



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2022 – 08:35 PM EDT

PDB ID : 5TCJ
Title : Crystal structure of tryptophan synthase from *M. tuberculosis* - aminoacrylate and BRD4592-bound form
Authors : Michalska, K.; Maltseva, N.; Jedrzejczak, R.; Wellington, S.; Nag, P.P.; Fisher, S.L.; Schreiber, S.L.; Hung, D.T.; Joachimiak, A.; Center for Structural 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.

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 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)	:	2.27

1 Overall quality at a glance

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

There are 8 unique types of molecules in this entry. The entry contains 20202 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	A	249	Total	C	N	O	S	0	1	0
			1814	1137	327	345	5			
1	G	248	Total	C	N	O	S	0	1	0
			1805	1132	326	342	5			
1	E	246	Total	C	N	O	S	0	1	0
			1793	1124	324	340	5			
1	C	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	HIS	-	expression tag	UNP P9WIFY1
A	272	HIS	-	expression tag	UNP P9WIFY1
A	273	HIS	-	expression tag	UNP P9WIFY1
A	274	HIS	-	expression tag	UNP P9WIFY1
A	275	HIS	-	expression tag	UNP P9WIFY1
A	276	HIS	-	expression tag	UNP P9WIFY1
G	271	HIS	-	expression tag	UNP P9WIFY1
G	272	HIS	-	expression tag	UNP P9WIFY1
G	273	HIS	-	expression tag	UNP P9WIFY1
G	274	HIS	-	expression tag	UNP P9WIFY1
G	275	HIS	-	expression tag	UNP P9WIFY1
G	276	HIS	-	expression tag	UNP P9WIFY1
E	271	HIS	-	expression tag	UNP P9WIFY1
E	272	HIS	-	expression tag	UNP P9WIFY1
E	273	HIS	-	expression tag	UNP P9WIFY1
E	274	HIS	-	expression tag	UNP P9WIFY1
E	275	HIS	-	expression tag	UNP P9WIFY1
E	276	HIS	-	expression tag	UNP P9WIFY1
C	271	HIS	-	expression tag	UNP P9WIFY1
C	272	HIS	-	expression tag	UNP P9WIFY1
C	273	HIS	-	expression tag	UNP P9WIFY1

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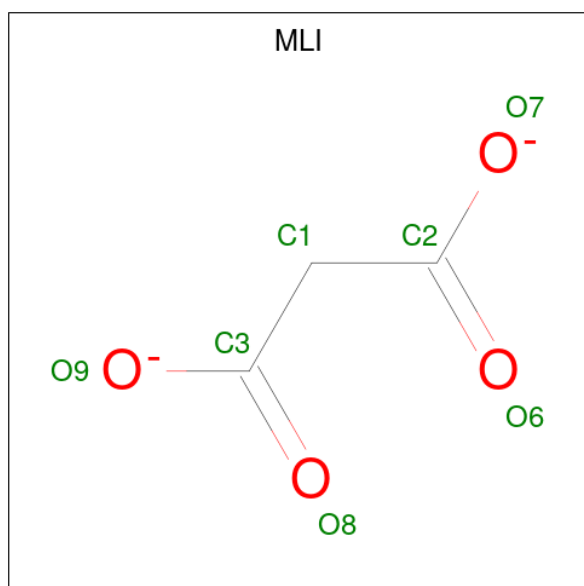
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Chain	Residue	Modelled	Actual	Comment	Reference
C	274	HIS	-	expression tag	UNP P9WFY1
C	275	HIS	-	expression tag	UNP P9WFY1
C	276	HIS	-	expression tag	UNP P9WFY1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			
2	H	401	Total	C	N	O	S	0	3	0
			3014	1882	545	573	14			
2	F	399	Total	C	N	O	S	0	3	0
			3000	1872	545	570	13			
2	D	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



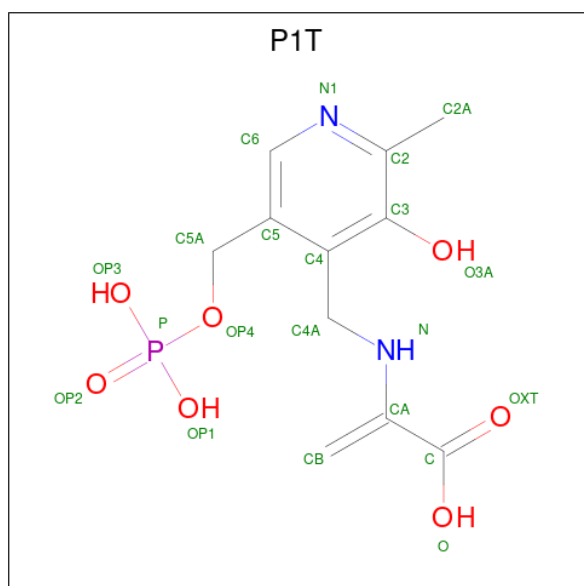
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	G	1	Total	C	O	0	0
			3	1	2		
4	G	1	Total	C	O	0	0
			3	1	2		
4	G	1	Total	C	O	0	0
			3	1	2		
4	H	1	Total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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

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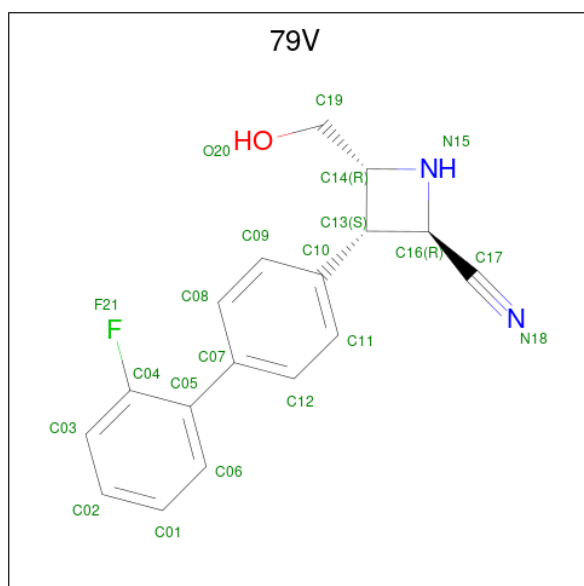
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
5	F	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
5	D	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Cs	0	0
			3	3		
6	H	1	Total	Cs	0	0
			1	1		
6	F	3	Total	Cs	0	0
			3	3		
6	D	2	Total	Cs	0	0
			2	2		

- Molecule 7 is (2R,3S,4R)-3-(2'-fluoro[1,1'-biphenyl]-4-yl)-4-(hydroxymethyl)azetidine-2-carbonitrile (three-letter code: 79V) (formula: C₁₇H₁₅FN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	F	N	O	0	0
			21	17	1	2	1		
7	H	1	Total	C	F	N	O	0	0
			21	17	1	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	F	1	Total	C	F	N	O	0	0
			21	17	1	2	1		
7	D	1	Total	C	F	N	O	0	0
			21	17	1	2	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	50	Total	O	0	0
			50	50		
8	B	147	Total	O	0	1
			147	147		
8	G	70	Total	O	0	2
			70	70		
8	H	140	Total	O	0	1
			141	141		
8	E	22	Total	O	0	0
			22	22		
8	F	120	Total	O	0	4
			120	120		
8	C	39	Total	O	0	0
			39	39		
8	D	132	Total	O	0	0
			132	132		

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.09Å 159.88Å 165.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	99.5 (30.00-2.40)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.180 , 0.211	Depositor
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.487	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k	Xtriage
Total number of atoms	20202	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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 43 ligands modelled in this entry, 9 are monoatomic - leaving 34 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
7	79V	D	504	-	22,23,23	2.71	6 (27%)	22,32,32	1.07	0
4	FMT	F	510	-	0,2,2	-	-	0,1,1	-	-
4	FMT	H	504	-	0,2,2	-	-	0,1,1	-	-
7	79V	H	503	-	22,23,23	2.93	10 (45%)	22,32,32	1.16	3 (13%)
4	FMT	H	505	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	507	-	0,2,2	-	-	0,1,1	-	-
4	FMT	H	506	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	509	-	0,2,2	-	-	0,1,1	-	-
5	P1T	D	501	-	18,21,21	2.88	4 (22%)	23,30,30	1.38	3 (13%)
4	FMT	A	302	-	0,2,2	-	-	0,1,1	-	-
7	79V	F	505	-	22,23,23	2.55	8 (36%)	22,32,32	1.08	2 (9%)
4	FMT	F	506	-	0,2,2	-	-	0,1,1	-	-
3	MLI	E	301	-	0,6,6	-	-	0,7,7	-	-
5	P1T	F	501	-	18,21,21	2.84	4 (22%)	23,30,30	1.40	3 (13%)
4	FMT	B	509	-	0,2,2	-	-	0,1,1	-	-
4	FMT	G	302	-	0,2,2	-	-	0,1,1	-	-
5	P1T	B	501	-	18,21,21	2.90	4 (22%)	23,30,30	1.45	3 (13%)
4	FMT	C	302	-	0,2,2	-	-	0,1,1	-	-
3	MLI	G	301	-	0,6,6	-	-	0,7,7	-	-
3	MLI	A	301	-	0,6,6	-	-	0,7,7	-	-
5	P1T	H	501	-	18,21,21	2.90	4 (22%)	23,30,30	1.40	4 (17%)
4	FMT	H	508	-	0,2,2	-	-	0,1,1	-	-
4	FMT	H	507	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	505	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	507	-	0,2,2	-	-	0,1,1	-	-
3	MLI	C	301	-	0,6,6	-	-	0,7,7	-	-
4	FMT	G	304	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	506	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	508	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	507	-	0,2,2	-	-	0,1,1	-	-
7	79V	B	505	-	22,23,23	2.74	9 (40%)	22,32,32	1.17	3 (13%)
4	FMT	B	506	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	508	-	0,2,2	-	-	0,1,1	-	-
4	FMT	G	303	-	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
7	79V	D	504	-	-	3/9/24/24	0/3/3/3
3	MLI	C	301	-	-	0/0/4/4	-
7	79V	H	503	-	-	3/9/24/24	0/3/3/3
5	P1T	B	501	-	-	3/10/15/15	0/1/1/1
5	P1T	D	501	-	-	3/10/15/15	0/1/1/1
7	79V	F	505	-	-	0/9/24/24	0/3/3/3
3	MLI	G	301	-	-	0/0/4/4	-
3	MLI	E	301	-	-	0/0/4/4	-
3	MLI	A	301	-	-	0/0/4/4	-
7	79V	B	505	-	-	3/9/24/24	0/3/3/3
5	P1T	H	501	-	-	3/10/15/15	0/1/1/1
5	P1T	F	501	-	-	3/10/15/15	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	504	79V	C14-N15	9.39	1.56	1.48
7	H	503	79V	C14-N15	9.08	1.56	1.48
7	B	505	79V	C14-N15	8.76	1.56	1.48
5	H	501	P1T	C3-C2	8.38	1.49	1.40
7	F	505	79V	C14-N15	7.81	1.55	1.48

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	501	P1T	C4A-C4-C3	3.44	123.73	120.04
5	B	501	P1T	C4A-C4-C3	3.42	123.71	120.04
5	F	501	P1T	C4A-C4-C3	3.28	123.56	120.04
5	D	501	P1T	C4A-C4-C3	3.23	123.50	120.04
5	B	501	P1T	C6-N1-C2	2.73	124.23	119.17

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	P1T	C5-C4-C4A-N
5	H	501	P1T	C5-C4-C4A-N
5	F	501	P1T	C5-C4-C4A-N

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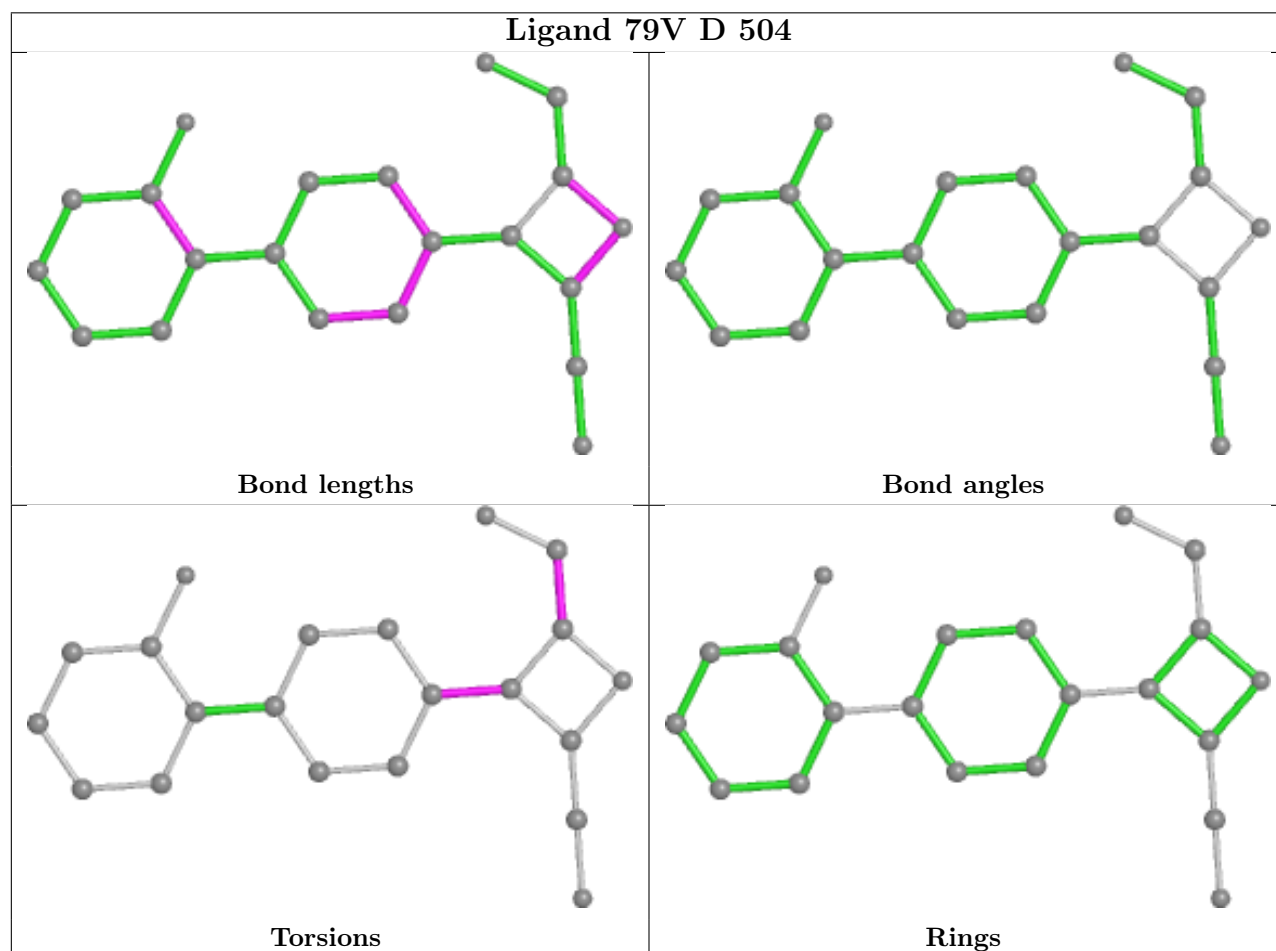
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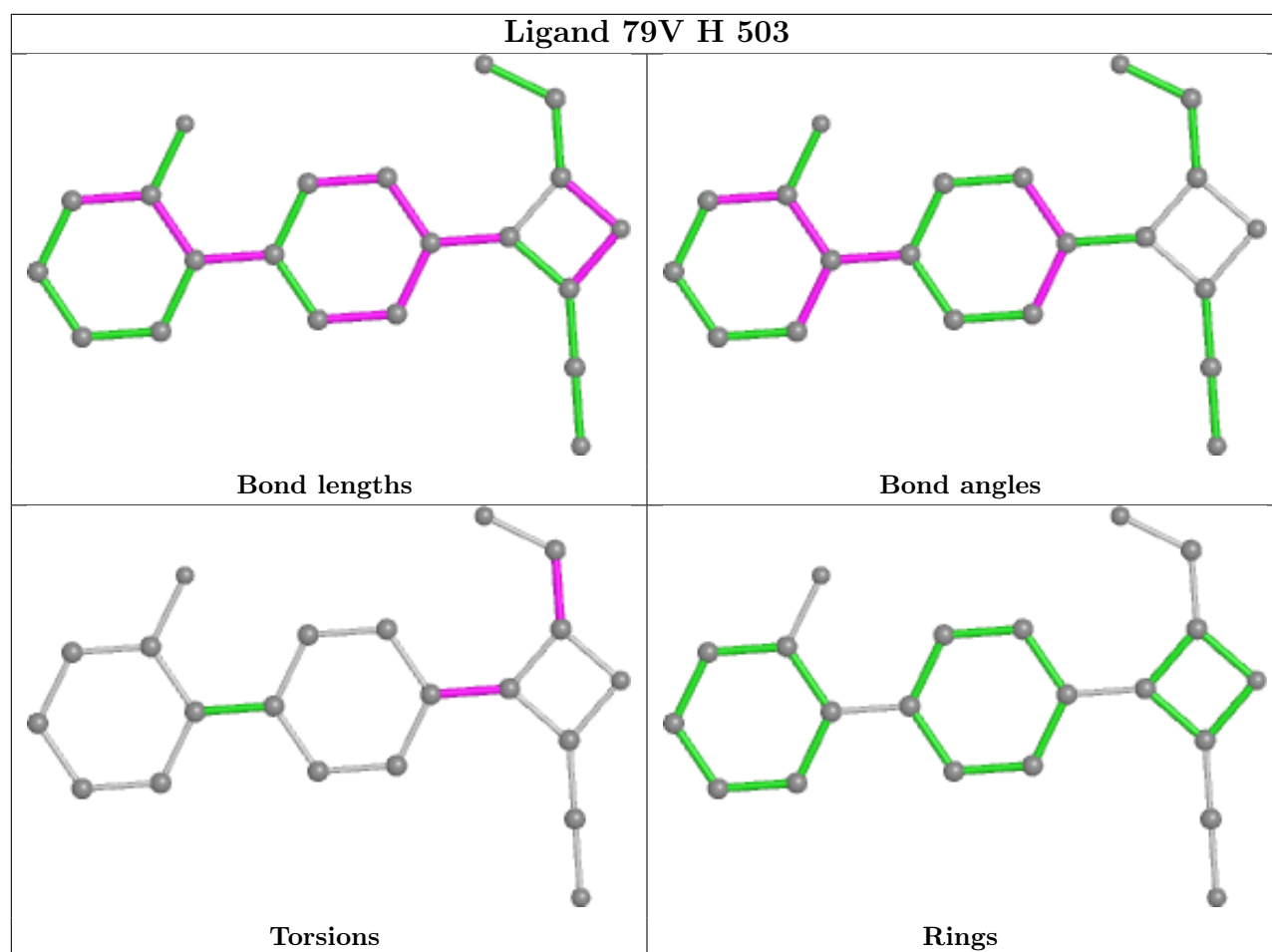
Mol	Chain	Res	Type	Atoms
5	D	501	P1T	C5-C4-C4A-N
5	D	501	P1T	C3-C4-C4A-N

There are no ring outliers.

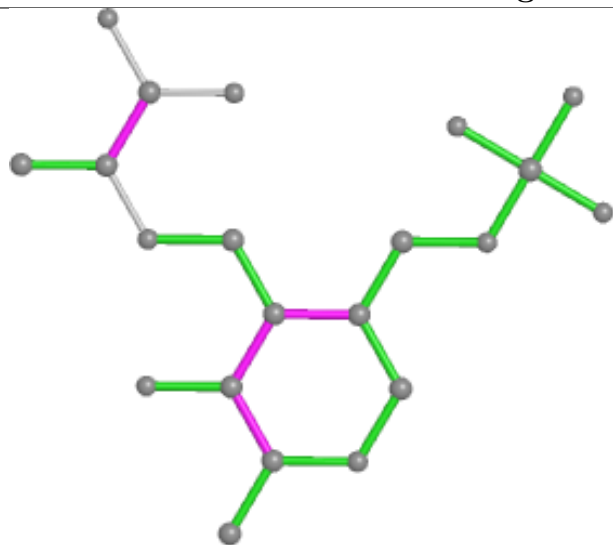
No monomer is involved in short contacts.

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 than 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.

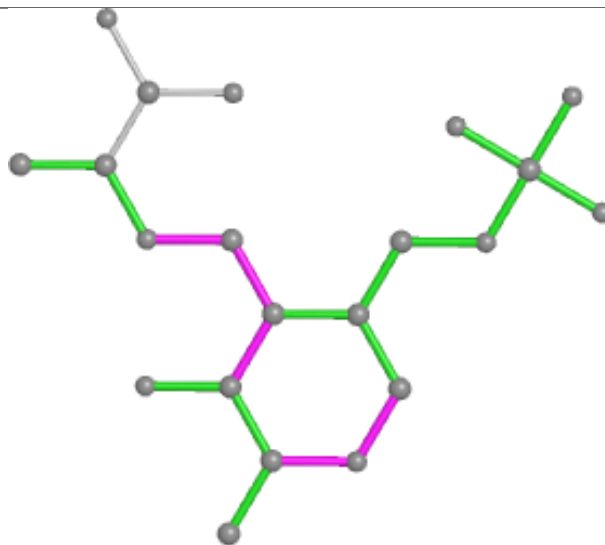




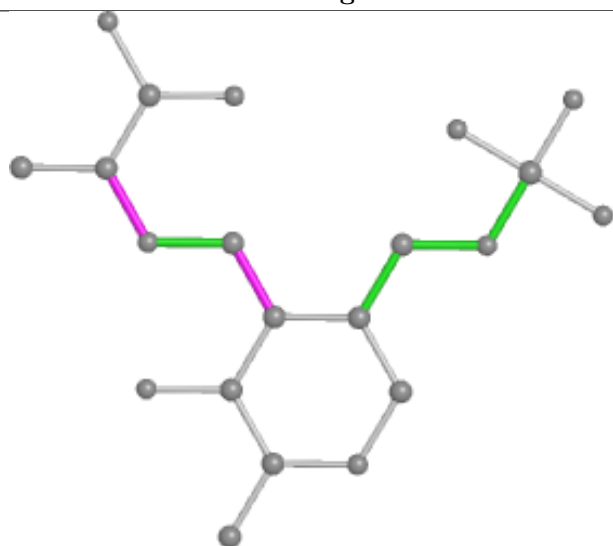
Ligand P1T D 501



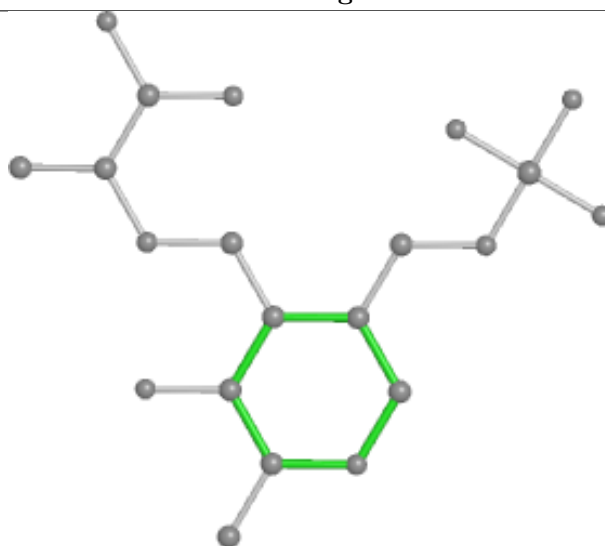
Bond lengths



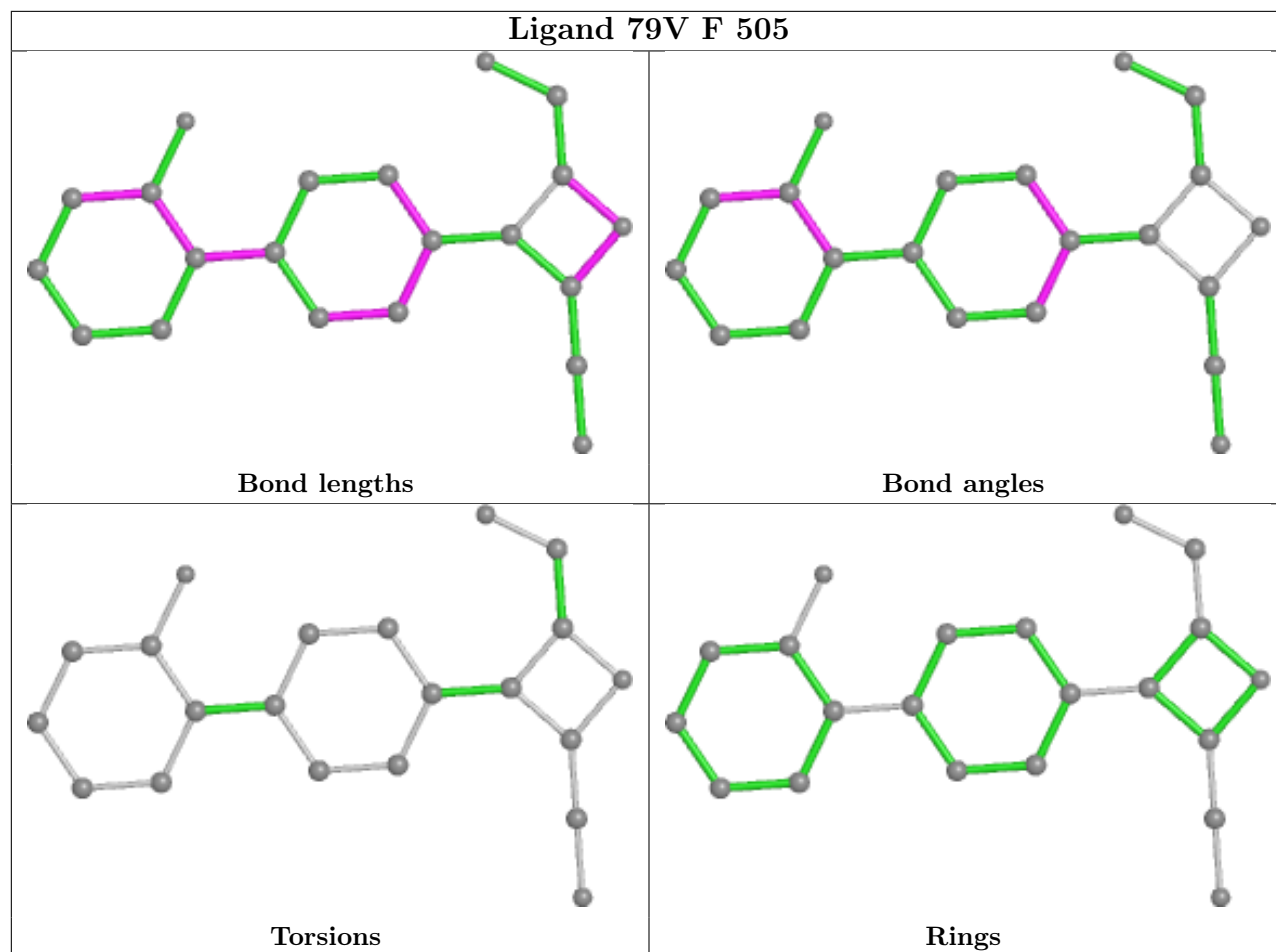
Bond angles



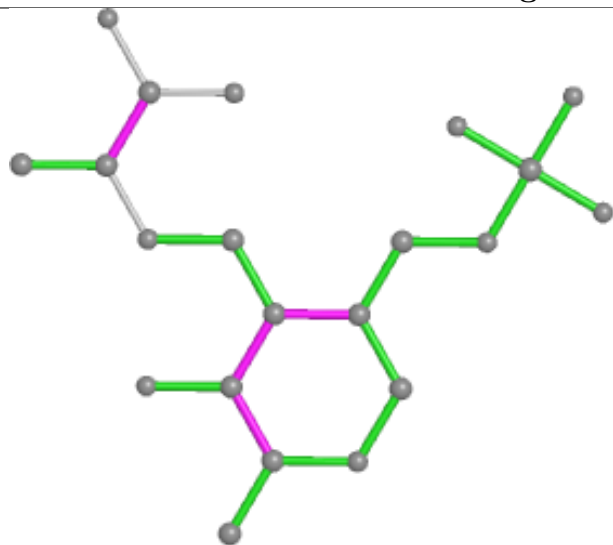
Torsions



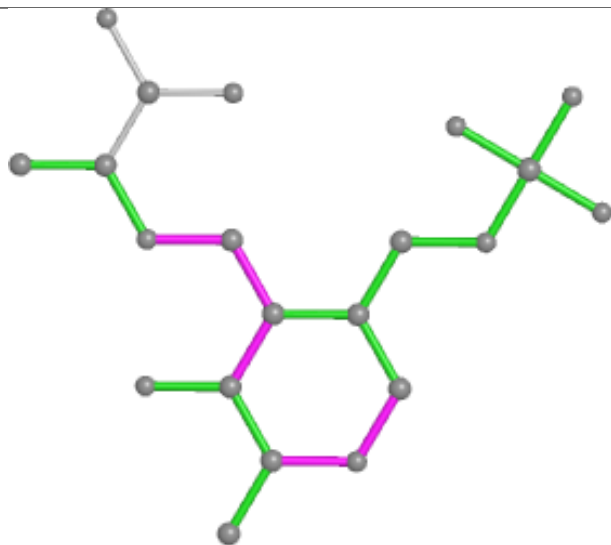
Rings



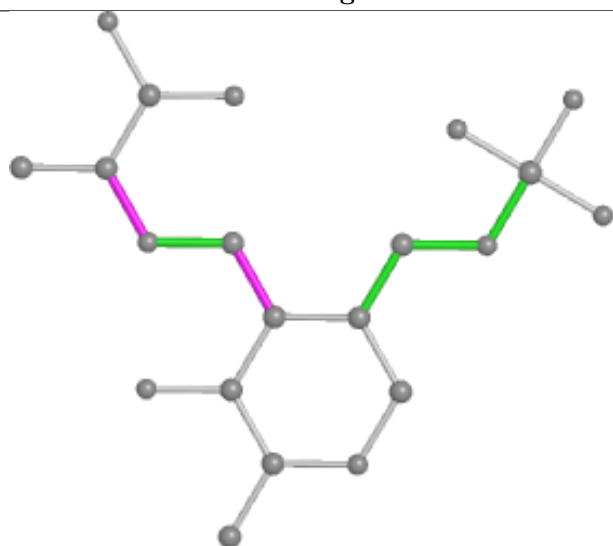
Ligand P1T F 501



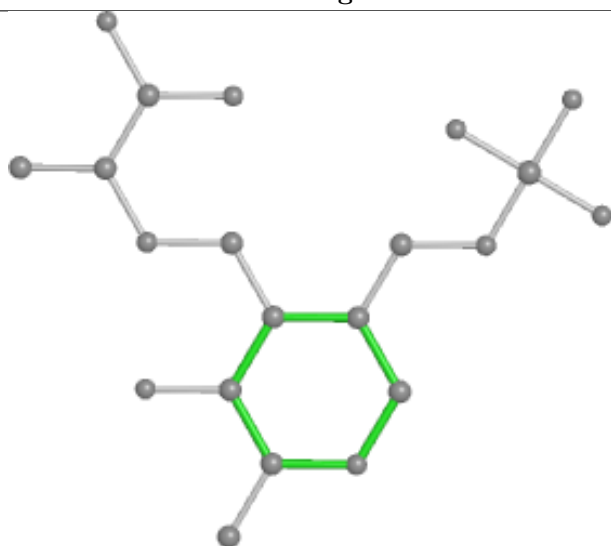
Bond lengths



Bond angles

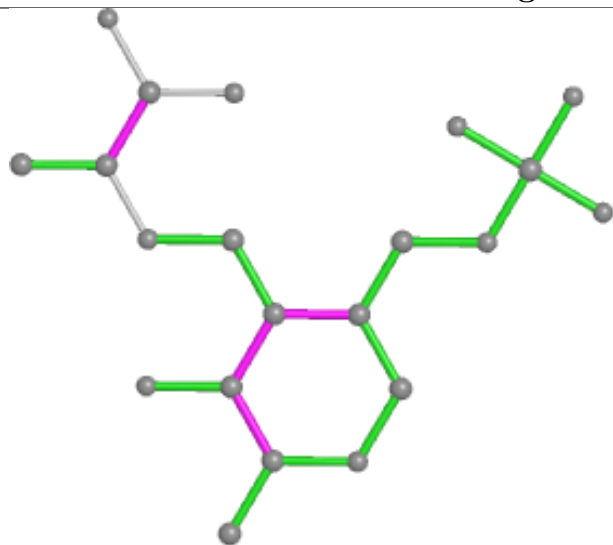


Torsions

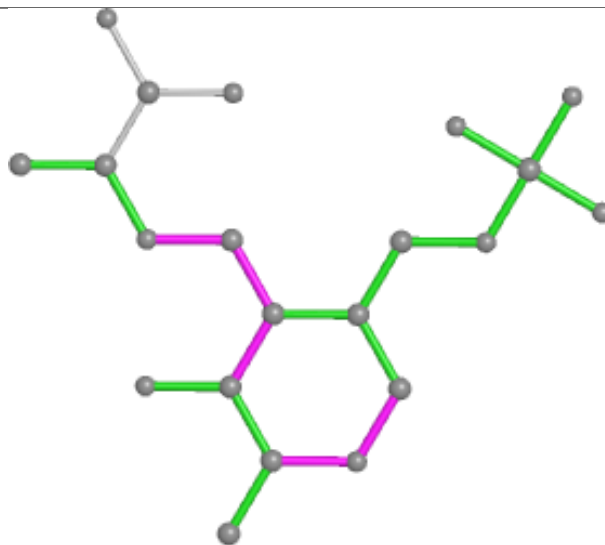


Rings

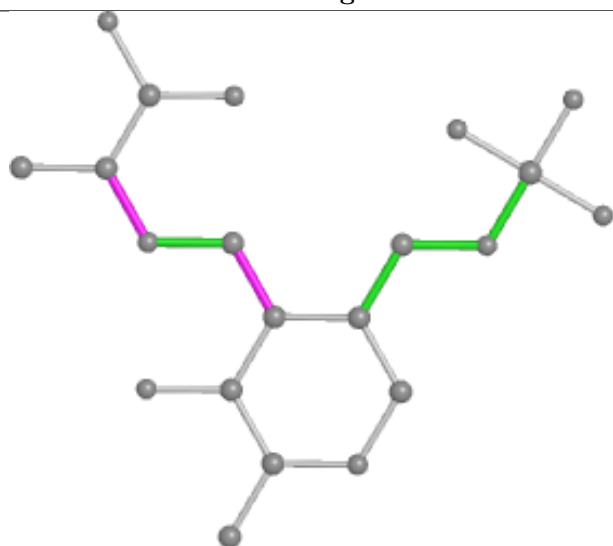
Ligand P1T B 501



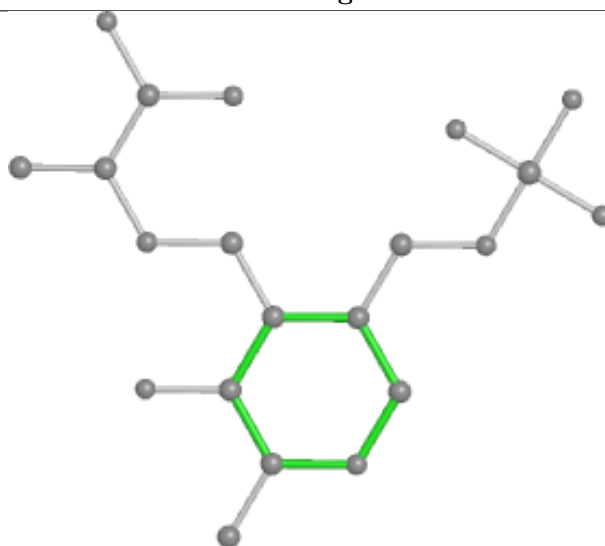
Bond lengths



Bond angles

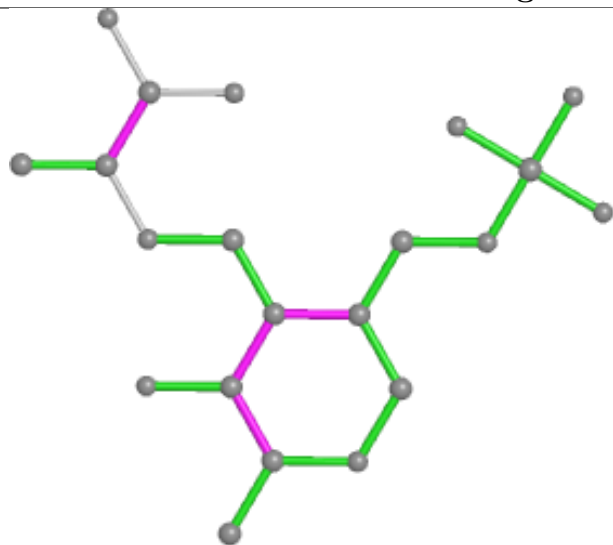


Torsions

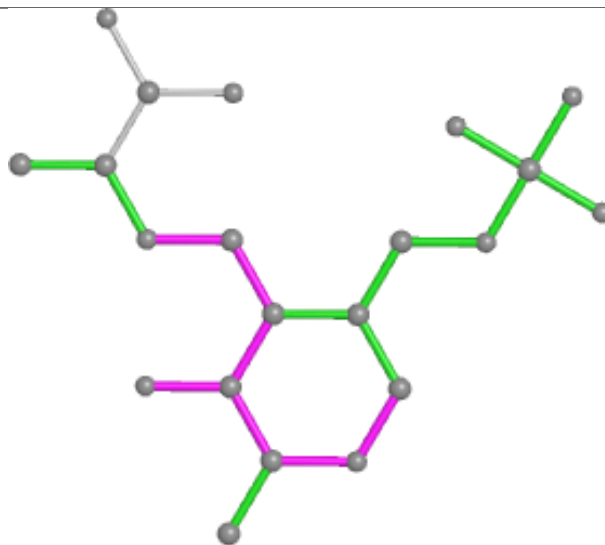


Rings

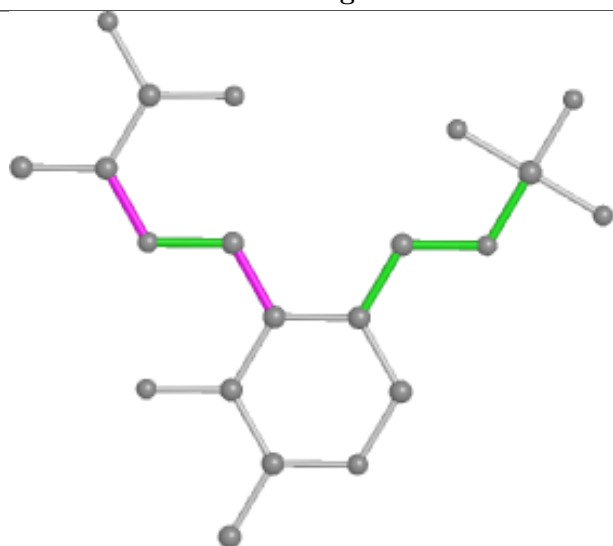
Ligand P1T H 501



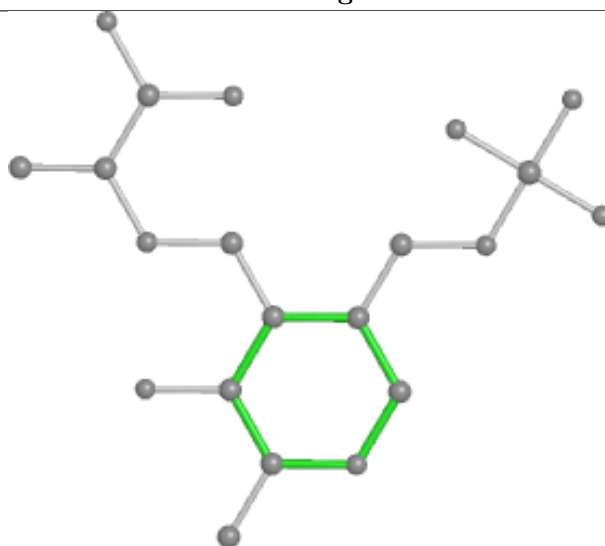
Bond lengths



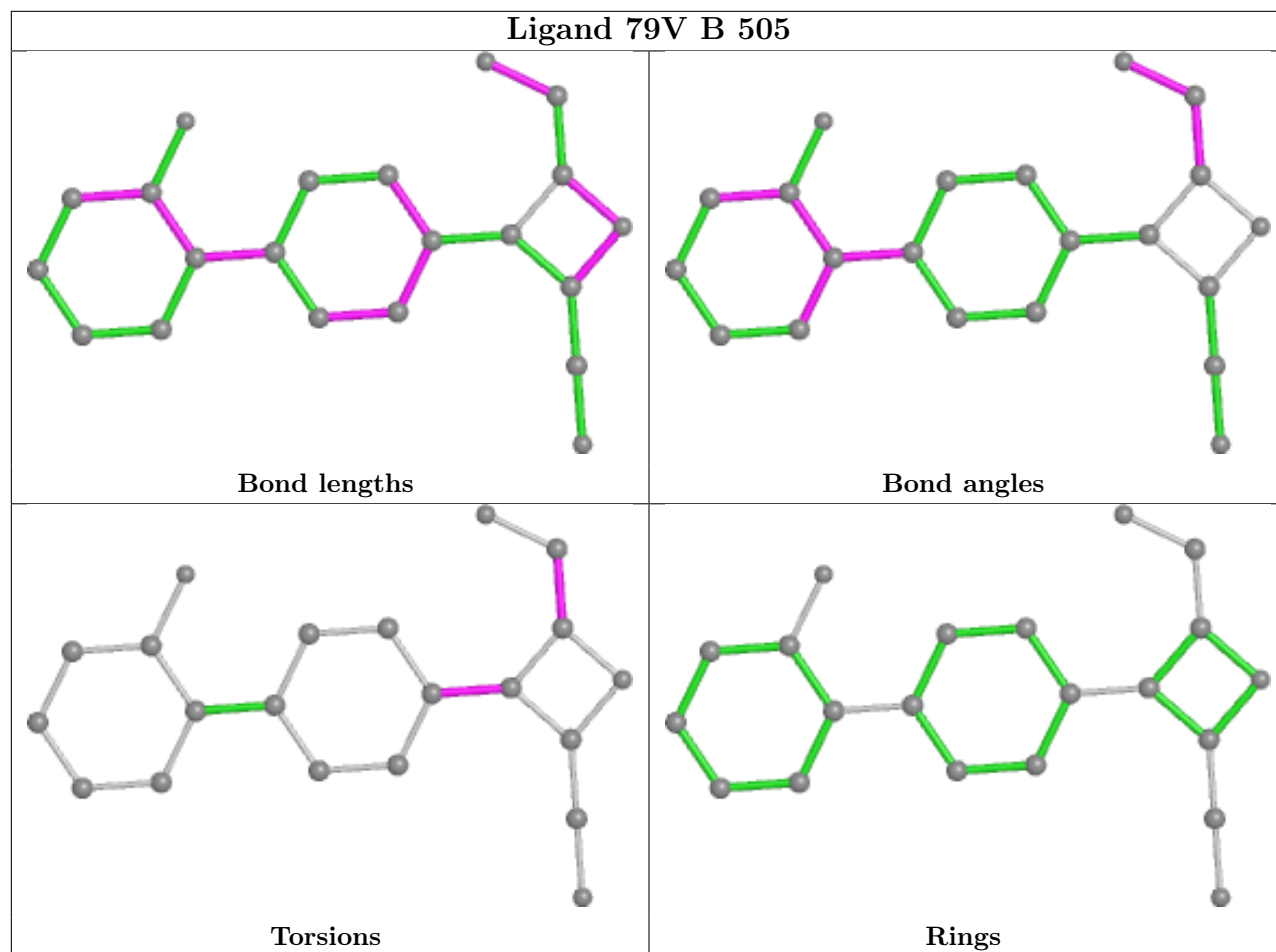
Bond angles



Torsions



Rings



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.