W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Jan 14, 2024 – 12:06 AM JST

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PDB ID	:	8JUL
EMDB ID	:	EMD-36661
Title	:	Cryo-EM structure of SIDT1 in complex with phosphatidic acid
Authors	:	Sun, C.R.; Xu, D.; Li, Q.; Zhou, C.Z.; Chen, Y.
Deposited on	:	2023-06-26
Resolution	:	2.92 Å(reported)

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 2.92 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		10
Ramachandran outliers		0
Sidechain outliers		0

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
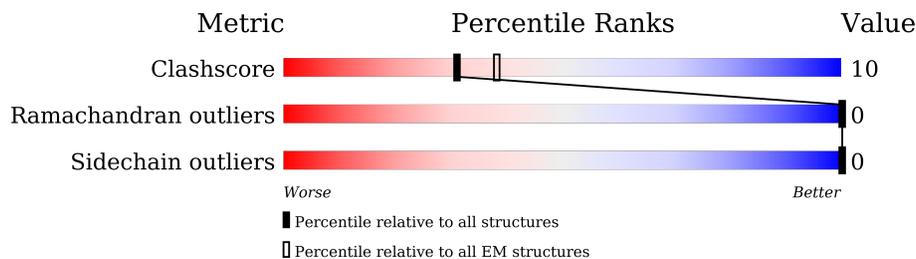
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	827	58% 17% 25%
1	B	827	60% 15% 25%

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PROTEIN DATA BANK

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9690 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 SID1 transmembrane family member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	623	Total	C	N	O	S	0	0
			4807	3142	782	857	26		
1	B	623	Total	C	N	O	S	0	0
			4807	3142	782	857	26		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	

- Molecule 3 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX2) (formula: $C_{27}H_{52}O_8P$) (labeled as "Ligand of Interest" by depositor).
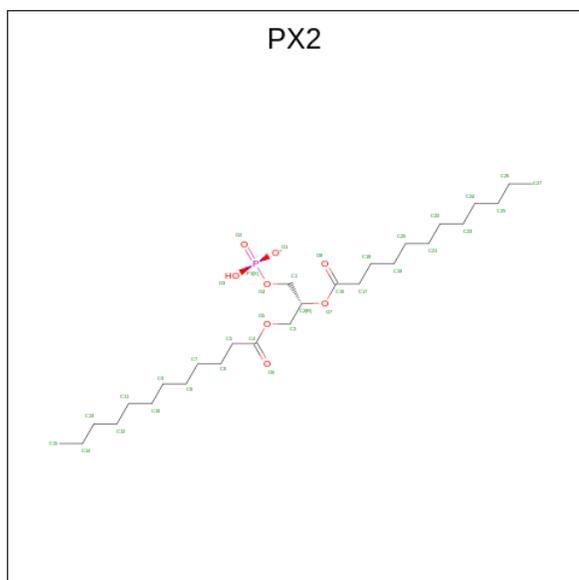
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 36	C 27	O 8	P 1	0
3	B	1	Total 36	C 27	O 8	P 1	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	O 1	0
4	B	1	Total 1	O 1	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: SID1 transmembrane family member 1

Chain A:

• Molecule 1: SID1 transmembrane family member 1

Chain B:

S239 M240 T241 A245 Q257 V261 F262 V263 I264 K265 P266 E267 D268 Y269 A270 C271 G272 G273 S274 F275 Q283 T284 W285 N286 L287 Q288 R289 K290 K291 S310 F320 Y321 L322 L326 Y332 LEU ARG PHE GLN ARG LYS SER ILE ASP GLY SER PHE GLY SER ASN ASP

GLY SER GLY ASN MET VAL ALA SER HIS PRO ILE ILE ALA ALA SER THR PRO GLU GLY SER ASN TYR GLY THR ILE ASP GLU GLU SER SER SER PRO GLY ARG GLN MET SER SER SER ASP GLY GLY PRO PRO GLY GLN GLN SER ASP THR ASP SER SER VAL GLU GLU GLU SER ASP PHE ASP THR MET

PRO ASP ILE GLU SER ASP LYS ASN ILE ILE ARG THR LYS MET PHE LEU TYR LEU SER ASP LEU SER ARG LYS ASP ARG ARG ILE VAL SER LYS LYS TYR K442 V463 I464 T465 Y466 Q467 V470 T473 G474 N475 Q476 D477 I478 C479 N482 C485 P488 V491 L492 S493

L499 S500 H504 L507 G508 R518 K529 ASP ILE PHE ALA VAL GLU TYR GLY ILE PRO K540 H541 F542 F545 L552 G556 V557 L558 Y562 C565 P566 N567 Y568 S569 N570 F571 Q572 F573 D574 A582 M586 L587 K588 Q591 T592 R593 HIS PRO ASP ILE

ASN ALA SER ALA TYR SER ALA TYR A606 G622 LYS ASN ASP V626 F660 ARG ARG ALA ALA MET VAL PHE TYR THR ASP CYS ILE GLN GLN CYS SER ARG PRO LEU TYR M681 A698 L699 F700 G701 L702 I703 Y704 R705 PRO R707 L722 K732 C746 Q763 P772

R776 N779 D790 H795 F806 L807 V819 R820 ARG ASP GLN ILE PRO VAL PHE

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	535389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	1800	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: PX2, ZN

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	0.53	0/4921	0.70	16/6694 (0.2%)
1	B	0.51	0/4921	0.65	12/6694 (0.2%)
All	All	0.52	0/9842	0.67	28/13388 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	705	ARG	CB-CA-C	-16.24	77.93	110.40
1	A	272	GLY	N-CA-C	13.15	145.97	113.10
1	B	272	GLY	N-CA-C	12.85	145.22	113.10
1	A	271	CYS	CB-CA-C	12.08	134.56	110.40
1	B	271	CYS	CB-CA-C	11.54	133.49	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	B	108	VAL	Peptide

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	4807	0	4580	96	0
1	B	4807	0	4580	91	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	51	5	0
3	B	36	0	51	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9690	0	9262	184	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 10.

The worst 5 of 184 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:B:700:PHE:CB	1:B:704:TYR:H	1.69	1.06
1:B:700:PHE:CB	1:B:704:TYR:N	2.36	0.88
1:B:571:PHE:O	1:B:572:GLN:HG2	1.77	0.84
1:A:225:TYR:HB3	1:A:230:ASN:HB3	1.60	0.84
1:A:571:PHE:O	1:A:572:GLN:HG2	1.78	0.83

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	609/827 (74%)	566 (93%)	43 (7%)	0	100	100
1	B	609/827 (74%)	563 (92%)	46 (8%)	0	100	100
All	All	1218/1654 (74%)	1129 (93%)	89 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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	492/732 (67%)	492 (100%)	0	100	100
1	B	492/732 (67%)	492 (100%)	0	100	100
All	All	984/1464 (67%)	984 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	67	ASN
1	B	763	GLN
1	B	83	ASN
1	B	229	HIS
1	B	74	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	PX2	A	902	-	35,35,35	1.37	6 (17%)	39,40,40	1.44	3 (7%)
3	PX2	B	902	-	35,35,35	1.34	5 (14%)	39,40,40	1.29	3 (7%)

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	PX2	A	902	-	-	25/37/37/37	-
3	PX2	B	902	-	-	20/37/37/37	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	PX2	P1-O2	4.51	1.65	1.50
3	A	902	PX2	P1-O2	4.04	1.63	1.50
3	A	902	PX2	O5-C3	-2.89	1.38	1.45
3	B	902	PX2	O7-C2	-2.78	1.39	1.46
3	A	902	PX2	O7-C2	-2.77	1.39	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	PX2	O7-C16-C17	4.12	120.38	111.50
3	B	902	PX2	O7-C16-C17	3.60	119.25	111.50
3	A	902	PX2	O5-C4-C5	3.33	122.37	111.91
3	B	902	PX2	O5-C4-C5	3.00	121.32	111.91
3	B	902	PX2	O4-P1-O2	2.18	112.60	106.47

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	PX2	C1-O4-P1-O1
3	A	902	PX2	C1-O4-P1-O2
3	A	902	PX2	C1-O4-P1-O3
3	B	902	PX2	C1-O4-P1-O1
3	B	902	PX2	C1-O4-P1-O2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	PX2	5	0
3	B	902	PX2	2	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 PX2 A 902

Bond lengths

Bond angles

Torsions

Rings

Ligand PX2 B 902

Bond lengths

Bond angles

Torsions

Rings
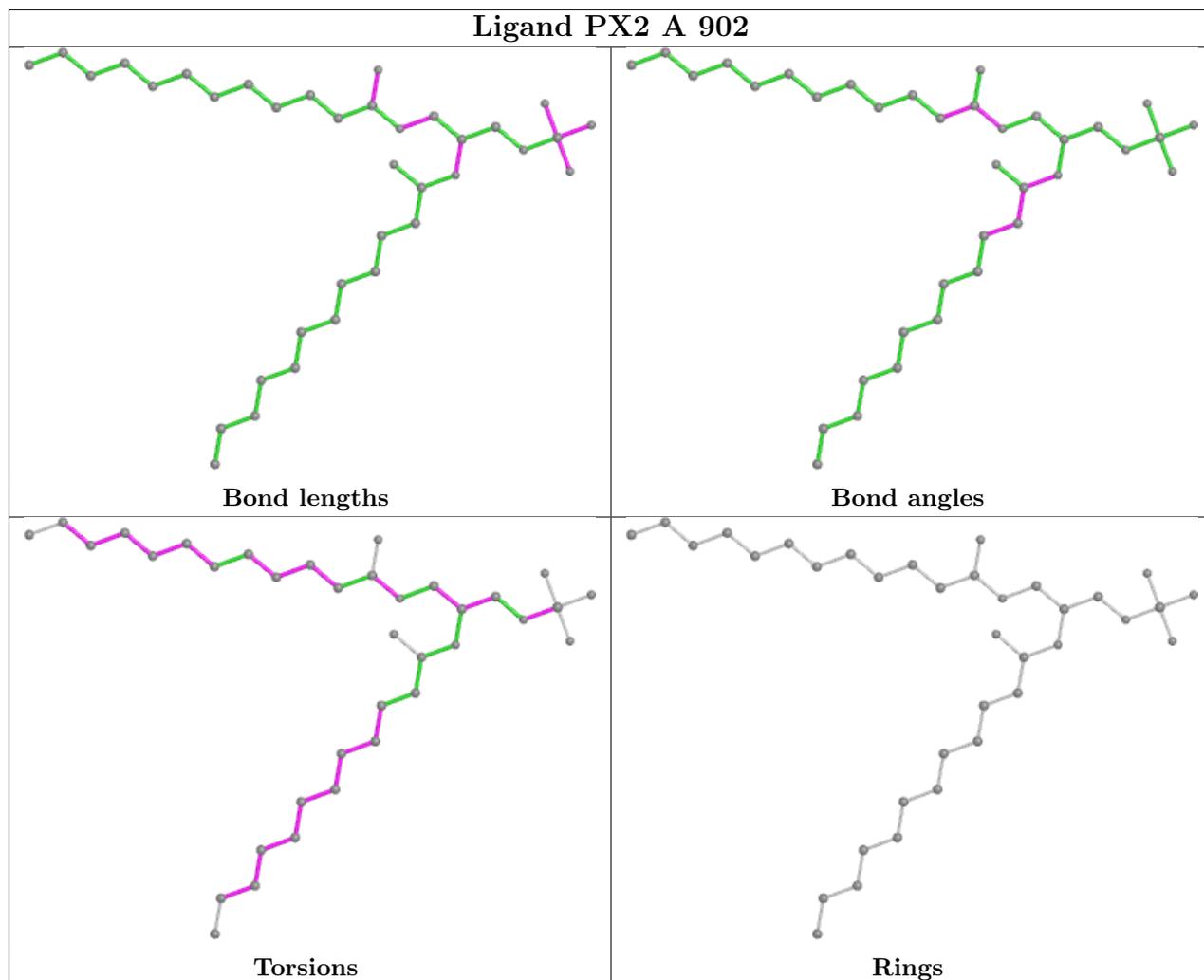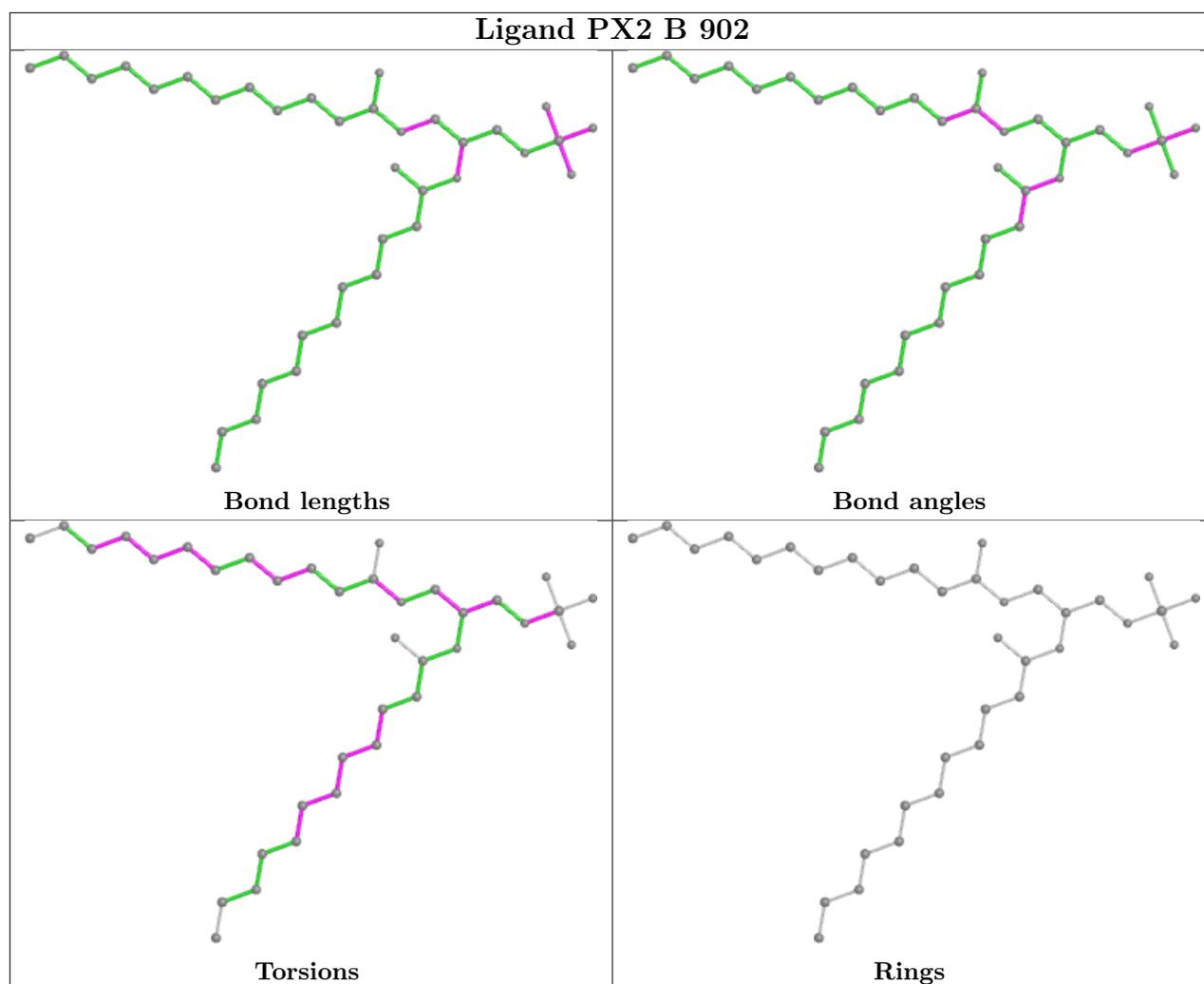
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.