Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 11:59 PM EDT

PDB ID	:	6N91
Title	:	Crystal Structure of Adenosine Deaminase from Vibrio cholerae Complexed with Pentostatin (Deoxycoformycin)
Authors	:	Maltseva, N.; Kim, Y.; Endres, M.; Welk, L.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2018-11-30
Resolution	:	2.05 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 2.05 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 11 unique types of molecules in this entry. The entry contains 5990 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.

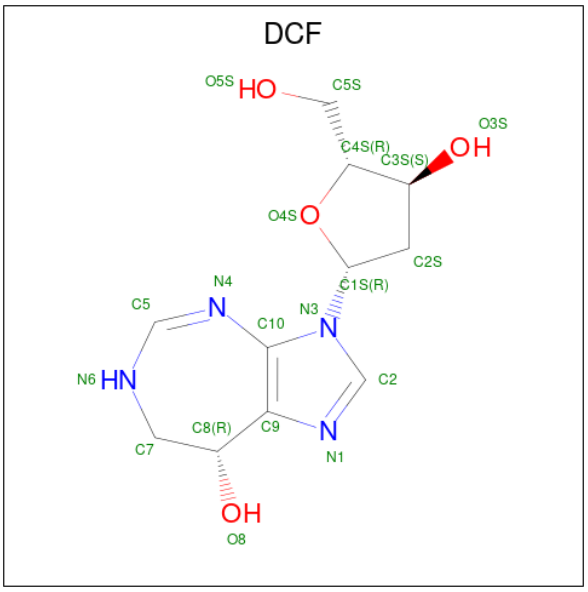
- Molecule 1 is a protein called Adenosine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	25	0
			2769	1743	490	525	11			
1	B	334	Total	C	N	O	S	0	19	0
			2716	1709	481	514	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	HIS	-	expression tag	UNP Q9KNI7
A	336	HIS	-	expression tag	UNP Q9KNI7
A	337	HIS	-	expression tag	UNP Q9KNI7
A	338	HIS	-	expression tag	UNP Q9KNI7
A	339	HIS	-	expression tag	UNP Q9KNI7
A	340	HIS	-	expression tag	UNP Q9KNI7
B	335	HIS	-	expression tag	UNP Q9KNI7
B	336	HIS	-	expression tag	UNP Q9KNI7
B	337	HIS	-	expression tag	UNP Q9KNI7
B	338	HIS	-	expression tag	UNP Q9KNI7
B	339	HIS	-	expression tag	UNP Q9KNI7
B	340	HIS	-	expression tag	UNP Q9KNI7

- Molecule 2 is 2'-DEOXYCOFORMYCIN (three-letter code: DCF) (formula: $C_{11}H_{16}N_4O_4$).

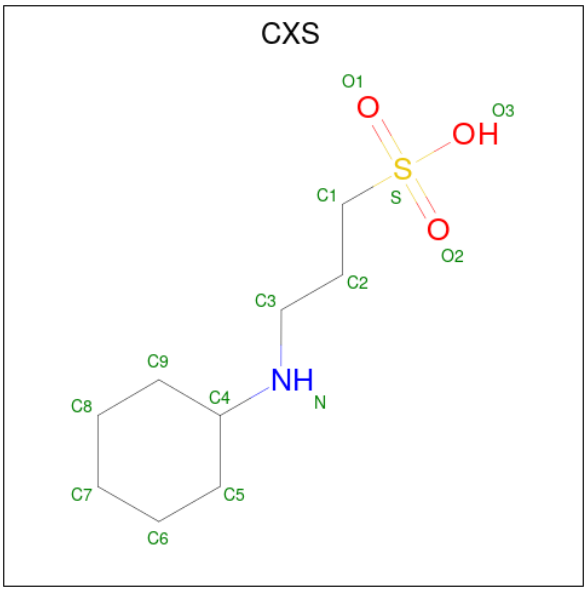


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 19 11 4 4	0	0
2	B	1	Total C N O 19 11 4 4	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

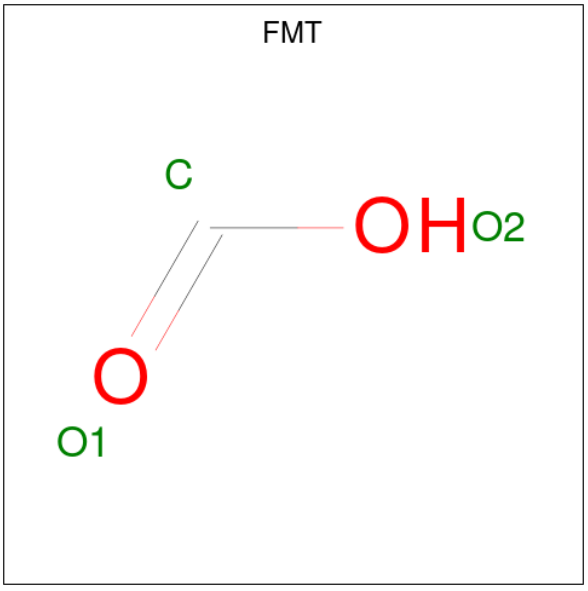
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: $C_9H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			3	1	2			

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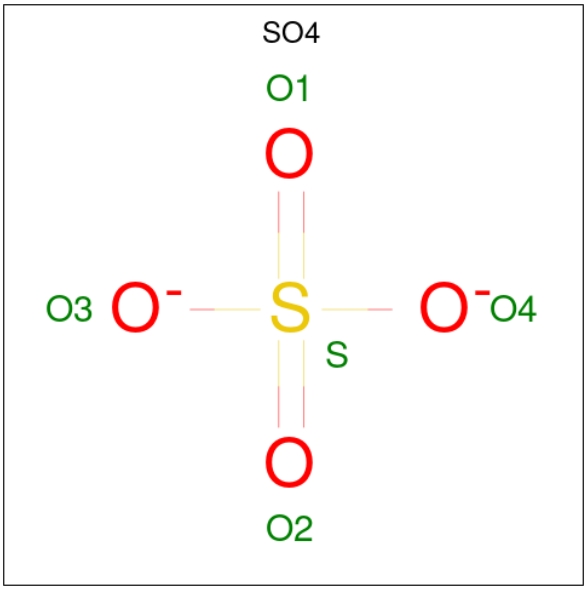
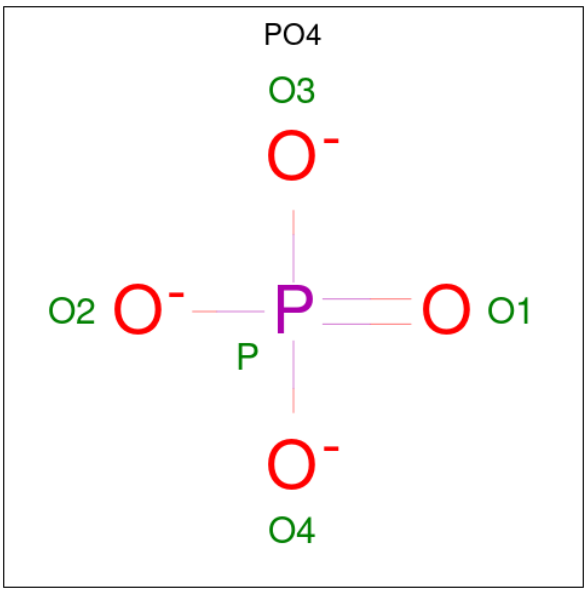
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 3 1 2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



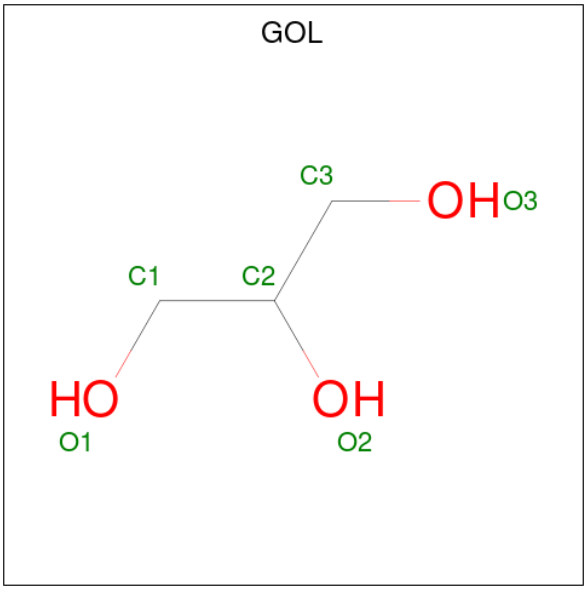
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

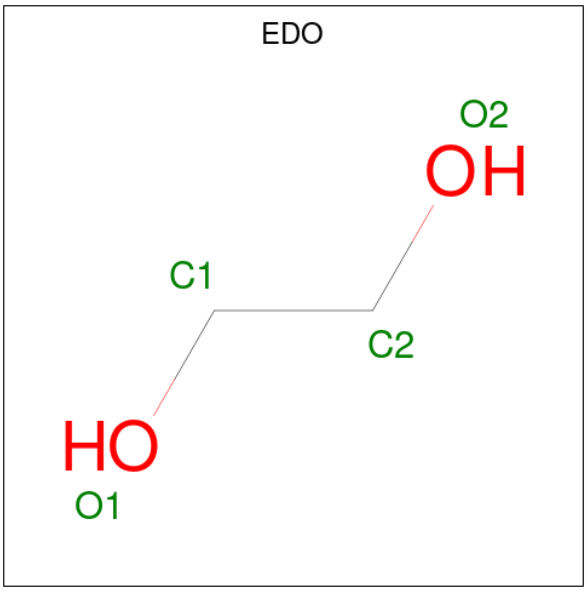


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Na 1 1	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	221	Total O 221 221	0	0
11	B	164	Total O 164 164	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 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	134.91Å 134.91Å 136.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.91 – 2.05	Depositor
% Data completeness (in resolution range)	99.8 (47.91-2.05)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.154 , 0.174	Depositor
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.092	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
Total number of atoms	5990	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 3.36% 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 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
5	FMT	B	404	-	2,2,2	0.64	0	1,1,1	0.11	0
5	FMT	A	404	-	2,2,2	0.66	0	1,1,1	0.21	0
7	PO4	A	406	-	4,4,4	0.84	0	6,6,6	0.47	0
4	CXS	A	403	-	14,14,14	2.46	2 (14%)	18,18,18	1.42	3 (16%)
8	GOL	A	407	-	5,5,5	1.05	0	5,5,5	0.73	0
6	SO4	A	405	-	4,4,4	0.14	0	6,6,6	0.12	0
2	DCF	B	401	3	14,21,21	1.01	1 (7%)	12,30,30	0.95	0
4	CXS	B	403	-	14,14,14	2.54	2 (14%)	18,18,18	1.70	2 (11%)
2	DCF	A	401	3	14,21,21	1.04	1 (7%)	12,30,30	0.79	0
10	EDO	B	406	-	3,3,3	0.42	0	2,2,2	0.49	0
4	CXS	B	409	-	14,14,14	2.62	2 (14%)	18,18,18	1.46	4 (22%)
7	PO4	B	408	-	4,4,4	0.81	0	6,6,6	0.45	0
8	GOL	B	407	-	5,5,5	1.11	0	5,5,5	0.95	0

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
4	CXS	A	403	-	-	1/8/16/16	0/1/1/1
8	GOL	A	407	-	-	0/4/4/4	-
2	DCF	B	401	3	-	0/2/29/29	0/2/3/3
4	CXS	B	403	-	-	3/8/16/16	0/1/1/1
2	DCF	A	401	3	-	0/2/29/29	0/2/3/3
10	EDO	B	406	-	-	1/1/1/1	-
4	CXS	B	409	-	-	5/8/16/16	0/1/1/1
8	GOL	B	407	-	-	4/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	409	CXS	C1-S	-7.39	1.67	1.77
4	B	403	CXS	C1-S	-6.85	1.67	1.77
4	A	403	CXS	C1-S	-6.50	1.68	1.77
4	B	403	CXS	O1-S	6.32	1.63	1.45
4	A	403	CXS	O1-S	6.20	1.63	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	409	CXS	O1-S	6.13	1.63	1.45
2	A	401	DCF	C10-N4	-2.80	1.38	1.41
2	B	401	DCF	C10-N4	-2.80	1.38	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	403	CXS	C3-N-C4	5.21	124.36	114.14
4	A	403	CXS	C3-N-C4	3.44	120.90	114.14
4	B	409	CXS	O1-S-C1	3.09	110.64	106.92
4	B	403	CXS	O3-S-C1	3.06	110.72	105.77
4	B	409	CXS	C2-C1-S	-2.93	108.75	113.25
4	B	409	CXS	C3-N-C4	2.67	119.37	114.14
4	A	403	CXS	O2-S-C1	2.47	109.88	106.92
4	A	403	CXS	O1-S-C1	2.13	109.48	106.92
4	B	409	CXS	O3-S-C1	2.01	109.02	105.77

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	CXS	C5-C4-N-C3
4	B	403	CXS	C5-C4-N-C3
4	B	409	CXS	C2-C1-S-O1
4	B	409	CXS	C2-C1-S-O2
4	B	409	CXS	C1-C2-C3-N
8	B	407	GOL	C1-C2-C3-O3
10	B	406	EDO	O1-C1-C2-O2
4	B	409	CXS	C2-C1-S-O3
8	B	407	GOL	O1-C1-C2-O2
8	B	407	GOL	O1-C1-C2-C3
8	B	407	GOL	O2-C2-C3-O3
4	B	403	CXS	C1-C2-C3-N
4	B	409	CXS	C2-C3-N-C4
4	B	403	CXS	C9-C4-N-C3

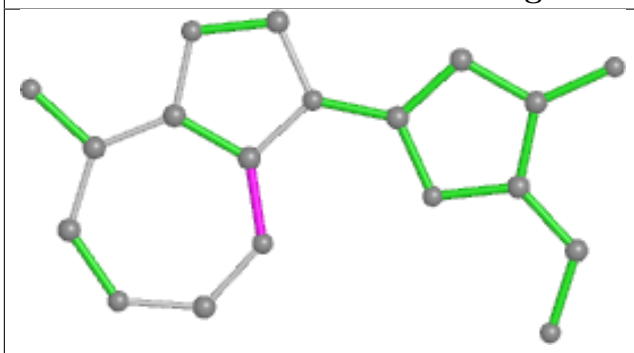
There are no ring outliers.

No monomer is involved in short contacts.

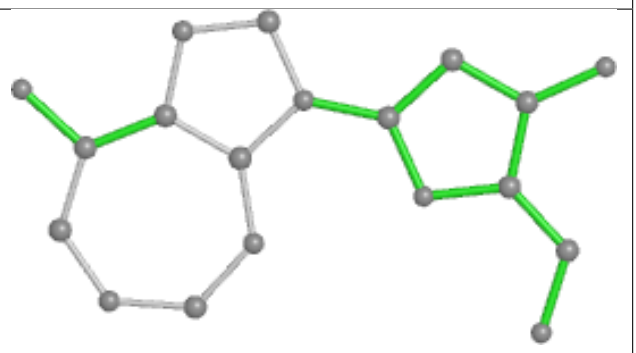
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

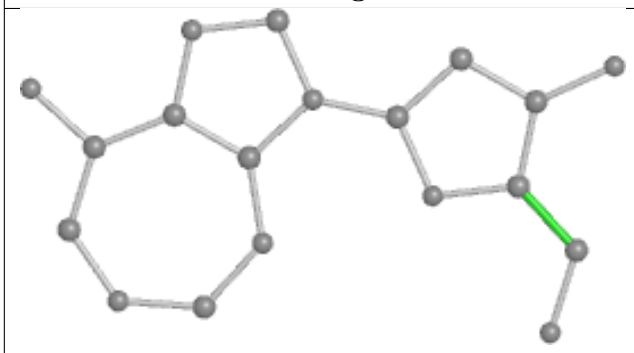
Ligand DCF B 401



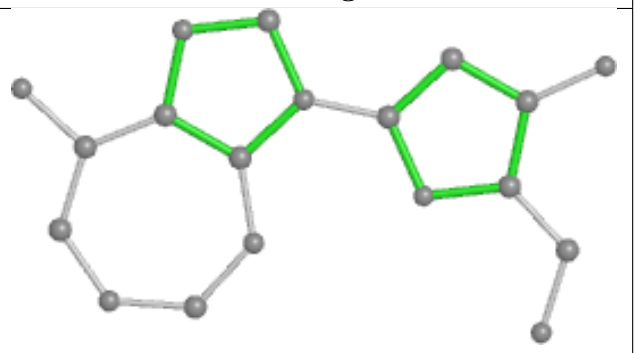
Bond lengths



Bond angles

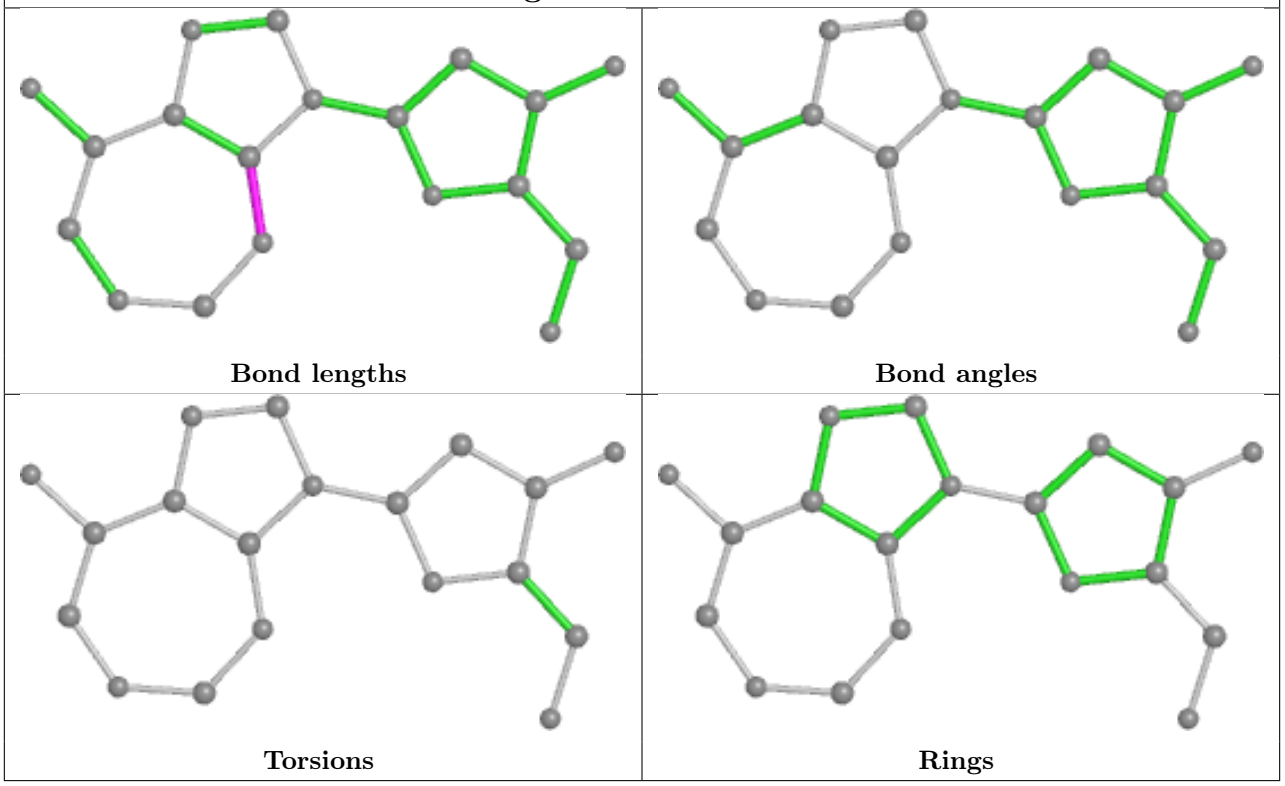


Torsions



Rings

Ligand DCF A 401



4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

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.