wwPDB X-ray Structure Validation Summary Report (i)

Mar 4, 2024 – 02:11 AM EST

PDB ID	:	1DO8
Title	:	CRYSTAL STRUCTURE OF A CLOSED FORM OF HUMAN MITOCHONDRIAL NAD(P)+-DEPENDENT MALIC ENZYME
Authors	:	Yang, Z.; Floyd, D.L.; Loeber, G.; Tong, L.
Deposited on	:	1999-12-19
Resolution	:	2.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

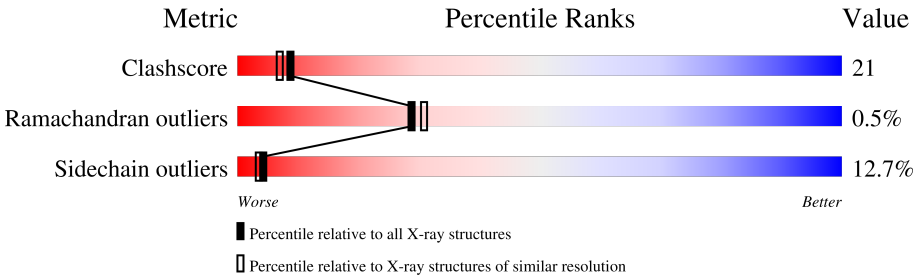
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	564	59% 31% 8% •
1	B	564	57% 35% 5% •
1	C	564	63% 30% 5% •
1	D	564	63% 28% 7% •

2 Entry composition (i)

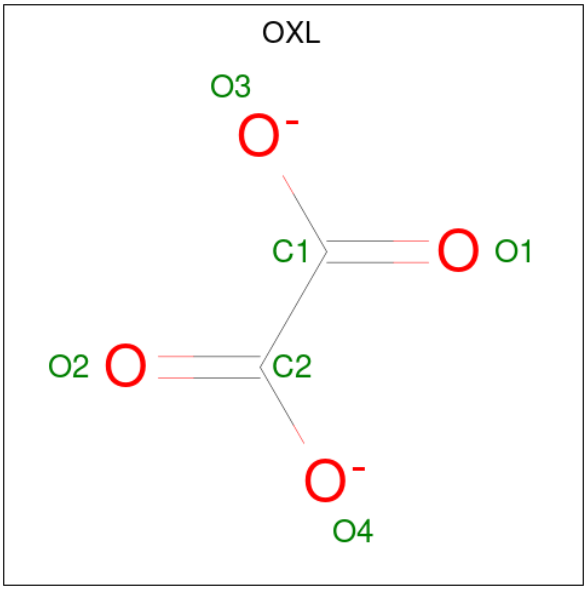
There are 5 unique types of molecules in this entry. The entry contains 18807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	B	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	C	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	D	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	2	4		
2	B	1	Total	C	O	0	0
			6	2	4		

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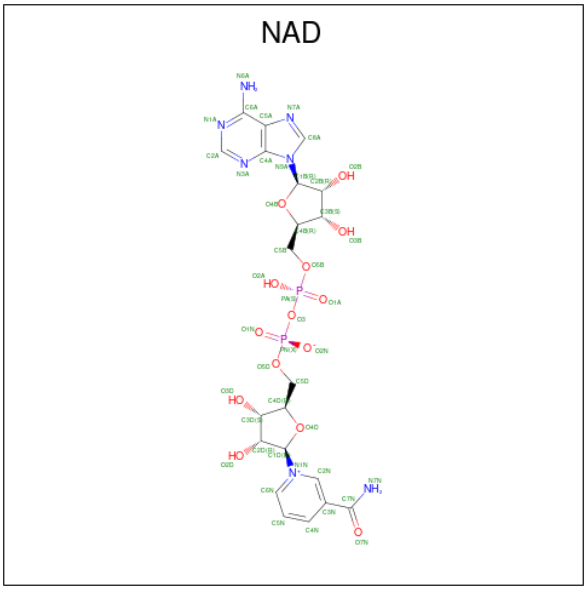
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 6 2 4	0	0
2	D	1	Total C O 6 2 4	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 44 21 7 14 2	0	0
4	A	1	Total C N O P 44 21 7 14 2	9	0
4	B	1	Total C N O P 44 21 7 14 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	9	0
			44	21	7	14	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total	O	0	0
			239	239		
5	B	199	Total	O	0	0
			199	199		
5	C	275	Total	O	0	0
			275	275		
5	D	246	Total	O	0	0
			246	246		

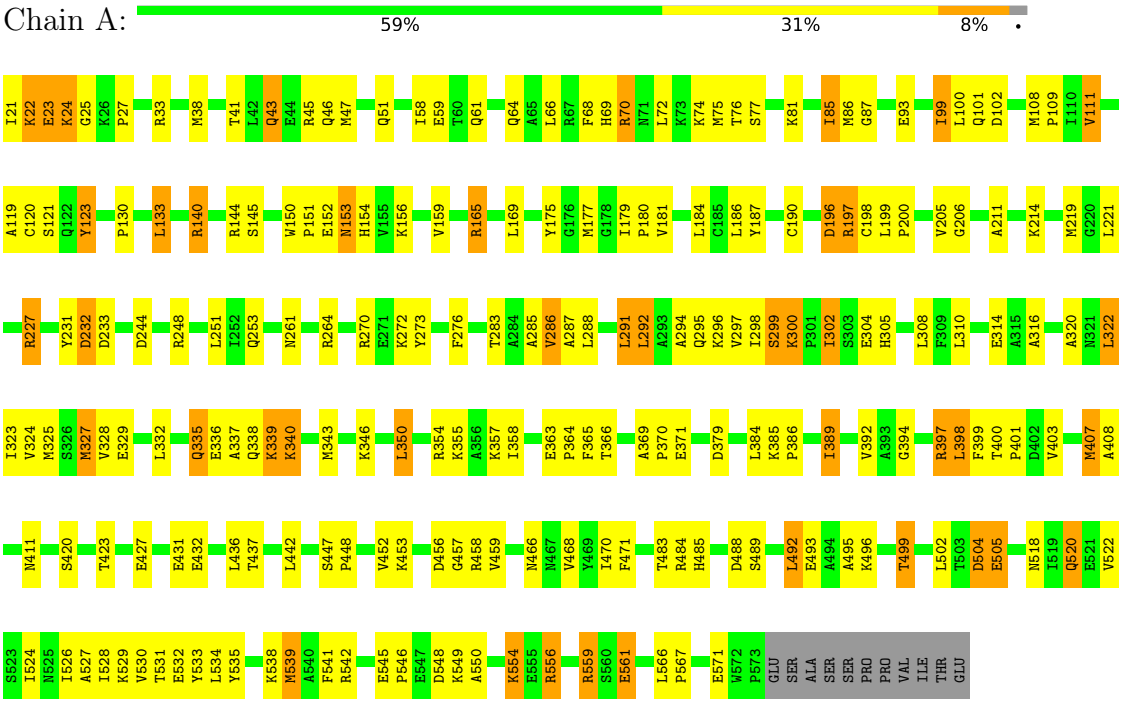
3 Residue-property plots (i)

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. 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.

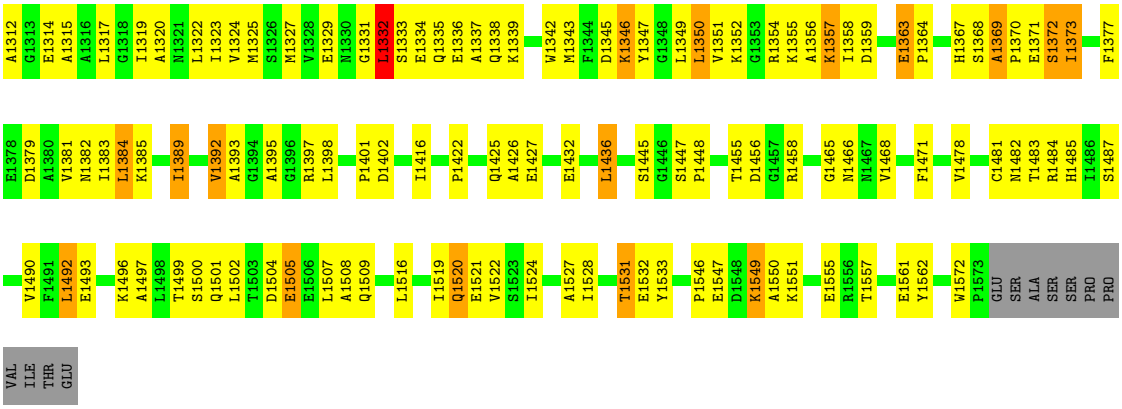
• Molecule 1: MALIC ENZYME

Chain A:



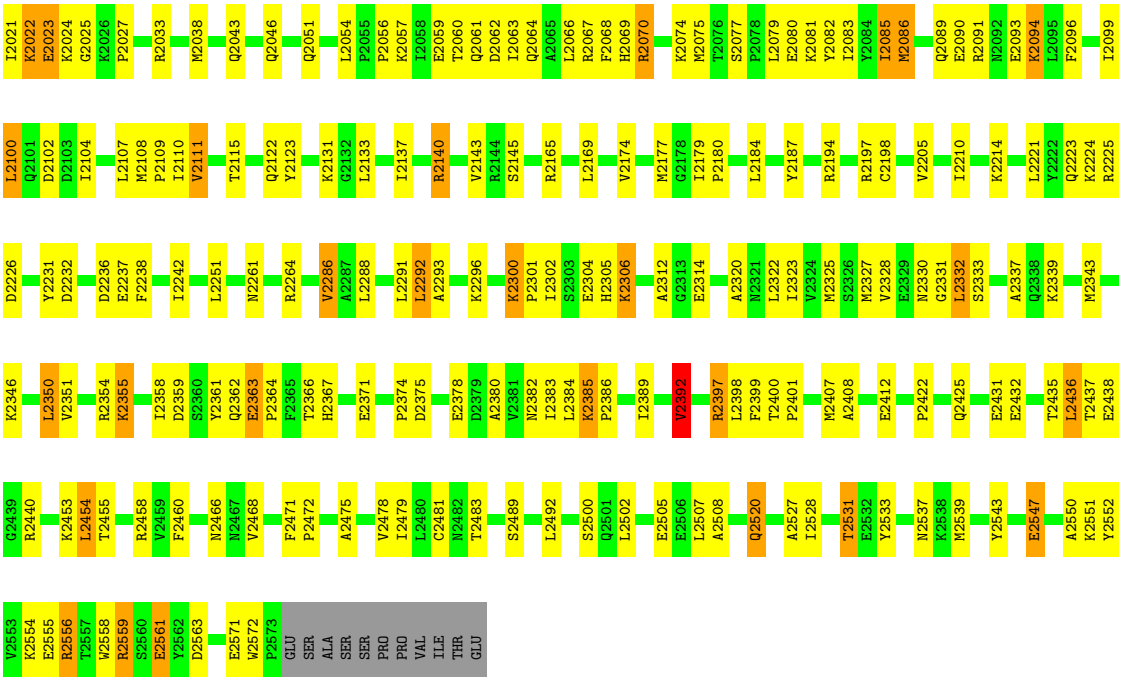
• Molecule 1: MALIC ENZYME

Chain B:



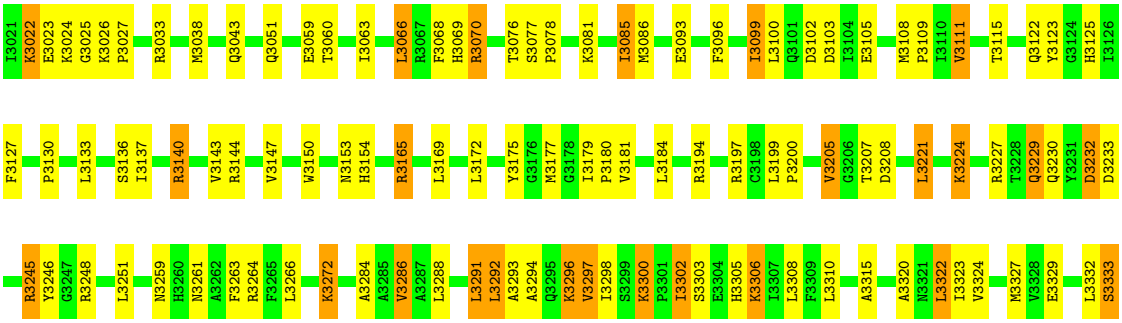
• Molecule 1: MALIC ENZYME

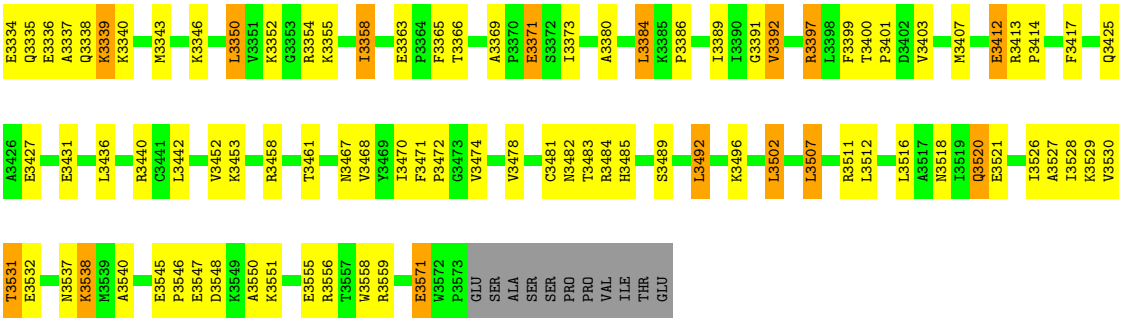
Chain C:



• Molecule 1: MALIC ENZYME

Chain D:




E3334 Q3335 E3336 A3337 Q3338 K3339 K3340 M3343 K3346 L3350 V3351 K3352 G3353 R3354 K3355 I3358 E3363 P3364 F3365 T3366 A3369 P3370 E3371 S3372 I3373 A3380 L3384 K3385 P3386 I3389 I3390 G3391 V3392 R3397 L3398 F3399 T3400 P3401 D3402 V3403 M3407 E3412 R3413 P3414 F3417 Q3425
A3426 E3427 E3431 L3436 R3440 C3441 L3442 V3452 K3453 R3458 T3461 N3467 V3468 Y3469 I3470 F3471 P3472 G3473 V3474 V3478 C3481 N3482 T3483 R3484 H3485 S3489 L3492 K3496 L3502 L3507 R3511 L3512 L3516 A3517 N3518 I3519 Q3520 E3521 I3526 A3527 I3528 K3529 V3530
T3531 E3532 N3537 K3538 M3539 A3540 E3545 P3546 E3547 D3548 K3549 A3550 K3551 E3555 R3556 T3557 W3558 R3559 E3571 W3572 P3573 GLU SER ALA SER SER PRO 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	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	229.00Å 118.70Å 113.00Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18807	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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: NAD, OXL, MN

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	0.37	0/4447	0.61	0/5998
1	B	0.37	0/4447	0.61	0/5998
1	C	0.38	0/4447	0.61	0/5998
1	D	0.38	0/4447	0.60	0/5998
All	All	0.37	0/17788	0.61	0/23992

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4367	0	4407	203	0
1	B	4367	0	4407	229	0
1	C	4367	0	4407	141	0
1	D	4367	0	4407	179	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	88	0	52	2	0
4	B	88	0	52	3	0
4	C	88	0	52	2	0
4	D	88	0	52	1	0
5	A	239	0	0	14	0
5	B	199	0	0	30	0
5	C	275	0	0	18	0
5	D	246	0	0	12	0
All	All	18807	0	17836	731	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 21.

The worst 5 of 731 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MSE:HE2	1:A:181:VAL:HG23	1.29	1.14
1:D:3177:MSE:HE2	1:D:3181:VAL:HG23	1.35	1.08
1:A:123:TYR:HD2	1:A:219:MSE:HE1	1.18	1.06
1:B:1358:ILE:HG22	5:B:4650:HOH:O	1.54	1.06
1:A:140:ARG:HH22	1:A:233:ASP:HB3	1.14	1.05

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	551/564 (98%)	530 (96%)	19 (3%)	2 (0%)	34 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	551/564 (98%)	522 (95%)	26 (5%)	3 (0%)	29	31
1	C	551/564 (98%)	530 (96%)	17 (3%)	4 (1%)	22	22
1	D	551/564 (98%)	528 (96%)	20 (4%)	3 (0%)	29	31
All	All	2204/2256 (98%)	2110 (96%)	82 (4%)	12 (0%)	29	31

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1332	LEU
1	C	2332	LEU
1	A	397	ARG
1	C	2392	VAL
1	D	3302	ILE

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	469/465 (101%)	406 (87%)	63 (13%)	4	3
1	B	469/465 (101%)	412 (88%)	57 (12%)	5	4
1	C	469/465 (101%)	409 (87%)	60 (13%)	4	3
1	D	469/465 (101%)	410 (87%)	59 (13%)	4	3
All	All	1876/1860 (101%)	1637 (87%)	239 (13%)	4	3

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1547	GLU
1	D	3363	GLU
1	C	2232	ASP
1	D	3355	LYS
1	D	3547	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2520	GLN
1	D	3261	ASN
1	D	3051	GLN
1	D	3125	HIS
1	D	3485	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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
2	OXL	A	603	3	5,5,5	1.67	2 (40%)	6,6,6	1.56	2 (33%)
4	NAD	C	2601	-	42,48,48	1.87	9 (21%)	50,73,73	1.29	4 (8%)
4	NAD	D	3602	-	42,48,48	2.08	9 (21%)	50,73,73	1.51	6 (12%)
2	OXL	B	1603	3	5,5,5	1.53	2 (40%)	6,6,6	1.71	2 (33%)
4	NAD	A	602	-	42,48,48	2.19	13 (30%)	50,73,73	1.48	6 (12%)
4	NAD	C	2602	-	42,48,48	2.79	12 (28%)	50,73,73	1.56	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAD	B	1602	-	42,48,48	2.18	11 (26%)	50,73,73	1.42	6 (12%)
4	NAD	A	601	-	42,48,48	2.04	12 (28%)	50,73,73	1.26	3 (6%)
2	OXL	D	3603	3	5,5,5	1.56	2 (40%)	6,6,6	1.61	2 (33%)
4	NAD	D	3601	-	42,48,48	2.04	11 (26%)	50,73,73	1.29	4 (8%)
2	OXL	C	2603	3	5,5,5	1.51	2 (40%)	6,6,6	1.66	2 (33%)
4	NAD	B	1601	-	42,48,48	1.94	13 (30%)	50,73,73	1.36	5 (10%)

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	OXL	A	603	3	-	0/4/4/4	-
4	NAD	C	2601	-	-	2/26/62/62	0/5/5/5
4	NAD	D	3602	-	-	6/26/62/62	0/5/5/5
2	OXL	B	1603	3	-	0/4/4/4	-
4	NAD	A	602	-	-	7/26/62/62	0/5/5/5
4	NAD	C	2602	-	-	7/26/62/62	0/5/5/5
4	NAD	B	1602	-	-	6/26/62/62	0/5/5/5
4	NAD	A	601	-	-	2/26/62/62	0/5/5/5
2	OXL	D	3603	3	-	0/4/4/4	-
4	NAD	D	3601	-	-	2/26/62/62	0/5/5/5
2	OXL	C	2603	3	-	0/4/4/4	-
4	NAD	B	1601	-	-	2/26/62/62	0/5/5/5

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2602	NAD	C2N-N1N	9.85	1.47	1.35
4	A	602	NAD	C2N-N1N	7.88	1.44	1.35
4	B	1602	NAD	C2N-N1N	7.15	1.43	1.35
4	B	1602	NAD	O4D-C1D	7.15	1.51	1.41
4	A	601	NAD	C2N-N1N	6.55	1.42	1.35

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	3602	NAD	N3A-C2A-N1A	-5.10	120.70	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	NAD	N3A-C2A-N1A	-5.06	120.76	128.68
4	B	1601	NAD	N3A-C2A-N1A	-5.06	120.77	128.68
4	C	2601	NAD	N3A-C2A-N1A	-5.05	120.79	128.68
4	B	1602	NAD	N3A-C2A-N1A	-5.02	120.83	128.68

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAD	O4D-C1D-N1N-C6N
4	A	602	NAD	C5B-O5B-PA-O1A
4	A	602	NAD	C5B-O5B-PA-O2A
4	B	1601	NAD	O4D-C1D-N1N-C6N
4	B	1602	NAD	C5B-O5B-PA-O2A

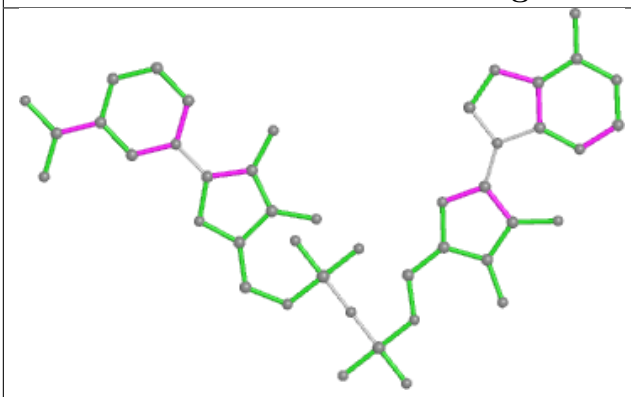
There are no ring outliers.

6 monomers are involved in 9 short contacts:

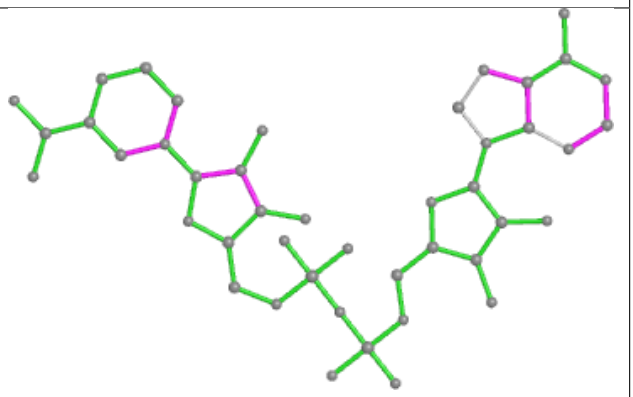
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2601	NAD	1	0
4	D	3602	NAD	1	0
4	C	2602	NAD	1	0
4	A	601	NAD	2	0
2	D	3603	OXL	1	0
4	B	1601	NAD	3	0

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

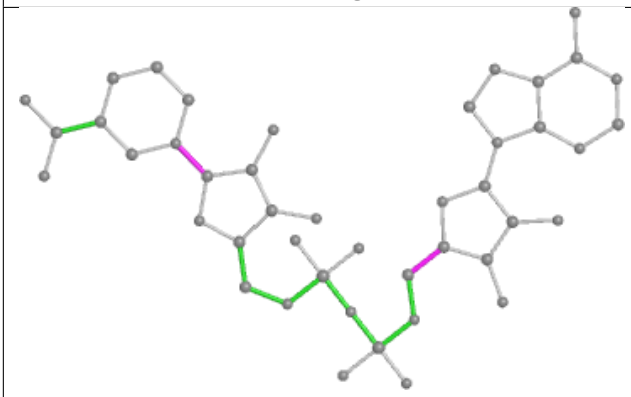
Ligand NAD C 2601



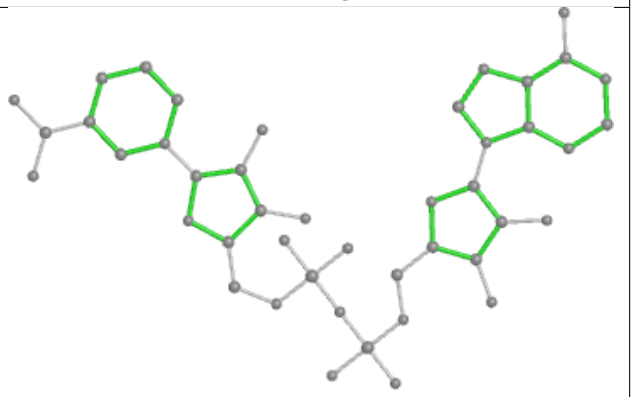
Bond lengths



Bond angles

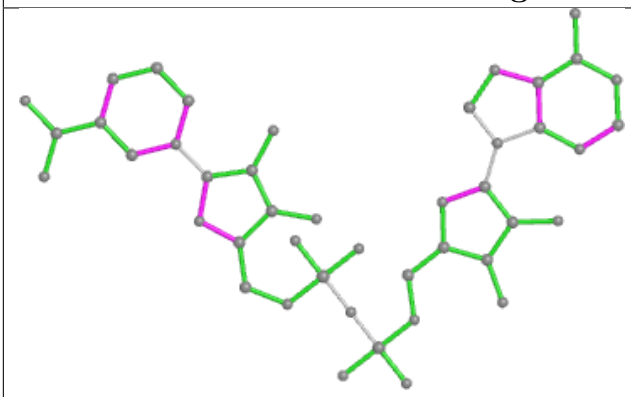


Torsions

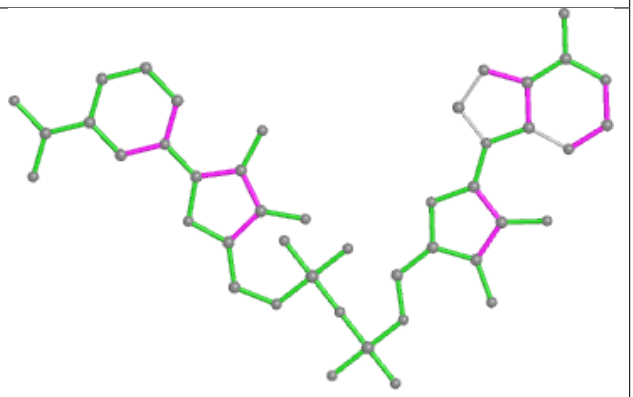


Rings

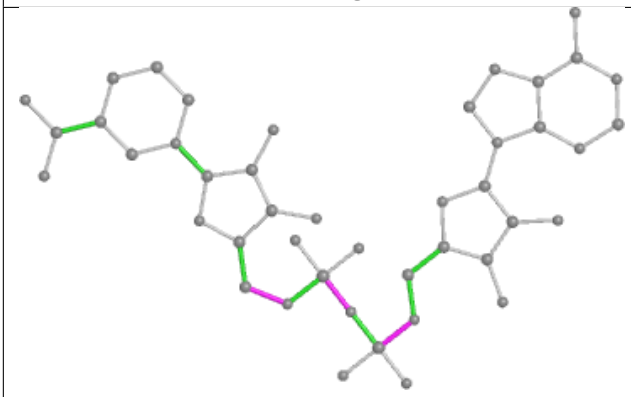
Ligand NAD D 3602



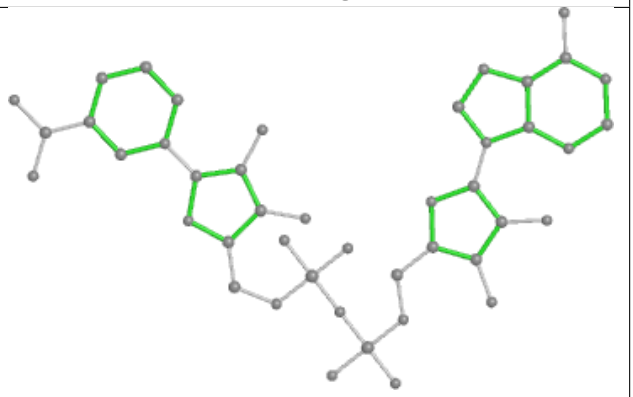
Bond lengths



Bond angles

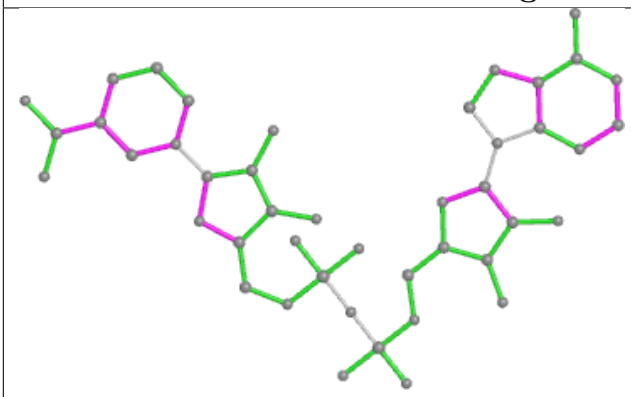


Torsions

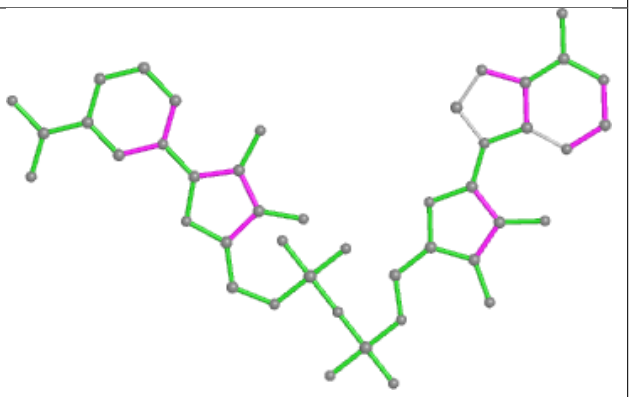


Rings

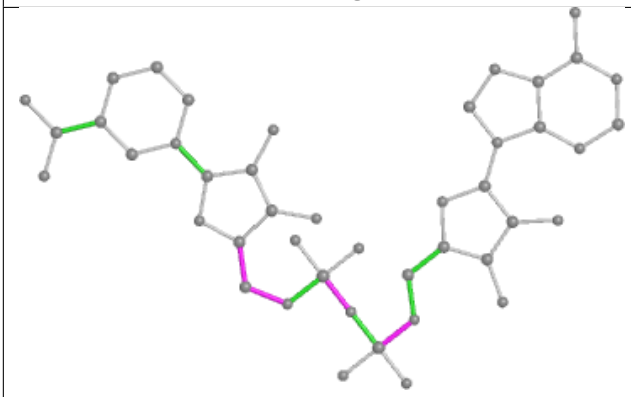
Ligand NAD A 602



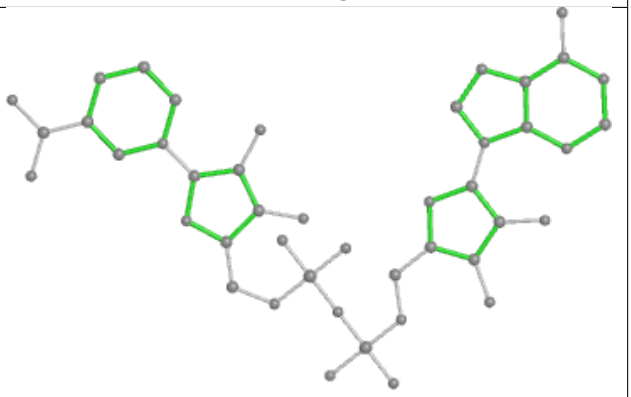
Bond lengths



Bond angles

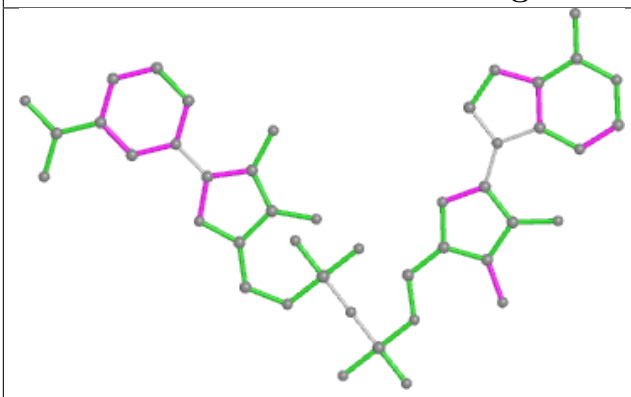


Torsions

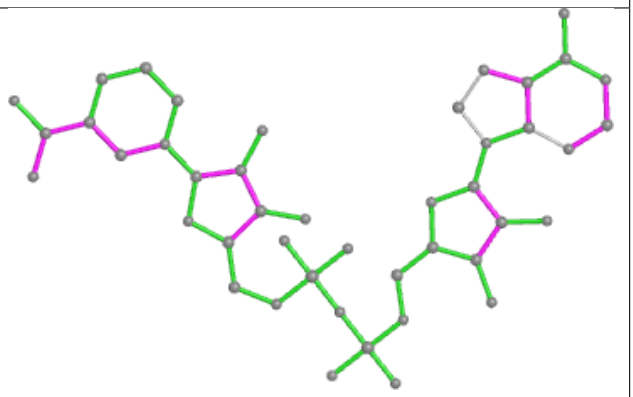


Rings

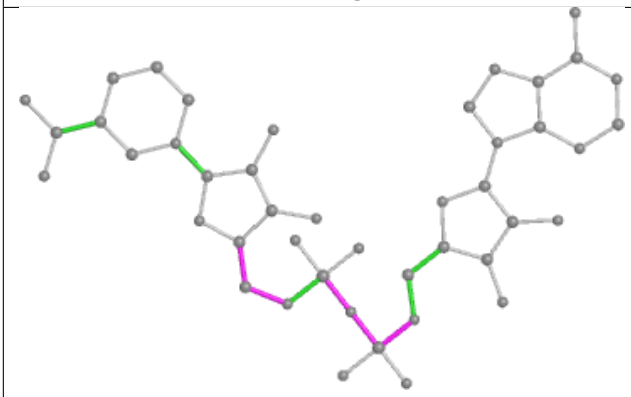
Ligand NAD C 2602



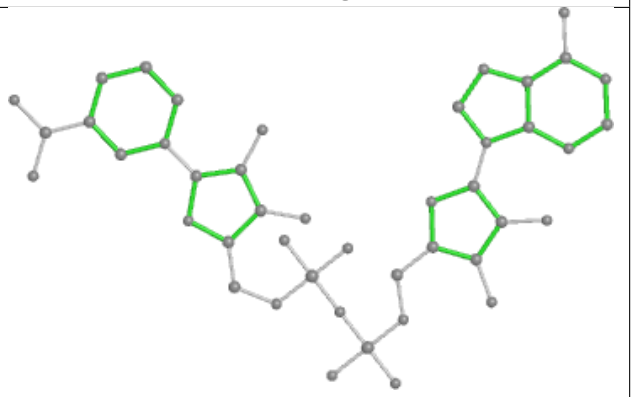
Bond lengths



Bond angles

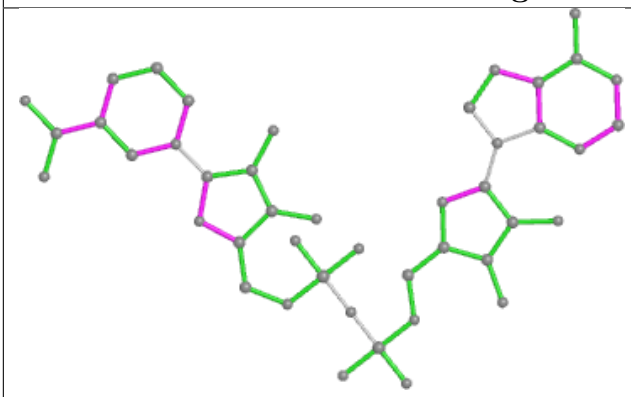


Torsions

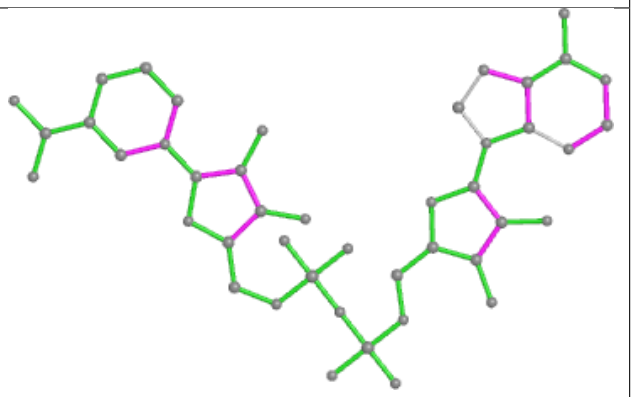


Rings

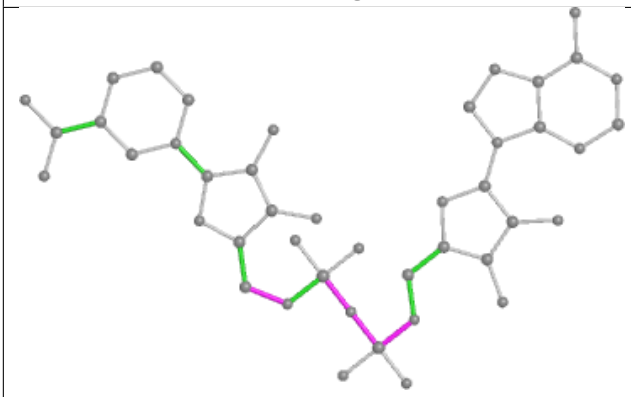
Ligand NAD B 1602



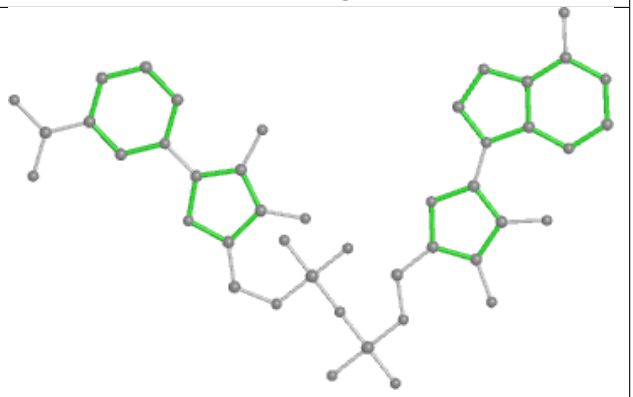
Bond lengths



Bond angles

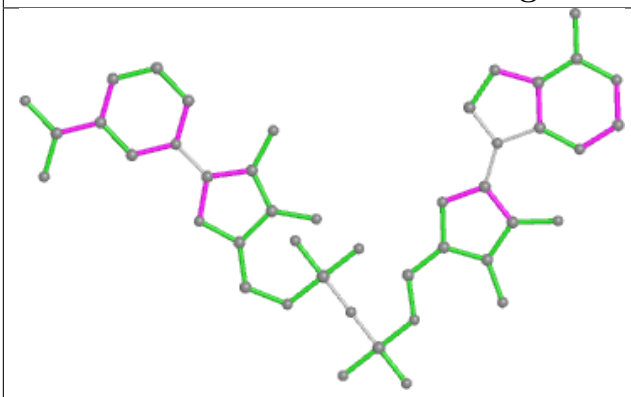


Torsions

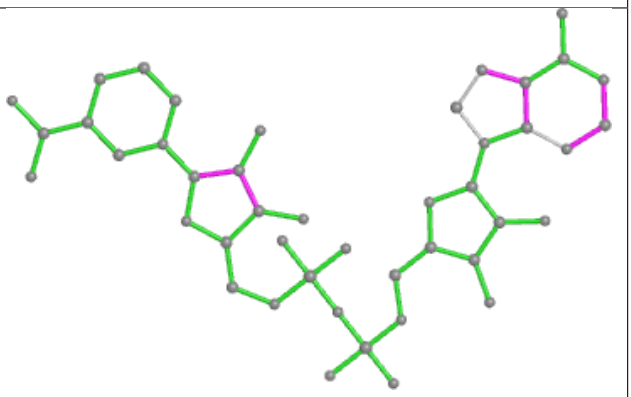


Rings

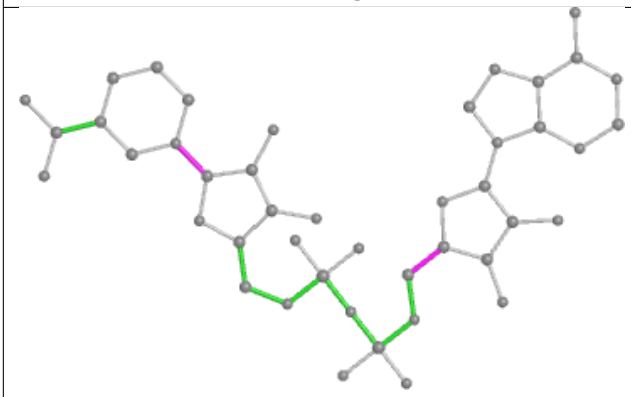
Ligand NAD A 601



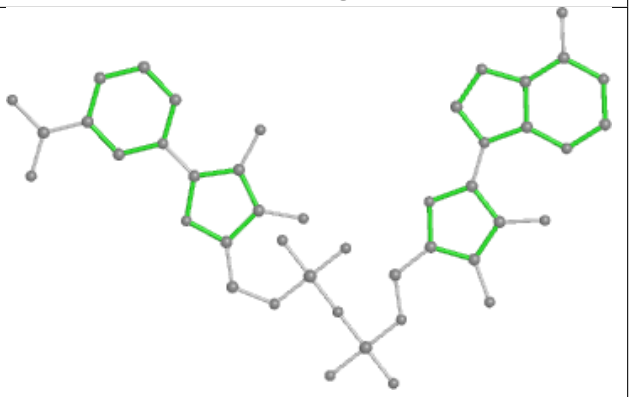
Bond lengths



Bond angles

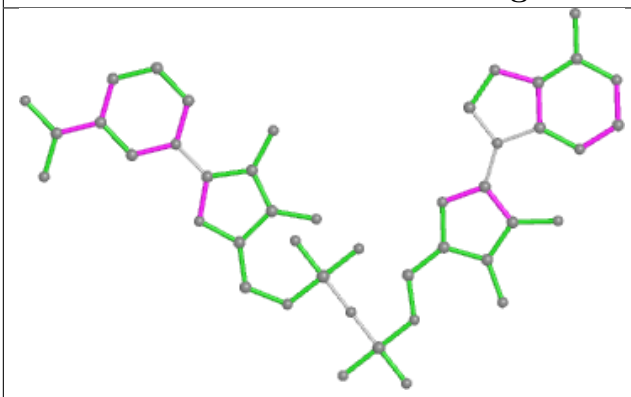


Torsions



Rings

Ligand NAD D 3601



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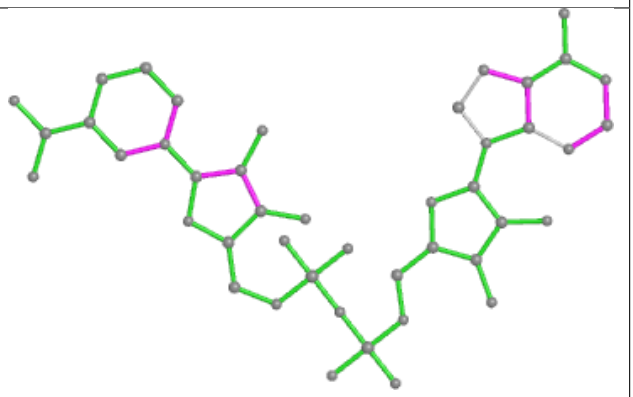
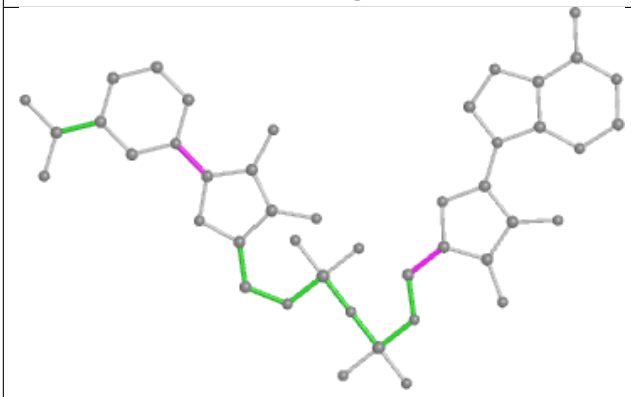
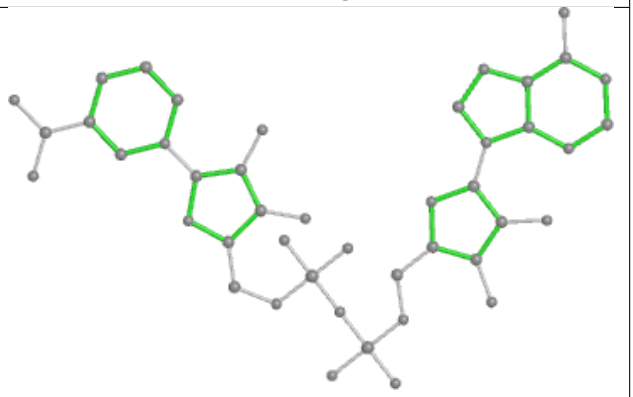


Bond angles

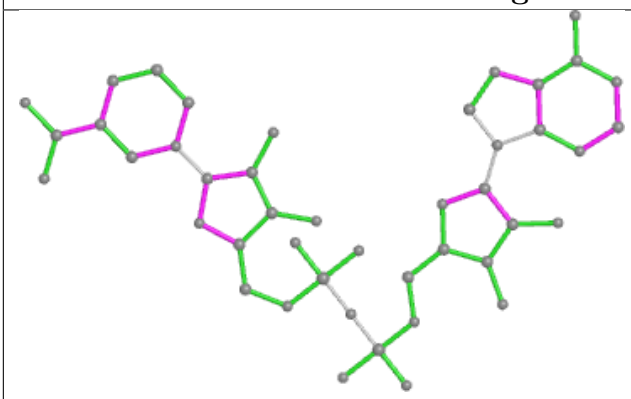


Torsions

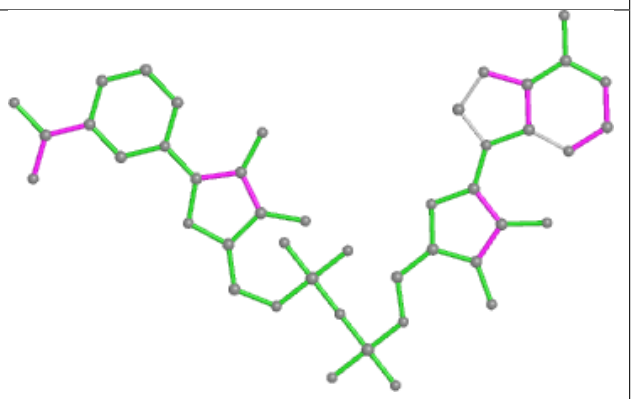


Rings

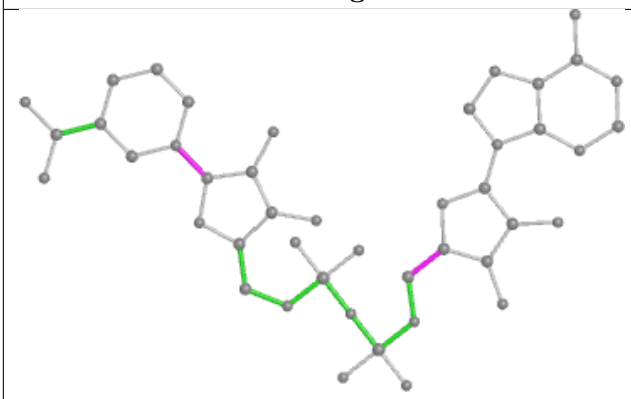
Ligand NAD B 1601



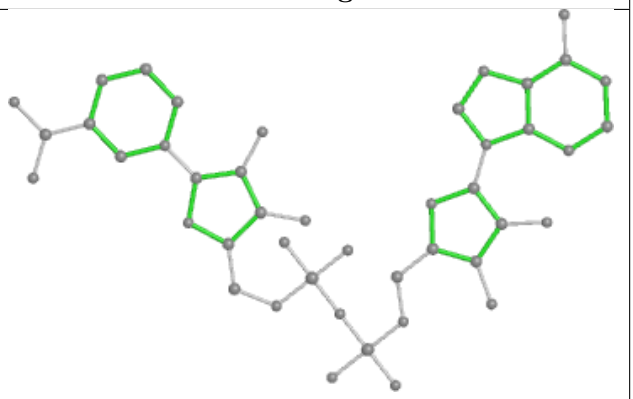
Bond lengths



Bond angles



Torsions



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.