



# wwPDB X-ray Structure Validation Summary Report

Mar 10, 2026 – 03:54 AM UTC

PDB ID : 2VBI / pdb\_00002vbi  
Title : Holostructure of pyruvate decarboxylase from *Acetobacter pasteurianus*  
Authors : Gocke, D.; Berthold, C.L.; Schneider, G.; Pohl, M.  
Deposited on : 2007-09-14  
Resolution : 2.75 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](mailto: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

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

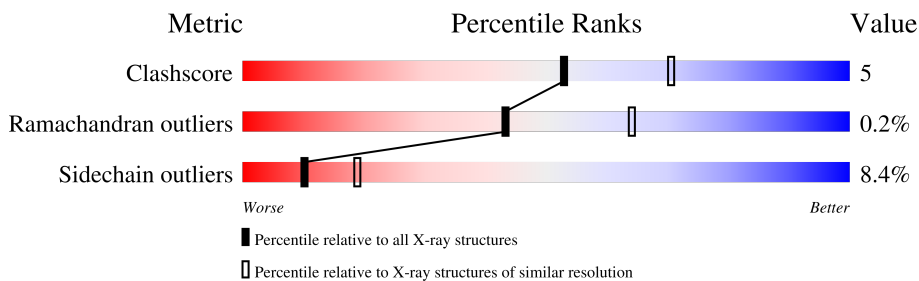
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	566	83% 14% ..
1	B	566	83% 13% ..
1	C	566	82% 13% ..
1	D	566	80% 16% ..
1	E	566	80% 15% ..
1	F	566	85% 13% .
1	G	566	87% 11% .
1	H	566	87% 11% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33860 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 PYRUVATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	554	4194	2637	731	801	25	0	1	0
1	B	554	4194	2637	731	801	25	0	1	0
1	C	554	4194	2637	731	801	25	0	1	0
1	D	554	4194	2637	731	801	25	0	1	0
1	E	554	4194	2637	731	801	25	0	1	0
1	F	554	4194	2637	731	801	25	0	1	0
1	G	554	4194	2637	731	801	25	0	1	0
1	H	554	4194	2637	731	801	25	0	1	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	GLY	conflict	UNP Q8L388
A	207	GLU	LYS	conflict	UNP Q8L388
A	208	LYS	ASN	conflict	UNP Q8L388
A	209	SER	ARG	conflict	UNP Q8L388
A	210	ALA	PRO	conflict	UNP Q8L388
A	211	SER	ALA	conflict	UNP Q8L388
A	297	ALA	GLY	conflict	UNP Q8L388
A	298	TRP	MET	conflict	UNP Q8L388
A	397	PRO	ALA	conflict	UNP Q8L388
B	25	ALA	GLY	conflict	UNP Q8L388
B	207	GLU	LYS	conflict	UNP Q8L388
B	208	LYS	ASN	conflict	UNP Q8L388
B	209	SER	ARG	conflict	UNP Q8L388

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Chain	Residue	Modelled	Actual	Comment	Reference
B	210	ALA	PRO	conflict	UNP Q8L388
B	211	SER	ALA	conflict	UNP Q8L388
B	297	ALA	GLY	conflict	UNP Q8L388
B	298	TRP	MET	conflict	UNP Q8L388
B	397	PRO	ALA	conflict	UNP Q8L388
C	25	ALA	GLY	conflict	UNP Q8L388
C	207	GLU	LYS	conflict	UNP Q8L388
C	208	LYS	ASN	conflict	UNP Q8L388
C	209	SER	ARG	conflict	UNP Q8L388
C	210	ALA	PRO	conflict	UNP Q8L388
C	211	SER	ALA	conflict	UNP Q8L388
C	297	ALA	GLY	conflict	UNP Q8L388
C	298	TRP	MET	conflict	UNP Q8L388
C	397	PRO	ALA	conflict	UNP Q8L388
D	25	ALA	GLY	conflict	UNP Q8L388
D	207	GLU	LYS	conflict	UNP Q8L388
D	208	LYS	ASN	conflict	UNP Q8L388
D	209	SER	ARG	conflict	UNP Q8L388
D	210	ALA	PRO	conflict	UNP Q8L388
D	211	SER	ALA	conflict	UNP Q8L388
D	297	ALA	GLY	conflict	UNP Q8L388
D	298	TRP	MET	conflict	UNP Q8L388
D	397	PRO	ALA	conflict	UNP Q8L388
E	25	ALA	GLY	conflict	UNP Q8L388
E	207	GLU	LYS	conflict	UNP Q8L388
E	208	LYS	ASN	conflict	UNP Q8L388
E	209	SER	ARG	conflict	UNP Q8L388
E	210	ALA	PRO	conflict	UNP Q8L388
E	211	SER	ALA	conflict	UNP Q8L388
E	297	ALA	GLY	conflict	UNP Q8L388
E	298	TRP	MET	conflict	UNP Q8L388
E	397	PRO	ALA	conflict	UNP Q8L388
F	25	ALA	GLY	conflict	UNP Q8L388
F	207	GLU	LYS	conflict	UNP Q8L388
F	208	LYS	ASN	conflict	UNP Q8L388
F	209	SER	ARG	conflict	UNP Q8L388
F	210	ALA	PRO	conflict	UNP Q8L388
F	211	SER	ALA	conflict	UNP Q8L388
F	297	ALA	GLY	conflict	UNP Q8L388
F	298	TRP	MET	conflict	UNP Q8L388
F	397	PRO	ALA	conflict	UNP Q8L388
G	25	ALA	GLY	conflict	UNP Q8L388

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Chain	Residue	Modelled	Actual	Comment	Reference
G	207	GLU	LYS	conflict	UNP Q8L388
G	208	LYS	ASN	conflict	UNP Q8L388
G	209	SER	ARG	conflict	UNP Q8L388
G	210	ALA	PRO	conflict	UNP Q8L388
G	211	SER	ALA	conflict	UNP Q8L388
G	297	ALA	GLY	conflict	UNP Q8L388
G	298	TRP	MET	conflict	UNP Q8L388
G	397	PRO	ALA	conflict	UNP Q8L388
H	25	ALA	GLY	conflict	UNP Q8L388
H	207	GLU	LYS	conflict	UNP Q8L388
H	208	LYS	ASN	conflict	UNP Q8L388
H	209	SER	ARG	conflict	UNP Q8L388
H	210	ALA	PRO	conflict	UNP Q8L388
H	211	SER	ALA	conflict	UNP Q8L388
H	297	ALA	GLY	conflict	UNP Q8L388
H	298	TRP	MET	conflict	UNP Q8L388
H	397	PRO	ALA	conflict	UNP Q8L388

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).

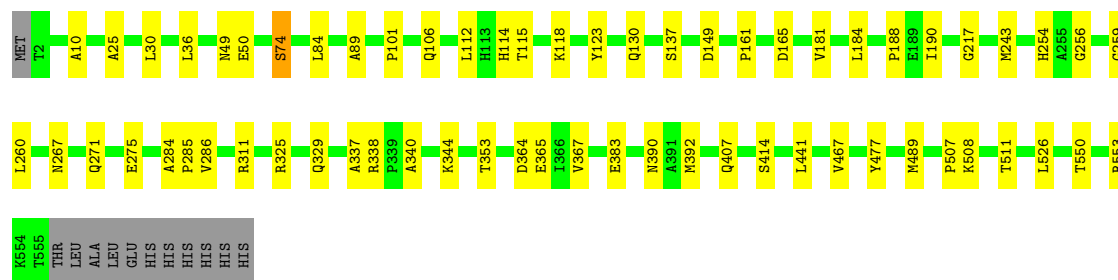


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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	E	20	Total 20	O 20	0	0
4	F	8	Total 8	O 8	0	0
4	G	11	Total 11	O 11	0	0
4	H	13	Total 13	O 13	0	0

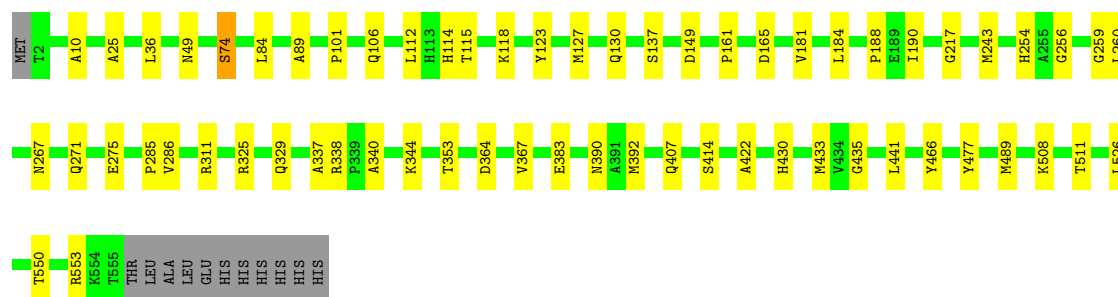






- Molecule 1: PYRUVATE DECARBOXYLASE

Chain H: 87% 11%



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.62Å 162.43Å 169.33Å 90.00° 102.71° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75	Depositor
% Data completeness (in resolution range)	97.1 (30.00-2.75)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.224 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	33860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.51	0/4282	0.82	0/5829
1	B	0.52	0/4282	0.83	0/5829
1	C	0.56	0/4282	0.83	0/5829
1	D	0.57	0/4282	0.84	0/5829
1	E	0.58	0/4282	0.86	2/5829 (0.0%)
1	F	0.55	0/4282	0.84	0/5829
1	G	0.52	0/4282	0.83	0/5829
1	H	0.53	0/4282	0.83	0/5829
All	All	0.54	0/34256	0.84	2/46632 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	283	ILE	N-CA-C	5.50	115.52	107.37
1	E	99	GLY	N-CA-C	-5.18	105.45	112.14

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4194	0	4148	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4194	0	4148	42	0
1	C	4194	0	4148	47	0
1	D	4194	0	4148	49	2
1	E	4194	0	4148	50	1
1	F	4194	0	4148	56	1
1	G	4194	0	4148	44	0
1	H	4194	0	4148	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	3	0
3	C	26	0	16	0	0
3	D	26	0	16	1	0
3	E	26	0	16	1	0
3	F	26	0	16	1	0
3	G	26	0	16	1	0
3	H	26	0	16	3	0
4	A	6	0	0	1	0
4	B	5	0	0	1	0
4	C	14	0	0	3	0
4	D	15	0	0	1	0
4	E	20	0	0	2	0
4	F	8	0	0	2	0
4	G	11	0	0	1	0
4	H	13	0	0	3	0
All	All	33860	0	33312	334	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 334 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:SER:HA	1:D:165:ASP:HB2	1.47	0.96
1:E:137:SER:HA	1:E:165:ASP:HB2	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:SER:HA	1:G:165:ASP:HB2	1.48	0.95
1:B:137:SER:HA	1:B:165:ASP:HB2	1.50	0.94
1:A:137:SER:HA	1:A:165:ASP:HB2	1.49	0.92

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:GLY:N	1:F:533:ARG:NH1[3_555]	1.95	0.25
1:D:509:GLU:OE2	1:E:496:GLU:CG[3_555]	2.09	0.11

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	43 64
1	B	553/566 (98%)	539 (98%)	13 (2%)	1 (0%)	43 64
1	C	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	43 64
1	D	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	43 64
1	E	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	43 64
1	F	553/566 (98%)	539 (98%)	13 (2%)	1 (0%)	43 64
1	G	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	43 64
1	H	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	43 64
All	All	4424/4528 (98%)	4306 (97%)	110 (2%)	8 (0%)	43 64

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	SER

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Mol	Chain	Res	Type
1	B	74	SER
1	C	74	SER
1	D	74	SER
1	E	74	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/450 (98%)	404 (92%)	36 (8%)	10	20
1	B	440/450 (98%)	403 (92%)	37 (8%)	10	19
1	C	440/450 (98%)	402 (91%)	38 (9%)	10	18
1	D	440/450 (98%)	403 (92%)	37 (8%)	10	19
1	E	440/450 (98%)	401 (91%)	39 (9%)	9	17
1	F	32/450 (7%)	31 (97%)	1 (3%)	35	59
All	All	2232/2700 (83%)	2044 (92%)	188 (8%)	10	19

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	130	GLN
1	D	511	THR
1	D	184	LEU
1	D	281	LEU
1	E	106	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	448	GLN
1	E	430	HIS
1	D	462	ASN
1	E	254	HIS

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Mol	Chain	Res	Type
1	E	462	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
3	TPP	C	2000	2	26,27,27	1.90	8 (30%)	38,40,40	1.60	8 (21%)
3	TPP	H	2000	2	26,27,27	1.83	8 (30%)	38,40,40	1.57	8 (21%)
3	TPP	D	2000	2	26,27,27	1.65	7 (26%)	38,40,40	1.88	12 (31%)
3	TPP	F	2000	2	26,27,27	1.70	7 (26%)	38,40,40	1.57	8 (21%)
3	TPP	E	2000	2	26,27,27	1.73	8 (30%)	38,40,40	1.54	10 (26%)
3	TPP	A	2000	2	26,27,27	1.79	7 (26%)	38,40,40	1.58	10 (26%)
3	TPP	B	2000	2	26,27,27	1.77	8 (30%)	38,40,40	1.51	8 (21%)
3	TPP	G	2000	2	26,27,27	1.68	7 (26%)	38,40,40	1.62	10 (26%)

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	TPP	C	2000	2	-	3/17/17/17	0/2/2/2
3	TPP	H	2000	2	-	1/17/17/17	0/2/2/2
3	TPP	D	2000	2	-	5/17/17/17	0/2/2/2
3	TPP	F	2000	2	-	2/17/17/17	0/2/2/2
3	TPP	E	2000	2	-	0/17/17/17	0/2/2/2
3	TPP	A	2000	2	-	0/17/17/17	0/2/2/2
3	TPP	B	2000	2	-	2/17/17/17	0/2/2/2
3	TPP	G	2000	2	-	3/17/17/17	0/2/2/2

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	TPP	C5-S1	-4.78	1.60	1.72
3	C	2000	TPP	C5-S1	-4.72	1.60	1.72
3	F	2000	TPP	C5-S1	-4.69	1.60	1.72
3	E	2000	TPP	C5-S1	-4.68	1.60	1.72
3	G	2000	TPP	C5-S1	-4.44	1.61	1.72

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2000	TPP	C2-N3-C4	-3.92	108.76	114.06
3	D	2000	TPP	C4-C5-S1	3.81	116.51	110.56
3	G	2000	TPP	CM2-C2'-N1'	3.60	121.03	117.20
3	H	2000	TPP	N1'-C2'-N3'	-3.52	119.67	125.53
3	E	2000	TPP	N1'-C2'-N3'	-3.34	119.97	125.53

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

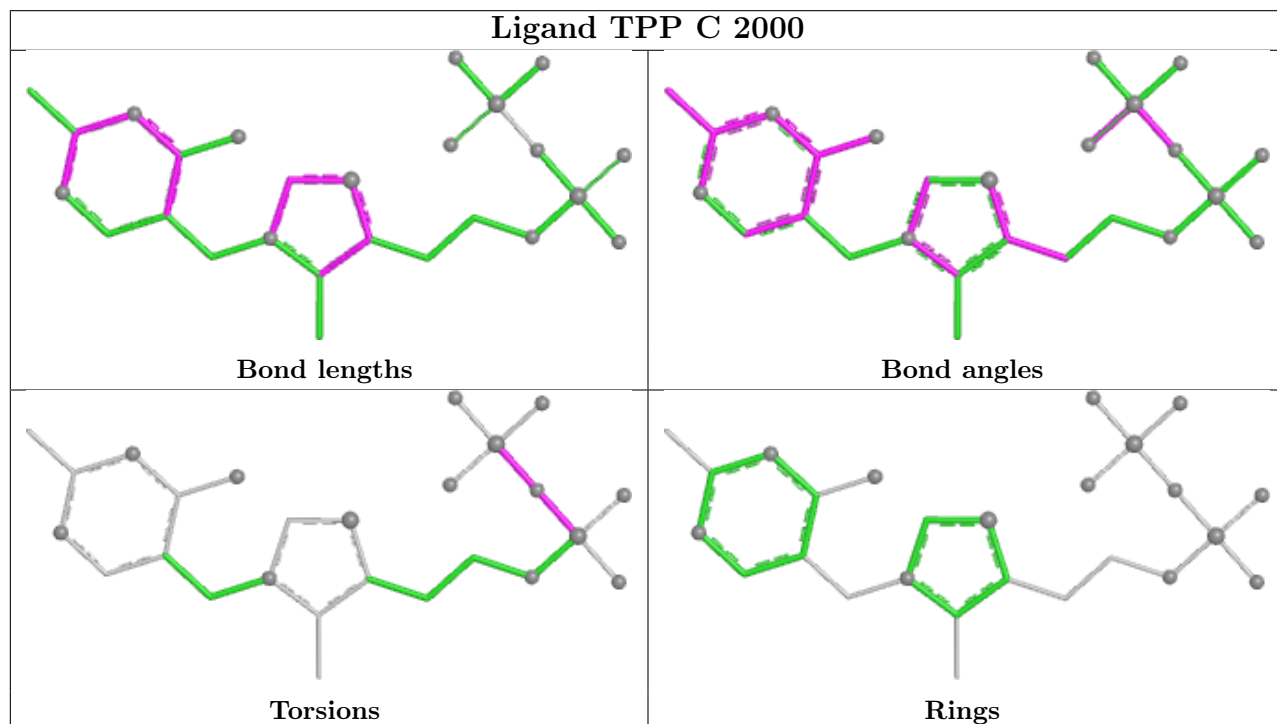
Mol	Chain	Res	Type	Atoms
3	C	2000	TPP	PA-O3A-PB-O3B
3	D	2000	TPP	C7-O7-PA-O1A
3	D	2000	TPP	C7-O7-PA-O2A
3	D	2000	TPP	C7-O7-PA-O3A
3	D	2000	TPP	PA-O3A-PB-O3B

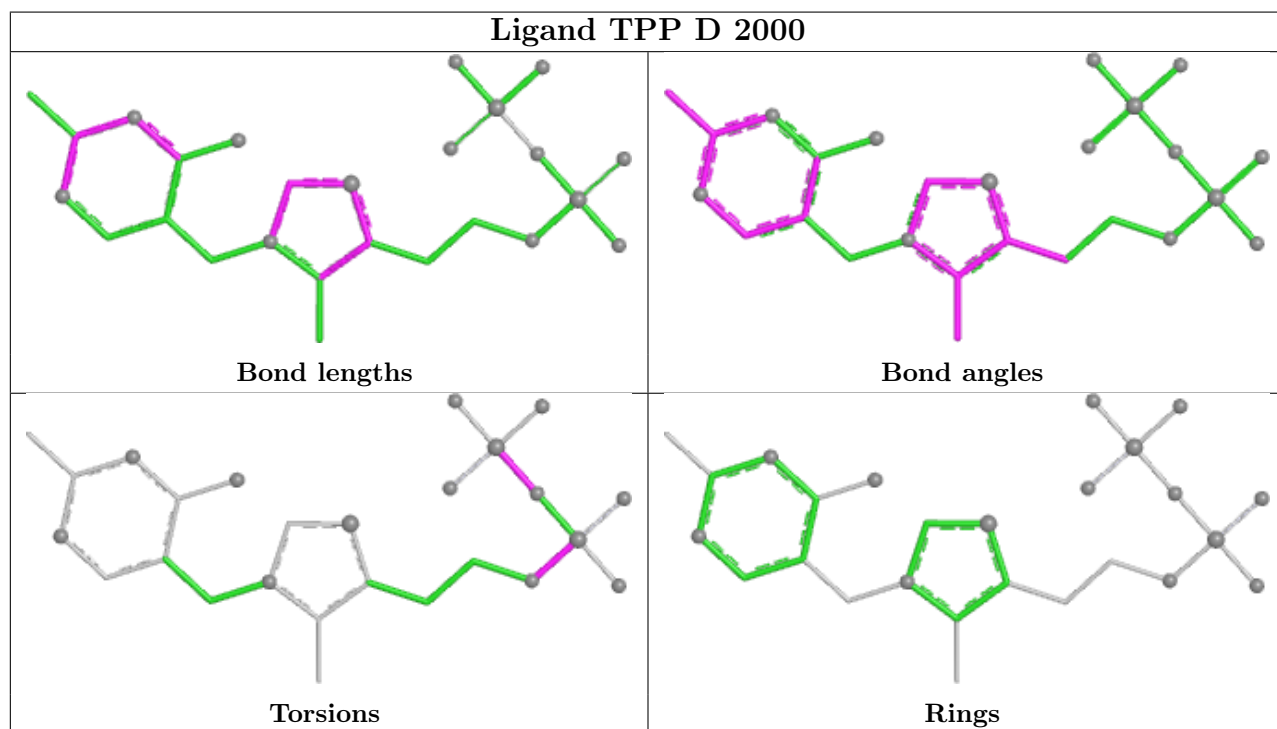
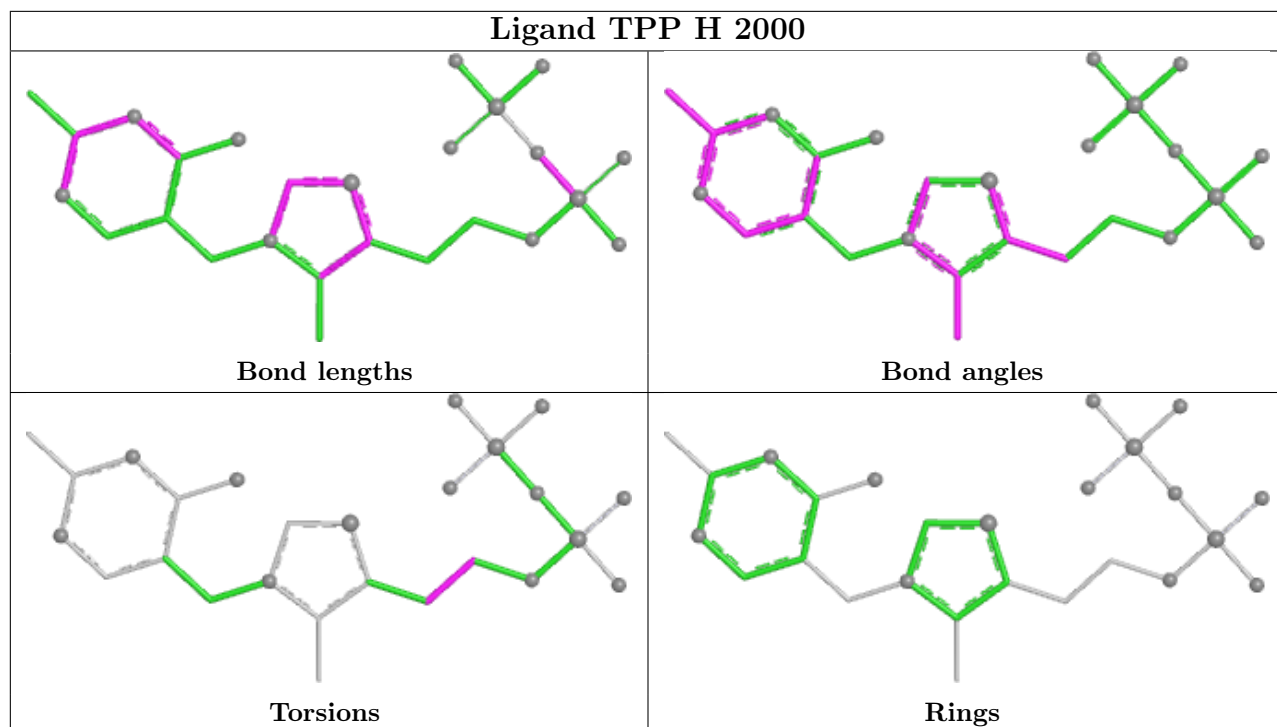
There are no ring outliers.

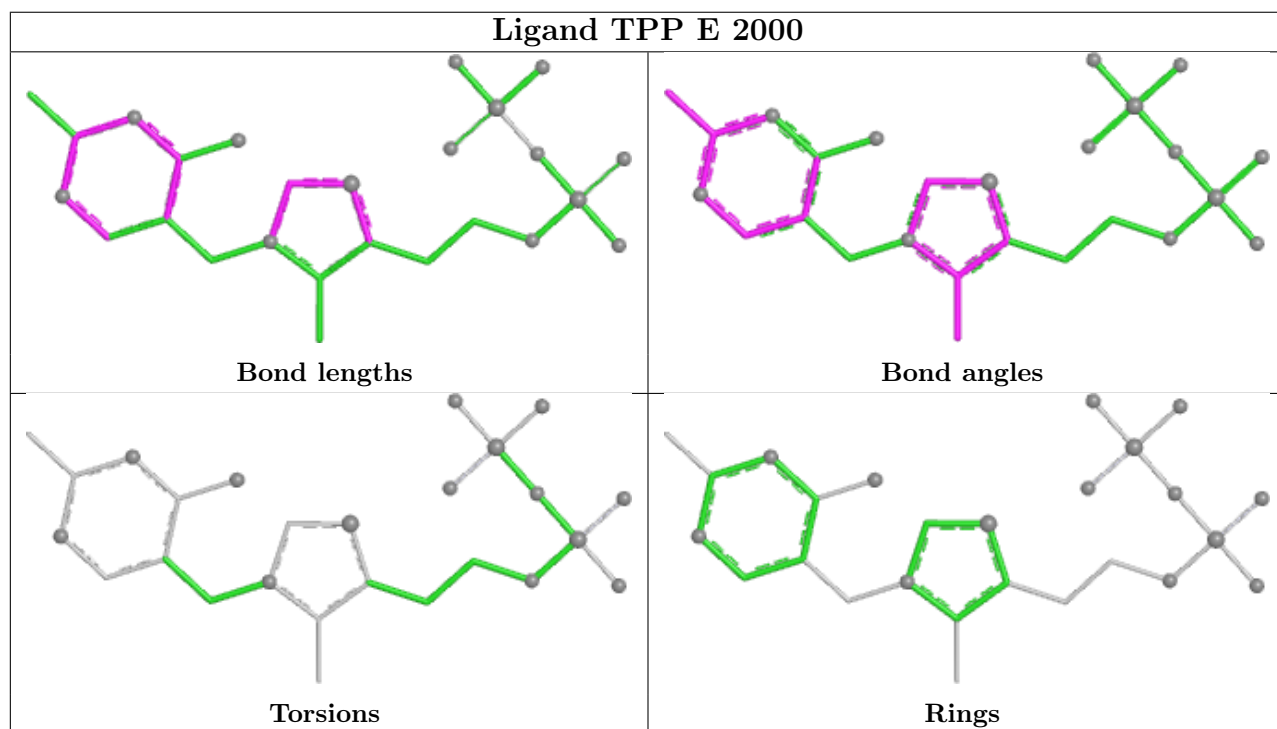
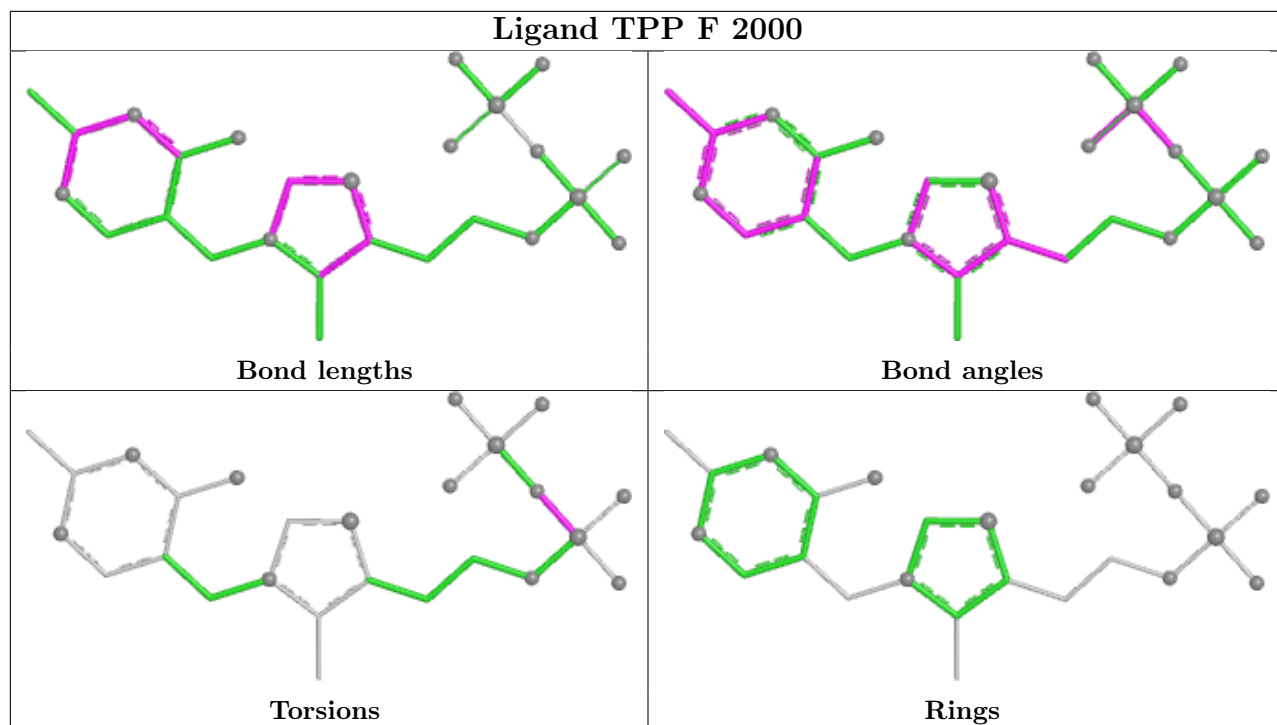
7 monomers are involved in 11 short contacts:

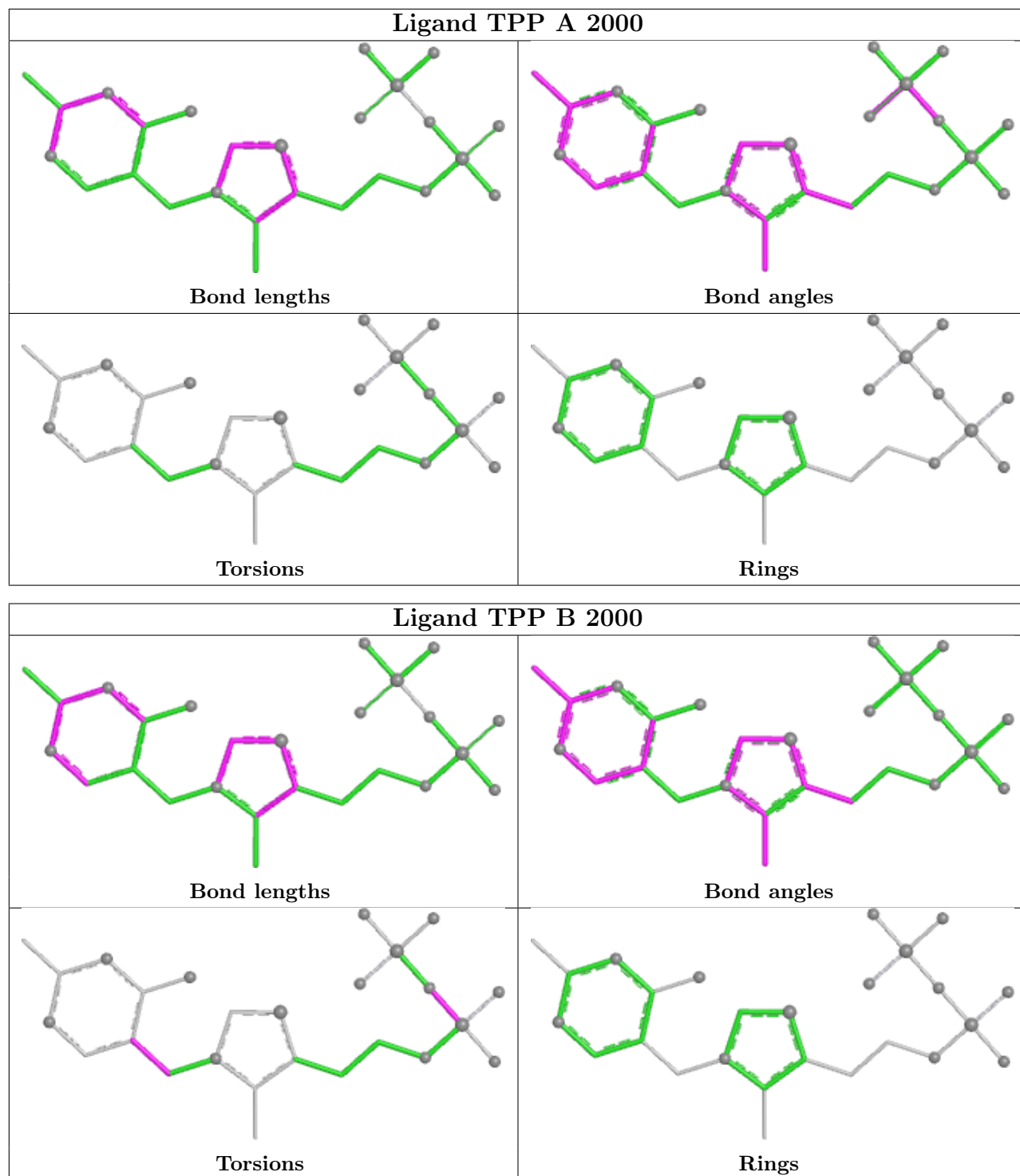
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2000	TPP	3	0
3	D	2000	TPP	1	0
3	F	2000	TPP	1	0
3	E	2000	TPP	1	0
3	A	2000	TPP	1	0
3	B	2000	TPP	3	0
3	G	2000	TPP	1	0

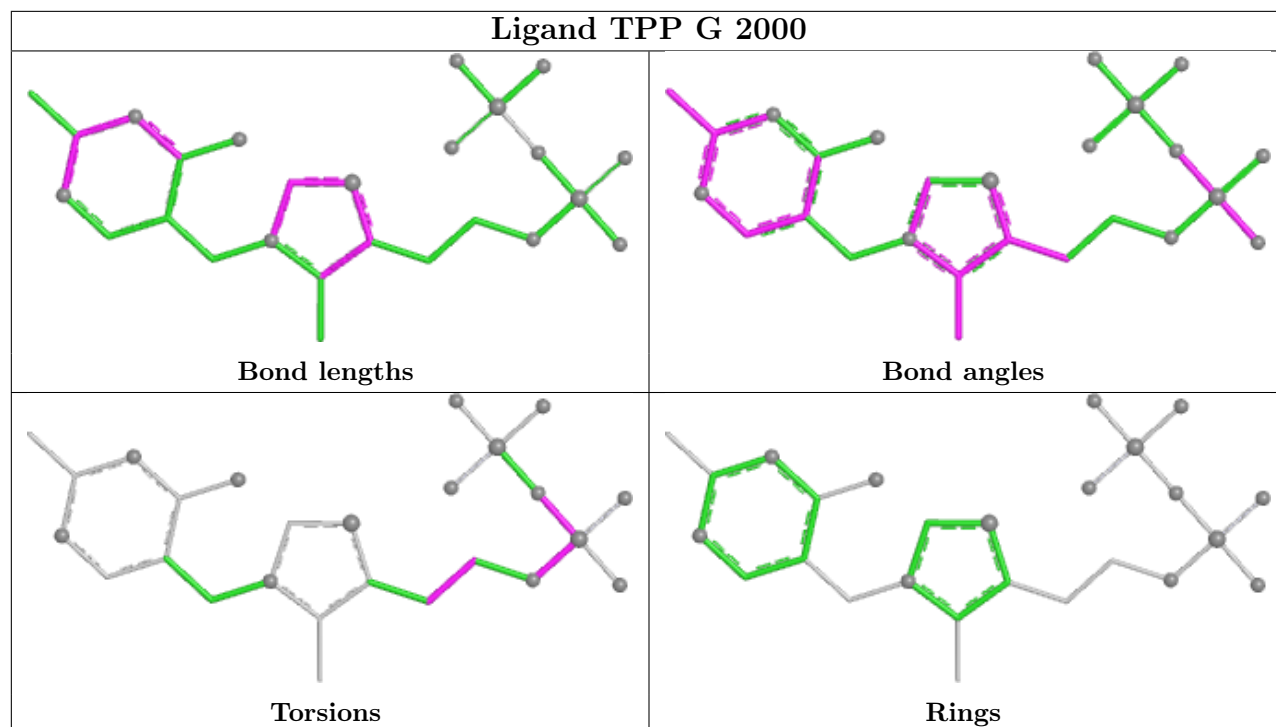
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.