



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Sep 16, 2019 – 12:49 PM EDT

PDB ID : 6PW4
EMDB ID: : EMD-20498
Title : Cryo-EM Structure of Thermo-Sensitive TRP Channel TRP1 from the Alga
Chlamydomonas reinhardtii in Detergent
Authors : McGoldrick, L.L.; Singh, A.K.; Sobolevsky, A.I.
Deposited on : 2019-07-22
Resolution : 3.53 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

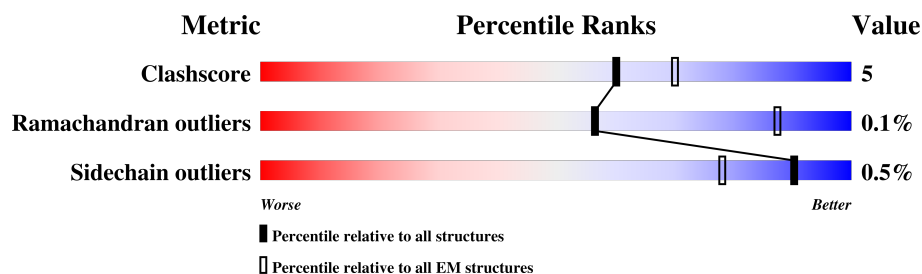
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	901	67% 10% 23%
1	B	901	64% 11% 25%
1	C	901	67% 10% 23%
1	D	901	65% 10% 25%

2 Entry composition i

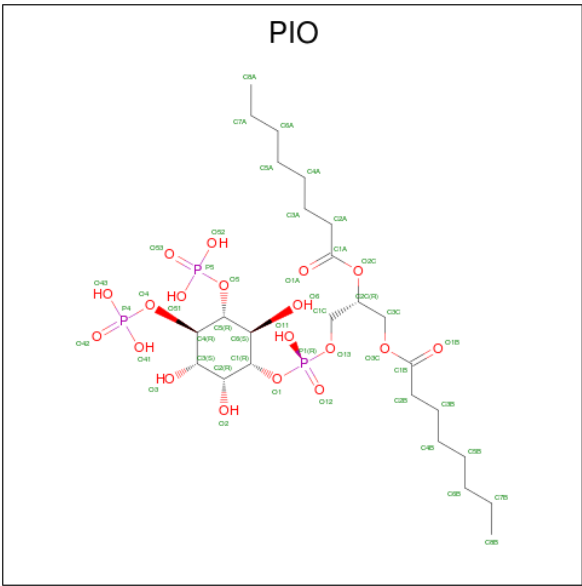
There are 5 unique types of molecules in this entry. The entry contains 22348 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

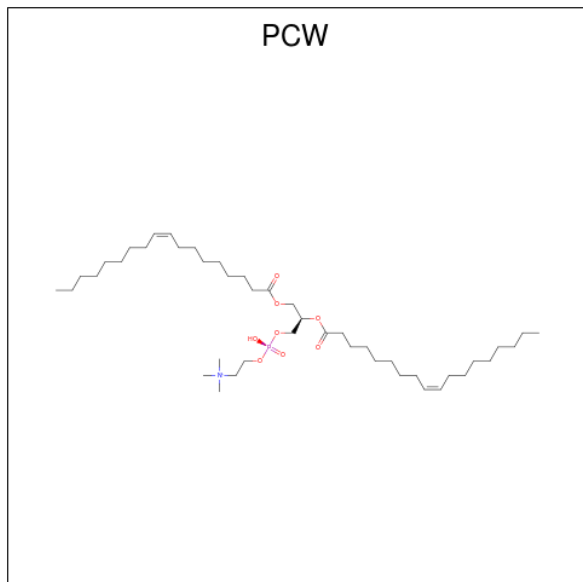
- Molecule 1 is a protein called TRP-like ion channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	696	Total	C	N	O	S	0	0
			5553	3604	923	981	45		
1	B	675	Total	C	N	O	S	0	0
			5372	3464	892	976	40		
1	C	696	Total	C	N	O	S	0	0
			5553	3604	923	981	45		
1	D	675	Total	C	N	O	S	0	0
			5372	3464	892	976	40		

- Molecule 2 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: PIO) (formula: C₂₅H₄₉O₁₉P₃).

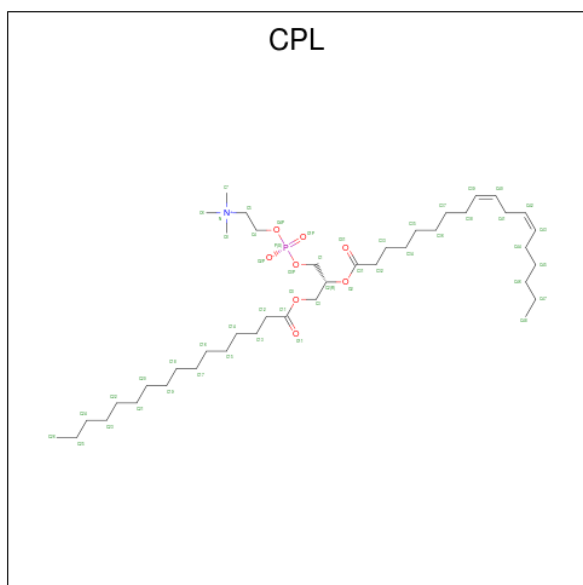


- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$) (labeled as "Ligand of Interest" by author).



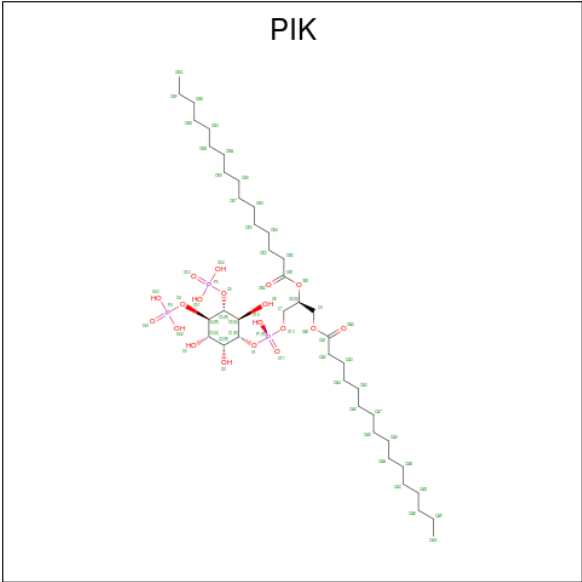
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	C	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 4 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: $C_{42}H_{80}NO_8P$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			26	16	1	8	1	
4	C	1	Total	C	N	O	P	0
			26	16	1	8	1	

- Molecule 5 is (2S)-3-{{[(R)-hydroxy{[(1R,2R,3S,4R,5R,6S)-2,3,6-trihydroxy-4,5-bis(phosphonoxy)cyclohexyl]oxy}phosphoryl]oxy}propane-1,2-diyl dihexadecanoate (three-letter code: PIK) (formula: C₄₁H₈₁O₁₉P₃).

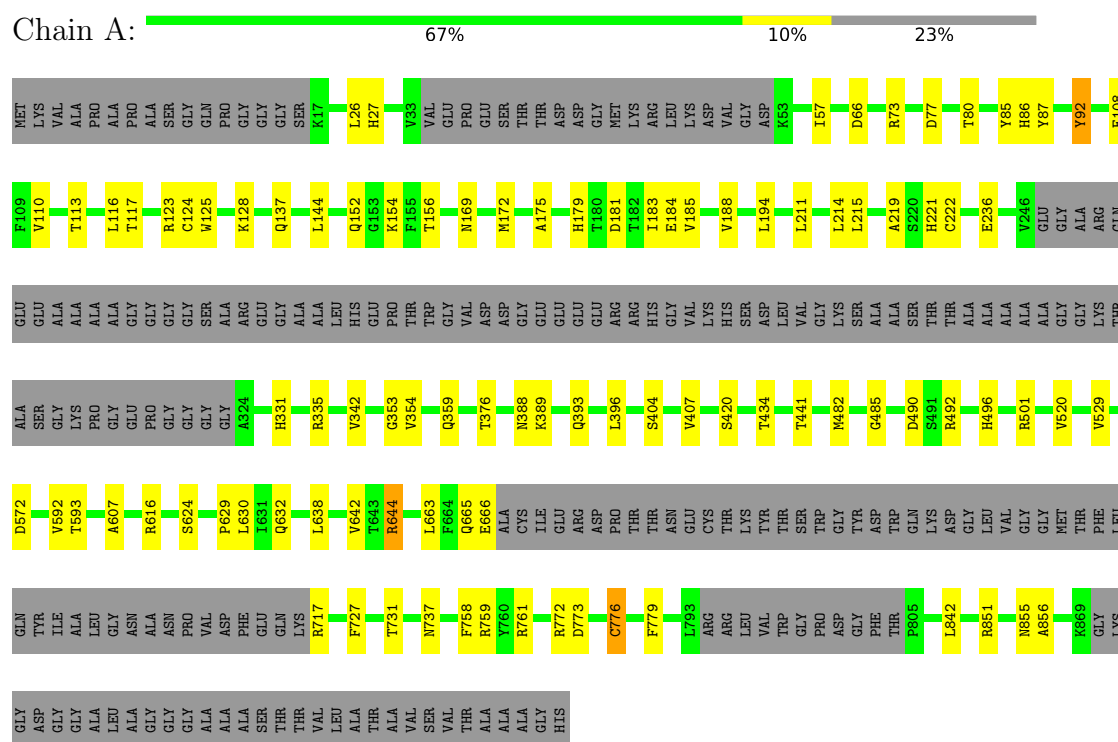


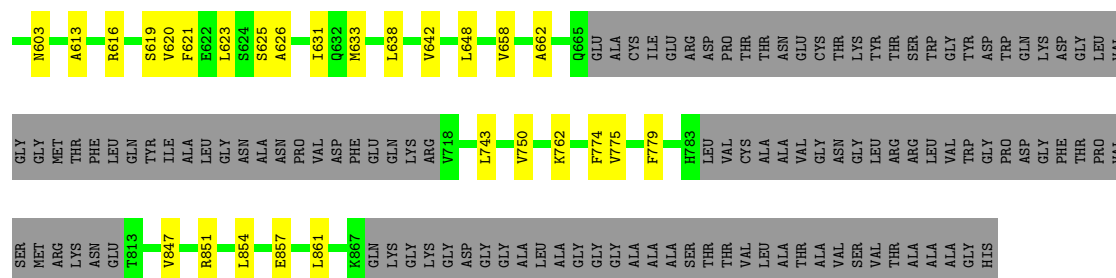
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	O	P	0
			126	82	38	6	
5	B	1	Total	C	O	P	0
			126	82	38	6	
5	D	1	Total	C	O	P	0
			126	82	38	6	
5	D	1	Total	C	O	P	0
			126	82	38	6	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

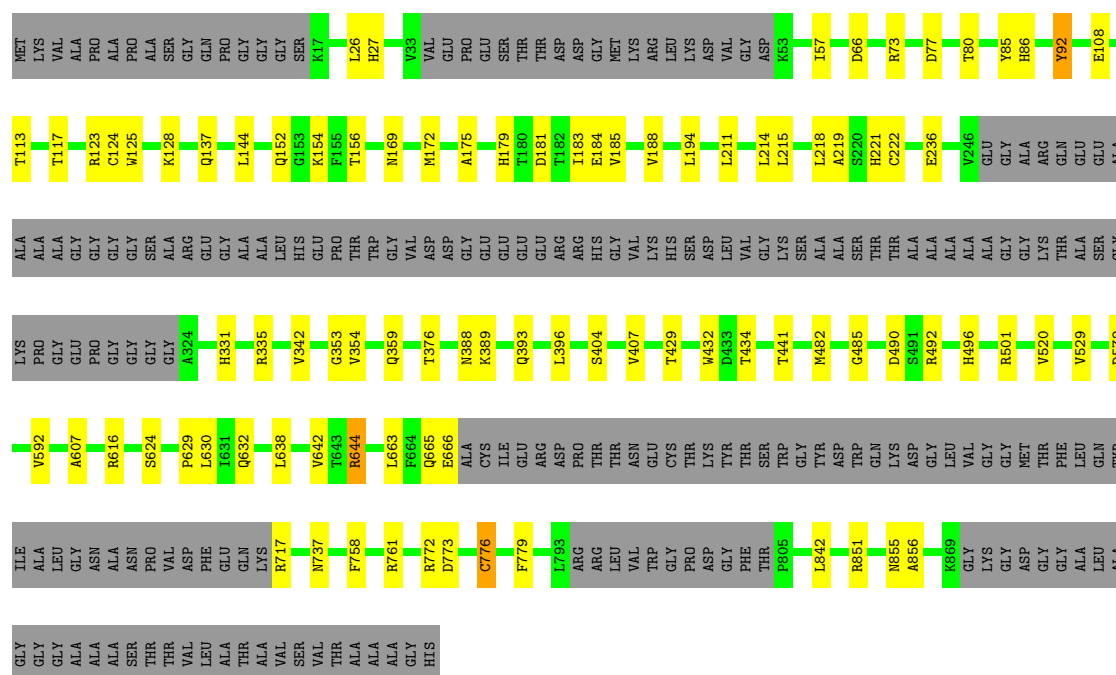
- Molecule 1: TRP-like ion channel





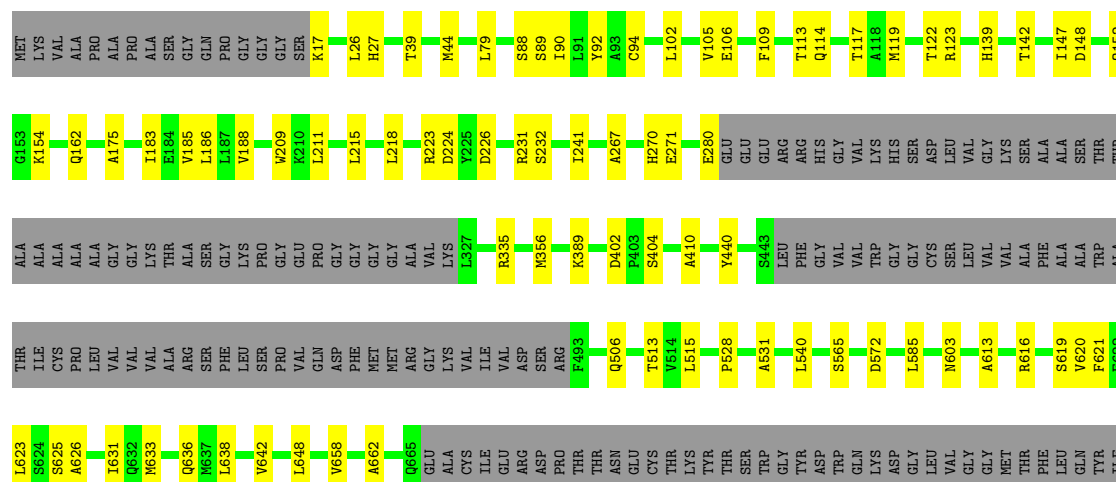
- Molecule 1: TRP-like ion channel

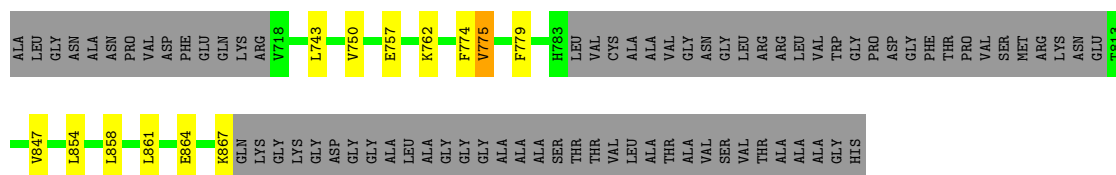
Chain C: 67% 10% 23%



- Molecule 1: TRP-like ion channel

Chain D: 65% 10% 25%





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	63018	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 ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: PIK, CPL, PCW, PIO

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 >2	RMSZ	# Z >2
1	A	0.35	0/5676	0.57	1/7704 (0.0%)
1	B	0.36	0/5489	0.59	0/7449
1	C	0.35	0/5676	0.57	1/7704 (0.0%)
1	D	0.36	0/5489	0.60	1/7449 (0.0%)
All	All	0.36	0/22330	0.58	3/30306 (0.0%)

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	3
1	C	0	1
1	D	0	3
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	CYS	CA-CB-SG	5.68	124.23	114.00
1	A	222	CYS	CA-CB-SG	5.67	124.20	114.00
1	D	775	VAL	C-N-CA	5.18	134.65	121.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	776	CYS	Peptide
1	B	223	ARG	Peptide
1	B	231	ARG	Peptide
1	B	232	SER	Peptide
1	C	776	CYS	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	5553	0	5632	68	0
1	B	5372	0	5381	63	0
1	C	5553	0	5632	64	0
1	D	5372	0	5381	62	0
2	A	47	0	44	3	0
2	C	47	0	44	3	0
3	A	50	0	71	0	0
3	C	50	0	71	1	0
4	A	26	0	23	3	0
4	C	26	0	23	3	0
5	B	126	0	153	2	0
5	D	126	0	153	3	0
All	All	22348	0	22608	230	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 5.

The worst 5 of 230 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:C:717:ARG:HH12	1:D:603:ASN:HD21	1.43	0.66
1:C:342:VAL:HG23	1:C:842:LEU:HD13	1.77	0.66
1:A:717:ARG:HH12	1:B:603:ASN:HD21	1.44	0.66
1:A:342:VAL:HG23	1:A:842:LEU:HD13	1.77	0.65
1:D:267:ALA:HB1	1:D:270:HIS:HB3	1.81	0.63

There are no symmetry-related clashes.

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 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	686/901 (76%)	622 (91%)	63 (9%)	1 (0%)	53	86
1	B	665/901 (74%)	585 (88%)	80 (12%)	0	100	100
1	C	686/901 (76%)	622 (91%)	63 (9%)	1 (0%)	53	86
1	D	665/901 (74%)	583 (88%)	82 (12%)	0	100	100
All	All	2702/3604 (75%)	2412 (89%)	288 (11%)	2 (0%)	56	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	THR
1	C	434	THR

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	606/740 (82%)	602 (99%)	4 (1%)	85	93
1	B	581/740 (78%)	579 (100%)	2 (0%)	93	98
1	C	606/740 (82%)	602 (99%)	4 (1%)	85	93
1	D	581/740 (78%)	579 (100%)	2 (0%)	93	98
All	All	2374/2960 (80%)	2362 (100%)	12 (0%)	90	95

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	585	LEU
1	C	85	TYR
1	C	644	ARG
1	B	17	LYS
1	C	123	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	569	ASN
1	C	359	GLN
1	D	506	GLN
1	C	152	GLN
1	C	179	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are 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
2	PIO	A	1001	-	47,47,47	1.20	6 (12%)	61,65,65	1.11	5 (8%)
3	PCW	A	1002	-	49,49,53	1.28	3 (6%)	55,57,61	0.97	2 (3%)
4	CPL	A	1003	-	25,25,51	1.29	2 (8%)	31,33,59	1.13	1 (3%)
5	PIK	B	1001	-	63,63,63	1.02	6 (9%)	77,81,81	1.10	5 (6%)
5	PIK	B	1002	-	63,63,63	1.04	5 (7%)	77,81,81	0.97	3 (3%)
2	PIO	C	1001	-	47,47,47	1.19	6 (12%)	61,65,65	1.11	5 (8%)
3	PCW	C	1002	-	49,49,53	1.28	4 (8%)	55,57,61	0.97	2 (3%)
4	CPL	C	1003	-	25,25,51	1.29	3 (12%)	31,33,59	1.12	1 (3%)
5	PIK	D	1001	-	63,63,63	1.02	6 (9%)	77,81,81	1.10	5 (6%)
5	PIK	D	1002	-	63,63,63	1.05	5 (7%)	77,81,81	0.97	3 (3%)

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
2	PIO	A	1001	-	-	15/44/68/68	0/1/1/1
3	PCW	A	1002	-	-	20/53/53/57	-
4	CPL	A	1003	-	-	12/28/28/55	-
5	PIK	B	1001	-	-	24/60/84/84	0/1/1/1
5	PIK	B	1002	-	-	19/60/84/84	0/1/1/1
2	PIO	C	1001	-	-	15/44/68/68	0/1/1/1
3	PCW	C	1002	-	-	20/53/53/57	-
4	CPL	C	1003	-	-	12/28/28/55	-
5	PIK	D	1001	-	-	24/60/84/84	0/1/1/1
5	PIK	D	1002	-	-	20/60/84/84	0/1/1/1

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	PCW	O2-C31	3.70	1.44	1.34
3	A	1002	PCW	O2-C31	3.68	1.44	1.34
3	A	1002	PCW	O3-C11	3.44	1.43	1.33
3	C	1002	PCW	O3-C11	3.43	1.43	1.33
5	B	1002	PIK	P4-O4	3.28	1.65	1.59

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	PIO	O2C-C1A-C2A	4.22	120.73	111.51
2	C	1001	PIO	O2C-C1A-C2A	4.20	120.67	111.51
5	B	1001	PIK	OB1-CB1-CB2	4.15	120.58	111.51
5	D	1001	PIK	OB1-CB1-CB2	4.15	120.56	111.51
4	A	1003	CPL	O2-C31-C32	3.99	120.23	111.51

There are no chirality outliers.

5 of 181 torsion outliers are listed below:

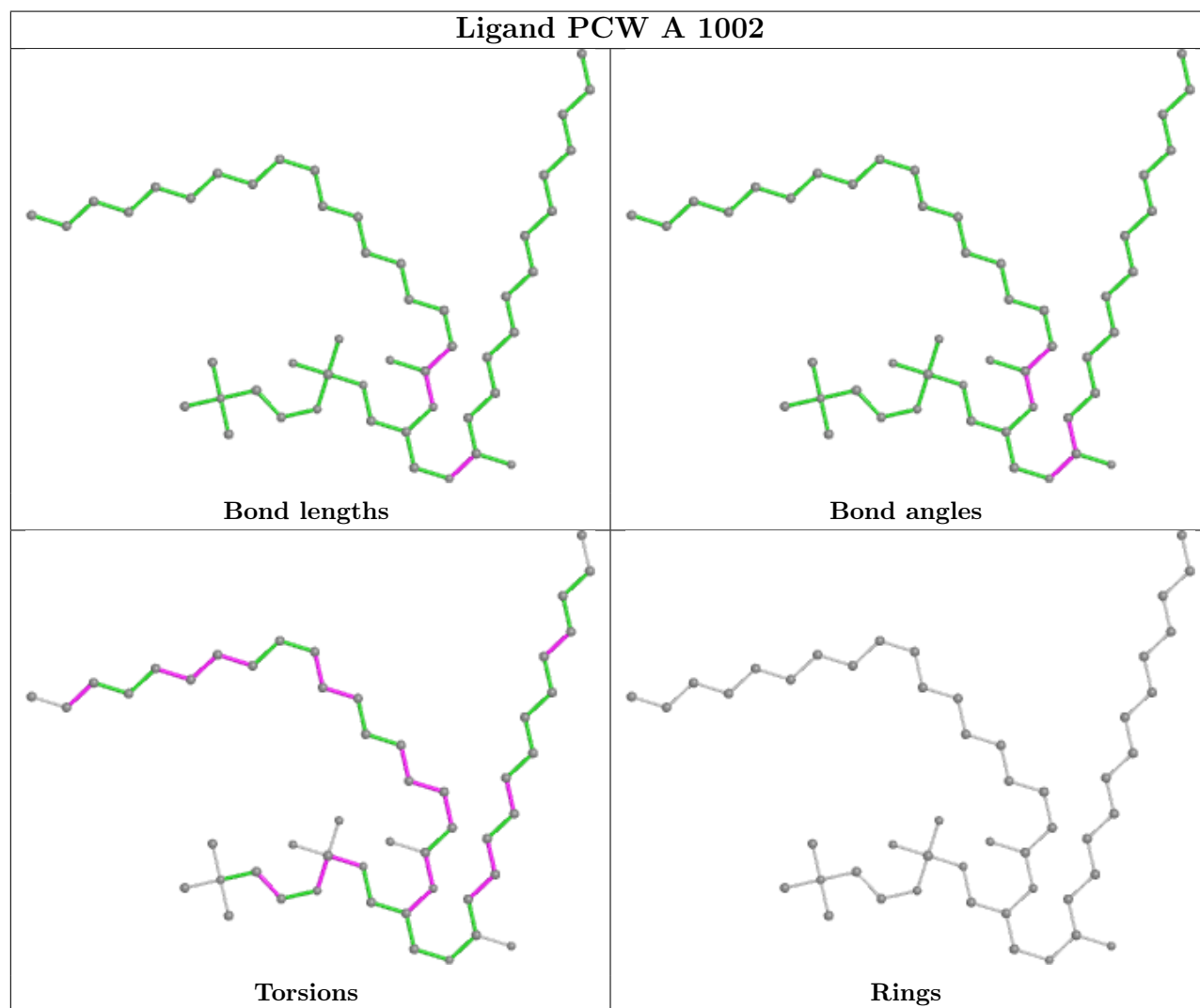
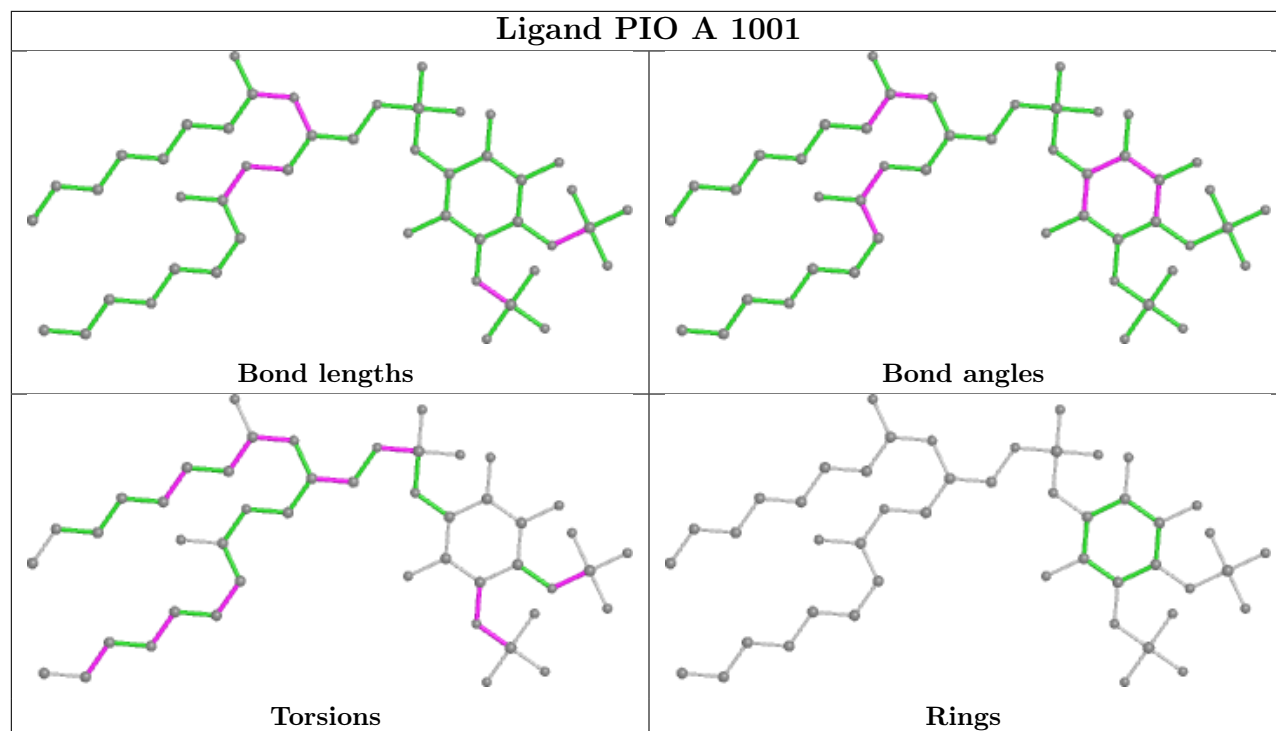
Mol	Chain	Res	Type	Atoms
5	B	1001	PIK	C8-C7-O13-P1
5	B	1001	PIK	CB2-CB1-OB1-C8
5	B	1001	PIK	C7-C8-OB1-CB1
5	B	1001	PIK	C6-C1-O1-P1
5	D	1001	PIK	C8-C7-O13-P1

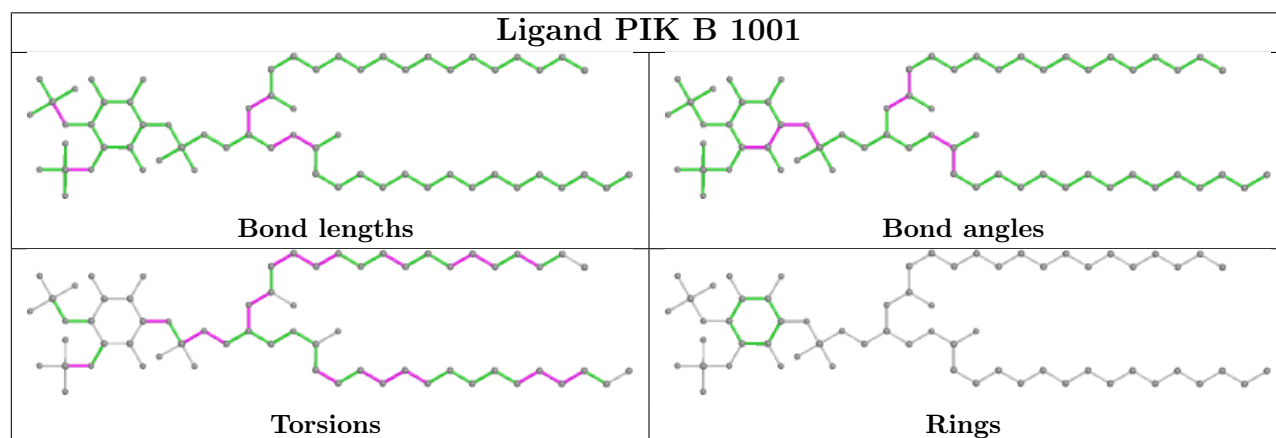
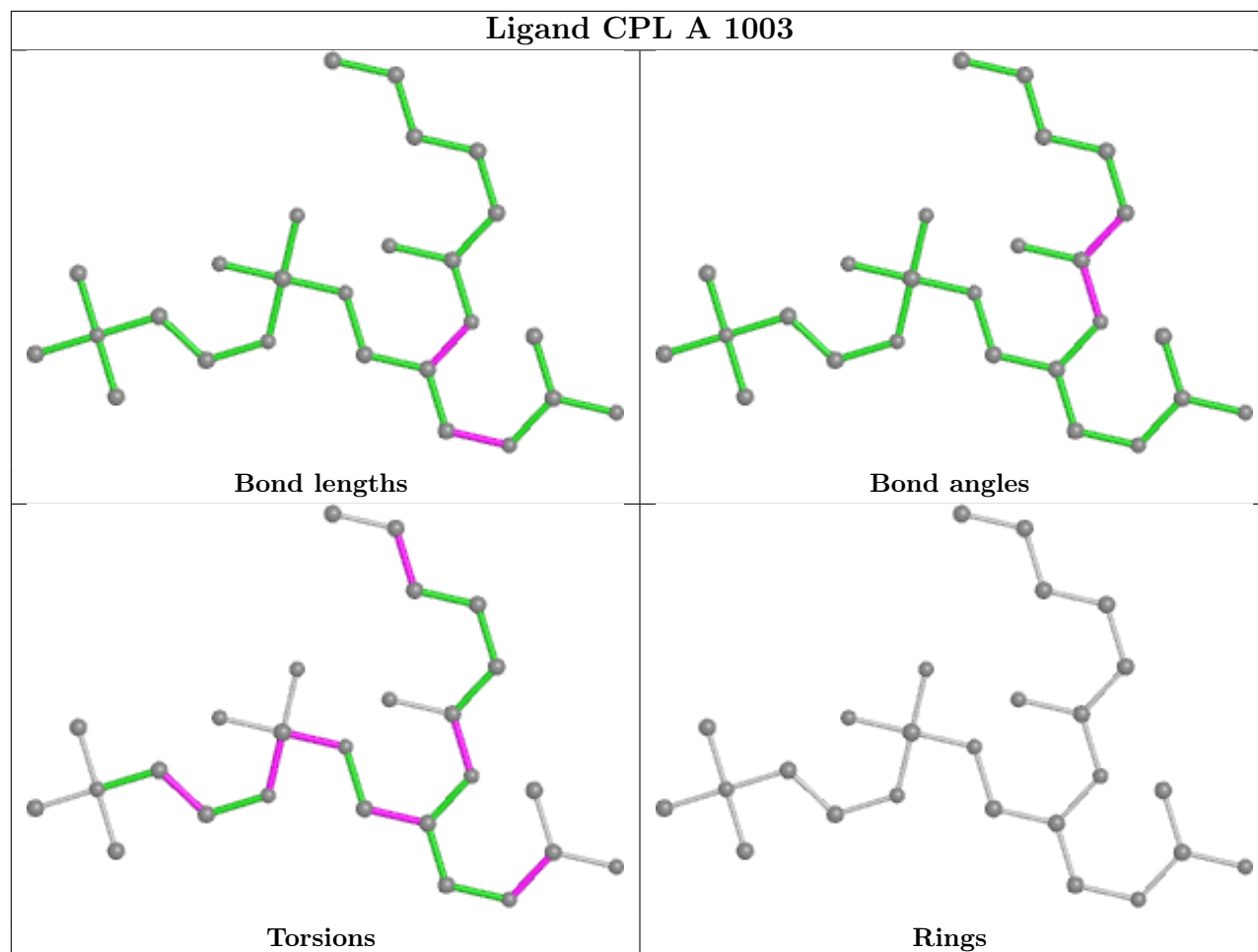
There are no ring outliers.

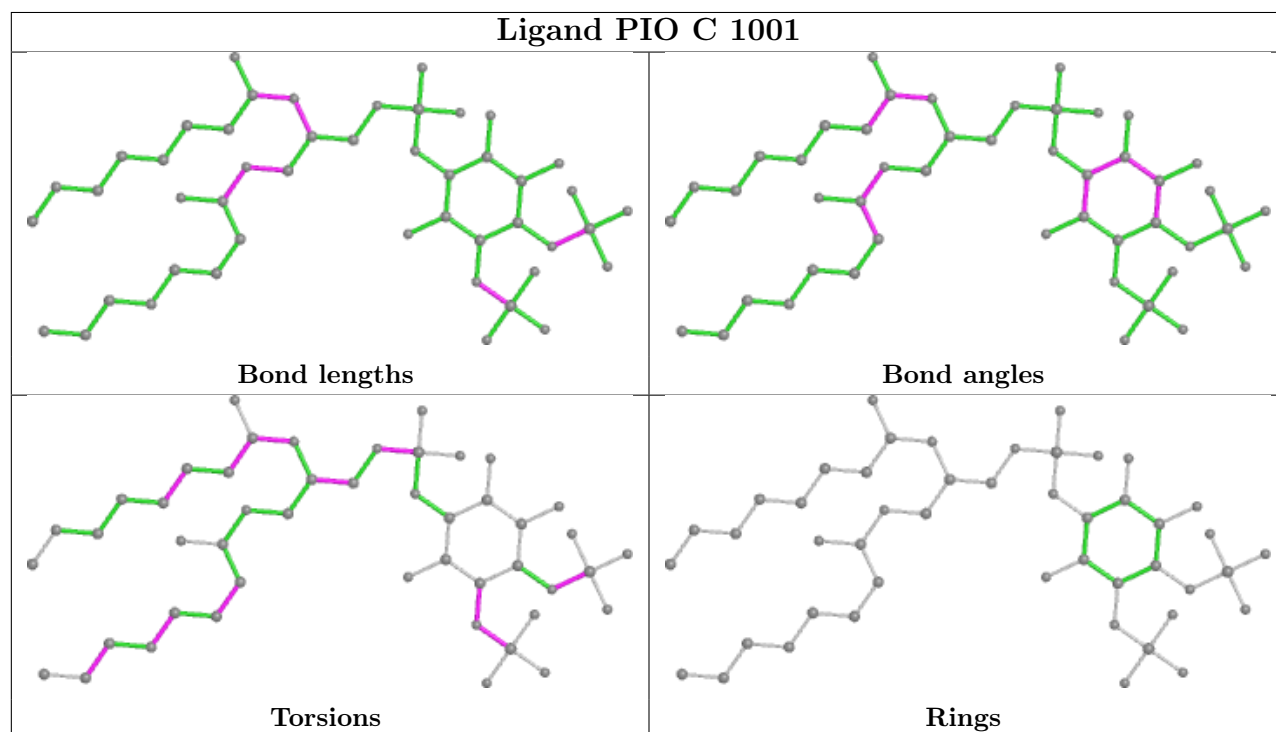
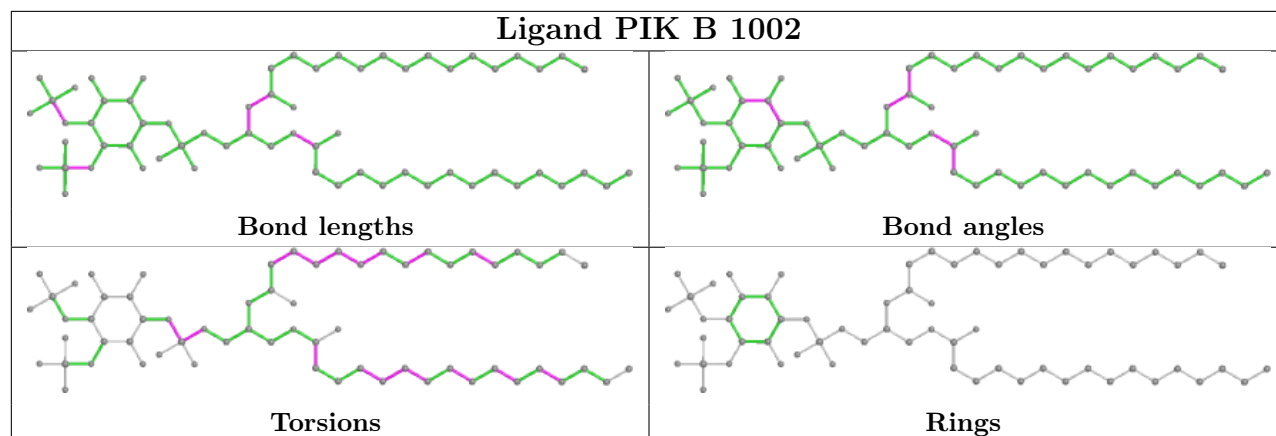
7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	PIO	3	0
4	A	1003	CPL	3	0
5	B	1001	PIK	2	0
2	C	1001	PIO	3	0
3	C	1002	PCW	1	0
4	C	1003	CPL	3	0
5	D	1001	PIK	3	0

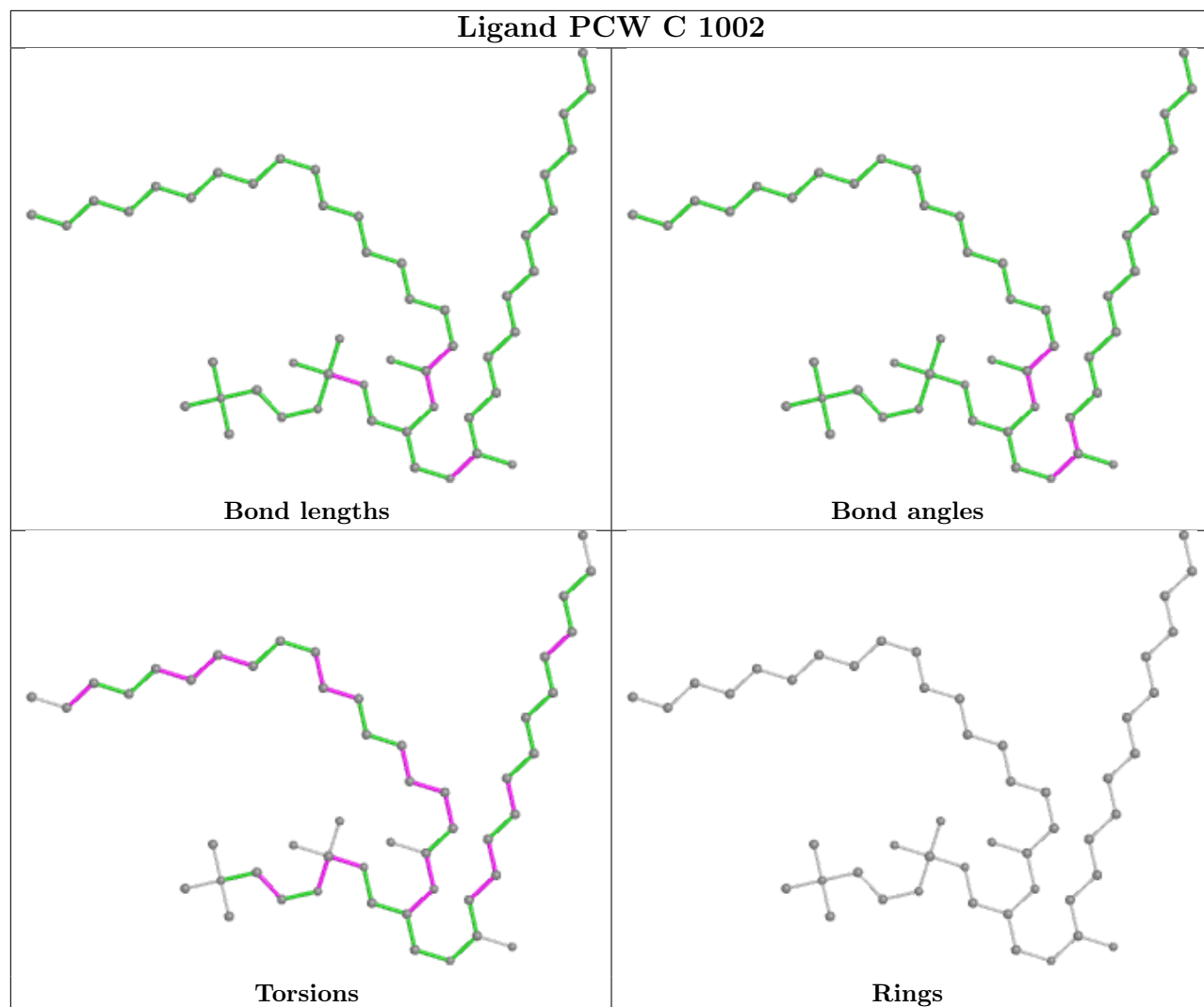
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

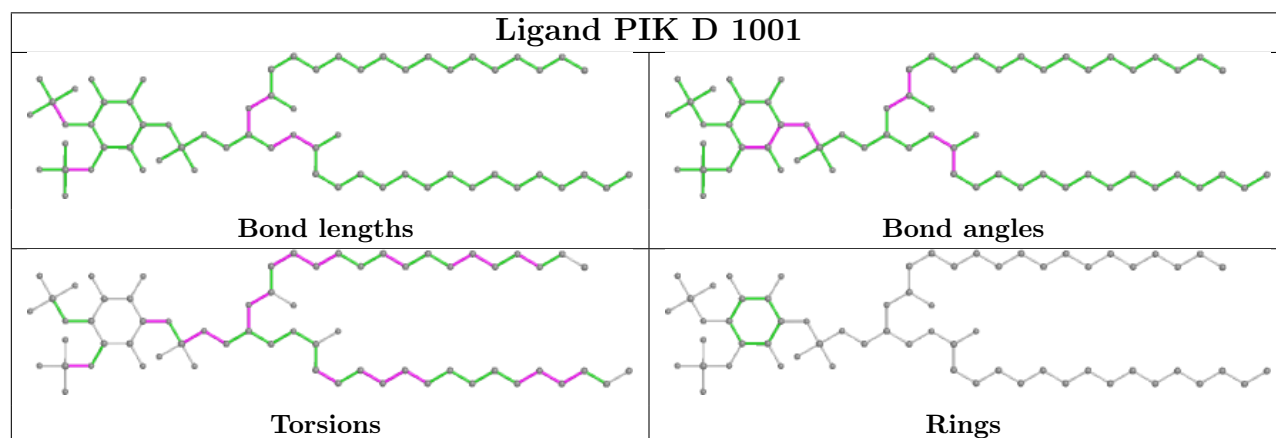
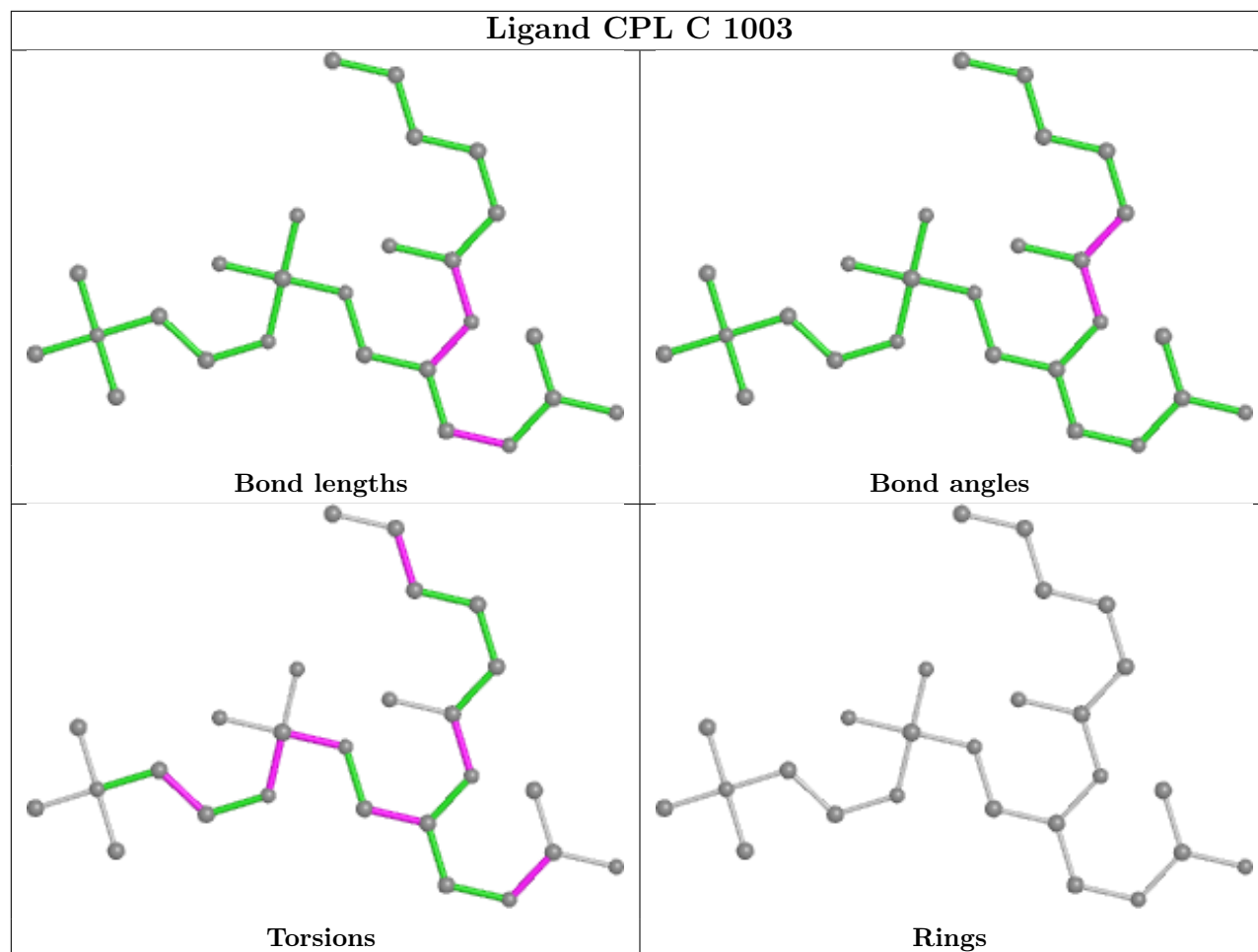


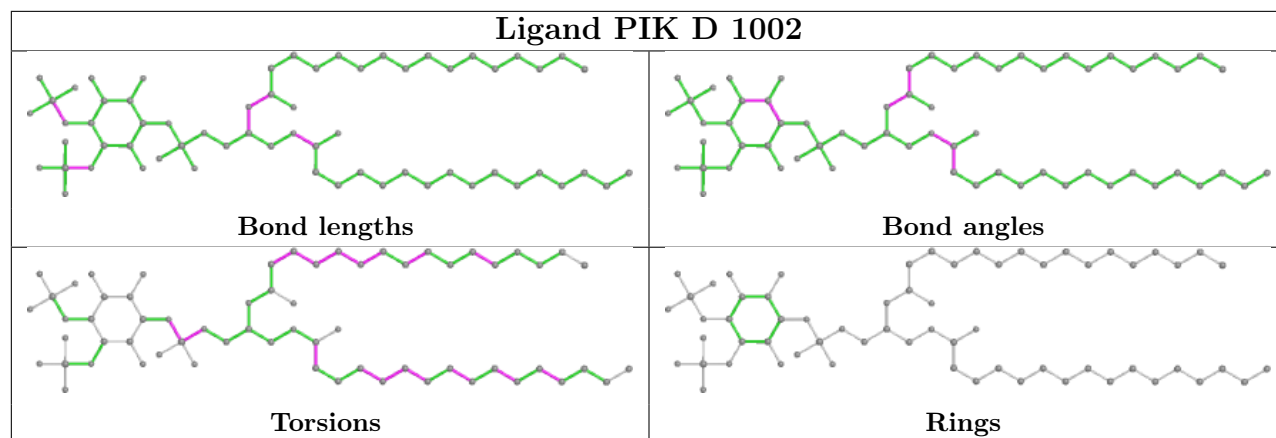




Ligand PCW C 1002







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.