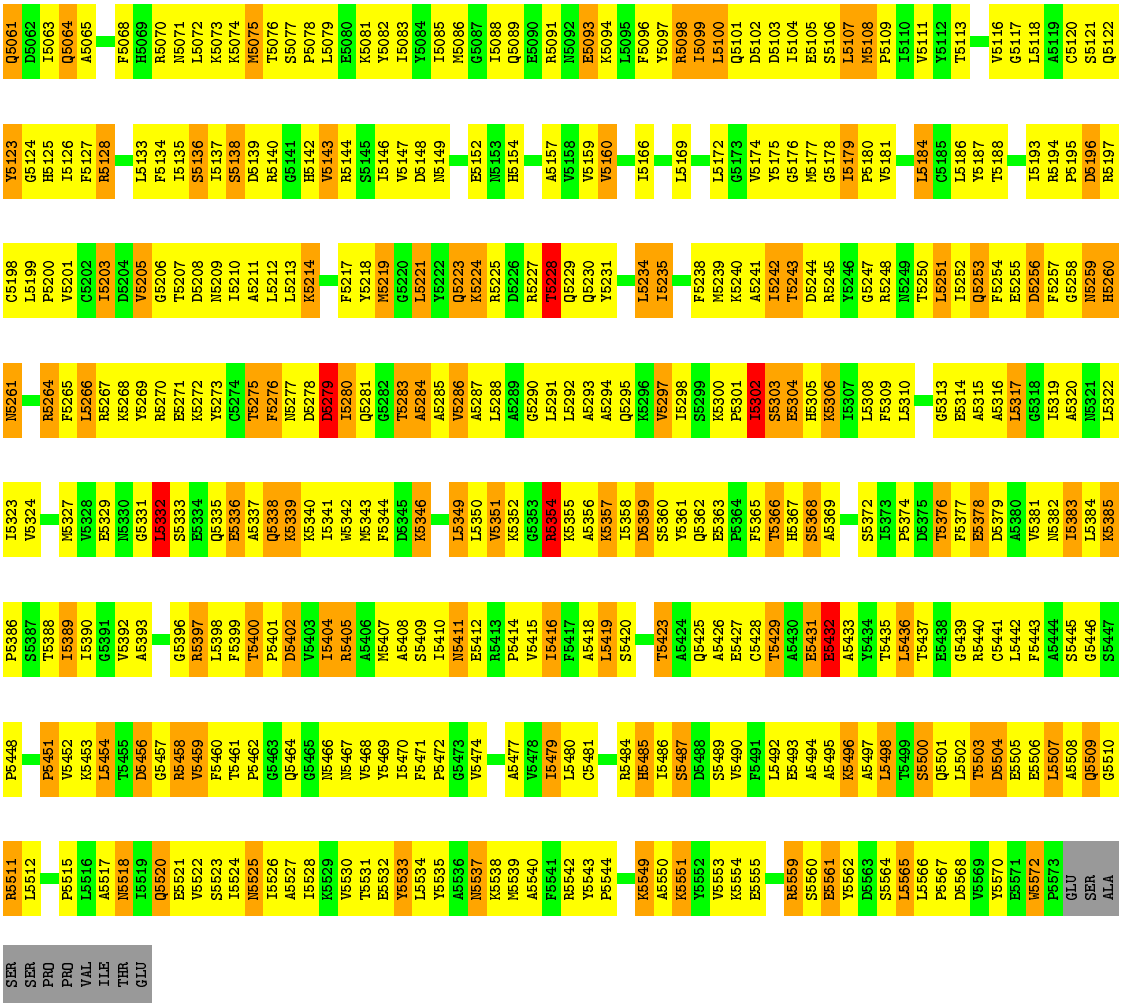


• Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain F:

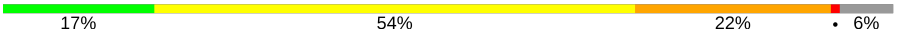


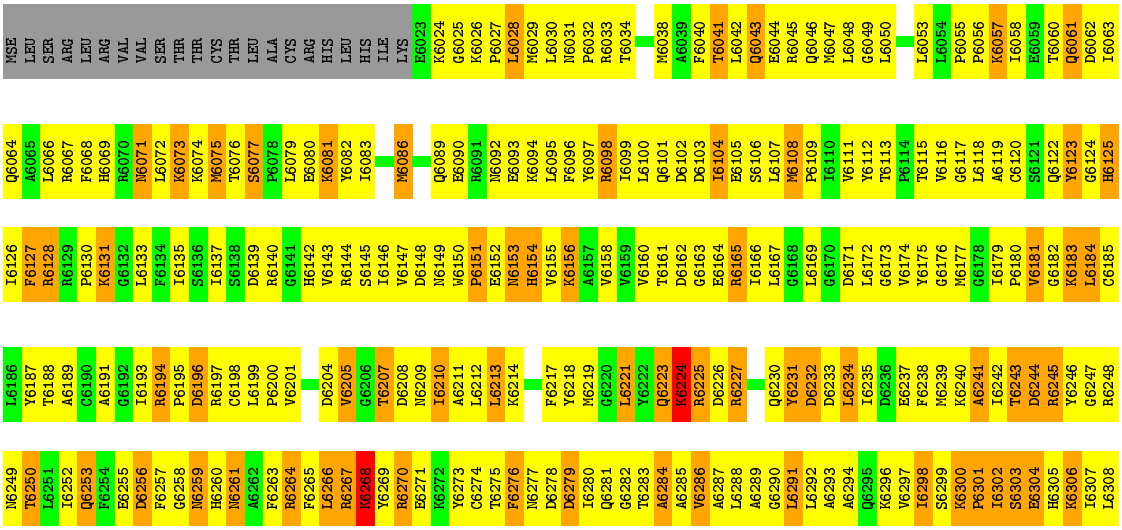


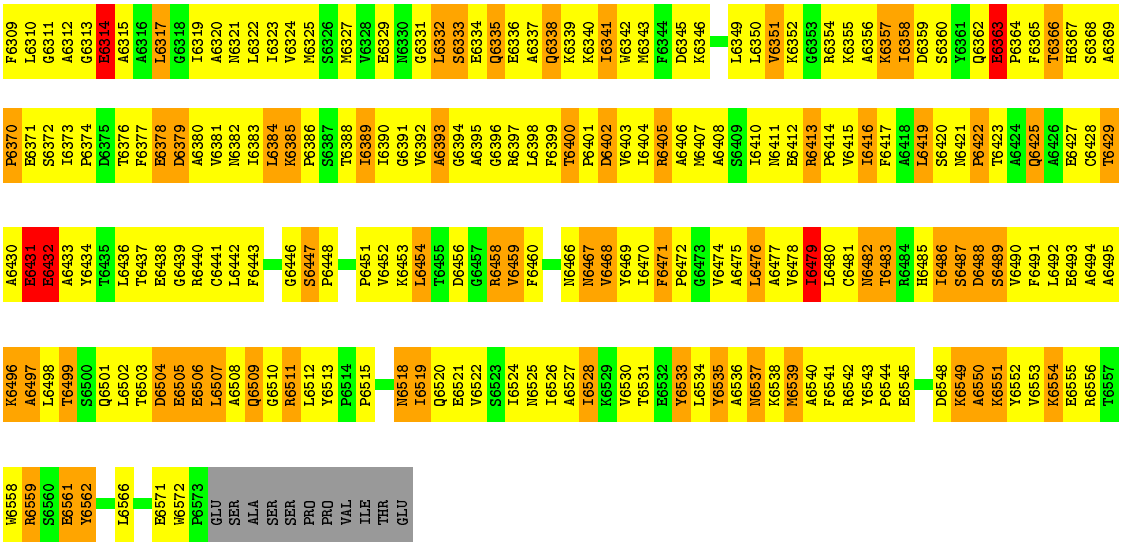


• Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain G:

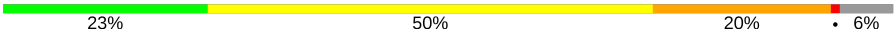


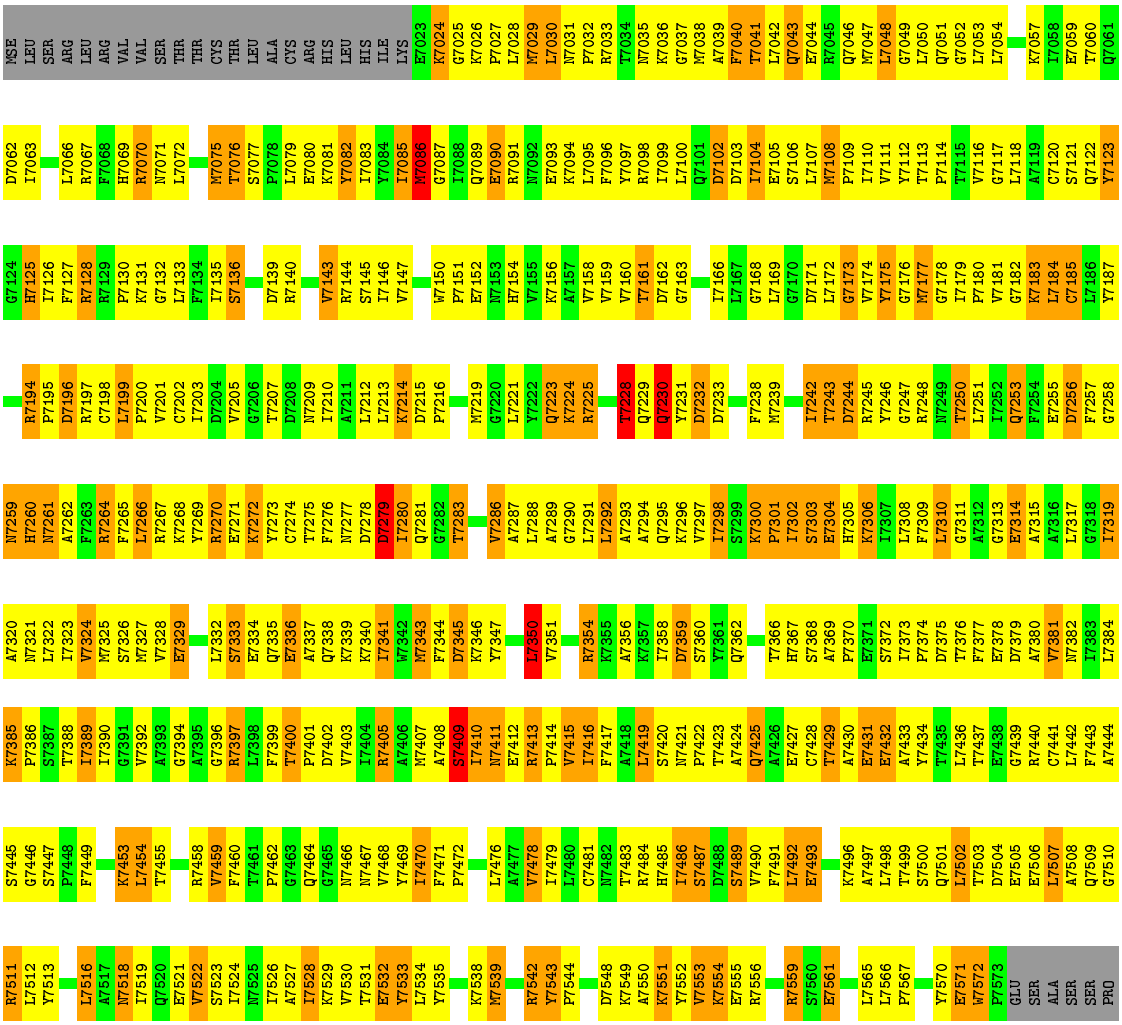




• Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain H:






PRO
VAL
ILE
THR
GLU

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	113.30Å 119.00Å 125.90Å 116.50° 94.80° 102.80°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.204 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	35527	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LU, 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	0.46	0/4424	0.67	0/5969
1	B	0.46	0/4424	0.66	0/5969
1	C	0.46	0/4424	0.66	0/5969
1	D	0.49	0/4424	0.69	0/5969
1	E	0.47	0/4424	0.68	1/5969 (0.0%)
1	F	0.47	0/4424	0.66	0/5969
1	G	0.46	0/4424	0.69	0/5969
1	H	0.46	0/4424	0.68	0/5969
All	All	0.47	0/35392	0.67	1/47752 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	4442	LEU	CA-CB-CG	-5.11	103.55	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	TYR	Sidechain

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	4344	0	4372	604	0
1	B	4344	0	4372	618	0
1	C	4344	0	4372	594	0
1	D	4344	0	4372	650	0
1	E	4344	0	4372	543	0
1	F	4344	0	4372	504	0
1	G	4344	0	4372	654	0
1	H	4344	0	4372	560	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	88	0	52	3	0
3	B	88	0	52	5	0
3	C	88	0	52	2	0
3	D	88	0	52	4	0
3	E	88	0	52	3	0
3	F	88	0	52	3	0
3	G	88	0	52	4	0
3	H	88	0	52	3	0
4	A	9	0	0	3	0
4	B	6	0	0	1	0
4	C	11	0	0	1	0
4	D	6	0	0	6	0
4	E	6	0	0	0	0
4	F	10	0	0	1	0
4	G	5	0	0	3	0
4	H	10	0	0	1	0
All	All	35527	0	35392	4647	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 66.

The worst 5 of 4647 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:D:3061:GLN:HA	1:D:3064:GLN:HE21	1.04	1.18
1:D:3388:THR:HG23	1:D:3415:VAL:HB	1.27	1.15
1:H:7388:THR:HG23	1:H:7415:VAL:HB	1.27	1.14
1:D:3253:GLN:HE22	1:D:3255:GLU:HG2	1.13	1.13
1:D:3263:PHE:HA	4:D:8022:HOH:O	1.48	1.13

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	549/584 (94%)	415 (76%)	99 (18%)	35 (6%)	1	4
1	B	549/584 (94%)	406 (74%)	107 (20%)	36 (7%)	1	3
1	C	549/584 (94%)	407 (74%)	102 (19%)	40 (7%)	1	3
1	D	549/584 (94%)	394 (72%)	119 (22%)	36 (7%)	1	3
1	E	549/584 (94%)	429 (78%)	94 (17%)	26 (5%)	2	8
1	F	549/584 (94%)	437 (80%)	83 (15%)	29 (5%)	2	6
1	G	549/584 (94%)	398 (72%)	111 (20%)	40 (7%)	1	3
1	H	549/584 (94%)	398 (72%)	120 (22%)	31 (6%)	2	5
All	All	4392/4672 (94%)	3284 (75%)	835 (19%)	273 (6%)	1	4

5 of 273 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ILE
1	A	167	LEU
1	A	256	ASP
1	A	259	ASN

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Mol	Chain	Res	Type
1	A	268	LYS

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	466/483 (96%)	332 (71%)	134 (29%)	0 1
1	B	466/483 (96%)	318 (68%)	148 (32%)	0 0
1	C	466/483 (96%)	327 (70%)	139 (30%)	0 1
1	D	466/483 (96%)	318 (68%)	148 (32%)	0 0
1	E	466/483 (96%)	340 (73%)	126 (27%)	0 1
1	F	466/483 (96%)	341 (73%)	125 (27%)	0 1
1	G	466/483 (96%)	335 (72%)	131 (28%)	0 1
1	H	466/483 (96%)	344 (74%)	122 (26%)	0 1
All	All	3728/3864 (96%)	2655 (71%)	1073 (29%)	0 1

5 of 1073 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3268	LYS
1	E	4183	LYS
1	H	7225	ARG
1	D	3306	LYS
1	D	3487	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3330	ASN
1	E	4125	HIS
1	H	7069	HIS
1	D	3335	GLN

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Mol	Chain	Res	Type
1	D	3509	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

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	NAD	C	2601	-	42,48,48	2.03	11 (26%)	50,73,73	1.42	7 (14%)
3	NAD	E	4602	-	42,48,48	2.01	11 (26%)	50,73,73	1.42	6 (12%)
3	NAD	D	3602	-	42,48,48	2.00	10 (23%)	50,73,73	1.49	6 (12%)
3	NAD	F	5602	-	42,48,48	1.98	10 (23%)	50,73,73	1.45	5 (10%)
3	NAD	H	7601	-	42,48,48	2.24	11 (26%)	50,73,73	1.39	6 (12%)
3	NAD	B	1602	-	42,48,48	2.08	9 (21%)	50,73,73	1.41	5 (10%)
3	NAD	G	6602	-	42,48,48	2.02	9 (21%)	50,73,73	1.41	5 (10%)
3	NAD	A	601	-	42,48,48	2.09	12 (28%)	50,73,73	1.49	6 (12%)
3	NAD	A	602	-	42,48,48	2.11	10 (23%)	50,73,73	1.41	4 (8%)
3	NAD	D	3601	-	42,48,48	2.38	14 (33%)	50,73,73	1.48	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAD	F	5601	-	42,48,48	1.94	11 (26%)	50,73,73	1.38	5 (10%)
3	NAD	E	4601	-	42,48,48	2.16	12 (28%)	50,73,73	1.33	4 (8%)
3	NAD	H	7602	-	42,48,48	1.99	9 (21%)	50,73,73	1.48	6 (12%)
3	NAD	B	1601	-	42,48,48	1.97	11 (26%)	50,73,73	1.40	4 (8%)
3	NAD	C	2602	-	42,48,48	2.10	9 (21%)	50,73,73	1.42	6 (12%)
3	NAD	G	6601	-	42,48,48	2.02	11 (26%)	50,73,73	1.49	6 (12%)

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
3	NAD	C	2601	-	-	5/26/62/62	0/5/5/5
3	NAD	E	4602	-	-	6/26/62/62	0/5/5/5
3	NAD	D	3602	-	-	8/26/62/62	0/5/5/5
3	NAD	F	5602	-	-	6/26/62/62	0/5/5/5
3	NAD	H	7601	-	-	1/26/62/62	0/5/5/5
3	NAD	B	1602	-	-	7/26/62/62	0/5/5/5
3	NAD	G	6602	-	-	7/26/62/62	0/5/5/5
3	NAD	A	601	-	-	1/26/62/62	0/5/5/5
3	NAD	A	602	-	-	6/26/62/62	0/5/5/5
3	NAD	D	3601	-	-	5/26/62/62	0/5/5/5
3	NAD	F	5601	-	-	2/26/62/62	0/5/5/5
3	NAD	E	4601	-	-	2/26/62/62	0/5/5/5
3	NAD	H	7602	-	-	6/26/62/62	0/5/5/5
3	NAD	B	1601	-	-	9/26/62/62	0/5/5/5
3	NAD	C	2602	-	-	5/26/62/62	0/5/5/5
3	NAD	G	6601	-	-	1/26/62/62	0/5/5/5

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1602	NAD	C2N-N1N	8.07	1.44	1.35
3	D	3601	NAD	C2N-N1N	7.62	1.44	1.35
3	C	2602	NAD	C2N-N1N	7.46	1.44	1.35
3	H	7601	NAD	C2N-N1N	7.25	1.43	1.35
3	D	3602	NAD	C2N-N1N	7.16	1.43	1.35

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	5601	NAD	N3A-C2A-N1A	-5.44	120.17	128.68
3	E	4601	NAD	N3A-C2A-N1A	-5.36	120.30	128.68
3	G	6601	NAD	N3A-C2A-N1A	-5.36	120.30	128.68
3	C	2601	NAD	N3A-C2A-N1A	-5.34	120.33	128.68
3	A	601	NAD	N3A-C2A-N1A	-5.31	120.37	128.68

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAD	C5B-O5B-PA-O1A
3	F	5601	NAD	PN-O3-PA-O5B
3	E	4602	NAD	C5B-O5B-PA-O1A
3	E	4602	NAD	C5D-O5D-PN-O1N
3	E	4602	NAD	C3D-C4D-C5D-O5D

There are no ring outliers.

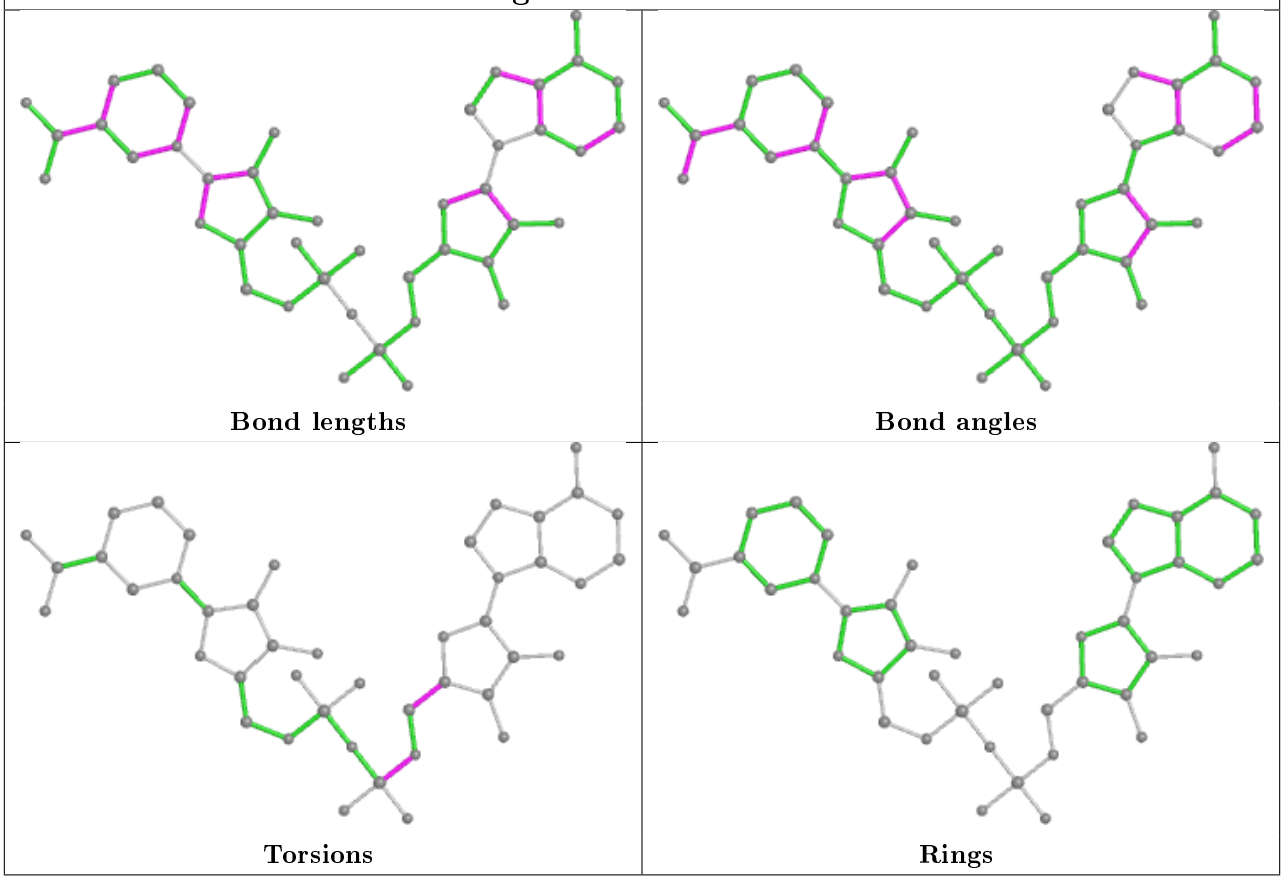
11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2601	NAD	2	0
3	D	3602	NAD	1	0
3	H	7601	NAD	2	0
3	B	1602	NAD	1	0
3	A	601	NAD	3	0
3	D	3601	NAD	3	0
3	F	5601	NAD	3	0
3	E	4601	NAD	3	0
3	H	7602	NAD	1	0
3	B	1601	NAD	4	0
3	G	6601	NAD	4	0

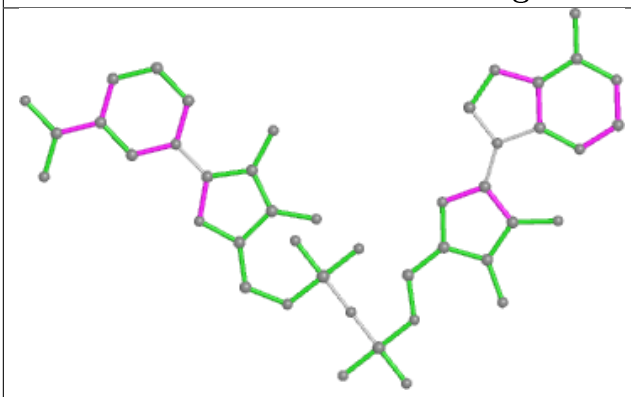
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

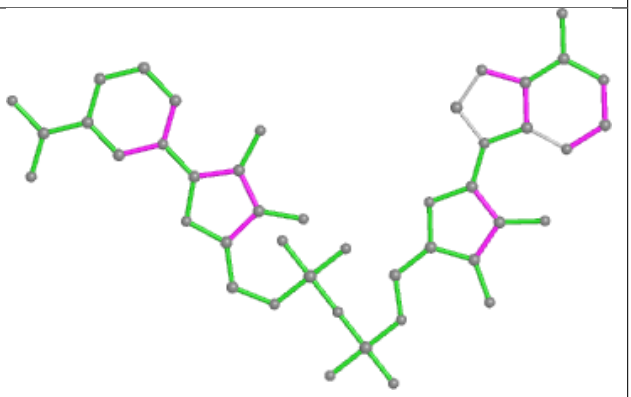
Ligand NAD C 2601



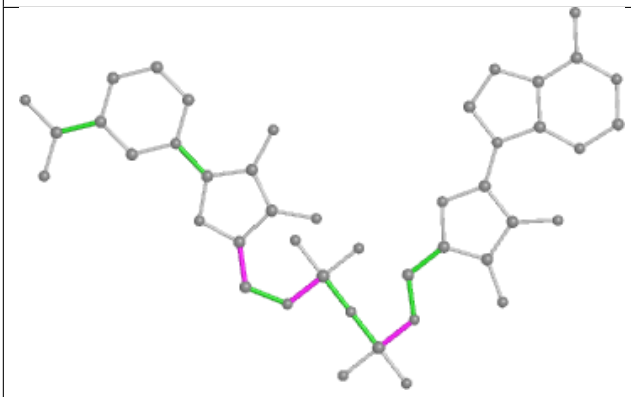
Ligand NAD E 4602



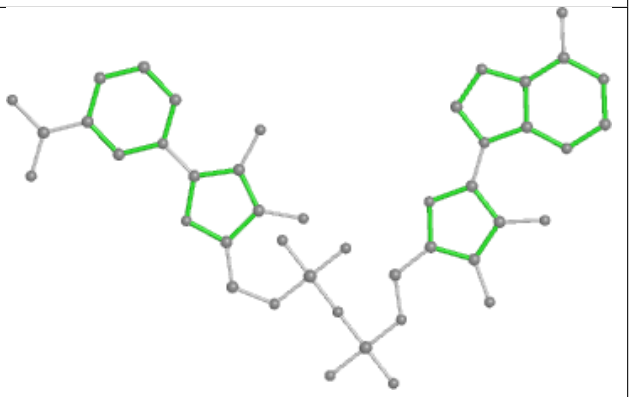
Bond lengths



Bond angles

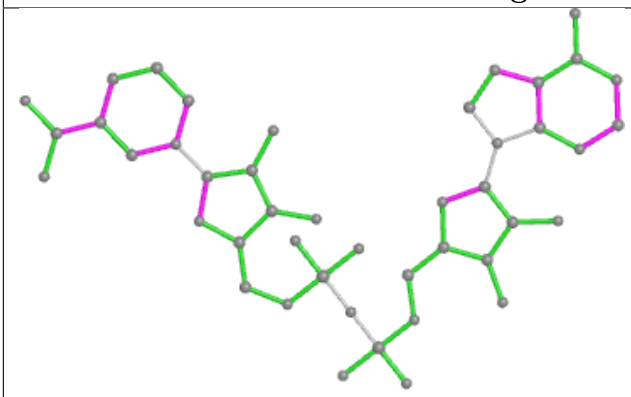


Torsions

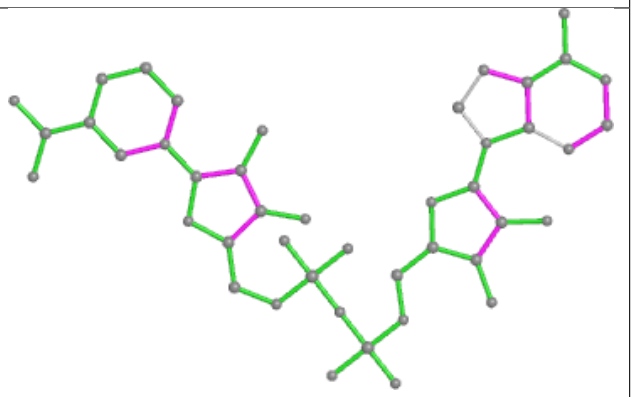


Rings

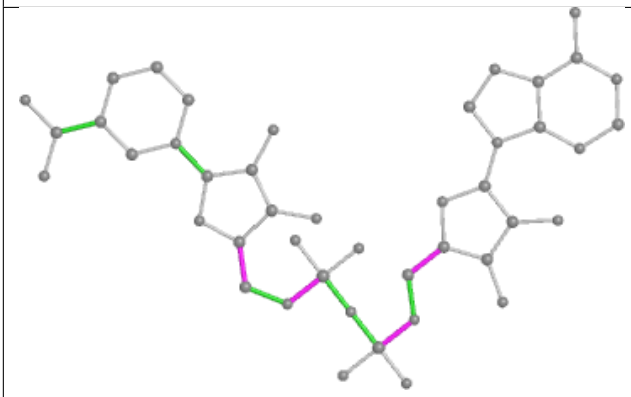
Ligand NAD D 3602



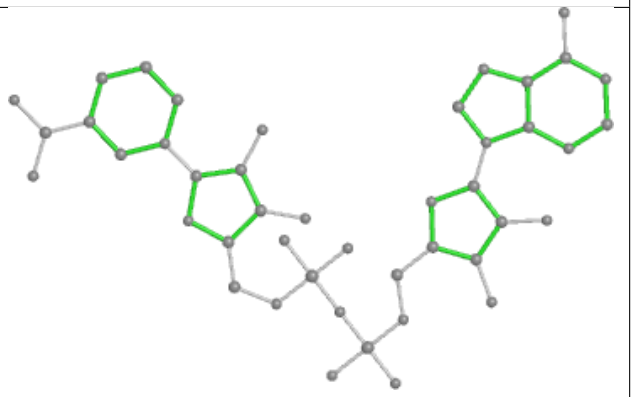
Bond lengths



Bond angles

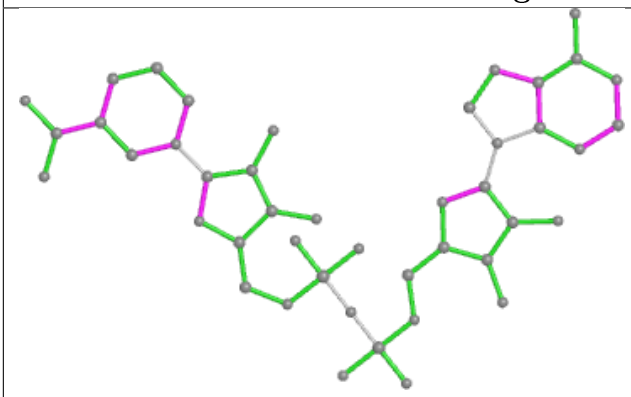


Torsions

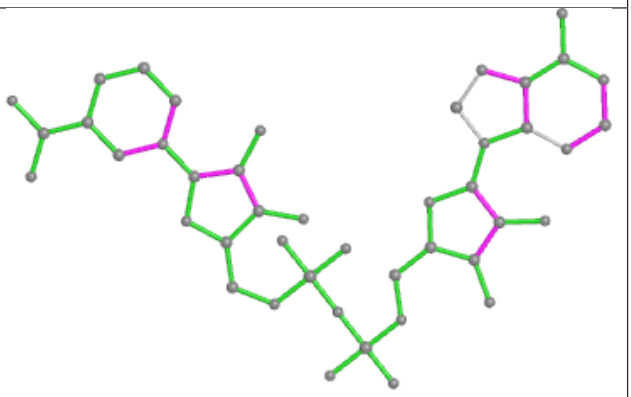


Rings

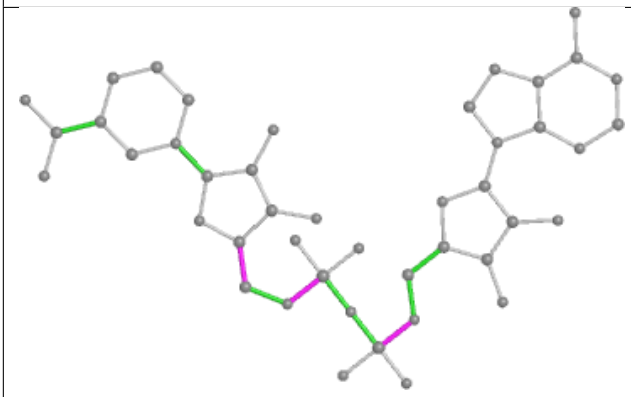
Ligand NAD F 5602



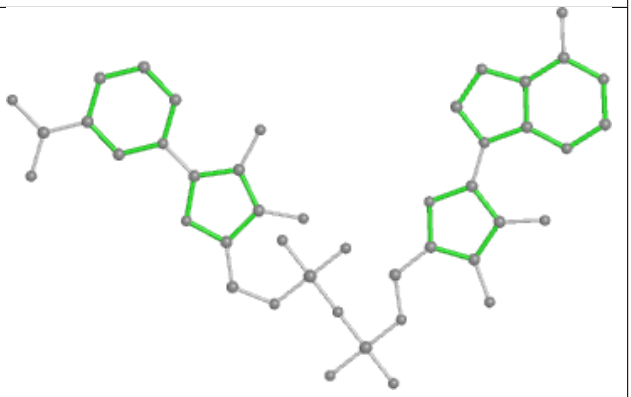
Bond lengths



Bond angles

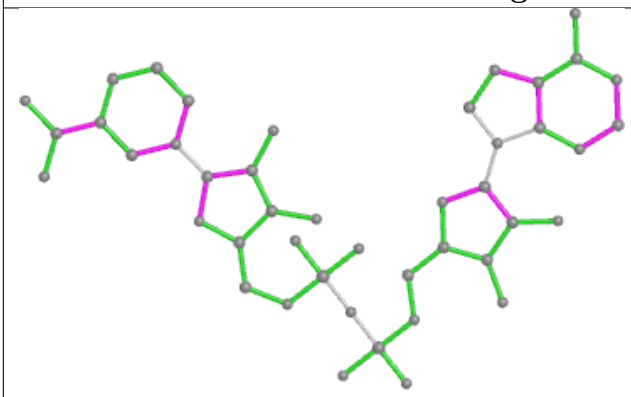


Torsions

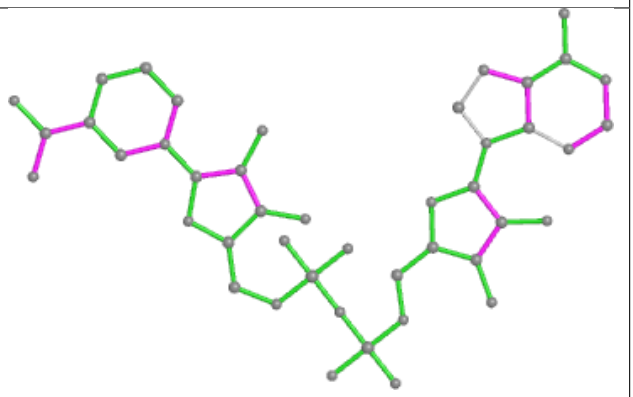


Rings

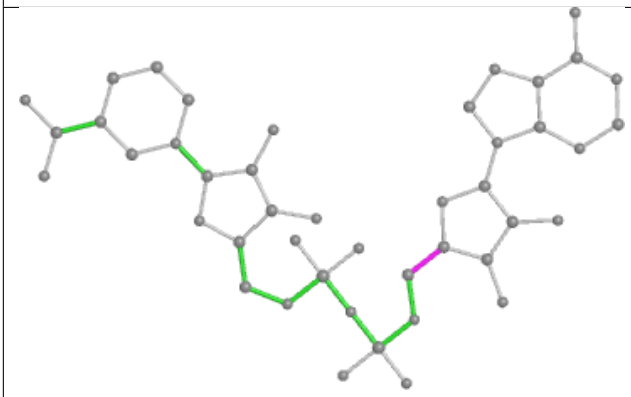
Ligand NAD H 7601



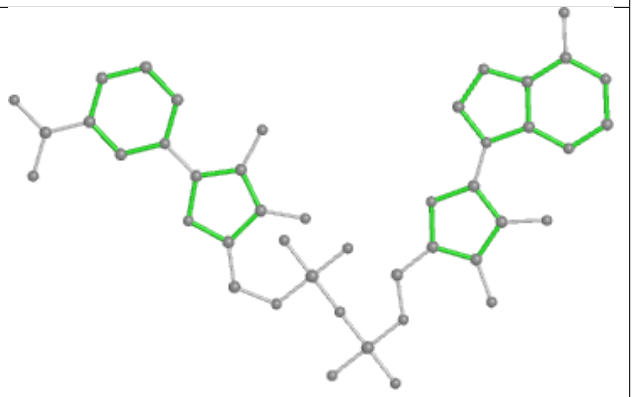
Bond lengths



Bond angles

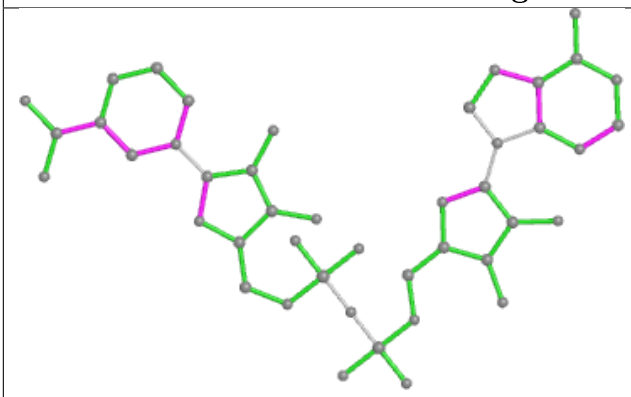


Torsions

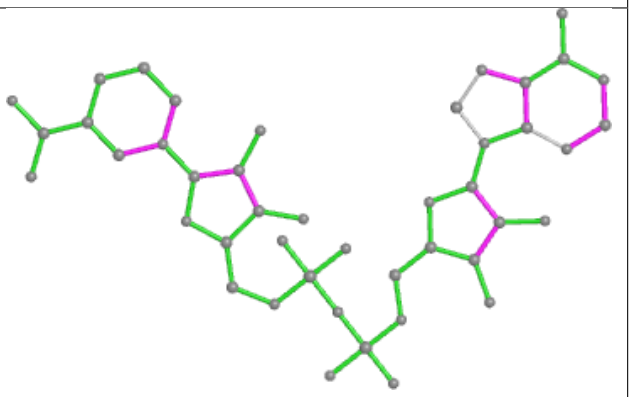


Rings

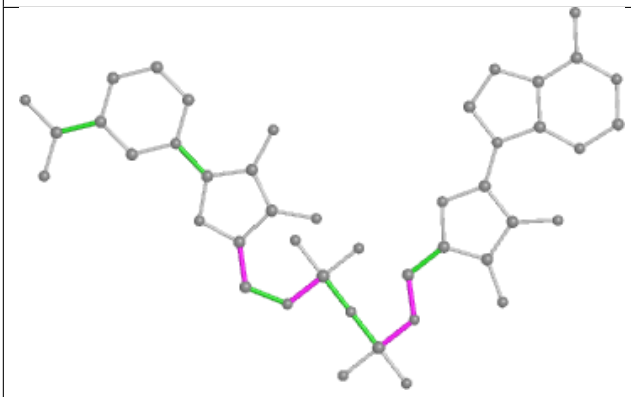
Ligand NAD B 1602



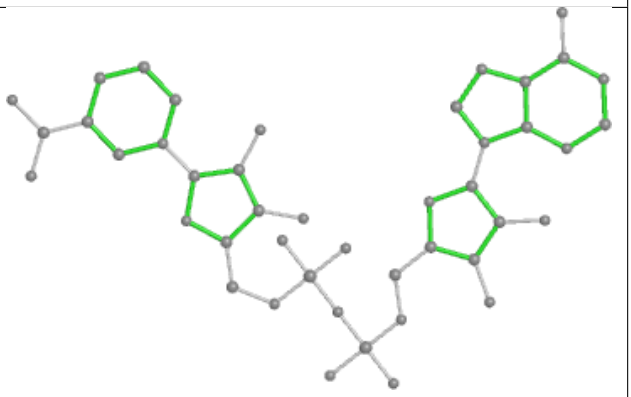
Bond lengths



Bond angles

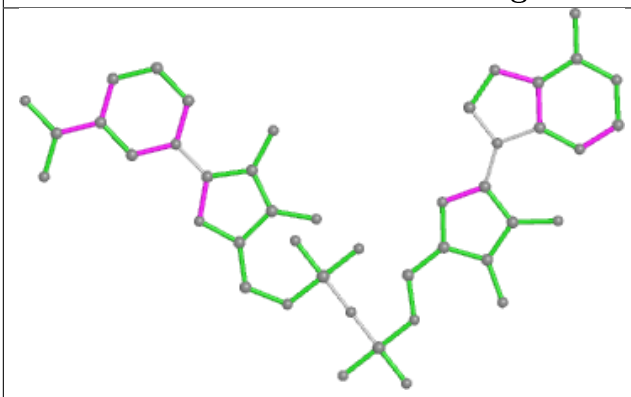


Torsions

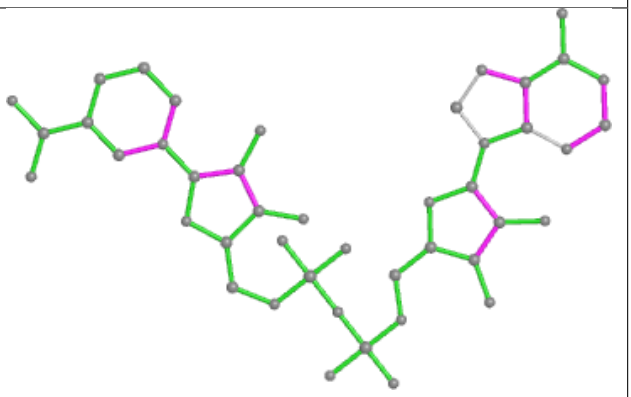


Rings

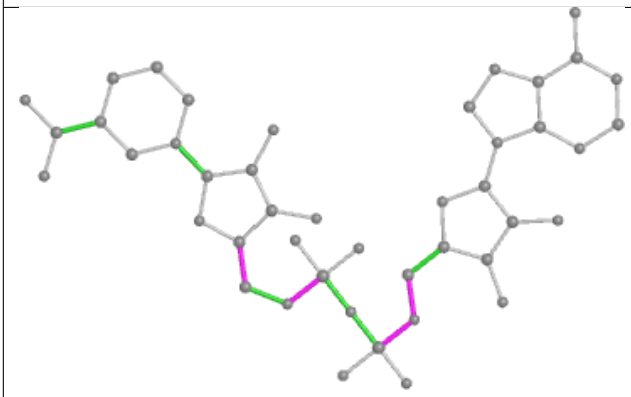
Ligand NAD G 6602



Bond lengths



Bond angles



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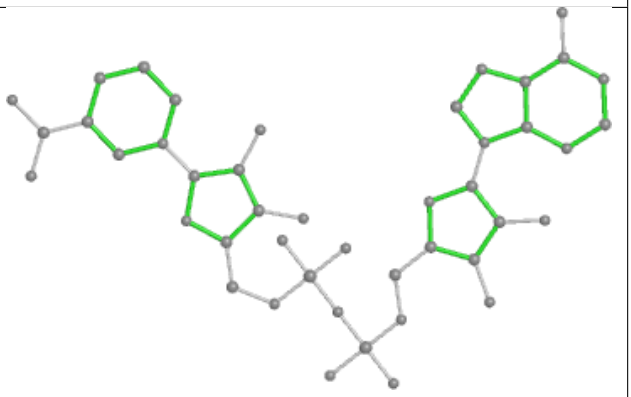
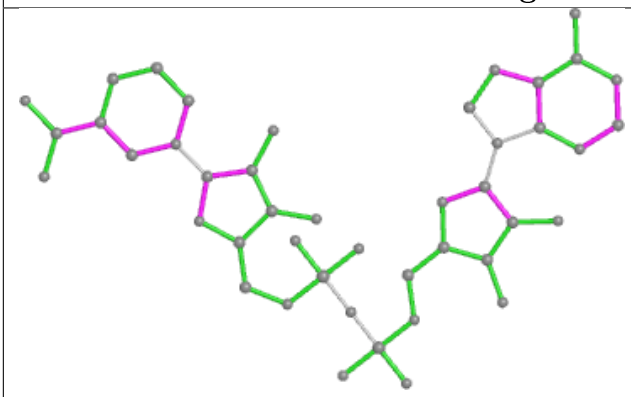
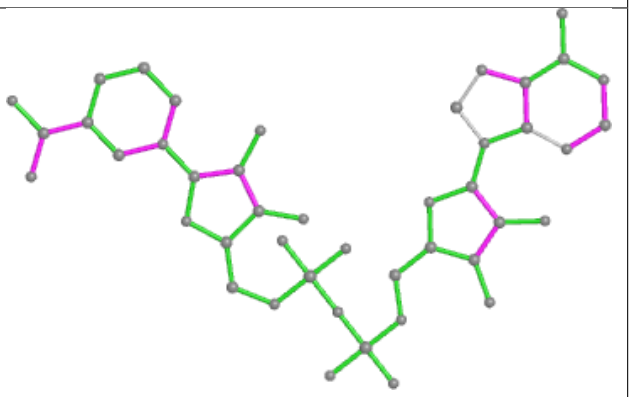


Rings

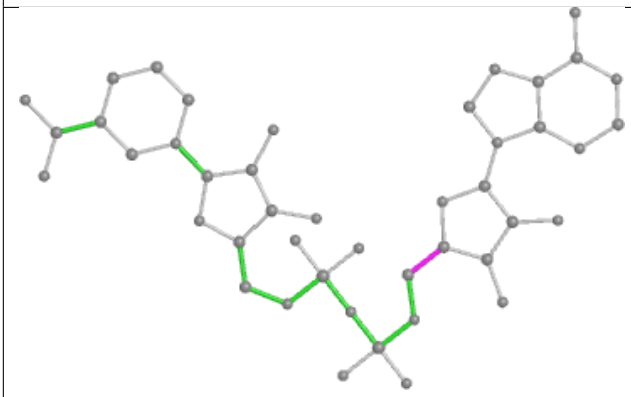
Ligand NAD A 601



Bond lengths



Bond angles



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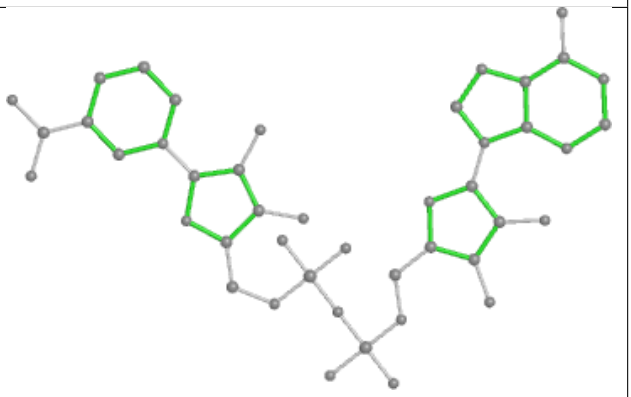
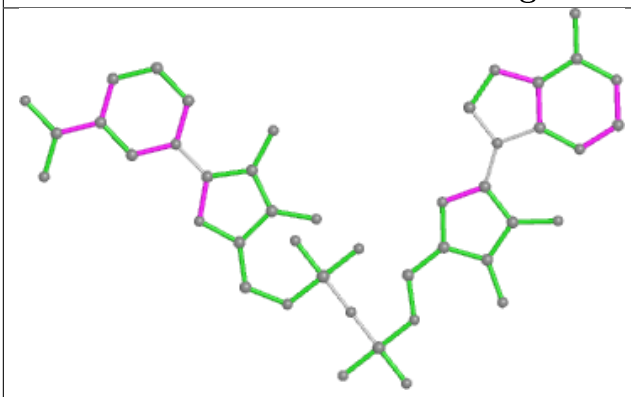
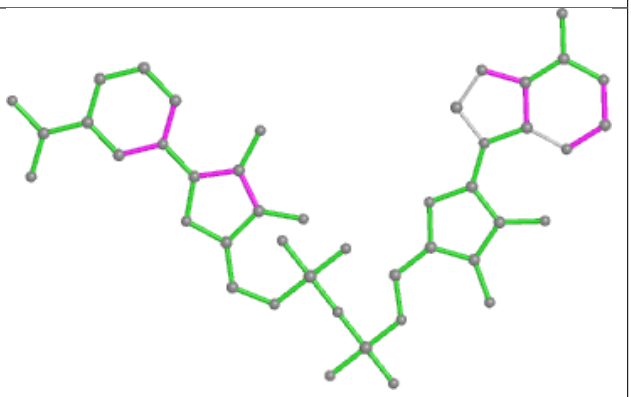


Rings

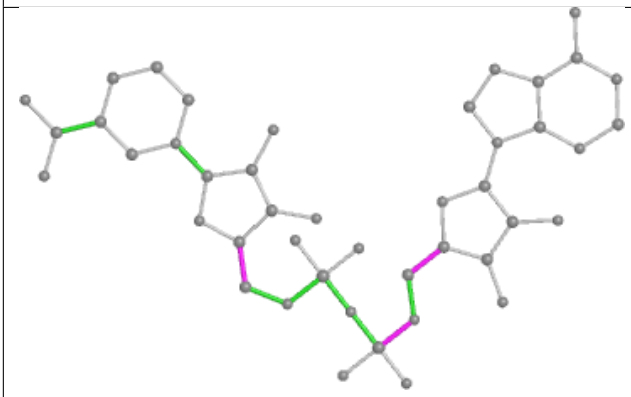
Ligand NAD A 602



Bond lengths



Bond angles



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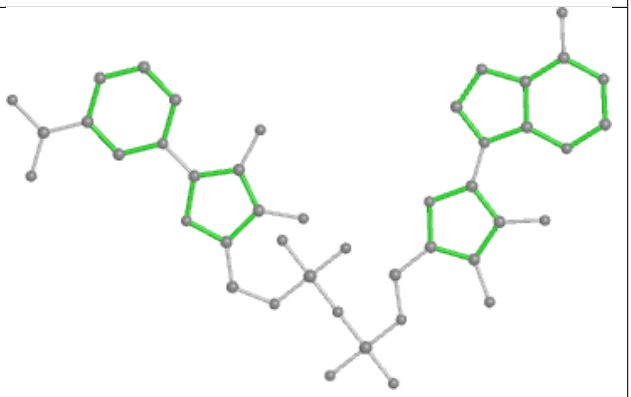
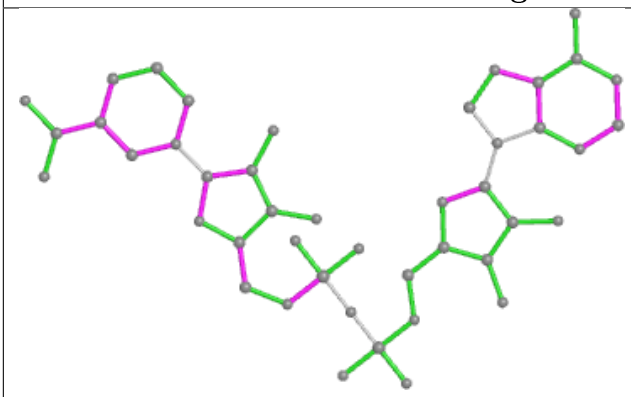
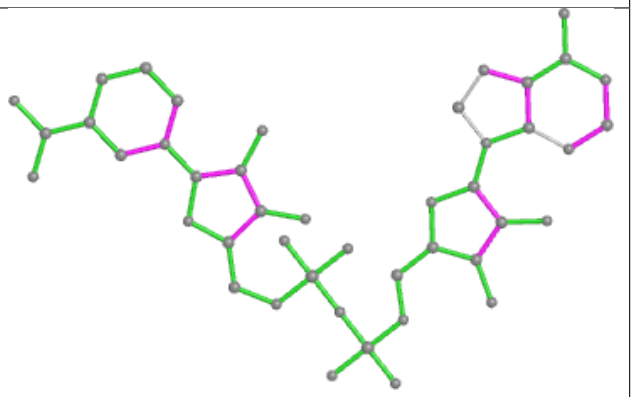


Rings

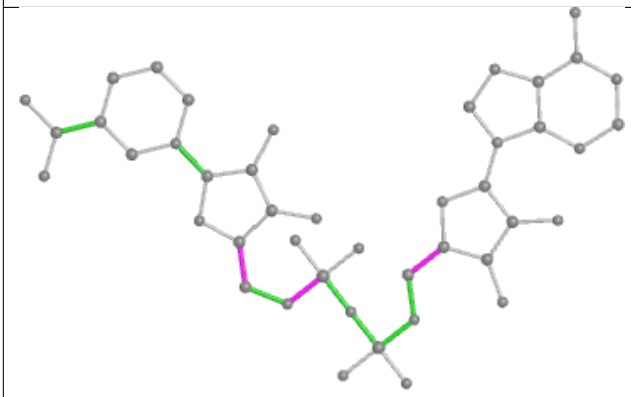
Ligand NAD D 3601



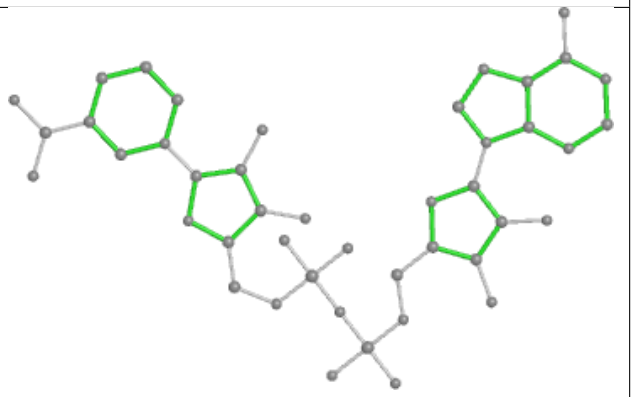
Bond lengths



Bond angles

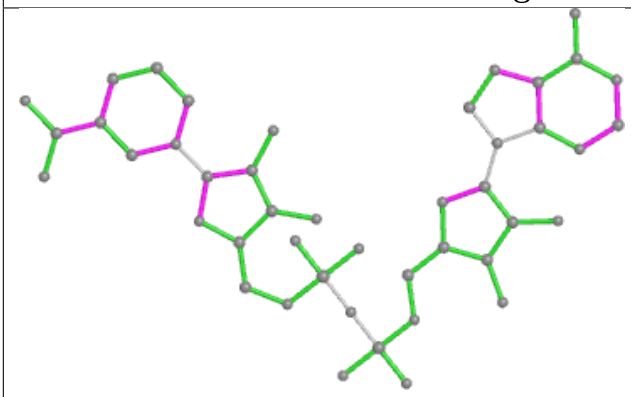


Torsions

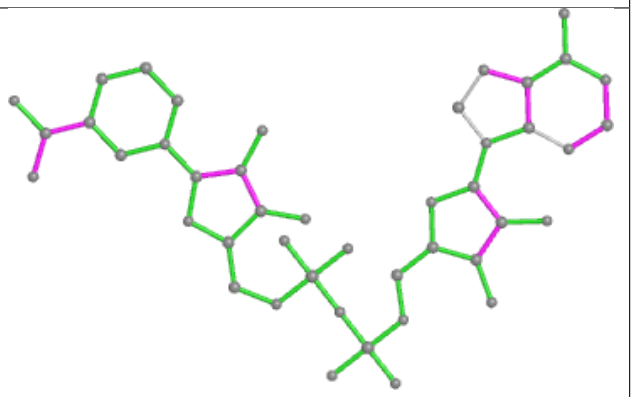


Rings

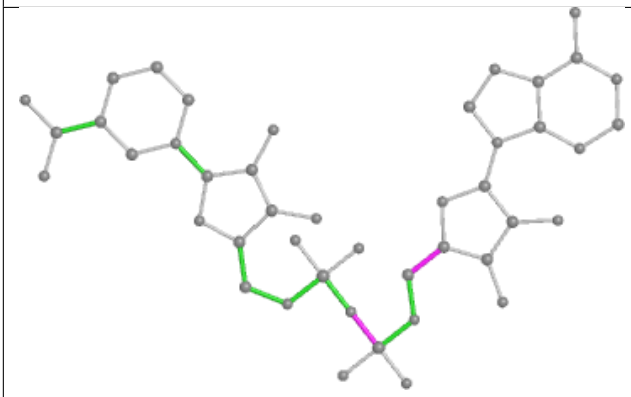
Ligand NAD F 5601



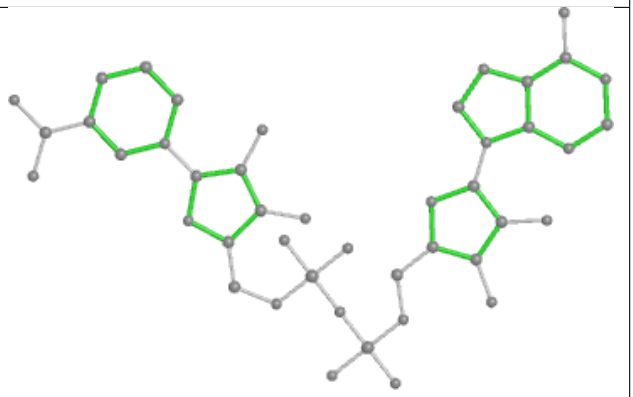
Bond lengths



Bond angles

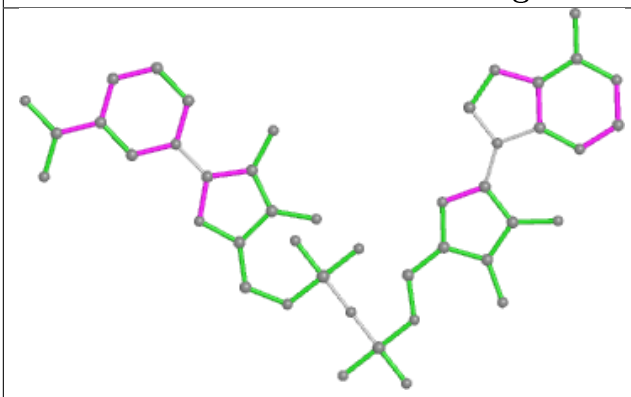


Torsions

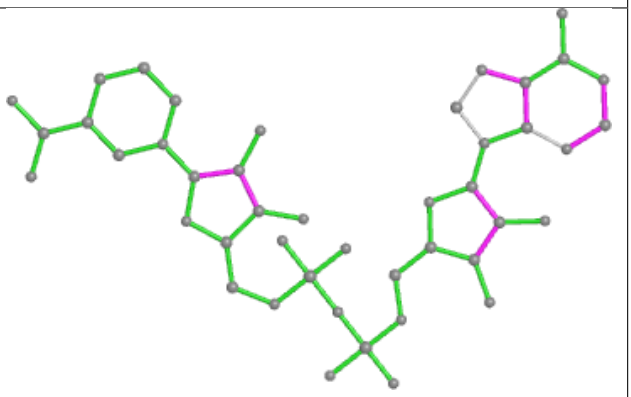


Rings

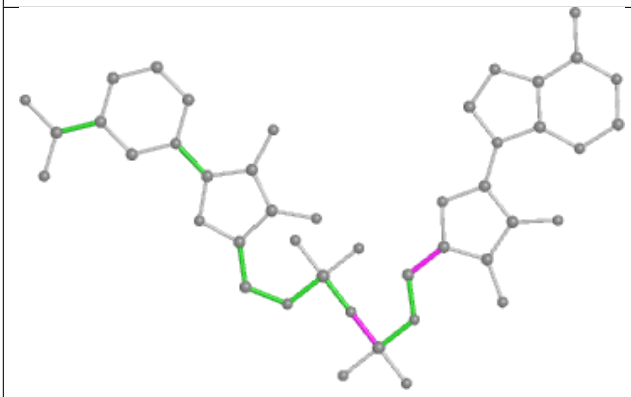
Ligand NAD E 4601



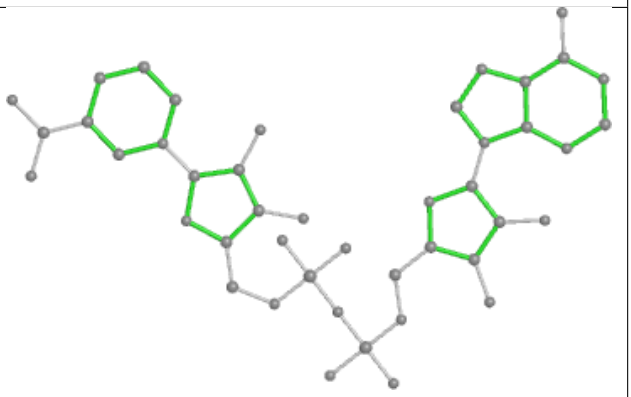
Bond lengths



Bond angles

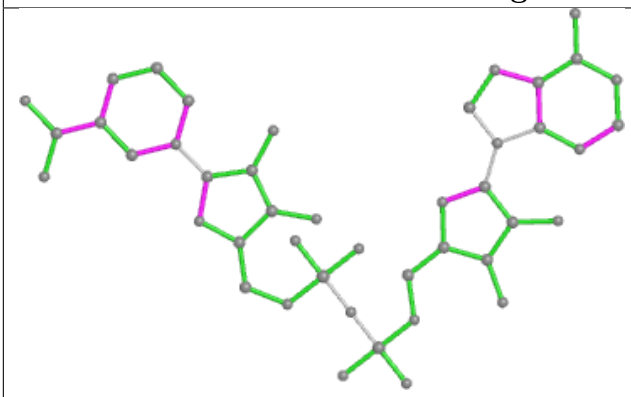


Torsions

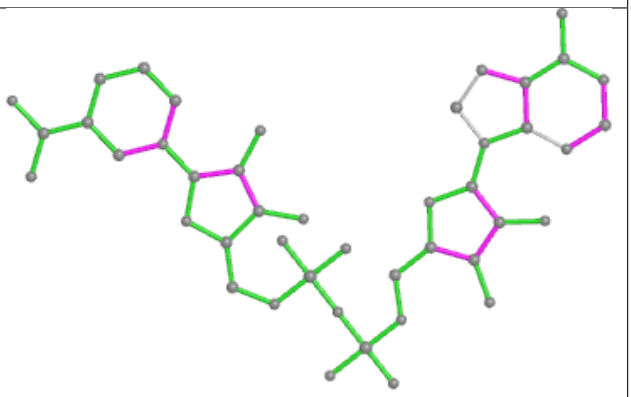


Rings

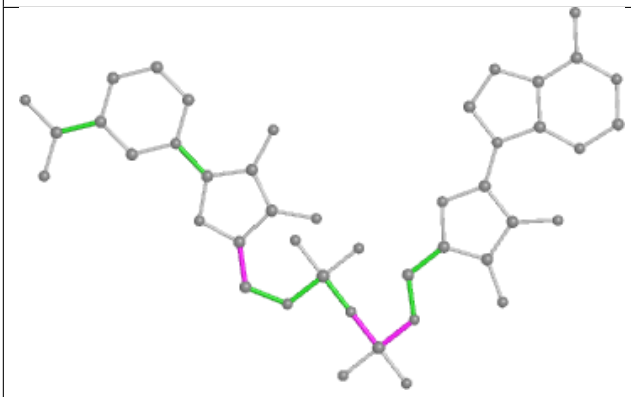
Ligand NAD H 7602



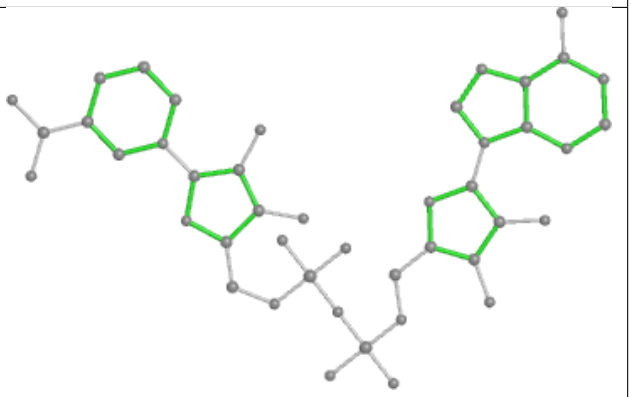
Bond lengths



Bond angles

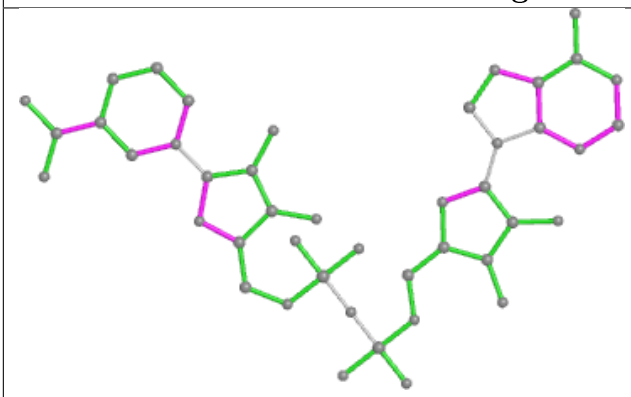


Torsions

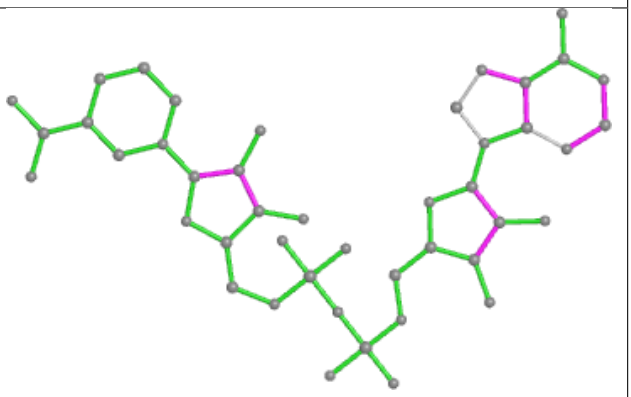


Rings

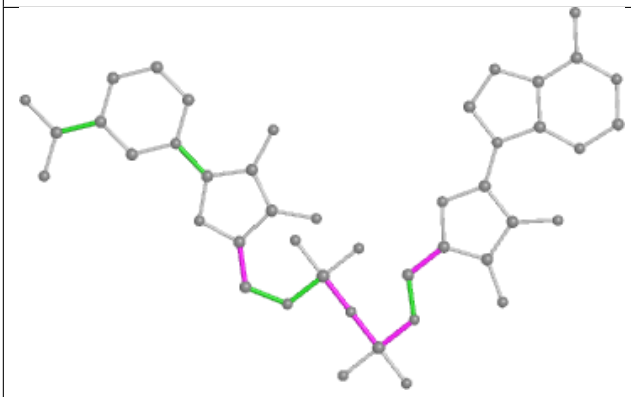
Ligand NAD B 1601



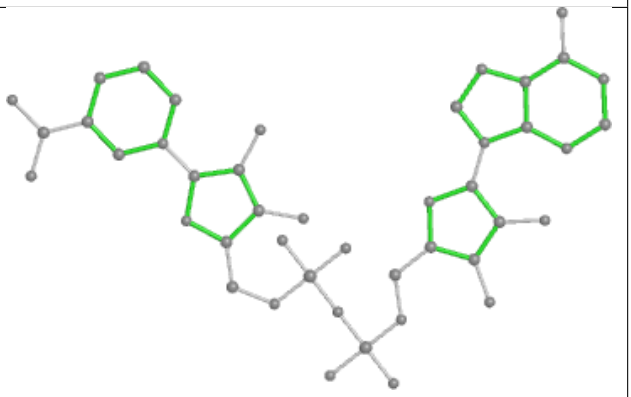
Bond lengths



Bond angles

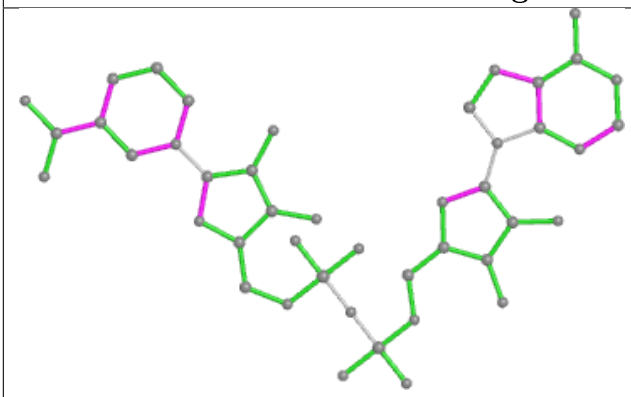


Torsions

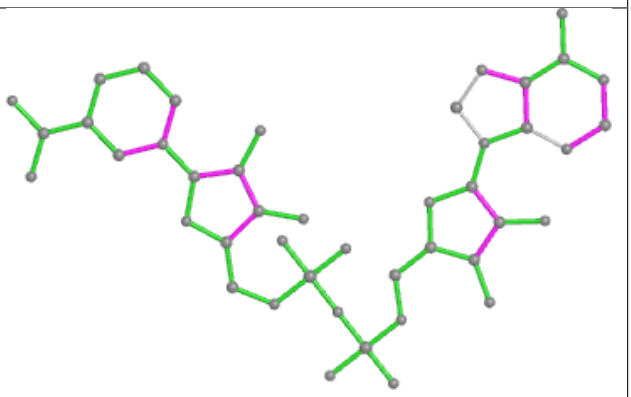


Rings

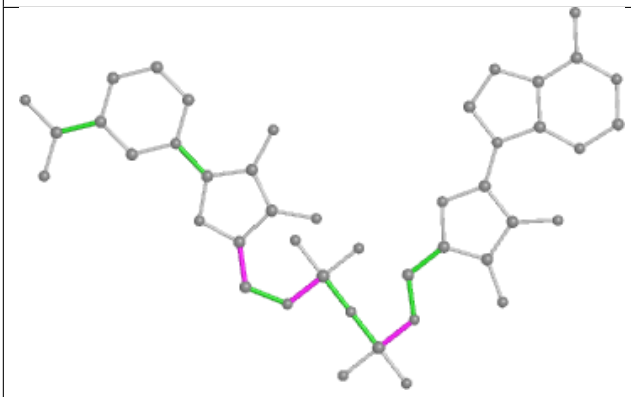
Ligand NAD C 2602



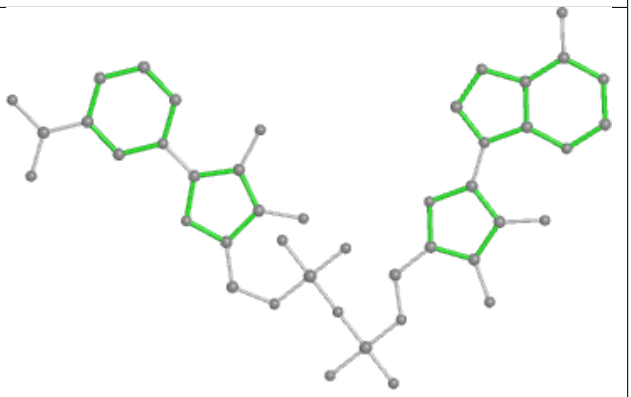
Bond lengths



Bond angles

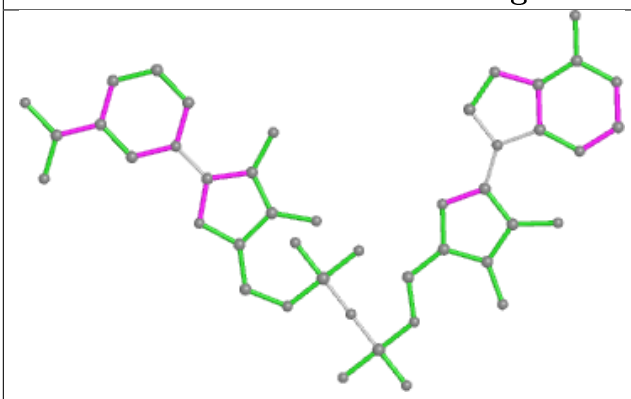


Torsions

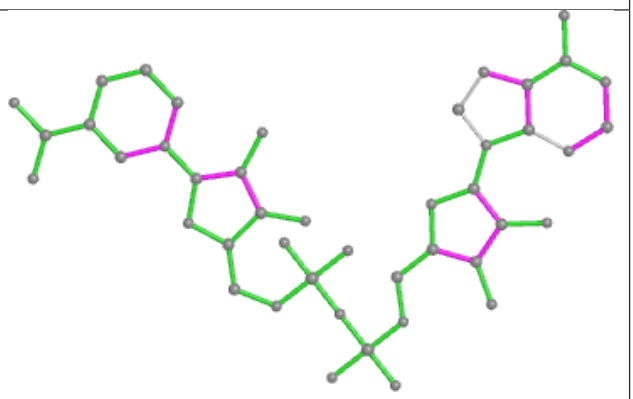


Rings

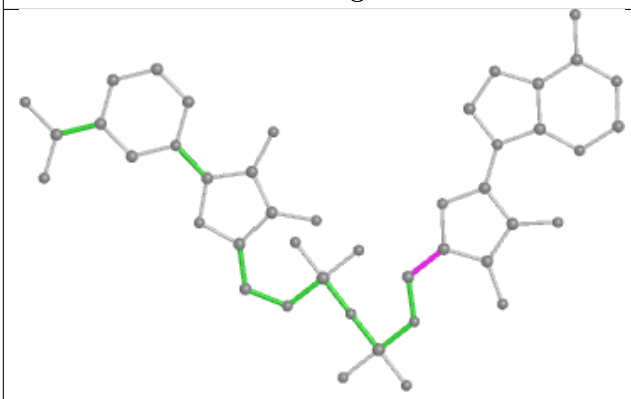
Ligand NAD G 6601



Bond lengths



Bond angles



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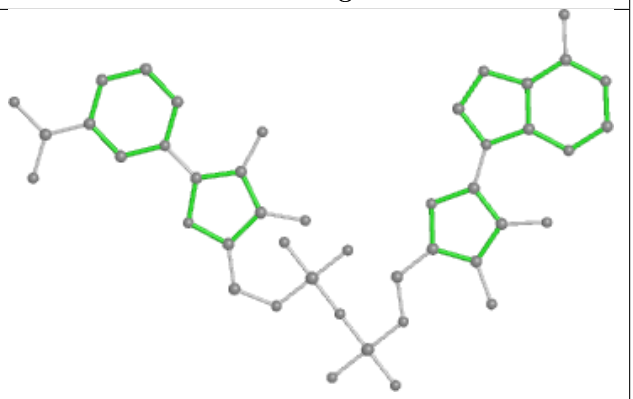

Rings

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.