Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 09:10 am GMT

PDB ID	:	3ZHT
Title	:	Crystal structure of the SucA domain of Mycobacterium smegmatis KGD, first post-decarboxylation intermediate from 2-oxoadipate
Authors	:	Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.
Deposited on	:	2012-12-24
Resolution	:	2.15 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	:	4.02b-467
Mogul	:	1.8.4, 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)	:	2.36

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 2.15 Å.

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

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	868	94% 6%
1	B	868	93% 7%
1	C	868	93% 7%
1	D	868	93% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26205 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.

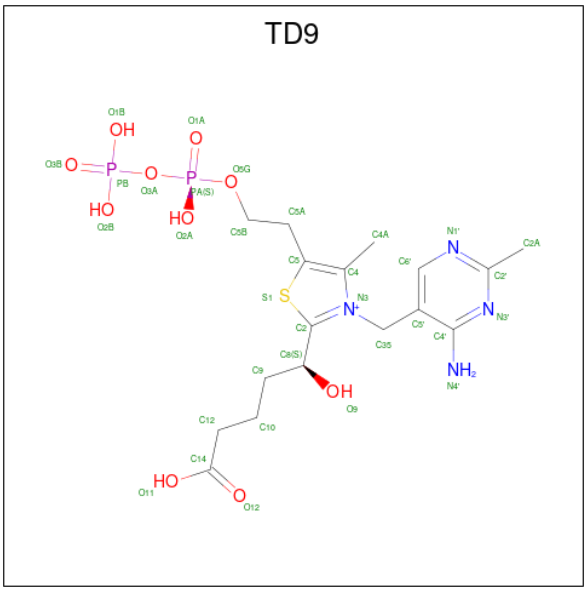
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	814	Total	C	N	O	S	0	1	0
			6292	3963	1111	1194	24			
1	B	809	Total	C	N	O	S	0	2	0
			6224	3922	1101	1176	25			
1	C	808	Total	C	N	O	S	0	0	0
			6258	3940	1104	1191	23			
1	D	807	Total	C	N	O	S	0	0	0
			6199	3905	1091	1180	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	expression tag	UNP A0R2B1
B	360	GLY	-	expression tag	UNP A0R2B1
C	360	GLY	-	expression tag	UNP A0R2B1
D	360	GLY	-	expression tag	UNP A0R2B1

- Molecule 2 is (5S)-5-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-4-methyl-5-(2-{[(phosphonatooxy)phosphinato]oxy}ethyl)-1,3-thiazol-3-ium-2-yl}-5-hydroxypentanoate (three-letter code: TD9) (formula: $C_{17}H_{27}N_4O_{10}P_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P S 34 17 4 10 2 1	0	0
2	B	1	Total C N O P S 34 17 4 10 2 1	0	0
2	C	1	Total C N O P S 34 17 4 10 2 1	0	0
2	D	1	Total C N O P S 34 17 4 10 2 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	339	Total O 339 339	0	0
5	B	223	Total O 223 223	0	0
5	C	305	Total O 305 305	0	0
5	D	221	Total O 221 221	0	0

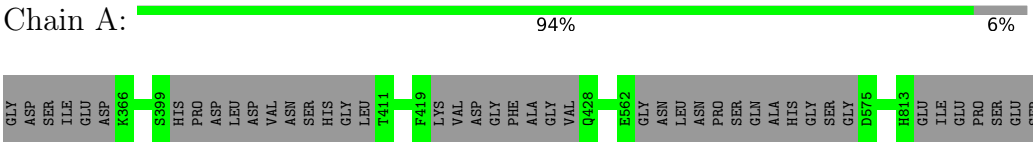
3 Residue-property plots (i)

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 failed to run properly.

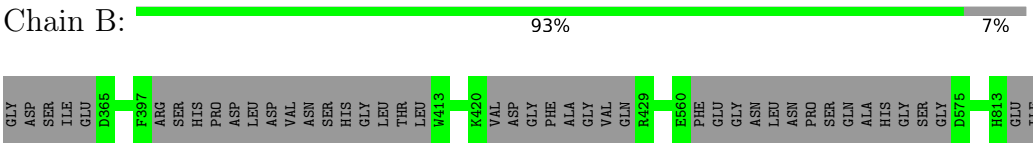
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

Chain A:



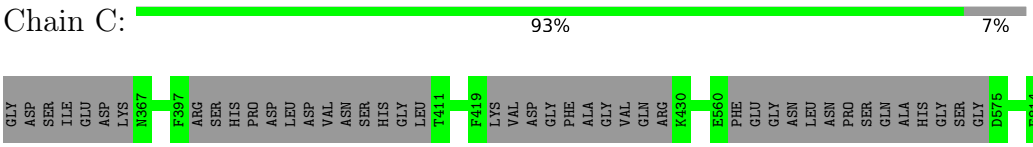
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

Chain B:



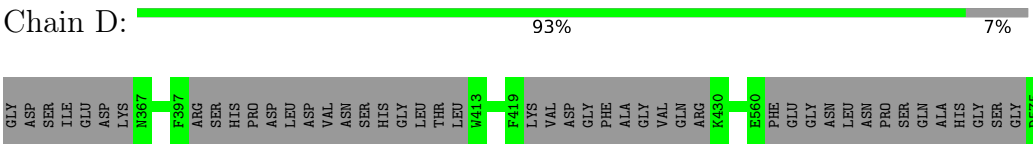
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

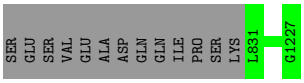
Chain C:



• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

Chain D:




SER
GLU
SER
VAL
GLU
ALA
ASP
GLN
GLN
ILE
PRO
SER
LYS
L831
G1227

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	80.37Å 83.80Å 159.51Å 99.76° 99.06° 100.61°	Depositor
Resolution (Å)	41.11 – 2.15	Depositor
% Data completeness (in resolution range)	97.5 (41.11-2.15)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.223 , 0.246	Depositor
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.172	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
Total number of atoms	26205	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1817e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG, TD9

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	0.50	0/6422	0.62	0/8710
1	B	0.48	0/6356	0.62	0/8627
1	C	0.50	0/6384	0.61	0/8657
1	D	0.48	0/6324	0.62	0/8584
All	All	0.49	0/25486	0.62	0/34578

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	TD9	B	2001	3	30,35,35	1.30	3 (10%)	36,51,51	1.36	4 (11%)
2	TD9	A	2001	3	30,35,35	1.37	2 (6%)	36,51,51	1.52	4 (11%)
2	TD9	D	2001	3	30,35,35	1.63	3 (10%)	36,51,51	1.36	4 (11%)
2	TD9	C	2001	3	30,35,35	1.41	3 (10%)	36,51,51	1.50	4 (11%)

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	TD9	B	2001	3	-	6/22/27/27	0/2/2/2
2	TD9	A	2001	3	-	4/22/27/27	0/2/2/2
2	TD9	D	2001	3	-	7/22/27/27	0/2/2/2
2	TD9	C	2001	3	-	4/22/27/27	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	TD9	C5-S1	-5.37	1.64	1.74
2	A	2001	TD9	C2-N3	5.28	1.47	1.35
2	D	2001	TD9	C5A-C5	5.25	1.53	1.50
2	A	2001	TD9	C5-S1	-4.97	1.64	1.74
2	D	2001	TD9	C2-N3	4.97	1.46	1.35
2	B	2001	TD9	C2-N3	4.85	1.46	1.35
2	C	2001	TD9	C2-N3	4.67	1.45	1.35
2	B	2001	TD9	C5-S1	-4.14	1.66	1.74
2	D	2001	TD9	C5-S1	-4.09	1.66	1.74
2	C	2001	TD9	C5A-C5	2.18	1.51	1.50
2	B	2001	TD9	C5A-C5	2.12	1.51	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2001	TD9	PA-O3A-PB	6.69	155.78	132.83
2	A	2001	TD9	PA-O3A-PB	6.52	155.20	132.83
2	D	2001	TD9	PA-O3A-PB	6.05	153.59	132.83
2	B	2001	TD9	PA-O3A-PB	5.80	152.72	132.83
2	A	2001	TD9	O1B-PB-O3A	-3.33	93.46	104.64
2	C	2001	TD9	O1B-PB-O3A	-3.08	94.30	104.64
2	D	2001	TD9	O1B-PB-O3A	-2.63	95.80	104.64
2	A	2001	TD9	C5A-C5-C4	-2.51	125.42	127.43
2	D	2001	TD9	C5-C4-N3	2.32	112.52	107.66
2	A	2001	TD9	C5-C4-N3	2.30	112.48	107.66
2	B	2001	TD9	O2B-PB-O3B	2.26	119.54	110.68
2	B	2001	TD9	C5-C4-N3	2.13	112.12	107.66
2	C	2001	TD9	C5A-C5-C4	-2.11	125.74	127.43
2	B	2001	TD9	O1B-PB-O3A	-2.09	97.63	104.64
2	D	2001	TD9	O5G-PA-O1A	2.07	117.17	109.07
2	C	2001	TD9	C5-C4-N3	2.07	111.98	107.66

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2001	TD9	C2-C8-C9-C10
2	B	2001	TD9	O9-C8-C9-C10
2	C	2001	TD9	PB-O3A-PA-O5G
2	D	2001	TD9	O9-C8-C9-C10
2	D	2001	TD9	N3-C35-C5'-C4'

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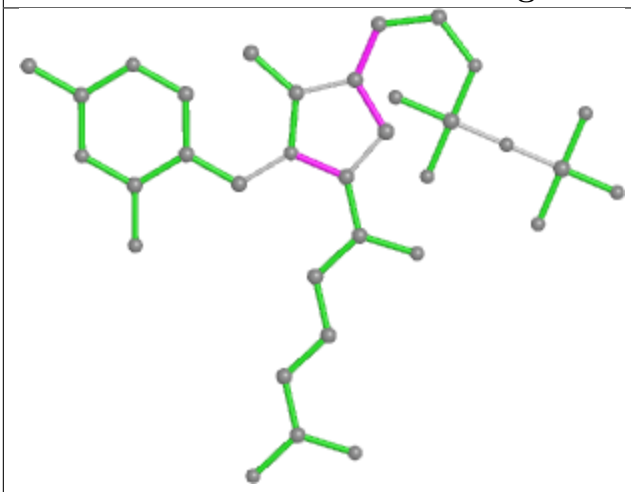
Mol	Chain	Res	Type	Atoms
2	D	2001	TD9	C9-C10-C12-C14
2	A	2001	TD9	PB-O3A-PA-O5G
2	B	2001	TD9	PB-O3A-PA-O5G
2	D	2001	TD9	PB-O3A-PA-O5G
2	D	2001	TD9	C12-C10-C9-C8
2	A	2001	TD9	C10-C12-C14-O12
2	C	2001	TD9	C10-C12-C14-O12
2	A	2001	TD9	C10-C12-C14-O11
2	C	2001	TD9	C10-C12-C14-O11
2	A	2001	TD9	C12-C10-C9-C8
2	C	2001	TD9	C12-C10-C9-C8
2	B	2001	TD9	C10-C12-C14-O11
2	B	2001	TD9	PA-O3A-PB-O2B
2	D	2001	TD9	PA-O3A-PB-O2B
2	B	2001	TD9	C10-C12-C14-O12
2	D	2001	TD9	C5B-O5G-PA-O1A

There are no ring outliers.

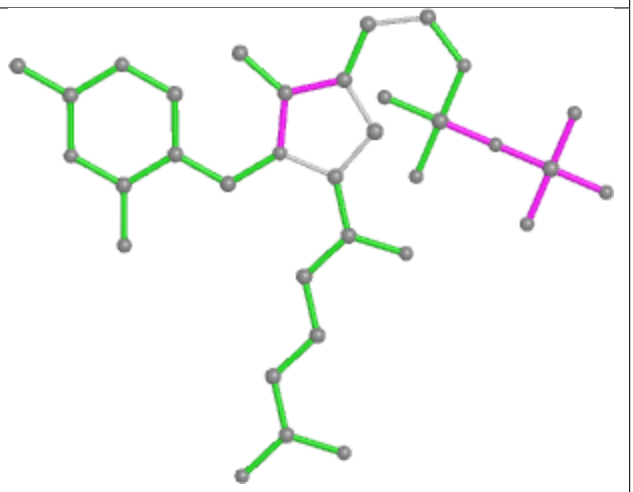
No monomer is involved in short contacts.

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.

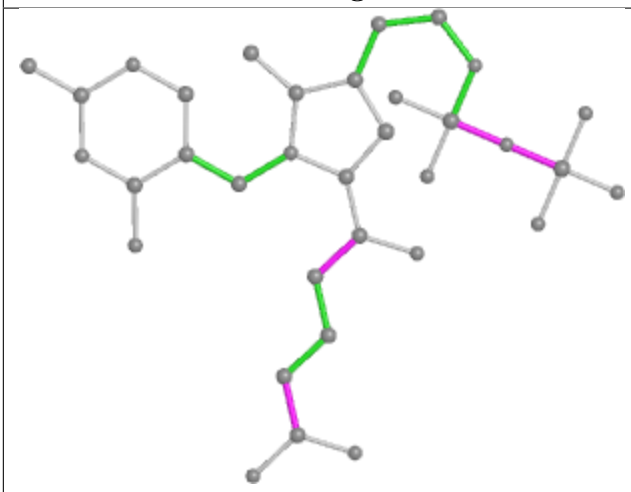
Ligand TD9 B 2001



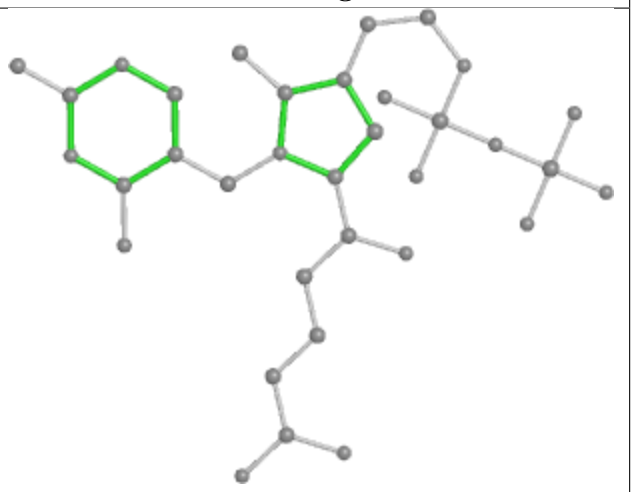
Bond lengths



Bond angles

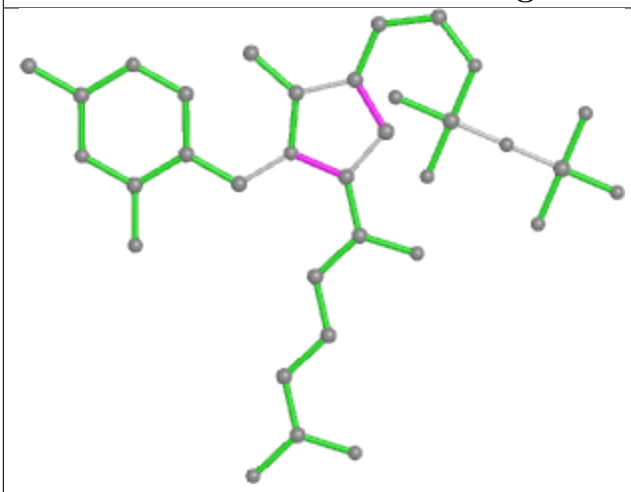


Torsions

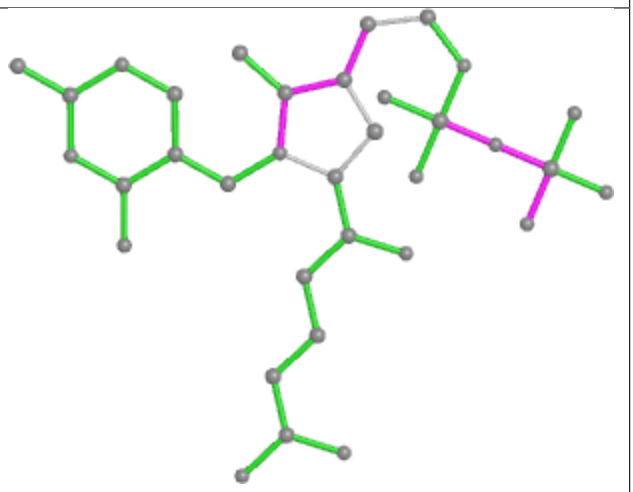


Rings

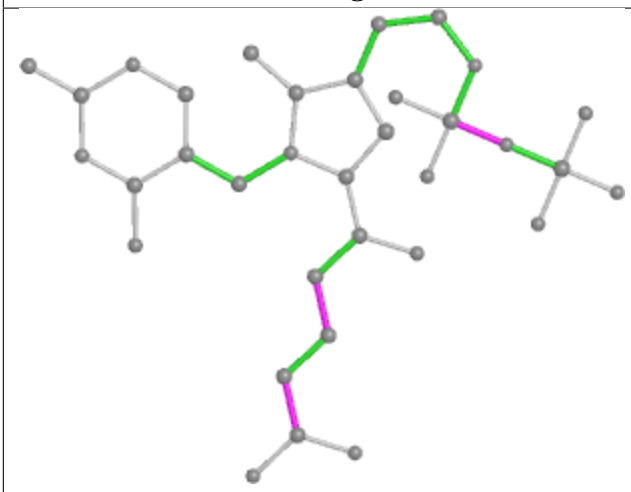
Ligand TD9 A 2001



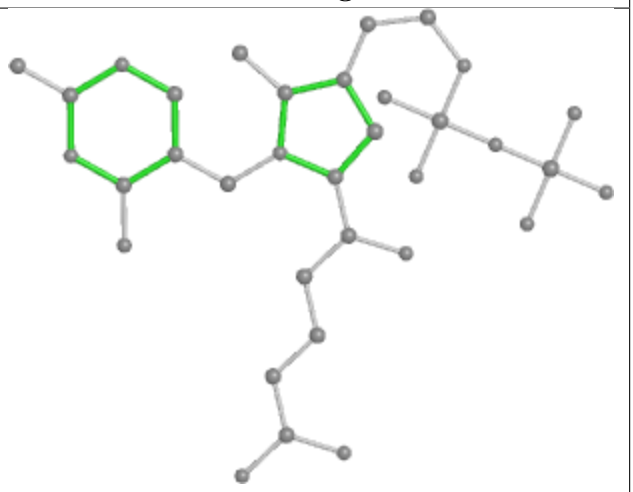
Bond lengths



Bond angles

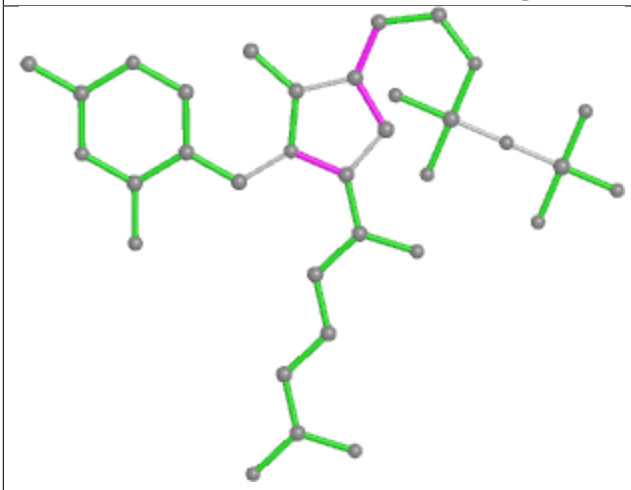


Torsions

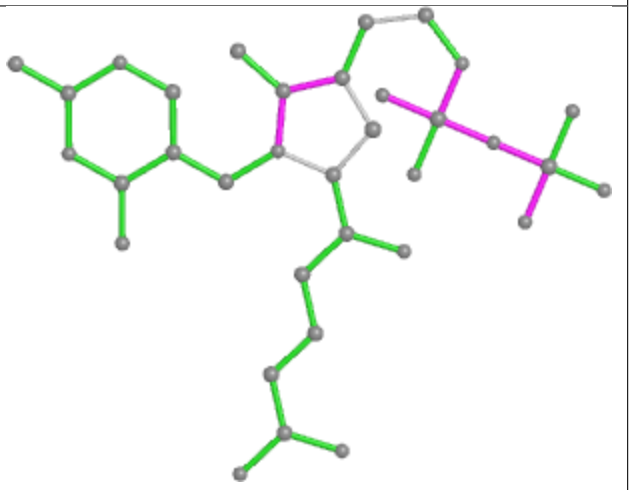


Rings

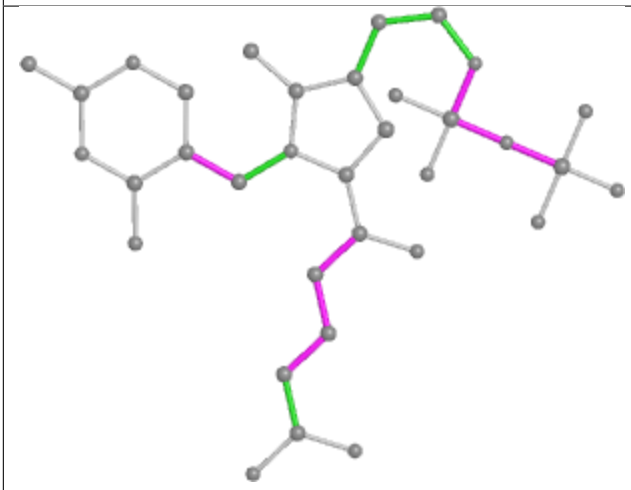
Ligand TD9 D 2001



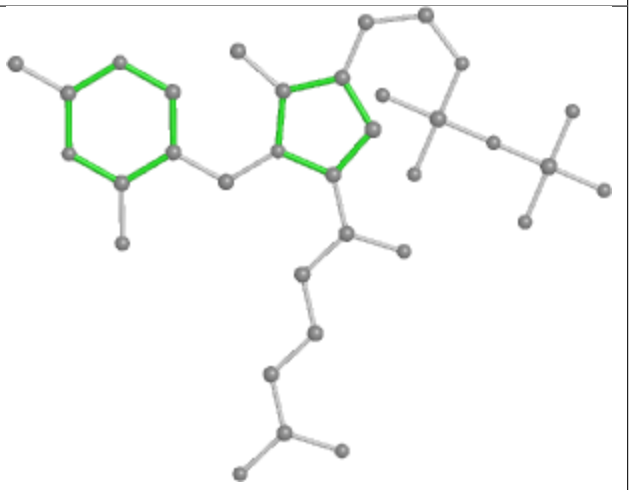
Bond lengths



Bond angles

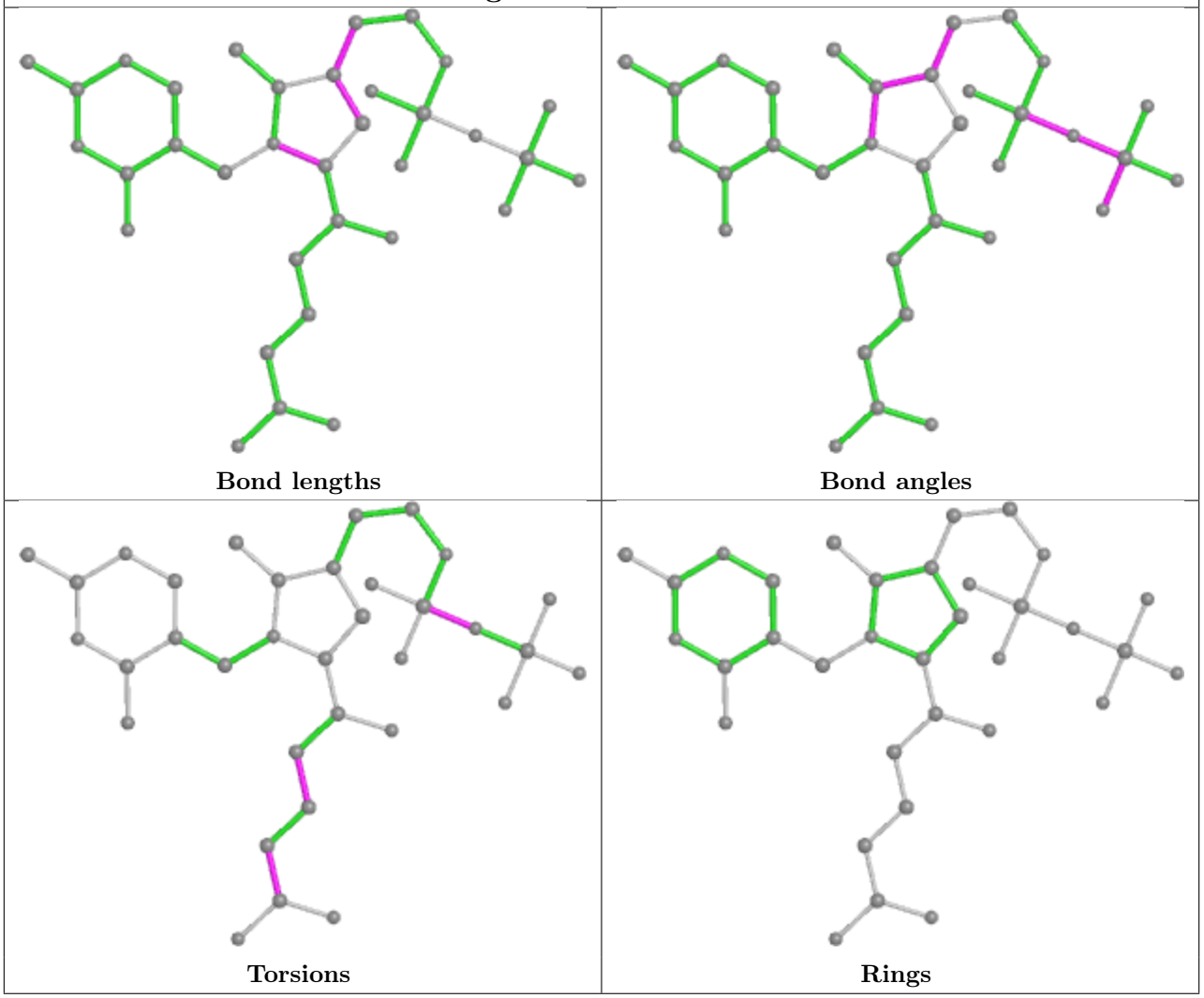


Torsions



Rings

Ligand TD9 C 2001



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 failed to run properly - this section is therefore empty.

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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