Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 01:20 AM EDT

PDB ID	:	6N7L
Title	:	Crystal structure of an alcohol dehydrogenase from Elizabethkingia anophelis NUHP1
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2018-11-27
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.35.1

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 2.10 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 33393 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 Alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	5	0
			2548	1622	425	483	18			
1	B	342	Total	C	N	O	S	0	4	0
			2524	1608	422	477	17			
1	C	344	Total	C	N	O	S	0	11	0
			2610	1672	437	483	18			
1	D	343	Total	C	N	O	S	0	3	0
			2549	1624	430	478	17			
1	E	340	Total	C	N	O	S	0	3	0
			2506	1595	423	471	17			
1	F	343	Total	C	N	O	S	0	4	0
			2532	1612	427	476	17			
1	G	340	Total	C	N	O	S	0	1	0
			2501	1593	419	472	17			
1	H	342	Total	C	N	O	S	0	3	0
			2525	1610	423	475	17			
1	I	341	Total	C	N	O	S	0	1	0
			2470	1571	420	462	17			
1	J	343	Total	C	N	O	S	0	3	0
			2517	1602	425	472	18			
1	K	342	Total	C	N	O	S	0	3	0
			2518	1602	424	475	17			
1	L	340	Total	C	N	O	S	0	1	0
			2423	1539	412	455	17			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP A0A077EGR8
A	-6	ALA	-	expression tag	UNP A0A077EGR8
A	-5	HIS	-	expression tag	UNP A0A077EGR8
A	-4	HIS	-	expression tag	UNP A0A077EGR8
A	-3	HIS	-	expression tag	UNP A0A077EGR8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	HIS	-	expression tag	UNP A0A077EGR8
A	-1	HIS	-	expression tag	UNP A0A077EGR8
A	0	HIS	-	expression tag	UNP A0A077EGR8
B	-7	MET	-	initiating methionine	UNP A0A077EGR8
B	-6	ALA	-	expression tag	UNP A0A077EGR8
B	-5	HIS	-	expression tag	UNP A0A077EGR8
B	-4	HIS	-	expression tag	UNP A0A077EGR8
B	-3	HIS	-	expression tag	UNP A0A077EGR8
B	-2	HIS	-	expression tag	UNP A0A077EGR8
B	-1	HIS	-	expression tag	UNP A0A077EGR8
B	0	HIS	-	expression tag	UNP A0A077EGR8
C	-7	MET	-	initiating methionine	UNP A0A077EGR8
C	-6	ALA	-	expression tag	UNP A0A077EGR8
C	-5	HIS	-	expression tag	UNP A0A077EGR8
C	-4	HIS	-	expression tag	UNP A0A077EGR8
C	-3	HIS	-	expression tag	UNP A0A077EGR8
C	-2	HIS	-	expression tag	UNP A0A077EGR8
C	-1	HIS	-	expression tag	UNP A0A077EGR8
C	0	HIS	-	expression tag	UNP A0A077EGR8
D	-7	MET	-	initiating methionine	UNP A0A077EGR8
D	-6	ALA	-	expression tag	UNP A0A077EGR8
D	-5	HIS	-	expression tag	UNP A0A077EGR8
D	-4	HIS	-	expression tag	UNP A0A077EGR8
D	-3	HIS	-	expression tag	UNP A0A077EGR8
D	-2	HIS	-	expression tag	UNP A0A077EGR8
D	-1	HIS	-	expression tag	UNP A0A077EGR8
D	0	HIS	-	expression tag	UNP A0A077EGR8
E	-7	MET	-	initiating methionine	UNP A0A077EGR8
E	-6	ALA	-	expression tag	UNP A0A077EGR8
E	-5	HIS	-	expression tag	UNP A0A077EGR8
E	-4	HIS	-	expression tag	UNP A0A077EGR8
E	-3	HIS	-	expression tag	UNP A0A077EGR8
E	-2	HIS	-	expression tag	UNP A0A077EGR8
E	-1	HIS	-	expression tag	UNP A0A077EGR8
E	0	HIS	-	expression tag	UNP A0A077EGR8
F	-7	MET	-	initiating methionine	UNP A0A077EGR8
F	-6	ALA	-	expression tag	UNP A0A077EGR8
F	-5	HIS	-	expression tag	UNP A0A077EGR8
F	-4	HIS	-	expression tag	UNP A0A077EGR8
F	-3	HIS	-	expression tag	UNP A0A077EGR8
F	-2	HIS	-	expression tag	UNP A0A077EGR8
F	-1	HIS	-	expression tag	UNP A0A077EGR8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP A0A077EGR8
G	-7	MET	-	initiating methionine	UNP A0A077EGR8
G	-6	ALA	-	expression tag	UNP A0A077EGR8
G	-5	HIS	-	expression tag	UNP A0A077EGR8
G	-4	HIS	-	expression tag	UNP A0A077EGR8
G	-3	HIS	-	expression tag	UNP A0A077EGR8
G	-2	HIS	-	expression tag	UNP A0A077EGR8
G	-1	HIS	-	expression tag	UNP A0A077EGR8
G	0	HIS	-	expression tag	UNP A0A077EGR8
H	-7	MET	-	initiating methionine	UNP A0A077EGR8
H	-6	ALA	-	expression tag	UNP A0A077EGR8
H	-5	HIS	-	expression tag	UNP A0A077EGR8
H	-4	HIS	-	expression tag	UNP A0A077EGR8
H	-3	HIS	-	expression tag	UNP A0A077EGR8
H	-2	HIS	-	expression tag	UNP A0A077EGR8
H	-1	HIS	-	expression tag	UNP A0A077EGR8
H	0	HIS	-	expression tag	UNP A0A077EGR8
I	-7	MET	-	initiating methionine	UNP A0A077EGR8
I	-6	ALA	-	expression tag	UNP A0A077EGR8
I	-5	HIS	-	expression tag	UNP A0A077EGR8
I	-4	HIS	-	expression tag	UNP A0A077EGR8
I	-3	HIS	-	expression tag	UNP A0A077EGR8
I	-2	HIS	-	expression tag	UNP A0A077EGR8
I	-1	HIS	-	expression tag	UNP A0A077EGR8
I	0	HIS	-	expression tag	UNP A0A077EGR8
J	-7	MET	-	initiating methionine	UNP A0A077EGR8
J	-6	ALA	-	expression tag	UNP A0A077EGR8
J	-5	HIS	-	expression tag	UNP A0A077EGR8
J	-4	HIS	-	expression tag	UNP A0A077EGR8
J	-3	HIS	-	expression tag	UNP A0A077EGR8
J	-2	HIS	-	expression tag	UNP A0A077EGR8
J	-1	HIS	-	expression tag	UNP A0A077EGR8
J	0	HIS	-	expression tag	UNP A0A077EGR8
K	-7	MET	-	initiating methionine	UNP A0A077EGR8
K	-6	ALA	-	expression tag	UNP A0A077EGR8
K	-5	HIS	-	expression tag	UNP A0A077EGR8
K	-4	HIS	-	expression tag	UNP A0A077EGR8
K	-3	HIS	-	expression tag	UNP A0A077EGR8
K	-2	HIS	-	expression tag	UNP A0A077EGR8
K	-1	HIS	-	expression tag	UNP A0A077EGR8
K	0	HIS	-	expression tag	UNP A0A077EGR8
L	-7	MET	-	initiating methionine	UNP A0A077EGR8

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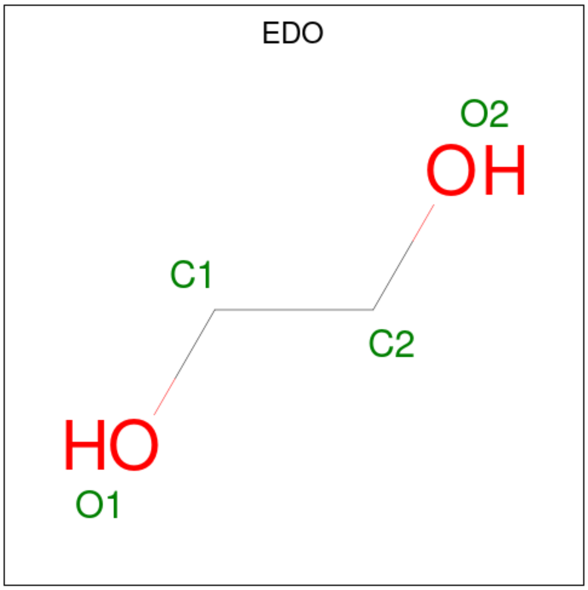
Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	ALA	-	expression tag	UNP A0A077EGR8
L	-5	HIS	-	expression tag	UNP A0A077EGR8
L	-4	HIS	-	expression tag	UNP A0A077EGR8
L	-3	HIS	-	expression tag	UNP A0A077EGR8
L	-2	HIS	-	expression tag	UNP A0A077EGR8
L	-1	HIS	-	expression tag	UNP A0A077EGR8
L	0	HIS	-	expression tag	UNP A0A077EGR8

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 8 4 4	0	1

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0

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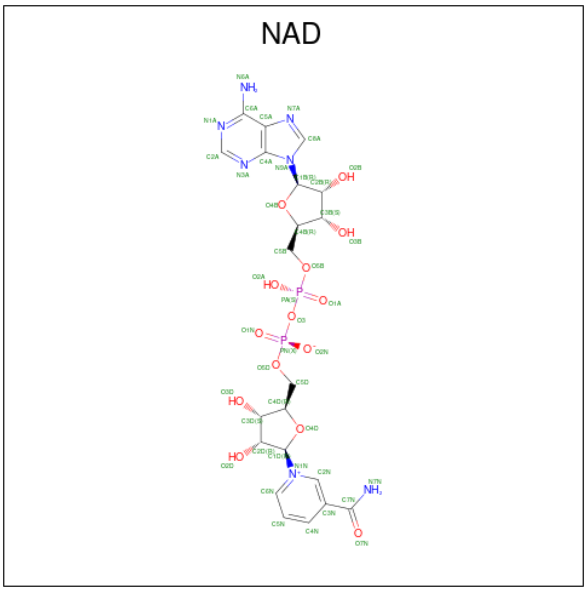
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	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	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0
4	B	2	Total Zn 2 2	0	0
4	C	2	Total Zn 2 2	0	0
4	D	2	Total Zn 2 2	0	0
4	E	2	Total Zn 2 2	0	0
4	F	2	Total Zn 2 2	0	0
4	G	2	Total Zn 2 2	0	0
4	H	2	Total Zn 2 2	0	0
4	I	2	Total Zn 2 2	0	0
4	J	2	Total Zn 2 2	0	0
4	K	2	Total Zn 2 2	0	0
4	L	2	Total Zn 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total Cl 1 1	0	0
5	J	1	Total Cl 1 1	0	0
5	K	1	Total Cl 1 1	0	0
5	L	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	231	Total O 231 231	0	0
6	B	237	Total O 238 238	0	1
6	C	284	Total O 284 284	0	0
6	D	221	Total O 221 221	0	0
6	E	196	Total O 197 197	0	1
6	F	210	Total O 210 210	0	0
6	G	195	Total O 197 197	0	2
6	H	198	Total O 198 198	0	0
6	I	90	Total O 90 90	0	0
6	J	157	Total O 157 157	0	0
6	K	149	Total O 149 149	0	0
6	L	70	Total O 70 70	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.15Å 168.29Å 199.73Å 90.00° 97.97° 90.00°	Depositor
Resolution (Å)	48.79 – 2.10	Depositor
% Data completeness (in resolution range)	95.2 (48.79-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.149 , 0.191	Depositor
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.022	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
Total number of atoms	33393	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 139 ligands modelled in this entry, 36 are monoatomic - leaving 103 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	EDO	B	401	-	3,3,3	0.58	0	2,2,2	0.21	0
2	EDO	C	404	-	3,3,3	0.37	0	2,2,2	0.64	0
2	EDO	D	502	-	3,3,3	0.48	0	2,2,2	0.22	0
2	EDO	L	404	-	3,3,3	0.44	0	2,2,2	0.41	0
2	EDO	D	505	-	3,3,3	0.43	0	2,2,2	0.50	0
2	EDO	B	406	-	3,3,3	0.40	0	2,2,2	0.63	0
2	EDO	G	508	-	3,3,3	0.43	0	2,2,2	0.59	0
2	EDO	C	405	-	3,3,3	0.50	0	2,2,2	0.28	0
2	EDO	H	705	-	3,3,3	0.48	0	2,2,2	0.17	0
3	NAD	H	703	-	42,48,48	0.51	0	50,73,73	0.71	1 (2%)
2	EDO	A	410	-	3,3,3	0.49	0	2,2,2	0.31	0
2	EDO	J	407	-	3,3,3	0.46	0	2,2,2	0.57	0
2	EDO	K	404	-	3,3,3	0.51	0	2,2,2	0.16	0
2	EDO	A	403	-	3,3,3	0.48	0	2,2,2	0.30	0
2	EDO	E	407	-	3,3,3	0.49	0	2,2,2	0.16	0
2	EDO	G	504	-	3,3,3	0.50	0	2,2,2	0.28	0
2	EDO	H	704	-	3,3,3	0.50	0	2,2,2	0.28	0
2	EDO	D	509	-	3,3,3	0.43	0	2,2,2	0.27	0
2	EDO	B	407	-	3,3,3	0.52	0	2,2,2	0.07	0
2	EDO	L	401	-	3,3,3	0.57	0	2,2,2	0.05	0
2	EDO	G	505	-	3,3,3	0.47	0	2,2,2	0.35	0
2	EDO	A	404	-	3,3,3	0.49	0	2,2,2	0.26	0
2	EDO	E	404	-	3,3,3	0.41	0	2,2,2	0.48	0
2	EDO	D	507	-	3,3,3	0.49	0	2,2,2	0.33	0
2	EDO	F	409	-	3,3,3	0.49	0	2,2,2	0.33	0
2	EDO	C	412	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	E	408	-	3,3,3	0.48	0	2,2,2	0.56	0
2	EDO	G	506	-	3,3,3	0.45	0	2,2,2	0.38	0
2	EDO	A	411	-	3,3,3	0.47	0	2,2,2	0.41	0
2	EDO	J	404	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	D	504	-	3,3,3	0.76	0	2,2,2	0.35	0
3	NAD	C	402	-	42,48,48	0.58	0	50,73,73	0.78	2 (4%)
3	NAD	K	402	-	42,48,48	0.54	0	50,73,73	0.67	2 (4%)
3	NAD	D	501	-	42,48,48	0.57	0	50,73,73	0.72	3 (6%)
2	EDO	D	503	-	3,3,3	0.47	0	2,2,2	0.38	0
2	EDO	H	701	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	F	401	-	3,3,3	0.60	0	2,2,2	0.13	0
2	EDO	E	410	-	3,3,3	0.41	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	C	406	-	3,3,3	0.57	0	2,2,2	0.11	0
2	EDO	E	403	-	3,3,3	0.42	0	2,2,2	0.46	0
2	EDO	K	401	-	3,3,3	0.55	0	2,2,2	0.20	0
2	EDO	C	401	-	3,3,3	0.71	0	2,2,2	0.59	0
2	EDO	F	408	-	3,3,3	0.42	0	2,2,2	0.53	0
2	EDO	A	409[B]	-	3,3,3	0.49	0	2,2,2	0.28	0
3	NAD	F	402	-	42,48,48	0.52	0	50,73,73	0.72	2 (4%)
3	NAD	J	402	-	42,48,48	0.57	0	50,73,73	0.74	3 (6%)
2	EDO	I	403	-	3,3,3	0.46	0	2,2,2	0.38	0
2	EDO	A	409[A]	-	3,3,3	0.52	0	2,2,2	0.19	0
2	EDO	E	409	-	3,3,3	0.36	0	2,2,2	0.70	0
2	EDO	H	707	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	B	403	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	F	410	-	3,3,3	0.53	0	2,2,2	0.13	0
2	EDO	B	405	-	3,3,3	0.44	0	2,2,2	0.48	0
2	EDO	F	406	-	3,3,3	0.48	0	2,2,2	0.35	0
2	EDO	G	502	-	3,3,3	0.44	0	2,2,2	0.38	0
2	EDO	J	405	-	3,3,3	0.54	0	2,2,2	0.10	0
2	EDO	B	404	-	3,3,3	0.41	0	2,2,2	0.52	0
2	EDO	C	408	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	J	401	-	3,3,3	0.60	0	2,2,2	0.11	0
2	EDO	L	403	-	3,3,3	0.44	0	2,2,2	0.34	0
2	EDO	A	405	-	3,3,3	0.52	0	2,2,2	0.29	0
2	EDO	B	408	-	3,3,3	0.49	0	2,2,2	0.43	0
2	EDO	E	405	-	3,3,3	0.48	0	2,2,2	0.24	0
2	EDO	J	406	-	3,3,3	0.41	0	2,2,2	0.60	0
2	EDO	C	410	-	3,3,3	0.47	0	2,2,2	0.35	0
2	EDO	D	508	-	3,3,3	0.47	0	2,2,2	0.10	0
2	EDO	F	407	-	3,3,3	0.47	0	2,2,2	0.15	0
2	EDO	A	401	-	3,3,3	0.70	0	2,2,2	0.62	0
2	EDO	C	411	-	3,3,3	0.46	0	2,2,2	0.23	0
3	NAD	E	402	-	42,48,48	0.55	0	50,73,73	0.74	3 (6%)
2	EDO	I	404	-	3,3,3	0.37	0	2,2,2	0.38	0
2	EDO	C	403	-	3,3,3	0.50	0	2,2,2	0.37	0
2	EDO	G	503	-	3,3,3	0.42	0	2,2,2	0.36	0
2	EDO	E	406	-	3,3,3	0.42	0	2,2,2	0.47	0
2	EDO	C	409	-	3,3,3	0.46	0	2,2,2	0.39	0
2	EDO	C	407	-	3,3,3	0.49	0	2,2,2	0.45	0
2	EDO	A	408	-	3,3,3	0.44	0	2,2,2	0.49	0
2	EDO	C	413	-	3,3,3	0.63	0	2,2,2	0.11	0
3	NAD	B	402	-	42,48,48	0.52	0	50,73,73	0.72	2 (4%)
2	EDO	J	408	-	3,3,3	0.44	0	2,2,2	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	I	406	-	3,3,3	0.42	0	2,2,2	0.61	0
2	EDO	G	507	-	3,3,3	0.48	0	2,2,2	0.27	0
2	EDO	D	506	-	3,3,3	0.47	0	2,2,2	0.27	0
2	EDO	F	403	-	3,3,3	0.47	0	2,2,2	0.45	0
2	EDO	A	406	-	3,3,3	0.37	0	2,2,2	0.86	0
2	EDO	H	702	-	3,3,3	0.69	0	2,2,2	0.23	0
3	NAD	I	402	-	42,48,48	0.54	0	50,73,73	0.65	2 (4%)
2	EDO	A	412	-	3,3,3	0.37	0	2,2,2	0.78	0
2	EDO	K	403	-	3,3,3	0.41	0	2,2,2	0.50	0
2	EDO	F	404	-	3,3,3	0.39	0	2,2,2	0.71	0
3	NAD	G	501	-	42,48,48	0.55	0	50,73,73	0.70	2 (4%)
2	EDO	E	401	-	3,3,3	0.68	0	2,2,2	0.17	0
3	NAD	A	402	-	42,48,48	0.56	0	50,73,73	0.76	2 (4%)
2	EDO	K	405	-	3,3,3	0.46	0	2,2,2	0.49	0
2	EDO	I	405	-	3,3,3	0.49	0	2,2,2	0.27	0
2	EDO	I	407	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	A	407	-	3,3,3	0.52	0	2,2,2	0.21	0
2	EDO	F	405	-	3,3,3	0.50	0	2,2,2	0.12	0
2	EDO	F	411	-	3,3,3	0.51	0	2,2,2	0.16	0
2	EDO	I	401	-	3,3,3	0.66	0	2,2,2	0.21	0
2	EDO	H	706	1	3,3,3	0.49	0	2,2,2	0.41	0
2	EDO	J	403	-	3,3,3	0.44	0	2,2,2	0.48	0
3	NAD	L	402	-	42,48,48	0.51	0	50,73,73	0.73	2 (4%)

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	EDO	B	401	-	-	0/1/1/1	-
2	EDO	C	404	-	-	0/1/1/1	-
2	EDO	D	502	-	-	0/1/1/1	-
2	EDO	L	404	-	-	1/1/1/1	-
2	EDO	D	505	-	-	0/1/1/1	-
2	EDO	B	406	-	-	1/1/1/1	-
2	EDO	G	508	-	-	0/1/1/1	-
2	EDO	C	405	-	-	0/1/1/1	-
2	EDO	H	705	-	-	0/1/1/1	-
3	NAD	H	703	-	-	5/26/62/62	0/5/5/5
2	EDO	A	410	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	J	407	-	-	1/1/1/1	-
2	EDO	K	404	-	-	0/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	E	407	-	-	0/1/1/1	-
2	EDO	G	504	-	-	1/1/1/1	-
2	EDO	H	704	-	-	0/1/1/1	-
2	EDO	D	509	-	-	0/1/1/1	-
2	EDO	B	407	-	-	0/1/1/1	-
2	EDO	L	401	-	-	0/1/1/1	-
2	EDO	G	505	-	-	0/1/1/1	-
2	EDO	A	404	-	-	0/1/1/1	-
2	EDO	E	404	-	-	0/1/1/1	-
2	EDO	D	507	-	-	0/1/1/1	-
2	EDO	F	409	-	-	0/1/1/1	-
2	EDO	C	412	-	-	1/1/1/1	-
2	EDO	E	408	-	-	1/1/1/1	-
2	EDO	G	506	-	-	0/1/1/1	-
2	EDO	A	411	-	-	1/1/1/1	-
2	EDO	J	404	-	-	1/1/1/1	-
2	EDO	D	504	-	-	0/1/1/1	-
3	NAD	C	402	-	-	5/26/62/62	0/5/5/5
3	NAD	K	402	-	-	5/26/62/62	0/5/5/5
3	NAD	D	501	-	-	5/26/62/62	0/5/5/5
2	EDO	D	503	-	-	0/1/1/1	-
2	EDO	H	701	-	-	0/1/1/1	-
2	EDO	F	401	-	-	0/1/1/1	-
2	EDO	E	410	-	-	0/1/1/1	-
2	EDO	C	406	-	-	1/1/1/1	-
2	EDO	E	403	-	-	0/1/1/1	-
2	EDO	K	401	-	-	1/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
2	EDO	F	408	-	-	0/1/1/1	-
2	EDO	A	409[B]	-	-	0/1/1/1	-
3	NAD	F	402	-	-	5/26/62/62	0/5/5/5
3	NAD	J	402	-	-	5/26/62/62	0/5/5/5
2	EDO	I	403	-	-	0/1/1/1	-
2	EDO	A	409[A]	-	-	0/1/1/1	-
2	EDO	E	409	-	-	0/1/1/1	-
2	EDO	H	707	-	-	0/1/1/1	-
2	EDO	B	403	-	-	0/1/1/1	-
2	EDO	F	410	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	405	-	-	0/1/1/1	-
2	EDO	F	406	-	-	0/1/1/1	-
2	EDO	G	502	-	-	0/1/1/1	-
2	EDO	J	405	-	-	1/1/1/1	-
2	EDO	B	404	-	-	0/1/1/1	-
2	EDO	C	408	-	-	0/1/1/1	-
2	EDO	J	401	-	-	0/1/1/1	-
2	EDO	L	403	-	-	1/1/1/1	-
2	EDO	A	405	-	-	0/1/1/1	-
2	EDO	B	408	-	-	1/1/1/1	-
2	EDO	E	405	-	-	0/1/1/1	-
2	EDO	J	406	-	-	1/1/1/1	-
2	EDO	C	410	-	-	0/1/1/1	-
2	EDO	D	508	-	-	0/1/1/1	-
2	EDO	F	407	-	-	0/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	C	411	-	-	0/1/1/1	-
3	NAD	E	402	-	-	5/26/62/62	0/5/5/5
2	EDO	I	404	-	-	1/1/1/1	-
2	EDO	C	403	-	-	1/1/1/1	-
2	EDO	G	503	-	-	0/1/1/1	-
2	EDO	E	406	-	-	1/1/1/1	-
2	EDO	C	409	-	-	0/1/1/1	-
2	EDO	C	407	-	-	0/1/1/1	-
2	EDO	A	408	-	-	0/1/1/1	-
2	EDO	C	413	-	-	1/1/1/1	-
3	NAD	B	402	-	-	5/26/62/62	0/5/5/5
2	EDO	J	408	-	-	1/1/1/1	-
2	EDO	I	406	-	-	1/1/1/1	-
2	EDO	G	507	-	-	0/1/1/1	-
2	EDO	D	506	-	-	0/1/1/1	-
2	EDO	F	403	-	-	0/1/1/1	-
2	EDO	A	406	-	-	1/1/1/1	-
2	EDO	H	702	-	-	0/1/1/1	-
3	NAD	I	402	-	-	5/26/62/62	0/5/5/5
2	EDO	A	412	-	-	1/1/1/1	-
2	EDO	K	403	-	-	1/1/1/1	-
2	EDO	F	404	-	-	0/1/1/1	-
3	NAD	G	501	-	-	5/26/62/62	0/5/5/5
2	EDO	E	401	-	-	0/1/1/1	-
3	NAD	A	402	-	-	5/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	K	405	-	-	0/1/1/1	-
2	EDO	I	405	-	-	0/1/1/1	-
2	EDO	I	407	-	-	1/1/1/1	-
2	EDO	A	407	-	-	0/1/1/1	-
2	EDO	F	405	-	-	0/1/1/1	-
2	EDO	F	411	-	-	0/1/1/1	-
2	EDO	I	401	-	-	0/1/1/1	-
2	EDO	H	706	1	-	0/1/1/1	-
2	EDO	J	403	-	-	1/1/1/1	-
3	NAD	L	402	-	-	5/26/62/62	0/5/5/5

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	NAD	C5A-C6A-N6A	2.46	124.10	120.35
3	C	402	NAD	O4B-C1B-C2B	-2.41	103.41	106.93
3	C	402	NAD	C5A-C6A-N6A	2.40	124.00	120.35
3	F	402	NAD	C5A-C6A-N6A	2.39	123.99	120.35
3	B	402	NAD	C5A-C6A-N6A	2.37	123.96	120.35
3	E	402	NAD	C5A-C6A-N6A	2.37	123.95	120.35
3	L	402	NAD	C5A-C6A-N6A	2.37	123.95	120.35
3	G	501	NAD	C5A-C6A-N6A	2.35	123.92	120.35
3	J	402	NAD	C5A-C6A-N6A	2.35	123.92	120.35
3	H	703	NAD	C5A-C6A-N6A	2.30	123.84	120.35
3	L	402	NAD	C2N-N1N-C1D	-2.30	114.02	119.14
3	D	501	NAD	C5A-C6A-N6A	2.24	123.76	120.35
3	I	402	NAD	C5A-C6A-N6A	2.21	123.71	120.35
3	E	402	NAD	C2N-N1N-C1D	-2.17	114.30	119.14
3	J	402	NAD	C2N-N1N-C1D	-2.17	114.31	119.14
3	D	501	NAD	C2N-N1N-C1D	-2.16	114.33	119.14
3	F	402	NAD	O4B-C1B-C2B	-2.15	103.79	106.93
3	A	402	NAD	C2N-N1N-C1D	-2.13	114.38	119.14
3	J	402	NAD	O4B-C1B-C2B	-2.09	103.87	106.93
3	K	402	NAD	C5A-C6A-N6A	2.07	123.49	120.35
3	D	501	NAD	O4B-C1B-C2B	-2.04	103.95	106.93
3	I	402	NAD	C2N-N1N-C1D	-2.04	114.60	119.14
3	E	402	NAD	O4B-C1B-C2B	-2.03	103.97	106.93
3	B	402	NAD	O4B-C1B-C2B	-2.02	103.97	106.93
3	K	402	NAD	O4B-C1B-C2B	-2.02	103.97	106.93
3	G	501	NAD	C2N-N1N-C1D	-2.01	114.66	119.14

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAD	O4D-C1D-N1N-C2N
3	A	402	NAD	O4D-C1D-N1N-C6N
3	A	402	NAD	C2D-C1D-N1N-C2N
3	A	402	NAD	C2D-C1D-N1N-C6N
3	B	402	NAD	O4D-C1D-N1N-C2N
3	B	402	NAD	O4D-C1D-N1N-C6N
3	B	402	NAD	C2D-C1D-N1N-C2N
3	B	402	NAD	C2D-C1D-N1N-C6N
3	C	402	NAD	O4D-C1D-N1N-C2N
3	C	402	NAD	O4D-C1D-N1N-C6N
3	C	402	NAD	C2D-C1D-N1N-C2N
3	C	402	NAD	C2D-C1D-N1N-C6N
3	D	501	NAD	O4D-C1D-N1N-C2N
3	D	501	NAD	O4D-C1D-N1N-C6N
3	D	501	NAD	C2D-C1D-N1N-C2N
3	D	501	NAD	C2D-C1D-N1N-C6N
3	E	402	NAD	O4D-C1D-N1N-C2N
3	E	402	NAD	O4D-C1D-N1N-C6N
3	E	402	NAD	C2D-C1D-N1N-C2N
3	E	402	NAD	C2D-C1D-N1N-C6N
3	F	402	NAD	O4D-C1D-N1N-C2N
3	F	402	NAD	O4D-C1D-N1N-C6N
3	F	402	NAD	C2D-C1D-N1N-C2N
3	F	402	NAD	C2D-C1D-N1N-C6N
3	G	501	NAD	O4D-C1D-N1N-C2N
3	G	501	NAD	O4D-C1D-N1N-C6N
3	G	501	NAD	C2D-C1D-N1N-C2N
3	G	501	NAD	C2D-C1D-N1N-C6N
3	H	703	NAD	O4D-C1D-N1N-C2N
3	H	703	NAD	O4D-C1D-N1N-C6N
3	H	703	NAD	C2D-C1D-N1N-C2N
3	H	703	NAD	C2D-C1D-N1N-C6N
3	I	402	NAD	O4D-C1D-N1N-C2N
3	I	402	NAD	O4D-C1D-N1N-C6N
3	I	402	NAD	C2D-C1D-N1N-C2N
3	I	402	NAD	C2D-C1D-N1N-C6N
3	J	402	NAD	O4D-C1D-N1N-C2N
3	J	402	NAD	O4D-C1D-N1N-C6N
3	J	402	NAD	C2D-C1D-N1N-C2N
3	J	402	NAD	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	K	402	NAD	O4D-C1D-N1N-C2N
3	K	402	NAD	O4D-C1D-N1N-C6N
3	K	402	NAD	C2D-C1D-N1N-C2N
3	K	402	NAD	C2D-C1D-N1N-C6N
3	L	402	NAD	O4D-C1D-N1N-C2N
3	L	402	NAD	O4D-C1D-N1N-C6N
3	L	402	NAD	C2D-C1D-N1N-C2N
3	L	402	NAD	C2D-C1D-N1N-C6N
2	A	406	EDO	O1-C1-C2-O2
2	C	403	EDO	O1-C1-C2-O2
2	C	401	EDO	O1-C1-C2-O2
2	E	406	EDO	O1-C1-C2-O2
2	C	406	EDO	O1-C1-C2-O2
2	J	407	EDO	O1-C1-C2-O2
3	H	703	NAD	O4B-C4B-C5B-O5B
2	A	401	EDO	O1-C1-C2-O2
2	C	412	EDO	O1-C1-C2-O2
2	J	405	EDO	O1-C1-C2-O2
2	J	406	EDO	O1-C1-C2-O2
2	A	411	EDO	O1-C1-C2-O2
2	J	408	EDO	O1-C1-C2-O2
2	L	404	EDO	O1-C1-C2-O2
2	A	412	EDO	O1-C1-C2-O2
2	E	408	EDO	O1-C1-C2-O2
2	I	406	EDO	O1-C1-C2-O2
2	K	401	EDO	O1-C1-C2-O2
3	L	402	NAD	O4B-C4B-C5B-O5B
3	E	402	NAD	O4B-C4B-C5B-O5B
2	B	406	EDO	O1-C1-C2-O2
2	B	408	EDO	O1-C1-C2-O2
2	C	413	EDO	O1-C1-C2-O2
2	G	504	EDO	O1-C1-C2-O2
2	I	407	EDO	O1-C1-C2-O2
2	J	403	EDO	O1-C1-C2-O2
2	J	404	EDO	O1-C1-C2-O2
3	B	402	NAD	O4B-C4B-C5B-O5B
3	C	402	NAD	O4B-C4B-C5B-O5B
3	D	501	NAD	O4B-C4B-C5B-O5B
3	F	402	NAD	O4B-C4B-C5B-O5B
3	I	402	NAD	O4B-C4B-C5B-O5B
3	A	402	NAD	O4B-C4B-C5B-O5B
3	G	501	NAD	O4B-C4B-C5B-O5B

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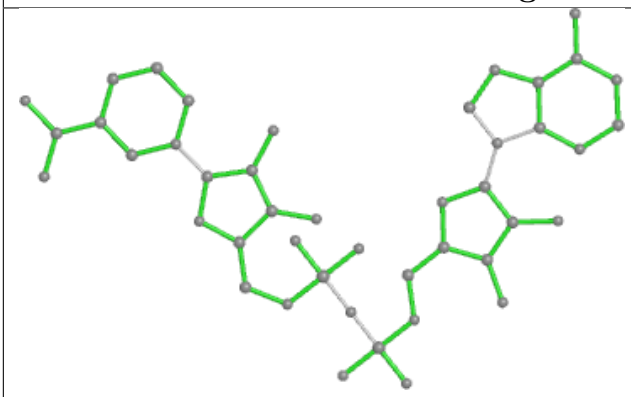
Mol	Chain	Res	Type	Atoms
3	J	402	NAD	O4B-C4B-C5B-O5B
3	K	402	NAD	O4B-C4B-C5B-O5B
2	I	404	EDO	O1-C1-C2-O2
2	K	403	EDO	O1-C1-C2-O2
2	L	403	EDO	O1-C1-C2-O2

There are no ring outliers.

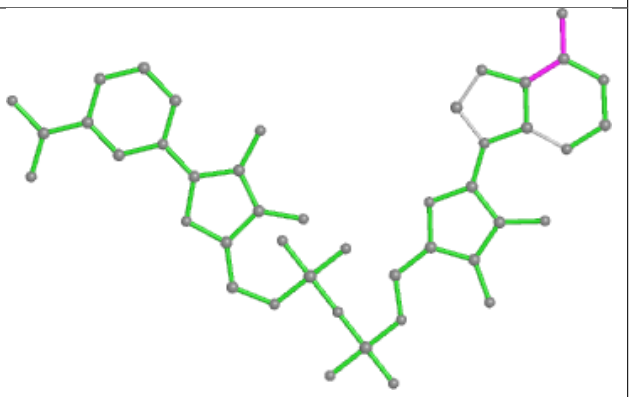
No monomer is involved in short contacts.

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.

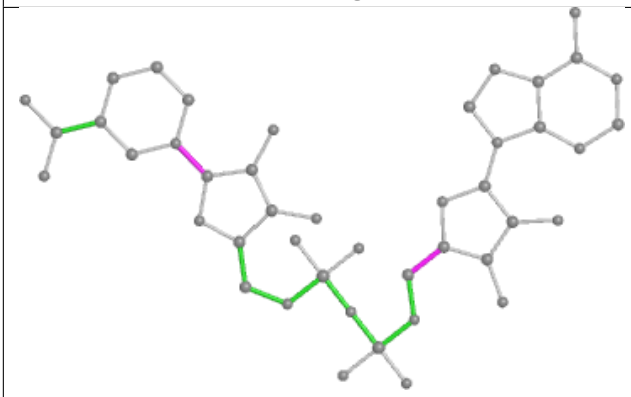
Ligand NAD H 703



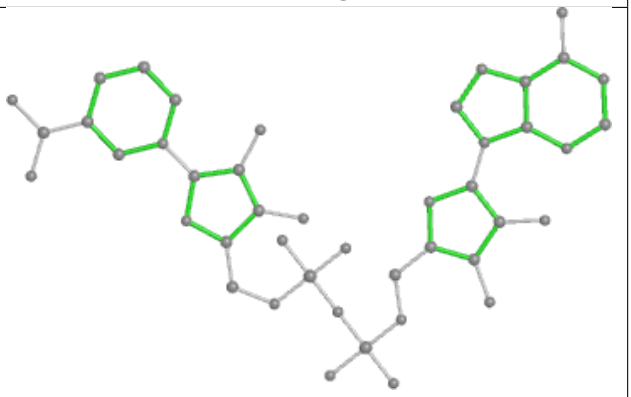
Bond lengths



Bond angles

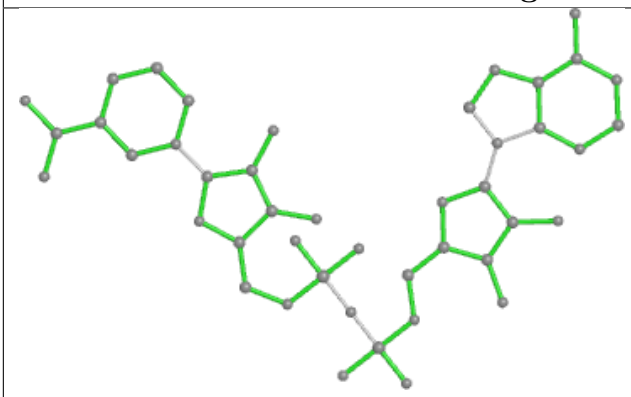


Torsions

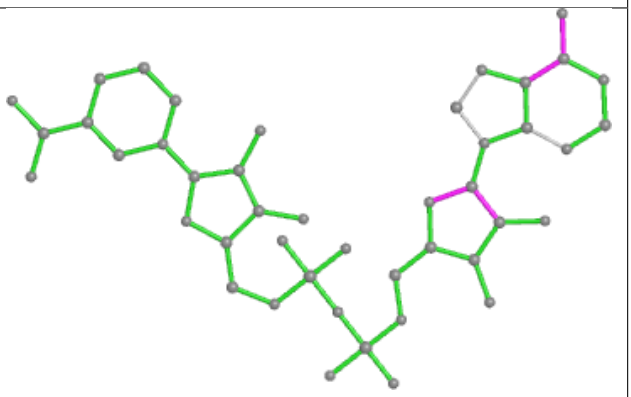


Rings

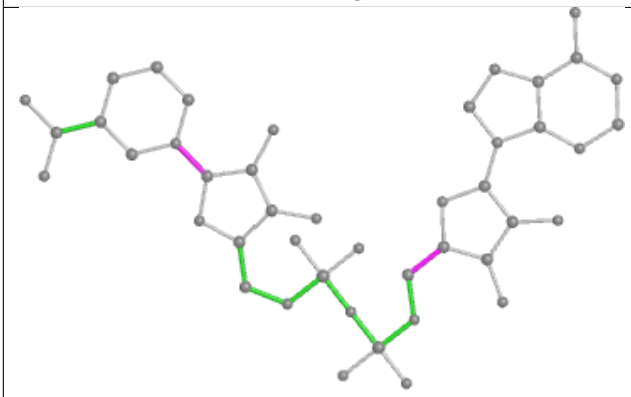
Ligand NAD C 402



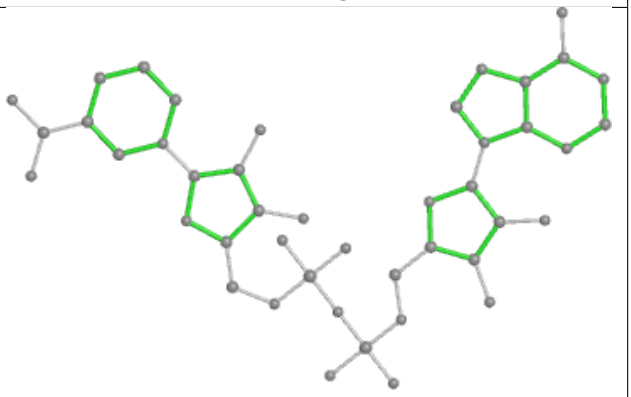
Bond lengths



Bond angles

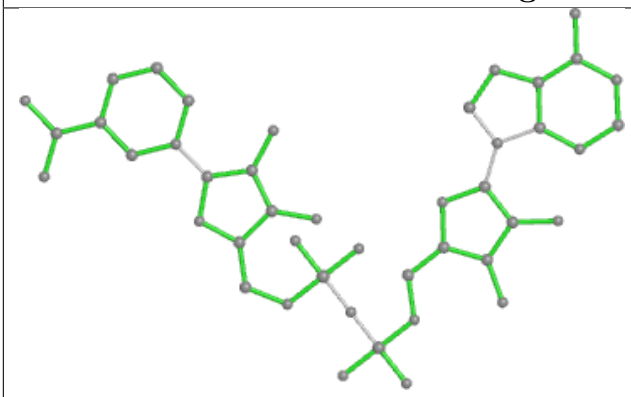


Torsions

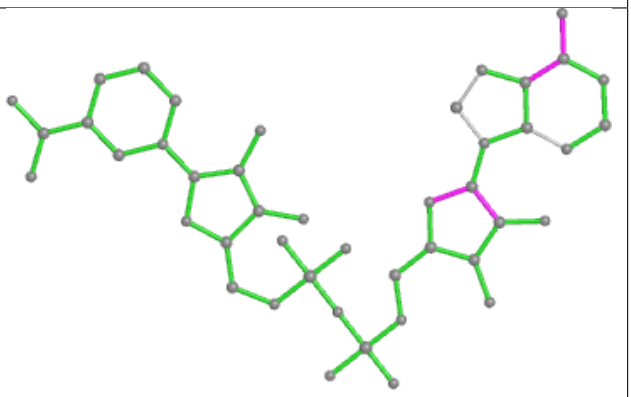


Rings

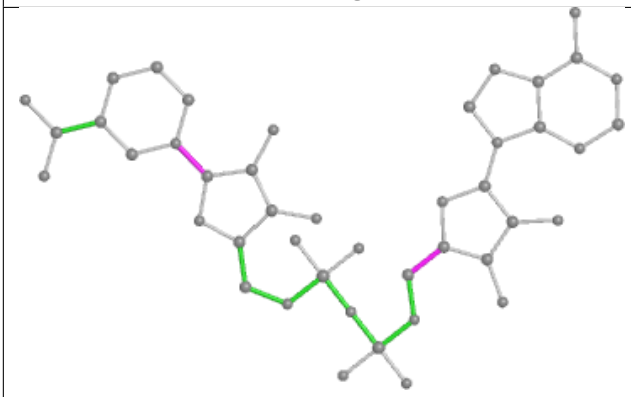
Ligand NAD K 402



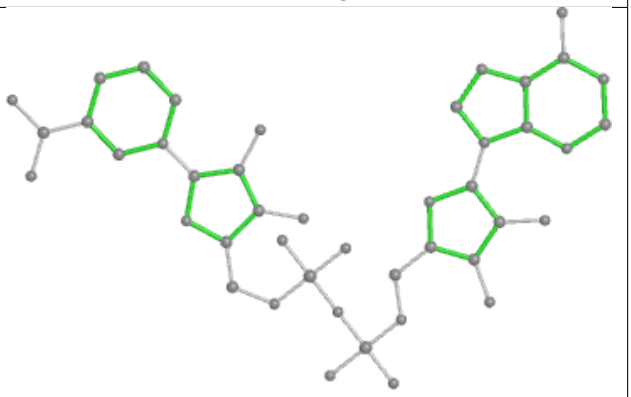
Bond lengths



Bond angles

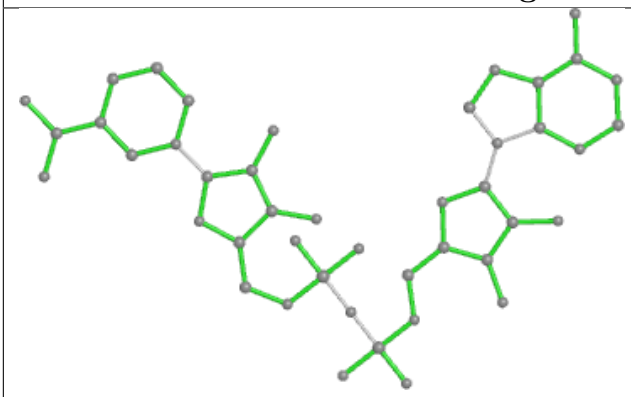


Torsions

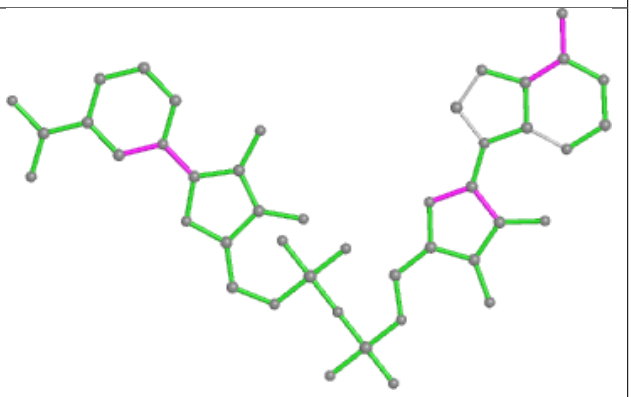


Rings

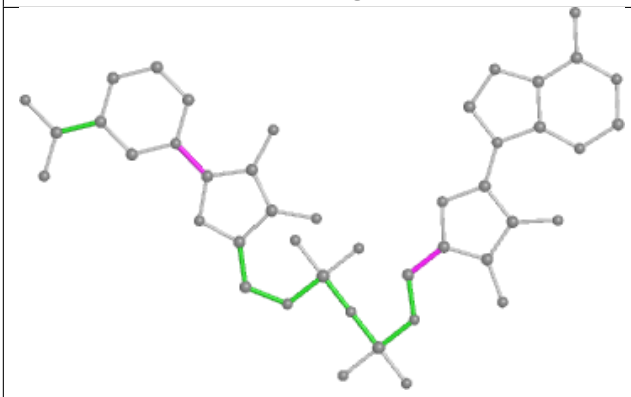
Ligand NAD D 501



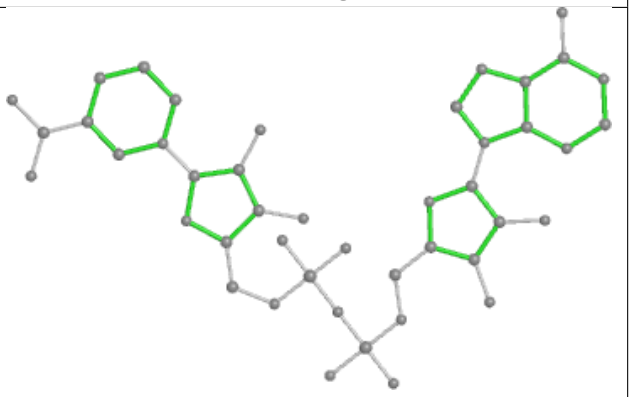
Bond lengths



Bond angles

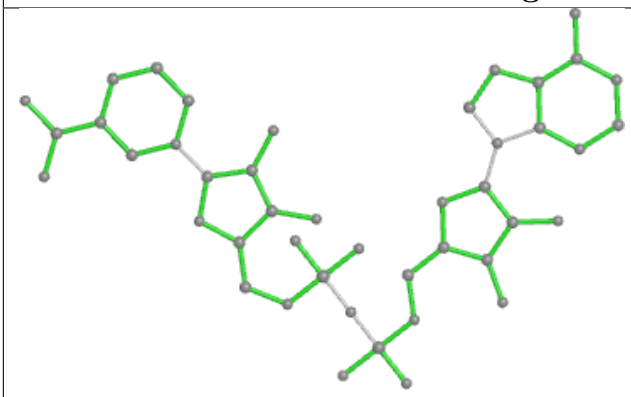


Torsions

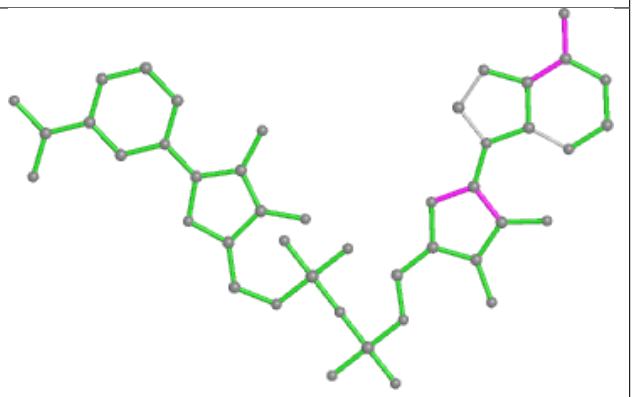


Rings

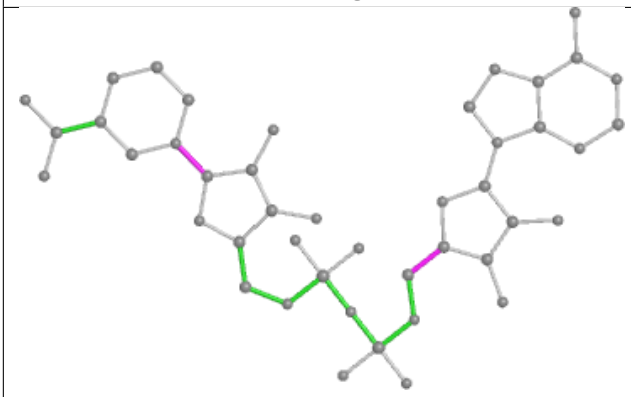
Ligand NAD F 402



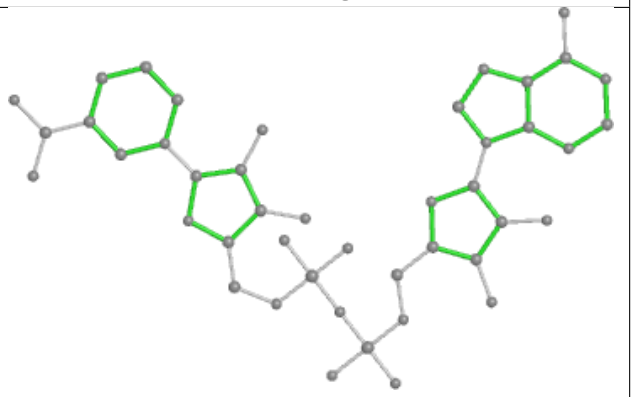
Bond lengths



Bond angles

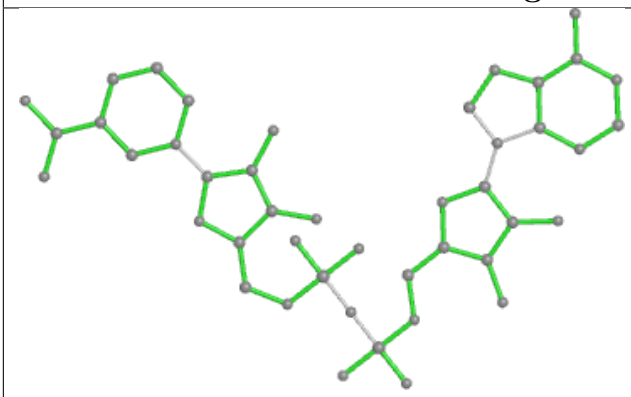


Torsions

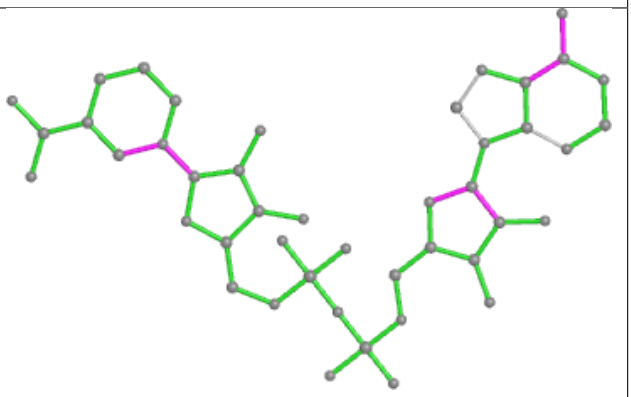


Rings

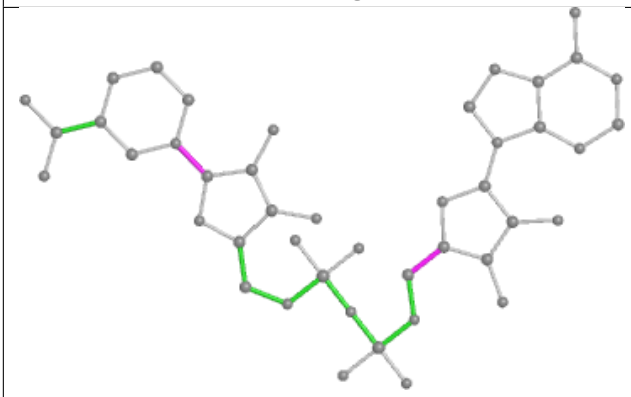
Ligand NAD J 402



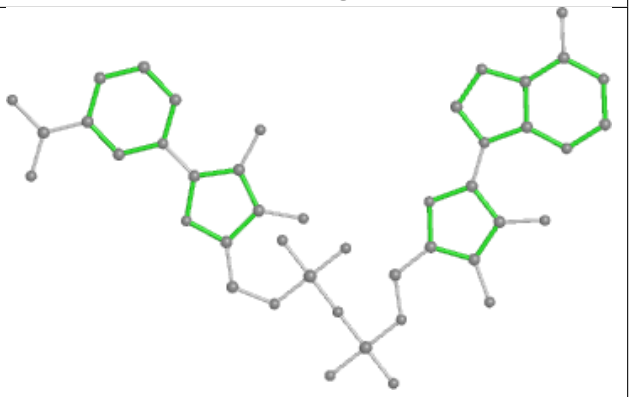
Bond lengths



Bond angles

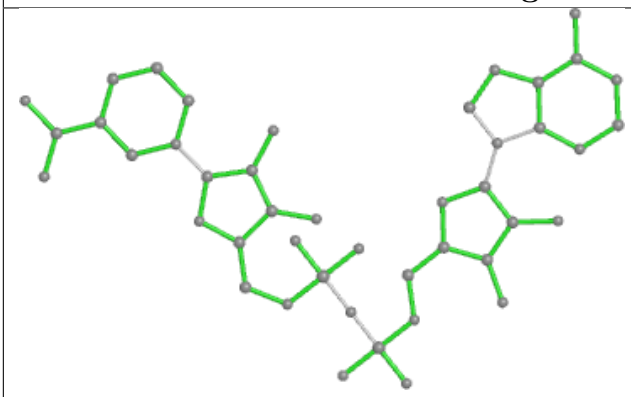


Torsions

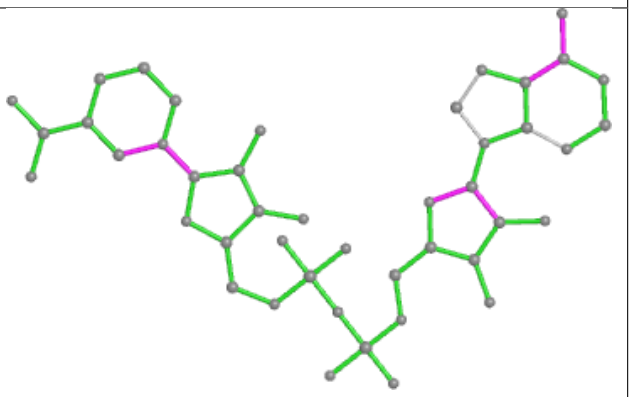


Rings

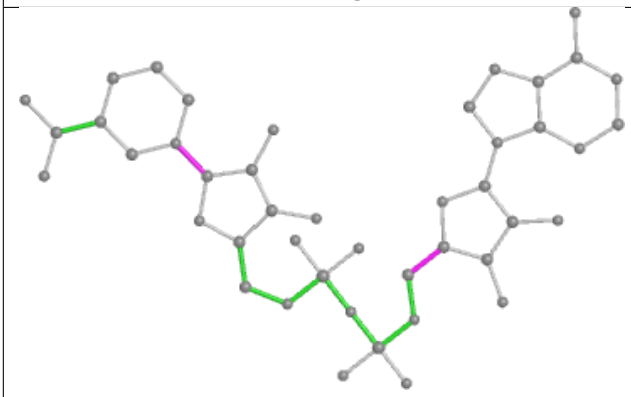
Ligand NAD E 402



Bond lengths



Bond angles



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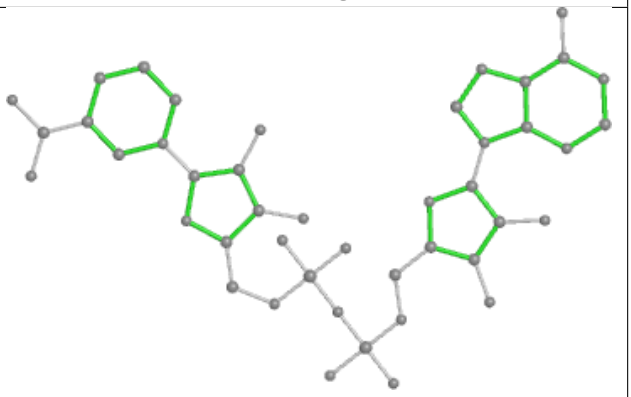
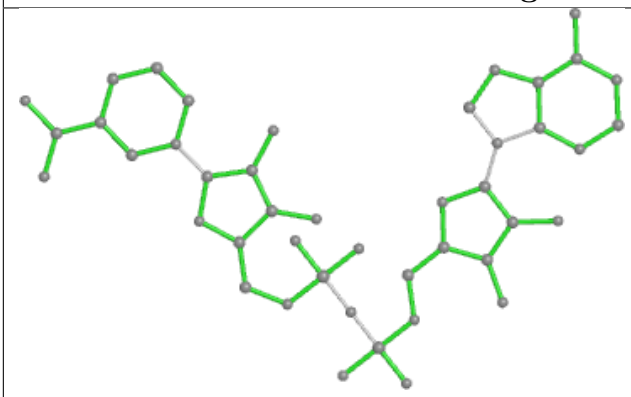
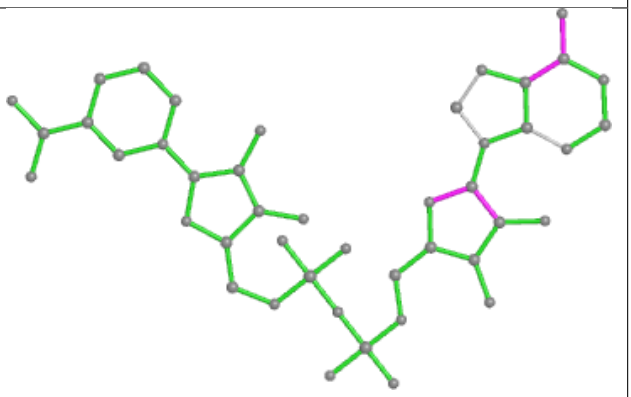


Rings

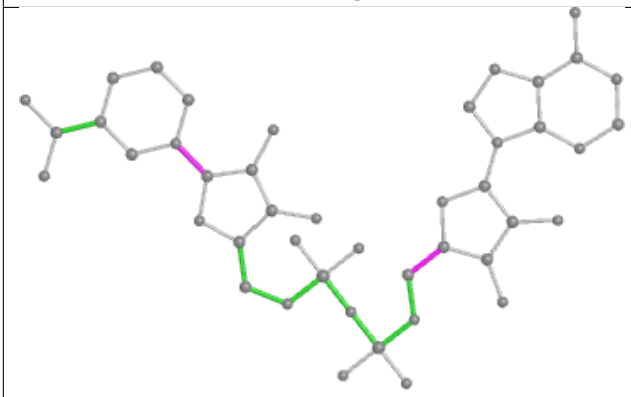
Ligand NAD B 402



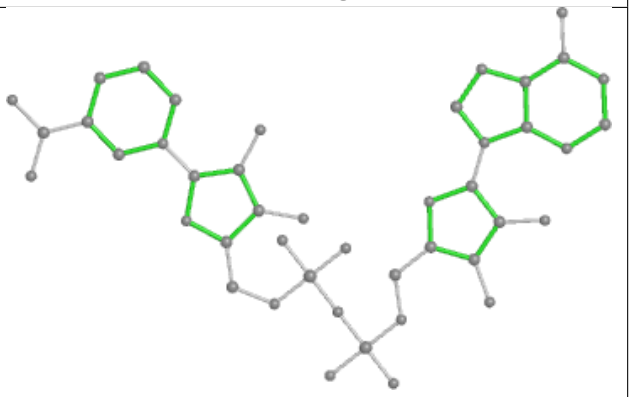
Bond lengths



Bond angles

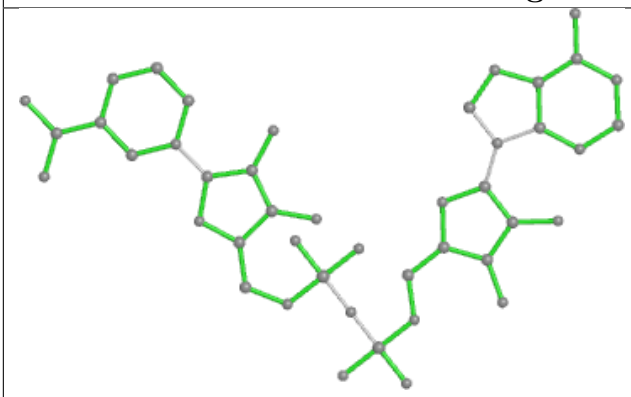


Torsions

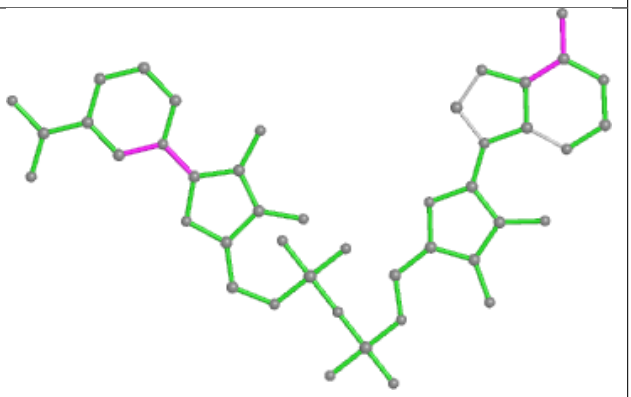


Rings

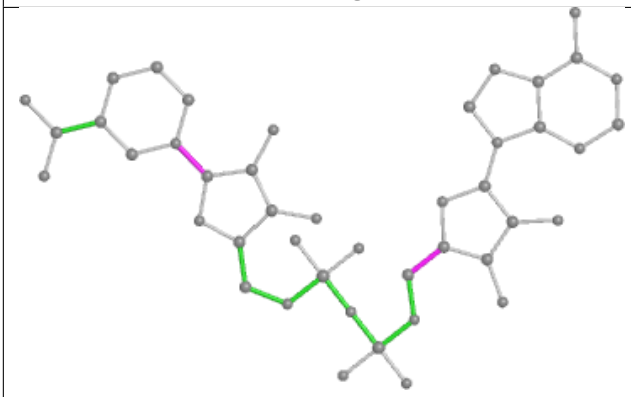
Ligand NAD I 402



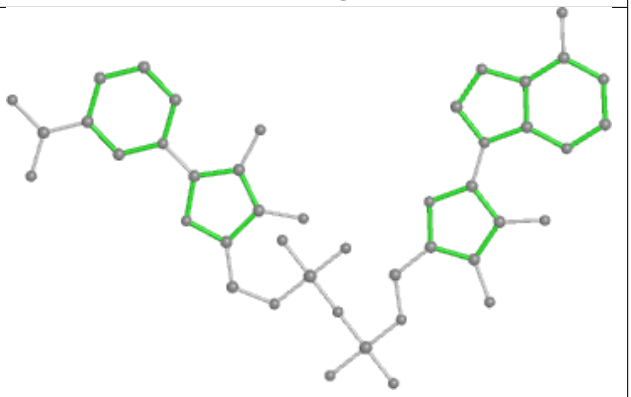
Bond lengths



Bond angles

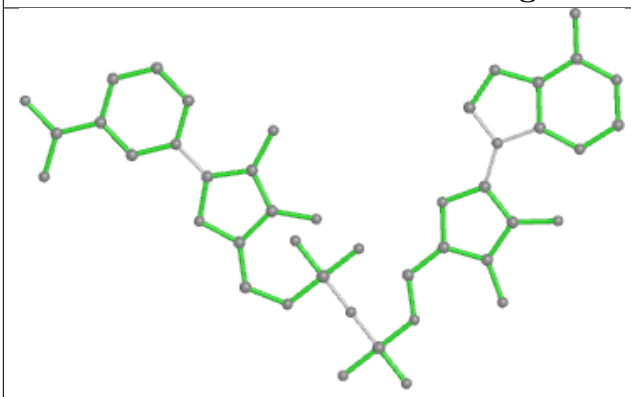


Torsions

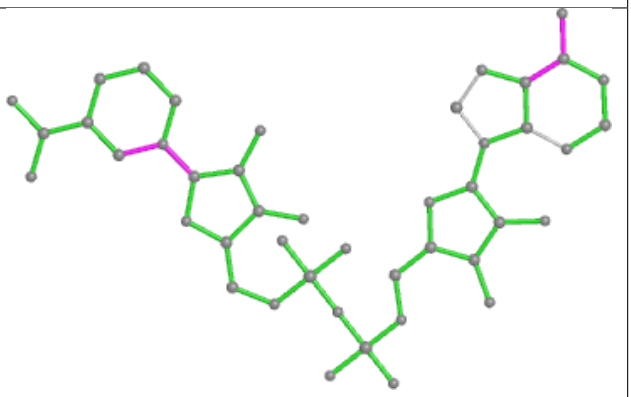


Rings

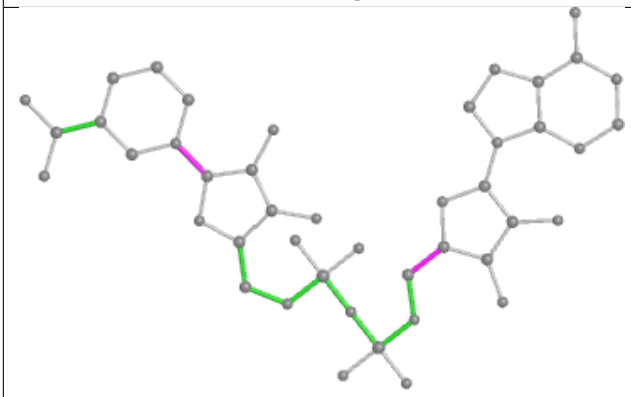
Ligand NAD G 501



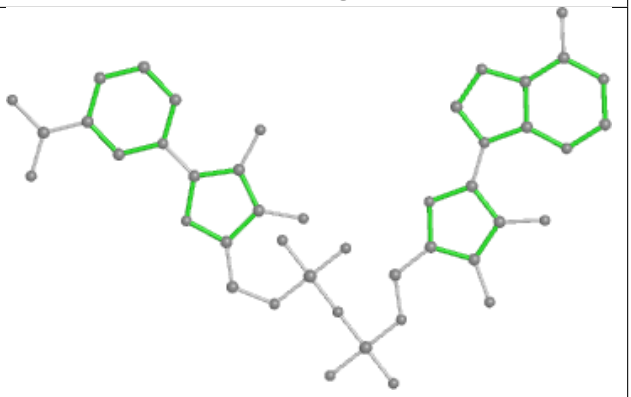
Bond lengths



Bond angles

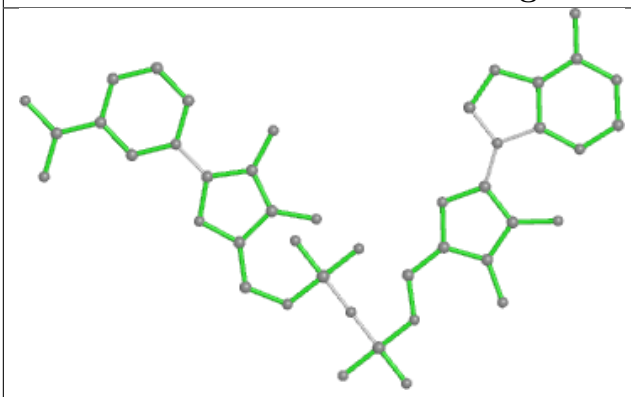


Torsions

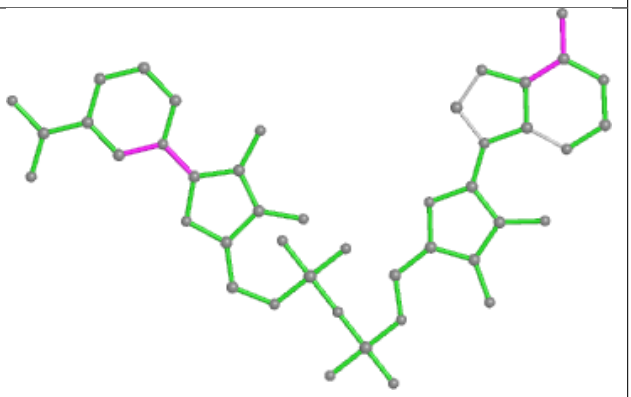


Rings

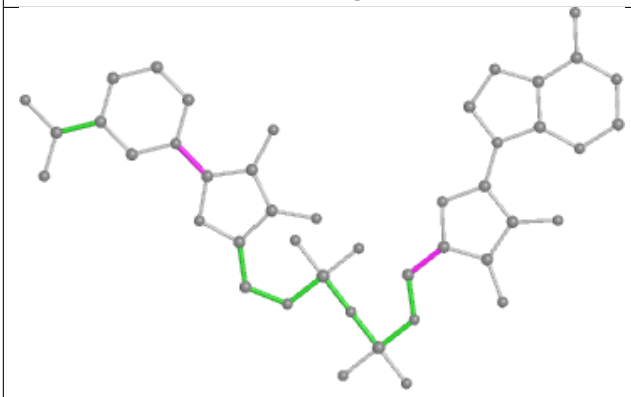
Ligand NAD A 402



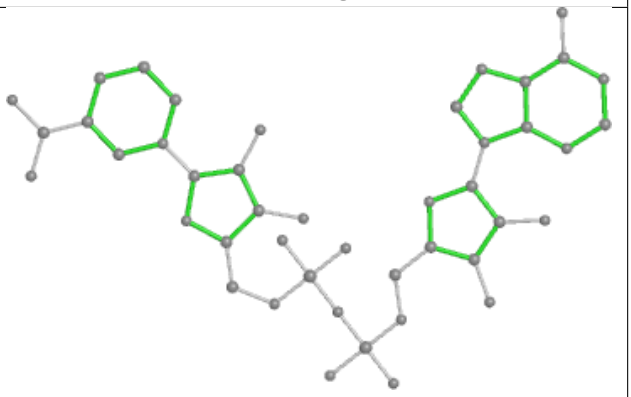
Bond lengths



Bond angles

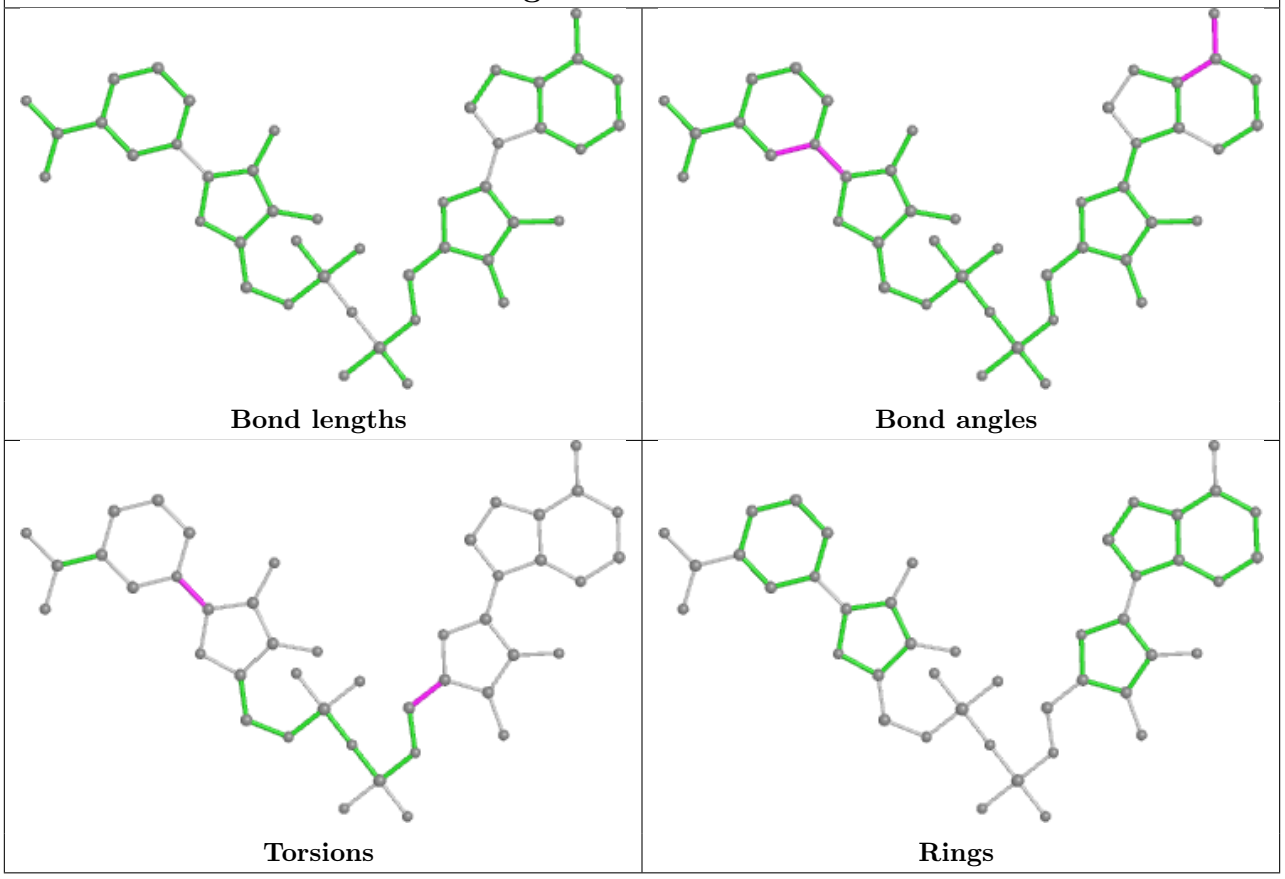


Torsions



Rings

Ligand NAD L 402



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.