

wwPDB X-ray Structure Validation Summary Report (i)

Apr 4, 2022 – 08:14 PM EDT

PDB ID : 5TCG

Title : Crystal structure of tryptophan synthase from M. tuberculosis - aminoacrylate-

bound form

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tural Genomics of Infectious Diseases (CSGID)

Deposited on : 2016-09-15

Resolution : 2.40 Å(reported)

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

The following versions of software and data (see references (1)) 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) : 2.27

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 2.40 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 7 unique types of molecules in this entry. The entry contains 20280 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 Tryptophan synthase alpha chain.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	Λ	249	Total	Cotal C N O S	1	0				
1	A	249	1812	1136	325	346	5	0	1	
1	G	248	Total	С	N	О	S	0	1	0
1	G	240	1802	1131	323	342	6	0	1	
1	Е	245	Total	С	N	О	S	0	1	0
1		240	1784	1120	320	338	6	0	1	
1	C	249	Total	С	N	О	S	0	1	0
1		249	1811	1136	324	345	6	0	1	

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	HIS	-	expression tag	UNP P9WFY1
A	272	HIS	-	expression tag	UNP P9WFY1
A	273	HIS	-	expression tag	UNP P9WFY1
A	274	HIS	-	expression tag	UNP P9WFY1
A	275	HIS	-	expression tag	UNP P9WFY1
A	276	HIS	-	expression tag	UNP P9WFY1
G	271	HIS	-	expression tag	UNP P9WFY1
G	272	HIS	-	expression tag	UNP P9WFY1
G	273	HIS	-	expression tag	UNP P9WFY1
G	274	HIS	-	expression tag	UNP P9WFY1
G	275	HIS	-	expression tag	UNP P9WFY1
G	276	HIS	-	expression tag	UNP P9WFY1
E	271	HIS	-	expression tag	UNP P9WFY1
E	272	HIS	_	expression tag	UNP P9WFY1
E	273	HIS	-	expression tag	UNP P9WFY1
Е	274	HIS	-	expression tag	UNP P9WFY1
Е	275	HIS	-	expression tag	UNP P9WFY1
Е	276	HIS	-	expression tag	UNP P9WFY1
С	271	HIS	-	expression tag	UNP P9WFY1
С	272	HIS	-	expression tag	UNP P9WFY1
С	273	HIS	-	expression tag	UNP P9WFY1

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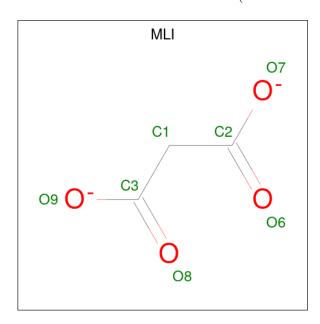
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Chain	Residue	Modelled	Actual	Comment	Reference
С	274	HIS	-	expression tag	UNP P9WFY1
С	275	HIS	-	expression tag	UNP P9WFY1
С	276	HIS	-	expression tag	UNP P9WFY1

• Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
2	В	399	Total	tal C N O S		0	3	0		
2	Б	399	3000	1873	544	569	14	0	3	
2	Н	399	Total	С	N	О	S	0	2	0
2	11	399	2989	1867	541	567	14	U		
2	F	399	Total	С	N	О	S	0	3	0
2	Г	399	3000	1872	545	570	13	U	3	U
2	D	399	Total	С	N	О	S	0	2	0
	ש	<u> </u>	2994	1869	546	566	13	U		U

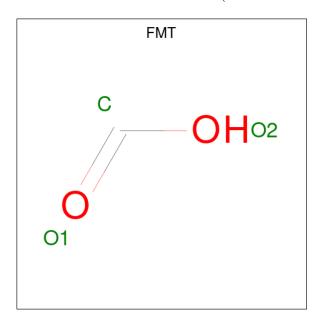
 \bullet Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: $\mathrm{C_3H_2O_4}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 3 4	0	0
3	G	1	Total C O 7 3 4	0	0
3	Ε	1	Total C O 7 3 4	0	0
3	С	1	Total C O 7 3 4	0	0



 \bullet Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: $\mathrm{CH_2O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	В	1	Total C O 3 1 2	0	0
4	В	1	Total C O 3 1 2	0	0
4	В	1	Total C O 3 1 2	0	0
4	В	1	Total C O 3 1 2	0	0
4	В	1	Total C O 3 1 2	0	0
4	G	1	Total C O 3 1 2	0	0
4	G	1	Total C O 3 1 2	0	0
4	G	1	Total C O 3 1 2	0	0
4	Н	1	Total C O 3 1 2	0	0
4	Н	1	Total C O 3 1 2	0	0
4	Н	1	Total C O 3 1 2	0	0
4	Н	1	Total C O 3 1 2	0	0
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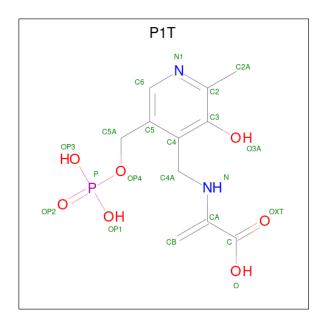


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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	1	Total C O 3 1 2	0	0
4	Н	1	Total C O 3 1 2	0	0
4	Н	1	Total C O 3 1 2	0	0
4	F	1	Total C O 3 1 2	0	0
4	F	1	Total C O 3 1 2	0	0
4	F	1	Total C O 3 1 2	0	0
4	F	1	Total C O 3 1 2	0	0
4	С	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0

• Molecule 5 is 2-[({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PY RIDIN-4-YL}METHYL)AMINO]ACRYLIC ACID (three-letter code: P1T) (formula: $C_{11}H_{15}N_2O_7P$).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
5	В	1	Total	С	N	О	Р	0	0
	Б	1	21	11	2	7	1	U	U
5	Н	1	Total	С	N	О	Р	0	0
9	11	1	21	11	2	7	1	U	
5	F	1	Total	С	N	О	Р	0	0
5	Г	1	21	11	2	7	1	U	0
5	D	1	Total	С	N	О	Р	0	0
	D	1	21	11	2	7	1	U	U

• Molecule 6 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	2	Total Cs 2 2	0	0
6	Н	1	Total Cs 1 1	0	0
6	F	3	Total Cs 3 3	0	0
6	D	3	Total Cs 3 3	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	57	Total O 57 57	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	170	Total O 170 170	0	0
7	G	82	Total O 82 82	0	2
7	Н	186	Total O 187 187	0	2
7	E	39	Total O 39 39	0	0
7	F	140	Total O 140 140	0	2
7	С	63	Total O 63 63	0	0
7	D	153	Total O 154 154	0	1

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 21 21 21	Depositor
Cell constants	135.18Å 159.43Å 165.23Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 - 2.40	Depositor
% Data completeness	99.5 (30.00-2.40)	Depositor
(in resolution range)	,	_
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.77 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.172 , 0.206	Depositor
Wilson B-factor $(Å^2)$	27.8	Xtriage
Anisotropy	0.248	Xtriage
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
Total number of atoms	20280	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 9 are monoatomic - leaving 33 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).

N / L - 1	Ф	Cl :	D	T : 1-	Во	Bond lengths		Bond angles		
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	
3	MLI	С	301	_	0,6,6	_	-	0,7,7	-	-
4	FMT	В	508	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	508	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	302	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	505	_	0,2,2	-	-	0,1,1	-	-
4	FMT	В	506	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	505	_	0,2,2	_	-	0,1,1	-	-
4	FMT	Н	505	-	0,2,2	-	-	0,1,1	-	-
4	FMT	G	302	-	0,2,2	-	-	0,1,1	-	-
4	FMT	Н	509	_	0,2,2	-	-	0,1,1	-	-
4	FMT	Н	504	-	0,2,2	-	-	0,1,1	-	-
3	MLI	A	301	-	0,6,6	-	-	0,7,7	-	-
4	FMT	F	507	-	0,2,2	-	-	0,1,1	-	-
5	P1T	D	501	-	18,21,21	3.02	4 (22%)	23,30,30	1.54	4 (17%)
4	FMT	В	505	_	0,2,2	-	-	0,1,1	-	-
3	MLI	G	301	_	0,6,6	_	-	0,7,7	-	-
5	P1T	Н	501	_	18,21,21	2.68	4 (22%)	23,30,30	1.43	4 (17%)
4	FMT	G	303	-	0,2,2	-	-	0,1,1	-	-
4	FMT	Н	507	-	0,2,2	-	-	0,1,1	-	-
4	FMT	Н	508	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	506	_	0,2,2	-	-	0,1,1	-	-
4	FMT	Н	503	-	0,2,2	-	-	0,1,1	-	-
4	FMT	В	504	_	0,2,2	-	-	0,1,1	-	-
4	FMT	Н	506	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	507	-	0,2,2	-	-	0,1,1	-	-
4	FMT	С	302	-	0,2,2	-	-	0,1,1	-	-
4	FMT	G	304	-	0,2,2	-	-	0,1,1	-	-
5	P1T	F	501	-	18,21,21	2.65	4 (22%)	23,30,30	1.52	4 (17%)
4	FMT	В	507	-	0,2,2	_	-	0,1,1	-	-
4	FMT	D	506	-	0,2,2	-	-	0,1,1	-	-
3	MLI	Е	301	-	0,6,6	-	-	0,7,7	-	-
5	P1T	В	501	-	18,21,21	2.75	4 (22%)	23,30,30	1.43	5 (21%)
4	FMT	F	508	-	0,2,2	-	-	0,1,1	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLI	С	301	-	-	0/0/4/4	-
3	MLI	A	301	-	-	0/0/4/4	-
5	P1T	F	501	-	-	3/10/15/15	0/1/1/1
5	P1T	В	501	-	-	3/10/15/15	0/1/1/1
5	P1T	D	501	-	-	3/10/15/15	0/1/1/1
3	MLI	Е	301	-	-	0/0/4/4	-
3	MLI	G	301	-	-	0/0/4/4	-
5	P1T	Н	501	-	-	3/10/15/15	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\mathring{A})$	Ideal(A)
5	D	501	P1T	C3-C2	8.07	1.49	1.40
5	Н	501	P1T	C3-C2	7.62	1.48	1.40
5	F	501	P1T	C3-C2	7.48	1.48	1.40
5	В	501	P1T	C3-C2	7.26	1.48	1.40
5	D	501	P1T	C3-C4	6.14	1.49	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$\operatorname{Ideal}(^{o})$
5	D	501	P1T	C4A-C4-C3	4.30	124.65	120.04
5	F	501	P1T	C4A-C4-C3	3.66	123.96	120.04
5	Н	501	P1T	C4A-C4-C3	3.31	123.58	120.04
5	В	501	P1T	C4A-C4-C3	3.13	123.40	120.04
5	В	501	P1T	C6-N1-C2	2.66	124.10	119.17

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	501	P1T	C5-C4-C4A-N
5	Н	501	P1T	C5-C4-C4A-N
5	F	501	P1T	C5-C4-C4A-N
5	F	501	P1T	C-CA-N-C4A
5	D	501	P1T	C5-C4-C4A-N

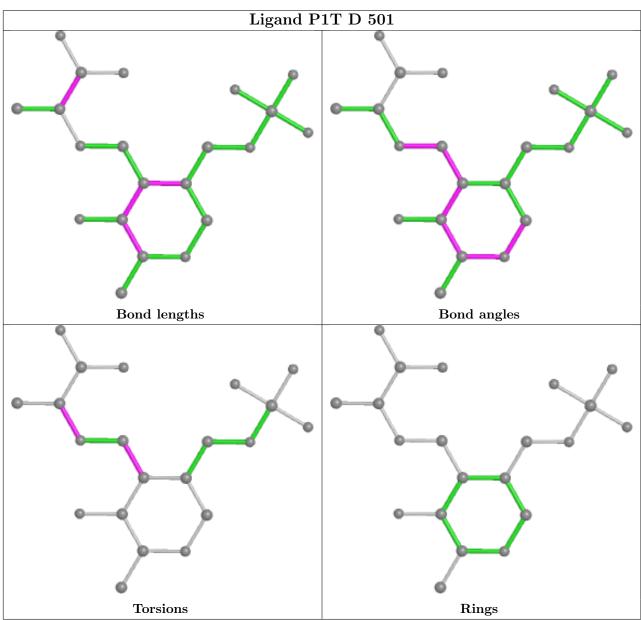
There are no ring outliers.

No monomer is involved in short contacts.

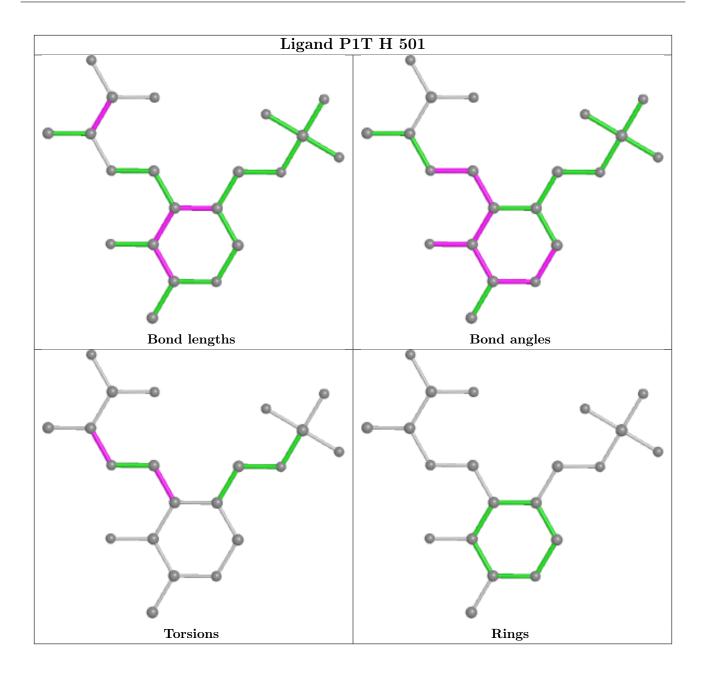
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In



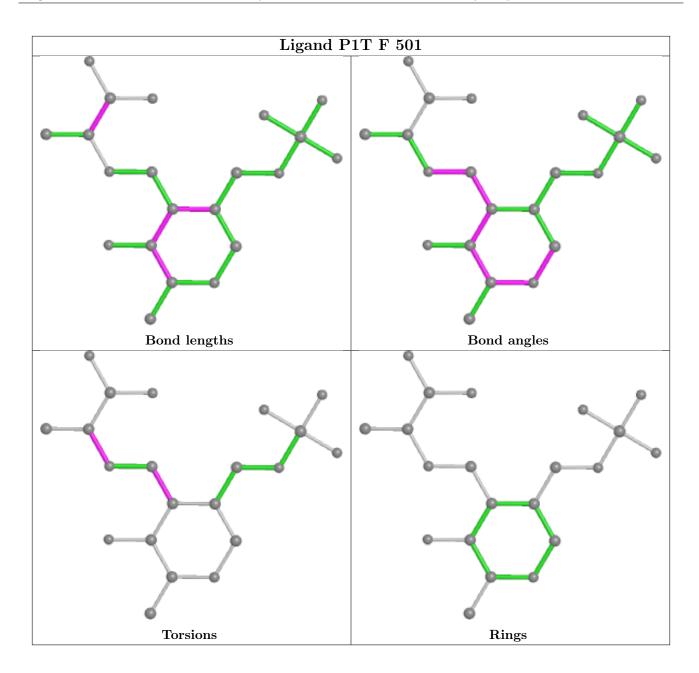
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



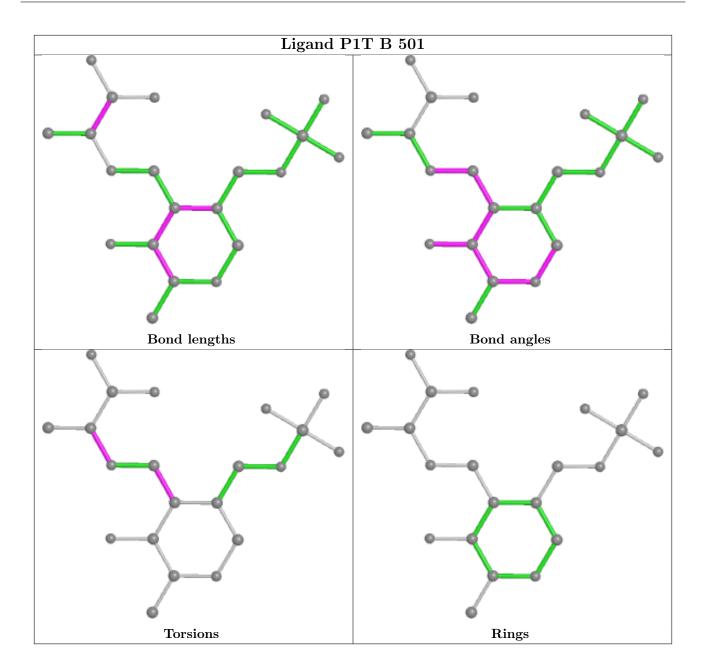












4.7 Other polymers (i)

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 (i)

5.1 Protein, DNA and RNA chains (i)

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

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

