WORLDWIDE PDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Jul 8, 2025 – 03:33 PM JST

PDB ID	:	9K9R / pdb_00009k9r
EMDB ID	:	EMD-62196
Title	:	MPXV DNA polymerase in complex with primer/5U template DNA
Authors	:	Xie, Y.F.; Kuai, L.; Peng, Q.; Wang, Q.; Wang, H.; Li, X.M.; Qi, J.X.; Ding, Q.; Shi, Y.; Gao, F.
Deposited on	:	2024-10-27
Resolution	:	2.61 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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:

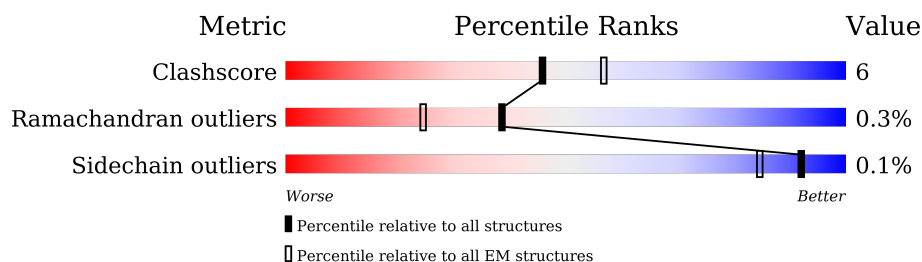|		
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.61 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	Percentile Ranks	Value
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		0.1%

Worse   *Better*

▊ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	1031	84% 13% •
2	B	218	89% 10%
3	C	426	72% 27% •
4	P	25	48% 8% 44%
5	T	38	55% 11% 34%

2   Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 14230 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1005	Total 8207	C 5242	N 1375	O 1535	S 55	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP A0A7H0DN44
A	-23	TRP	-	expression tag	UNP A0A7H0DN44
A	-22	SER	-	expression tag	UNP A0A7H0DN44
A	-21	HIS	-	expression tag	UNP A0A7H0DN44
A	-20	PRO	-	expression tag	UNP A0A7H0DN44
A	-19	GLN	-	expression tag	UNP A0A7H0DN44
A	-18	PHE	-	expression tag	UNP A0A7H0DN44
A	-17	GLU	-	expression tag	UNP A0A7H0DN44
A	-16	LYS	-	expression tag	UNP A0A7H0DN44
A	-15	GLY	-	expression tag	UNP A0A7H0DN44
A	-14	SER	-	expression tag	UNP A0A7H0DN44
A	-13	GLY	-	expression tag	UNP A0A7H0DN44
A	-12	SER	-	expression tag	UNP A0A7H0DN44
A	-11	TRP	-	expression tag	UNP A0A7H0DN44
A	-10	SER	-	expression tag	UNP A0A7H0DN44
A	-9	HIS	-	expression tag	UNP A0A7H0DN44
A	-8	PRO	-	expression tag	UNP A0A7H0DN44
A	-7	GLN	-	expression tag	UNP A0A7H0DN44
A	-6	PHE	-	expression tag	UNP A0A7H0DN44
A	-5	GLU	-	expression tag	UNP A0A7H0DN44
A	-4	LYS	-	expression tag	UNP A0A7H0DN44
A	-3	GLY	-	expression tag	UNP A0A7H0DN44
A	-2	SER	-	expression tag	UNP A0A7H0DN44
A	-1	GLY	-	expression tag	UNP A0A7H0DN44
A	0	SER	-	expression tag	UNP A0A7H0DN44
A	108	PHE	LEU	conflict	UNP A0A7H0DN44
A	166	ALA	ASP	engineered mutation	UNP A0A7H0DN44
A	168	ALA	GLU	engineered mutation	UNP A0A7H0DN44

- Molecule 2 is a protein called E4R.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	218	Total 1767	C 1146	N 289	O 326	S 6	0	0

- Molecule 3 is a protein called DNA polymerase processivity factor component A20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	419	Total 3415	C 2203	N 552	O 650	S 10	0	0

- Molecule 4 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	14	Total 287	C 138	N 51	O 84	P 14	0	0

- Molecule 5 is a DNA chain called DNA (5U 38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	25	Total 524	C 250	N 94	O 154	P 26	1	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total 1	Mg 1	0

- Molecule 7 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).

TTP

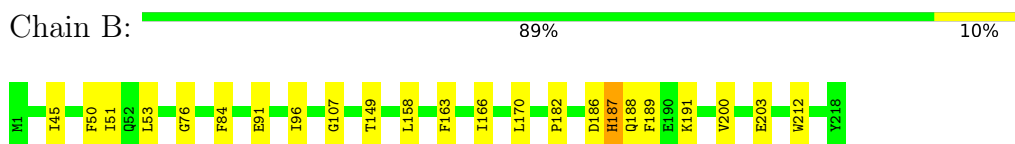| Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	29	10	2	14	3	0

3 Residue-property plots ⓘ

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.
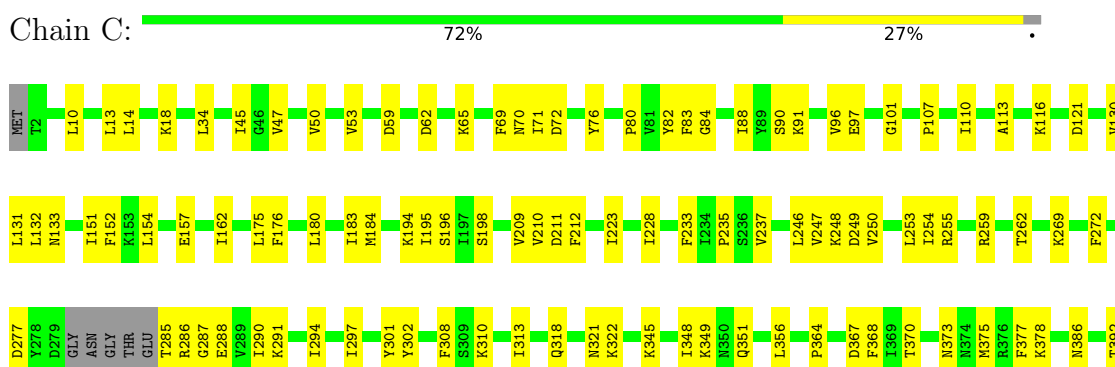
• Molecule 1: DNA polymerase
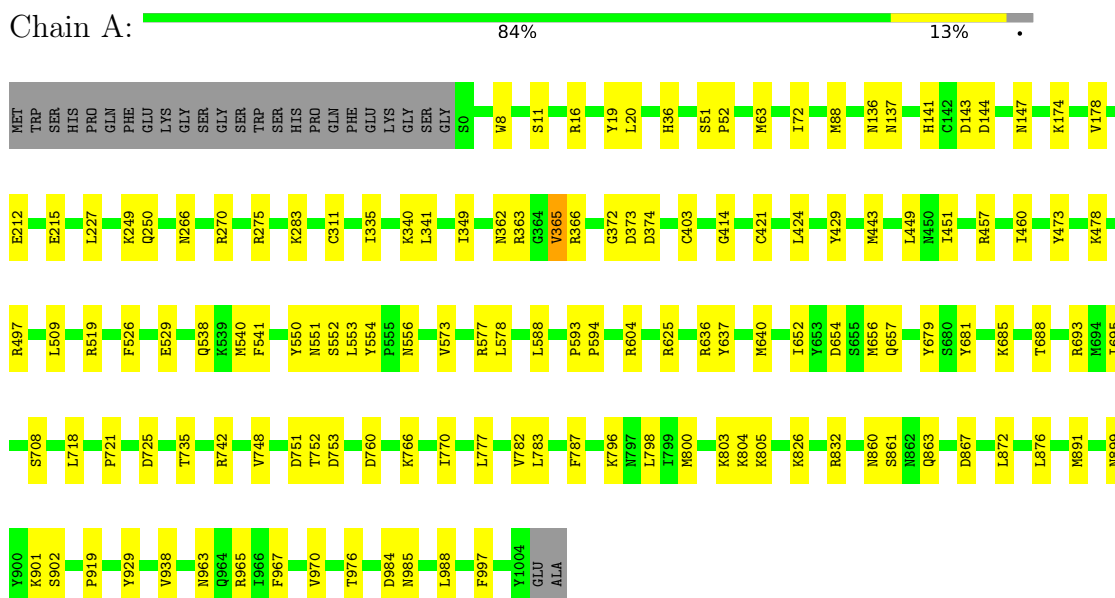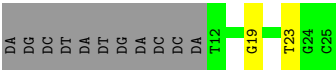

• Molecule 2: E4R

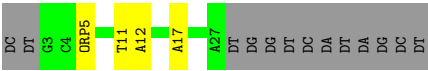• Molecule 3: DNA polymerase processivity factor component A20

L395 I400 E401 T402 Q409 F410 V411 F414 N415 T418 K421 L424 F425 GLU

• Molecule 4: DNA (25-MER)

Chain P:

48%   8%   44%

DA DG DC DT DA DT DG DA DC DC DA T12 G19 T23 G24 C25

• Molecule 5: DNA (5U 38-MER)

Chain T:

55%   11%   34%

DC DT G3 C4 ORP5 T11 A12 A17 A27 DT DG DG DT DC DA DT DA DG DC DT

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	307468	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	0.21	0/8383	0.34	0/11319
2	B	0.22	0/1817	0.38	0/2472
3	C	0.15	0/3481	0.33	0/4697
4	P	0.28	0/321	0.39	0/493
5	T	0.26	0/573	0.35	0/879
All	All	0.20	0/14575	0.34	0/19860

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 ⓘ

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	8207	0	8172	82	0
2	B	1767	0	1753	13	0
3	C	3415	0	3421	77	0
4	P	287	0	158	2	0
5	T	524	0	291	3	0
6	A	1	0	0	0	0
7	A	29	0	13	1	0
All	All	14230	0	13808	168	0

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 6.

The worst 5 of 168 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)
3:C:84:GLY:HA3	3:C:131:LEU:O	1.66	0.96
1:A:373:ASP:OD1	1:A:374:ASP:N	2.12	0.82
3:C:249:ASP:OD1	3:C:250:VAL:N	2.16	0.78
3:C:97:GLU:H	3:C:101:GLY:HA2	1.52	0.75
3:C:313:ILE:O	3:C:409:GLN:NE2	2.22	0.72

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1003/1031 (97%)	955 (95%)	46 (5%)	2 (0%)	44	65
2	B	216/218 (99%)	204 (94%)	11 (5%)	1 (0%)	25	45
3	C	415/426 (97%)	400 (96%)	13 (3%)	2 (0%)	25	45
All	All	1634/1675 (98%)	1559 (95%)	70 (4%)	5 (0%)	38	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	VAL
2	B	187	HIS
3	C	72	ASP
1	A	902	SER
3	C	53	VAL

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 PDB entries followed by that with respect to all EM entries.

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	926/947 (98%)	926 (100%)	0	100	100
2	B	199/200 (100%)	199 (100%)	0	100	100
3	C	390/396 (98%)	389 (100%)	1 (0%)	91	97
All	All	1515/1543 (98%)	1514 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	50	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	899	ASN
1	A	918	ASN
3	C	304	ASN
3	C	48	GLN
3	C	115	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	ORP	T	5	5	9,12,13	4.36	5 (55%)	8,16,19	0.65	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
5	ORP	T	5	5	-	1/3/17/18	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	5	ORP	O4-C4	7.28	1.61	1.45
5	T	5	ORP	O4-C1	-6.78	1.29	1.41
5	T	5	ORP	C3-C4	-6.60	1.34	1.53
5	T	5	ORP	C2-C1	4.34	1.58	1.52
5	T	5	ORP	O3-C3	2.67	1.49	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	T	5	ORP	C3-C4-C5-O5

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	TTP	A	1102	6	26,30,30	0.58	0	39,47,47	0.52	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
7	TTP	A	1102	6	-	2/22/34/34	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1102	TTP	PG-O3B-PB-O2B
7	A	1102	TTP	PG-O3B-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1102	TTP	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 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 TTP A 1102

Bond lengths

Bond angles

Torsions

Rings
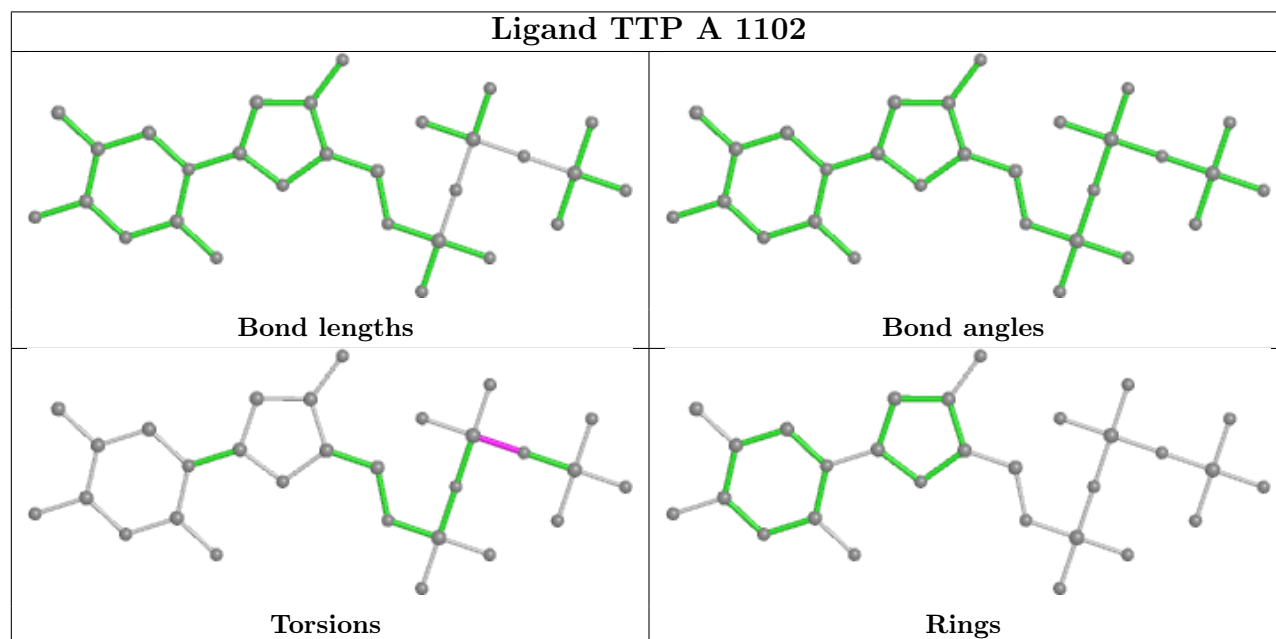
5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.