



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 16, 2020 – 09:55 am BST

PDB ID : 2MSC  
Title : NMR data-driven model of GTPase KRas-GDP tethered to a lipid-bilayer nanodisc  
Authors : Mazhab-Jafari, M.; Stathopoulos, P.; Marshall, C.; Ikura, M.  
Deposited on : 2014-07-29

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

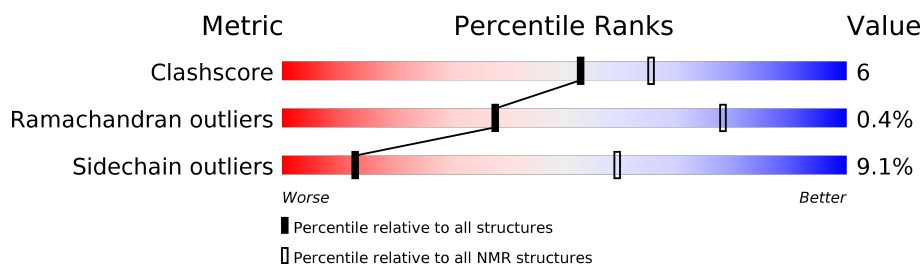
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 0%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	200	80% 17% ...
1	C	200	79% 17% ...
2	B	187	67% 10% 22% .

## 2 Ensemble composition and analysis i

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:201-A:395, C:402-C:593 (387)	0.26	4
2	B:3-B:146 (144)	0.33	8

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	5, 6, 7, 10
2	1, 2, 4
Single-model clusters	3; 8; 9

### 3 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9134 atoms, of which 62 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	198	1645	1019	22	287	314	3	0
1	C	198	1646	1019	22	287	315	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	-	expression tag	UNP P02647
A	200	PRO	-	expression tag	UNP P02647
C	397	GLY	-	expression tag	UNP P02647
C	398	PRO	-	expression tag	UNP P02647

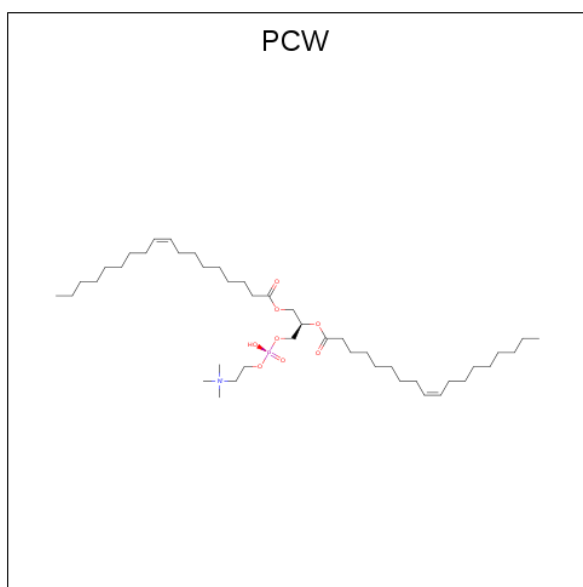
- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	185	1494	923	18	257	287	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P01116
B	0	SER	-	expression tag	UNP P01116

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1

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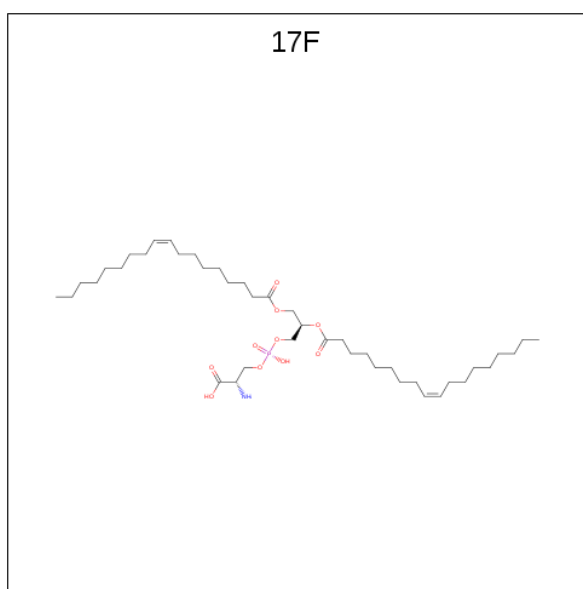




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Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1

- Molecule 4 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: C<sub>42</sub>H<sub>78</sub>NO<sub>10</sub>P).



Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1

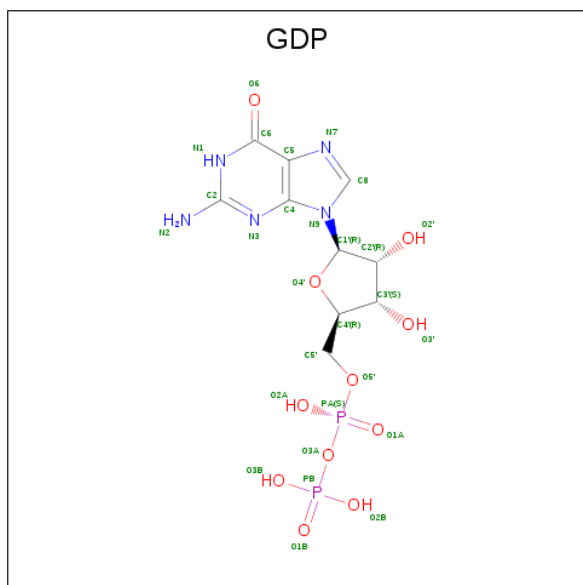
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Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1
4	A	1	54	42	1	10	1

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
5	B	1	28	10	5	11	2

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

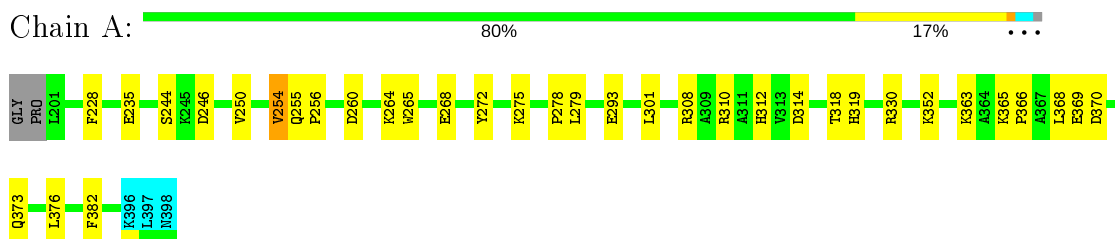
Mol	Chain	Residues	Atoms	
			Total	Mg
6	B	1	1	1

## 4 Residue-property plots [i](#)

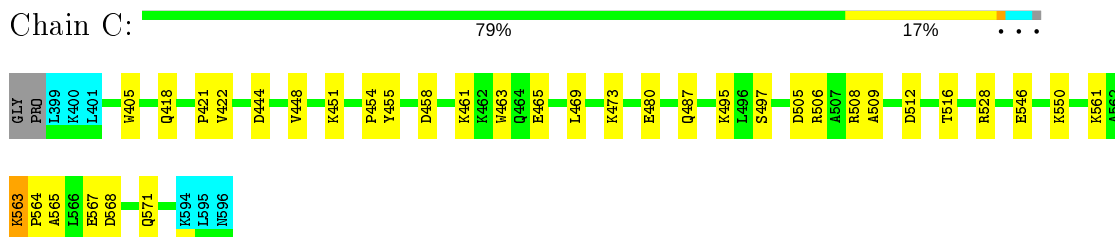
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

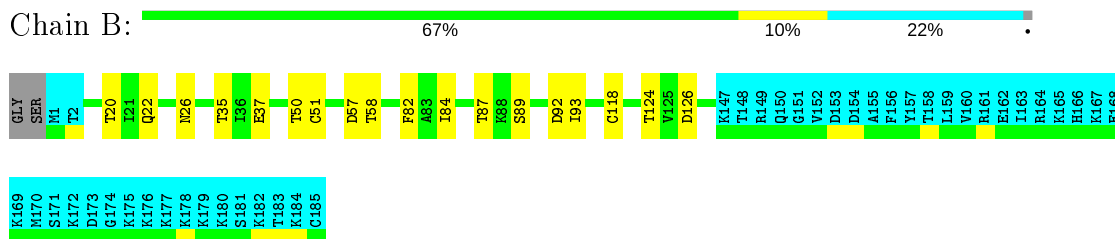
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



### 4.2 Scores per residue for each member of the ensemble

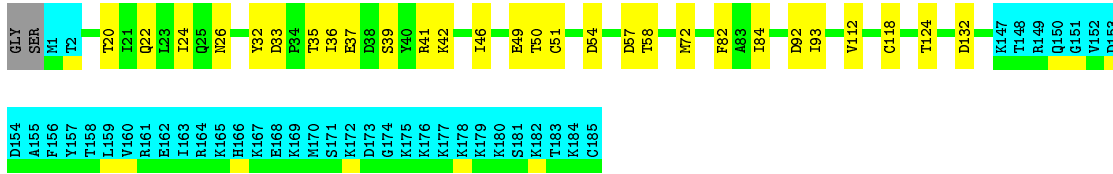
Colouring as in section 4.1 above.





- Molecule 2: GTPase KRas

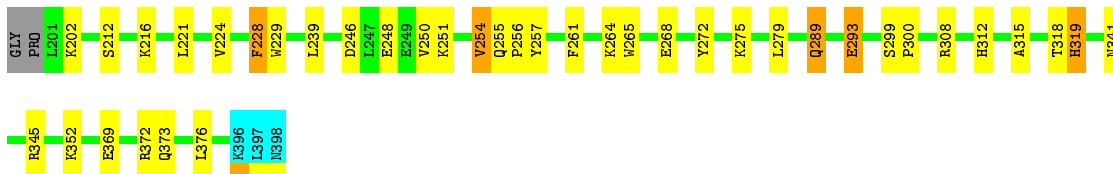
Chain B: 62% 15% 22%



### 4.2.3 Score per residue for model 3

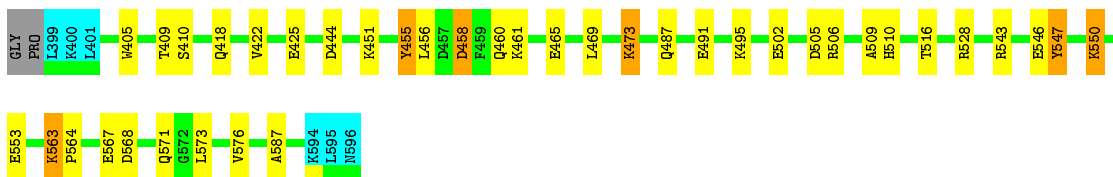
- Molecule 1: Apolipoprotein A-I

Chain A: 78% 17%



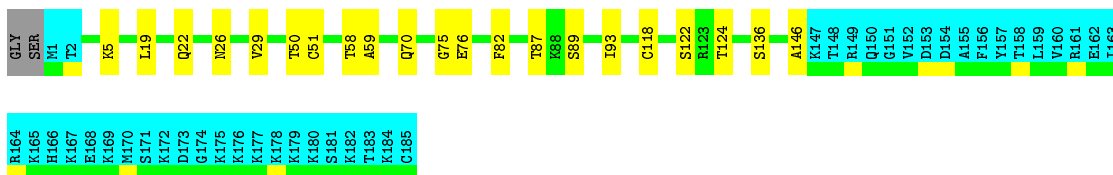
- Molecule 1: Apolipoprotein A-I

Chain C: 77% 17%



- Molecule 2: GTPase KRas

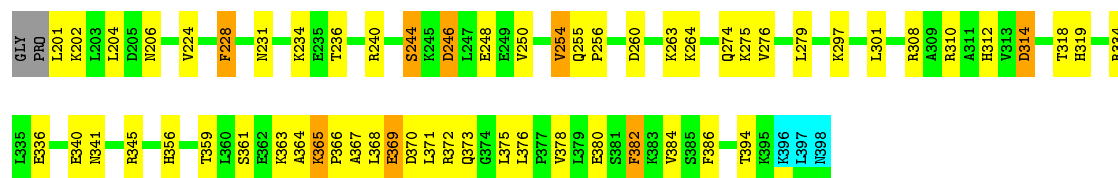
Chain B: 66% 11% 22%



### 4.2.4 Score per residue for model 4 (medoid)

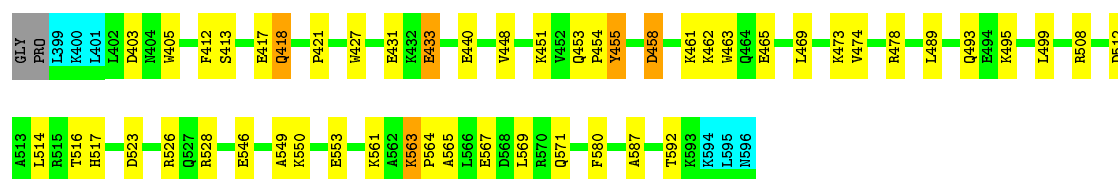
- Molecule 1: Apolipoprotein A-I

Chain A:  68% 26%



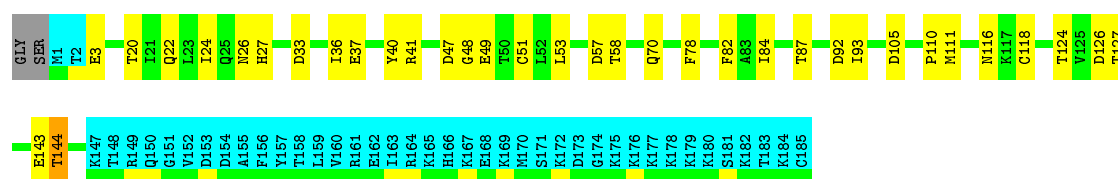
- Molecule 1: Apolipoprotein A-I

Chain C:  71% 23%



- Molecule 2: GTPase KRas

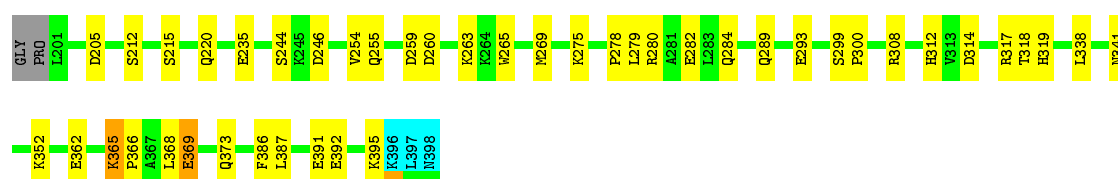
Chain B:  58% 18% 22%



#### 4.2.5 Score per residue for model 5

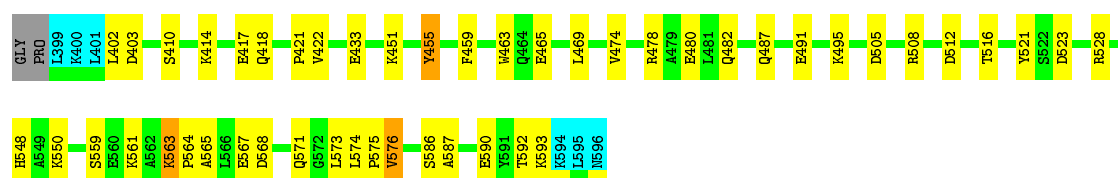
- Molecule 1: Apolipoprotein A-I

Chain A:  76% 21%

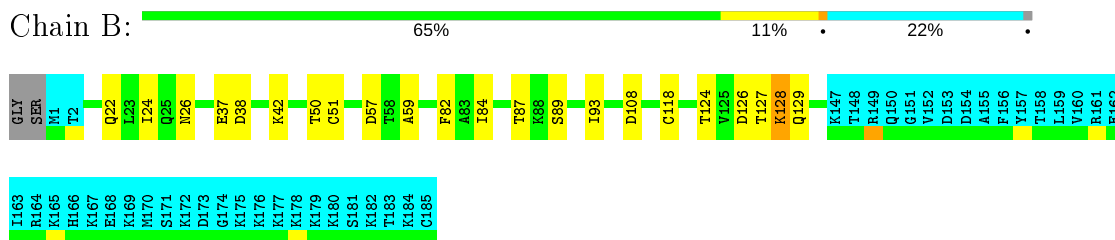


- Molecule 1: Apolipoprotein A-I

Chain C:  72% 23%

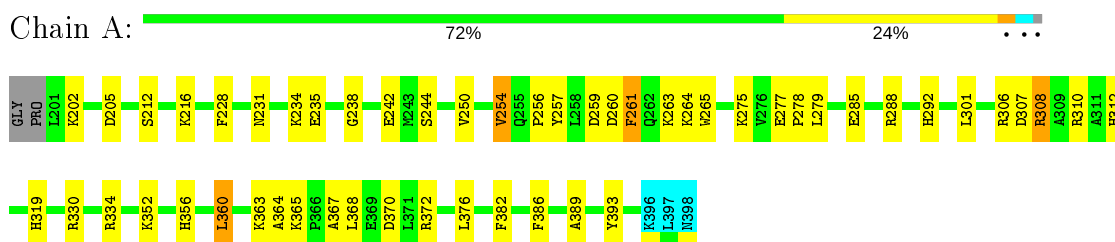


- Molecule 2: GTPase KRas

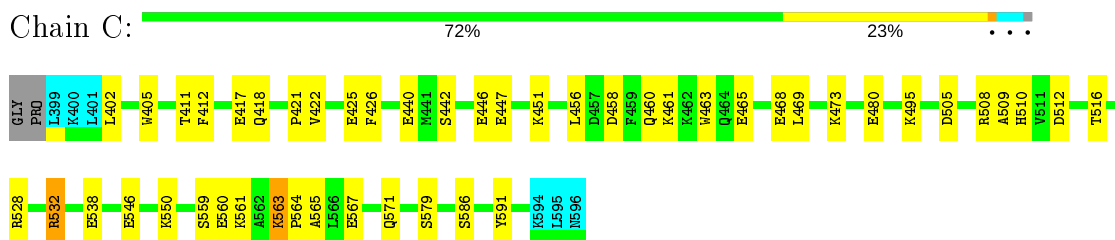


#### 4.2.6 Score per residue for model 6

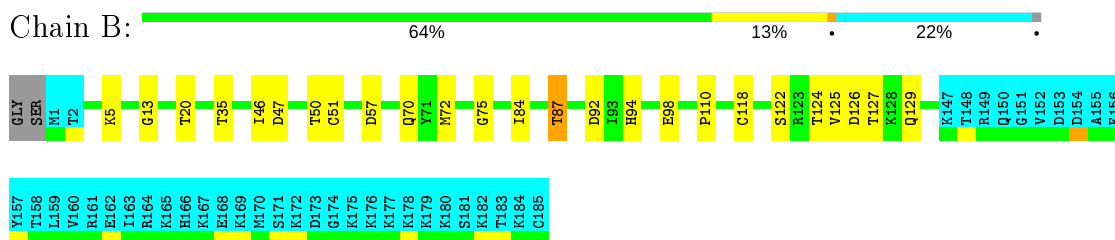
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

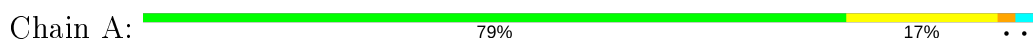


- Molecule 2: GTPase KRas



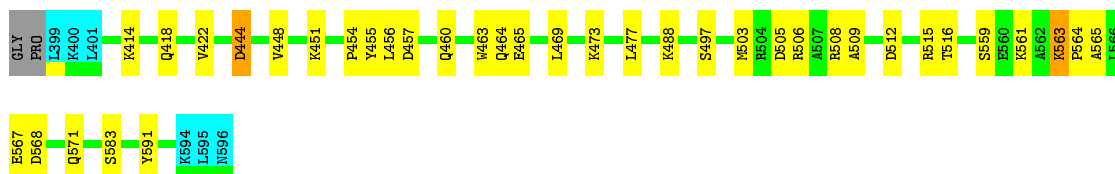
#### 4.2.7 Score per residue for model 7

- Molecule 1: Apolipoprotein A-I

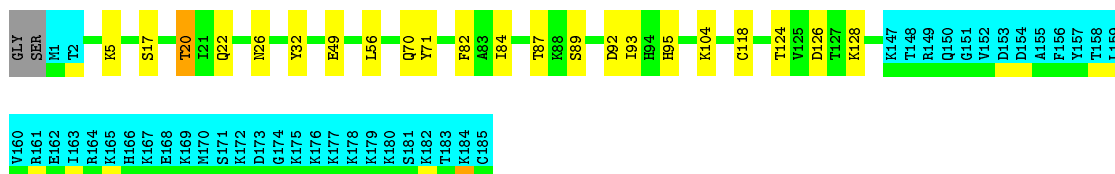




• Molecule 1: Apolipoprotein A-I

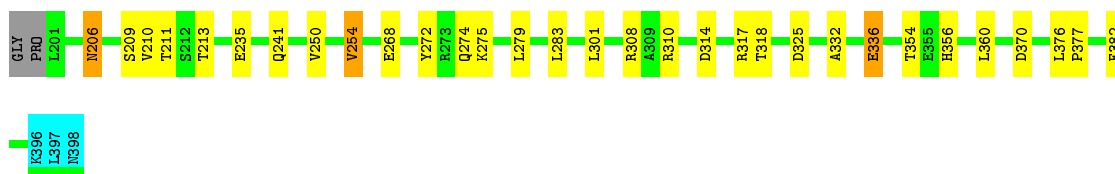
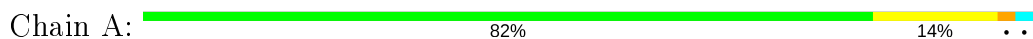


• Molecule 2: GTPase KRas

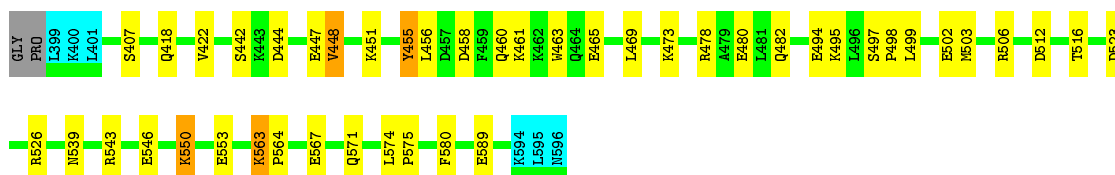


### 4.2.8 Score per residue for model 8

• Molecule 1: Apolipoprotein A-I

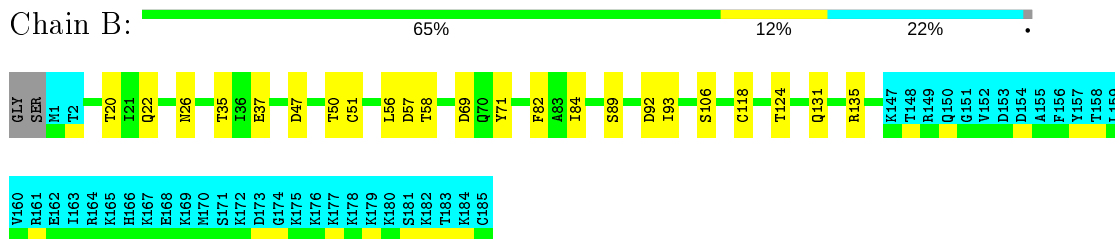


• Molecule 1: Apolipoprotein A-I



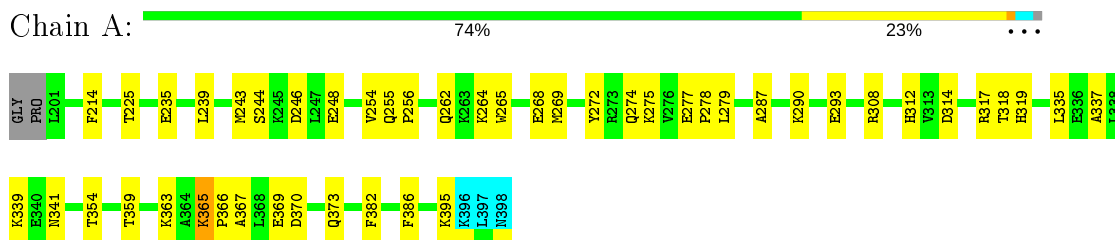
• Molecule 2: GTPase KRas



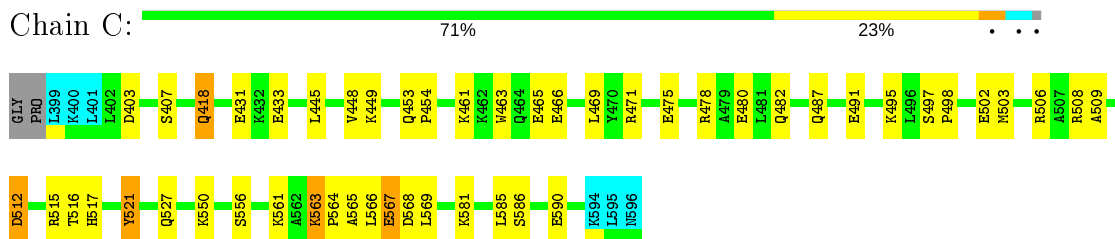


#### 4.2.9 Score per residue for model 9

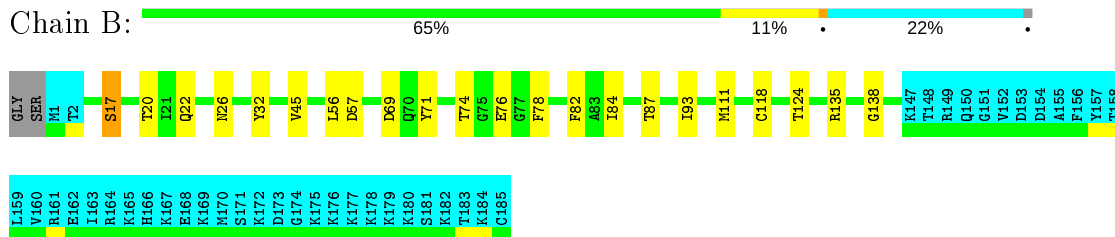
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

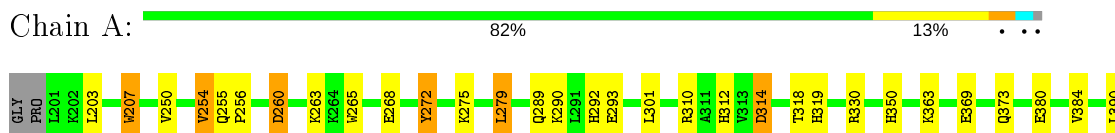


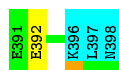
- Molecule 2: GTPase KRAs



#### 4.2.10 Score per residue for model 10

- Molecule 1: Apolipoprotein A-I





- Molecule 1: Apolipoprotein A-I

Chain C: 81% 15%



- Molecule 2: GTPase KRas

Chain B: 67% 10% 22%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 3000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	structure solution	
HADDOCK	structure solution	
CHARMM-GUI	structure solution	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	44
Number of shifts mapped to atoms	44
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 17F, MG, PCW

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1598	22	1596	25±7
1	C	1573	22	1562	27±7
2	B	1137	16	1109	8±2
3	A	3456	0	5376	54±5
4	A	864	0	1216	22±4
All	All	86570	600	108711	1101

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.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ARG:HD2	1:C:469:LEU:CD2	1.30	1.57	9	1
1:C:465:GLU:O	1:C:469:LEU:CG	1.29	1.78	9	9
1:C:567:GLU:O	1:C:571:GLN:HG3	1.25	1.23	2	9
1:C:465:GLU:O	1:C:469:LEU:HG	1.25	1.26	7	9
1:A:308:ARG:CD	1:C:469:LEU:HD11	1.21	1.66	9	1
1:A:308:ARG:CD	1:C:469:LEU:HD21	1.15	1.71	9	1
1:A:308:ARG:HD3	1:C:469:LEU:HD11	1.04	1.06	9	1
1:C:567:GLU:O	1:C:571:GLN:CG	1.01	2.09	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:369:GLU:O	1:A:373:GLN:HG3	0.98	1.58	7	7
1:A:308:ARG:CD	1:C:469:LEU:CD1	0.95	2.43	9	1
3:A:30:PCW:H71	4:A:37:17F:HN1A	0.91	1.24	10	1
4:A:38:17F:HN1	2:B:131:GLN:HE21	0.89	1.05	8	1
1:A:308:ARG:HG3	1:C:469:LEU:HD11	0.89	1.43	5	3
3:A:70:PCW:H31	3:A:71:PCW:H32	0.86	1.43	9	1
1:A:260:ASP:HA	1:A:263:LYS:HE2	0.86	1.45	6	3
4:A:40:17F:H4	4:A:40:17F:HN1	0.85	1.30	4	1
1:C:563:LYS:HB2	1:C:564:PRO:HD3	0.85	1.46	2	8
1:A:389:ALA:O	1:A:393:TYR:CD2	0.84	2.30	6	1
1:A:308:ARG:HG3	1:C:469:LEU:HD21	0.84	1.47	7	7
1:C:465:GLU:O	1:C:469:LEU:CD1	0.83	2.26	1	3
1:C:458:ASP:HA	1:C:461:LYS:HE2	0.83	1.50	4	1
3:A:15:PCW:H71	4:A:39:17F:H2	0.82	1.49	3	1
1:A:308:ARG:CD	1:C:469:LEU:CD2	0.82	2.47	9	1
1:A:308:ARG:HD2	1:C:469:LEU:HD21	0.82	0.83	9	1
1:A:308:ARG:HD2	1:C:469:LEU:CG	0.80	2.05	9	1
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.80	1.50	9	5
3:A:63:PCW:P	4:A:75:17F:HN1A	0.80	2.00	3	1
3:A:45:PCW:H71	3:A:71:PCW:H20	0.79	1.54	8	1
3:A:32:PCW:H331	4:A:35:17F:H11	0.79	1.52	7	1
1:A:369:GLU:O	1:A:373:GLN:CG	0.79	2.30	7	3
1:A:308:ARG:HD3	1:C:469:LEU:CD1	0.79	2.00	9	1
3:A:32:PCW:H61	4:A:38:17F:HN1A	0.79	1.38	8	1
1:C:465:GLU:O	1:C:469:LEU:CB	0.78	2.31	1	4
1:A:389:ALA:O	1:A:393:TYR:HD2	0.78	1.60	6	1
3:A:51:PCW:H41	3:A:71:PCW:H382	0.75	1.56	3	1
3:A:42:PCW:H341	3:A:52:PCW:H331	0.75	1.59	1	1
3:A:57:PCW:H82	4:A:80:17F:HN1A	0.74	1.42	5	1
1:A:352:LYS:HG2	1:C:422:VAL:HG13	0.73	1.60	5	3
3:A:16:PCW:H19	4:A:39:17F:H5	0.73	1.59	6	1
1:A:308:ARG:CG	1:C:469:LEU:HD11	0.72	2.12	5	4
3:A:10:PCW:H62	4:A:36:17F:H2	0.72	1.61	6	1
3:A:17:PCW:H132	3:A:17:PCW:H332	0.70	1.63	7	1
1:A:250:VAL:O	1:A:254:VAL:HB	0.70	1.85	1	8
3:A:19:PCW:H41	3:A:23:PCW:H411	0.70	1.64	2	1
3:A:7:PCW:H73	4:A:35:17F:HN1A	0.69	1.46	1	1
4:A:33:17F:H8	4:A:35:17F:H9A	0.68	1.65	1	1
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.67	1.64	8	3
1:C:453:GLN:HB2	1:C:454:PRO:HD3	0.67	1.65	2	4
4:A:38:17F:HN1	2:B:131:GLN:NE2	0.67	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:279:LEU:HD22	1:C:495:LYS:HG2	0.67	1.66	3	6
3:A:20:PCW:H32	3:A:24:PCW:H352	0.67	1.66	6	2
4:A:74:17F:H34	4:A:79:17F:H6A	0.67	1.67	7	1
3:A:59:PCW:H61	4:A:77:17F:H6A	0.67	1.65	4	1
3:A:70:PCW:H39	3:A:71:PCW:H152	0.66	1.66	10	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.66	1.90	4	9
3:A:47:PCW:H12	4:A:73:17F:H1	0.66	1.68	8	1
3:A:5:PCW:H31	3:A:17:PCW:H382	0.66	1.67	9	1
1:C:418:GLN:O	1:C:422:VAL:HB	0.65	1.91	6	6
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.65	1.69	7	9
4:A:33:17F:P1	4:A:33:17F:HN1	0.65	2.14	9	3
3:A:51:PCW:H51	3:A:71:PCW:H382	0.65	1.69	4	1
3:A:14:PCW:H51	2:B:48:GLY:HA2	0.65	1.68	4	1
4:A:38:17F:O2	2:B:135:ARG:HD3	0.65	1.90	8	1
3:A:47:PCW:H231	4:A:76:17F:H5	0.65	1.67	9	1
3:A:13:PCW:H62	4:A:34:17F:HN1	0.65	1.52	10	1
1:A:231:ASN:HA	1:A:234:LYS:HE2	0.65	1.69	1	2
3:A:57:PCW:H19	4:A:76:17F:H40	0.65	1.68	5	1
3:A:58:PCW:H372	3:A:60:PCW:H141	0.65	1.67	10	1
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.65	1.67	10	7
3:A:11:PCW:H81	3:A:25:PCW:H31	0.64	1.69	4	1
1:A:308:ARG:HG3	1:C:469:LEU:CD1	0.64	2.20	5	3
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.64	1.67	3	2
3:A:14:PCW:H121	4:A:34:17F:H20	0.64	1.69	8	2
1:C:465:GLU:O	1:C:469:LEU:HD12	0.64	1.92	1	1
3:A:46:PCW:H322	3:A:71:PCW:H352	0.64	1.69	5	1
1:A:352:LYS:HZ2	1:C:425:GLU:HB3	0.64	1.52	3	2
3:A:9:PCW:H51	4:A:34:17F:H4	0.64	1.69	4	1
1:C:508:ARG:O	1:C:512:ASP:HB2	0.63	1.94	6	2
1:C:590:GLU:HA	1:C:593:LYS:HE3	0.63	1.70	5	1
1:C:505:ASP:HA	1:C:508:ARG:HD2	0.63	1.71	7	2
3:A:6:PCW:H341	3:A:16:PCW:H342	0.63	1.70	3	1
3:A:32:PCW:H332	4:A:35:17F:H62	0.63	1.70	9	1
3:A:41:PCW:H131	3:A:52:PCW:H39	0.63	1.70	7	1
1:A:301:LEU:HD22	1:C:473:LYS:HG2	0.63	1.68	10	2
1:A:301:LEU:HB3	1:C:473:LYS:HD2	0.63	1.68	2	1
3:A:27:PCW:H41	4:A:37:17F:O1	0.63	1.94	3	1
1:C:557:THR:HA	1:C:560:GLU:HG2	0.62	1.71	1	1
3:A:70:PCW:H73	3:A:70:PCW:H19	0.62	1.72	2	1
3:A:48:PCW:H61	3:A:61:PCW:H39	0.62	1.71	9	1
3:A:30:PCW:H61	4:A:37:17F:N1	0.62	2.10	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:376:LEU:HB2	1:A:377:PRO:HD3	0.62	1.72	1	2
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.62	1.69	2	3
3:A:66:PCW:H212	3:A:67:PCW:H61	0.61	1.70	8	1
1:C:474:VAL:O	1:C:478:ARG:HB2	0.61	1.96	4	2
3:A:46:PCW:H31	3:A:71:PCW:H382	0.61	1.72	8	1
3:A:3:PCW:H142	3:A:3:PCW:H372	0.61	1.72	5	1
4:A:33:17F:HN1	4:A:33:17F:P1	0.61	2.18	2	4
3:A:27:PCW:H73	4:A:37:17F:HN1	0.61	1.56	1	1
2:B:24:ILE:HA	2:B:42:LYS:HD2	0.61	1.73	5	2
3:A:4:PCW:H321	3:A:7:PCW:H12	0.61	1.71	3	1
3:A:49:PCW:H322	3:A:57:PCW:H2	0.61	1.71	7	1
1:C:574:LEU:HB2	1:C:575:PRO:HD3	0.60	1.71	5	2
3:A:25:PCW:H131	3:A:31:PCW:H31	0.60	1.71	3	1
3:A:14:PCW:H232	3:A:14:PCW:H452	0.60	1.73	7	1
3:A:13:PCW:H431	3:A:18:PCW:H172	0.60	1.72	2	1
3:A:47:PCW:H232	4:A:76:17F:H33	0.60	1.74	3	1
1:C:458:ASP:HA	1:C:461:LYS:HE3	0.60	1.72	1	1
3:A:59:PCW:H121	4:A:77:17F:H10A	0.60	1.73	3	1
1:C:563:LYS:HB2	1:C:564:PRO:CD	0.60	2.27	7	5
3:A:1:PCW:H283	3:A:5:PCW:H241	0.60	1.73	2	1
3:A:48:PCW:H20	3:A:58:PCW:H151	0.60	1.74	2	1
3:A:20:PCW:H42	3:A:31:PCW:O2P	0.59	1.97	2	1
4:A:73:17F:H58	4:A:76:17F:H19	0.59	1.73	3	1
1:A:352:LYS:NZ	1:C:425:GLU:HB3	0.59	2.12	6	2
1:C:503:MET:HA	1:C:506:ARG:HD2	0.59	1.74	9	4
3:A:48:PCW:H322	3:A:54:PCW:H152	0.59	1.73	2	1
1:A:341:ASN:HD21	1:C:433:GLU:HA	0.59	1.56	4	1
1:A:314:ASP:HA	1:A:317:ARG:HD2	0.59	1.74	9	3
1:A:256:PRO:HA	1:A:259:ASP:HB3	0.59	1.74	6	1
1:C:451:LYS:O	1:C:455:TYR:HB2	0.58	1.98	4	4
3:A:26:PCW:H132	3:A:26:PCW:H352	0.58	1.73	2	1
2:B:5:LYS:HB3	2:B:75:GLY:HA2	0.58	1.75	3	1
3:A:42:PCW:H162	3:A:52:PCW:H331	0.58	1.76	6	1
1:A:301:LEU:HB3	1:C:473:LYS:HE3	0.58	1.76	6	1
3:A:43:PCW:H422	3:A:43:PCW:H181	0.58	1.76	2	1
3:A:9:PCW:H351	3:A:14:PCW:H122	0.58	1.74	2	1
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.58	1.76	7	2
3:A:44:PCW:H122	4:A:77:17F:H1A	0.58	1.74	9	1
1:A:264:LYS:HE2	1:C:509:ALA:HB1	0.58	1.75	9	3
3:A:13:PCW:H41	4:A:34:17F:O1	0.58	1.99	8	1
3:A:16:PCW:H182	4:A:39:17F:H33	0.58	1.76	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:66:PCW:H451	4:A:79:17F:H10	0.57	1.76	10	1
1:A:264:LYS:HG2	1:C:509:ALA:HB1	0.57	1.76	6	2
1:A:342:GLY:HA2	1:A:345:ARG:HD2	0.57	1.76	7	1
3:A:11:PCW:H142	3:A:28:PCW:H341	0.57	1.74	1	1
3:A:47:PCW:H73	3:A:71:PCW:H19	0.57	1.75	4	1
1:C:448:VAL:O	1:C:452:VAL:HB	0.57	1.99	2	1
4:A:40:17F:H4	4:A:40:17F:N1	0.57	2.10	4	1
3:A:25:PCW:H11	3:A:31:PCW:H41	0.57	1.76	6	2
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.57	1.76	9	2
3:A:60:PCW:H421	3:A:63:PCW:H371	0.57	1.76	7	1
3:A:51:PCW:H132	3:A:71:PCW:H431	0.57	1.74	8	1
3:A:51:PCW:H62	3:A:71:PCW:H39	0.57	1.75	10	1
3:A:30:PCW:H71	4:A:34:17F:N1	0.57	2.15	8	1
1:A:288:ARG:O	1:A:292:HIS:HB2	0.57	2.00	6	2
3:A:45:PCW:H412	3:A:57:PCW:H61	0.57	1.77	6	1
2:B:22:GLN:O	2:B:26:ASN:HA	0.57	2.00	5	8
3:A:68:PCW:O2P	3:A:69:PCW:H41	0.57	2.00	9	1
3:A:43:PCW:H83	3:A:68:PCW:O1P	0.57	1.99	3	1
3:A:6:PCW:H39	3:A:16:PCW:H11	0.56	1.76	7	1
3:A:46:PCW:H322	3:A:71:PCW:H372	0.56	1.77	2	1
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.56	2.30	10	7
3:A:30:PCW:H71	4:A:37:17F:N1	0.56	2.07	10	1
4:A:79:17F:H9	4:A:79:17F:H18A	0.56	1.76	9	1
3:A:57:PCW:H72	4:A:80:17F:HN1A	0.56	1.59	4	1
1:A:279:LEU:HD13	1:C:495:LYS:HG2	0.56	1.76	4	1
3:A:2:PCW:H62	4:A:36:17F:H1A	0.56	1.77	6	1
1:C:502:GLU:HG2	1:C:506:ARG:HE	0.56	1.61	9	2
3:A:10:PCW:H331	3:A:21:PCW:H321	0.56	1.78	10	1
3:A:53:PCW:H321	3:A:68:PCW:H372	0.56	1.76	10	1
3:A:1:PCW:H39	4:A:33:17F:H39	0.56	1.77	6	1
3:A:15:PCW:H41	3:A:16:PCW:H131	0.56	1.77	1	1
3:A:19:PCW:H322	3:A:23:PCW:H332	0.56	1.77	6	1
1:C:454:PRO:HA	1:C:457:ASP:HB3	0.56	1.78	7	1
2:B:37:GLU:HG3	2:B:58:THR:HA	0.56	1.78	4	4
3:A:62:PCW:H351	3:A:72:PCW:H332	0.56	1.77	5	1
3:A:6:PCW:O1P	3:A:16:PCW:H11	0.56	2.01	9	1
3:A:57:PCW:H142	4:A:80:17F:H8A	0.56	1.76	9	1
1:C:465:GLU:O	1:C:469:LEU:HB2	0.56	2.01	1	1
3:A:49:PCW:H62	4:A:80:17F:HN1	0.55	1.60	8	1
3:A:66:PCW:H20	3:A:67:PCW:H71	0.55	1.77	10	1
3:A:14:PCW:H131	3:A:23:PCW:H41	0.55	1.78	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:9:PCW:O2P	3:A:14:PCW:H11	0.55	2.01	7	1
4:A:39:17F:H33	4:A:39:17F:H8	0.55	1.77	2	1
3:A:63:PCW:P	4:A:75:17F:N1	0.55	2.76	3	1
3:A:65:PCW:H121	4:A:80:17F:H62	0.55	1.78	5	1
3:A:3:PCW:H361	3:A:18:PCW:H12	0.55	1.78	4	1
3:A:6:PCW:H332	3:A:28:PCW:H41	0.55	1.77	3	1
1:A:308:ARG:CD	1:C:469:LEU:CG	0.55	2.76	9	1
3:A:10:PCW:H81	4:A:36:17F:N1	0.55	2.17	9	1
4:A:74:17F:H5	4:A:74:17F:H20A	0.55	1.78	9	1
1:C:495:LYS:O	1:C:499:LEU:HB2	0.55	2.01	2	3
1:A:244:SER:O	1:A:248:GLU:HB2	0.55	2.02	4	3
3:A:9:PCW:H142	3:A:11:PCW:H132	0.55	1.78	3	1
4:A:36:17F:H44	4:A:40:17F:H38	0.55	1.78	1	1
3:A:49:PCW:H151	3:A:57:PCW:H322	0.55	1.78	1	1
2:B:118:CYS:HB3	2:B:143:GLU:HG2	0.55	1.77	4	1
2:B:19:LEU:HD23	2:B:146:ALA:HB2	0.54	1.77	3	1
3:A:25:PCW:H2	3:A:31:PCW:H41	0.54	1.79	2	1
3:A:23:PCW:H39	3:A:29:PCW:H372	0.54	1.79	2	1
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.54	1.80	6	2
3:A:58:PCW:H31	3:A:61:PCW:H432	0.54	1.79	2	1
4:A:75:17F:H8	4:A:75:17F:H20A	0.54	1.79	9	1
1:C:466:GLU:HA	1:C:469:LEU:HD12	0.54	1.80	9	2
1:A:231:ASN:HA	1:A:234:LYS:CE	0.54	2.33	1	1
1:A:364:ALA:O	1:A:368:LEU:HB2	0.54	2.03	1	3
3:A:9:PCW:H252	3:A:11:PCW:H421	0.54	1.80	9	1
3:A:9:PCW:O4P	3:A:14:PCW:H322	0.54	2.03	2	1
3:A:53:PCW:H352	3:A:64:PCW:H141	0.54	1.79	1	1
1:C:528:ARG:HB3	1:C:532:ARG:NH2	0.53	2.17	6	1
3:A:26:PCW:H131	3:A:26:PCW:H372	0.53	1.78	9	1
3:A:42:PCW:O31	3:A:42:PCW:H41	0.53	2.03	4	1
3:A:5:PCW:H381	3:A:17:PCW:H81	0.53	1.80	1	1
3:A:16:PCW:H382	4:A:39:17F:H8A	0.53	1.80	10	1
3:A:4:PCW:H11	3:A:16:PCW:H62	0.53	1.79	9	1
3:A:58:PCW:H171	3:A:61:PCW:H381	0.53	1.78	9	1
3:A:53:PCW:H321	3:A:68:PCW:H332	0.53	1.80	9	1
3:A:63:PCW:H322	3:A:63:PCW:H51	0.53	1.80	4	1
1:A:212:SER:O	1:A:216:LYS:HG2	0.53	2.03	6	2
3:A:12:PCW:O2P	3:A:22:PCW:H32	0.53	2.03	9	1
1:C:517:HIS:O	1:C:521:TYR:HB2	0.53	2.04	9	1
3:A:54:PCW:H332	3:A:72:PCW:H132	0.53	1.80	3	1
3:A:6:PCW:H322	3:A:28:PCW:H2	0.53	1.78	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:447:GLU:OE1	1:C:451:LYS:HE2	0.53	2.03	8	2
3:A:43:PCW:H131	3:A:69:PCW:H332	0.53	1.79	6	1
4:A:33:17F:H39	4:A:35:17F:H32	0.53	1.81	7	1
4:A:36:17F:H4	4:A:36:17F:H1A	0.53	1.78	10	1
3:A:10:PCW:H371	3:A:10:PCW:H121	0.53	1.79	2	1
3:A:53:PCW:H382	3:A:64:PCW:H461	0.53	1.80	2	1
3:A:42:PCW:H31	3:A:69:PCW:H132	0.53	1.81	1	1
4:A:36:17F:H70	3:A:46:PCW:H451	0.53	1.81	6	1
3:A:66:PCW:H352	4:A:79:17F:H9A	0.53	1.80	1	1
2:B:33:ASP:HB3	2:B:36:ILE:HG13	0.52	1.81	4	3
3:A:58:PCW:H352	3:A:61:PCW:H382	0.52	1.80	5	1
3:A:1:PCW:H241	4:A:38:17F:H59	0.52	1.80	4	1
3:A:54:PCW:H142	3:A:72:PCW:H151	0.52	1.81	8	1
4:A:33:17F:H35	4:A:35:17F:H30	0.52	1.82	10	1
3:A:45:PCW:H381	3:A:57:PCW:H71	0.52	1.80	6	1
3:A:1:PCW:H222	4:A:38:17F:H33	0.52	1.81	4	1
3:A:15:PCW:H63	4:A:39:17F:O2	0.52	2.04	1	1
3:A:6:PCW:H31	3:A:16:PCW:H371	0.52	1.81	1	1
3:A:53:PCW:H121	3:A:56:PCW:H321	0.52	1.81	6	1
3:A:18:PCW:H42	3:A:23:PCW:O2P	0.52	2.05	5	1
3:A:13:PCW:H61	4:A:34:17F:O1	0.52	2.04	7	1
3:A:68:PCW:H63	3:A:70:PCW:H122	0.52	1.81	8	1
1:A:268:GLU:O	1:A:272:TYR:HB2	0.52	2.04	10	3
3:A:41:PCW:H121	3:A:61:PCW:H322	0.52	1.81	7	1
3:A:48:PCW:H121	3:A:54:PCW:H182	0.52	1.81	2	1
1:A:308:ARG:CG	1:C:469:LEU:CD1	0.52	2.87	9	1
3:A:58:PCW:H362	3:A:61:PCW:H382	0.52	1.81	7	1
3:A:58:PCW:H11	3:A:61:PCW:H412	0.52	1.81	2	1
1:A:334:ARG:HD3	1:C:440:GLU:HB3	0.52	1.82	6	1
1:A:236:THR:O	1:A:240:ARG:HB2	0.52	2.04	4	1
1:A:326:GLU:O	1:A:330:ARG:HG3	0.52	2.05	1	2
3:A:20:PCW:H412	3:A:31:PCW:H20	0.52	1.81	3	1
4:A:80:17F:H32	4:A:80:17F:H8	0.52	1.82	10	1
3:A:47:PCW:H61	3:A:57:PCW:O1P	0.52	2.04	8	1
1:A:310:ARG:O	1:A:314:ASP:HB2	0.52	2.05	10	3
1:C:561:LYS:HA	1:C:565:ALA:HB3	0.52	1.81	5	5
3:A:44:PCW:H321	3:A:68:PCW:H332	0.52	1.80	6	1
3:A:22:PCW:H42	3:A:27:PCW:H41	0.51	1.82	8	1
3:A:2:PCW:H51	3:A:5:PCW:H11	0.51	1.81	10	1
2:B:82:PHE:HB2	2:B:89:SER:HB2	0.51	1.82	10	1
1:A:334:ARG:HA	1:C:440:GLU:HG2	0.51	1.80	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:26:PCW:H322	3:A:28:PCW:H32	0.51	1.81	5	1
3:A:24:PCW:H121	4:A:39:17F:H31	0.51	1.83	6	1
3:A:17:PCW:H142	3:A:21:PCW:H32	0.51	1.83	1	1
3:A:25:PCW:H32	3:A:31:PCW:H321	0.51	1.82	1	1
3:A:28:PCW:H72	2:B:47:ASP:HB3	0.51	1.82	8	1
3:A:14:PCW:H382	4:A:34:17F:H10	0.51	1.82	7	1
3:A:25:PCW:H2	3:A:31:PCW:H73	0.51	1.80	8	1
3:A:27:PCW:H412	3:A:27:PCW:H142	0.51	1.81	2	1
1:A:315:ALA:O	1:A:319:HIS:HB2	0.51	2.06	3	1
3:A:60:PCW:H40	3:A:72:PCW:H261	0.51	1.82	3	1
1:A:249:GLU:O	1:A:253:LYS:HB2	0.51	2.04	1	1
3:A:49:PCW:H321	4:A:80:17F:H31	0.51	1.80	2	1
3:A:21:PCW:O1P	4:A:36:17F:H1	0.51	2.06	6	1
3:A:27:PCW:H73	4:A:37:17F:N1	0.51	2.21	1	1
1:A:279:LEU:HB3	1:C:495:LYS:HE3	0.51	1.83	8	2
3:A:1:PCW:H61	3:A:26:PCW:O2P	0.51	2.05	5	1
3:A:45:PCW:H162	4:A:74:17F:H11A	0.51	1.83	2	1
3:A:11:PCW:H371	3:A:16:PCW:H39	0.51	1.82	3	1
3:A:26:PCW:H121	4:A:40:17F:H33	0.51	1.83	5	1
3:A:49:PCW:H342	3:A:57:PCW:H382	0.51	1.82	6	1
3:A:27:PCW:H321	4:A:37:17F:H33	0.51	1.81	7	1
3:A:29:PCW:H122	3:A:31:PCW:H342	0.51	1.82	3	1
1:A:249:GLU:HB2	1:C:528:ARG:NH2	0.51	2.21	1	1
1:A:308:ARG:CB	1:C:469:LEU:HD11	0.51	2.36	5	2
1:C:508:ARG:O	1:C:512:ASP:HB3	0.51	2.06	4	2
3:A:55:PCW:H11	3:A:64:PCW:H2	0.51	1.83	9	1
3:A:4:PCW:H381	3:A:7:PCW:H262	0.51	1.83	4	1
1:A:224:VAL:O	1:A:228:PHE:HB2	0.51	2.05	3	3
3:A:15:PCW:H412	3:A:20:PCW:H232	0.51	1.83	2	1
1:C:410:SER:O	1:C:414:LYS:HG2	0.51	2.05	2	1
4:A:74:17F:H12	4:A:79:17F:H49	0.51	1.82	1	1
3:A:13:PCW:H141	3:A:18:PCW:H141	0.50	1.82	5	1
3:A:46:PCW:H82	4:A:73:17F:O1	0.50	2.07	6	1
3:A:72:PCW:H412	4:A:78:17F:H51	0.50	1.83	1	1
1:A:362:GLU:HB3	1:C:414:LYS:HD3	0.50	1.83	5	1
3:A:68:PCW:H2	3:A:69:PCW:H321	0.50	1.81	5	1
3:A:15:PCW:H321	3:A:16:PCW:H211	0.50	1.84	2	1
1:A:231:ASN:HA	1:A:234:LYS:HD2	0.50	1.84	6	1
3:A:20:PCW:H19	3:A:31:PCW:H241	0.50	1.83	9	1
3:A:10:PCW:H83	4:A:36:17F:N1	0.50	2.21	7	1
3:A:72:PCW:O31	3:A:72:PCW:H42	0.50	2.07	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:9:PCW:H63	3:A:30:PCW:O2P	0.50	2.07	5	1
2:B:5:LYS:HD2	2:B:75:GLY:HA2	0.50	1.82	6	1
3:A:25:PCW:H2	3:A:31:PCW:H42	0.50	1.82	7	1
3:A:58:PCW:H381	3:A:60:PCW:H122	0.50	1.84	4	1
3:A:42:PCW:H72	3:A:63:PCW:O1P	0.50	2.06	2	1
3:A:17:PCW:H322	3:A:17:PCW:H41	0.50	1.81	10	1
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.50	2.37	4	5
3:A:55:PCW:H63	3:A:64:PCW:O1P	0.50	2.07	6	1
1:C:469:LEU:O	1:C:473:LYS:HB2	0.50	2.06	2	2
4:A:39:17F:O4	2:B:136:SER:HA	0.50	2.06	3	1
3:A:63:PCW:H83	4:A:75:17F:O4	0.50	2.07	3	1
1:A:360:LEU:HA	1:A:363:LYS:HD2	0.50	1.82	6	1
3:A:7:PCW:H82	4:A:35:17F:N1	0.50	2.22	1	1
3:A:54:PCW:H2	3:A:60:PCW:H11	0.50	1.83	10	1
3:A:12:PCW:H82	3:A:22:PCW:O2P	0.50	2.07	5	1
1:A:372:ARG:O	1:A:376:LEU:HG	0.50	2.05	4	3
3:A:12:PCW:H62	3:A:22:PCW:O2P	0.50	2.06	9	1
3:A:9:PCW:H81	4:A:34:17F:O5	0.50	2.06	3	1
3:A:49:PCW:H2	3:A:57:PCW:H62	0.50	1.83	5	1
1:A:330:ARG:HH22	1:C:448:VAL:HG23	0.50	1.66	10	1
1:A:289:GLN:O	1:A:293:GLU:HG2	0.50	2.07	5	1
4:A:33:17F:H1	4:A:33:17F:C4	0.50	2.37	9	4
3:A:3:PCW:H361	3:A:18:PCW:H342	0.49	1.82	6	1
3:A:1:PCW:H472	3:A:43:PCW:H262	0.49	1.83	7	1
3:A:18:PCW:O1P	3:A:23:PCW:H61	0.49	2.07	2	1
4:A:35:17F:H33	4:A:35:17F:H11A	0.49	1.83	2	1
3:A:14:PCW:H252	4:A:37:17F:H48	0.49	1.85	8	1
3:A:6:PCW:P	3:A:16:PCW:O1P	0.49	2.70	10	1
1:A:363:LYS:HD2	1:C:411:THR:HG23	0.49	1.82	10	1
2:B:37:GLU:HB2	2:B:59:ALA:HB2	0.49	1.84	5	1
4:A:33:17F:N1	4:A:33:17F:P1	0.49	2.84	9	3
3:A:48:PCW:H372	3:A:54:PCW:H231	0.49	1.84	4	1
3:A:25:PCW:H321	3:A:25:PCW:H51	0.49	1.84	2	1
3:A:14:PCW:O11	3:A:23:PCW:H42	0.49	2.06	8	2
4:A:33:17F:H35	4:A:35:17F:H34	0.49	1.84	6	1
3:A:62:PCW:O1P	3:A:72:PCW:H83	0.49	2.08	7	1
4:A:76:17F:H20A	4:A:76:17F:H11A	0.49	1.83	10	1
1:C:421:PRO:O	1:C:425:GLU:HG2	0.49	2.06	10	1
3:A:58:PCW:H12	3:A:61:PCW:H351	0.49	1.85	2	1
3:A:24:PCW:H121	3:A:25:PCW:H141	0.49	1.84	8	1
3:A:32:PCW:H61	4:A:38:17F:N1	0.49	2.14	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:25:PCW:H222	3:A:67:PCW:H472	0.49	1.84	10	1
2:B:126:ASP:OD2	2:B:128:LYS:HG3	0.49	2.07	5	1
3:A:55:PCW:H2	4:A:77:17F:H2	0.49	1.85	3	1
1:C:461:LYS:O	1:C:465:GLU:HG3	0.49	2.07	8	1
3:A:50:PCW:H39	3:A:72:PCW:H81	0.49	1.83	5	1
3:A:41:PCW:H81	3:A:59:PCW:O1P	0.49	2.07	7	1
4:A:33:17F:C4	4:A:33:17F:H1	0.49	2.37	2	1
3:A:5:PCW:H411	3:A:17:PCW:H331	0.49	1.83	3	1
3:A:7:PCW:H82	4:A:35:17F:HN1A	0.49	1.67	1	1
3:A:53:PCW:H81	3:A:69:PCW:O1P	0.49	2.08	3	1
1:A:365:LYS:HB2	1:A:366:PRO:CD	0.49	2.31	9	1
3:A:48:PCW:H71	3:A:61:PCW:H411	0.49	1.82	7	1
3:A:17:PCW:H72	4:A:38:17F:O2	0.49	2.08	2	1
3:A:49:PCW:H472	4:A:80:17F:H47	0.49	1.85	2	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.49	1.85	8	3
3:A:7:PCW:H42	4:A:33:17F:H4	0.49	1.85	10	1
3:A:50:PCW:H121	4:A:78:17F:H4A	0.49	1.85	5	1
3:A:70:PCW:H421	3:A:71:PCW:H472	0.49	1.84	6	1
3:A:17:PCW:H81	4:A:38:17F:O1	0.49	2.07	9	1
2:B:17:SER:HB3	2:B:32:TYR:CE1	0.49	2.43	9	1
3:A:50:PCW:H352	4:A:78:17F:H62	0.49	1.84	7	1
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.48	1.84	5	2
3:A:8:PCW:H81	3:A:22:PCW:O1P	0.48	2.07	4	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.48	1.85	1	1
1:A:359:THR:HA	1:A:362:GLU:HB2	0.48	1.84	7	1
3:A:25:PCW:H152	3:A:31:PCW:H322	0.48	1.83	4	1
3:A:46:PCW:H361	3:A:70:PCW:H40	0.48	1.84	4	1
3:A:66:PCW:H32	4:A:79:17F:O1	0.48	2.08	2	1
4:A:38:17F:H10	4:A:38:17F:H60	0.48	1.85	3	1
1:C:465:GLU:HB3	1:C:469:LEU:HD11	0.48	1.84	10	1
3:A:49:PCW:H332	3:A:57:PCW:H371	0.48	1.84	5	1
3:A:10:PCW:H332	3:A:21:PCW:H341	0.48	1.85	4	1
1:C:458:ASP:O	1:C:462:LYS:HG2	0.48	2.08	1	2
3:A:22:PCW:H182	3:A:27:PCW:H431	0.48	1.85	4	1
3:A:53:PCW:H82	3:A:68:PCW:H332	0.48	1.85	2	1
3:A:4:PCW:H242	3:A:32:PCW:H252	0.48	1.86	4	1
3:A:6:PCW:H132	3:A:11:PCW:H322	0.48	1.85	1	1
3:A:20:PCW:H332	3:A:31:PCW:H132	0.48	1.85	10	1
3:A:3:PCW:H122	3:A:3:PCW:H352	0.48	1.85	5	1
4:A:74:17F:H12	4:A:79:17F:H8	0.48	1.84	5	1
1:C:586:SER:O	1:C:590:GLU:HG3	0.48	2.07	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:514:LEU:HA	1:C:517:HIS:HB2	0.48	1.85	4	1
3:A:55:PCW:H71	3:A:64:PCW:O1P	0.48	2.09	3	1
3:A:67:PCW:H172	4:A:75:17F:H56	0.48	1.86	3	1
1:A:234:LYS:HE3	1:C:539:ASN:OD1	0.48	2.09	1	1
3:A:5:PCW:H51	3:A:5:PCW:H2	0.48	1.84	8	1
3:A:14:PCW:H211	4:A:34:17F:H19	0.48	1.85	4	1
1:A:327:LEU:HD23	1:A:330:ARG:HD3	0.48	1.86	1	1
4:A:74:17F:H9	4:A:74:17F:H18A	0.48	1.86	9	1
3:A:12:PCW:H32	3:A:22:PCW:H12	0.48	1.85	8	1
3:A:24:PCW:O1P	3:A:25:PCW:H31	0.48	2.09	8	1
3:A:47:PCW:H411	4:A:73:17F:H9	0.48	1.86	8	1
3:A:12:PCW:H73	3:A:22:PCW:O2P	0.48	2.09	5	1
1:A:335:LEU:O	1:A:339:LYS:HB2	0.48	2.08	9	1
3:A:3:PCW:H61	3:A:19:PCW:O2P	0.48	2.08	7	1
3:A:29:PCW:H182	3:A:31:PCW:H71	0.48	1.86	2	1
4:A:33:17F:P1	4:A:33:17F:N1	0.48	2.87	2	2
1:C:455:TYR:O	1:C:459:PHE:HB2	0.48	2.08	2	2
1:A:341:ASN:HD21	1:C:433:GLU:HG2	0.48	1.69	5	1
1:C:491:GLU:O	1:C:495:LYS:HG3	0.48	2.09	5	2
1:A:242:GLU:HB3	1:C:532:ARG:NH2	0.48	2.24	6	1
3:A:55:PCW:H381	3:A:55:PCW:H142	0.48	1.84	6	1
3:A:21:PCW:H361	3:A:21:PCW:H122	0.48	1.86	9	1
3:A:13:PCW:H141	3:A:18:PCW:H122	0.48	1.86	7	1
3:A:7:PCW:O2P	3:A:16:PCW:H42	0.48	2.08	4	1
3:A:30:PCW:H321	4:A:40:17F:H20A	0.48	1.85	2	1
1:A:301:LEU:HB3	1:C:473:LYS:HE2	0.47	1.86	8	1
4:A:77:17F:H9	4:A:77:17F:O10	0.47	2.09	8	1
3:A:68:PCW:H2	3:A:69:PCW:H342	0.47	1.85	6	1
3:A:10:PCW:H362	3:A:22:PCW:H432	0.47	1.85	2	1
3:A:17:PCW:H252	4:A:36:17F:H63	0.47	1.85	1	1
3:A:25:PCW:H132	3:A:31:PCW:H321	0.47	1.85	8	1
1:C:458:ASP:HA	1:C:461:LYS:HD2	0.47	1.85	6	2
3:A:13:PCW:H62	4:A:34:17F:O9	0.47	2.08	2	1
3:A:48:PCW:H362	3:A:54:PCW:H382	0.47	1.86	5	1
3:A:9:PCW:H81	3:A:30:PCW:O2P	0.47	2.10	1	1
1:C:483:GLU:O	1:C:487:GLN:HG3	0.47	2.09	10	1
3:A:11:PCW:H83	3:A:24:PCW:O2P	0.47	2.09	5	1
3:A:5:PCW:H132	3:A:17:PCW:H342	0.47	1.84	5	1
3:A:42:PCW:H52	4:A:75:17F:H2	0.47	1.85	9	1
3:A:8:PCW:H171	3:A:27:PCW:H241	0.47	1.85	9	1
3:A:45:PCW:H211	3:A:49:PCW:H162	0.47	1.86	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:48:PCW:H162	3:A:54:PCW:H182	0.47	1.86	1	1
1:C:444:ASP:O	1:C:448:VAL:HB	0.47	2.09	7	2
3:A:55:PCW:H142	3:A:55:PCW:H381	0.47	1.86	10	1
3:A:70:PCW:H2	3:A:70:PCW:O4P	0.47	2.09	5	1
3:A:51:PCW:H361	3:A:70:PCW:H182	0.47	1.85	4	1
3:A:58:PCW:H12	3:A:61:PCW:H412	0.47	1.87	3	1
3:A:13:PCW:H19	3:A:18:PCW:H262	0.47	1.86	10	1
3:A:17:PCW:O1P	4:A:36:17F:H6	0.47	2.10	10	1
3:A:57:PCW:H121	4:A:80:17F:H6	0.47	1.87	5	1
3:A:15:PCW:H31	3:A:16:PCW:H181	0.47	1.86	7	1
3:A:17:PCW:H162	4:A:36:17F:H32	0.47	1.86	3	1
3:A:15:PCW:H81	4:A:39:17F:N1	0.47	2.25	3	1
3:A:65:PCW:H221	4:A:80:17F:H37	0.47	1.85	1	1
1:A:356:HIS:O	1:A:360:LEU:HB2	0.47	2.09	6	2
3:A:41:PCW:H71	4:A:77:17F:HN1A	0.47	1.70	9	1
2:B:41:ARG:HA	2:B:53:LEU:O	0.47	2.09	4	1
3:A:12:PCW:H371	3:A:21:PCW:H321	0.47	1.84	2	1
3:A:10:PCW:H61	3:A:12:PCW:O31	0.47	2.08	3	1
3:A:20:PCW:H452	3:A:31:PCW:H261	0.47	1.86	3	1
3:A:6:PCW:H73	3:A:28:PCW:H73	0.47	1.86	3	1
3:A:50:PCW:H12	4:A:78:17F:H4	0.47	1.86	3	1
3:A:27:PCW:H41	4:A:37:17F:P1	0.47	2.49	1	1
1:A:387:LEU:O	1:A:391:GLU:HG3	0.47	2.09	2	2
1:C:563:LYS:O	1:C:567:GLU:HG2	0.47	2.09	7	2
2:B:126:ASP:HB3	2:B:129:GLN:HG3	0.47	1.85	6	1
1:A:287:ALA:HA	1:A:290:LYS:HD2	0.47	1.86	9	1
3:A:27:PCW:H82	4:A:37:17F:O2	0.47	2.10	6	1
3:A:16:PCW:H152	4:A:39:17F:H58	0.47	1.87	9	1
3:A:48:PCW:H142	3:A:54:PCW:H181	0.47	1.85	7	1
3:A:9:PCW:H152	4:A:34:17F:H37	0.47	1.85	4	1
3:A:9:PCW:H41	2:B:49:GLU:HG3	0.47	1.86	2	1
3:A:68:PCW:O31	3:A:69:PCW:H61	0.47	2.09	6	1
3:A:60:PCW:H472	3:A:63:PCW:H422	0.47	1.87	9	1
3:A:30:PCW:H83	4:A:34:17F:HN1	0.47	1.70	4	1
3:A:49:PCW:H351	4:A:80:17F:H31	0.47	1.86	4	1
4:A:75:17F:H11	4:A:75:17F:H20	0.47	1.85	3	1
1:C:473:LYS:O	1:C:477:LEU:HB2	0.46	2.11	10	2
4:A:74:17F:H46	4:A:75:17F:H36	0.46	1.86	6	1
1:C:442:SER:O	1:C:446:GLU:HG3	0.46	2.09	6	1
3:A:1:PCW:H322	3:A:5:PCW:H371	0.46	1.88	7	1
3:A:59:PCW:H82	3:A:59:PCW:O31	0.46	2.10	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:24:PCW:H62	4:A:39:17F:O1	0.46	2.11	1	1
3:A:72:PCW:H431	4:A:78:17F:H47	0.46	1.87	10	1
3:A:32:PCW:H342	4:A:33:17F:H60	0.46	1.87	5	1
3:A:9:PCW:H31	3:A:14:PCW:H361	0.46	1.87	5	1
3:A:30:PCW:H142	3:A:30:PCW:H382	0.46	1.87	9	1
3:A:31:PCW:H52	3:A:31:PCW:O31	0.46	2.10	2	2
1:A:308:ARG:HG3	1:C:469:LEU:CD2	0.46	2.39	2	2
3:A:48:PCW:H321	3:A:54:PCW:H132	0.46	1.87	10	1
1:A:260:ASP:HA	1:A:263:LYS:HE3	0.46	1.87	5	1
3:A:9:PCW:H72	3:A:30:PCW:O2P	0.46	2.11	3	2
3:A:45:PCW:H241	4:A:74:17F:H40	0.46	1.87	3	1
1:A:310:ARG:O	1:A:314:ASP:HB3	0.46	2.11	1	1
3:A:13:PCW:H182	3:A:23:PCW:H162	0.46	1.88	8	1
3:A:16:PCW:H121	4:A:39:17F:H9A	0.46	1.87	6	1
3:A:13:PCW:H121	3:A:23:PCW:H142	0.46	1.87	9	1
1:A:337:ALA:O	1:A:341:ASN:HB2	0.46	2.10	9	1
2:B:78:PHE:O	2:B:111:MET:HA	0.46	2.10	9	3
1:C:478:ARG:O	1:C:482:GLN:HB2	0.46	2.10	5	3
3:A:59:PCW:H2	4:A:77:17F:H8	0.46	1.88	5	1
3:A:15:PCW:H51	4:A:39:17F:N1	0.46	2.26	6	1
3:A:26:PCW:H441	4:A:33:17F:H46	0.46	1.86	7	1
4:A:39:17F:H58	4:A:39:17F:H10	0.46	1.86	2	1
3:A:67:PCW:H41	3:A:67:PCW:C31	0.46	2.41	2	1
4:A:74:17F:H38	4:A:75:17F:H10	0.46	1.88	8	1
2:B:17:SER:HA	2:B:20:THR:OG1	0.46	2.11	7	1
1:A:203:LEU:O	1:A:207:TRP:HB2	0.46	2.11	10	2
1:A:255:GLN:HB2	1:A:256:PRO:HD3	0.46	1.88	4	4
2:B:94:HIS:O	2:B:98:GLU:HG2	0.46	2.11	6	1
3:A:48:PCW:H371	3:A:54:PCW:H382	0.46	1.88	3	1
3:A:14:PCW:H162	4:A:34:17F:H18A	0.46	1.88	9	1
4:A:37:17F:O5	2:B:135:ARG:HD3	0.46	2.10	9	1
3:A:5:PCW:H12	3:A:17:PCW:H321	0.46	1.88	3	2
3:A:10:PCW:N	4:A:36:17F:N1	0.46	2.61	3	1
3:A:49:PCW:O2P	3:A:57:PCW:H62	0.46	2.10	3	1
3:A:60:PCW:H411	3:A:62:PCW:H481	0.46	1.87	6	1
3:A:47:PCW:H61	4:A:74:17F:O1	0.46	2.10	9	1
1:A:312:HIS:HE1	1:C:465:GLU:HB2	0.46	1.71	1	2
3:A:52:PCW:H441	3:A:69:PCW:H442	0.46	1.88	7	1
3:A:56:PCW:O1P	3:A:70:PCW:H41	0.45	2.11	8	1
3:A:30:PCW:H332	4:A:40:17F:H57	0.45	1.88	10	1
3:A:7:PCW:H41	4:A:33:17F:H8	0.45	1.88	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:6:PCW:H342	3:A:16:PCW:H321	0.45	1.87	6	1
3:A:10:PCW:H83	4:A:36:17F:HN1	0.45	1.69	7	1
2:B:92:ASP:O	2:B:95:HIS:HB3	0.45	2.11	7	1
3:A:3:PCW:H342	3:A:23:PCW:H322	0.45	1.86	4	1
2:B:24:ILE:HG13	2:B:40:TYR:HB3	0.45	1.87	4	1
1:C:560:GLU:O	1:C:564:PRO:HD2	0.45	2.10	2	1
3:A:5:PCW:H332	4:A:38:17F:O9	0.45	2.11	8	1
3:A:1:PCW:H71	3:A:26:PCW:O2P	0.45	2.11	5	1
3:A:41:PCW:H71	4:A:77:17F:H1A	0.45	1.87	6	1
3:A:4:PCW:H51	3:A:7:PCW:O1P	0.45	2.11	6	1
3:A:22:PCW:H52	3:A:22:PCW:H2	0.45	1.88	4	1
1:C:559:SER:HA	1:C:562:ALA:HB3	0.45	1.88	2	1
3:A:16:PCW:H271	3:A:24:PCW:H452	0.45	1.88	1	1
3:A:57:PCW:H19	4:A:80:17F:H12	0.45	1.88	1	1
3:A:46:PCW:H62	4:A:73:17F:N1	0.45	2.27	8	1
3:A:2:PCW:H342	3:A:5:PCW:H151	0.45	1.87	6	1
3:A:49:PCW:H321	3:A:57:PCW:H322	0.45	1.88	9	1
3:A:17:PCW:H42	2:B:45:VAL:HB	0.45	1.88	9	1
3:A:15:PCW:H81	4:A:39:17F:HN1A	0.45	1.71	3	1
1:A:246:ASP:HA	1:C:528:ARG:CZ	0.45	2.41	3	1
3:A:51:PCW:H2	3:A:71:PCW:H422	0.45	1.87	1	1
3:A:45:PCW:H152	4:A:74:17F:H11A	0.45	1.87	10	1
3:A:16:PCW:H122	4:A:39:17F:H9A	0.45	1.88	5	1
1:A:272:TYR:O	1:A:276:VAL:HB	0.45	2.11	7	1
3:A:55:PCW:H71	3:A:64:PCW:H12	0.45	1.87	3	1
3:A:16:PCW:O31	3:A:16:PCW:H41	0.45	2.11	5	1
3:A:47:PCW:H171	4:A:73:17F:H32	0.45	1.87	2	1
3:A:41:PCW:H242	3:A:58:PCW:H422	0.45	1.88	1	1
2:B:56:LEU:HB2	2:B:71:TYR:CD2	0.45	2.46	7	3
1:C:565:ALA:O	1:C:569:LEU:HG	0.45	2.10	4	1
3:A:43:PCW:H482	3:A:70:PCW:H152	0.45	1.87	2	1
1:A:330:ARG:NH2	1:C:444:ASP:HA	0.45	2.27	1	1
3:A:25:PCW:O31	3:A:31:PCW:H82	0.45	2.11	10	1
3:A:17:PCW:H232	4:A:36:17F:H33	0.45	1.87	5	1
3:A:48:PCW:H81	3:A:61:PCW:H411	0.45	1.89	6	1
3:A:62:PCW:H451	3:A:72:PCW:H231	0.45	1.88	6	1
3:A:11:PCW:H251	3:A:67:PCW:H442	0.45	1.89	9	1
3:A:2:PCW:O1P	3:A:17:PCW:H11	0.45	2.11	7	1
3:A:66:PCW:H20	3:A:67:PCW:H81	0.45	1.88	7	1
3:A:67:PCW:H181	4:A:75:17F:H58	0.45	1.88	1	1
3:A:10:PCW:H71	4:A:36:17F:HN1A	0.45	1.71	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:4:PCW:H52	3:A:7:PCW:O1P	0.45	2.12	3	1
1:C:491:GLU:HB3	1:C:495:LYS:HE2	0.45	1.87	3	1
1:C:554:HIS:HA	1:C:557:THR:OG1	0.45	2.12	1	1
1:A:257:TYR:O	1:A:261:PHE:HB2	0.45	2.12	6	1
1:C:535:ALA:O	1:C:539:ASN:HB2	0.45	2.12	2	1
3:A:26:PCW:H142	3:A:28:PCW:H122	0.45	1.89	1	1
3:A:32:PCW:H122	4:A:33:17F:H20	0.45	1.86	1	1
3:A:3:PCW:H81	3:A:19:PCW:O11	0.45	2.11	6	1
3:A:42:PCW:N	4:A:75:17F:N1	0.45	2.64	6	1
3:A:48:PCW:H42	3:A:58:PCW:O2P	0.45	2.12	4	1
3:A:3:PCW:H181	3:A:19:PCW:H251	0.45	1.89	3	1
3:A:5:PCW:H52	3:A:5:PCW:O31	0.45	2.12	3	1
3:A:69:PCW:O11	3:A:69:PCW:H82	0.45	2.12	3	1
3:A:7:PCW:H483	3:A:52:PCW:H40	0.44	1.89	8	1
3:A:2:PCW:H51	3:A:5:PCW:C1	0.44	2.41	10	1
1:A:277:GLU:HB2	1:A:278:PRO:CD	0.44	2.42	6	2
3:A:6:PCW:H31	3:A:11:PCW:O2P	0.44	2.12	7	1
3:A:64:PCW:H161	3:A:64:PCW:H412	0.44	1.89	4	1
1:C:427:TRP:O	1:C:431:GLU:HG2	0.44	2.12	1	2
3:A:42:PCW:H462	3:A:52:PCW:H421	0.44	1.89	3	1
3:A:43:PCW:O11	3:A:43:PCW:H82	0.44	2.12	1	1
3:A:3:PCW:O2P	3:A:23:PCW:H51	0.44	2.12	4	1
1:C:475:GLU:HB2	1:C:476:PRO:HD3	0.44	1.89	2	1
2:B:6:LEU:O	2:B:55:ILE:HA	0.44	2.12	10	1
1:A:330:ARG:NH2	1:C:451:LYS:HD2	0.44	2.27	7	1
1:A:378:VAL:O	1:A:382:PHE:HB2	0.44	2.12	4	1
3:A:49:PCW:H322	3:A:57:PCW:H352	0.44	1.88	4	1
3:A:1:PCW:N	4:A:35:17F:N1	0.44	2.64	6	1
3:A:42:PCW:H421	3:A:52:PCW:H471	0.44	1.88	9	1
3:A:55:PCW:H72	3:A:64:PCW:O11	0.44	2.12	9	1
3:A:6:PCW:O2P	3:A:6:PCW:N	0.44	2.50	4	2
3:A:57:PCW:H152	4:A:76:17F:H29	0.44	1.90	1	1
1:C:570:ARG:O	1:C:574:LEU:HG	0.44	2.11	1	1
3:A:46:PCW:H121	3:A:71:PCW:H39	0.44	1.88	2	1
3:A:8:PCW:H332	3:A:27:PCW:H172	0.44	1.90	3	1
1:C:456:LEU:O	1:C:460:GLN:HB2	0.44	2.11	8	4
1:C:550:LYS:HA	1:C:553:GLU:OE1	0.44	2.13	8	2
3:A:11:PCW:H82	3:A:24:PCW:O2P	0.44	2.12	10	1
3:A:30:PCW:H63	4:A:34:17F:O2	0.44	2.13	10	1
3:A:67:PCW:O31	3:A:67:PCW:H42	0.44	2.12	10	1
4:A:39:17F:H12	4:A:39:17F:H65	0.44	1.89	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:43:PCW:O11	3:A:43:PCW:H41	0.44	2.13	6	1
3:A:16:PCW:H151	4:A:39:17F:H11A	0.44	1.88	8	1
3:A:42:PCW:H122	3:A:67:PCW:H212	0.44	1.89	5	1
3:A:52:PCW:H232	3:A:58:PCW:H461	0.44	1.89	5	1
3:A:5:PCW:H83	4:A:38:17F:H6	0.44	1.88	2	1
3:A:18:PCW:H441	3:A:23:PCW:H221	0.44	1.89	3	1
3:A:6:PCW:P	4:A:39:17F:O2	0.44	2.75	3	1
1:A:363:LYS:HD3	1:C:411:THR:HG23	0.44	1.87	1	1
3:A:3:PCW:H321	3:A:23:PCW:H12	0.44	1.90	6	1
1:A:260:ASP:HA	1:A:263:LYS:CE	0.44	2.30	6	1
1:A:363:LYS:O	1:A:367:ALA:HB3	0.44	2.11	4	3
3:A:29:PCW:H232	3:A:31:PCW:H382	0.44	1.90	9	1
3:A:14:PCW:H152	4:A:34:17F:H1A	0.44	1.90	9	1
3:A:1:PCW:H281	3:A:17:PCW:H441	0.44	1.88	2	1
2:B:116:ASN:HA	2:B:144:THR:O	0.44	2.13	4	1
3:A:12:PCW:O1P	3:A:22:PCW:H11	0.44	2.13	2	1
3:A:10:PCW:H122	3:A:10:PCW:H372	0.44	1.89	1	1
1:A:268:GLU:OE1	1:C:506:ARG:HD3	0.43	2.13	8	1
1:A:336:GLU:O	1:A:340:GLU:HG2	0.43	2.12	4	1
3:A:4:PCW:H83	4:A:33:17F:HN1A	0.43	1.73	4	1
3:A:53:PCW:O2P	3:A:55:PCW:H62	0.43	2.13	2	1
3:A:13:PCW:H81	4:A:37:17F:H1	0.43	1.89	3	1
1:C:539:ASN:HB3	1:C:543:ARG:HH21	0.43	1.73	8	1
3:A:42:PCW:O11	3:A:42:PCW:H51	0.43	2.14	10	1
3:A:2:PCW:H73	3:A:21:PCW:O1P	0.43	2.13	5	1
3:A:52:PCW:O1P	3:A:60:PCW:H73	0.43	2.12	5	1
3:A:50:PCW:H82	4:A:78:17F:O1	0.43	2.13	6	1
3:A:12:PCW:H121	3:A:30:PCW:H211	0.43	1.89	9	1
3:A:68:PCW:O2P	3:A:69:PCW:H73	0.43	2.12	9	1
3:A:7:PCW:H362	4:A:33:17F:H11	0.43	1.89	9	1
3:A:52:PCW:H131	3:A:60:PCW:H11	0.43	1.89	7	1
3:A:6:PCW:P	3:A:11:PCW:O2P	0.43	2.76	2	1
3:A:41:PCW:H242	3:A:61:PCW:H481	0.43	1.89	5	1
3:A:5:PCW:H381	3:A:17:PCW:H61	0.43	1.89	7	1
3:A:51:PCW:H11	3:A:71:PCW:H421	0.43	1.90	7	1
3:A:48:PCW:H361	3:A:54:PCW:H431	0.43	1.90	2	1
3:A:68:PCW:H331	3:A:69:PCW:H342	0.43	1.89	2	1
3:A:14:PCW:H121	4:A:34:17F:H34	0.43	1.90	1	1
1:A:275:LYS:O	1:A:279:LEU:HB2	0.43	2.12	10	1
3:A:43:PCW:H83	4:A:74:17F:HN1A	0.43	1.73	10	1
1:A:278:PRO:O	1:A:282:GLU:HG3	0.43	2.13	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:3:PCW:H382	3:A:3:PCW:H161	0.43	1.90	6	1
1:C:560:GLU:O	1:C:564:PRO:HG2	0.43	2.13	6	1
3:A:58:PCW:H362	3:A:61:PCW:H351	0.43	1.91	9	1
1:A:338:LEU:HA	1:A:345:ARG:HH12	0.43	1.72	7	1
3:A:16:PCW:O11	3:A:16:PCW:H51	0.43	2.14	4	1
3:A:70:PCW:H181	3:A:70:PCW:H332	0.43	1.90	4	1
3:A:7:PCW:H73	4:A:35:17F:N1	0.43	2.24	1	1
3:A:12:PCW:H73	3:A:30:PCW:O11	0.43	2.14	8	1
1:C:417:GLU:O	1:C:421:PRO:HD2	0.43	2.12	6	4
3:A:21:PCW:H331	3:A:22:PCW:H441	0.43	1.91	9	1
3:A:17:PCW:O1P	3:A:17:PCW:H31	0.43	2.12	4	1
1:A:254:VAL:HA	1:A:257:TYR:HB2	0.43	1.89	3	1
3:A:31:PCW:O31	3:A:31:PCW:H62	0.43	2.14	8	1
3:A:3:PCW:C7	3:A:19:PCW:H2	0.43	2.43	5	1
1:A:264:LYS:CG	1:C:509:ALA:HB1	0.43	2.43	6	1
3:A:25:PCW:O2P	3:A:31:PCW:H51	0.43	2.14	9	1
3:A:62:PCW:H122	3:A:72:PCW:H131	0.43	1.91	7	1
1:C:561:LYS:O	1:C:565:ALA:HB3	0.43	2.14	7	1
1:A:349:TYR:HB3	3:A:2:PCW:H252	0.43	1.90	2	1
3:A:63:PCW:H32	4:A:75:17F:N1	0.43	2.29	10	1
3:A:18:PCW:H371	3:A:19:PCW:H172	0.43	1.89	5	1
3:A:25:PCW:O31	3:A:31:PCW:H12	0.43	2.13	9	1
1:A:359:THR:HG21	1:C:418:GLN:HB2	0.43	1.89	9	2
3:A:27:PCW:H161	3:A:27:PCW:H371	0.43	1.90	4	1
3:A:20:PCW:H31	3:A:31:PCW:H12	0.43	1.90	2	1
3:A:13:PCW:H122	3:A:23:PCW:C3	0.43	2.44	8	1
3:A:7:PCW:O2P	3:A:16:PCW:H83	0.43	2.13	8	1
1:C:426:PHE:O	1:C:430:LEU:HG	0.43	2.14	10	1
3:A:57:PCW:H452	4:A:79:17F:H38	0.43	1.90	6	1
3:A:30:PCW:H71	2:B:138:GLY:O	0.43	2.13	9	1
3:A:71:PCW:H342	3:A:71:PCW:H131	0.43	1.91	4	1
2:B:41:ARG:HG2	2:B:54:ASP:HA	0.43	1.91	2	1
3:A:20:PCW:H172	3:A:20:PCW:H411	0.43	1.90	1	1
3:A:26:PCW:H342	4:A:40:17F:H56	0.43	1.91	1	1
3:A:68:PCW:O1P	3:A:69:PCW:H41	0.43	2.14	6	1
3:A:53:PCW:H371	3:A:68:PCW:H422	0.43	1.89	7	1
1:A:289:GLN:O	1:A:293:GLU:HB2	0.43	2.14	3	1
1:C:502:GLU:O	1:C:506:ARG:HG3	0.43	2.14	3	2
1:A:202:LYS:NZ	1:C:576:VAL:HG21	0.43	2.29	3	1
4:A:38:17F:H18	4:A:38:17F:H9A	0.43	1.91	8	1
1:A:280:ARG:O	1:A:284:GLN:HB2	0.43	2.13	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:43:PCW:H411	3:A:47:PCW:H71	0.43	1.89	7	1
3:A:3:PCW:H251	3:A:19:PCW:H211	0.42	1.91	6	1
1:A:308:ARG:HD3	1:C:465:GLU:HB3	0.42	1.90	9	1
1:C:445:LEU:O	1:C:449:LYS:HG3	0.42	2.13	9	1
3:A:14:PCW:H121	4:A:34:17F:O10	0.42	2.14	7	1
1:C:489:LEU:O	1:C:493:GLN:HG3	0.42	2.14	4	1
3:A:42:PCW:H41	3:A:42:PCW:O31	0.42	2.13	2	1
2:B:35:THR:HG22	2:B:61:GLN:HG2	0.42	1.90	1	1
3:A:32:PCW:H63	4:A:35:17F:O1	0.42	2.14	8	1
3:A:54:PCW:H72	3:A:62:PCW:O2P	0.42	2.13	8	1
3:A:41:PCW:H31	3:A:52:PCW:H352	0.42	1.90	4	1
1:C:524:GLU:HB3	1:C:528:ARG:NH2	0.42	2.29	2	1
1:C:543:ARG:O	1:C:547:TYR:HB2	0.42	2.13	3	1
1:A:293:GLU:O	1:A:297:LYS:HG2	0.42	2.15	2	1
3:A:5:PCW:H481	4:A:36:17F:H45	0.42	1.91	1	1
4:A:39:17F:H8	4:A:39:17F:H33	0.42	1.91	8	1
3:A:50:PCW:H31	4:A:78:17F:H4	0.42	1.92	10	1
3:A:42:PCW:H121	3:A:67:PCW:H283	0.42	1.90	5	1
3:A:5:PCW:H451	3:A:17:PCW:H141	0.42	1.92	5	1
1:A:383:LYS:O	1:A:387:LEU:HB2	0.42	2.14	2	1
3:A:54:PCW:H352	3:A:72:PCW:H132	0.42	1.90	2	1
4:A:79:17F:H31	4:A:79:17F:H11A	0.42	1.91	2	1
3:A:48:PCW:H422	3:A:54:PCW:H261	0.42	1.91	1	1
3:A:48:PCW:H362	3:A:54:PCW:H172	0.42	1.91	10	1
2:B:6:LEU:HA	2:B:77:GLY:O	0.42	2.14	10	1
3:A:32:PCW:H63	4:A:38:17F:O4	0.42	2.14	9	1
1:C:563:LYS:O	1:C:567:GLU:HB2	0.42	2.14	9	1
3:A:4:PCW:H51	3:A:7:PCW:O11	0.42	2.14	7	1
2:B:56:LEU:HB2	2:B:71:TYR:HD2	0.42	1.74	7	1
4:A:36:17F:H73	3:A:51:PCW:H232	0.42	1.91	4	1
3:A:32:PCW:H332	4:A:35:17F:H10A	0.42	1.91	2	1
1:C:574:LEU:HB2	1:C:575:PRO:CD	0.42	2.44	1	1
1:A:380:GLU:O	1:A:384:VAL:HG23	0.42	2.15	4	3
3:A:5:PCW:H12	3:A:17:PCW:O2P	0.42	2.15	5	1
3:A:23:PCW:N	4:A:34:17F:N1	0.42	2.67	9	1
3:A:9:PCW:H462	4:A:34:17F:H67	0.42	1.92	6	1
3:A:49:PCW:H131	4:A:79:17F:H50	0.42	1.91	7	1
3:A:30:PCW:H142	4:A:40:17F:H4	0.42	1.91	2	1
1:A:251:LYS:O	1:A:254:VAL:HG12	0.42	2.15	3	1
3:A:41:PCW:H372	3:A:59:PCW:H351	0.42	1.91	1	1
3:A:7:PCW:H72	4:A:33:17F:H4	0.42	1.92	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:37:17F:H11	4:A:37:17F:H32	0.42	1.90	10	1
1:A:306:ARG:O	1:A:310:ARG:HG3	0.42	2.14	6	1
1:A:221:LEU:HA	1:A:224:VAL:HB	0.42	1.92	3	1
3:A:53:PCW:O11	3:A:64:PCW:H51	0.42	2.14	3	1
3:A:65:PCW:O2P	3:A:66:PCW:H62	0.42	2.15	10	1
3:A:13:PCW:H41	4:A:34:17F:HN1A	0.42	1.74	5	1
3:A:16:PCW:H51	3:A:16:PCW:H31	0.42	1.92	6	1
3:A:10:PCW:H452	3:A:21:PCW:H432	0.42	1.92	6	1
3:A:45:PCW:H381	3:A:57:PCW:C7	0.42	2.45	6	1
1:C:469:LEU:O	1:C:473:LYS:HD3	0.42	2.15	6	1
3:A:51:PCW:H51	3:A:71:PCW:H39	0.42	1.92	7	1
1:A:341:ASN:O	1:A:345:ARG:HB2	0.42	2.15	3	1
3:A:42:PCW:H222	3:A:52:PCW:H162	0.42	1.91	3	1
3:A:22:PCW:H51	3:A:22:PCW:H2	0.42	1.91	8	1
3:A:22:PCW:H52	4:A:37:17F:H4A	0.42	1.91	8	1
3:A:4:PCW:H331	3:A:4:PCW:H131	0.42	1.92	8	1
3:A:60:PCW:H41	3:A:63:PCW:H42	0.42	1.92	8	1
3:A:6:PCW:H331	3:A:28:PCW:H61	0.42	1.90	10	1
3:A:10:PCW:H181	3:A:12:PCW:H222	0.42	1.91	6	1
3:A:45:PCW:H211	4:A:79:17F:H48	0.42	1.91	6	1
3:A:28:PCW:H122	3:A:28:PCW:H361	0.42	1.91	7	1
3:A:19:PCW:O1P	3:A:29:PCW:H62	0.42	2.14	7	1
3:A:62:PCW:H341	4:A:78:17F:H38	0.42	1.92	7	1
3:A:65:PCW:H281	1:C:488:LYS:HG2	0.42	1.90	7	1
4:A:38:17F:H11A	4:A:38:17F:H34	0.42	1.92	4	1
3:A:68:PCW:H42	3:A:69:PCW:O1P	0.41	2.14	5	1
3:A:25:PCW:H441	3:A:25:PCW:H272	0.41	1.91	4	1
3:A:65:PCW:H272	3:A:65:PCW:H432	0.41	1.91	4	1
3:A:6:PCW:H362	3:A:28:PCW:H132	0.41	1.93	2	1
3:A:60:PCW:H162	3:A:62:PCW:H271	0.41	1.92	2	1
1:A:279:LEU:O	1:A:283:LEU:HG	0.41	2.15	8	2
3:A:31:PCW:H2	3:A:31:PCW:O4P	0.41	2.15	8	1
3:A:51:PCW:H32	3:A:71:PCW:H40	0.41	1.91	8	1
3:A:4:PCW:C1	3:A:16:PCW:H62	0.41	2.46	9	1
1:A:264:LYS:O	1:A:268:GLU:HG3	0.41	2.15	9	2
4:A:77:17F:HN1	4:A:77:17F:P1	0.41	2.38	2	1
3:A:6:PCW:H351	3:A:16:PCW:H12	0.41	1.92	8	1
3:A:43:PCW:H321	3:A:71:PCW:H283	0.41	1.92	8	1
1:A:238:GLY:O	1:A:242:GLU:HG2	0.41	2.15	6	1
3:A:24:PCW:H81	3:A:31:PCW:O1P	0.41	2.16	6	1
4:A:74:17F:H12	4:A:79:17F:H45	0.41	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:9:PCW:H282	3:A:28:PCW:H251	0.41	1.92	9	1
3:A:1:PCW:H151	4:A:38:17F:H18	0.41	1.92	9	1
3:A:47:PCW:H262	4:A:76:17F:H58	0.41	1.91	4	1
3:A:30:PCW:H81	4:A:37:17F:N1	0.41	2.31	10	1
3:A:6:PCW:H162	3:A:11:PCW:H331	0.41	1.92	5	1
1:A:308:ARG:HH12	1:C:468:GLU:HB2	0.41	1.76	6	1
3:A:13:PCW:H11	3:A:14:PCW:H19	0.41	1.93	9	1
1:A:239:LEU:O	1:A:243:MET:HG2	0.41	2.15	9	1
3:A:15:PCW:H431	3:A:24:PCW:H451	0.41	1.93	7	1
2:B:126:ASP:OD2	2:B:128:LYS:HB2	0.41	2.15	7	1
3:A:6:PCW:O11	3:A:24:PCW:H11	0.41	2.15	4	1
1:C:404:ASN:O	1:C:408:VAL:HG23	0.41	2.15	2	1
1:A:239:LEU:HA	1:A:242:GLU:HB2	0.41	1.92	1	1
1:A:332:ALA:O	1:A:336:GLU:HB2	0.41	2.14	8	1
3:A:12:PCW:H42	3:A:22:PCW:O2P	0.41	2.15	5	1
3:A:10:PCW:C7	4:A:36:17F:HN1A	0.41	2.28	9	1
1:A:202:LYS:O	1:A:206:ASN:HB2	0.41	2.16	4	1
3:A:21:PCW:H122	4:A:36:17F:H31	0.41	1.93	4	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.41	2.42	2	1
3:A:41:PCW:H462	3:A:61:PCW:H211	0.41	1.92	2	1
3:A:17:PCW:H52	2:B:135:ARG:HD2	0.41	1.92	8	1
3:A:63:PCW:H142	3:A:67:PCW:H182	0.41	1.91	10	1
3:A:3:PCW:H42	3:A:23:PCW:O2P	0.41	2.15	6	1
3:A:14:PCW:H42	3:A:23:PCW:O1P	0.41	2.14	10	1
3:A:67:PCW:H121	4:A:74:17F:H57	0.41	1.91	10	1
3:A:30:PCW:H372	4:A:34:17F:H10A	0.41	1.93	5	1
3:A:51:PCW:H121	3:A:56:PCW:H271	0.41	1.93	5	1
1:C:563:LYS:CB	1:C:564:PRO:HD3	0.41	2.38	5	1
3:A:16:PCW:H12	3:A:16:PCW:H73	0.41	1.92	9	1
1:A:308:ARG:CG	1:C:469:LEU:CD2	0.41	2.98	9	1
1:A:330:ARG:HH12	1:C:448:VAL:HG23	0.41	1.75	7	1
3:A:50:PCW:H41	4:A:78:17F:C6	0.41	2.46	8	1
3:A:57:PCW:H2	3:A:57:PCW:C4	0.41	2.46	10	1
1:C:567:GLU:OE1	1:C:567:GLU:HA	0.41	2.16	5	1
1:A:201:LEU:HA	1:A:204:LEU:HD12	0.41	1.92	4	2
3:A:43:PCW:H341	3:A:45:PCW:H132	0.41	1.91	4	1
3:A:41:PCW:H162	3:A:59:PCW:H412	0.41	1.91	4	1
3:A:20:PCW:H142	3:A:20:PCW:H371	0.41	1.91	2	1
3:A:57:PCW:H332	3:A:57:PCW:H132	0.41	1.92	1	1
2:B:37:GLU:HA	2:B:57:ASP:O	0.41	2.16	1	1
3:A:30:PCW:H72	4:A:34:17F:O2	0.41	2.15	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:246:ASP:OD2	1:C:528:ARG:HD3	0.41	2.16	5	1
1:A:391:GLU:O	1:A:395:LYS:HB2	0.41	2.16	5	1
1:A:255:GLN:O	1:A:259:ASP:HB3	0.41	2.16	5	1
3:A:9:PCW:H51	3:A:14:PCW:O31	0.41	2.15	9	1
3:A:43:PCW:O11	3:A:43:PCW:H62	0.41	2.14	4	1
3:A:42:PCW:H83	3:A:63:PCW:O1P	0.41	2.15	2	1
3:A:46:PCW:O11	3:A:51:PCW:H51	0.41	2.16	2	1
3:A:53:PCW:O2P	3:A:55:PCW:H83	0.41	2.16	2	1
3:A:5:PCW:H31	3:A:17:PCW:H342	0.41	1.93	3	1
3:A:32:PCW:H121	4:A:33:17F:H20	0.41	1.93	3	1
1:A:358:SER:O	1:A:362:GLU:HG3	0.41	2.15	1	1
1:C:511:VAL:O	1:C:515:ARG:HG3	0.41	2.16	1	1
3:A:50:PCW:H41	4:A:78:17F:H6A	0.41	1.93	8	1
3:A:59:PCW:O31	3:A:59:PCW:H41	0.41	2.16	8	1
1:A:299:SER:HB2	1:A:300:PRO:CD	0.41	2.46	5	1
3:A:54:PCW:N	3:A:62:PCW:O1P	0.41	2.54	5	1
3:A:9:PCW:H332	3:A:14:PCW:H351	0.41	1.92	7	1
3:A:54:PCW:H41	3:A:54:PCW:H322	0.41	1.93	7	1
3:A:16:PCW:H251	3:A:24:PCW:H362	0.41	1.92	4	1
3:A:11:PCW:H62	3:A:24:PCW:O2P	0.41	2.16	4	1
4:A:33:17F:H37	4:A:35:17F:H31	0.41	1.94	3	1
3:A:41:PCW:H431	3:A:41:PCW:H211	0.41	1.93	3	1
3:A:43:PCW:O31	3:A:45:PCW:H83	0.40	2.16	8	1
3:A:59:PCW:O2P	3:A:61:PCW:H63	0.40	2.17	10	1
3:A:16:PCW:H73	3:A:16:PCW:O31	0.40	2.15	5	1
1:A:243:MET:HA	1:A:246:ASP:HB3	0.40	1.93	9	1
1:C:423:THR:HG22	1:C:427:TRP:HD1	0.40	1.76	2	1
1:A:268:GLU:OE2	1:C:510:HIS:NE2	0.40	2.55	3	1
1:A:206:ASN:O	1:A:210:VAL:HG23	0.40	2.17	8	1
3:A:23:PCW:H71	4:A:34:17F:H1	0.40	1.93	8	1
3:A:42:PCW:H431	3:A:69:PCW:H19	0.40	1.93	8	1
4:A:36:17F:H1A	4:A:36:17F:C4	0.40	2.46	10	1
3:A:72:PCW:H431	4:A:78:17F:H50	0.40	1.92	5	1
3:A:43:PCW:H41	3:A:68:PCW:O1P	0.40	2.17	9	1
1:A:324:SER:O	1:A:328:ARG:HG3	0.40	2.16	7	1
1:A:334:ARG:HD3	1:C:440:GLU:CD	0.40	2.37	4	1
1:A:246:ASP:CG	1:C:528:ARG:HD3	0.40	2.37	4	1
1:C:549:ALA:O	1:C:553:GLU:HG3	0.40	2.17	4	1
3:A:56:PCW:H472	3:A:56:PCW:H211	0.40	1.93	2	1
1:A:305:MET:SD	1:C:469:LEU:HD13	0.40	2.56	2	1
1:C:523:ASP:O	1:C:526:ARG:HB2	0.40	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:6:PCW:H122	3:A:16:PCW:H341	0.40	1.93	5	1
3:A:9:PCW:H382	3:A:14:PCW:H82	0.40	1.92	6	1
1:C:566:LEU:HD23	1:C:569:LEU:HD12	0.40	1.93	9	1
3:A:25:PCW:O31	3:A:31:PCW:H42	0.40	2.17	7	1
1:A:371:LEU:O	1:A:375:LEU:HG	0.40	2.16	4	1
3:A:69:PCW:O31	3:A:69:PCW:H52	0.40	2.16	4	1
3:A:1:PCW:H122	4:A:35:17F:H19	0.40	1.91	2	1
3:A:71:PCW:O11	3:A:71:PCW:H51	0.40	2.16	10	1
3:A:3:PCW:H322	3:A:3:PCW:H83	0.40	1.92	6	1
2:B:87:THR:HG23	2:B:125:VAL:HG22	0.40	1.91	6	1
4:A:74:17F:H49	4:A:75:17F:H44	0.40	1.92	9	1
1:C:581:LYS:O	1:C:585:LEU:HG	0.40	2.17	9	1
1:A:225:THR:O	1:A:229:TRP:HB2	0.40	2.17	7	1
1:A:218:ARG:HA	1:A:221:LEU:HB2	0.40	1.93	2	1
1:C:471:ARG:O	1:C:475:GLU:HB2	0.40	2.16	9	1
3:A:23:PCW:H411	4:A:34:17F:H70	0.40	1.92	7	1
3:A:28:PCW:H2	3:A:28:PCW:H41	0.40	1.93	7	1
3:A:1:PCW:H412	4:A:36:17F:H35	0.40	1.92	1	1

## 6.3 Torsion angles [i](#)

### 6.3.1 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 NMR 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	194/200 (97%)	190±2 (98±1%)	4±1 (2±1%)	1±0 (0±0%)	44	80
1	C	192/200 (96%)	188±2 (98±1%)	3±1 (2±1%)	1±0 (0±0%)	38	78
2	B	144/187 (77%)	138±2 (96±1%)	6±2 (4±2%)	1±1 (0±1%)	32	76
All	All	5300/5870 (90%)	5155 (97%)	124 (2%)	21 (0%)	38	78

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	563	LYS	8

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Mol	Chain	Res	Type	Models (Total)
1	A	365	LYS	6
2	B	58	THR	2
2	B	110	PRO	2
2	B	59	ALA	1
2	B	47	ASP	1
2	B	13	GLY	1

### 6.3.2 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 NMR 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	171/175 (98%)	154±2 (90±1%)	17±2 (10±1%)	11	57
1	C	168/175 (96%)	153±2 (91±1%)	15±2 (9±1%)	13	60
2	B	126/165 (76%)	116±2 (92±1%)	10±2 (8±1%)	15	62
All	All	4650/5150 (90%)	4227 (91%)	423 (9%)	13	59

All 171 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	254	VAL	10
1	C	516	THR	9
1	C	550	LYS	9
2	B	124	THR	9
1	A	312	HIS	8
1	A	318	THR	8
2	B	51	CYS	7
2	B	50	THR	7
2	B	57	ASP	7
1	A	319	HIS	7
2	B	87	THR	7
1	C	463	TRP	7
2	B	20	THR	7
1	C	455	TYR	6
2	B	89	SER	6
1	A	382	PHE	6
1	C	480	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	272	TYR	6
1	A	265	TRP	6
1	A	235	GLU	6
1	C	568	ASP	5
1	C	546	GLU	5
2	B	92	ASP	5
1	A	370	ASP	5
1	C	405	TRP	5
1	A	386	PHE	4
1	C	407	SER	4
1	A	274	GLN	4
1	C	592	THR	4
2	B	35	THR	4
1	A	228	PHE	4
2	B	70	GLN	4
1	A	293	GLU	4
1	C	505	ASP	4
1	A	361	SER	4
1	C	448	VAL	4
1	C	487	GLN	4
1	A	369	GLU	3
1	C	410	SER	3
1	A	285	GLU	3
1	C	412	PHE	3
2	B	32	TYR	3
1	A	261	PHE	3
1	C	418	GLN	3
1	A	229	TRP	3
1	C	458	ASP	3
1	A	354	THR	3
1	C	559	SER	3
1	C	444	ASP	3
2	B	122	SER	3
2	B	127	THR	3
1	C	403	ASP	3
1	A	244	SER	3
1	A	394	THR	3
1	A	205	ASP	3
1	C	521	TYR	3
1	A	264	LYS	2
1	C	589	GLU	2
1	C	591	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	C	402	LEU	2
2	B	76	GLU	2
1	C	433	GLU	2
1	C	512	ASP	2
1	C	413	SER	2
1	A	241	GLN	2
2	B	132	ASP	2
1	A	212	SER	2
1	A	206	ASN	2
1	C	473	LYS	2
1	A	314	ASP	2
1	C	426	PHE	2
1	A	297	LYS	2
1	A	292	HIS	2
1	A	249	GLU	2
2	B	72	MET	2
1	C	457	ASP	2
1	C	459	PHE	2
1	C	497	SER	2
2	B	3	GLU	2
2	B	69	ASP	2
1	A	207	TRP	2
1	A	211	THR	2
1	A	289	GLN	2
1	C	580	PHE	2
1	A	246	ASP	2
2	B	126	ASP	2
1	A	368	LEU	2
1	A	299	SER	2
1	A	269	MET	2
1	A	220	GLN	2
1	A	325	ASP	1
2	B	108	ASP	1
1	A	262	GLN	1
1	C	414	LYS	1
2	B	17	SER	1
1	A	345	ARG	1
1	A	209	SER	1
1	C	510	HIS	1
1	C	431	GLU	1
1	C	583	SER	1
2	B	135	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	327	LEU	1
1	C	452	VAL	1
1	C	451	LYS	1
1	A	215	SER	1
2	B	29	VAL	1
1	A	237	GLU	1
2	B	128	LYS	1
1	A	214	PHE	1
1	A	225	THR	1
1	C	467	MET	1
1	A	239	LEU	1
1	C	461	LYS	1
1	C	586	SER	1
1	C	547	TYR	1
1	A	279	LEU	1
2	B	74	THR	1
1	C	567	GLU	1
1	C	409	THR	1
1	A	350	HIS	1
1	C	538	GLU	1
1	A	290	LYS	1
1	C	466	GLU	1
2	B	118	CYS	1
1	C	488	LYS	1
1	A	276	VAL	1
1	C	579	SER	1
1	A	356	HIS	1
1	A	260	ASP	1
1	C	576	VAL	1
2	B	47	ASP	1
1	C	442	SER	1
2	B	106	SER	1
2	B	104	LYS	1
2	B	39	SER	1
2	B	37	GLU	1
2	B	105	ASP	1
2	B	5	LYS	1
1	A	385	SER	1
1	C	555	LEU	1
2	B	49	GLU	1
1	C	552	THR	1
1	C	527	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	390	LEU	1
1	C	494	GLU	1
2	B	144	THR	1
1	C	548	HIS	1
1	A	213	THR	1
1	C	554	HIS	1
1	C	532	ARG	1
1	C	523	ASP	1
1	A	336	GLU	1
2	B	96	TYR	1
2	B	129	GLN	1
1	A	395	LYS	1
1	A	308	ARG	1
2	B	38	ASP	1
1	A	202	LYS	1
2	B	27	HIS	1
1	C	411	THR	1
1	A	392	GLU	1
1	C	464	GLN	1
1	C	447	GLU	1
1	A	248	GLU	1
1	C	556	SER	1
1	A	330	ARG	1
1	A	338	LEU	1
1	A	357	LEU	1
1	C	522	SER	1
1	A	393	TYR	1
1	A	360	LEU	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 82 ligands modelled in this entry, 1 is monoatomic - leaving 81 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	A	57	-	53,53,53	1.02±0.01	0±0 (0±0%)
4	17F	A	79	-	50,53,53	0.91±0.01	0±0 (0±0%)
4	17F	A	39	-	50,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	A	72	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	60	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	6	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	71	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	42	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	17F	A	77	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	73	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	33	-	50,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	A	54	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	14	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	53	-	53,53,53	1.02±0.01	0±0 (0±0%)
4	17F	A	75	-	50,53,53	0.92±0.00	0±0 (0±0%)
3	PCW	A	63	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	A	61	-	53,53,53	1.03±0.00	0±0 (0±0%)
3	PCW	A	19	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	17F	A	35	-	50,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	A	26	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	45	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	52	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	A	4	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	59	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	50	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	5	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	67	-	53,53,53	1.03±0.00	0±0 (0±0%)
3	PCW	A	8	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	25	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	32	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	17F	A	36	-	50,53,53	0.91±0.00	0±0 (0±0%)
3	PCW	A	30	-	53,53,53	1.03±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	A	7	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	62	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	13	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	51	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	41	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	A	29	-	53,53,53	1.03±0.00	0±0 (0±0%)
4	17F	A	34	-	50,53,53	0.91±0.00	0±0 (0±0%)
3	PCW	A	3	-	53,53,53	1.03±0.00	0±0 (0±0%)
3	PCW	A	24	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	1	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	56	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	46	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	17F	A	38	-	50,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	A	2	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	17F	A	76	-	50,53,53	0.92±0.01	0±0 (0±0%)
3	PCW	A	17	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	15	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	64	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	66	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	20	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	17F	A	78	-	50,53,53	0.92±0.01	0±0 (0±0%)
3	PCW	A	49	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	21	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	43	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	A	18	-	53,53,53	1.02±0.01	0±0 (0±0%)
4	17F	A	40	-	50,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	A	28	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	9	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	47	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	17F	A	74	-	50,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	A	10	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	22	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	23	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	A	55	-	53,53,53	1.05±0.01	0±0 (0±0%)
3	PCW	A	16	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	69	-	53,53,53	1.03±0.01	0±0 (0±0%)
5	GDP	B	201	-	24,30,30	1.27±0.02	0±0 (0±0%)
3	PCW	A	58	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	48	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	17F	A	37	-	50,53,53	0.91±0.00	0±0 (0±0%)
3	PCW	A	11	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	31	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	44	-	53,53,53	1.03±0.00	0±0 (0±0%)



Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	A	68	-	53,53,53	1.03±0.00	0±0 (0±0%)
4	17F	A	80	-	50,53,53	0.91±0.00	0±0 (0±0%)
3	PCW	A	65	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	12	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	70	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	27	-	53,53,53	1.05±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	A	57	-	59,61,61	2.35±0.00	3±0 (5±0%)
4	17F	A	79	-	52,60,60	0.96±0.01	0±0 (0±0%)
4	17F	A	39	-	52,60,60	0.97±0.02	0±0 (0±0%)
3	PCW	A	72	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	A	60	-	59,61,61	2.35±0.01	3±0 (5±0%)
3	PCW	A	6	-	59,61,61	2.78±0.01	6±0 (10±0%)
3	PCW	A	71	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	42	-	59,61,61	2.35±0.01	3±0 (5±0%)
4	17F	A	77	-	52,60,60	1.69±0.02	2±0 (3±0%)
4	17F	A	73	-	52,60,60	0.95±0.01	0±0 (0±0%)
4	17F	A	33	-	52,60,60	1.74±0.02	2±0 (3±0%)
3	PCW	A	54	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	14	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	53	-	59,61,61	2.35±0.00	3±0 (5±0%)
4	17F	A	75	-	52,60,60	0.95±0.02	0±0 (0±0%)
3	PCW	A	63	-	59,61,61	2.78±0.00	6±0 (10±0%)
3	PCW	A	61	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	19	-	59,61,61	0.84±0.00	0±0 (0±0%)
4	17F	A	35	-	52,60,60	0.96±0.02	0±0 (0±0%)
3	PCW	A	26	-	59,61,61	2.35±0.01	3±0 (5±0%)
3	PCW	A	45	-	59,61,61	2.34±0.00	3±0 (5±0%)
3	PCW	A	52	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	4	-	59,61,61	2.35±0.01	3±0 (5±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	A	59	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	50	-	59,61,61	0.84±0.00	0±0 (0±0%)
3	PCW	A	5	-	59,61,61	2.35±0.01	3±0 (5±0%)
3	PCW	A	67	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	8	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	A	25	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	32	-	59,61,61	0.83±0.00	0±0 (0±0%)
4	17F	A	36	-	52,60,60	0.96±0.03	0±0 (0±0%)
3	PCW	A	30	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	A	7	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	A	62	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	13	-	59,61,61	2.35±0.01	3±0 (5±0%)
3	PCW	A	51	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	41	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	29	-	59,61,61	2.35±0.00	3±0 (5±0%)
4	17F	A	34	-	52,60,60	0.96±0.02	0±0 (0±0%)
3	PCW	A	3	-	59,61,61	2.35±0.01	3±0 (5±0%)
3	PCW	A	24	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	1	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	56	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	46	-	59,61,61	2.35±0.00	3±0 (5±0%)
4	17F	A	38	-	52,60,60	0.94±0.01	0±0 (0±0%)
3	PCW	A	2	-	59,61,61	2.35±0.00	3±0 (5±0%)
4	17F	A	76	-	52,60,60	0.95±0.02	0±0 (0±0%)
3	PCW	A	17	-	59,61,61	2.34±0.01	3±0 (5±0%)
3	PCW	A	15	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	A	64	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	66	-	59,61,61	0.84±0.00	0±0 (0±0%)
3	PCW	A	20	-	59,61,61	2.35±0.00	3±0 (5±0%)
4	17F	A	78	-	52,60,60	0.95±0.02	0±0 (0±0%)
3	PCW	A	49	-	59,61,61	2.34±0.00	3±0 (5±0%)
3	PCW	A	21	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	43	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	18	-	59,61,61	2.35±0.00	3±0 (5±0%)
4	17F	A	40	-	52,60,60	0.95±0.03	0±0 (0±0%)
3	PCW	A	28	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	9	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	A	47	-	59,61,61	0.84±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
4	17F	A	74	-	52,60,60	0.97±0.02	0±0 (0±0%)
3	PCW	A	10	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	22	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	23	-	59,61,61	2.35±0.01	3±0 (5±0%)
3	PCW	A	55	-	59,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	A	16	-	59,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	A	69	-	59,61,61	2.35±0.00	3±0 (5±0%)
5	GDP	B	201	-	31,47,47	2.06±0.02	1±1 (1±1%)
3	PCW	A	58	-	59,61,61	2.35±0.01	3±0 (5±0%)
3	PCW	A	48	-	59,61,61	0.84±0.01	0±0 (0±0%)
4	17F	A	37	-	52,60,60	0.96±0.02	0±0 (0±0%)
3	PCW	A	11	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	A	31	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	44	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	68	-	59,61,61	2.35±0.00	3±0 (5±0%)
4	17F	A	80	-	52,60,60	0.93±0.02	0±0 (0±0%)
3	PCW	A	65	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	A	12	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	A	70	-	59,61,61	2.35±0.00	3±0 (5±0%)
3	PCW	A	27	-	59,61,61	0.83±0.01	0±0 (0±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
4	17F	A	79	-	-	0±0,55,59,59	-
3	PCW	A	25	-	-	0±0,57,57,57	-
3	PCW	A	71	-	-	0±0,57,57,57	-
3	PCW	A	41	-	-	0±0,57,57,57	-
3	PCW	A	56	-	-	0±0,57,57,57	-
3	PCW	A	63	-	-	0±0,57,57,57	-
3	PCW	A	46	-	-	0±0,57,57,57	-
4	17F	A	34	-	-	0±0,55,59,59	-
4	17F	A	35	-	-	0±0,55,59,59	-
3	PCW	A	13	-	-	0±0,57,57,57	-
4	17F	A	76	-	-	0±0,55,59,59	-
3	PCW	A	47	-	-	0±0,57,57,57	-
4	17F	A	40	-	-	0±0,55,59,59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	14	-	-	0±0,57,57,57	-
3	PCW	A	60	-	-	0±0,57,57,57	-
3	PCW	A	55	-	-	0±0,57,57,57	-
3	PCW	A	16	-	-	0±0,57,57,57	-
4	17F	A	38	-	-	0±0,55,59,59	-
3	PCW	A	61	-	-	0±0,57,57,57	-
4	17F	A	39	-	-	0±0,55,59,59	-
4	17F	A	37	-	-	0±0,55,59,59	-
3	PCW	A	11	-	-	0±0,57,57,57	-
3	PCW	A	20	-	-	0±0,57,57,57	-
3	PCW	A	43	-	-	0±0,57,57,57	-
3	PCW	A	30	-	-	0±0,57,57,57	-
3	PCW	A	44	-	-	0±0,57,57,57	-
3	PCW	A	69	-	-	0±0,57,57,57	-
3	PCW	A	17	-	-	0±0,57,57,57	-
3	PCW	A	10	-	-	0±0,57,57,57	-
3	PCW	A	49	-	-	0±0,57,57,57	-
3	PCW	A	65	-	-	0±0,57,57,57	-
3	PCW	A	62	-	-	0±0,57,57,57	-
4	17F	A	77	-	-	0±0,55,59,59	-
3	PCW	A	3	-	-	0±0,57,57,57	-
3	PCW	A	7	-	-	0±0,57,57,57	-
3	PCW	A	4	-	-	0±0,57,57,57	-
3	PCW	A	70	-	-	0±0,57,57,57	-
3	PCW	A	31	-	-	0±0,57,57,57	-
3	PCW	A	2	-	-	0±0,57,57,57	-
4	17F	A	75	-	-	0±0,55,59,59	-
3	PCW	A	48	-	-	0±0,57,57,57	-
3	PCW	A	66	-	-	0±0,57,57,57	-
4	17F	A	73	-	-	0±0,55,59,59	-
3	PCW	A	42	-	-	0±0,57,57,57	-
3	PCW	A	8	-	-	0±0,57,57,57	-
3	PCW	A	23	-	-	0±0,57,57,57	-
3	PCW	A	53	-	-	0±0,57,57,57	-
3	PCW	A	59	-	-	0±0,57,57,57	-
3	PCW	A	19	-	-	0±0,57,57,57	-
4	17F	A	74	-	-	0±0,55,59,59	-
3	PCW	A	1	-	-	0±0,57,57,57	-
5	GDP	B	201	-	-	0±0,12,32,32	0±0,3,3,3
3	PCW	A	72	-	-	0±0,57,57,57	-
3	PCW	A	24	-	-	0±0,57,57,57	-
3	PCW	A	54	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	50	-	-	0±0,57,57,57	-
3	PCW	A	22	-	-	0±0,57,57,57	-
3	PCW	A	52	-	-	0±0,57,57,57	-
3	PCW	A	5	-	-	0±0,57,57,57	-
3	PCW	A	28	-	-	0±0,57,57,57	-
4	17F	A	36	-	-	0±0,55,59,59	-
3	PCW	A	9	-	-	0±0,57,57,57	-
3	PCW	A	12	-	-	0±0,57,57,57	-
4	17F	A	33	-	-	0±0,55,59,59	-
4	17F	A	78	-	-	0±0,55,59,59	-
3	PCW	A	57	-	-	0±0,57,57,57	-
3	PCW	A	21	-	-	0±0,57,57,57	-
3	PCW	A	58	-	-	0±0,57,57,57	-
3	PCW	A	32	-	-	0±0,57,57,57	-
3	PCW	A	6	-	-	0±0,57,57,57	-
3	PCW	A	51	-	-	0±0,57,57,57	-
3	PCW	A	45	-	-	0±0,57,57,57	-
3	PCW	A	64	-	-	0±0,57,57,57	-
3	PCW	A	27	-	-	0±0,57,57,57	-
3	PCW	A	15	-	-	0±0,57,57,57	-
4	17F	A	80	-	-	0±0,55,59,59	-
3	PCW	A	29	-	-	0±0,57,57,57	-
3	PCW	A	26	-	-	0±0,57,57,57	-
3	PCW	A	68	-	-	0±0,57,57,57	-
3	PCW	A	67	-	-	0±0,57,57,57	-
3	PCW	A	18	-	-	0±0,57,57,57	-

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	13	PCW	C8-N-C7	12.24	77.49	108.97	10	10
3	A	46	PCW	C8-N-C7	12.23	77.53	108.97	6	10
3	A	3	PCW	C8-N-C7	12.22	77.55	108.97	5	10
3	A	2	PCW	C8-N-C7	12.22	77.56	108.97	5	10
3	A	20	PCW	C8-N-C7	12.21	77.57	108.97	4	10
3	A	67	PCW	C8-N-C7	12.20	77.62	108.97	8	10
3	A	24	PCW	C8-N-C7	12.19	77.63	108.97	5	10
3	A	64	PCW	C8-N-C7	12.19	77.63	108.97	6	10
3	A	52	PCW	C8-N-C7	12.19	77.64	108.97	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	59	PCW	C8-N-C7	12.19	77.64	108.97	4	10
3	A	21	PCW	C8-N-C7	12.19	77.64	108.97	10	10
3	A	69	PCW	C8-N-C7	12.18	77.65	108.97	8	10
3	A	68	PCW	C8-N-C7	12.18	77.67	108.97	9	10
3	A	70	PCW	C8-N-C7	12.17	77.67	108.97	4	10
3	A	4	PCW	C8-N-C7	12.17	77.68	108.97	4	10
3	A	56	PCW	C8-N-C7	12.17	77.68	108.97	8	10
3	A	63	PCW	C8-N-C7	12.17	77.69	108.97	4	10
3	A	58	PCW	C8-N-C7	12.16	77.70	108.97	6	10
3	A	18	PCW	C8-N-C7	12.16	77.71	108.97	7	10
3	A	6	PCW	C8-N-C7	12.16	77.72	108.97	1	10
3	A	71	PCW	C8-N-C7	12.15	77.73	108.97	9	10
3	A	51	PCW	C8-N-C7	12.15	77.73	108.97	10	10
3	A	41	PCW	C8-N-C7	12.15	77.73	108.97	4	10
3	A	42	PCW	C8-N-C7	12.15	77.74	108.97	4	10
3	A	10	PCW	C8-N-C7	12.15	77.74	108.97	1	10
3	A	23	PCW	C8-N-C7	12.15	77.74	108.97	4	10
3	A	31	PCW	C8-N-C7	12.15	77.74	108.97	9	10
3	A	57	PCW	C8-N-C7	12.14	77.75	108.97	5	10
3	A	44	PCW	C8-N-C7	12.14	77.75	108.97	7	10
3	A	28	PCW	C8-N-C7	12.14	77.75	108.97	3	10
3	A	29	PCW	C8-N-C7	12.13	77.78	108.97	1	10
3	A	5	PCW	C8-N-C7	12.13	77.79	108.97	9	10
3	A	25	PCW	C8-N-C7	12.13	77.79	108.97	8	10
3	A	17	PCW	C8-N-C7	12.13	77.79	108.97	7	10
3	A	61	PCW	C8-N-C7	12.13	77.79	108.97	6	10
3	A	14	PCW	C8-N-C7	12.12	77.80	108.97	5	10
3	A	53	PCW	C8-N-C7	12.12	77.80	108.97	2	10
3	A	43	PCW	C8-N-C7	12.12	77.80	108.97	6	10
3	A	60	PCW	C8-N-C7	12.12	77.82	108.97	6	10
3	A	54	PCW	C8-N-C7	12.12	77.82	108.97	9	10
3	A	26	PCW	C8-N-C7	12.12	77.82	108.97	4	10
3	A	22	PCW	C8-N-C7	12.11	77.83	108.97	1	10
3	A	62	PCW	C8-N-C7	12.11	77.84	108.97	6	10
3	A	1	PCW	C8-N-C7	12.10	77.87	108.97	5	10
3	A	45	PCW	C8-N-C7	12.09	77.88	108.97	10	10
3	A	49	PCW	C8-N-C7	12.06	77.96	108.97	8	10
3	A	23	PCW	C8-N-C6	10.49	82.01	108.97	3	10
3	A	58	PCW	C8-N-C6	10.37	82.31	108.97	2	10
3	A	42	PCW	C8-N-C6	10.34	82.38	108.97	3	10
3	A	60	PCW	C8-N-C6	10.30	82.49	108.97	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	10	PCW	C8-N-C6	10.29	82.50	108.97	6	10
3	A	52	PCW	C8-N-C6	10.29	82.52	108.97	4	10
3	A	57	PCW	C8-N-C6	10.29	82.52	108.97	6	10
3	A	21	PCW	C8-N-C6	10.28	82.54	108.97	5	10
3	A	29	PCW	C8-N-C6	10.28	82.55	108.97	7	10
3	A	4	PCW	C8-N-C6	10.27	82.56	108.97	8	10
3	A	54	PCW	C8-N-C6	10.27	82.56	108.97	7	10
3	A	63	PCW	C8-N-C6	10.27	82.57	108.97	3	10
3	A	43	PCW	C8-N-C6	10.27	82.57	108.97	2	10
3	A	53	PCW	C8-N-C6	10.26	82.58	108.97	10	10
3	A	17	PCW	C8-N-C6	10.26	82.58	108.97	4	10
3	A	24	PCW	C8-N-C6	10.26	82.59	108.97	4	10
3	A	61	PCW	C8-N-C6	10.26	82.60	108.97	8	10
3	A	5	PCW	C8-N-C6	10.26	82.60	108.97	10	10
3	A	2	PCW	C8-N-C6	10.25	82.62	108.97	10	10
3	A	59	PCW	C8-N-C6	10.25	82.62	108.97	6	10
3	A	1	PCW	C8-N-C6	10.25	82.62	108.97	8	10
3	A	6	PCW	C8-N-C6	10.25	82.63	108.97	3	10
3	A	51	PCW	C8-N-C6	10.25	82.63	108.97	4	10
3	A	22	PCW	C8-N-C6	10.25	82.63	108.97	7	10
3	A	67	PCW	C8-N-C6	10.24	82.64	108.97	3	10
3	A	18	PCW	C8-N-C6	10.24	82.64	108.97	8	10
3	A	25	PCW	C8-N-C6	10.24	82.64	108.97	9	10
3	A	41	PCW	C8-N-C6	10.24	82.64	108.97	6	10
3	A	46	PCW	C8-N-C6	10.24	82.64	108.97	5	10
3	A	45	PCW	C8-N-C6	10.24	82.64	108.97	8	10
3	A	62	PCW	C8-N-C6	10.24	82.64	108.97	10	10
3	A	28	PCW	C8-N-C6	10.24	82.65	108.97	9	10
3	A	68	PCW	C8-N-C6	10.24	82.66	108.97	8	10
3	A	3	PCW	C8-N-C6	10.23	82.67	108.97	10	10
3	A	14	PCW	C8-N-C6	10.23	82.68	108.97	1	10
3	A	71	PCW	C8-N-C6	10.23	82.68	108.97	9	10
3	A	69	PCW	C8-N-C6	10.23	82.68	108.97	10	10
3	A	26	PCW	C8-N-C6	10.22	82.69	108.97	10	10
3	A	64	PCW	C8-N-C6	10.22	82.69	108.97	7	10
3	A	49	PCW	C8-N-C6	10.22	82.69	108.97	9	10
3	A	31	PCW	C8-N-C6	10.22	82.71	108.97	5	10
3	A	44	PCW	C8-N-C6	10.21	82.72	108.97	7	10
3	A	70	PCW	C8-N-C6	10.21	82.72	108.97	5	10
3	A	13	PCW	C8-N-C6	10.21	82.72	108.97	1	10
3	A	56	PCW	C8-N-C6	10.18	82.79	108.97	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	20	PCW	C8-N-C6	10.17	82.84	108.97	6	10
3	A	6	PCW	O4P-P-O2P	7.84	78.43	109.07	4	10
3	A	63	PCW	O4P-P-O2P	7.80	78.60	109.07	2	10
4	A	33	17F	O2-P1-O6	6.21	78.89	107.75	2	10
4	A	77	17F	O2-P1-O6	6.21	78.91	107.75	9	10
4	A	33	17F	O2-P1-O3	6.05	79.67	107.75	6	10
4	A	77	17F	O2-P1-O3	6.03	79.73	107.75	7	10
3	A	6	PCW	O3P-P-O2P	5.94	85.84	109.07	10	10
3	A	63	PCW	O3P-P-O2P	5.88	86.08	109.07	3	10
3	A	63	PCW	O1P-P-O2P	5.48	85.16	112.24	4	10
3	A	6	PCW	O1P-P-O2P	5.48	85.17	112.24	10	10
3	A	58	PCW	C8-N-C5	5.29	88.29	109.92	4	10
3	A	52	PCW	C8-N-C5	5.27	88.35	109.92	6	10
3	A	45	PCW	C8-N-C5	5.26	88.39	109.92	7	10
3	A	4	PCW	C8-N-C5	5.25	88.43	109.92	6	10
3	A	13	PCW	C8-N-C5	5.25	88.43	109.92	2	10
3	A	25	PCW	C8-N-C5	5.24	88.47	109.92	3	10
3	A	31	PCW	C8-N-C5	5.24	88.47	109.92	3	10
3	A	14	PCW	C8-N-C5	5.24	88.48	109.92	7	10
3	A	41	PCW	C8-N-C5	5.24	88.49	109.92	7	10
3	A	24	PCW	C8-N-C5	5.24	88.48	109.92	1	10
3	A	10	PCW	C8-N-C5	5.24	88.48	109.92	9	10
3	A	53	PCW	C8-N-C5	5.24	88.50	109.92	1	10
3	A	49	PCW	C8-N-C5	5.23	88.52	109.92	4	10
5	B	201	GDP	C2-N3-C4	5.23	121.33	115.36	4	5
3	A	1	PCW	C8-N-C5	5.23	88.53	109.92	9	10
3	A	43	PCW	C8-N-C5	5.23	88.53	109.92	1	10
3	A	62	PCW	C8-N-C5	5.22	88.55	109.92	2	10
3	A	42	PCW	C8-N-C5	5.22	88.56	109.92	10	10
3	A	70	PCW	C8-N-C5	5.22	88.56	109.92	10	10
3	A	21	PCW	C8-N-C5	5.22	88.57	109.92	3	10
3	A	44	PCW	C8-N-C5	5.22	88.57	109.92	8	10
3	A	29	PCW	C8-N-C5	5.21	88.58	109.92	10	10
3	A	3	PCW	C8-N-C5	5.22	88.58	109.92	2	10
3	A	28	PCW	C8-N-C5	5.21	88.58	109.92	6	10
3	A	69	PCW	C8-N-C5	5.21	88.58	109.92	6	10
3	A	54	PCW	C8-N-C5	5.21	88.60	109.92	6	10
3	A	67	PCW	C8-N-C5	5.21	88.60	109.92	7	10
3	A	56	PCW	C8-N-C5	5.21	88.59	109.92	3	10
3	A	46	PCW	C8-N-C5	5.21	88.60	109.92	8	10
3	A	17	PCW	C8-N-C5	5.21	88.60	109.92	2	10

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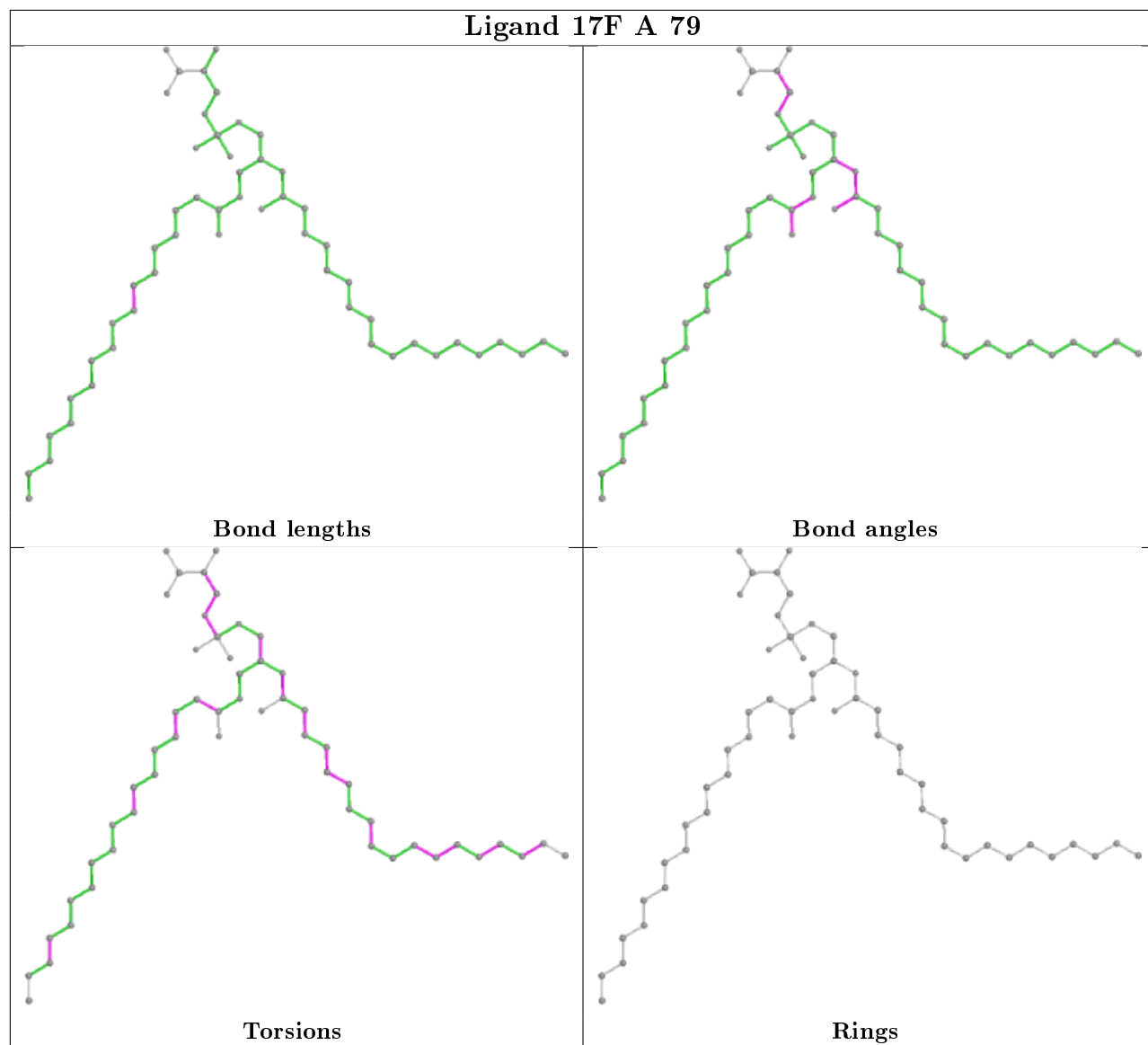
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	64	PCW	C8-N-C5	5.21	88.60	109.92	4	10
3	A	26	PCW	C8-N-C5	5.21	88.61	109.92	7	10
3	A	20	PCW	C8-N-C5	5.21	88.62	109.92	3	10
3	A	60	PCW	C8-N-C5	5.20	88.62	109.92	3	10
3	A	51	PCW	C8-N-C5	5.20	88.62	109.92	5	10
3	A	59	PCW	C8-N-C5	5.20	88.64	109.92	10	10
3	A	5	PCW	C8-N-C5	5.20	88.64	109.92	6	10
3	A	22	PCW	C8-N-C5	5.20	88.65	109.92	8	10
3	A	57	PCW	C8-N-C5	5.20	88.66	109.92	9	10
3	A	71	PCW	C8-N-C5	5.19	88.67	109.92	10	10
3	A	63	PCW	C8-N-C5	5.19	88.67	109.92	7	10
3	A	6	PCW	C8-N-C5	5.19	88.69	109.92	4	10
3	A	61	PCW	C8-N-C5	5.19	88.69	109.92	2	10
3	A	2	PCW	C8-N-C5	5.19	88.70	109.92	4	10
3	A	68	PCW	C8-N-C5	5.19	88.69	109.92	9	10
3	A	18	PCW	C8-N-C5	5.19	88.70	109.92	2	10
3	A	23	PCW	C8-N-C5	5.17	88.76	109.92	10	10

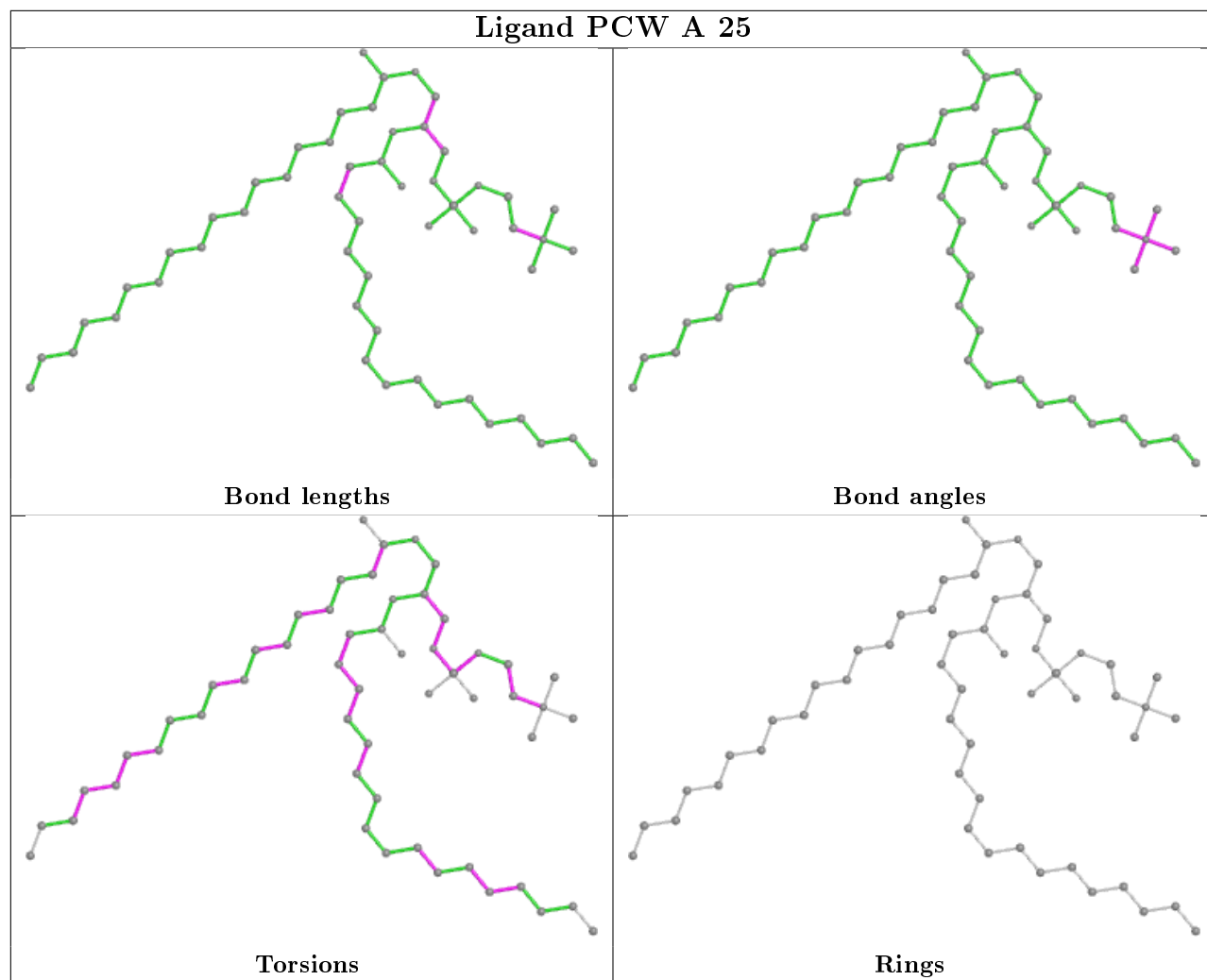
There are no chirality outliers.

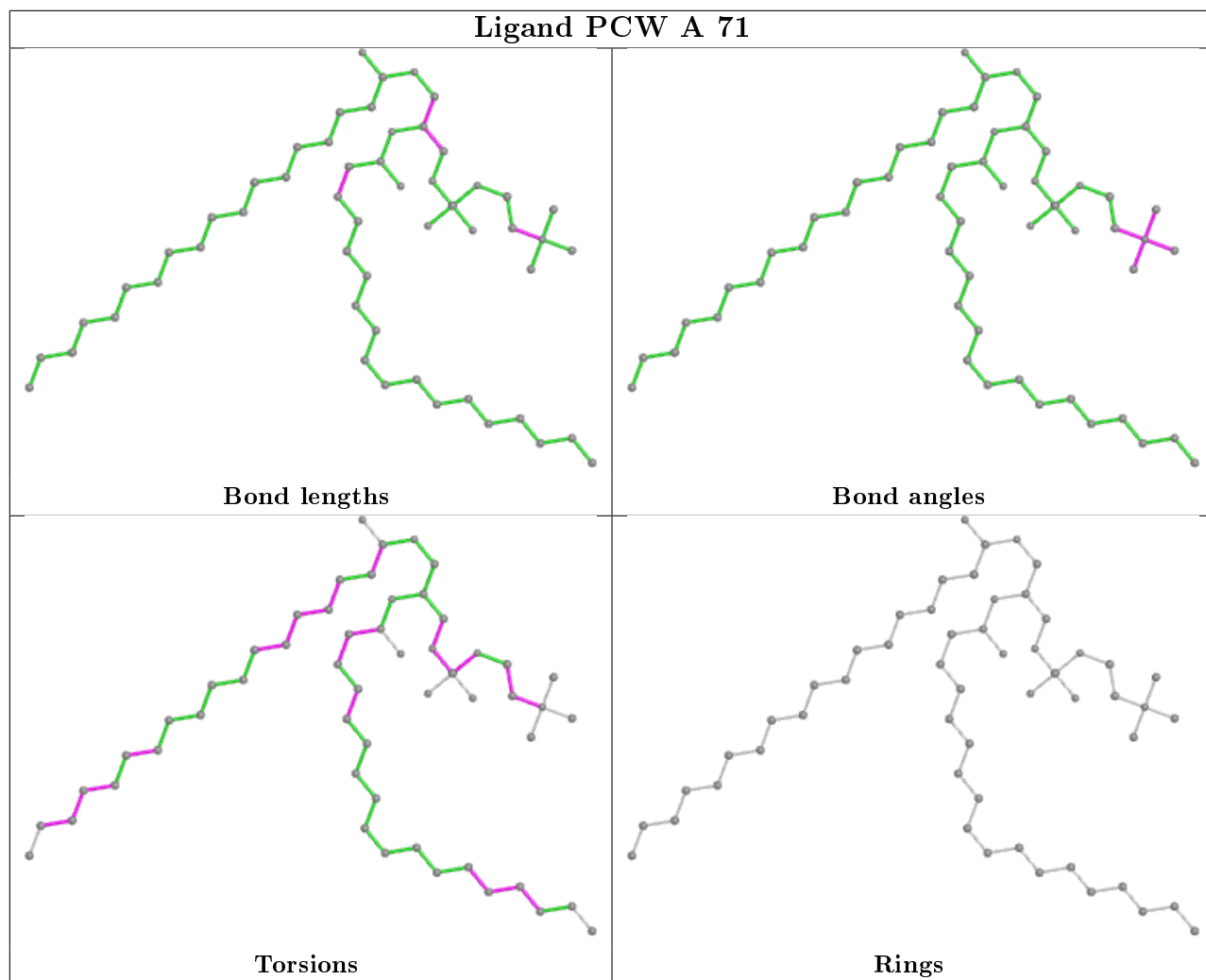
There are no torsion outliers.

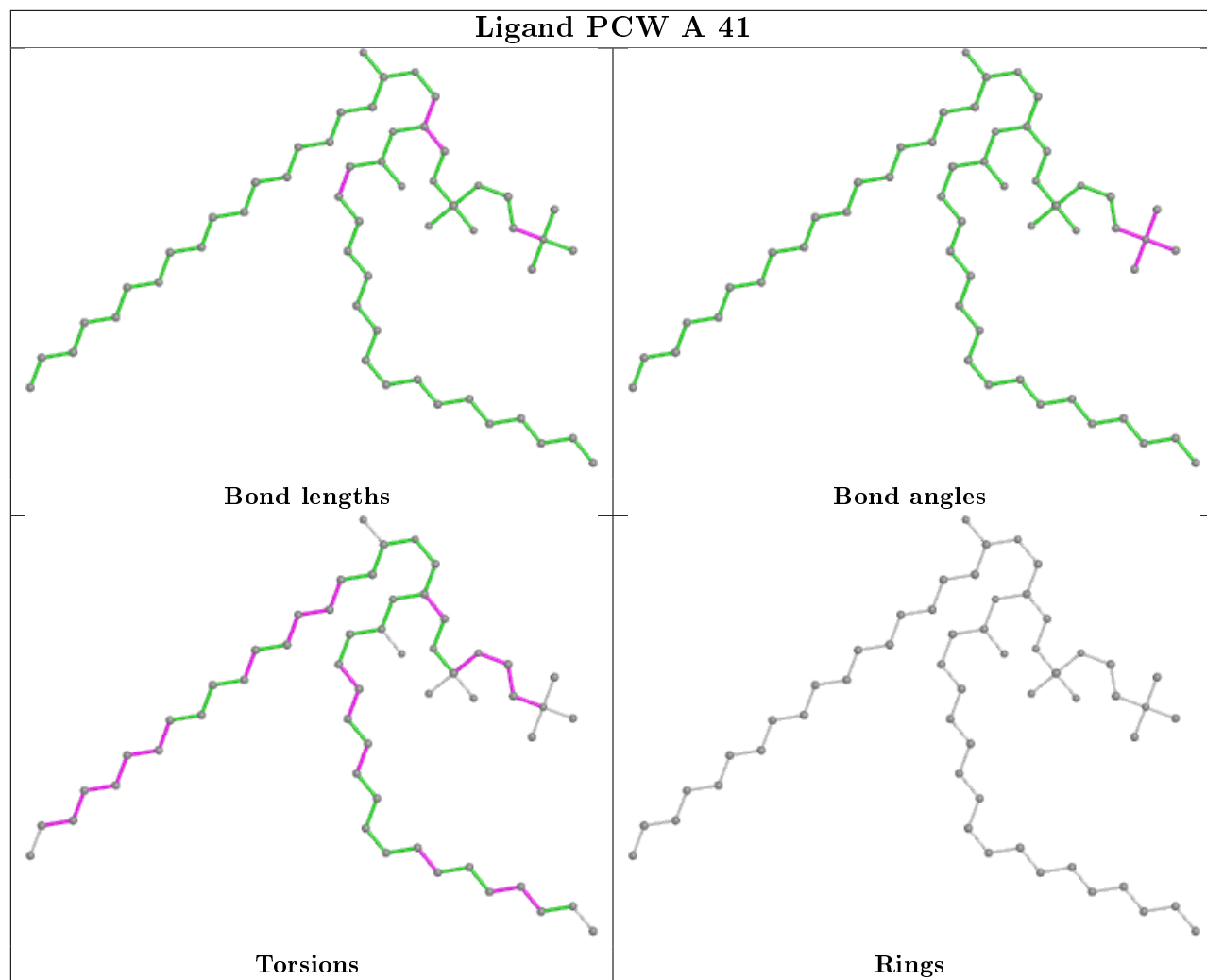
There are no ring outliers.

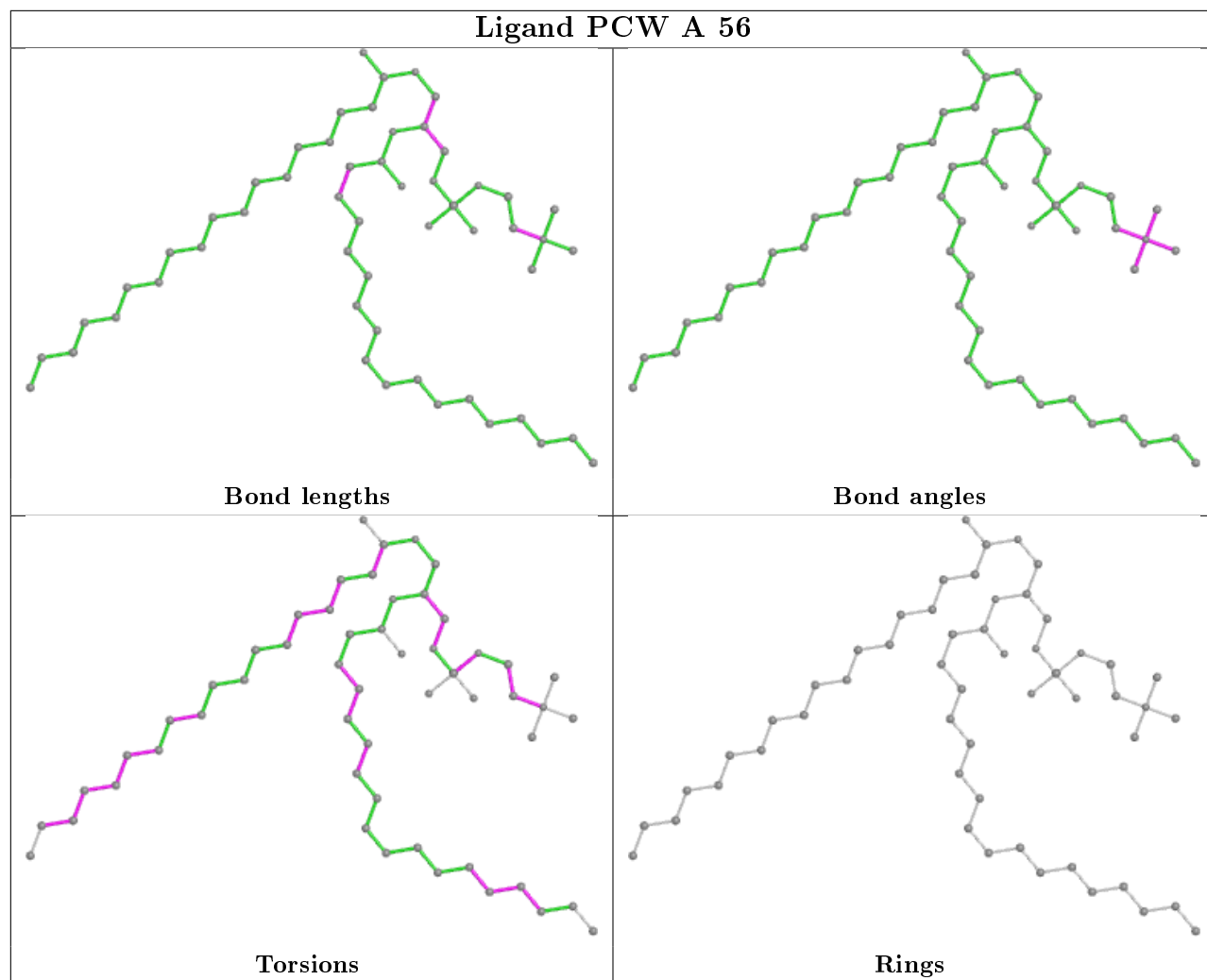
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

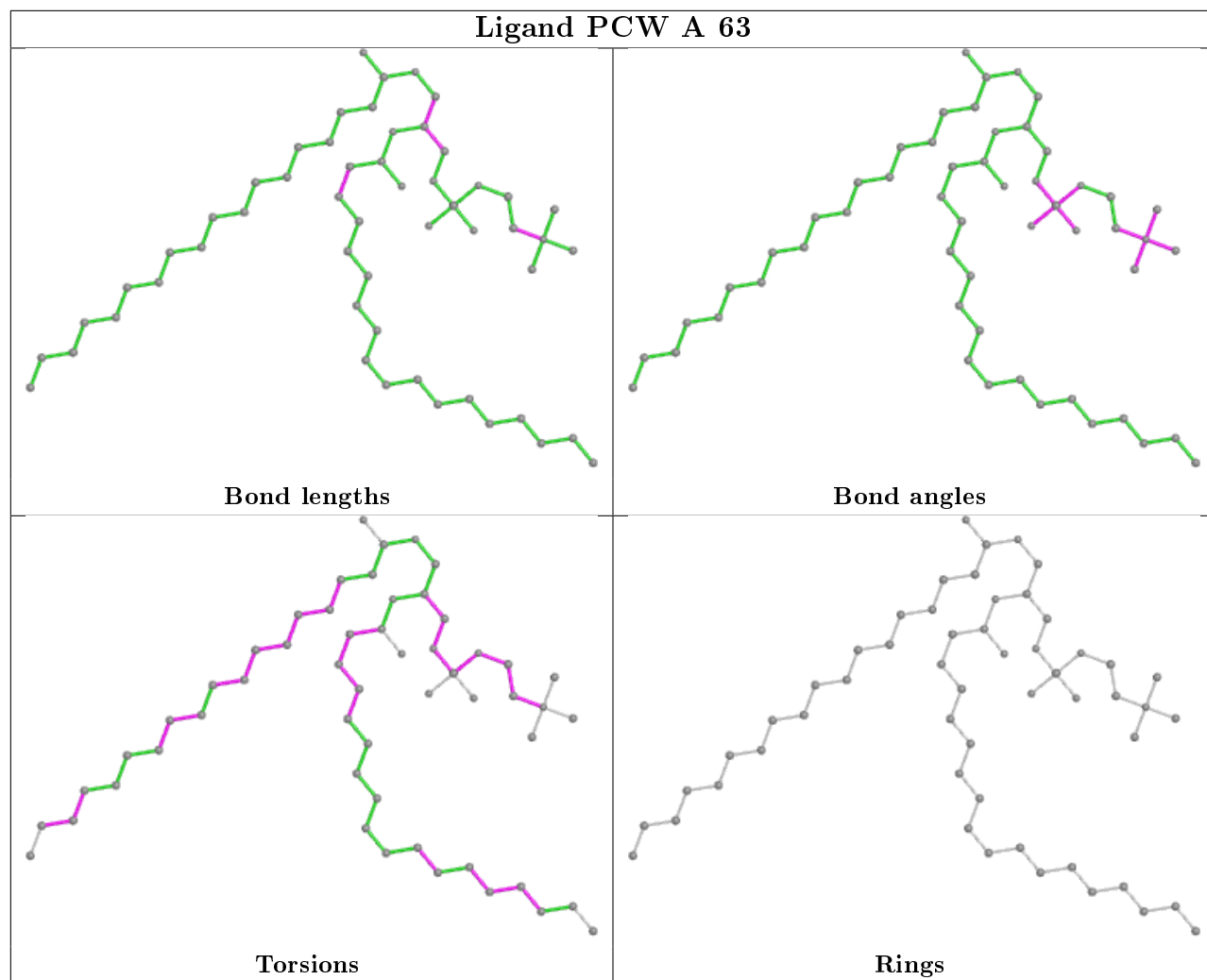


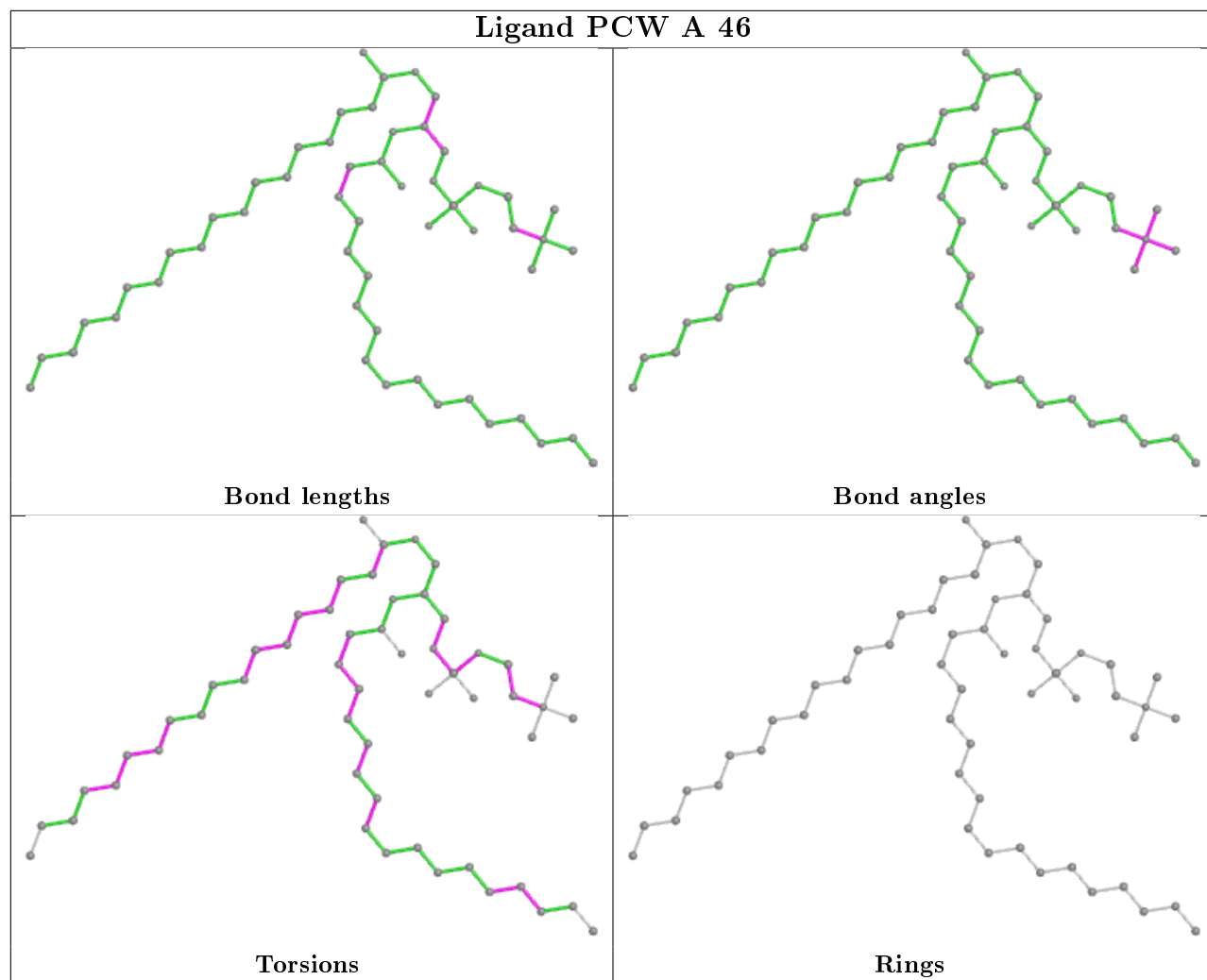




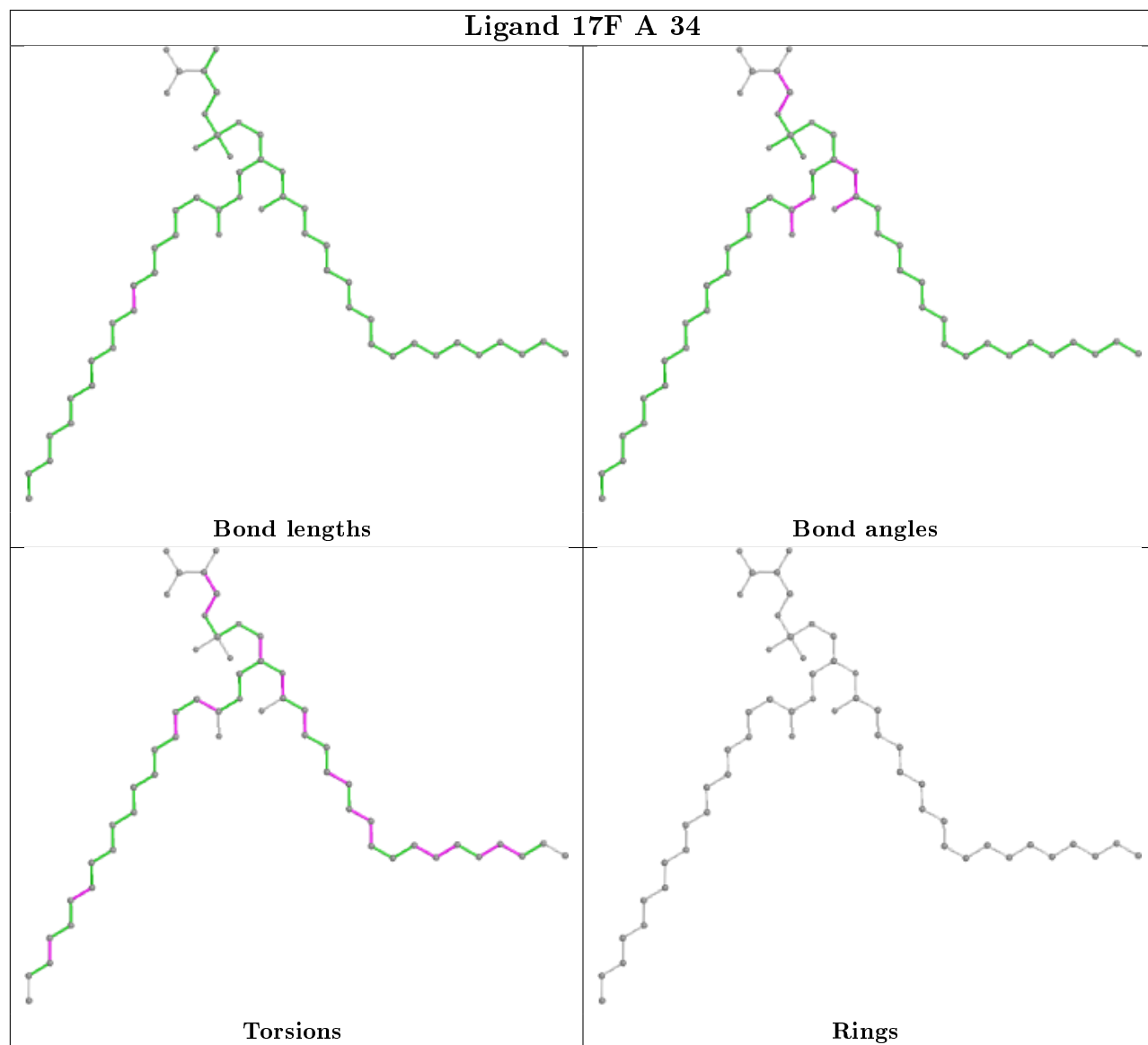


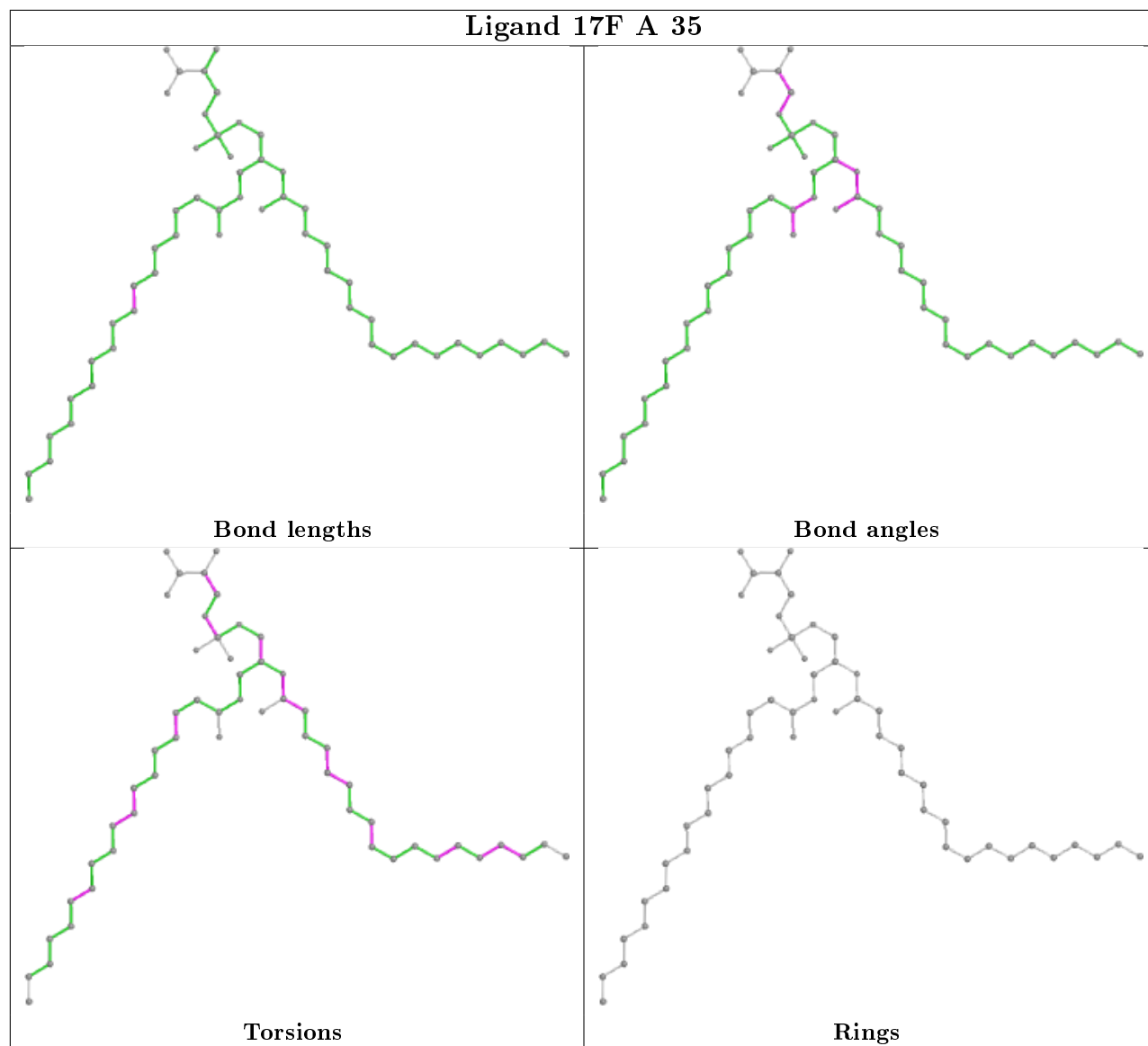


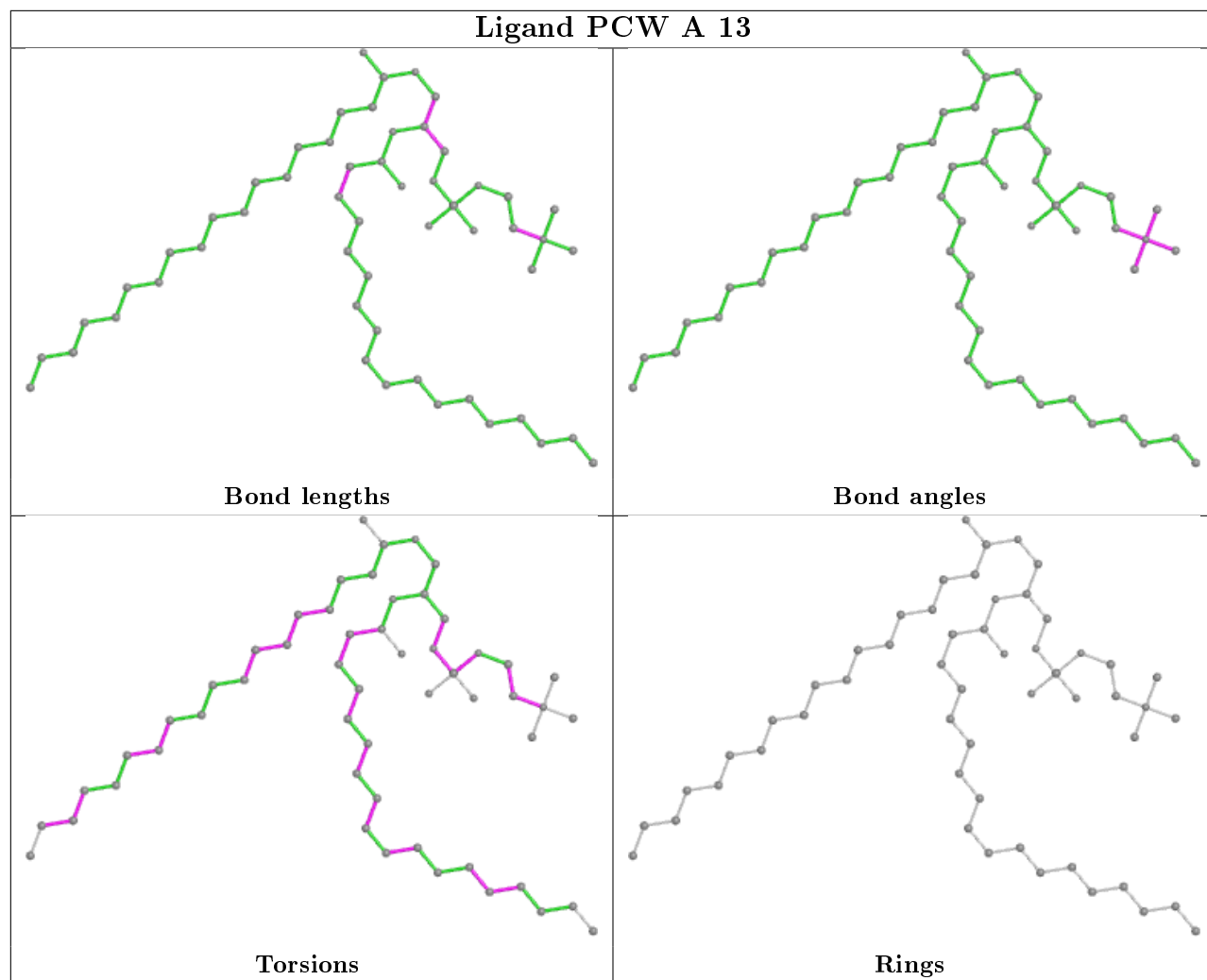


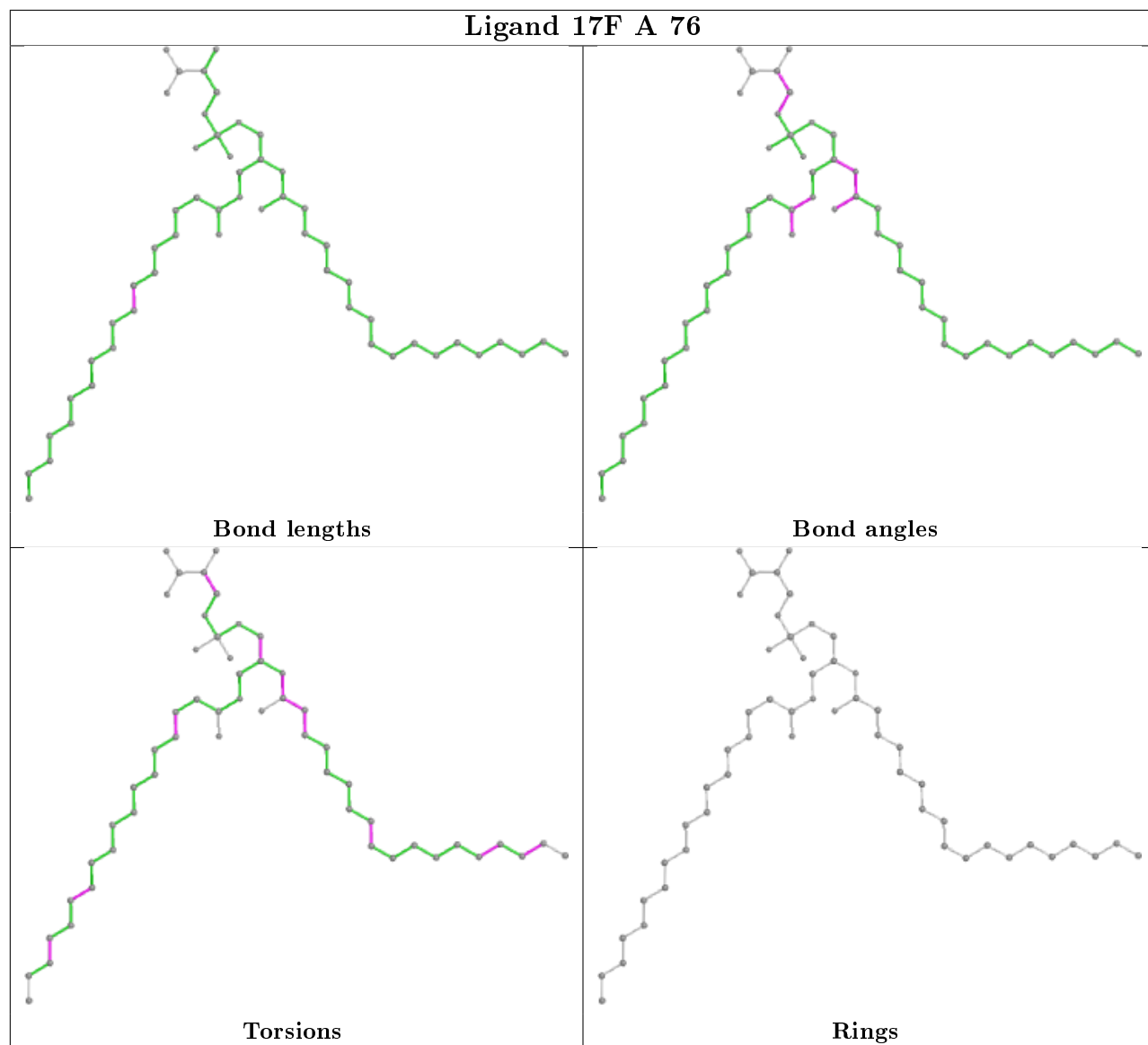


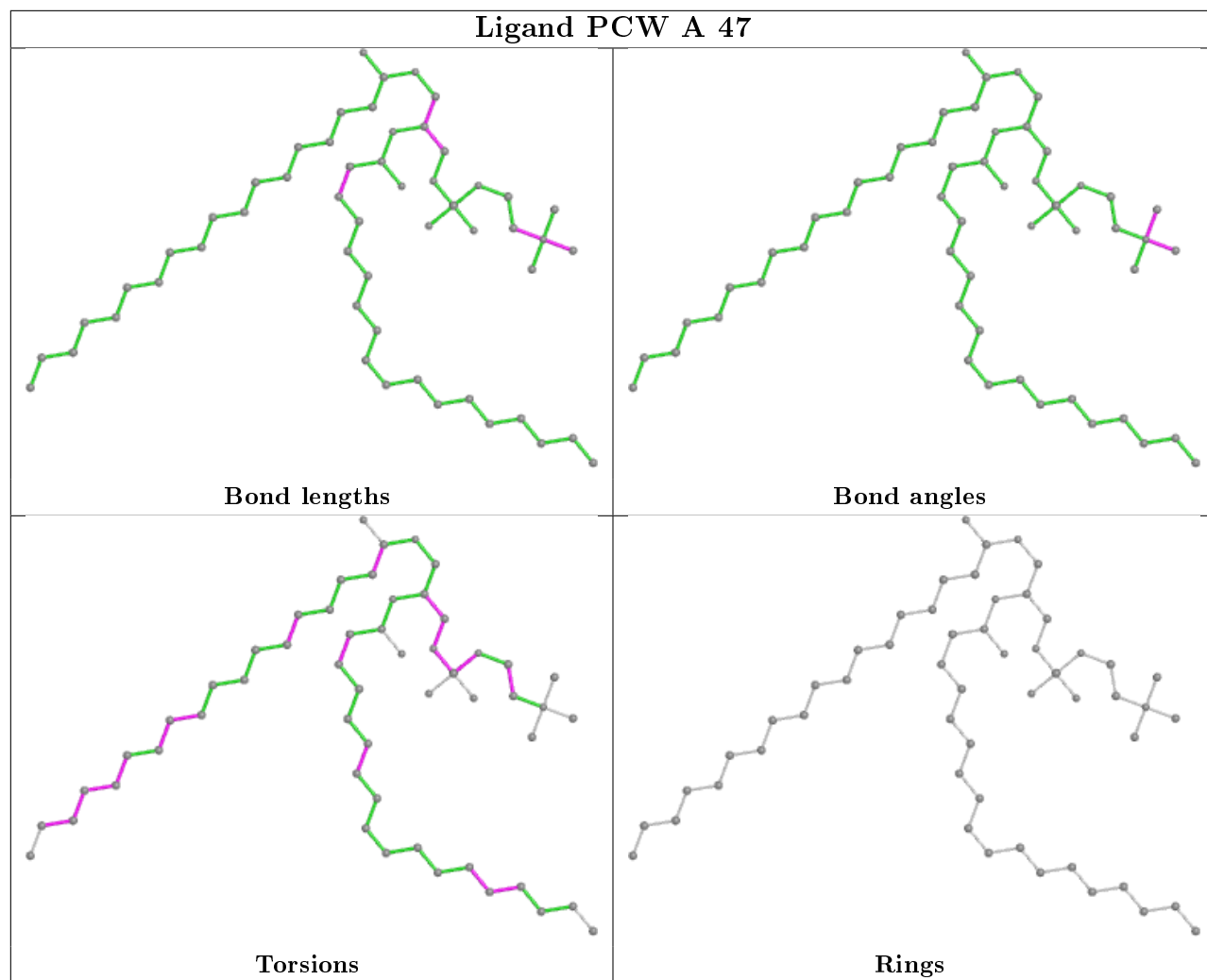


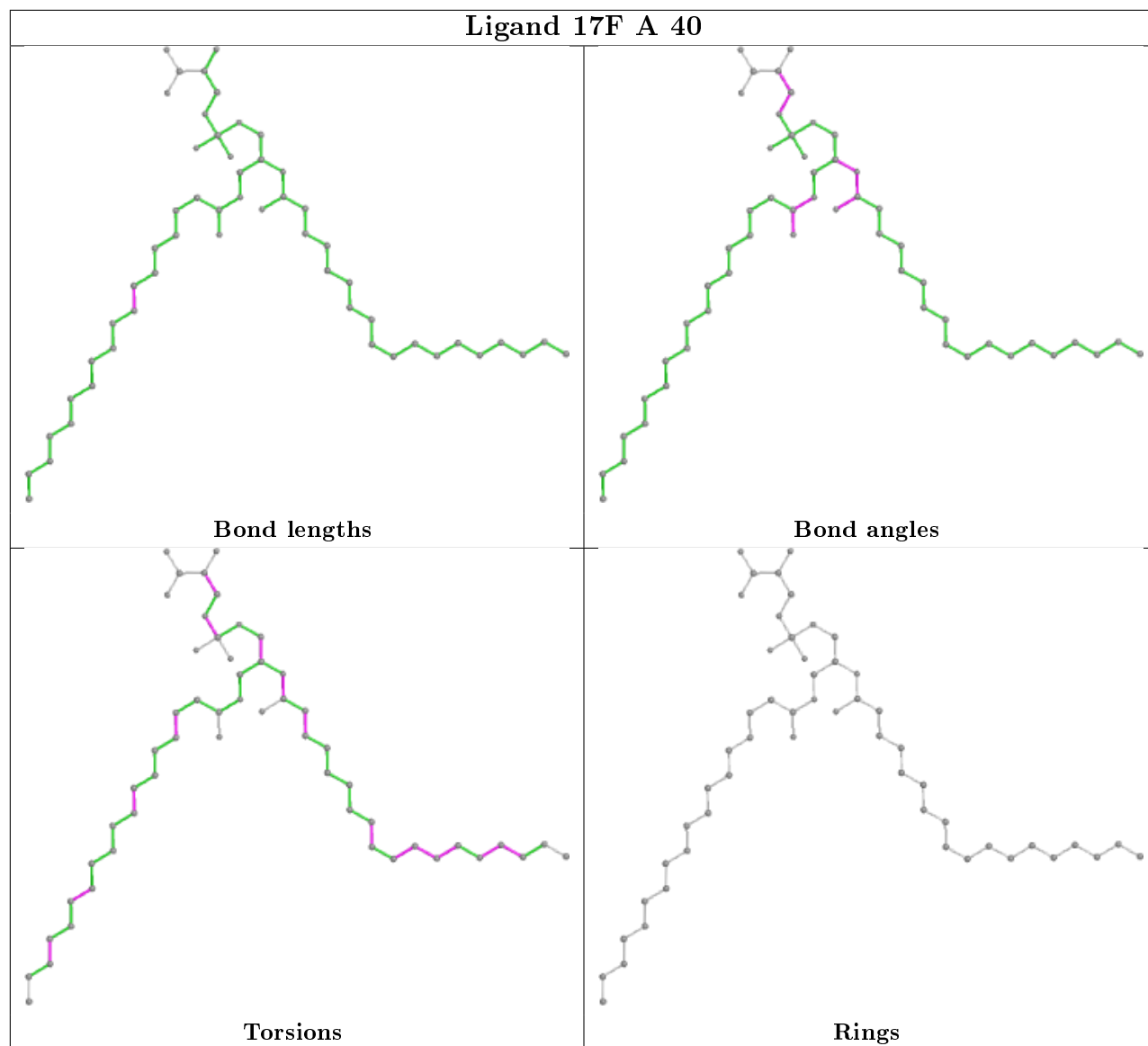


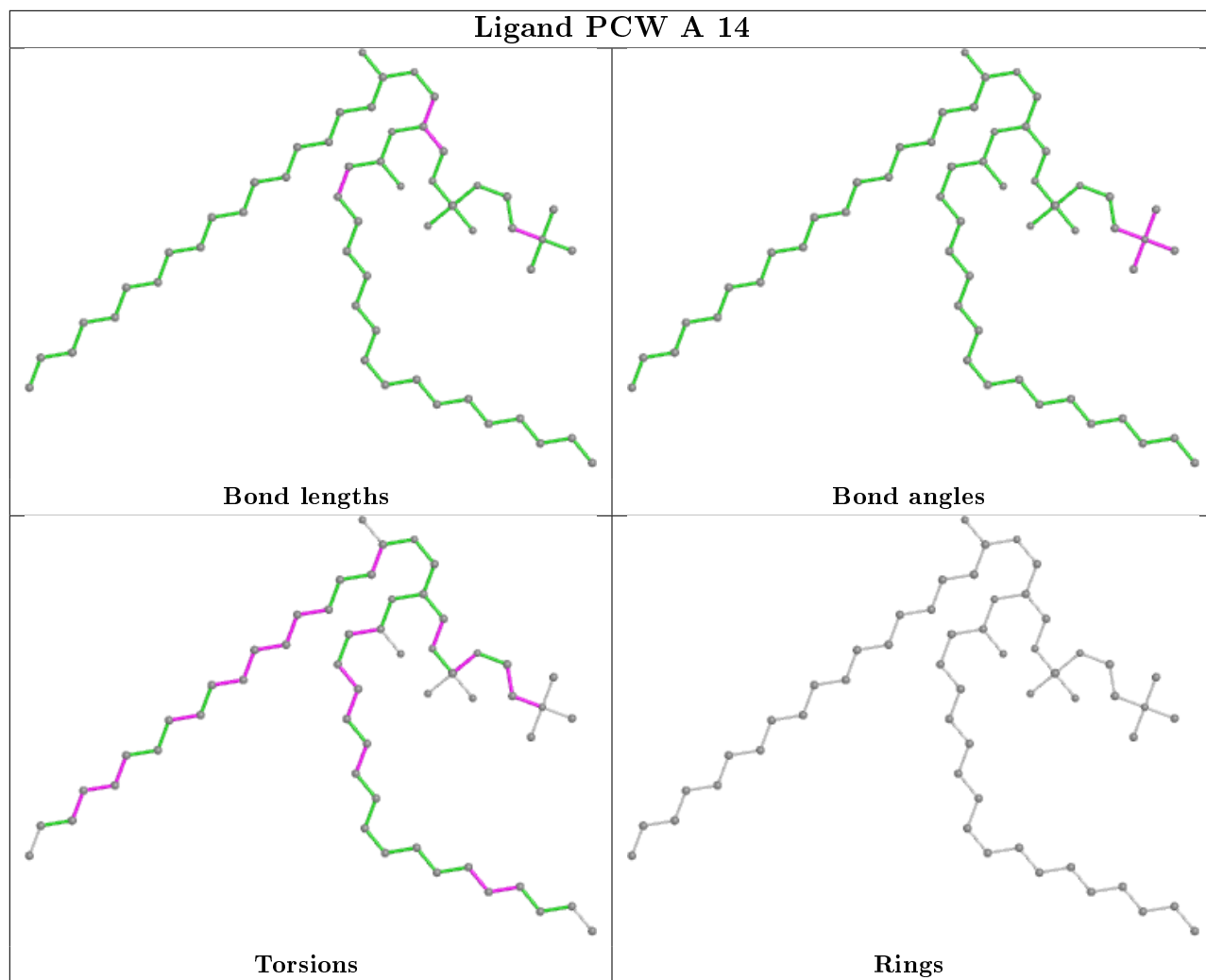


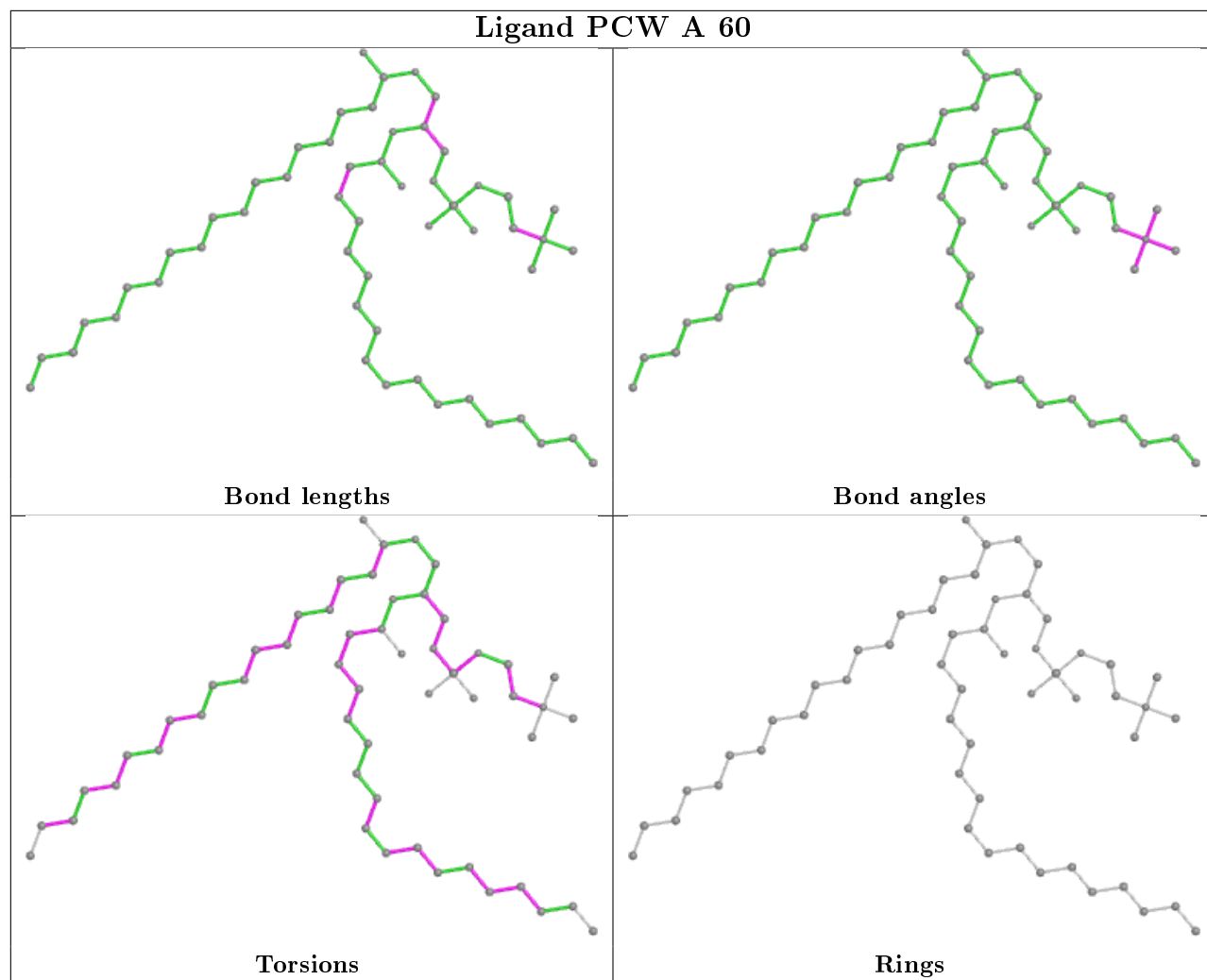




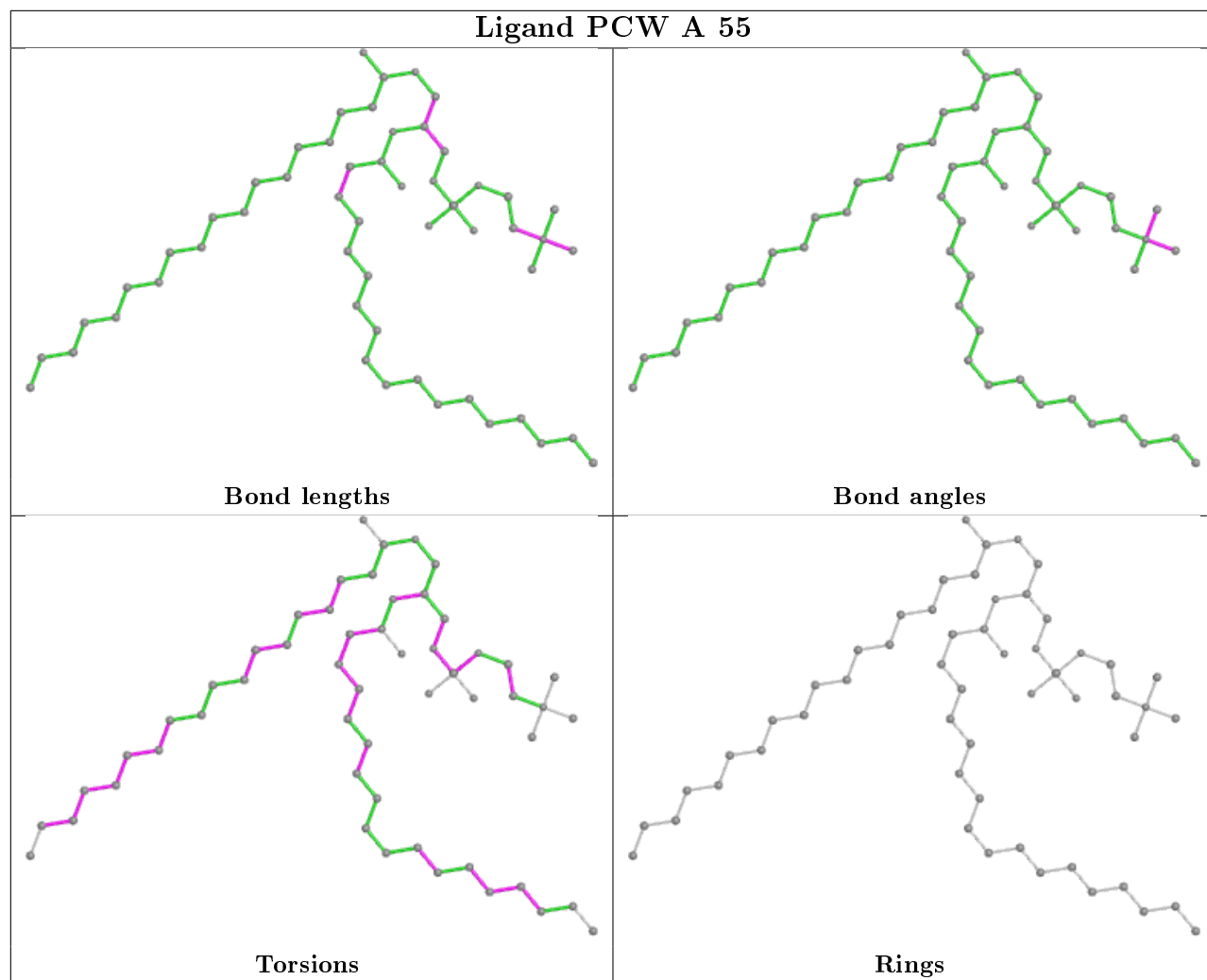


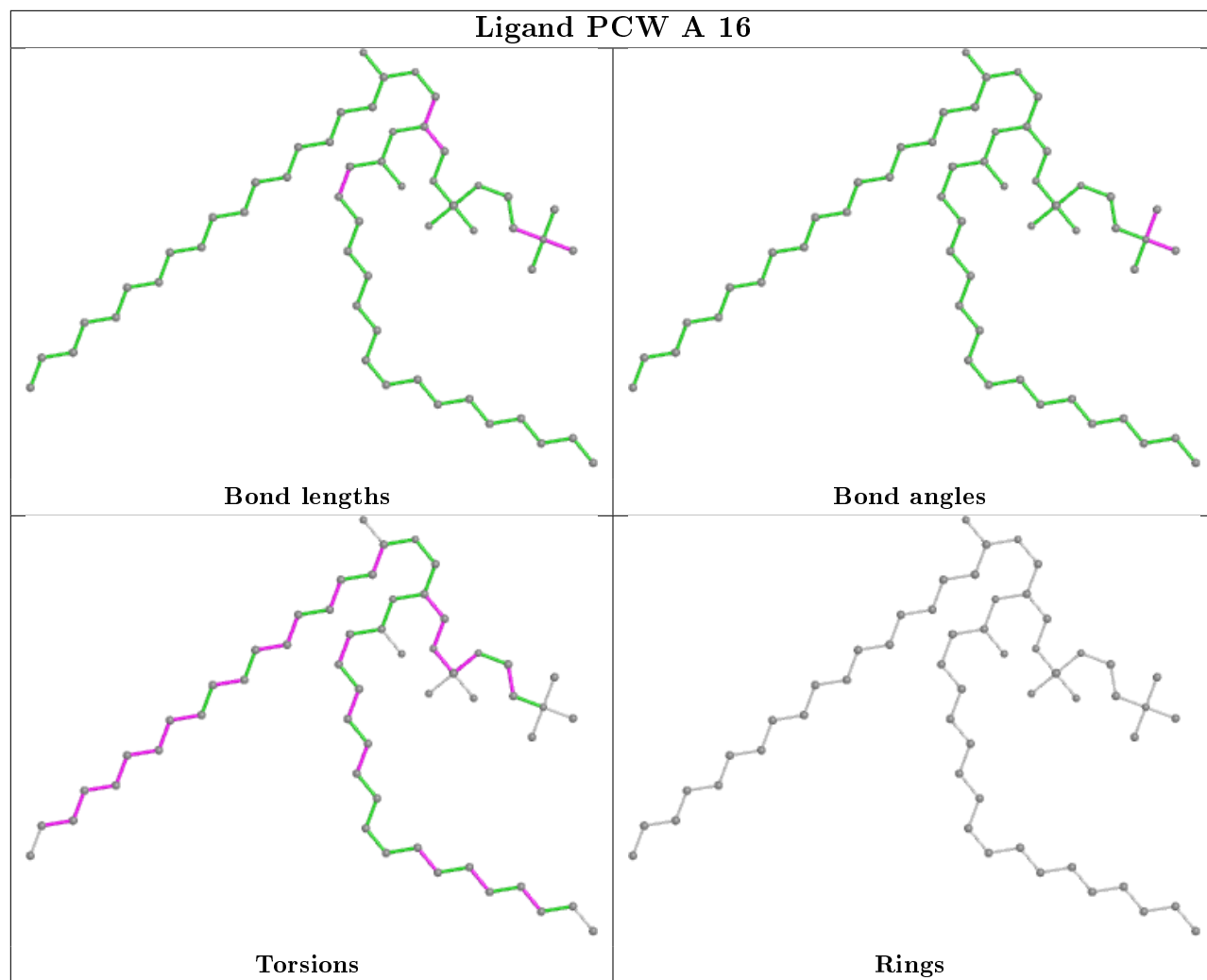


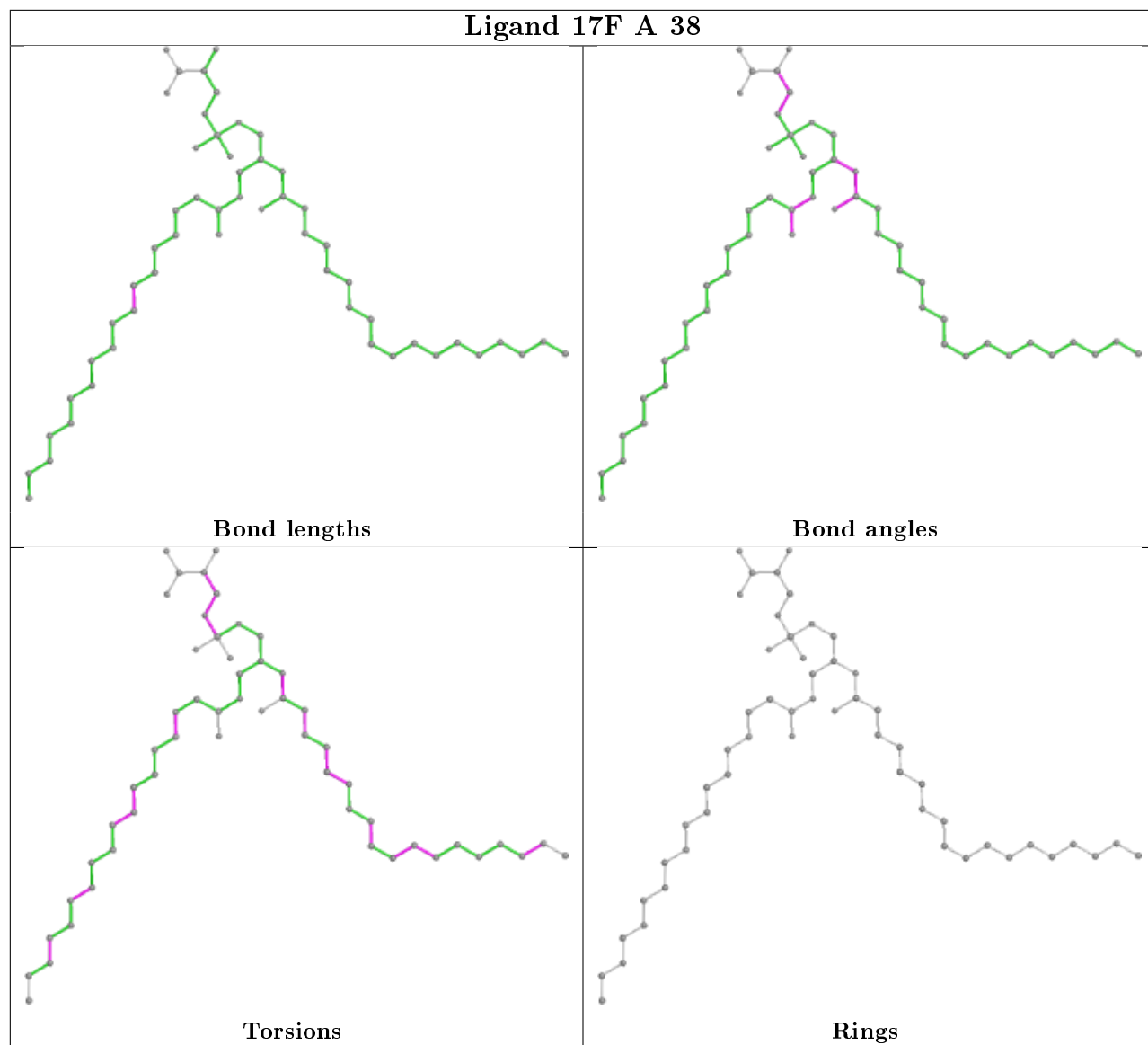


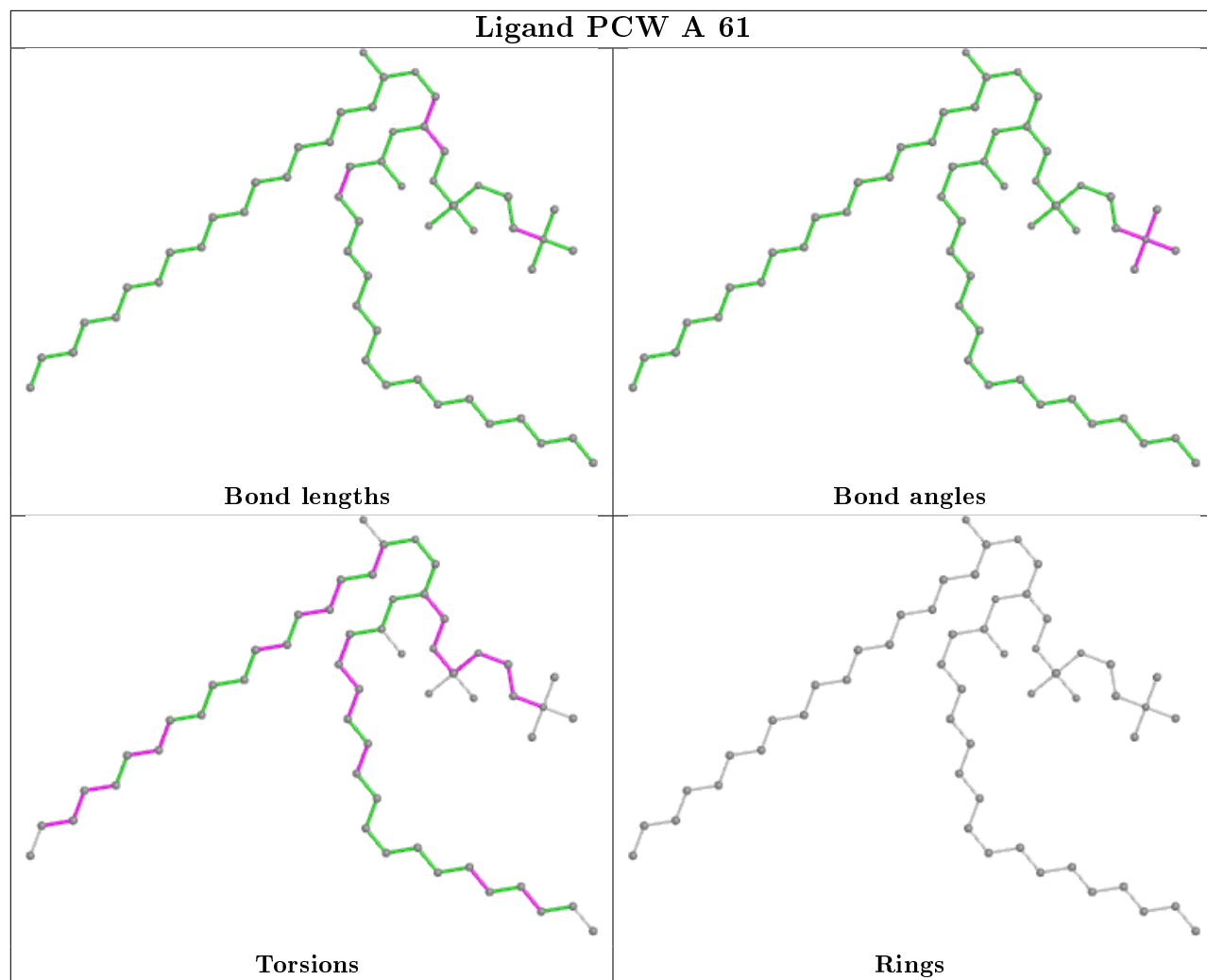


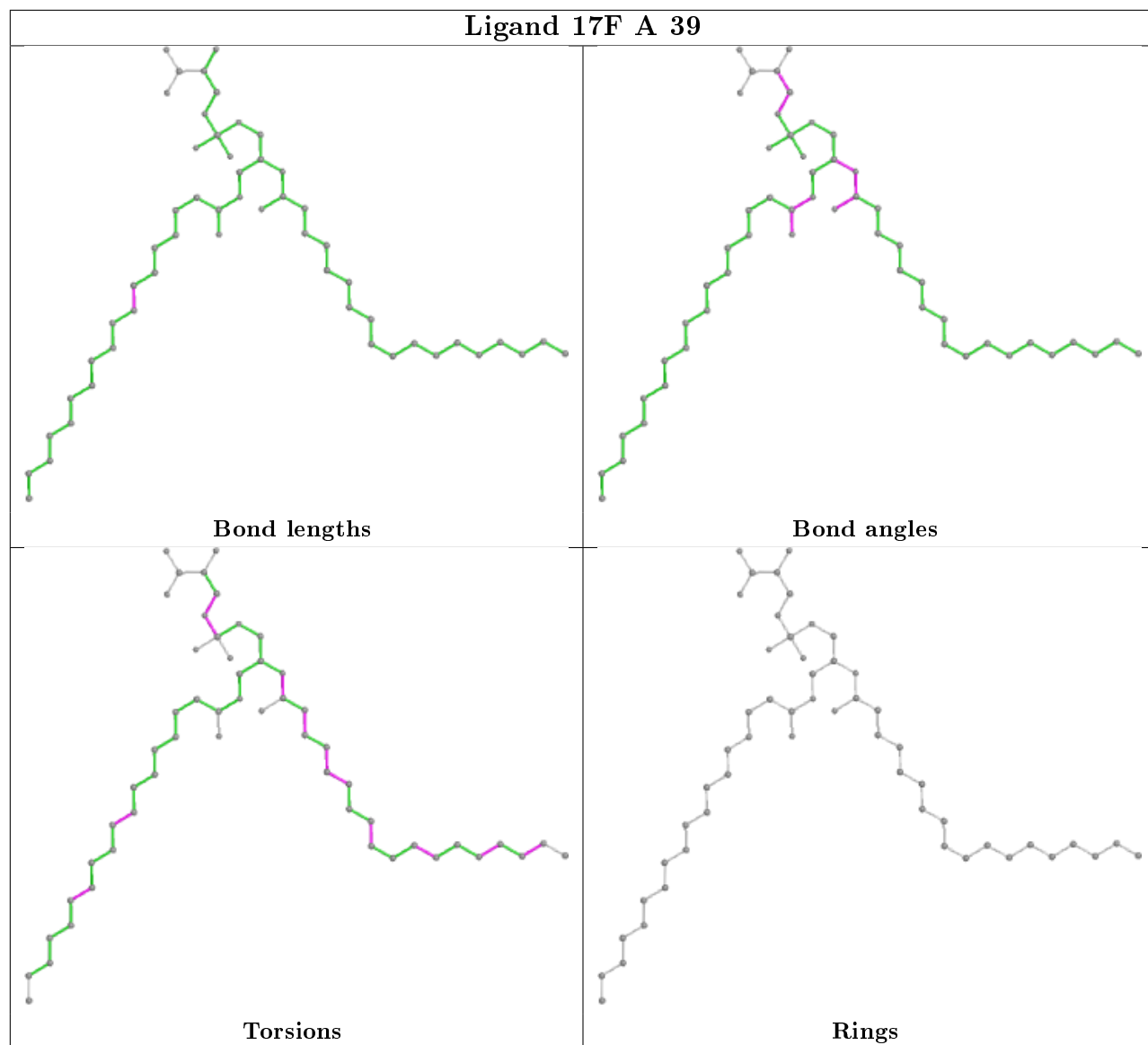


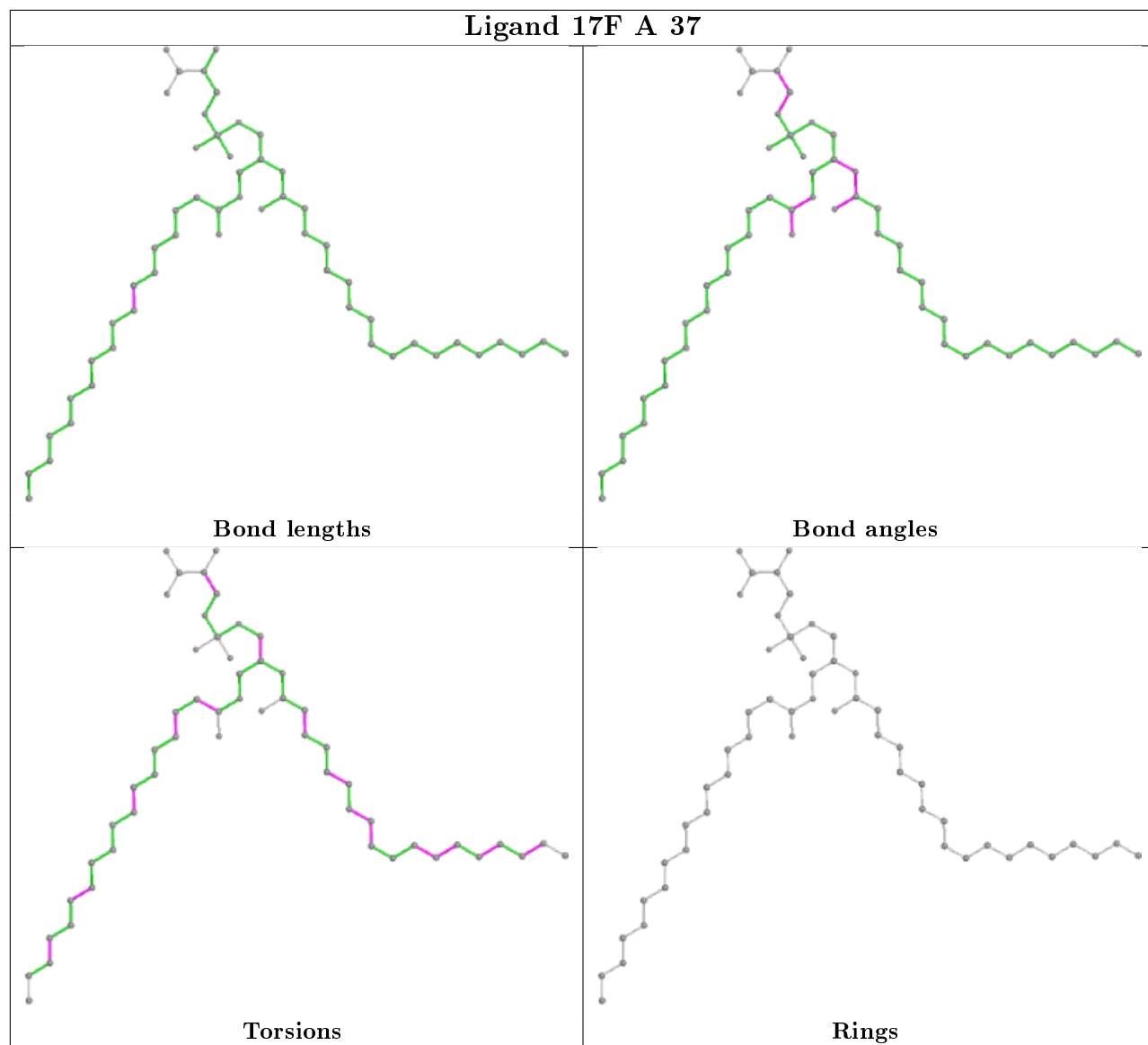


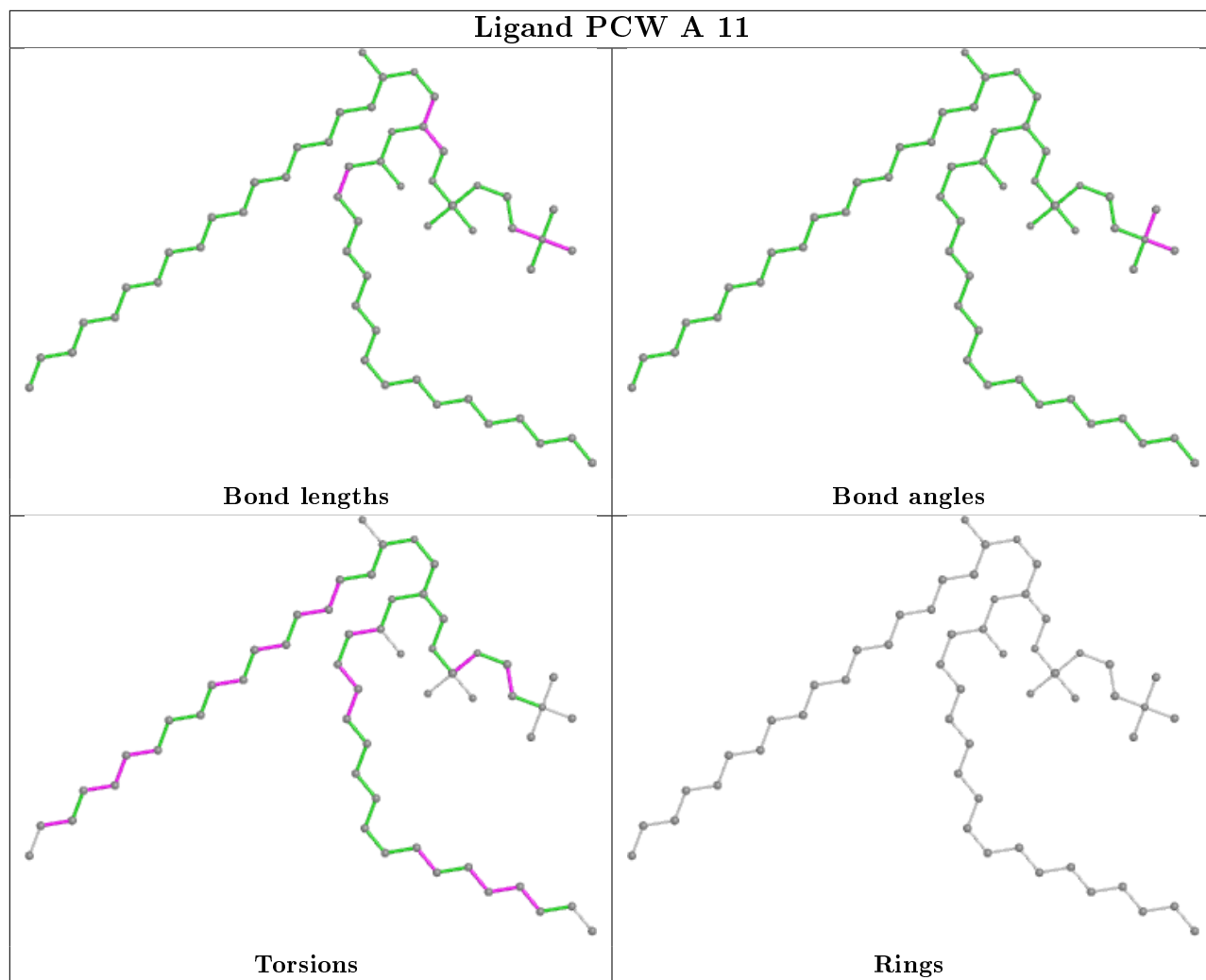


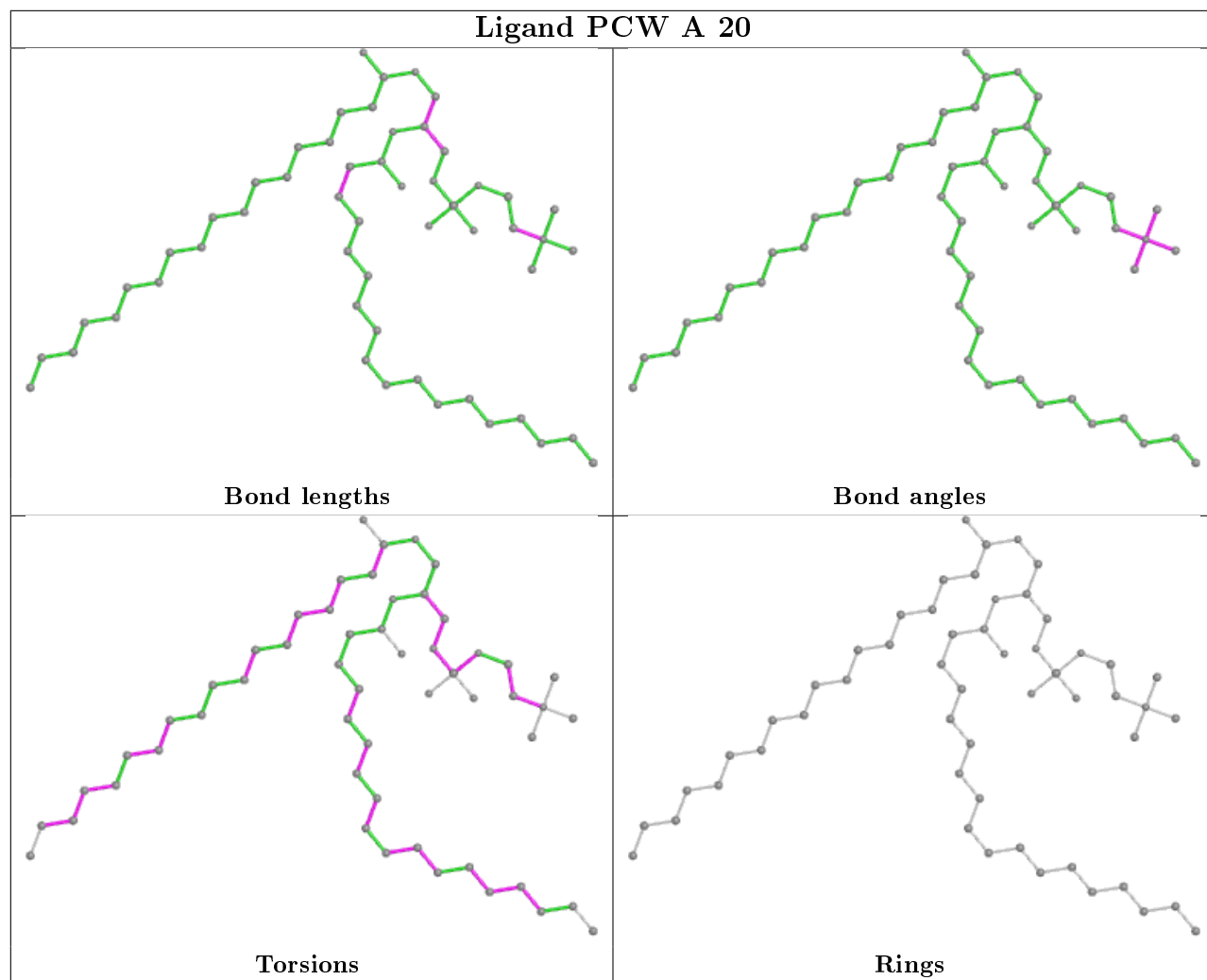




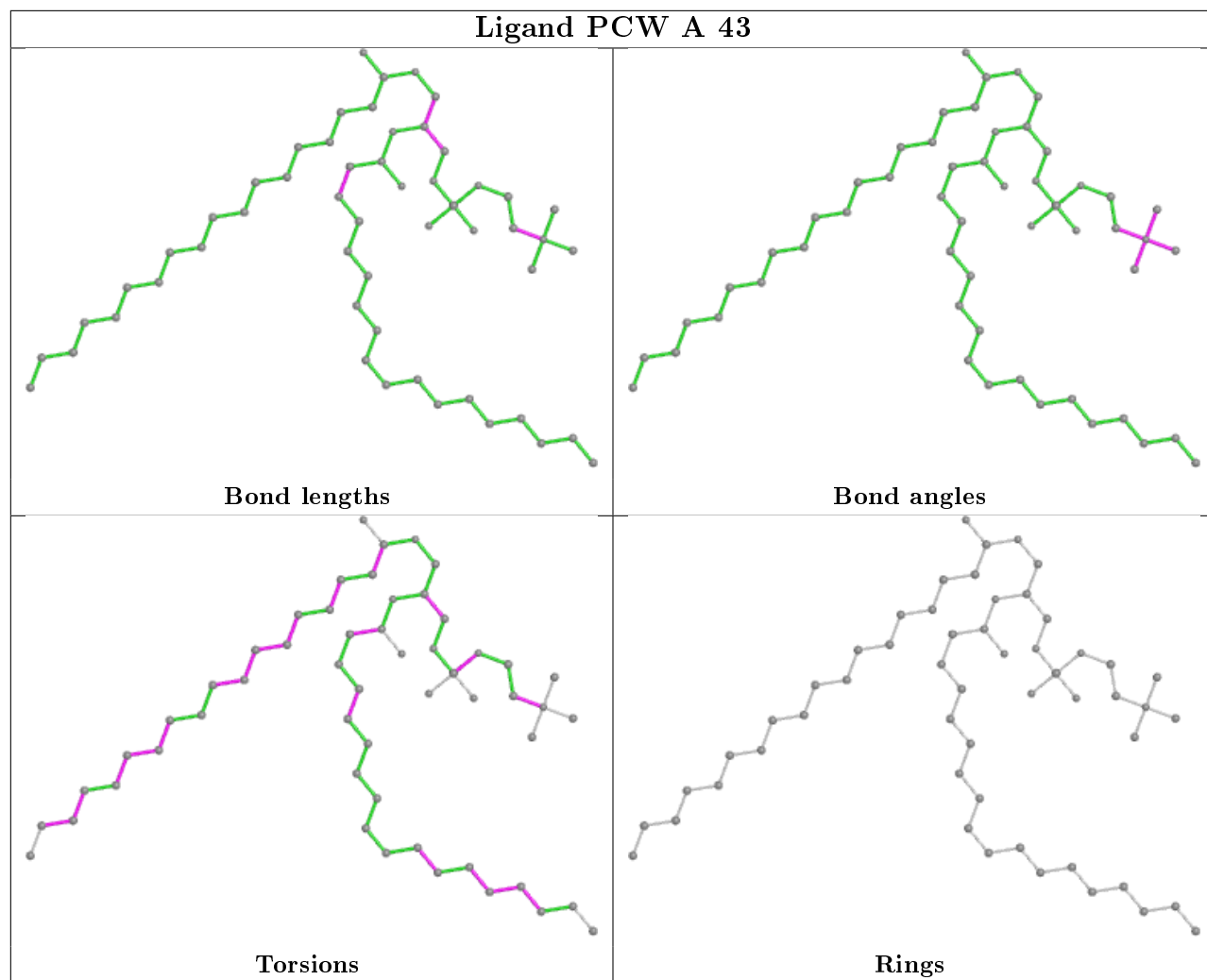


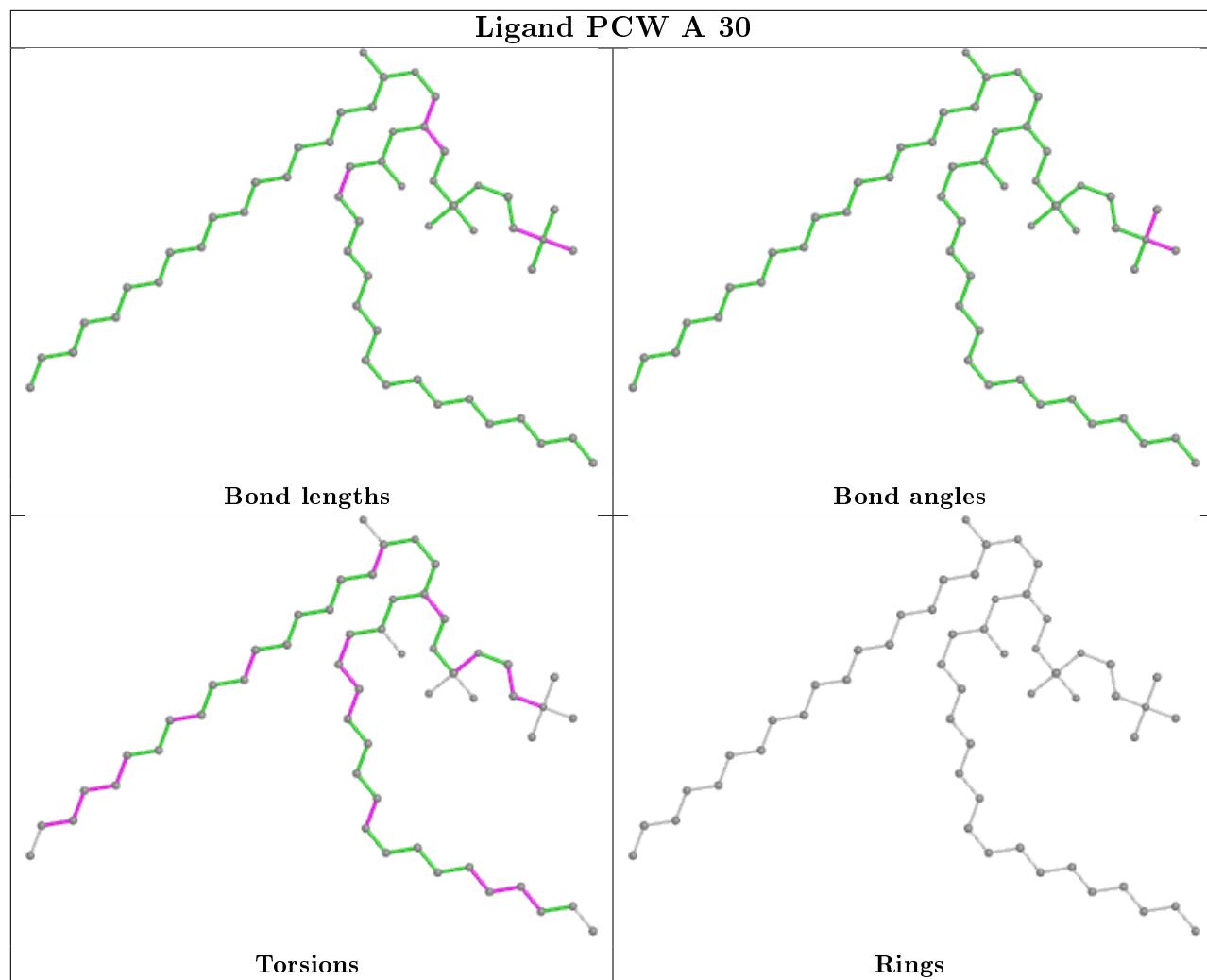


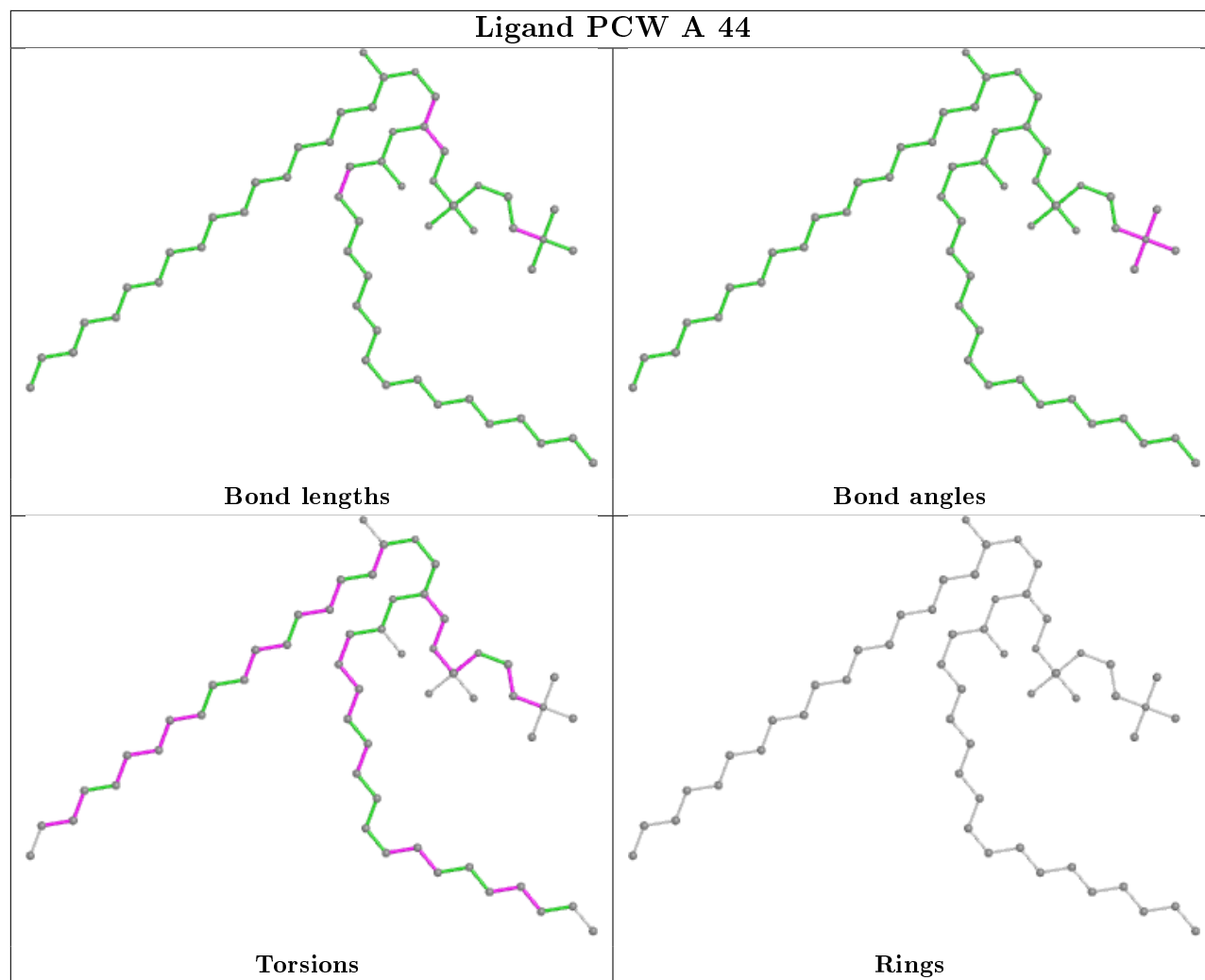


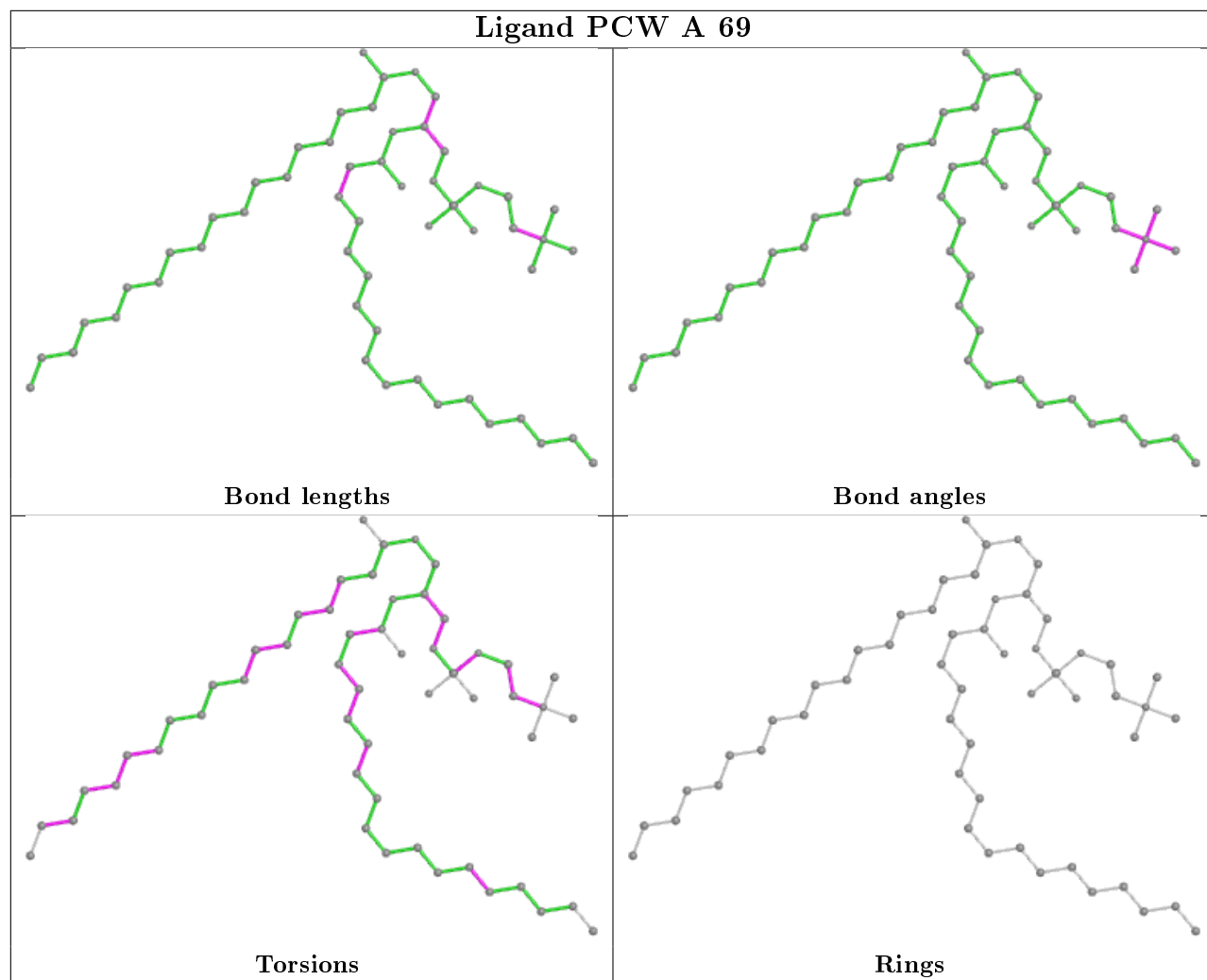


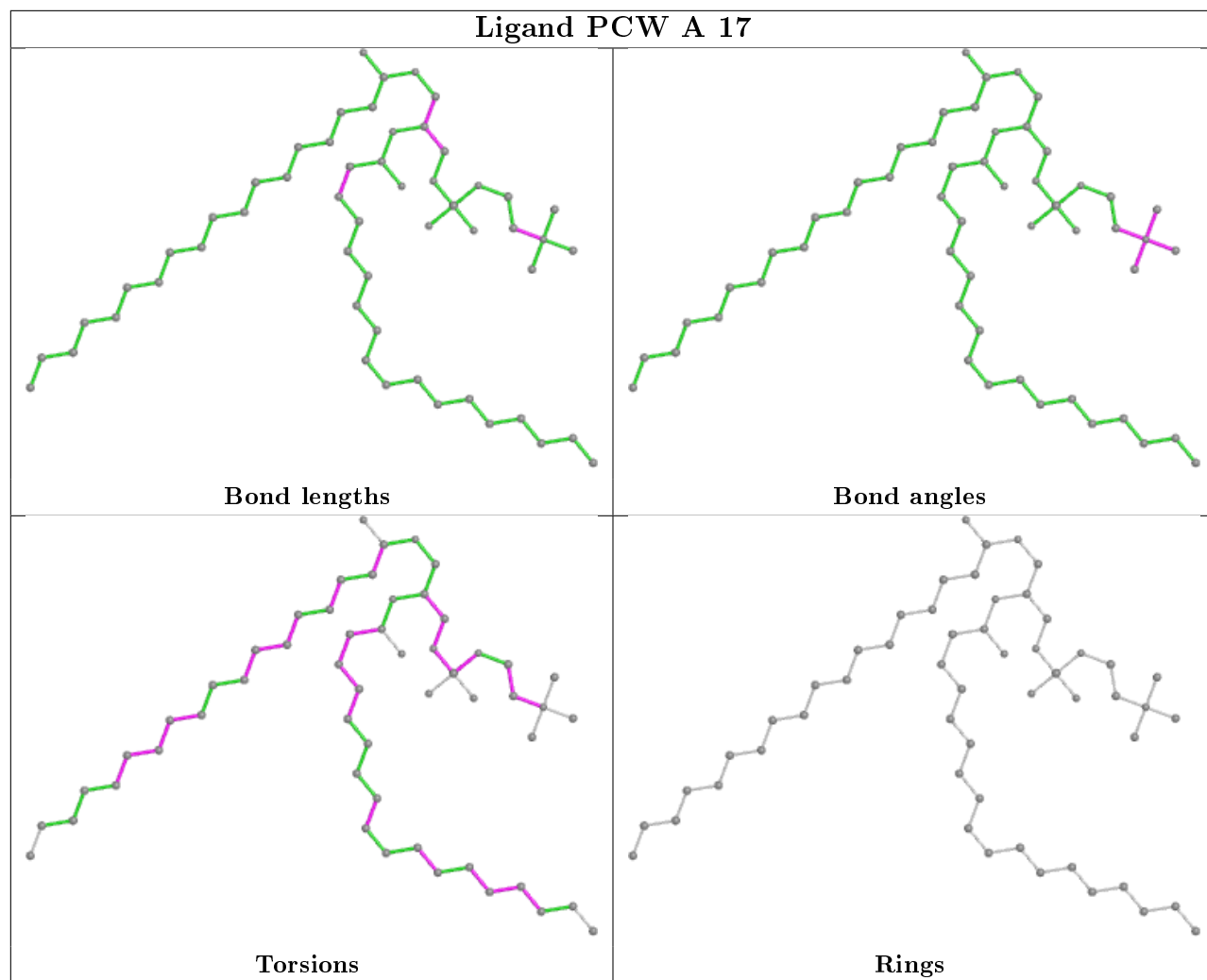


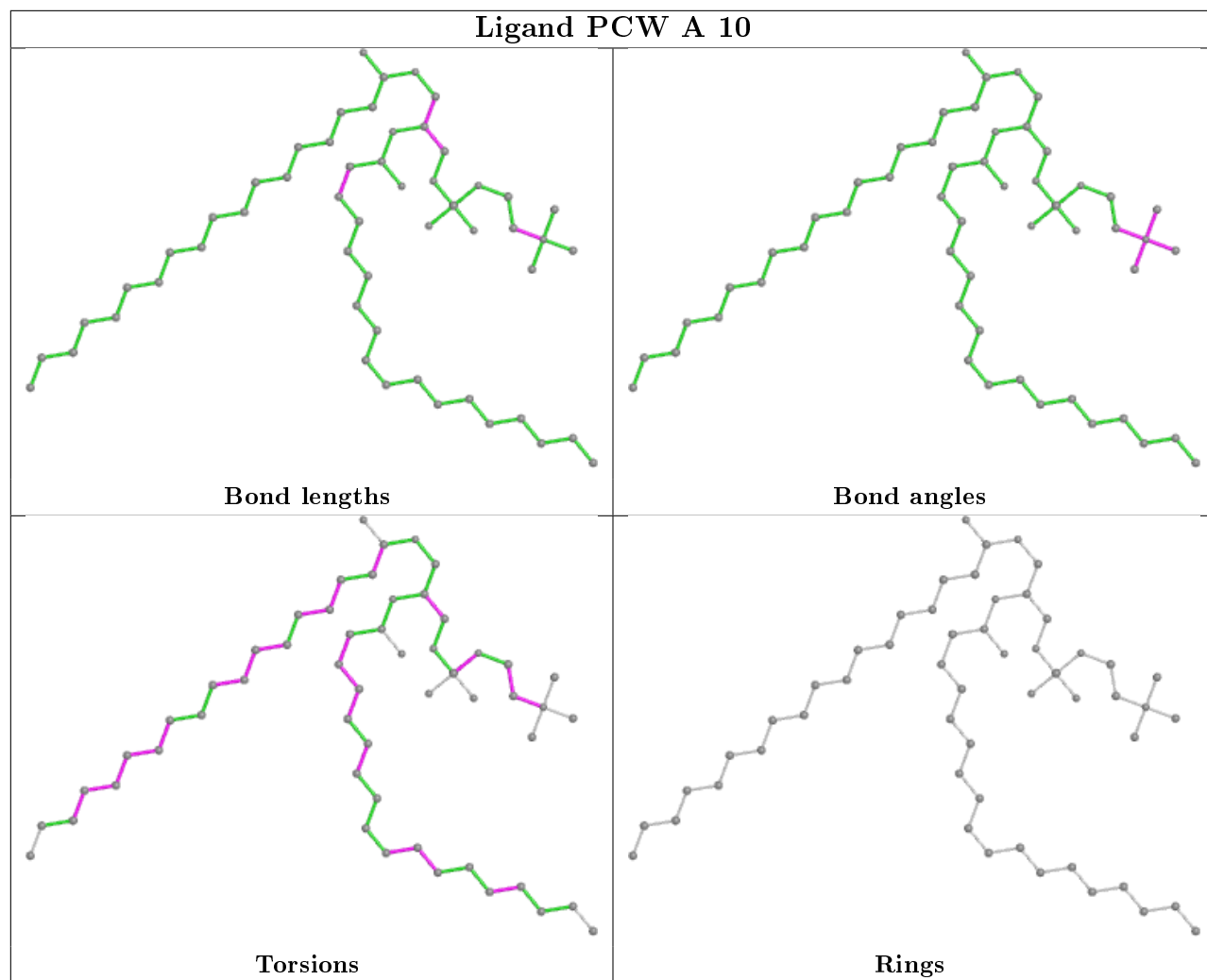


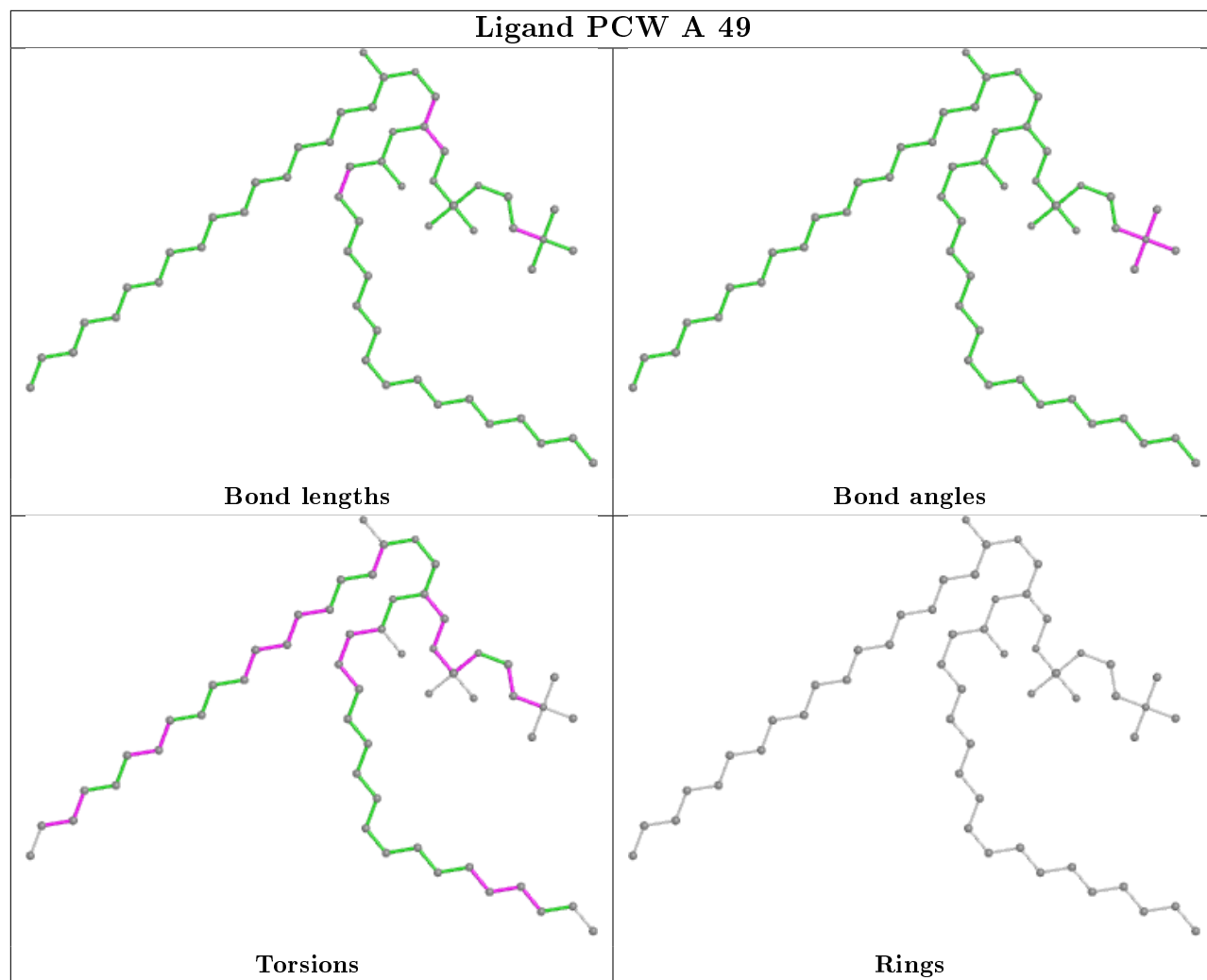


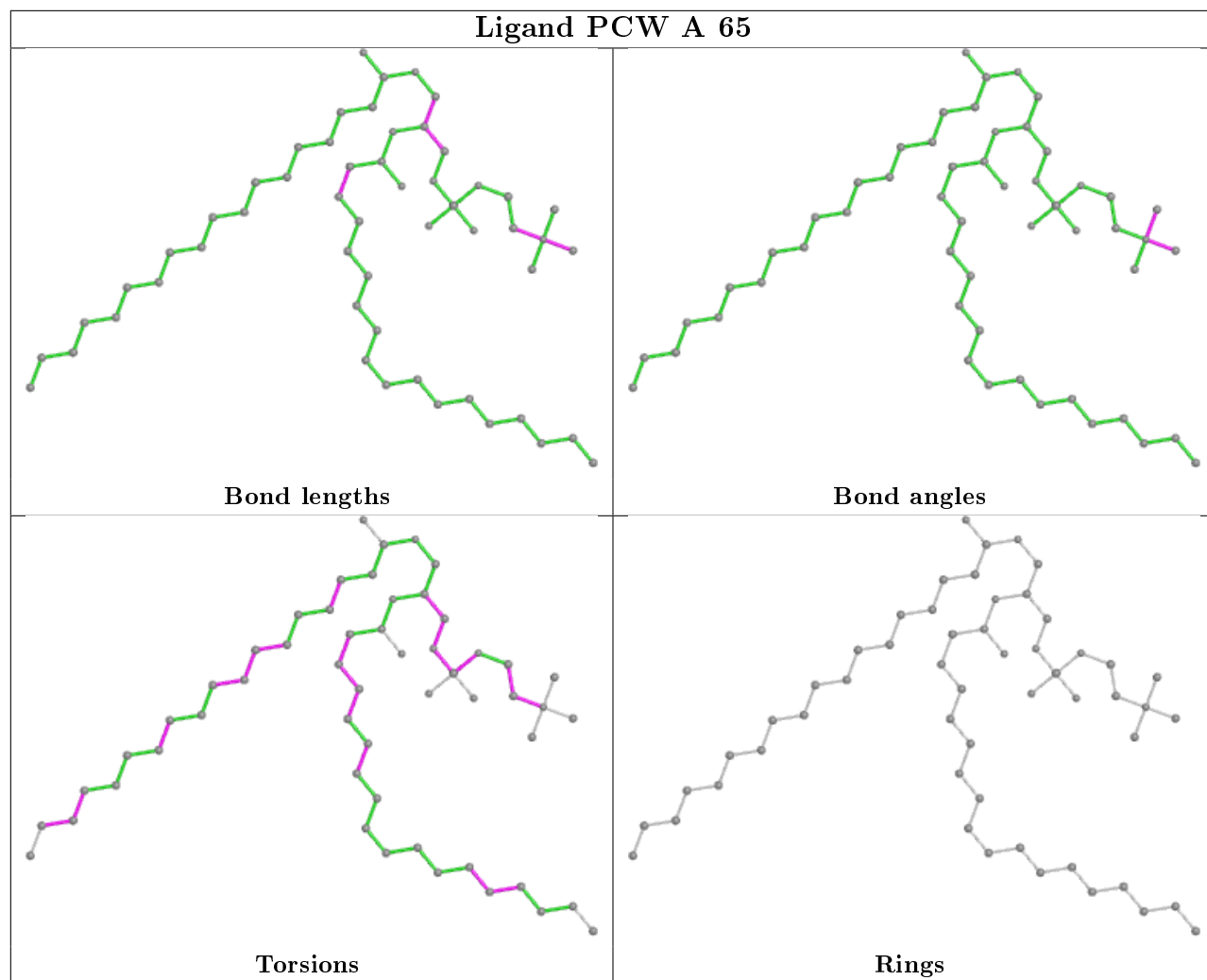




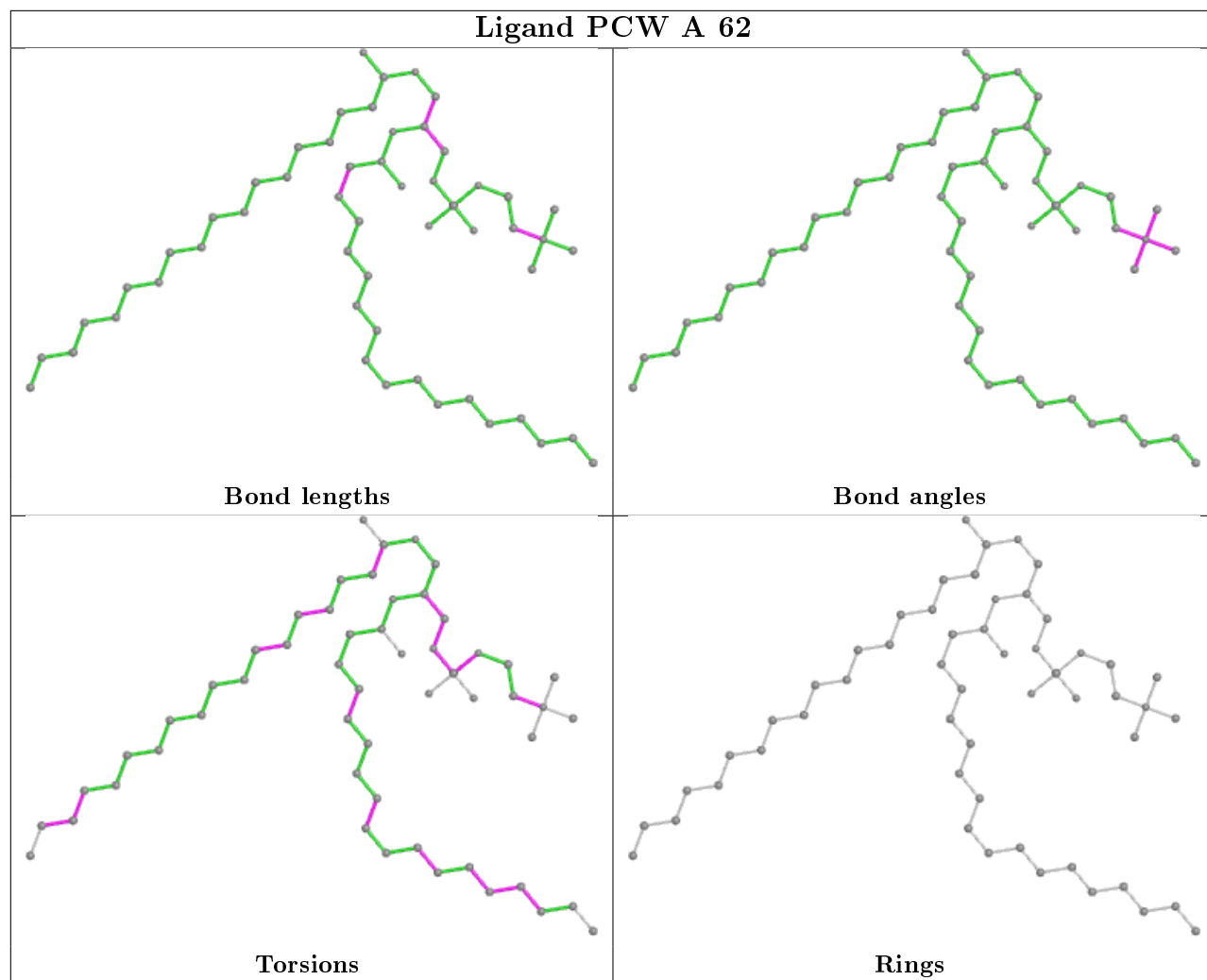


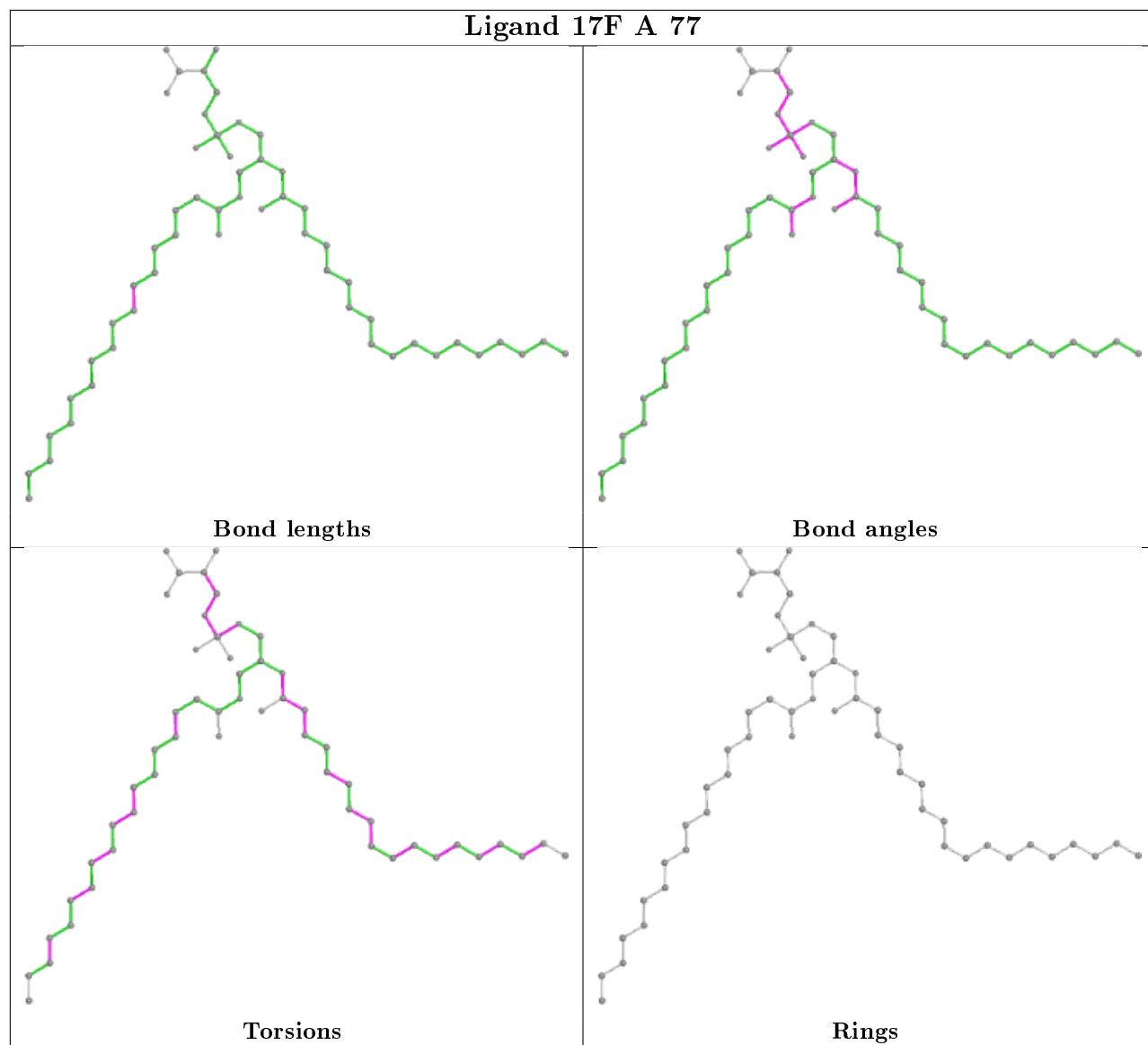


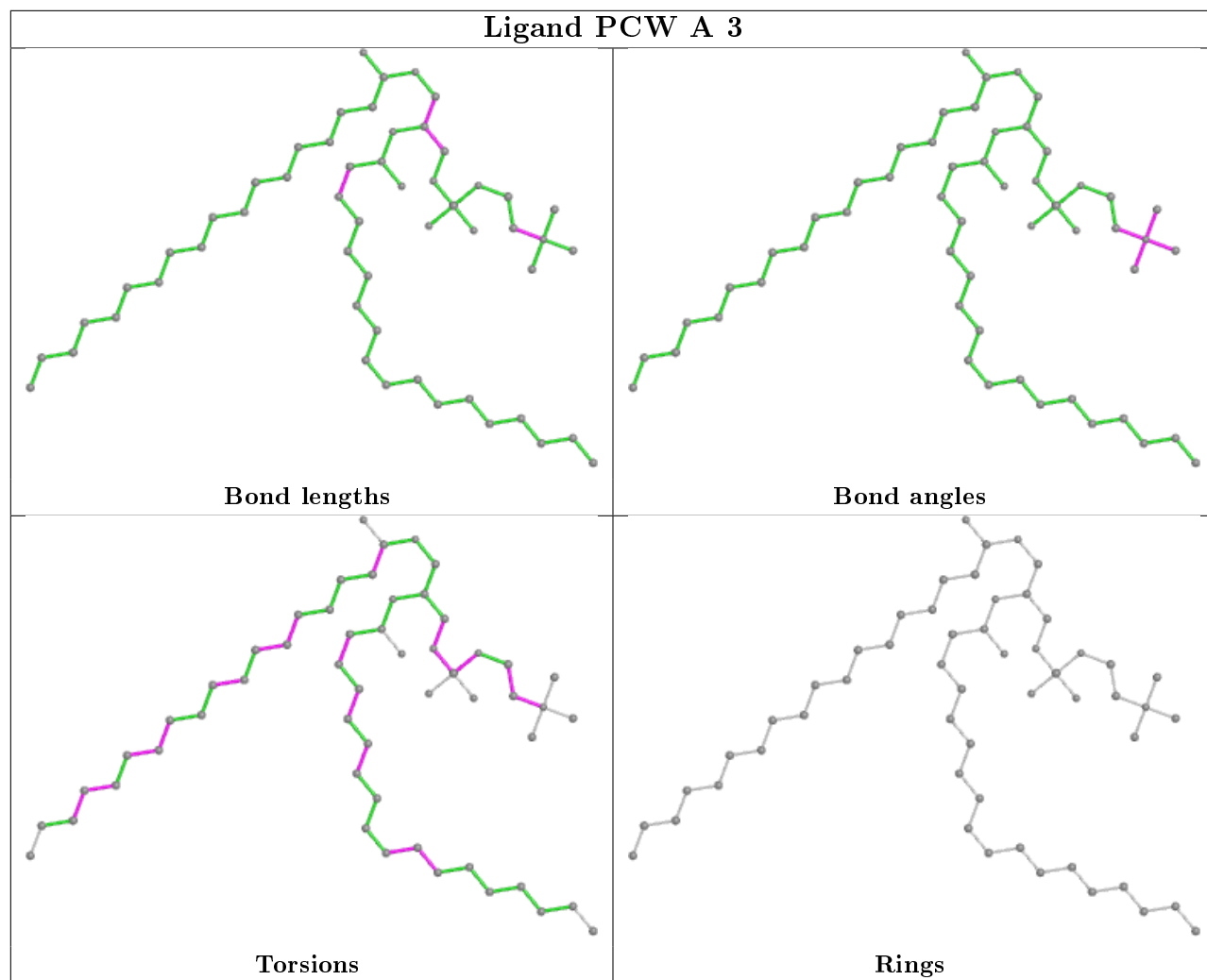


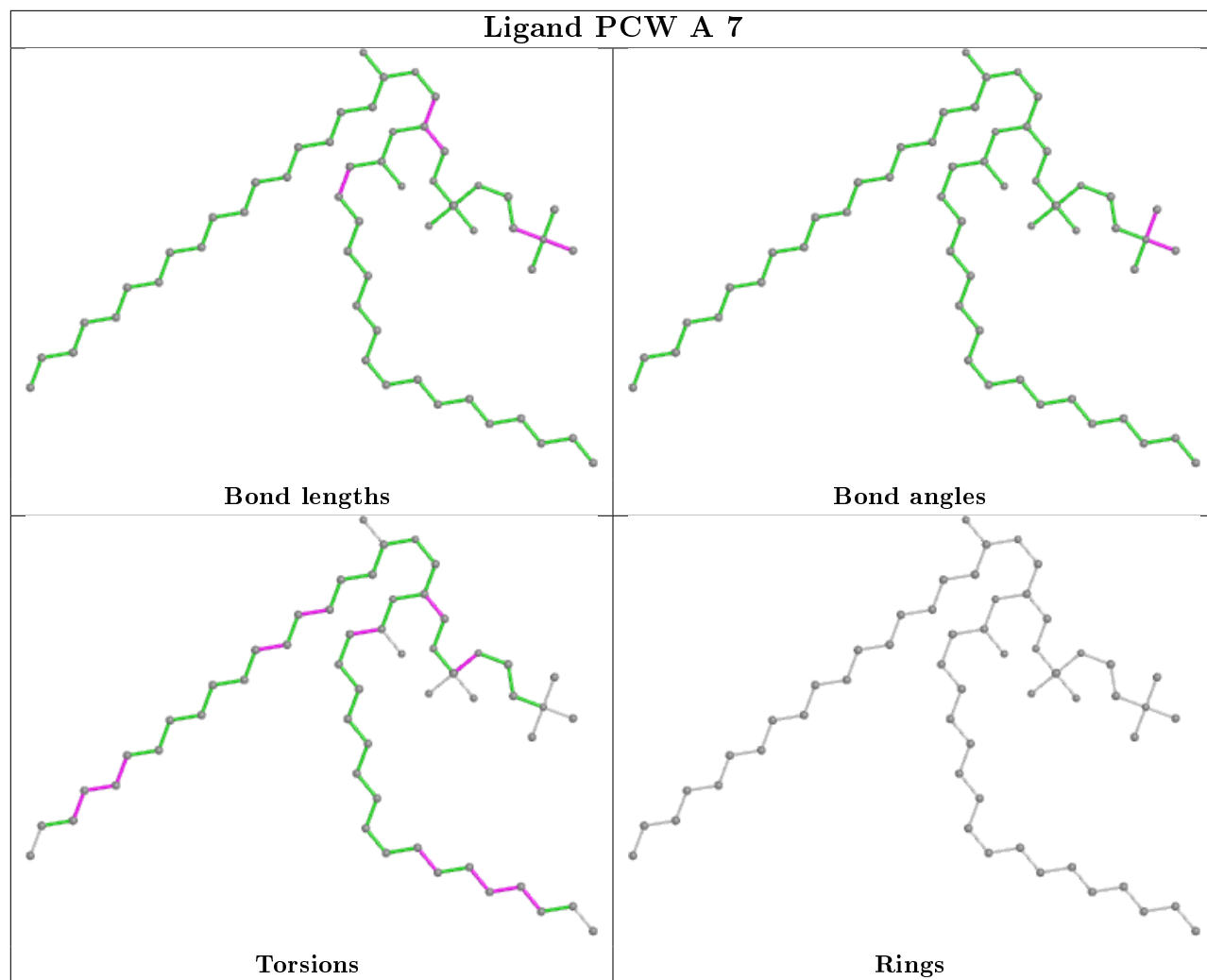


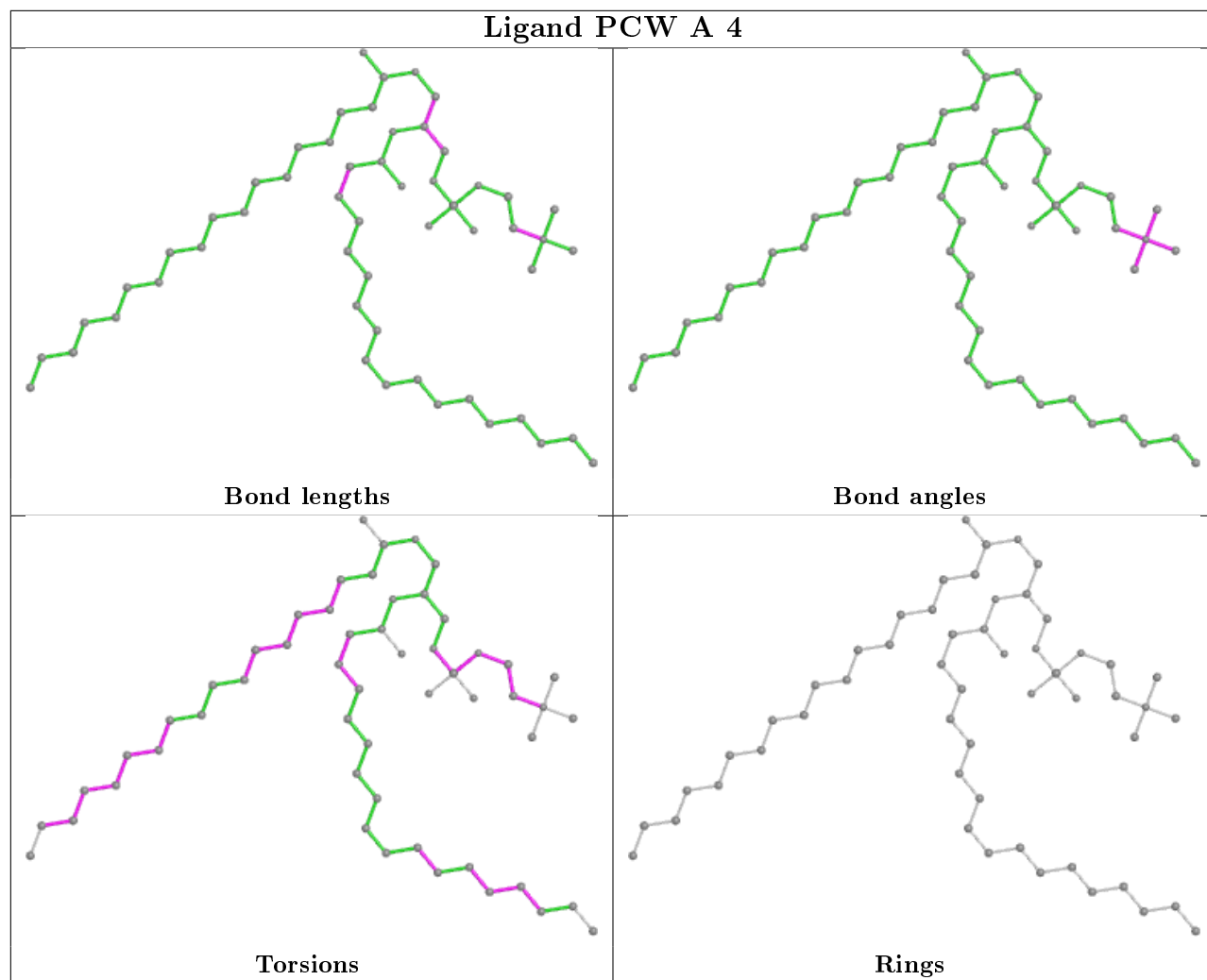


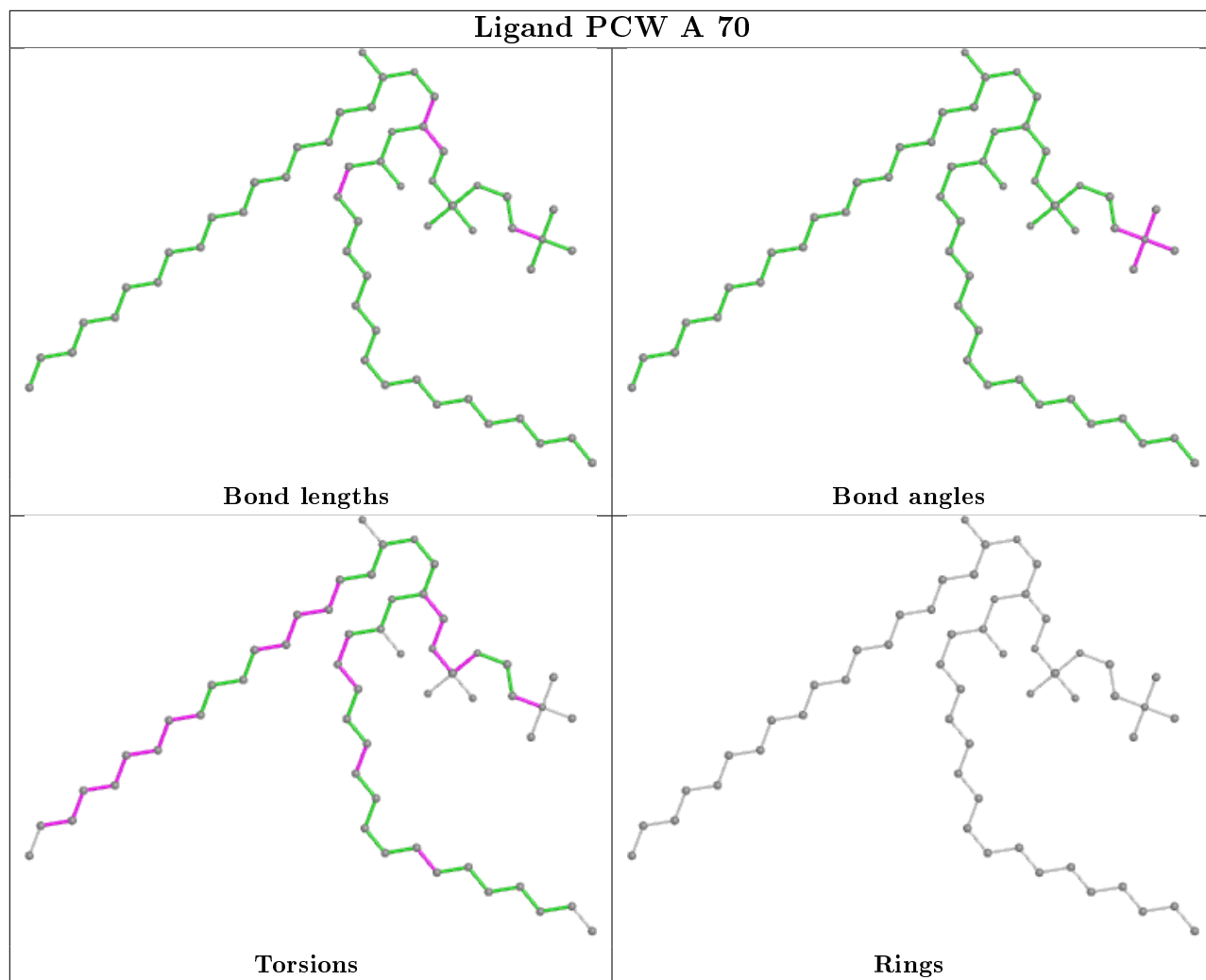


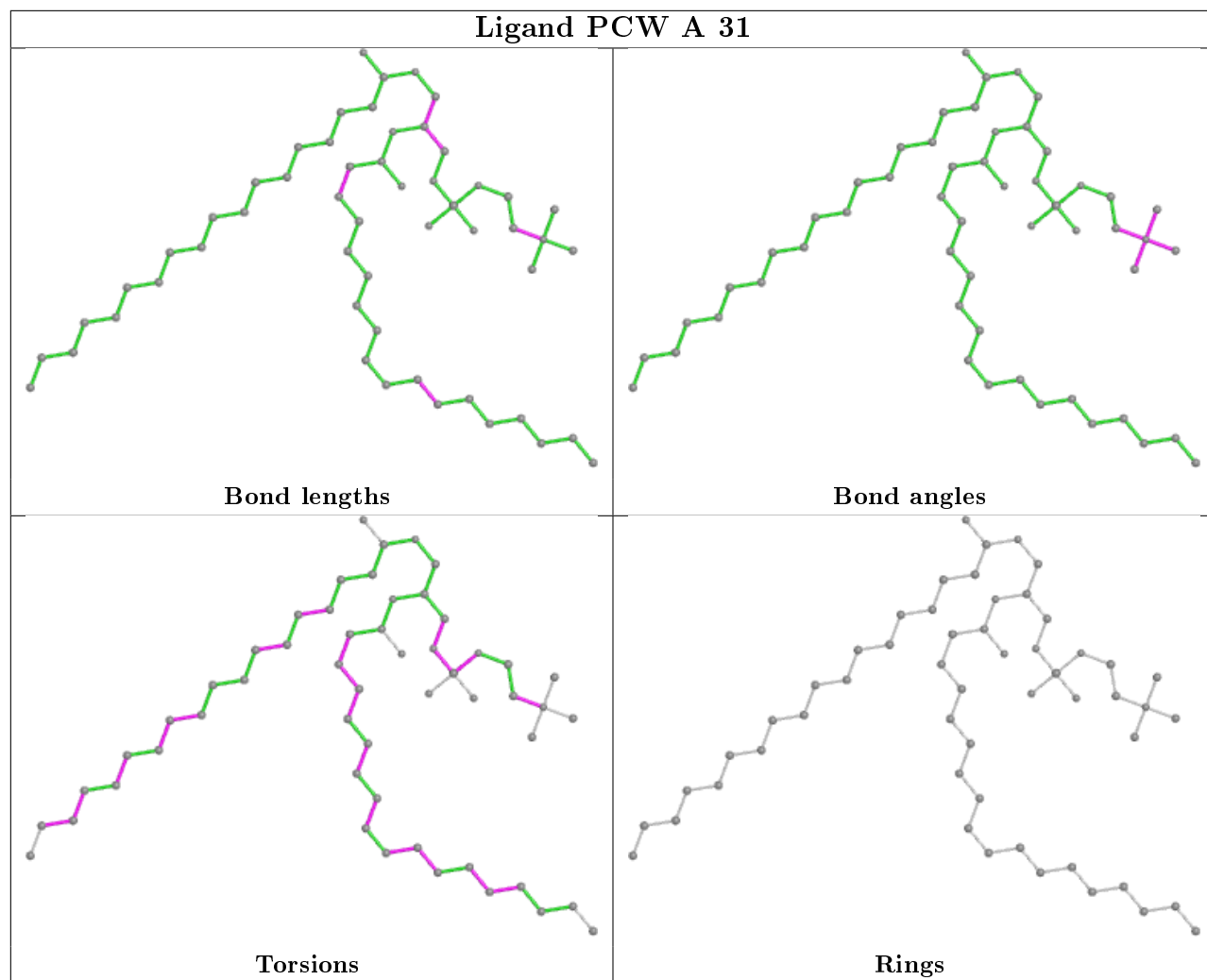


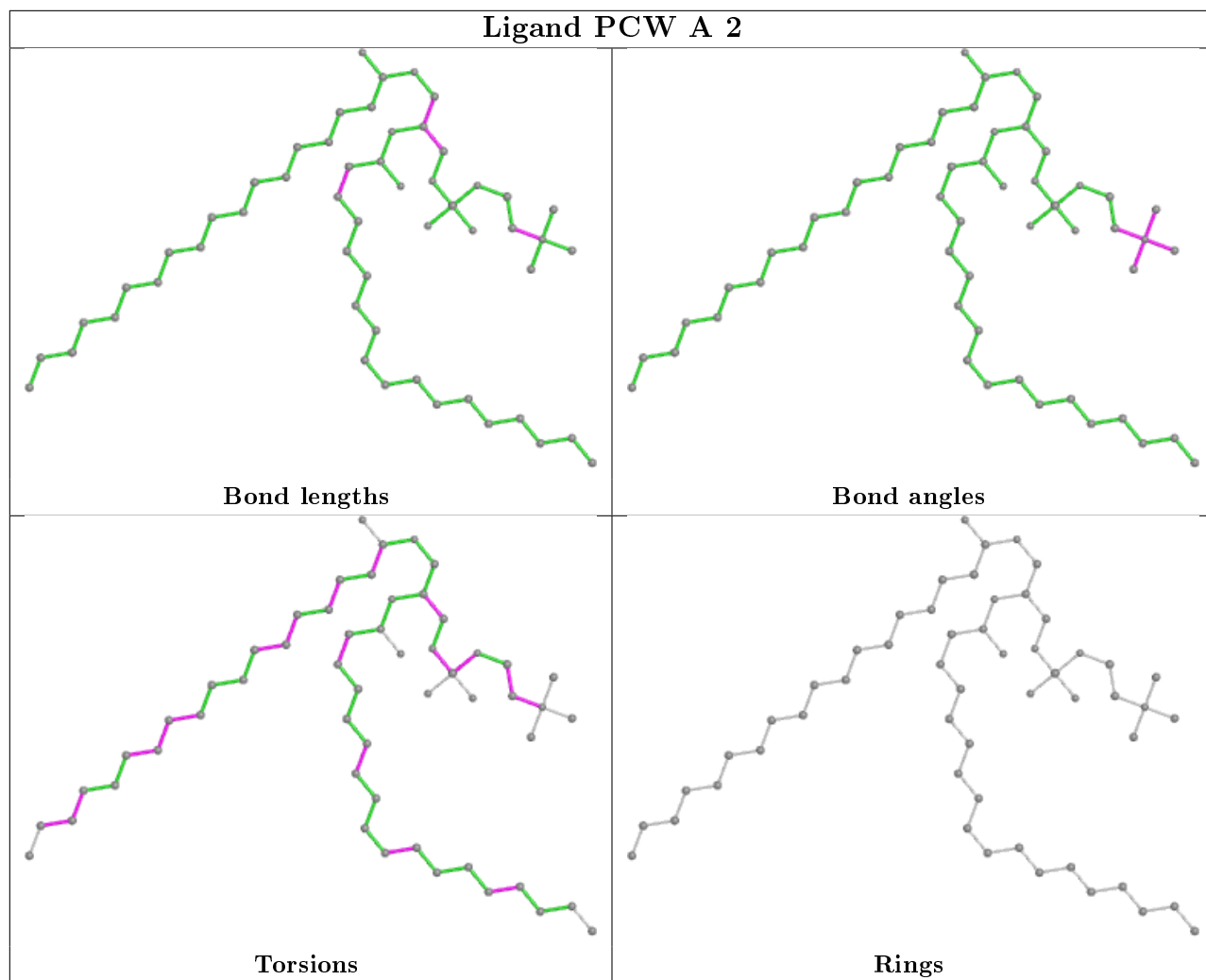




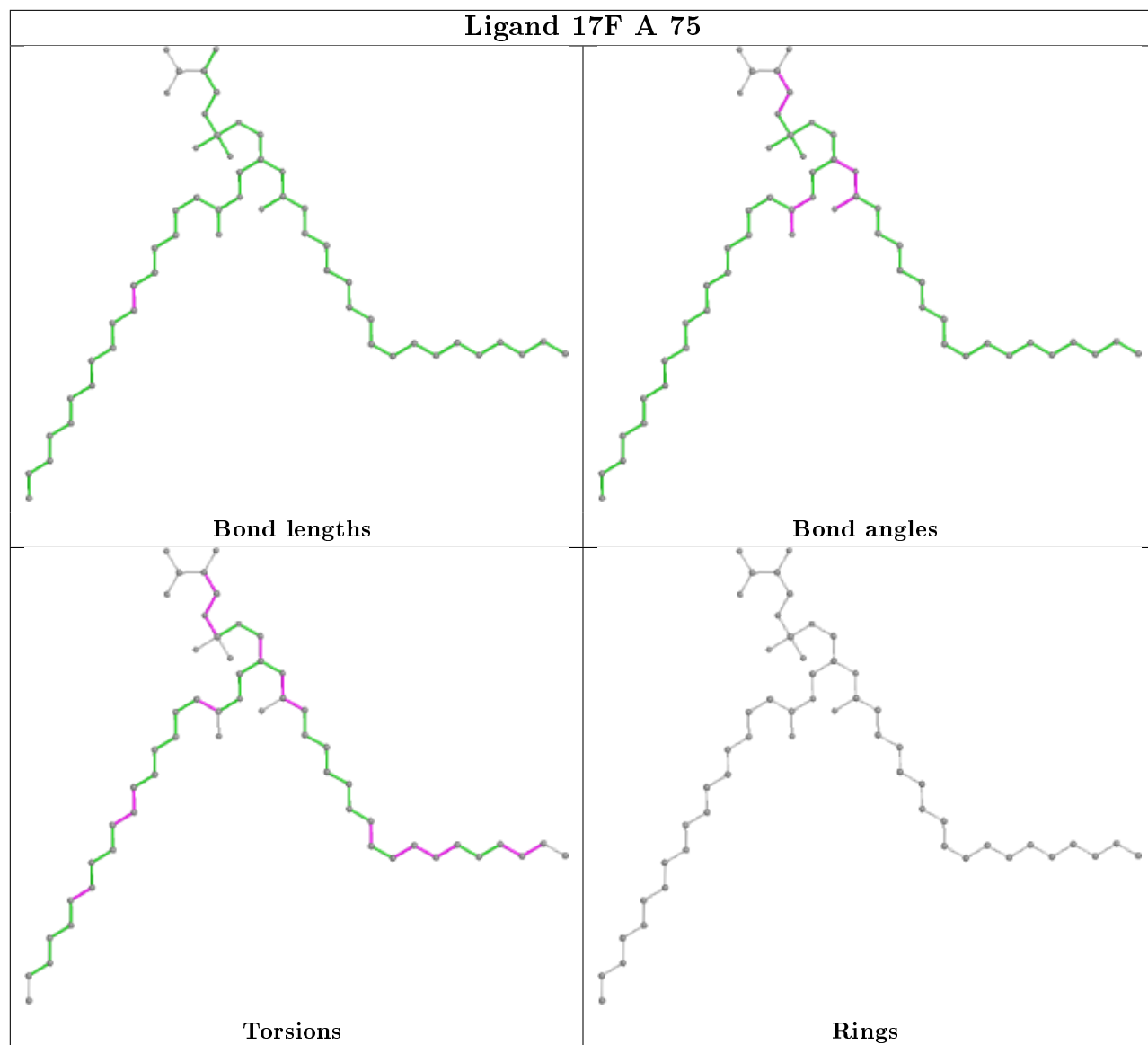


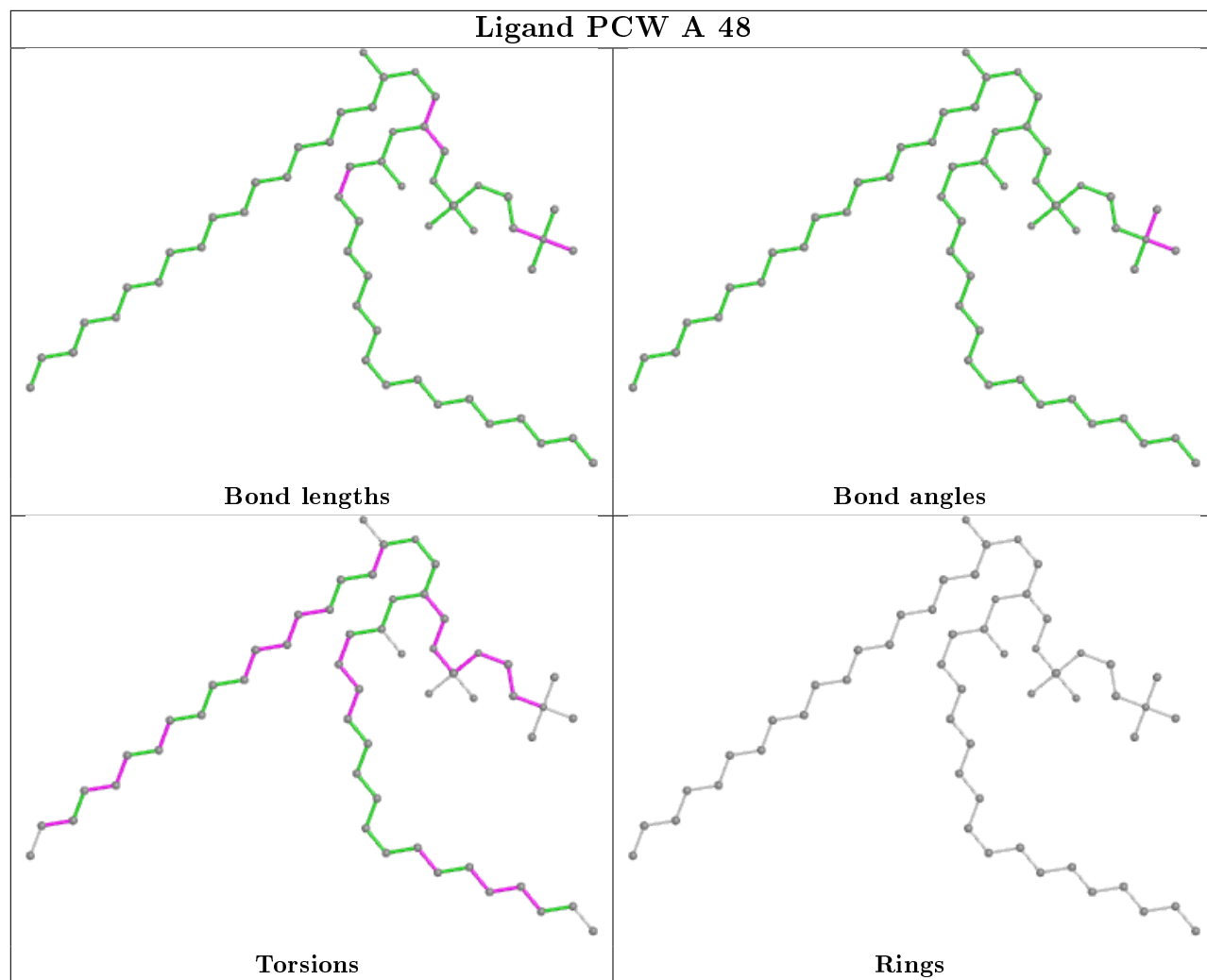


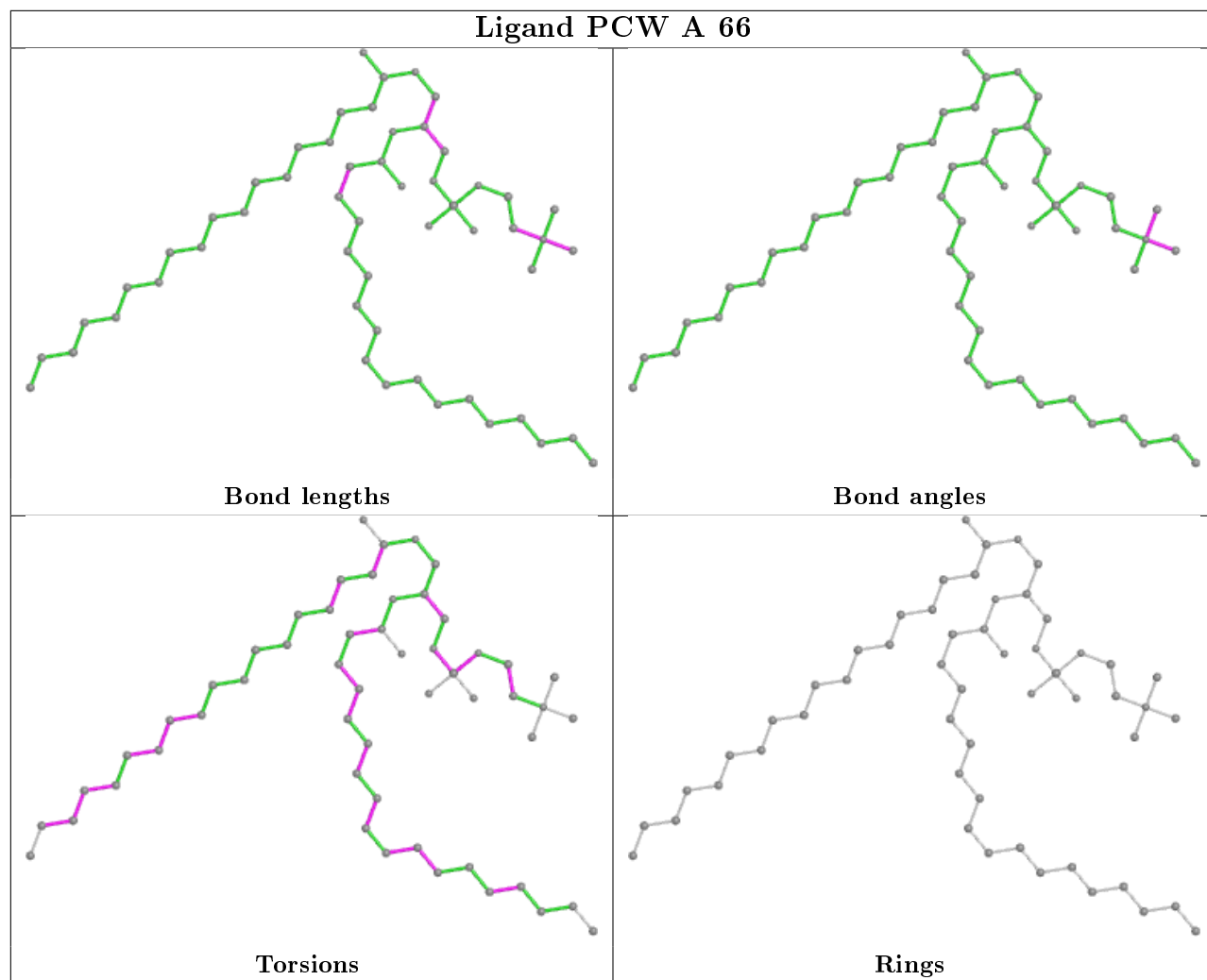


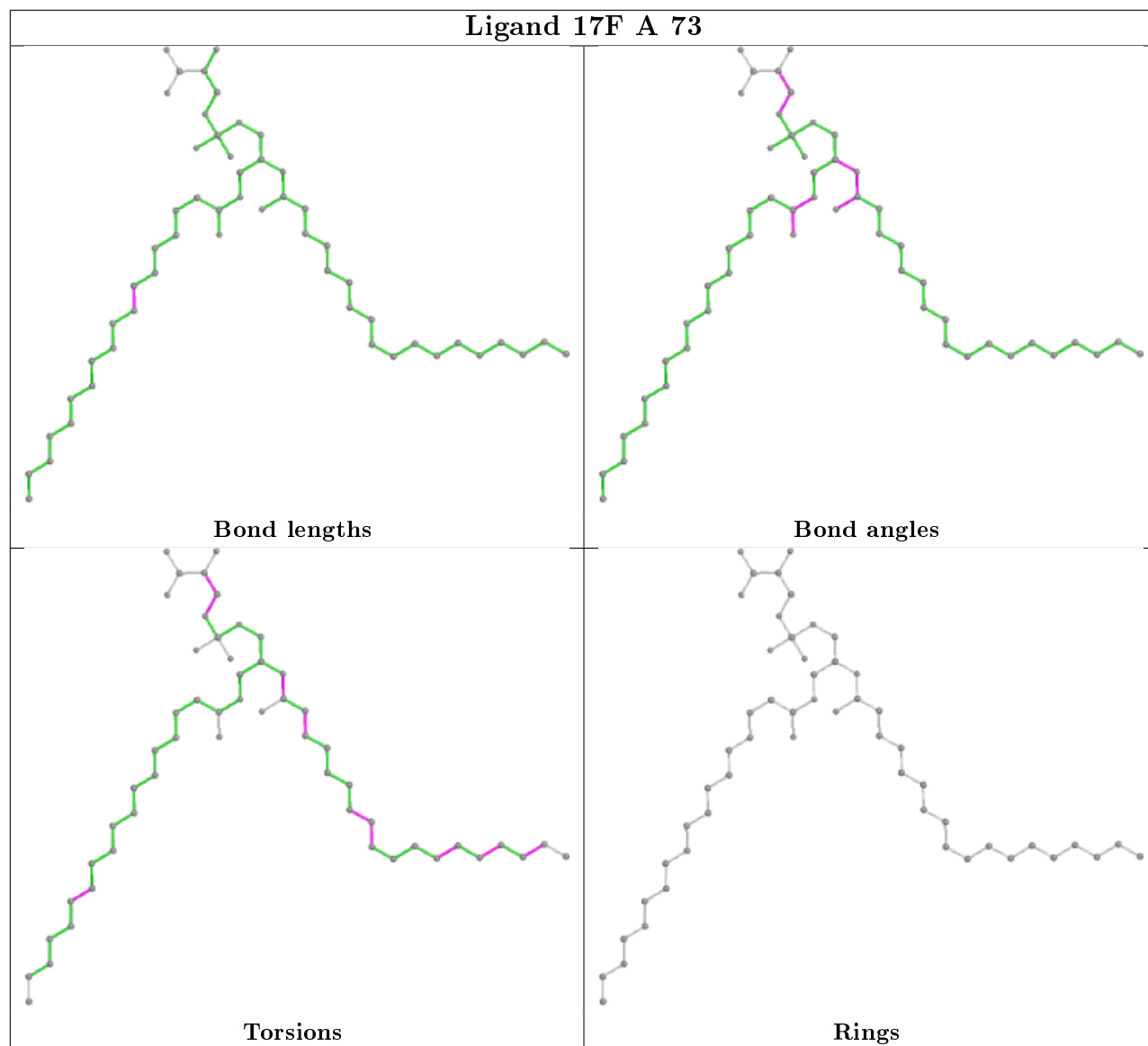


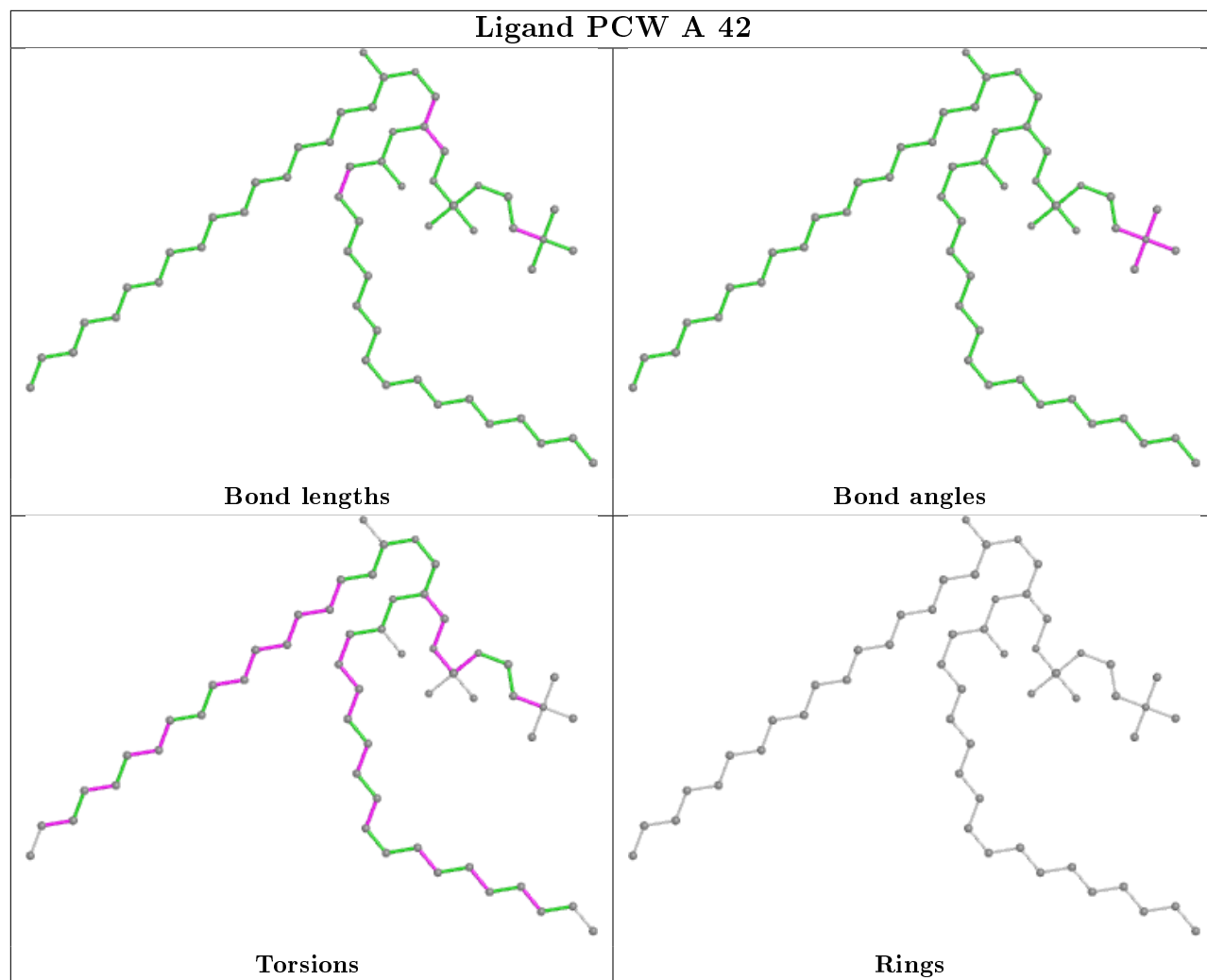


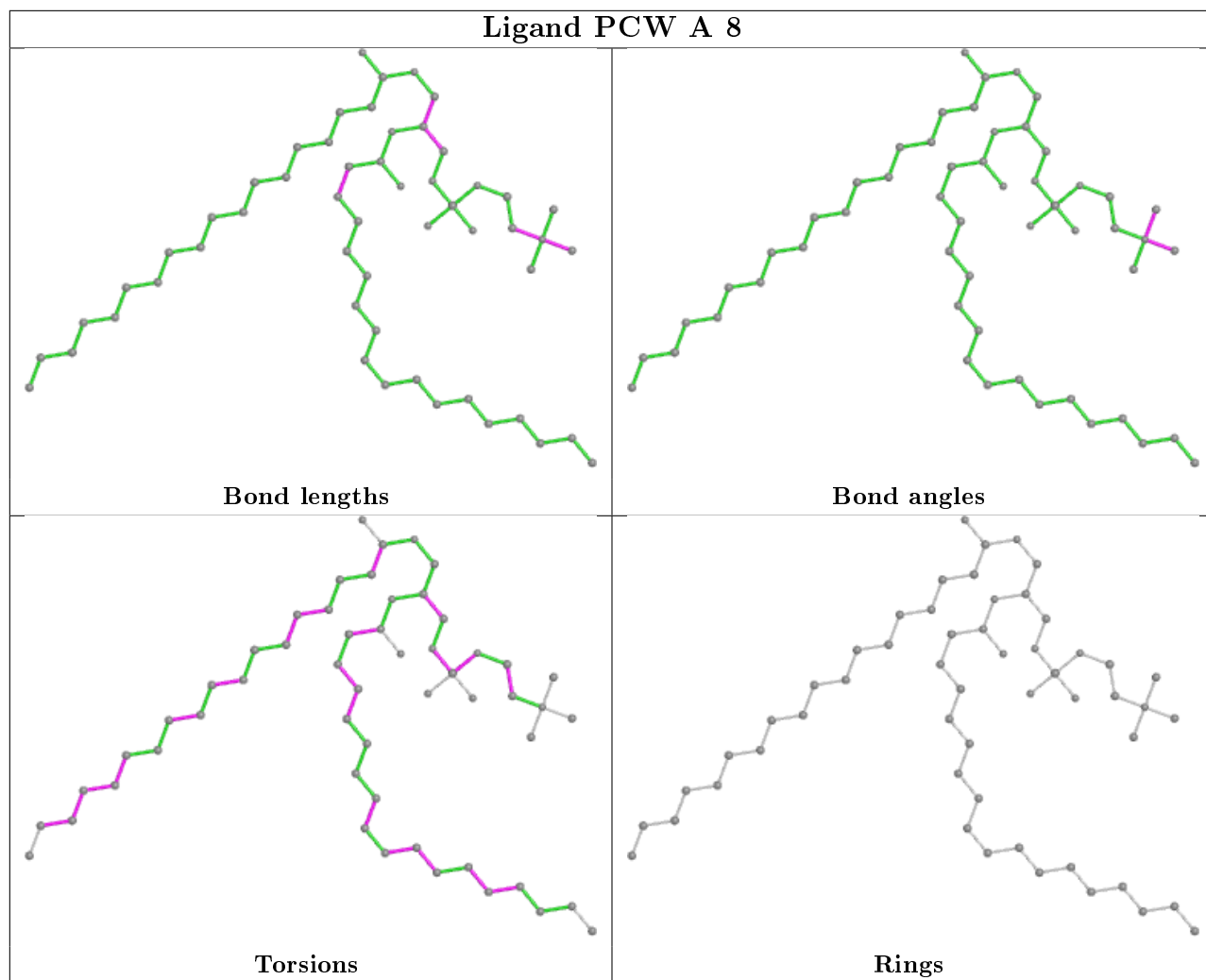


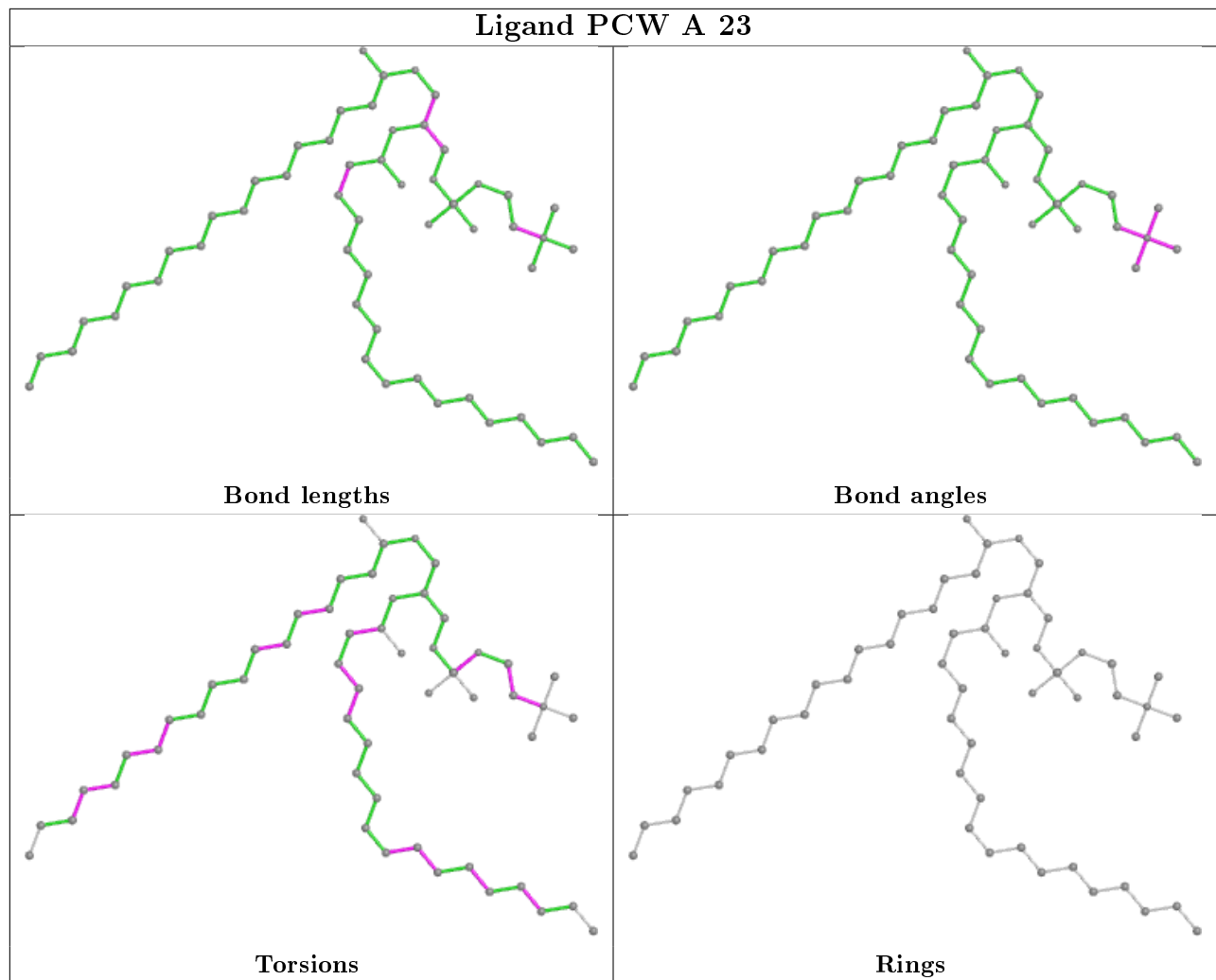


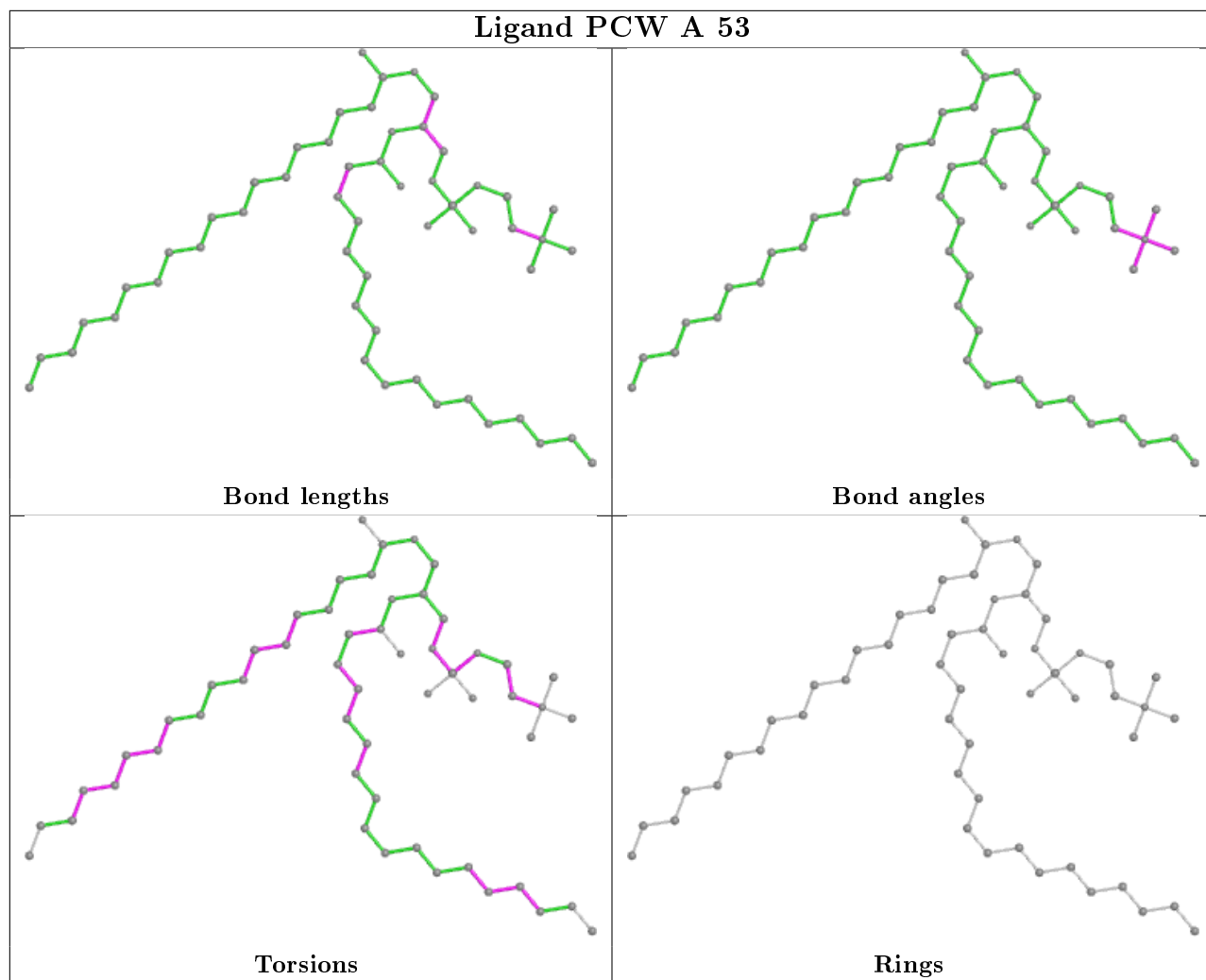




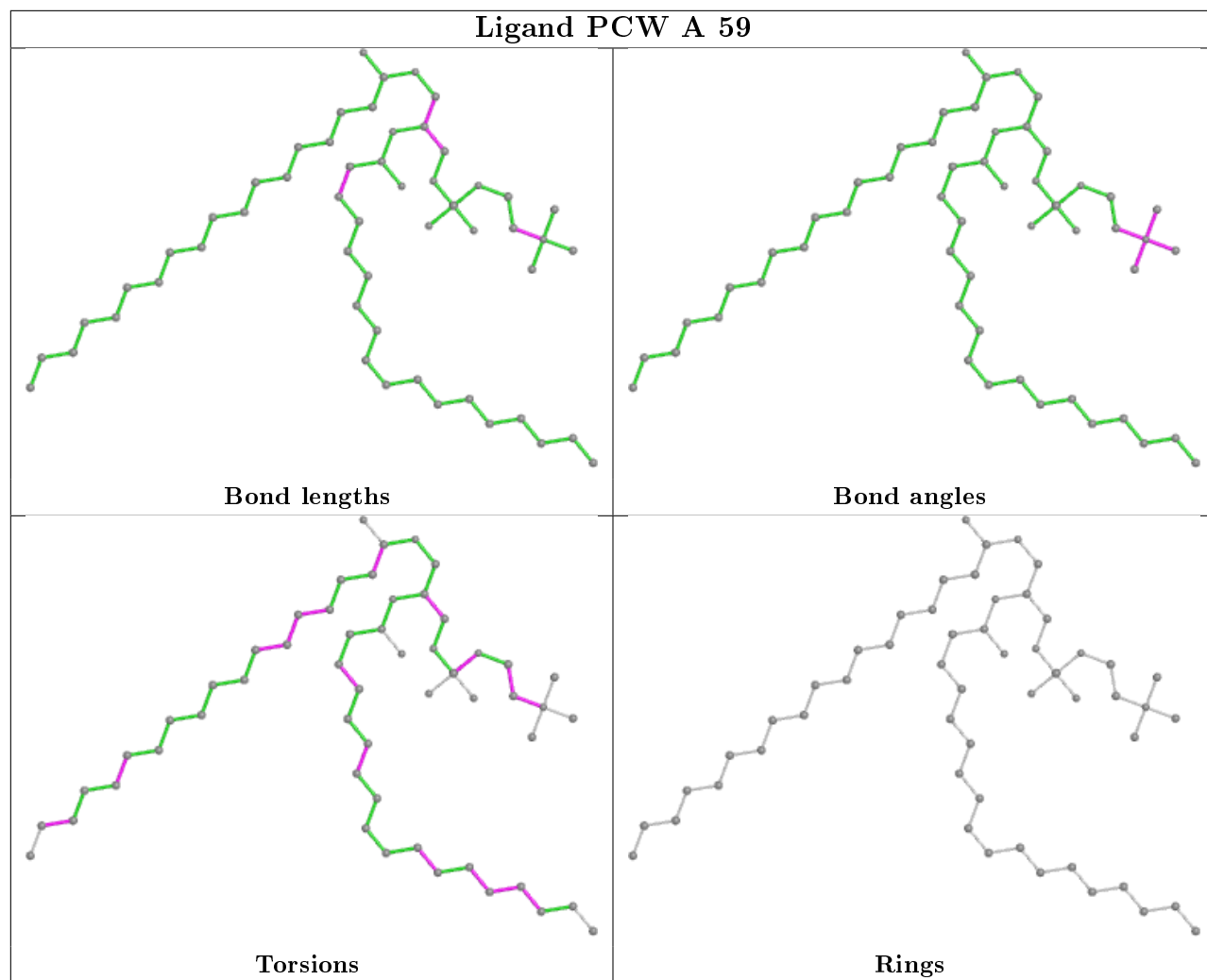


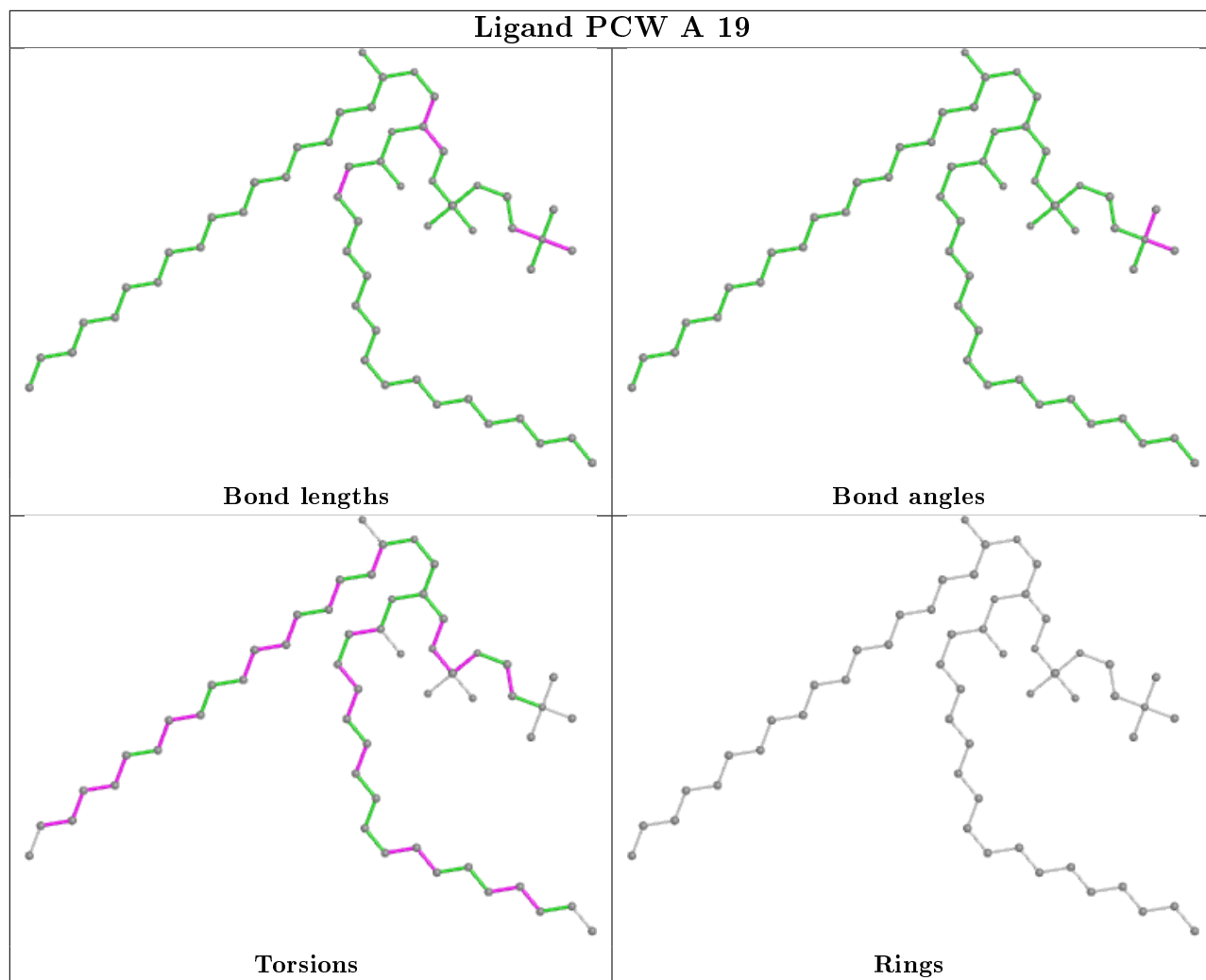


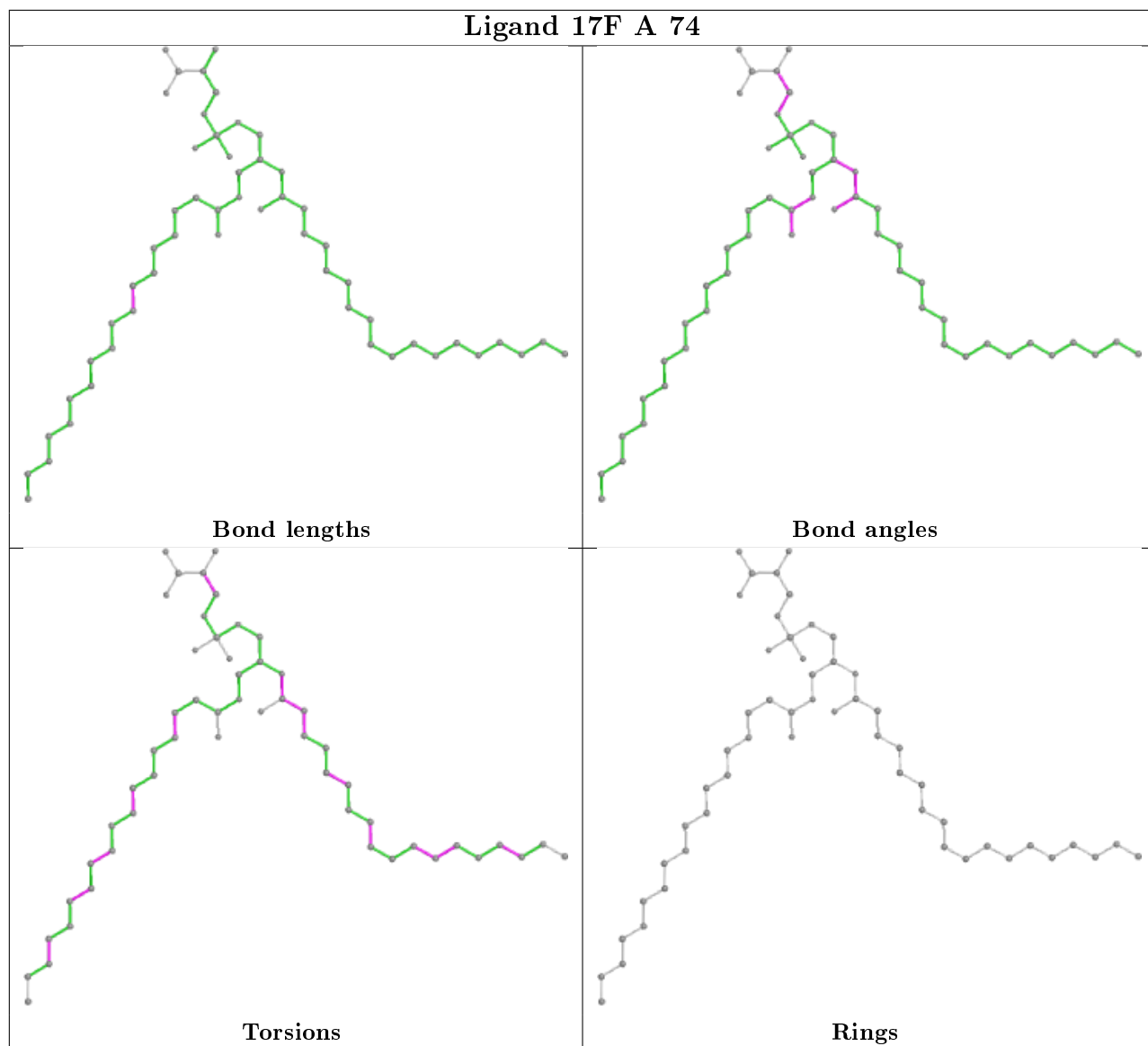


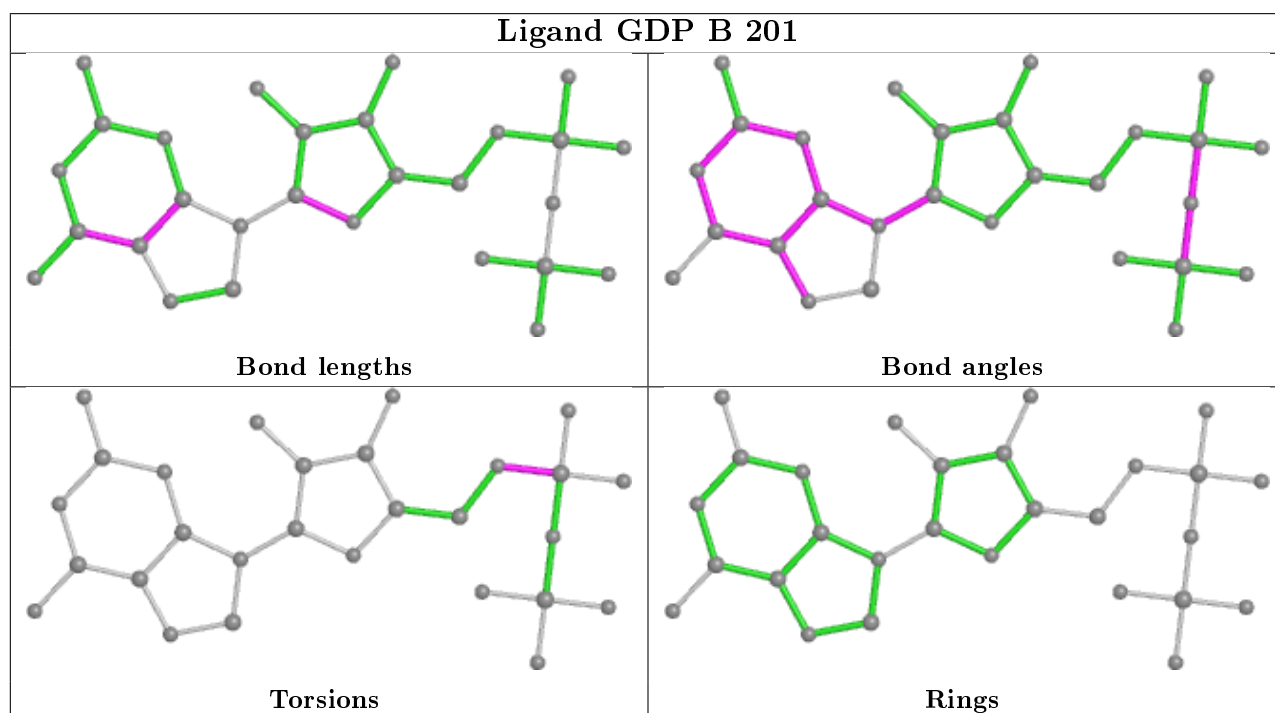
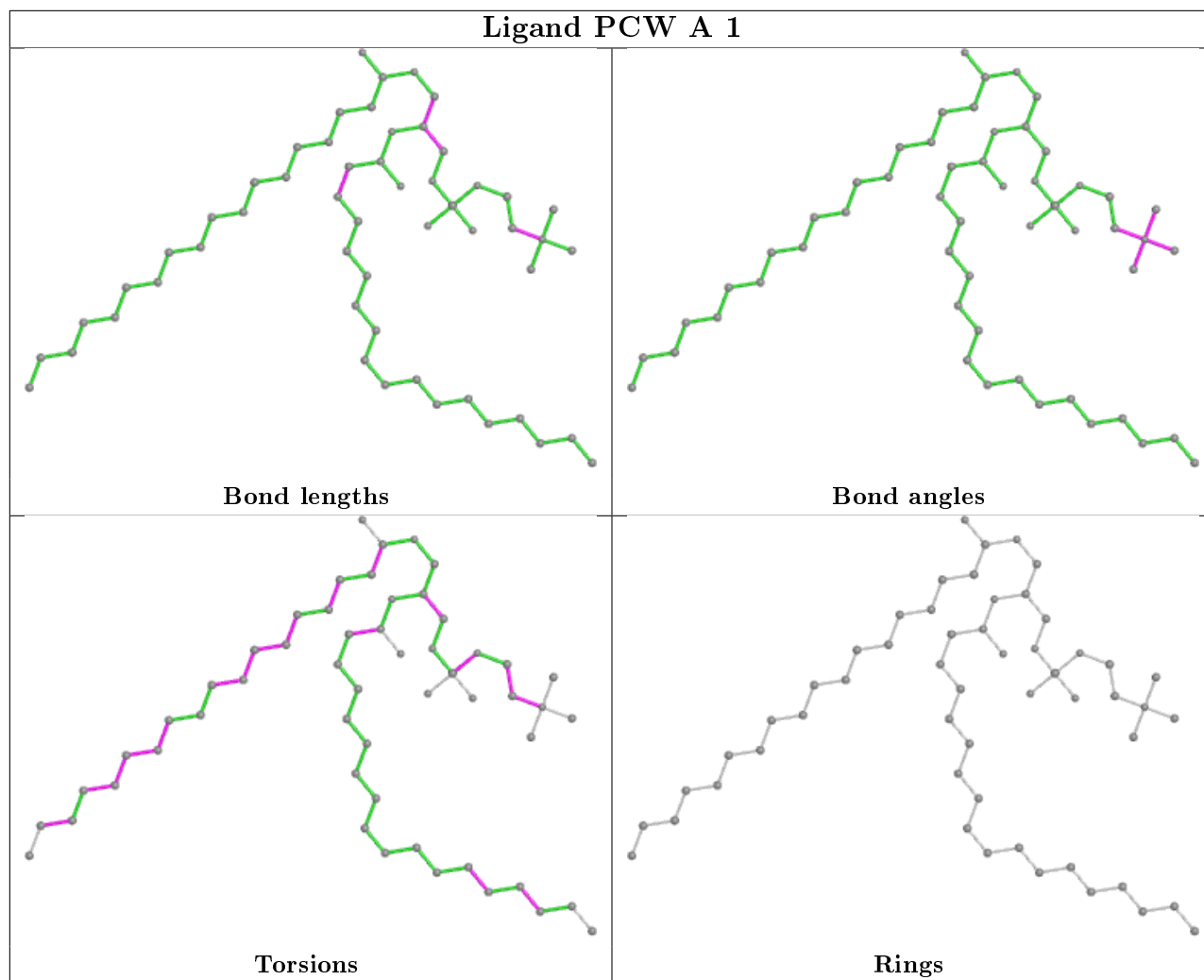


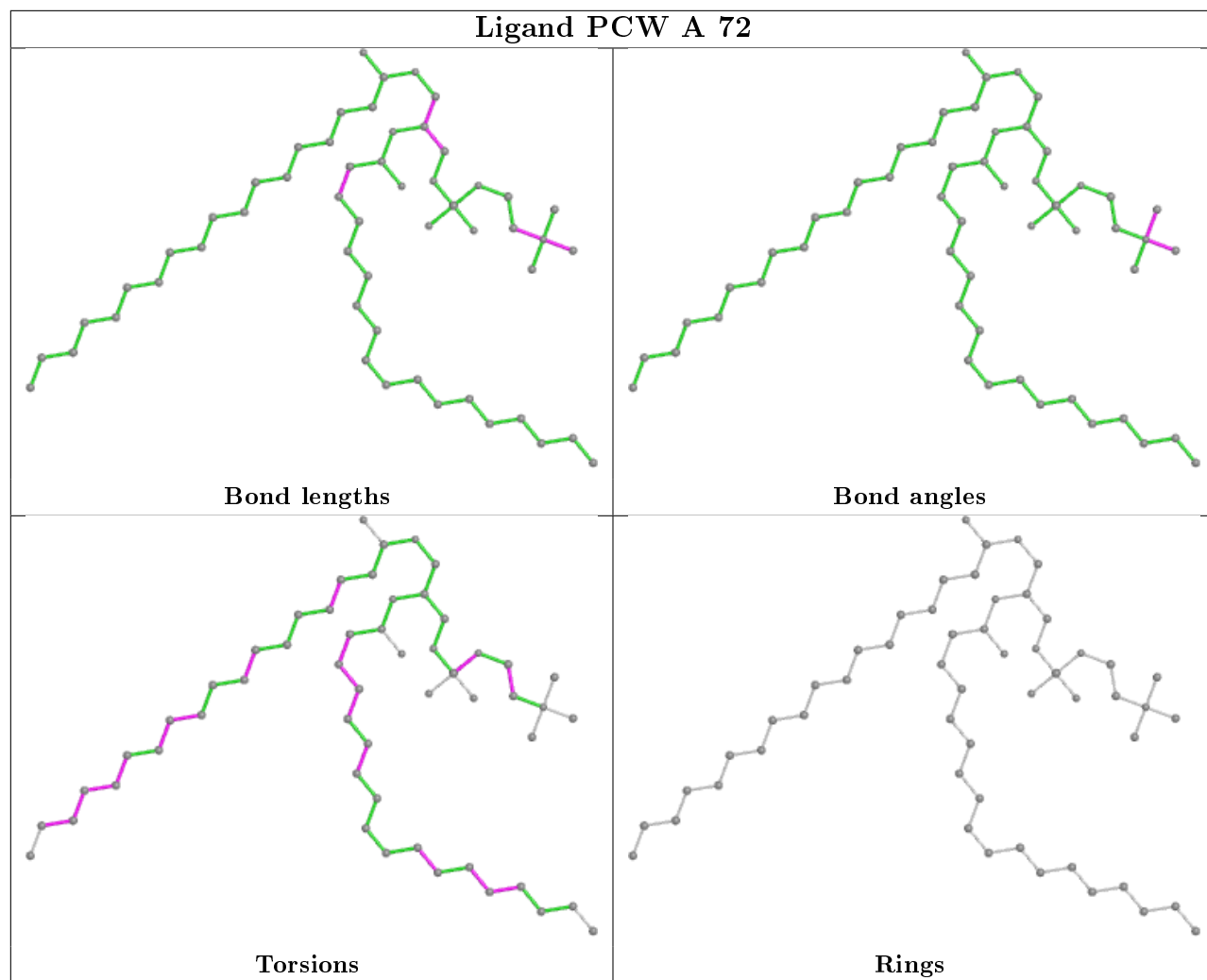


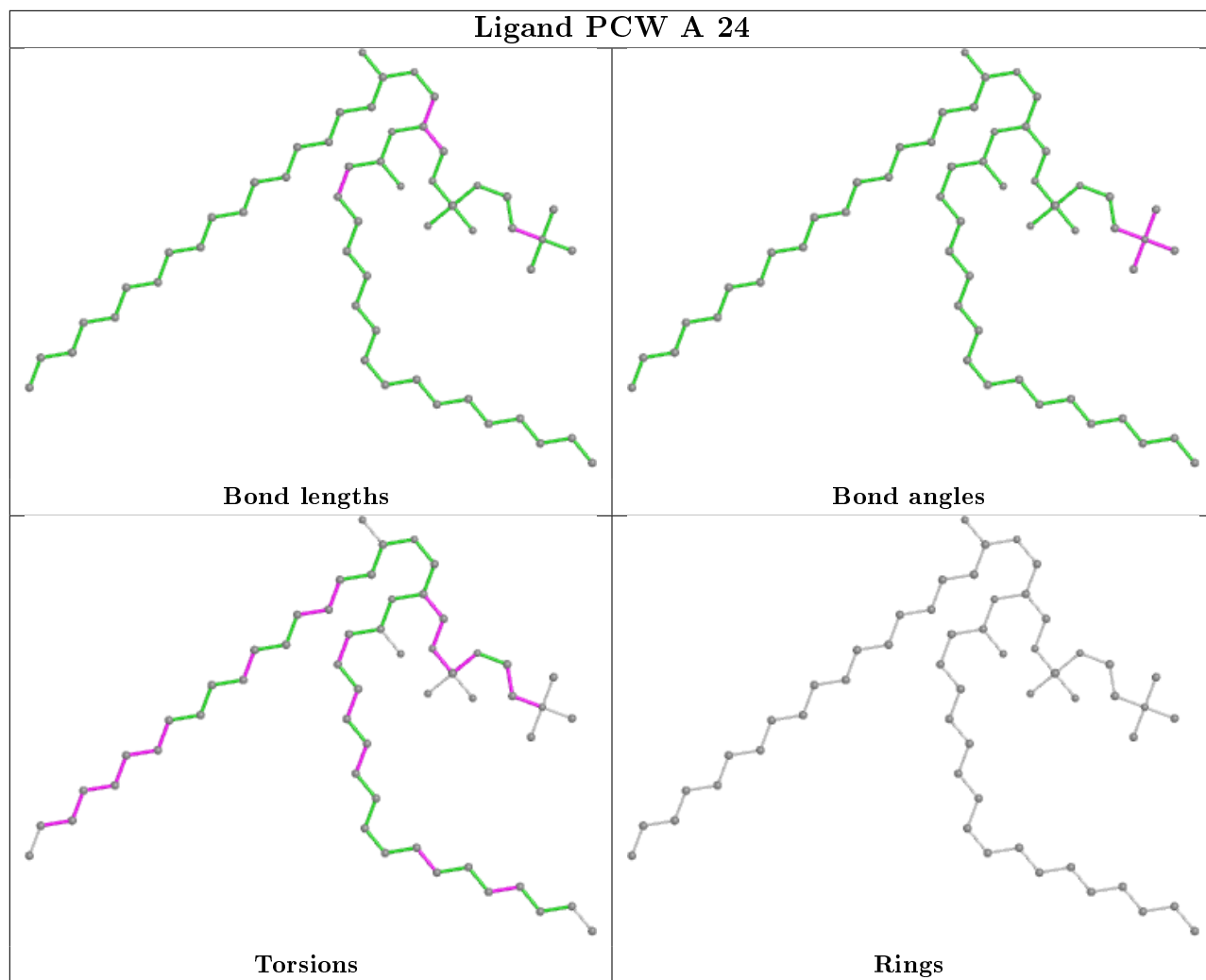


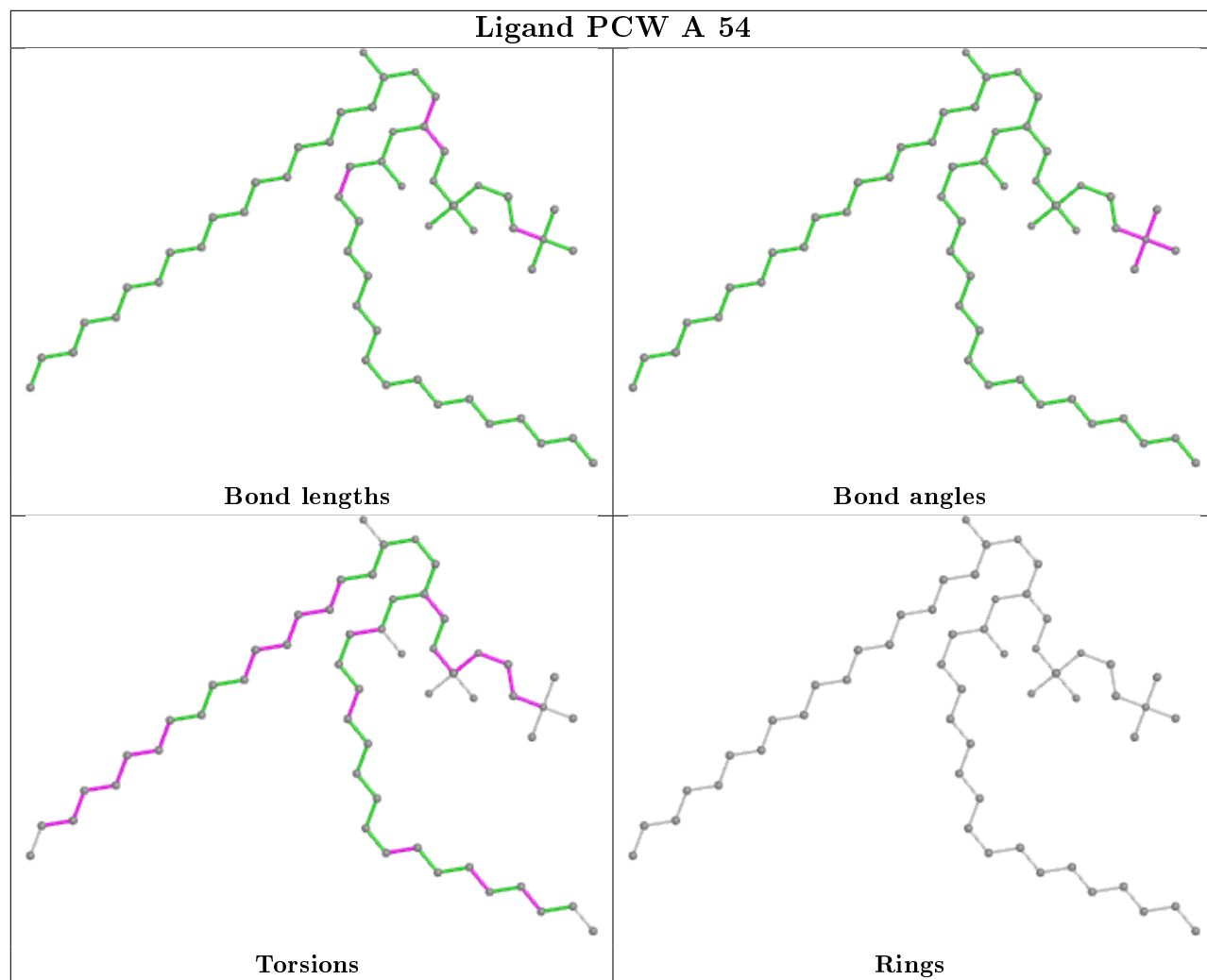


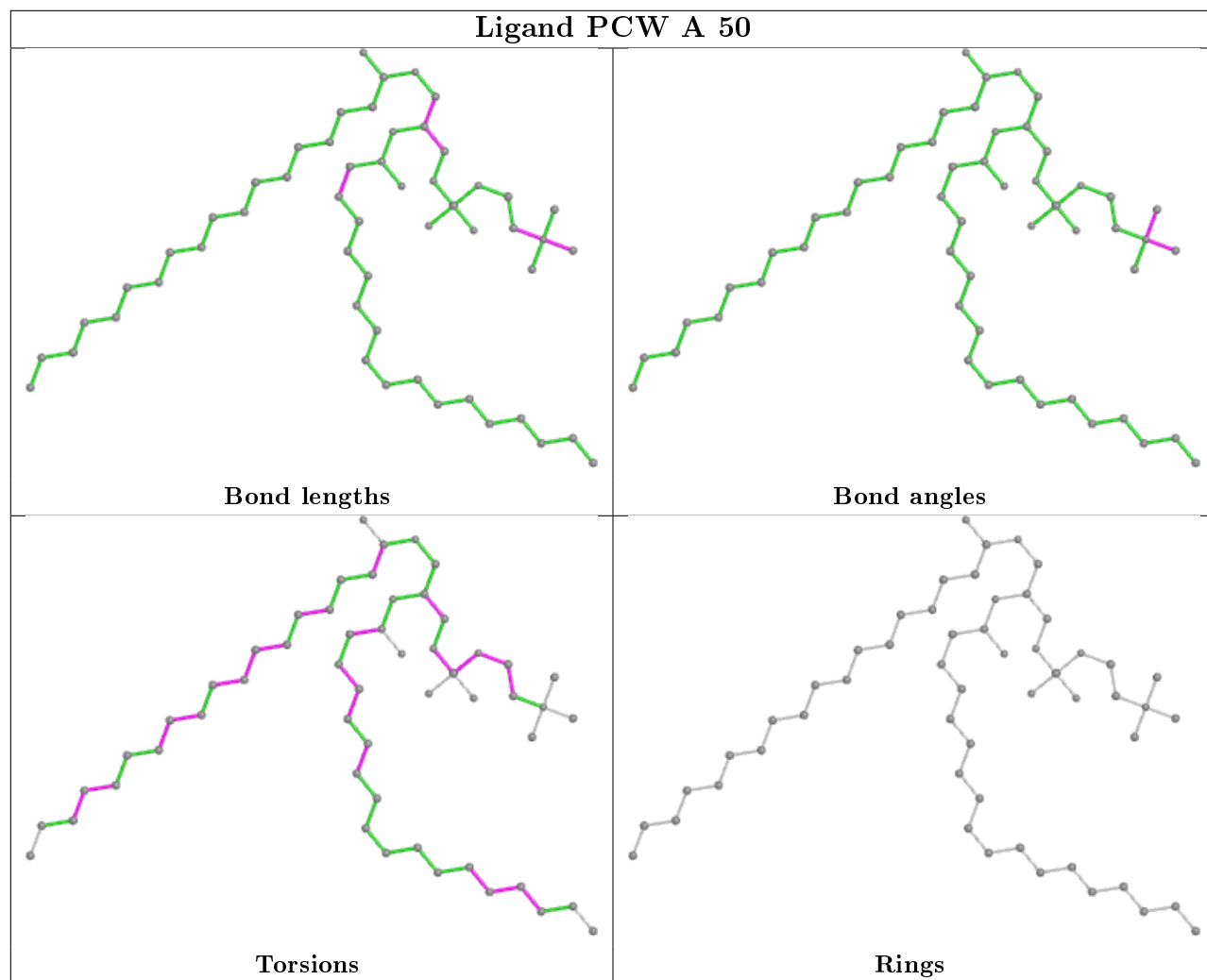




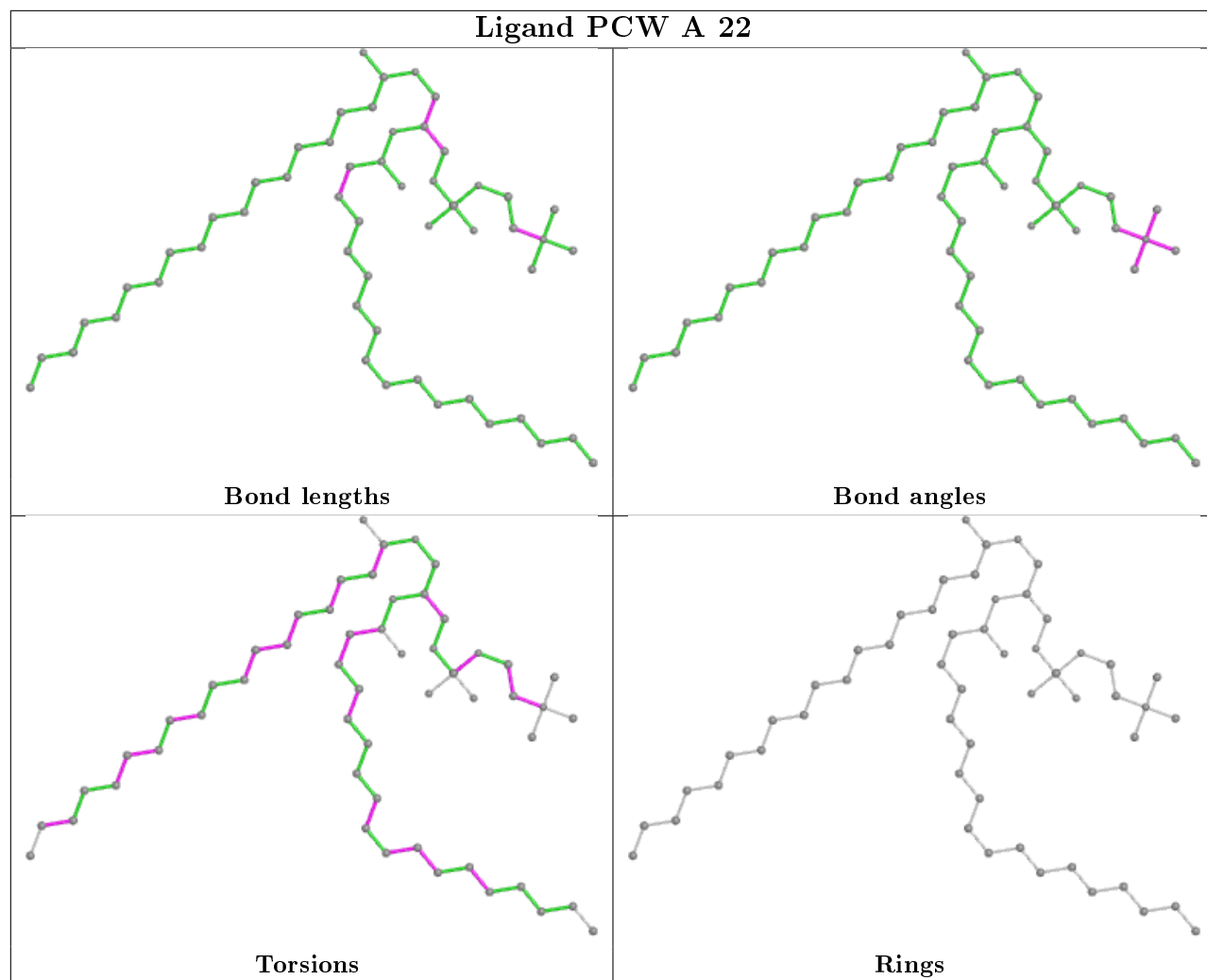


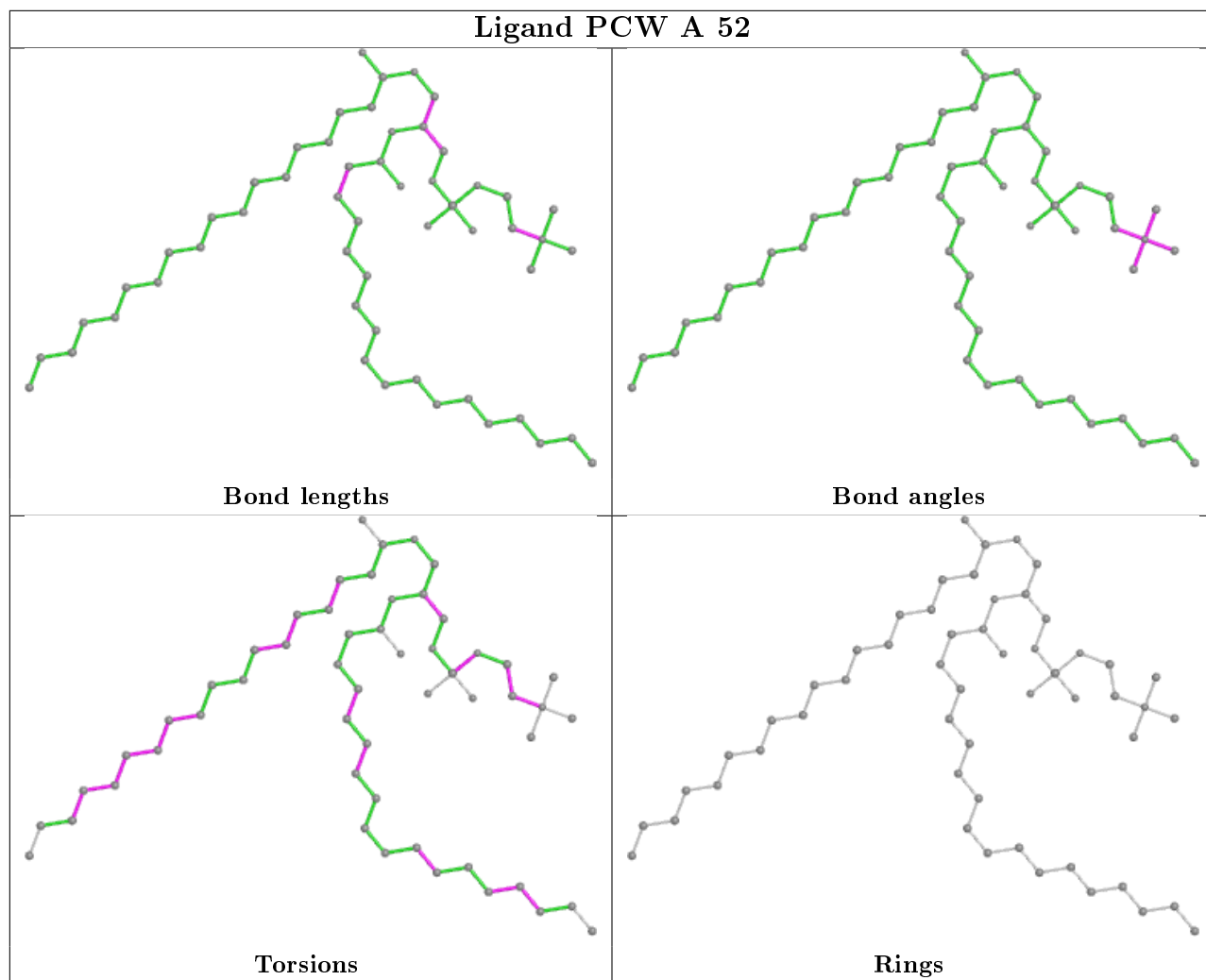


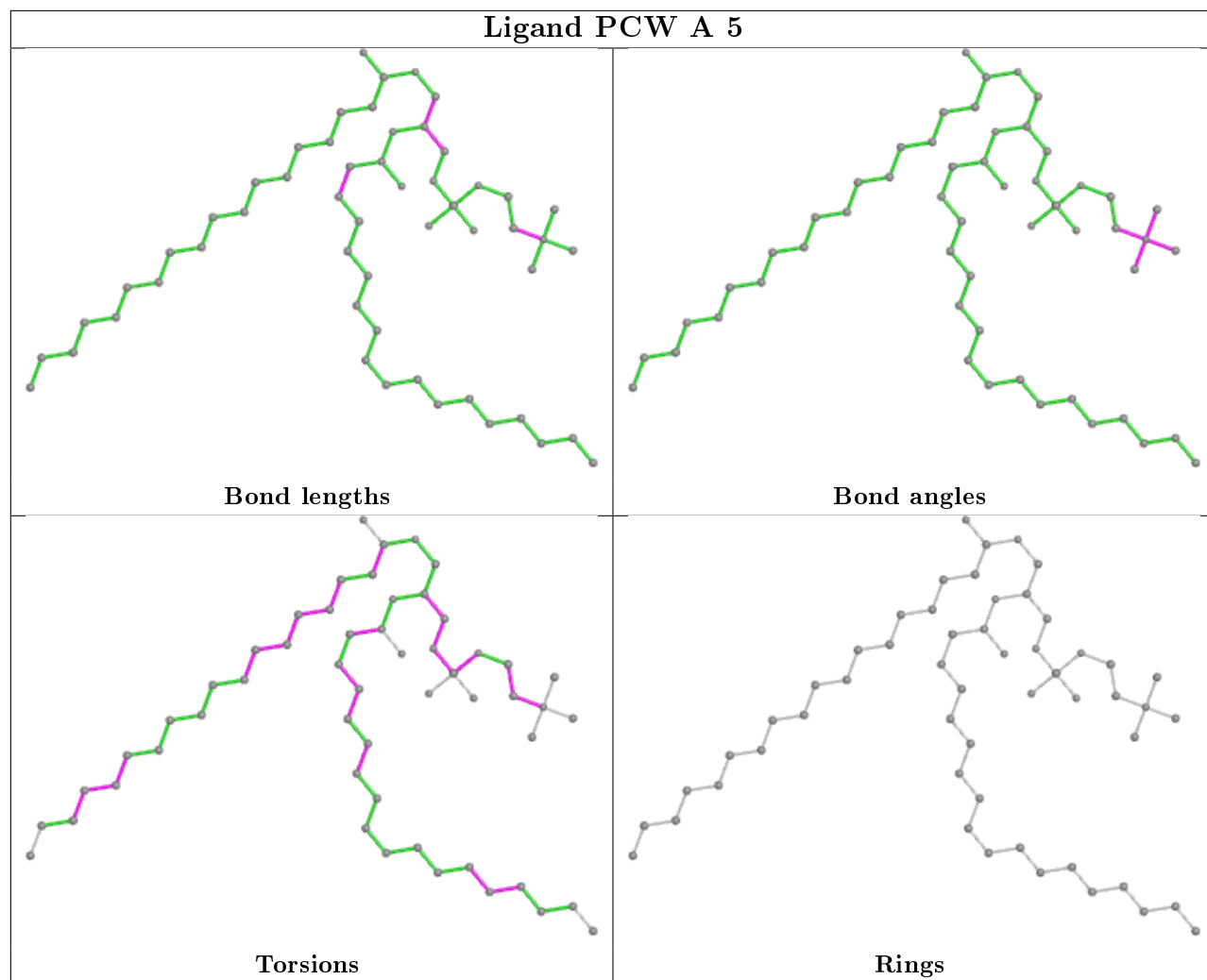


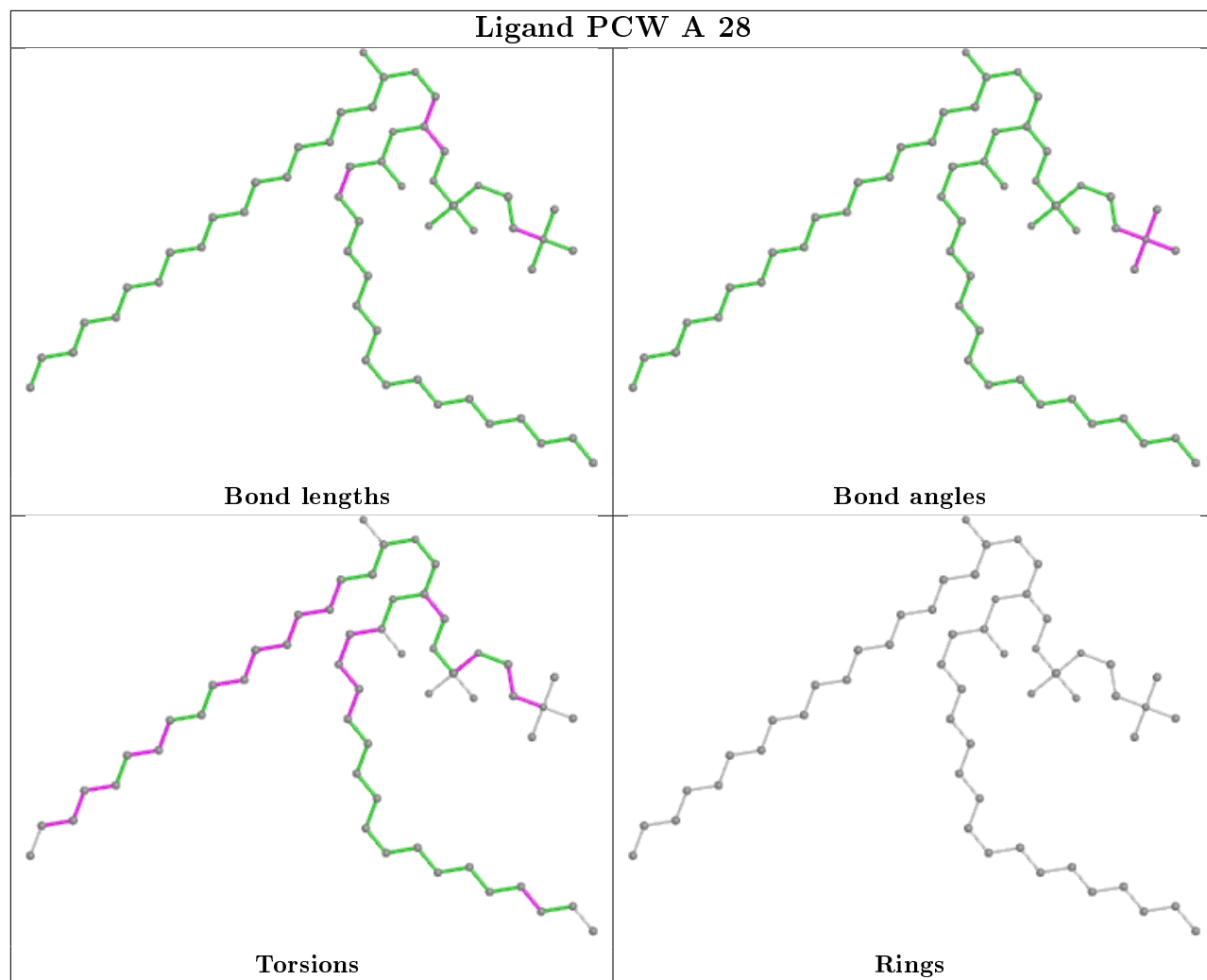


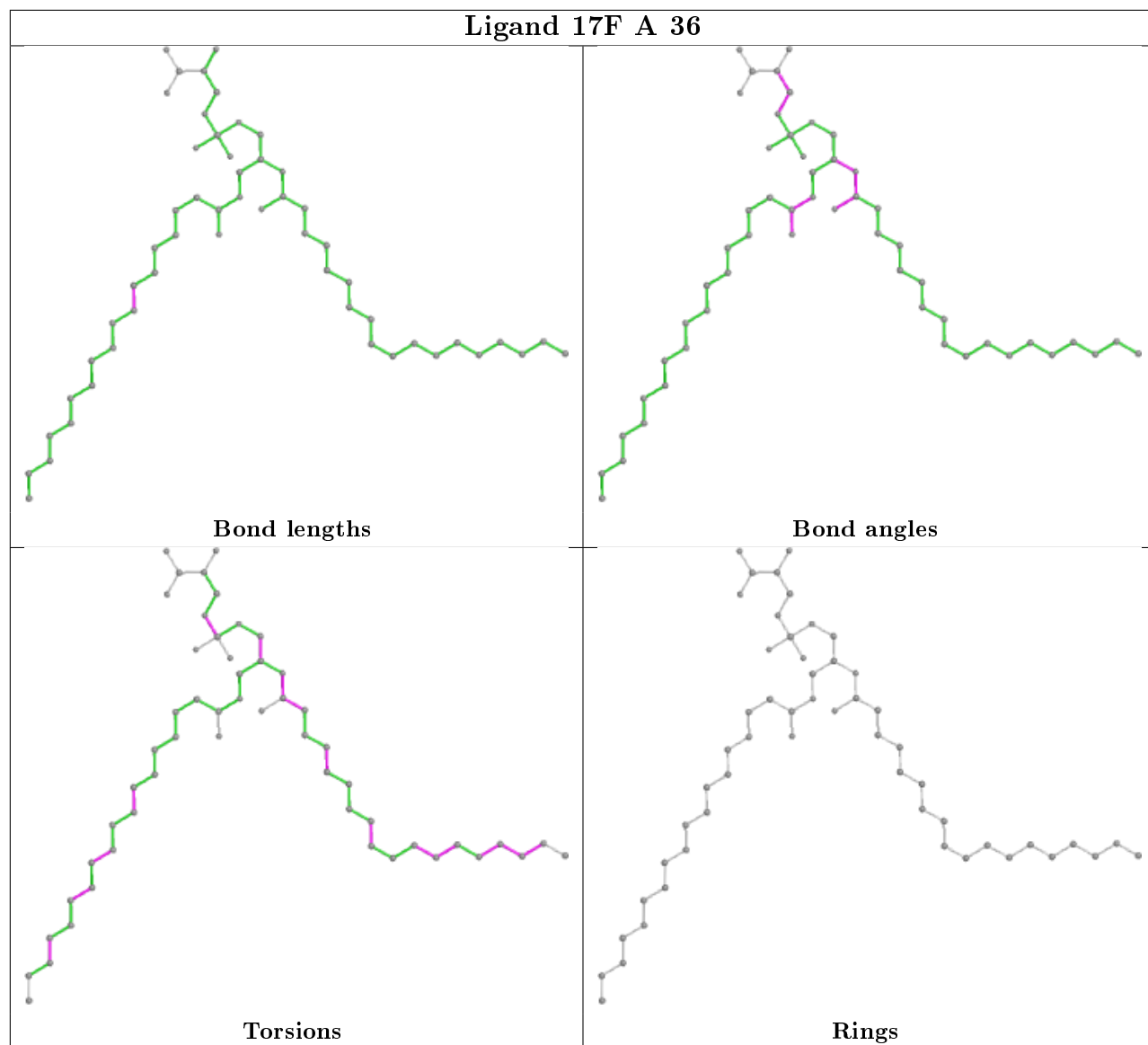


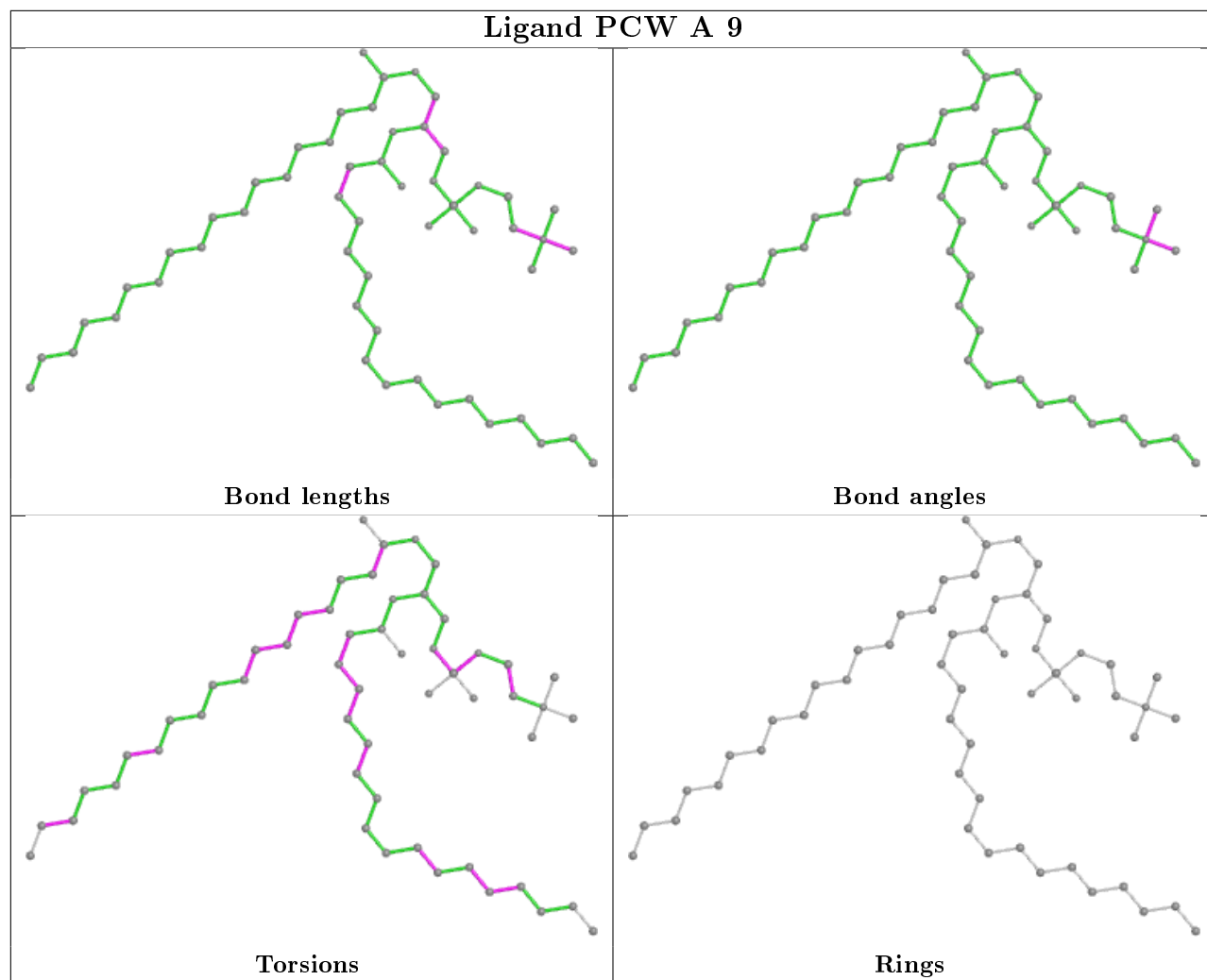


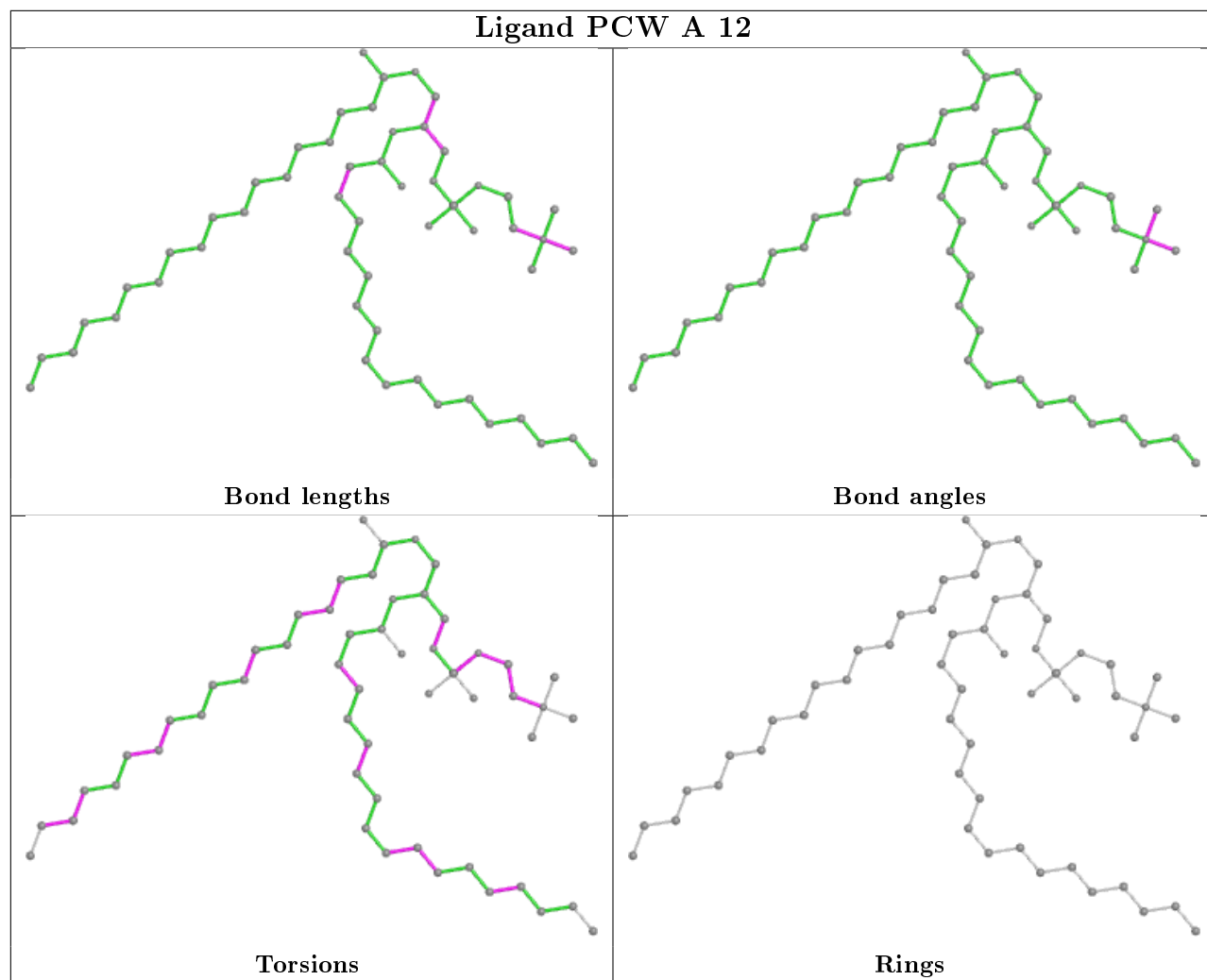


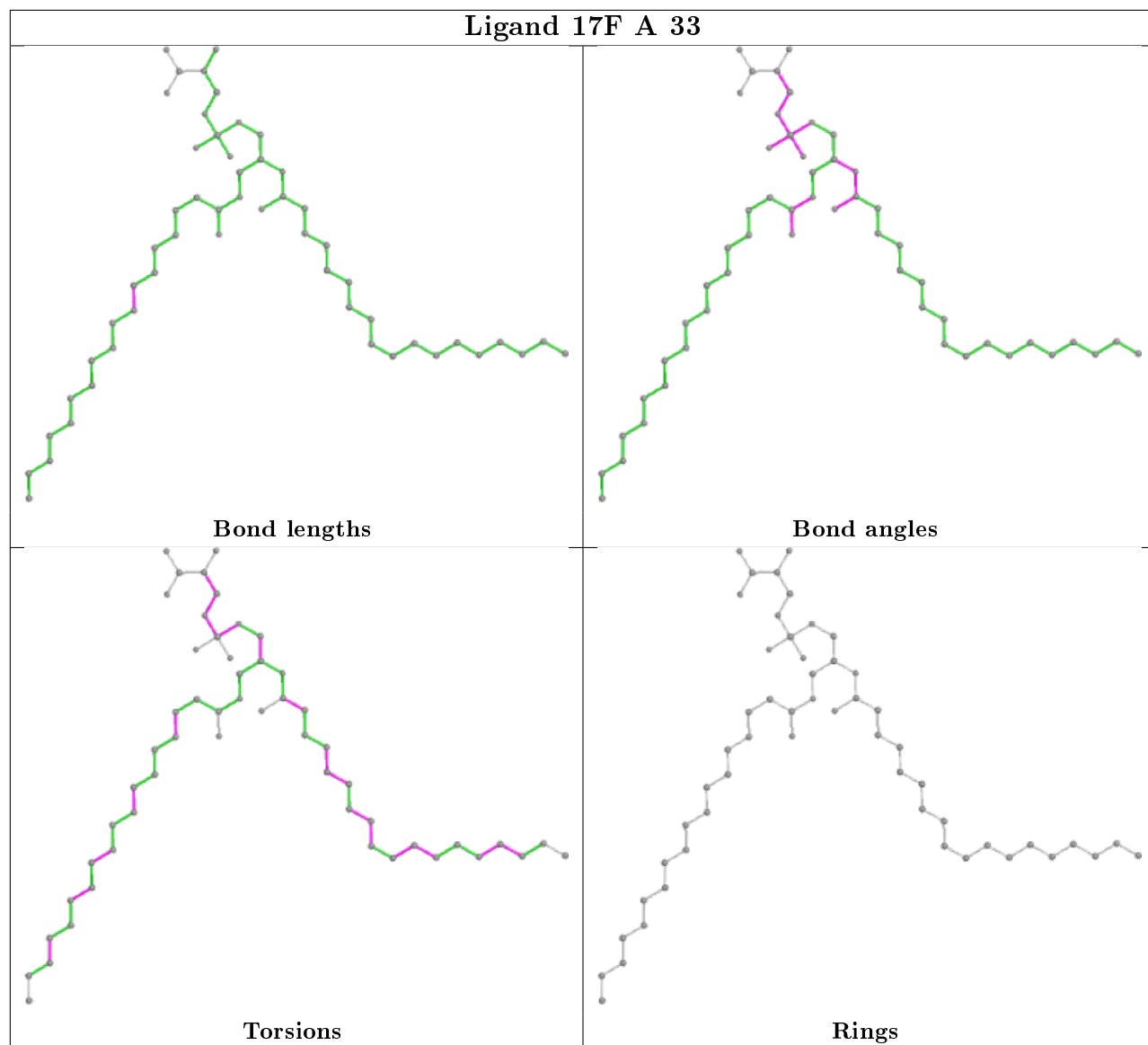




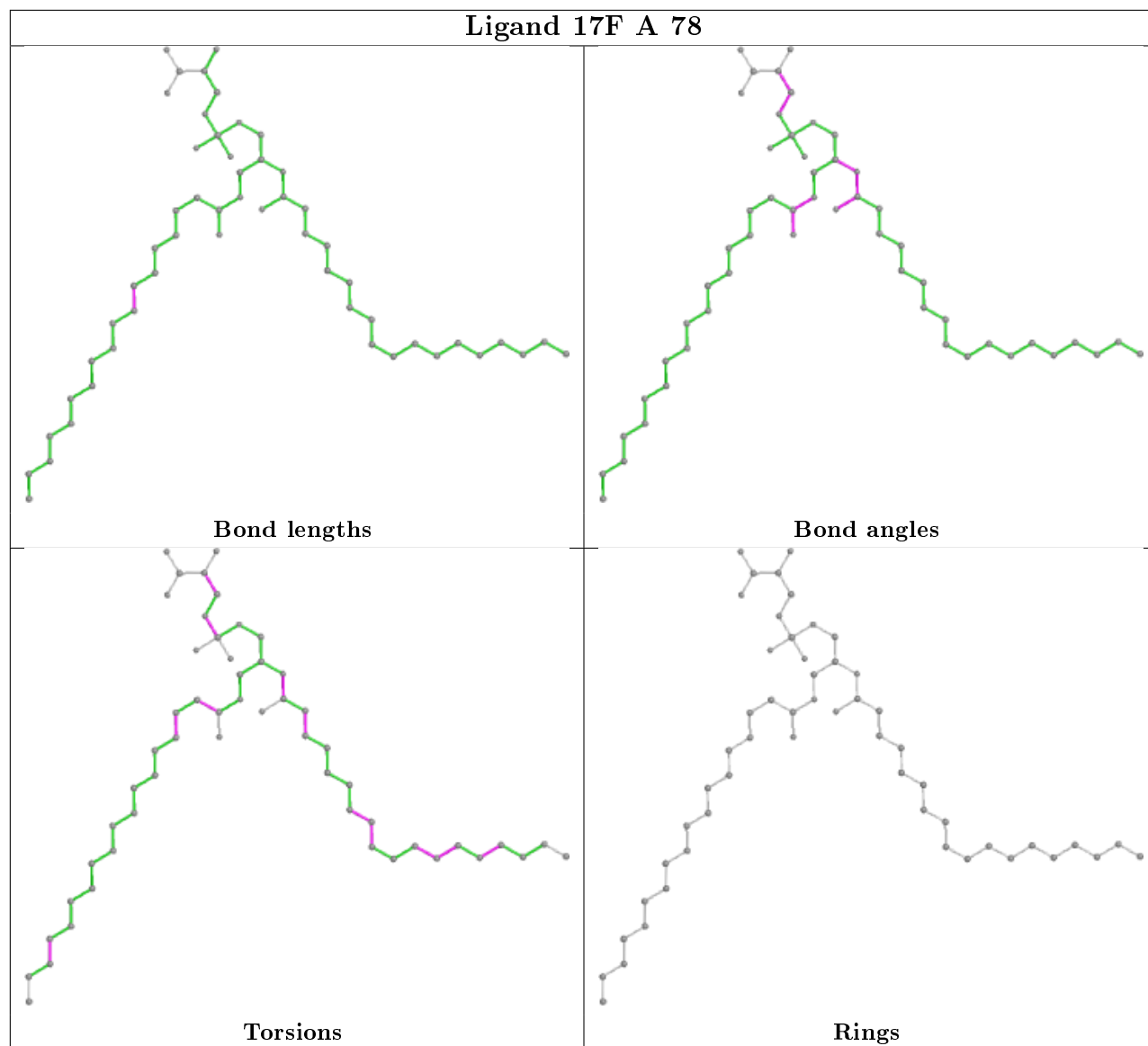


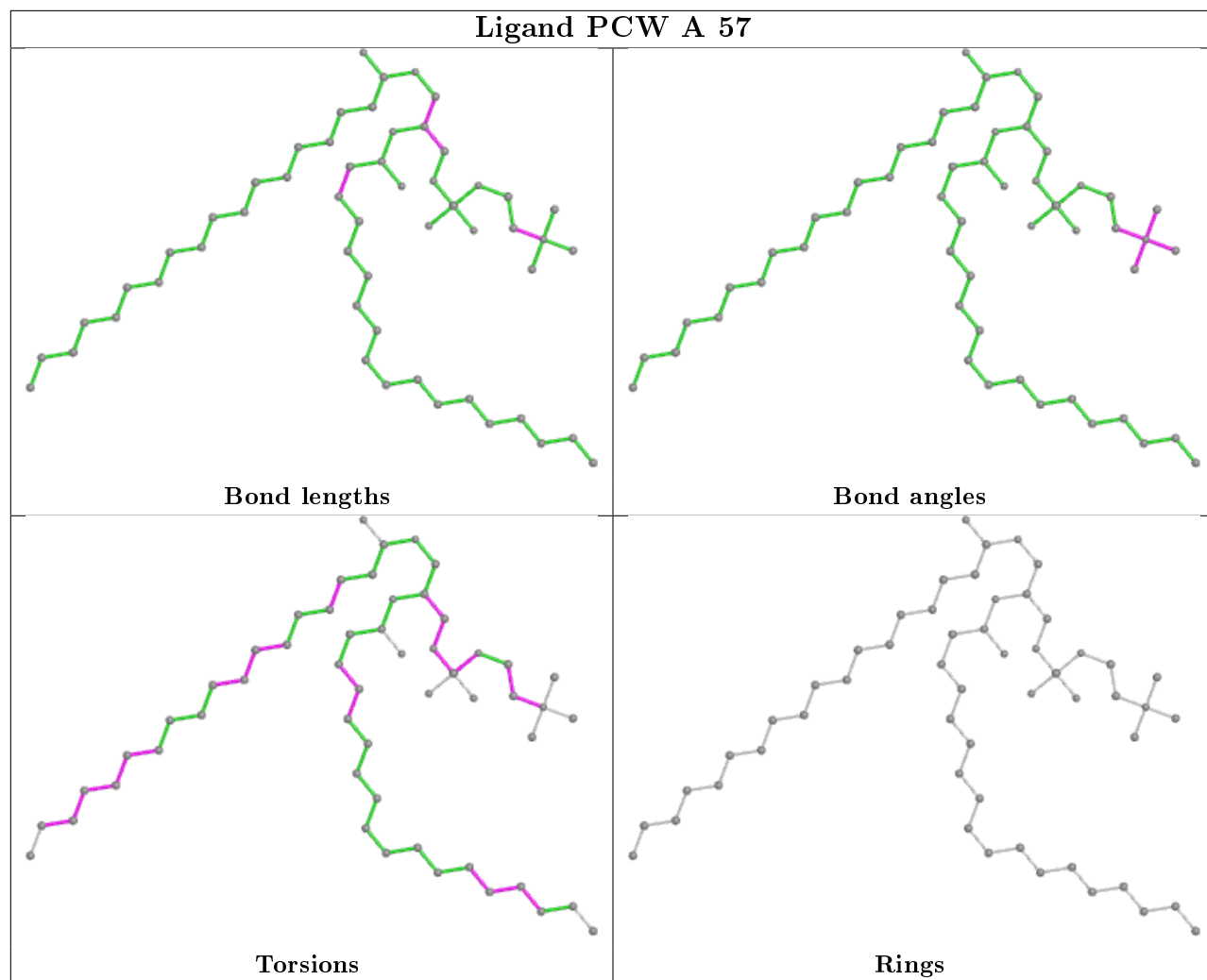


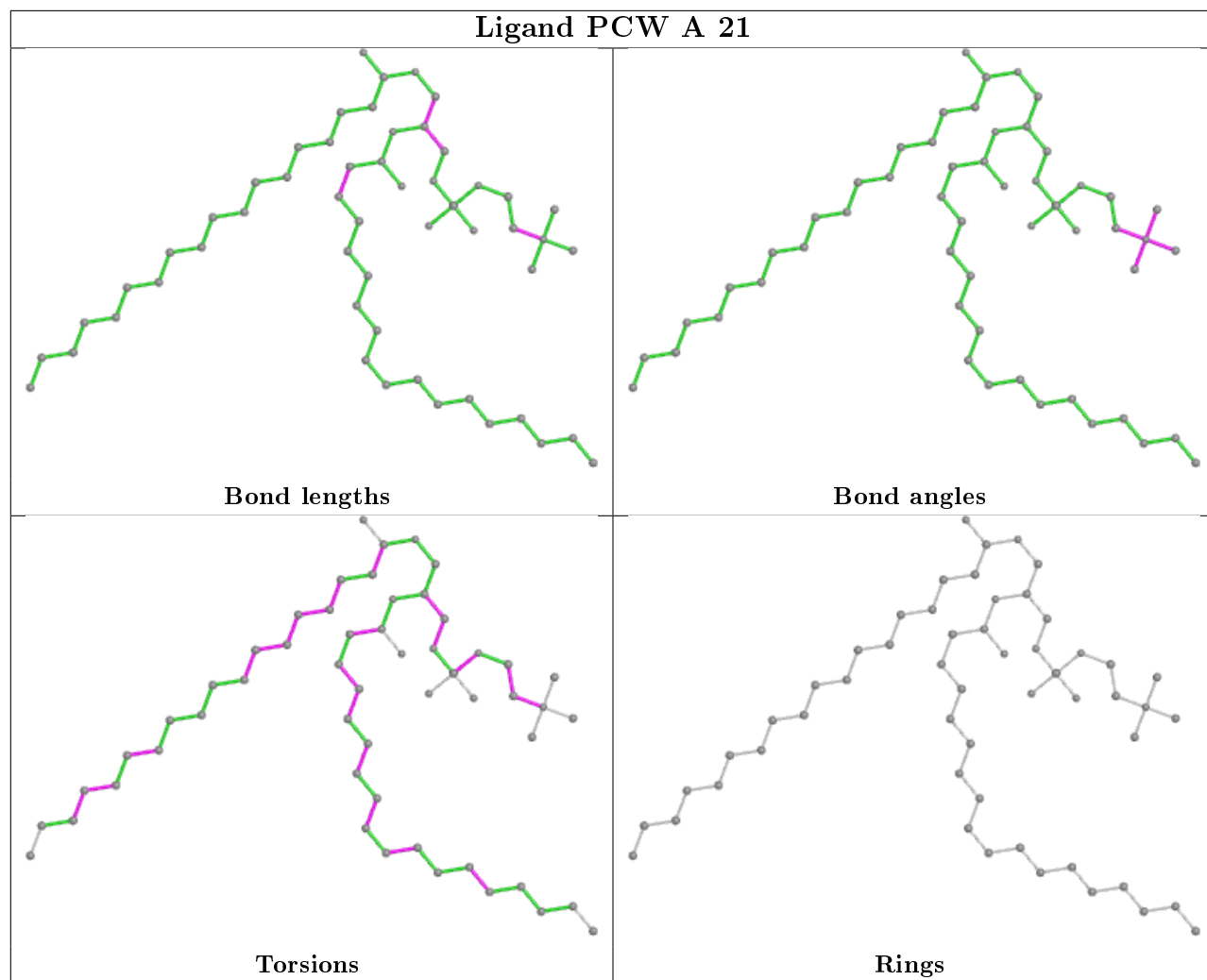


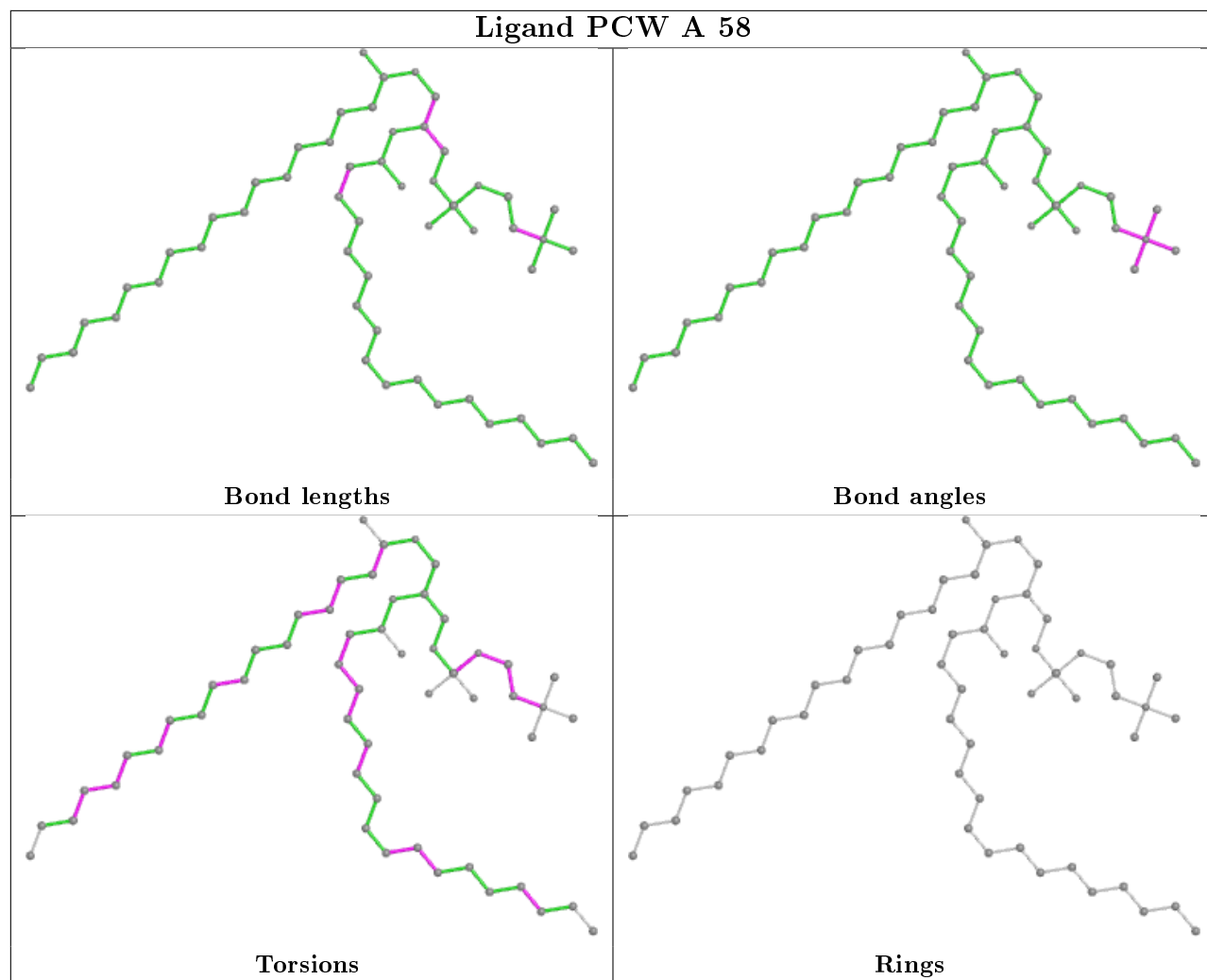


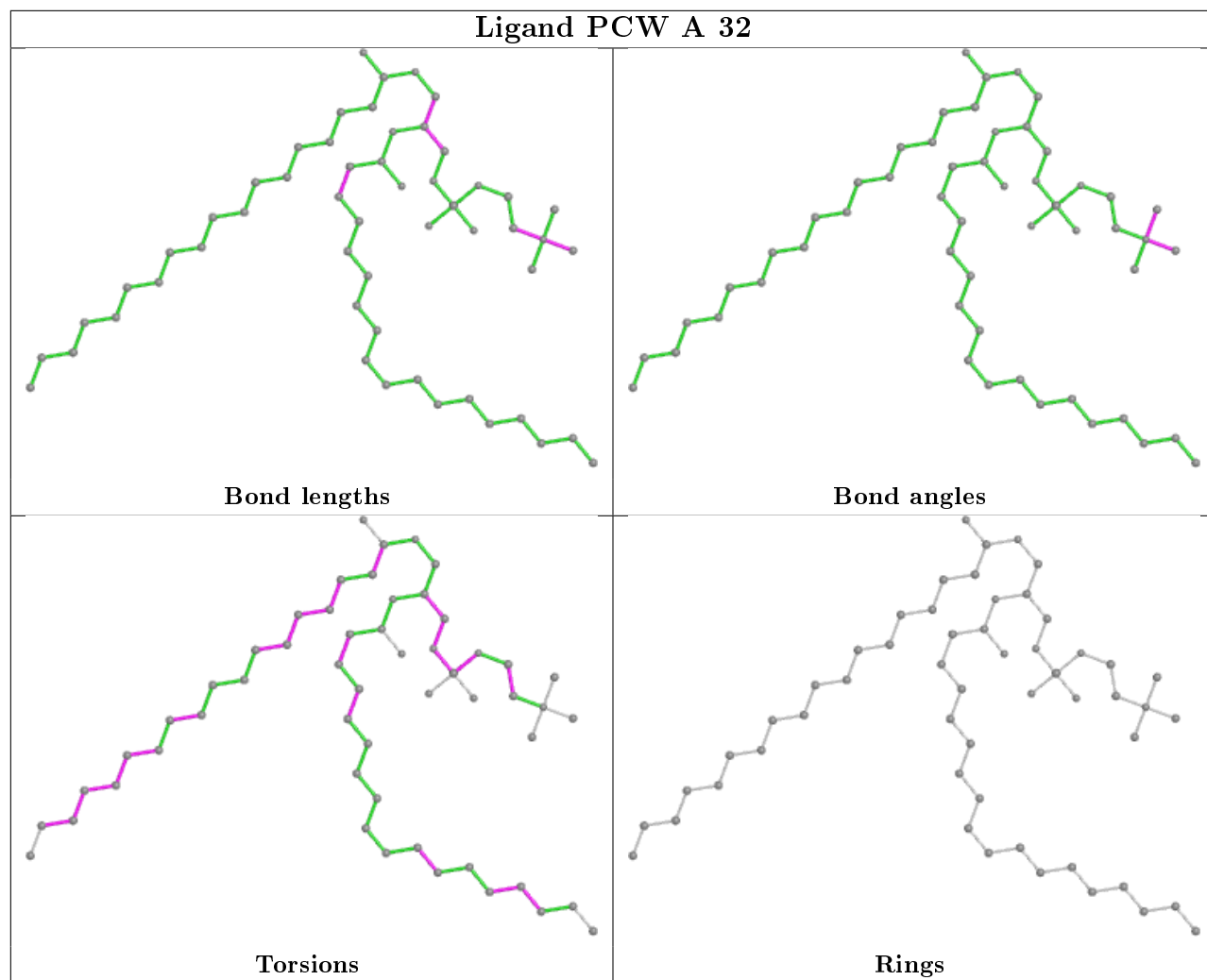


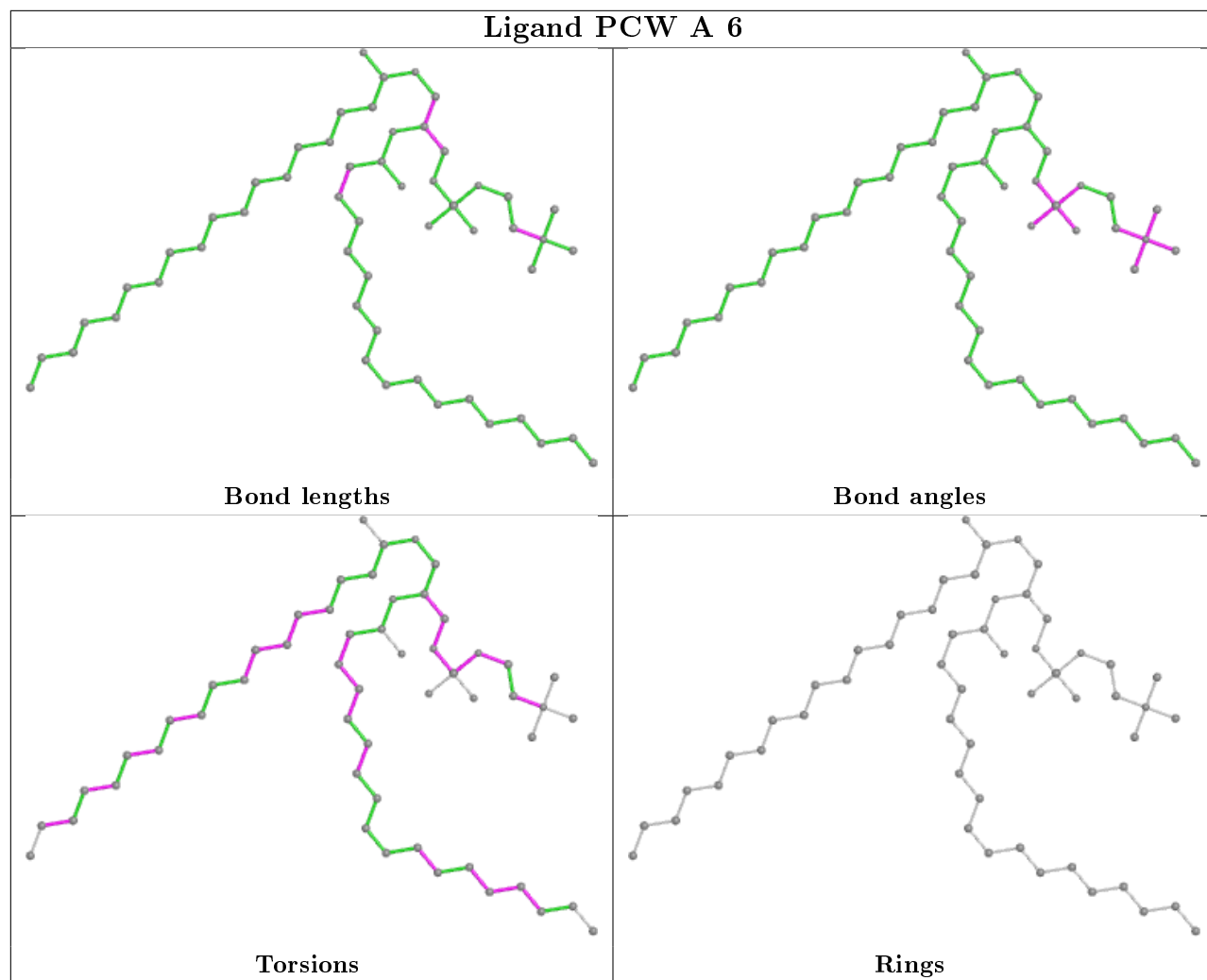


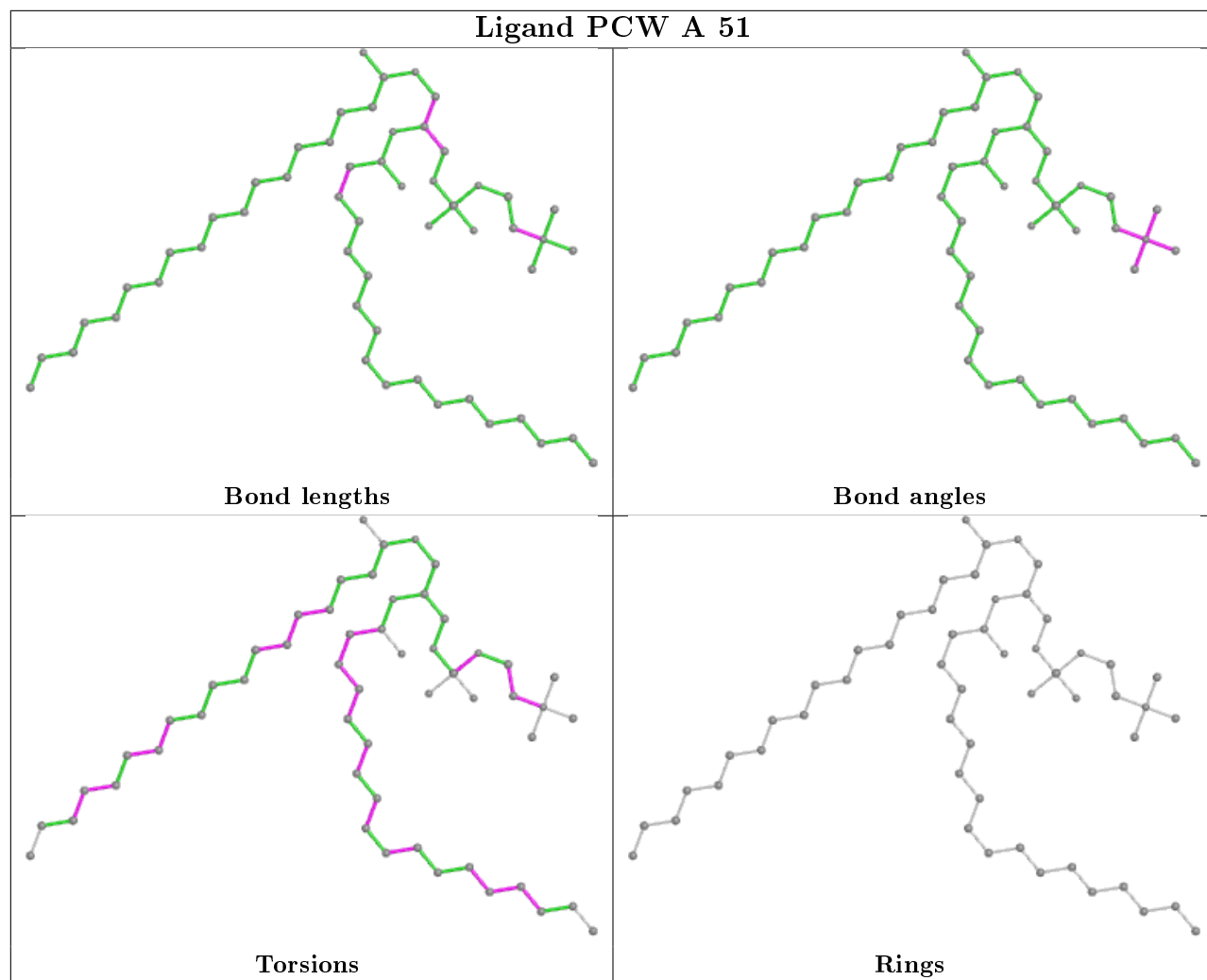


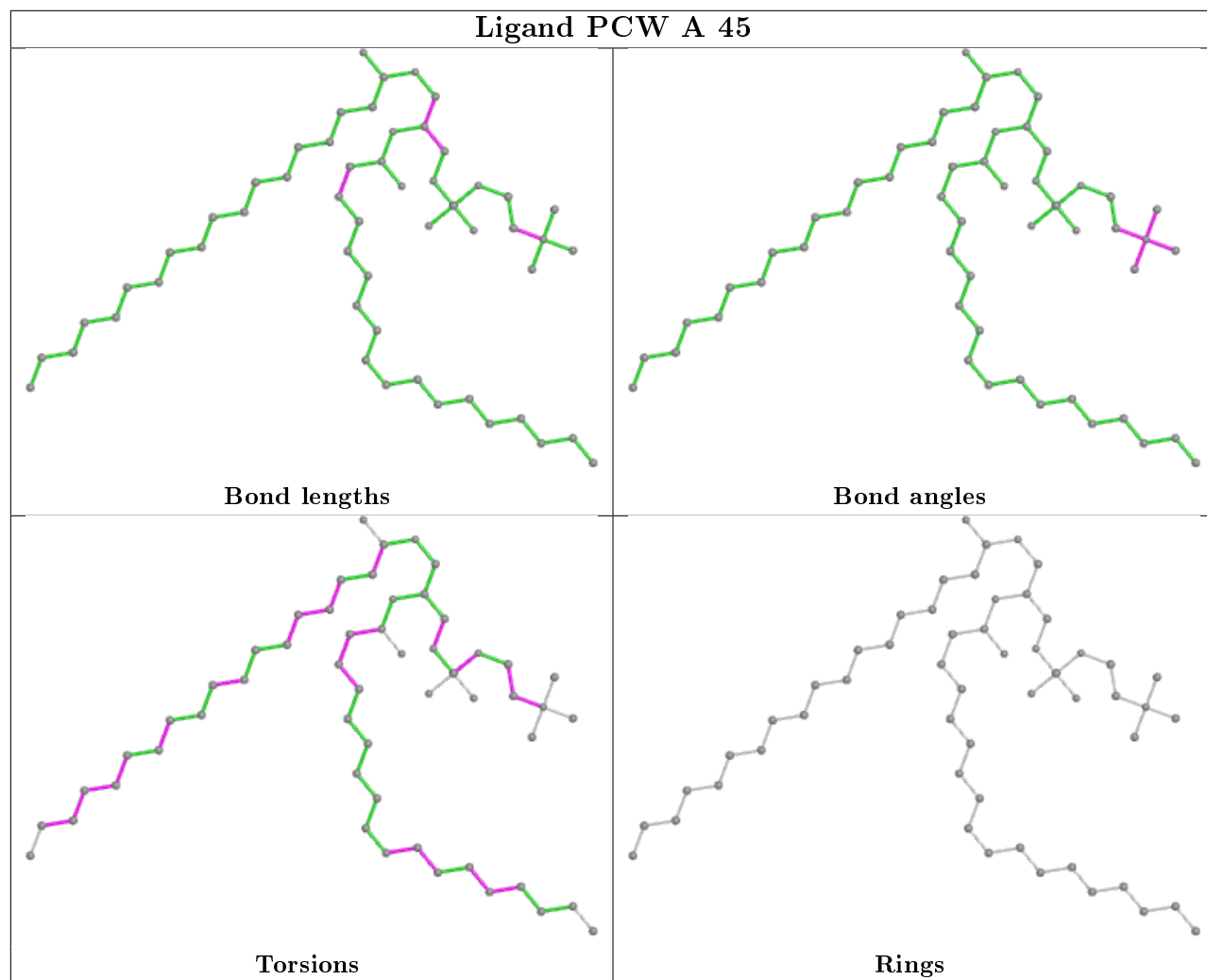




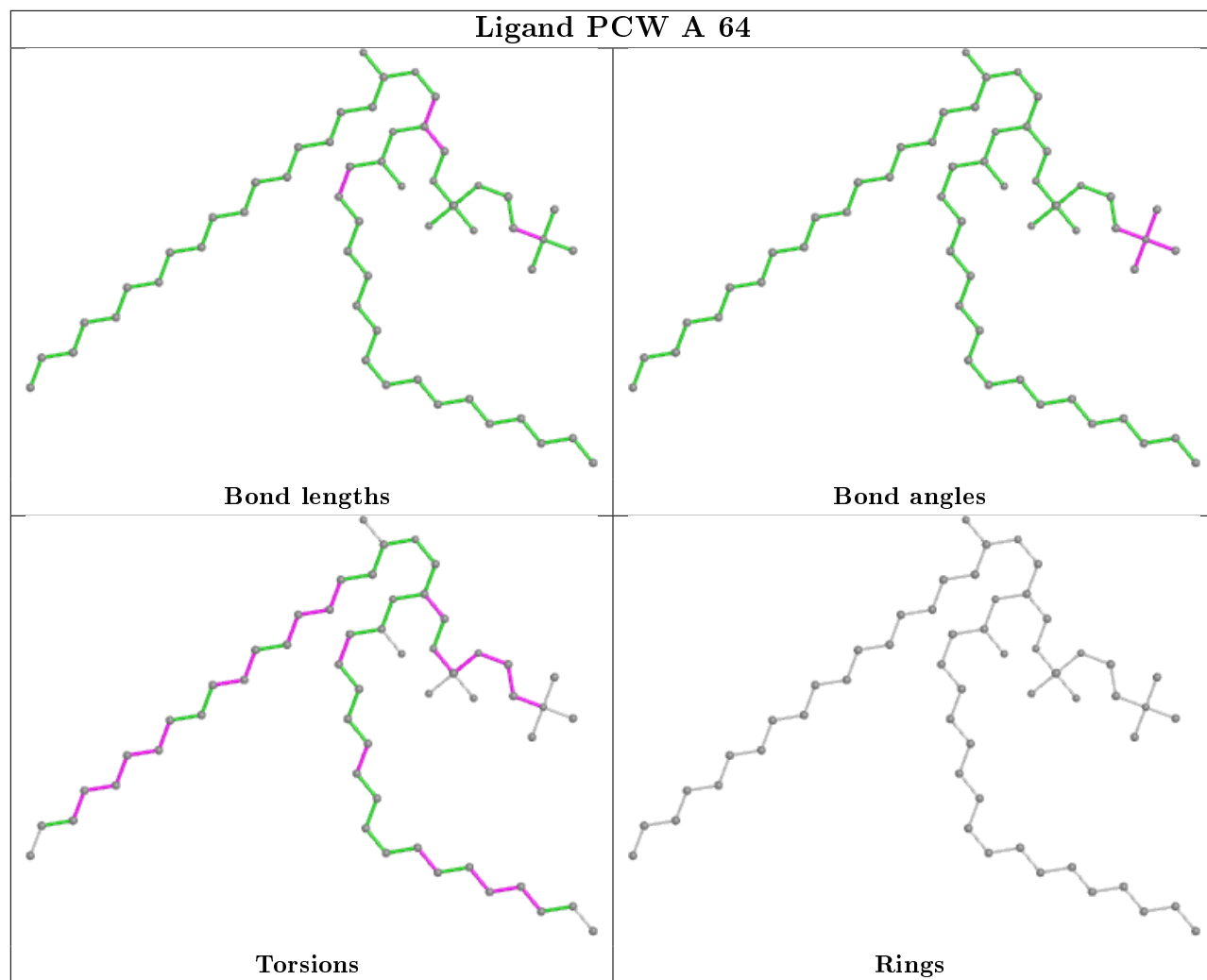


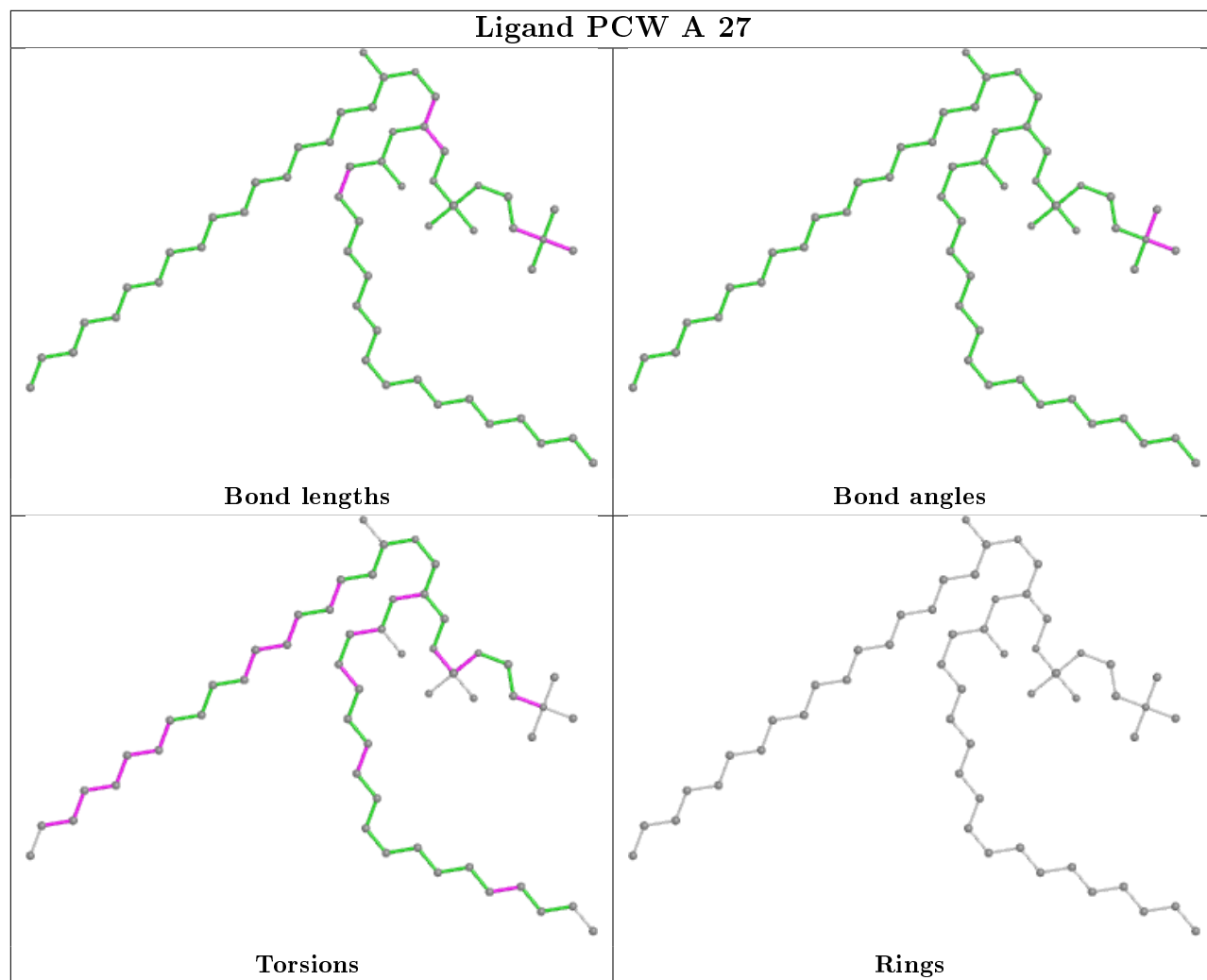


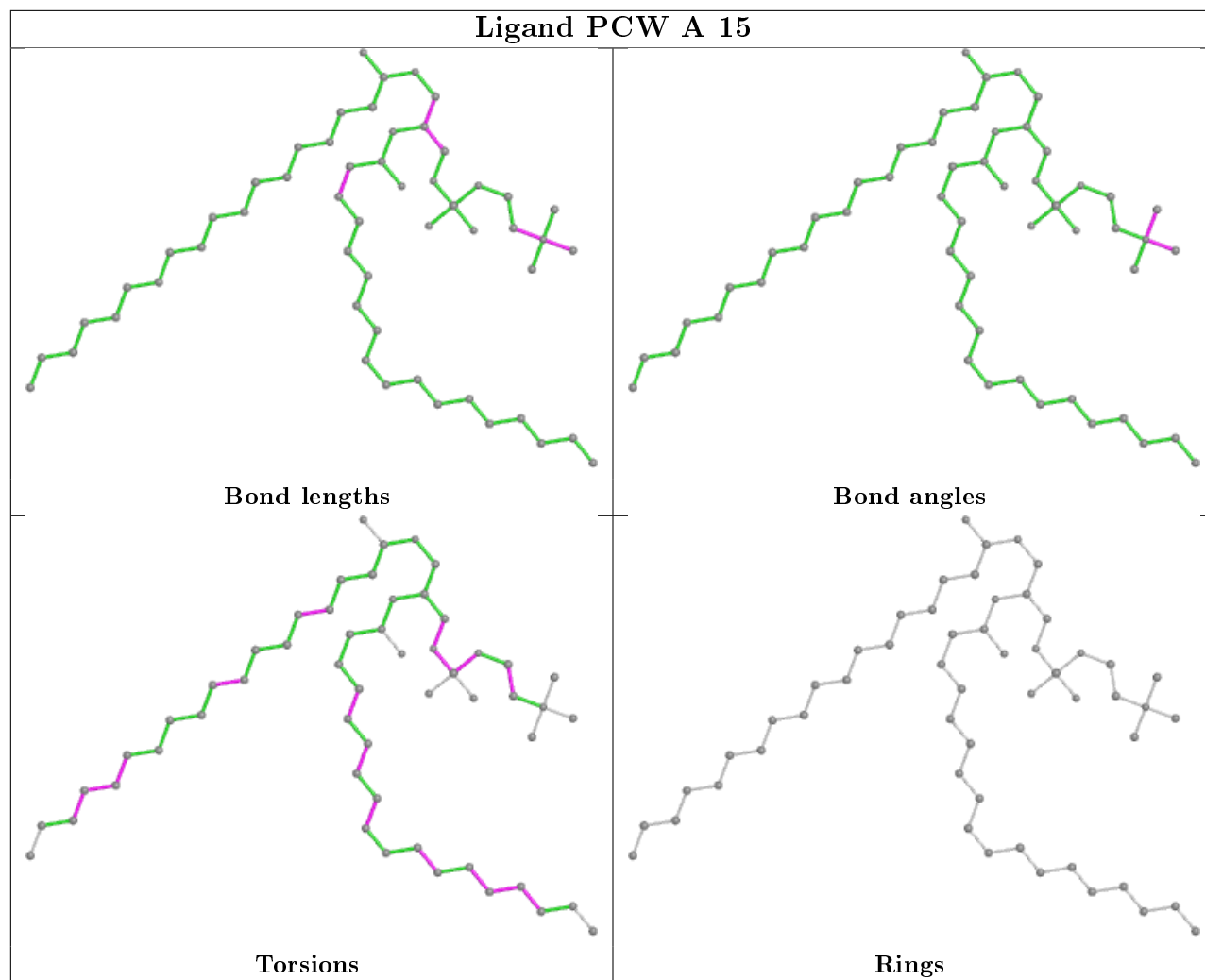


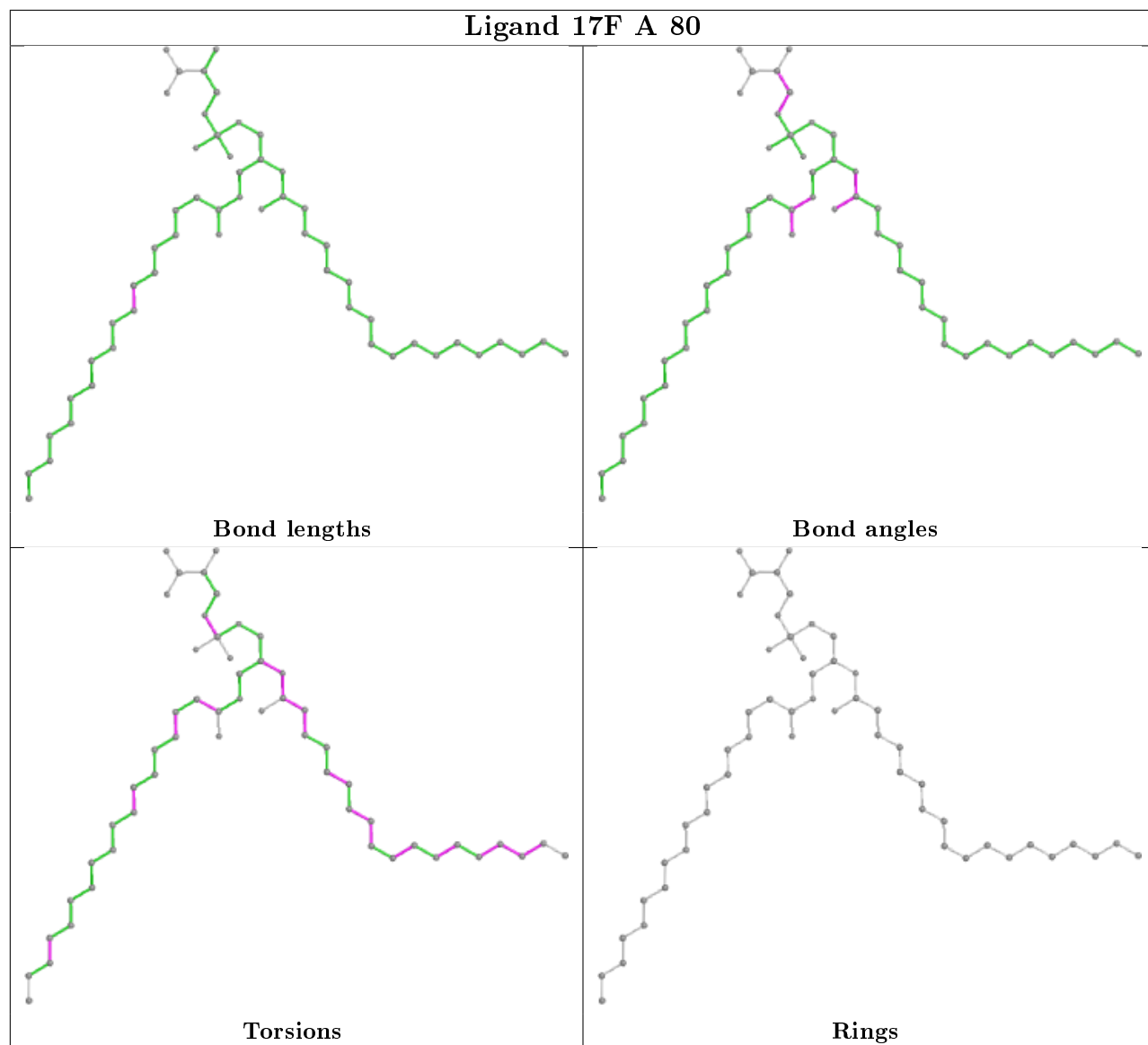


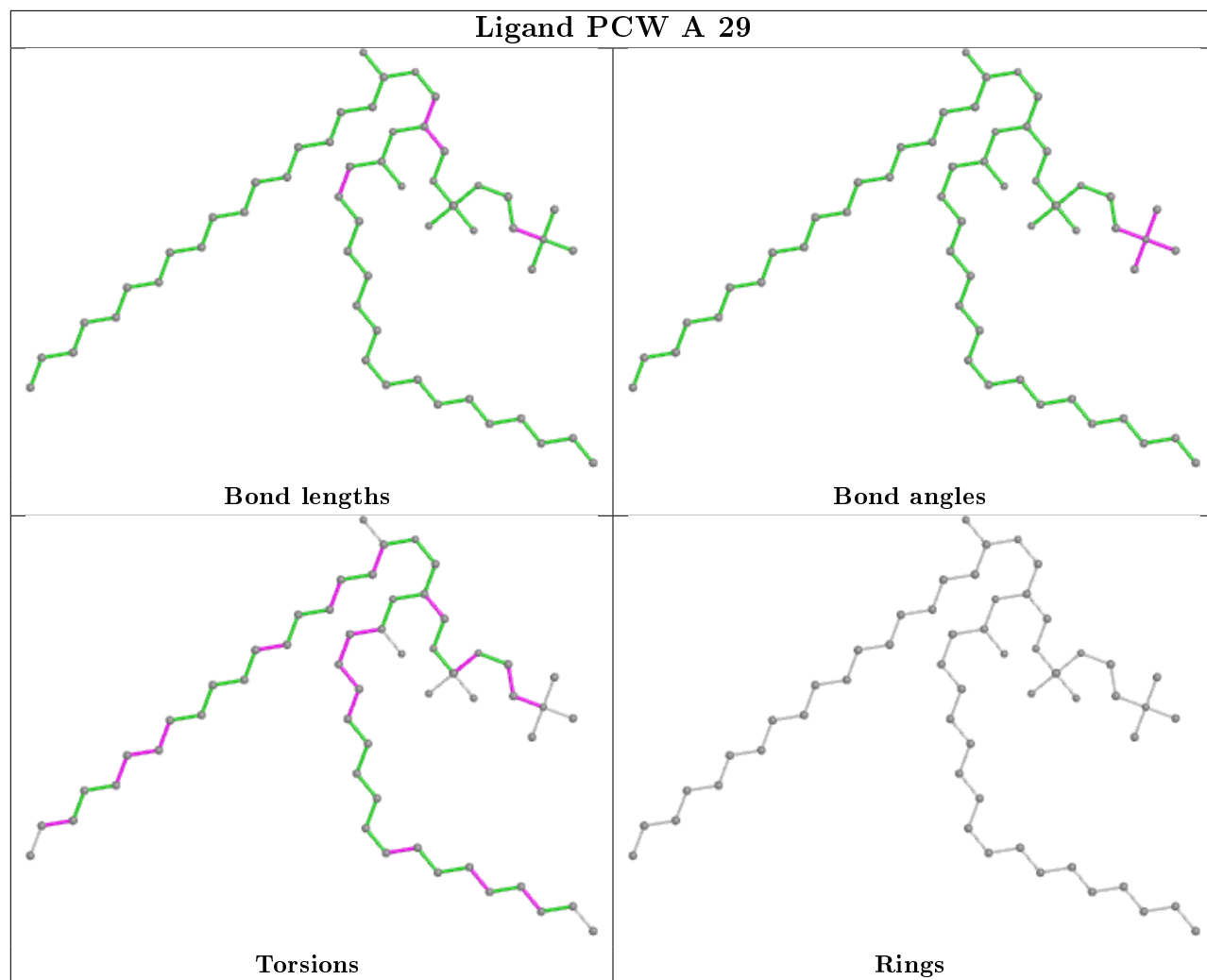


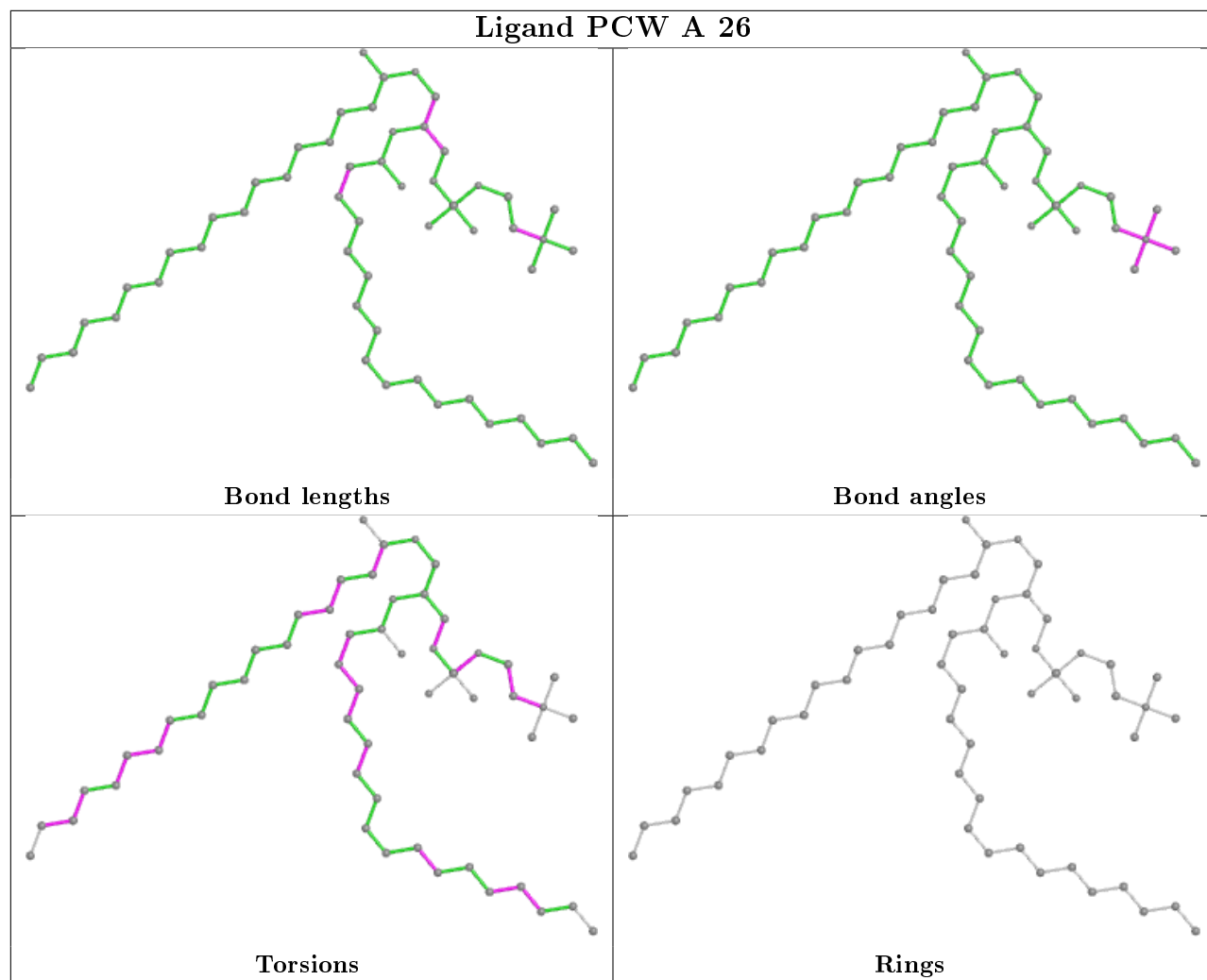


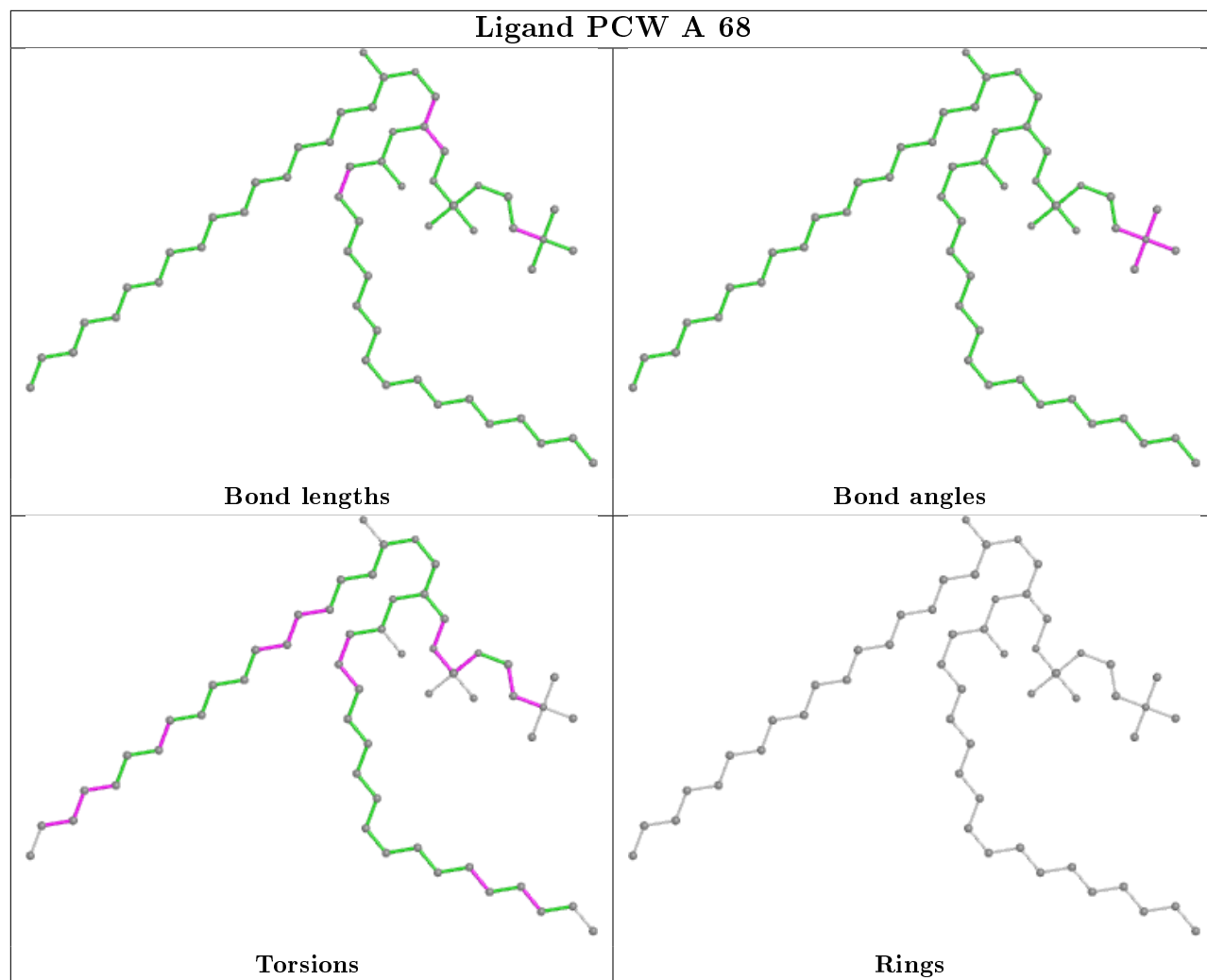


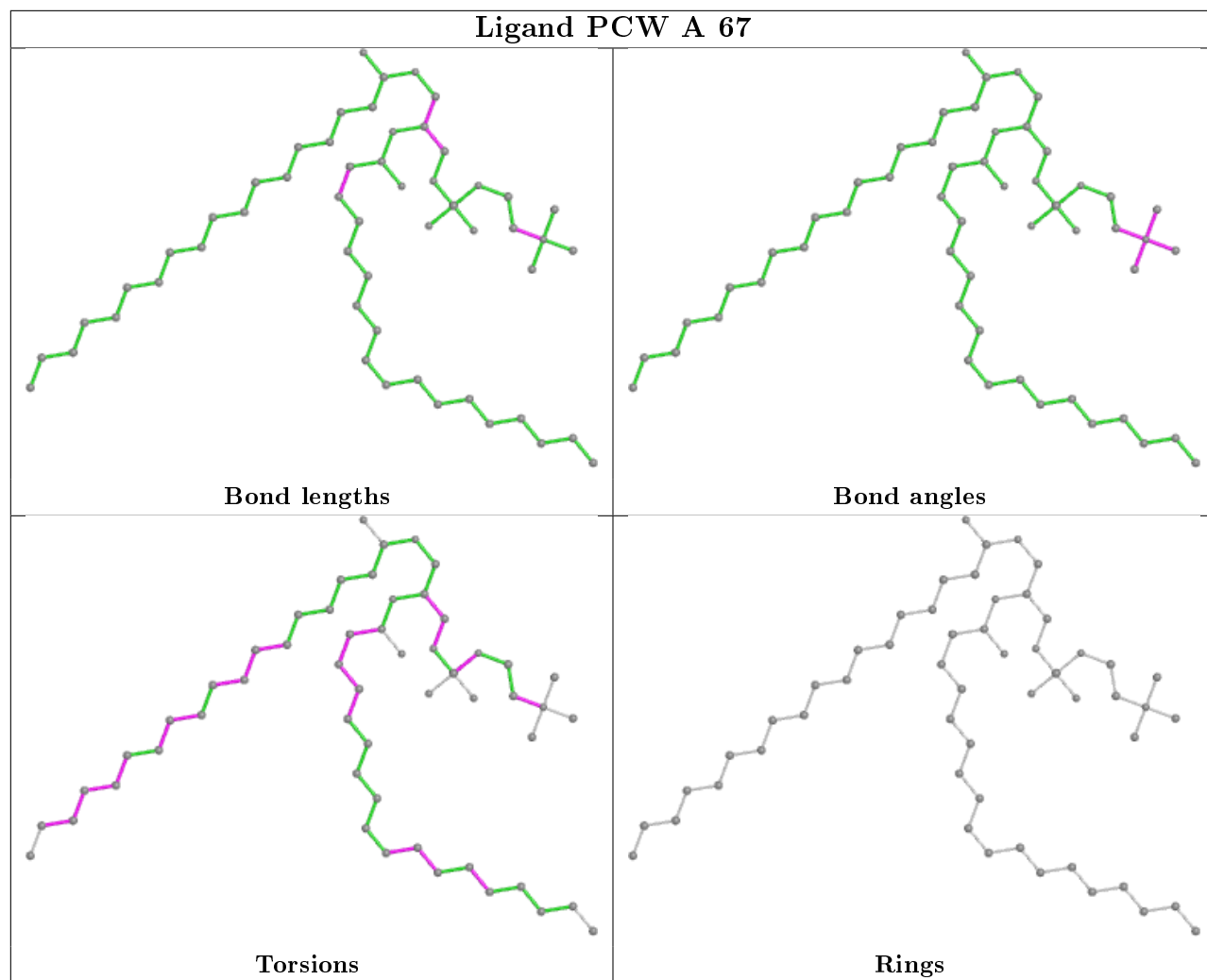




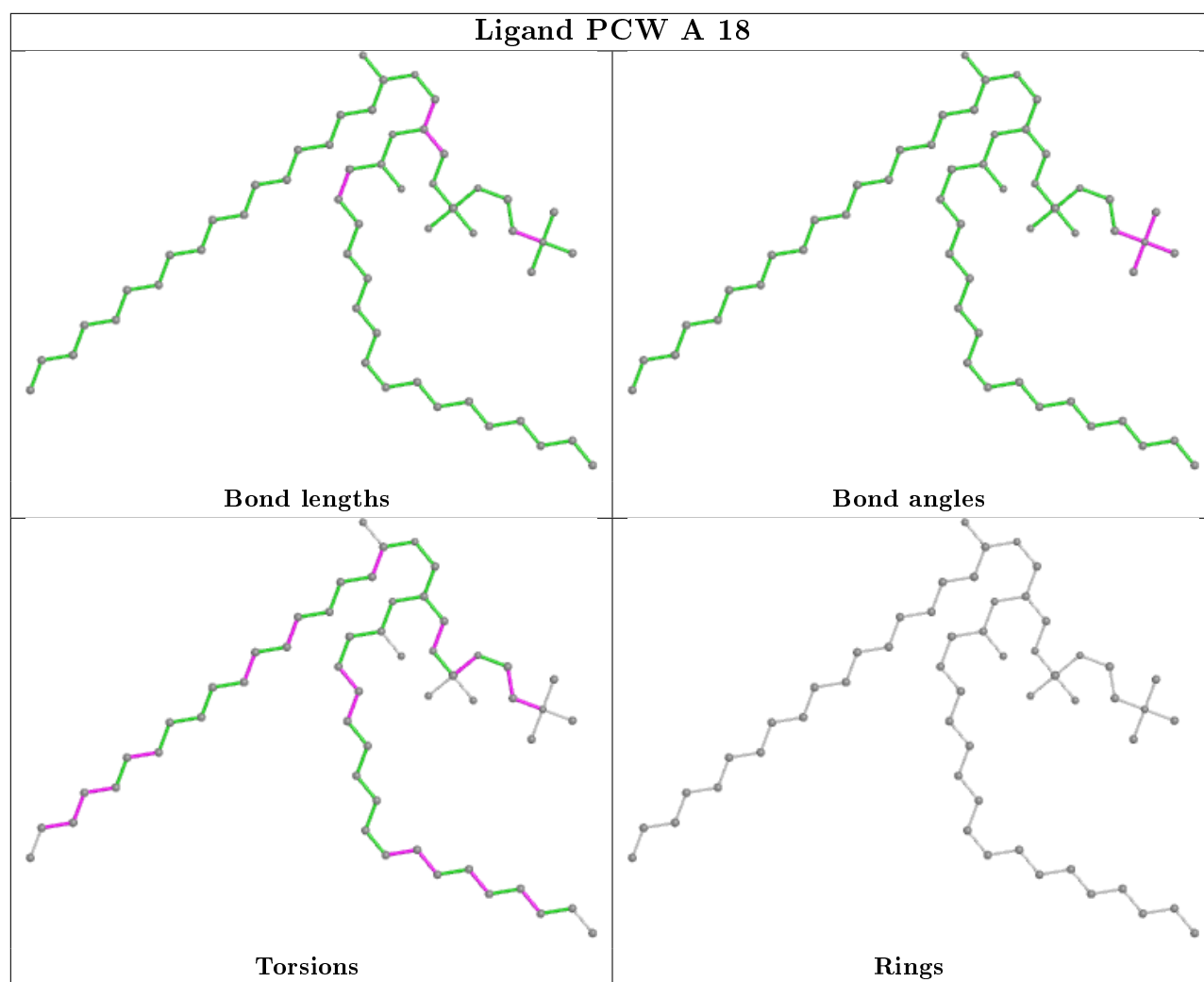












## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	44
Number of shifts mapped to atoms	44
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 20 atoms were assigned a chemical shift out of a possible 6770. 0 out of 101 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/2619 (0%)	0/1044 (0%)	0/1062 (0%)	0/513 (0%)
Sidechain	20/3736 (1%)	10/2189 (0%)	10/1359 (1%)	0/188 (0%)
Aromatic	0/415 (0%)	0/231 (0%)	0/184 (0%)	0/0 (—%)
Overall	20/6770 (0%)	10/3464 (0%)	10/2605 (0%)	0/701 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 22 atoms were assigned a chemical shift out of a possible 7473. 0 out of 108 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	0/2869 (0%)	0/1144 (0%)	0/1162 (0%)	0/563 (0%)
Sidechain	22/4166 (1%)	11/2445 (0%)	11/1505 (1%)	0/216 (0%)
Aromatic	0/438 (0%)	0/244 (0%)	0/194 (0%)	0/0 (—%)
Overall	22/7473 (0%)	11/3833 (0%)	11/2861 (0%)	0/779 (0%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned\_chem\_shift\_list\_1). RCI is only applicable to proteins.