



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 12, 2026 – 09:05 PM UTC

PDB ID : 2MSD / pdb\_00002msd  
BMRB ID : 25115  
Title : NMR data-driven model of GTPase KRas-GNP 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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

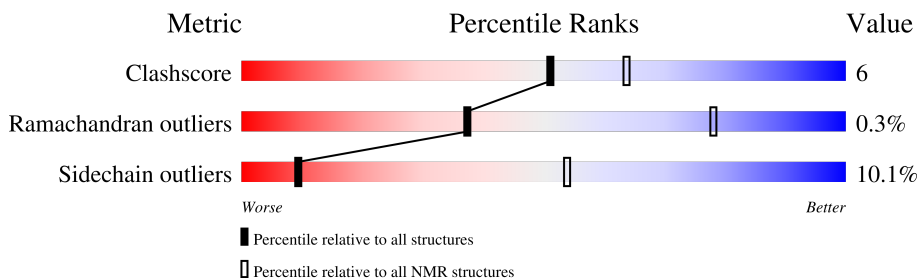
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 1%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	86% 12% ...
1	C	200	84% 13% ..
2	B	187	81% 10% 8% .

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:396, C:401-C:595 (391)	0.45	1
2	B:3-B:172 (170)	0.79	3

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 6, 7, 10
2	5, 8, 9
3	1, 2, 4

### 3 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9138 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

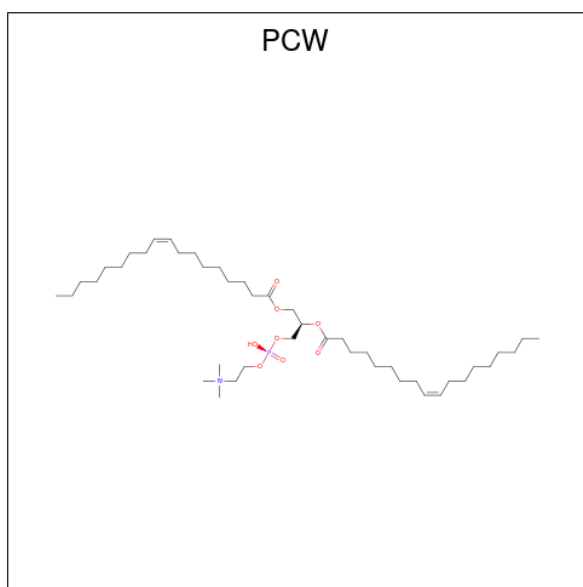
- Molecule 2 is a protein called GTPase KRas.

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 (CCD ID: 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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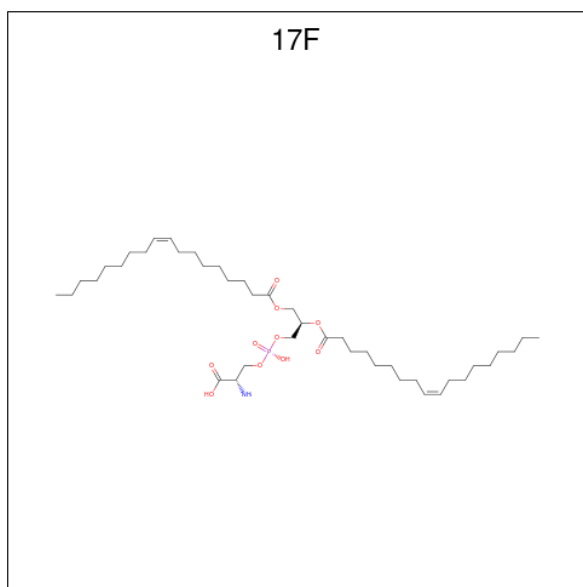




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Mol	Chain	Residues	Atoms				
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1

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



Mol	Chain	Residues	Atoms				
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

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).

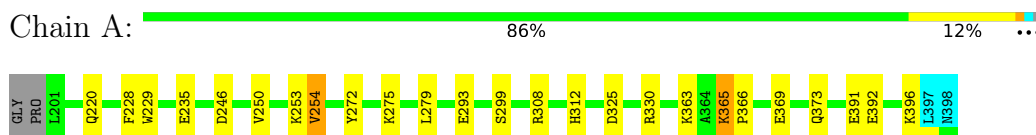


## 4 Residue-property plots i

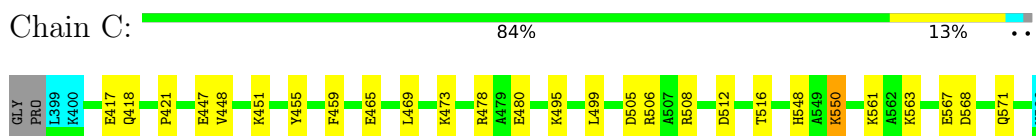
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

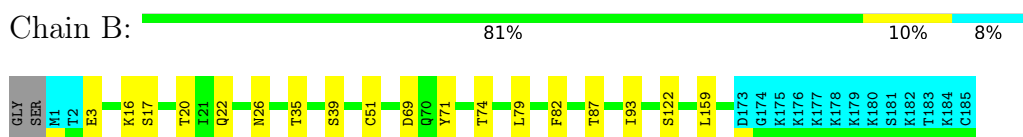
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas

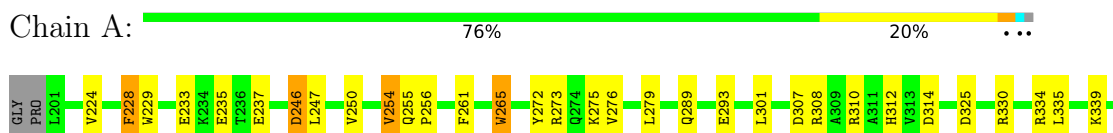


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

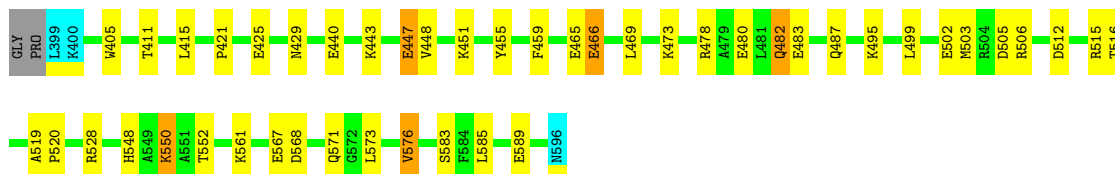
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Apolipoprotein A-I

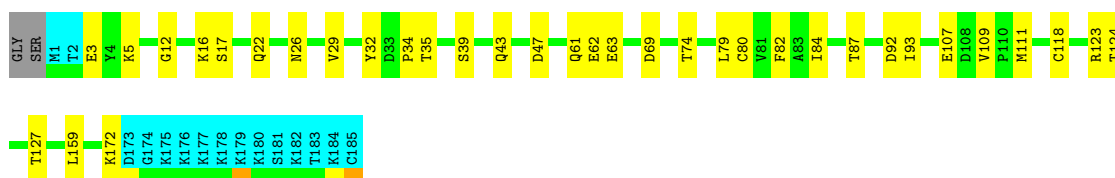




- Molecule 1: Apolipoprotein A-I

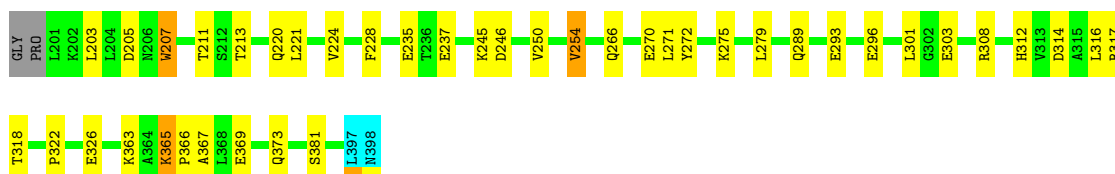
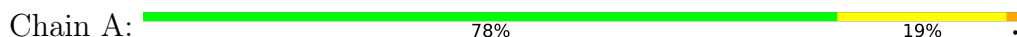


- Molecule 2: GTPase KRas

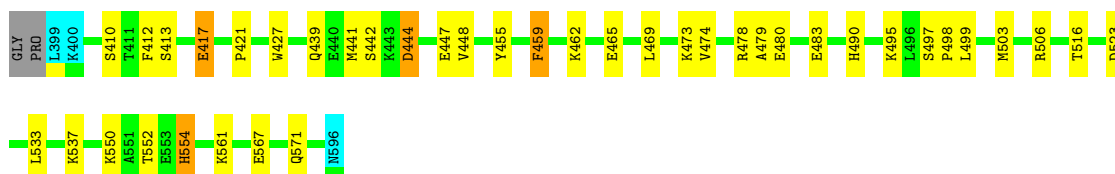
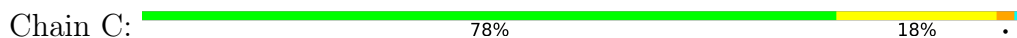


#### 4.2.2 Score per residue for model 2

- Molecule 1: Apolipoprotein A-I

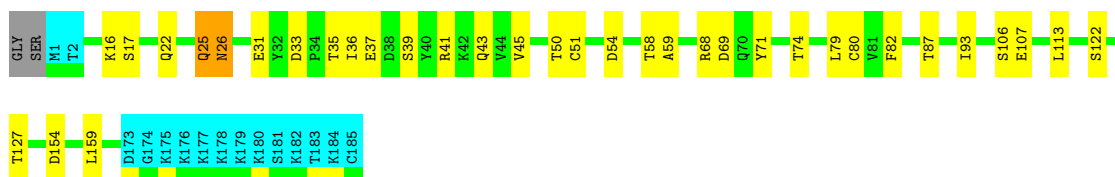


- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas

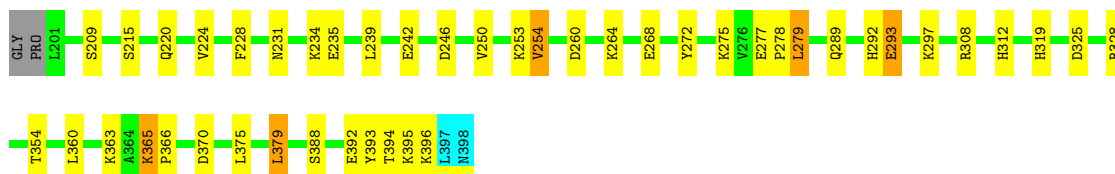




### 4.2.3 Score per residue for model 3

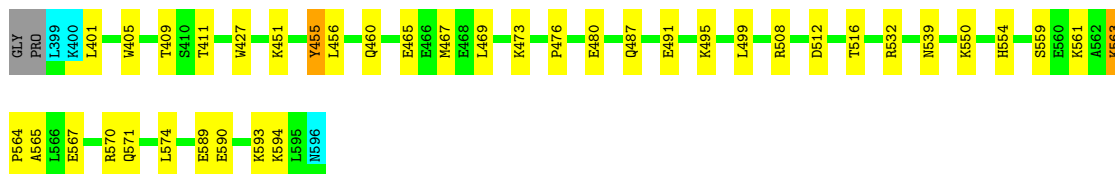
- Molecule 1: Apolipoprotein A-I

Chain A: 76% 20%



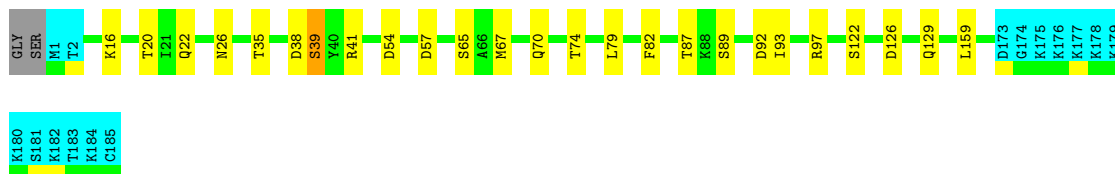
- Molecule 1: Apolipoprotein A-I

Chain C: 78% 18%



- Molecule 2: GTPase KRas

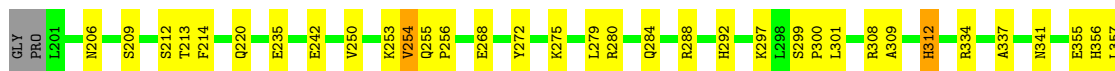
Chain B: 78% 13% 8%



### 4.2.4 Score per residue for model 4

- Molecule 1: Apolipoprotein A-I

Chain A: 74% 22%





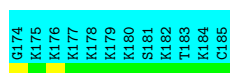
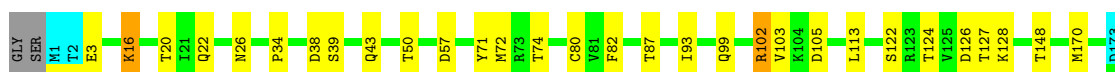
- Molecule 1: Apolipoprotein A-I

Chain C: 72% 24%



- Molecule 2: GTPase KRas

Chain B: 75% 15% 8%



#### 4.2.5 Score per residue for model 5

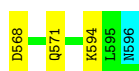
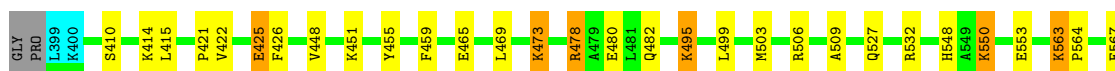
- Molecule 1: Apolipoprotein A-I

Chain A: 80% 16%



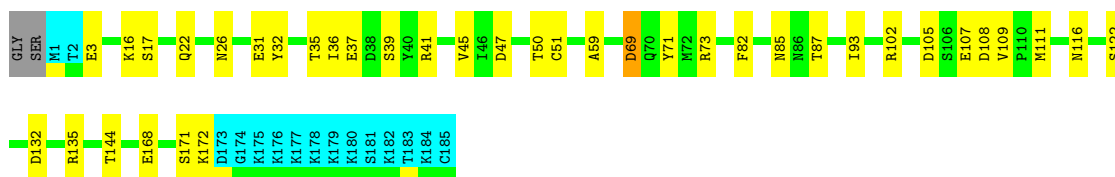
- Molecule 1: Apolipoprotein A-I

Chain C: 81% 14%



- Molecule 2: GTPase KRas

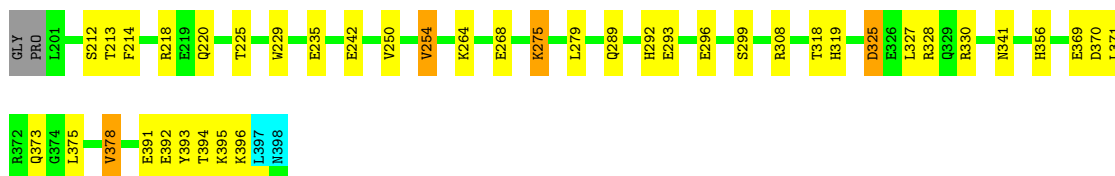
Chain B: 71% 20% 8%



#### 4.2.6 Score per residue for model 6

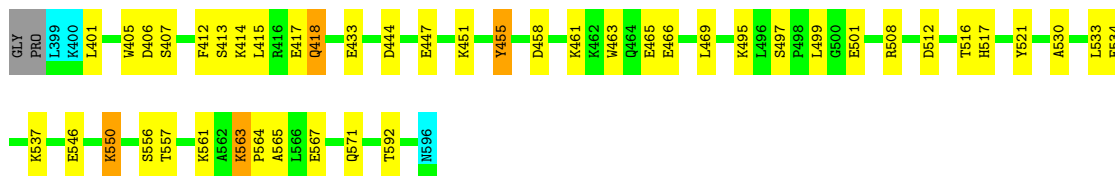
- Molecule 1: Apolipoprotein A-I

Chain A: 78% 18%



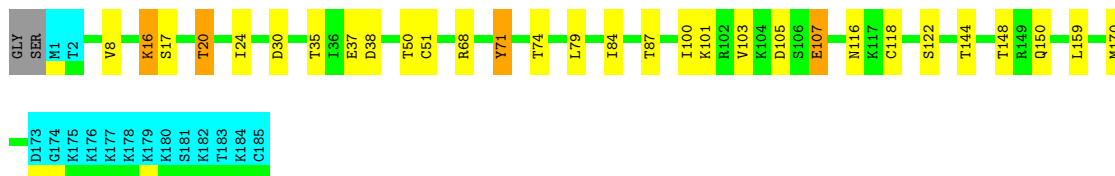
- Molecule 1: Apolipoprotein A-I

Chain C: 75% 20%



- Molecule 2: GTPase KRas

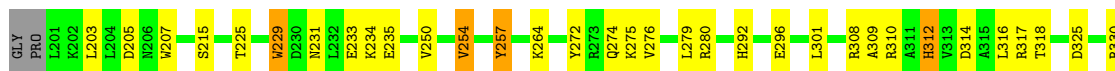
Chain B: 75% 14% 8%

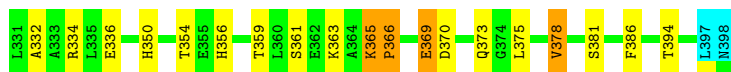


#### 4.2.7 Score per residue for model 7

- Molecule 1: Apolipoprotein A-I

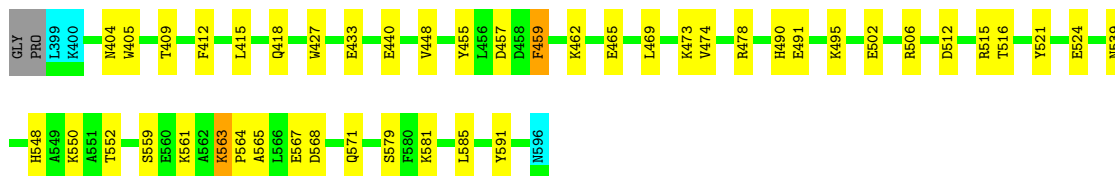
Chain A: 72% 22%





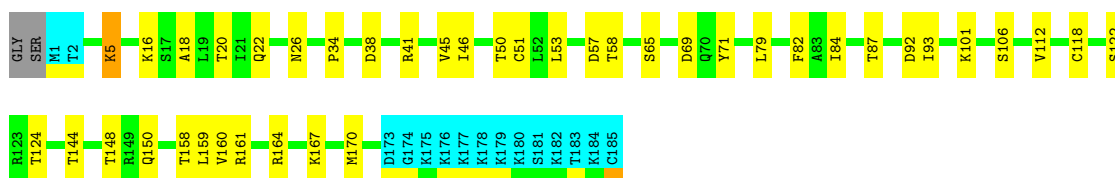
- Molecule 1: Apolipoprotein A-I

Chain C: 75% 22%



- Molecule 2: GTPase KRas

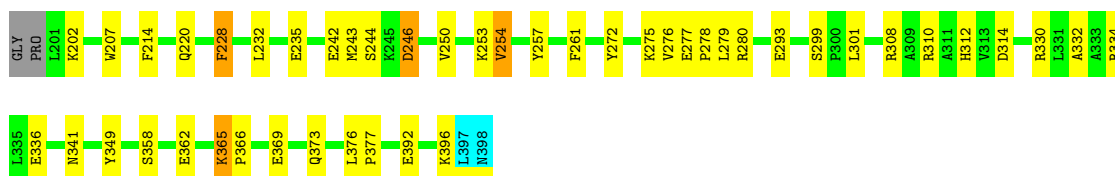
Chain B: 69% 21% 8%



#### 4.2.8 Score per residue for model 8

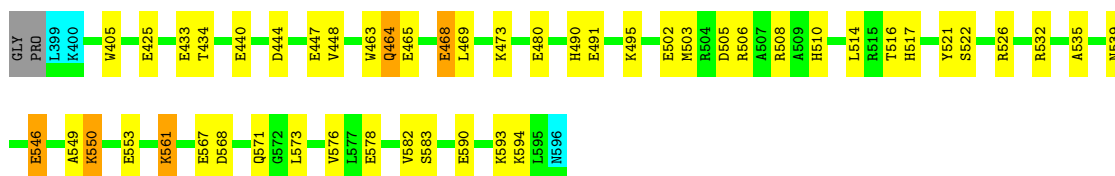
- Molecule 1: Apolipoprotein A-I

Chain A: 75% 21%



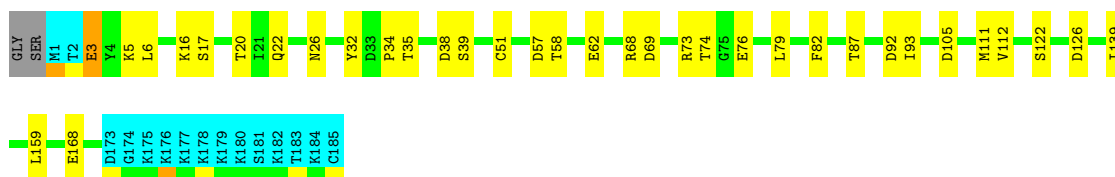
- Molecule 1: Apolipoprotein A-I

Chain C: 73% 22%



- Molecule 2: GTPase KRas

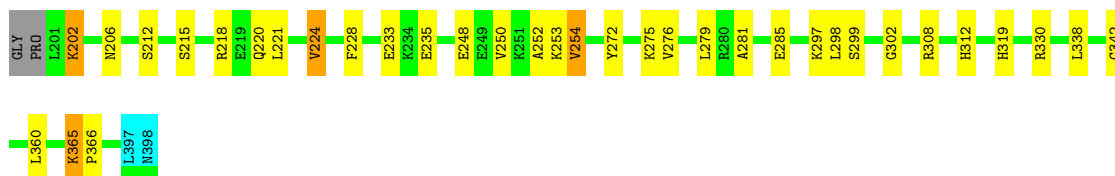
Chain B: 72% 18% 8%



#### 4.2.9 Score per residue for model 9

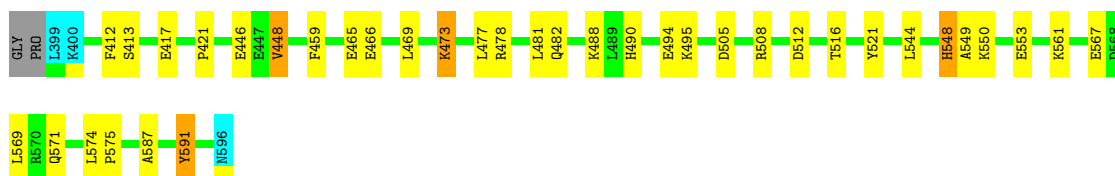
- Molecule 1: Apolipoprotein A-I

Chain A: 80% 16%



- Molecule 1: Apolipoprotein A-I

Chain C: 79% 16%



- Molecule 2: GTPase KRas

Chain B: 72% 19% 8%



#### 4.2.10 Score per residue for model 10

- Molecule 1: Apolipoprotein A-I

Chain A: 72% 24%





- Molecule 1: Apolipoprotein A-I

Chain C: 68% 26%



- Molecule 2: GTPase KRas

Chain B: 72% 19% 8%



## 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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	44
Number of shifts mapped to atoms	11
Number of unparsed shifts	0
Number of shifts with mapping errors	33
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

## 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: GNP, 17F, PCW, MG

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	1607	22	1609	26±6
1	C	1598	22	1597	28±6
2	B	1358	18	1342	14±4
3	A	3456	0	5376	52±4
4	A	864	0	1216	20±5
5	B	32	0	13	1±1
All	All	89160	620	111525	1111

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:CG	1:C:469:LEU:HD11	1.44	1.42	5	2
1:C:465:GLU:O	1:C:469:LEU:CG	1.27	1.82	1	8
1:A:308:ARG:HG2	1:C:469:LEU:CD1	1.27	1.59	5	1
1:C:465:GLU:O	1:C:469:LEU:HG	1.21	1.30	7	10
1:A:391:GLU:O	1:A:395:LYS:HG3	1.10	1.46	6	1
1:C:567:GLU:O	1:C:571:GLN:HG3	1.05	1.50	9	10
1:A:308:ARG:CD	1:C:469:LEU:HD21	1.00	1.86	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ARG:HG3	1:C:469:LEU:HD21	0.98	1.32	10	7
1:A:392:GLU:OE1	1:A:395:LYS:HD2	0.94	1.62	6	1
1:C:567:GLU:O	1:C:571:GLN:CG	0.93	2.17	9	4
1:A:369:GLU:OE1	1:A:373:GLN:NE2	0.92	2.02	2	1
1:A:369:GLU:O	1:A:373:GLN:HG3	0.88	1.67	10	7
1:A:308:ARG:HD2	1:C:469:LEU:HD21	0.88	1.43	7	1
4:A:35:17F:HN1A	2:B:73:ARG:HH12	0.88	1.11	5	1
1:A:392:GLU:CD	1:A:395:LYS:HD2	0.87	1.93	6	1
1:A:308:ARG:HG3	1:C:469:LEU:CD2	0.84	2.01	10	4
1:A:392:GLU:OE1	1:A:395:LYS:CD	0.84	2.25	6	1
2:B:38:ASP:HB2	2:B:57:ASP:HB3	0.83	1.46	7	4
1:A:279:LEU:HD22	1:C:495:LYS:HG2	0.82	1.51	7	2
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.81	1.52	2	8
1:C:465:GLU:O	1:C:469:LEU:CB	0.81	2.27	7	2
3:A:68:PCW:H122	3:A:69:PCW:H331	0.80	1.53	1	2
1:A:308:ARG:CB	1:C:469:LEU:HD11	0.80	2.06	5	2
1:A:314:ASP:HA	1:A:317:ARG:HD2	0.79	1.52	2	3
4:A:36:17F:HN1A	2:B:73:ARG:HH11	0.79	1.19	10	1
1:A:308:ARG:CG	1:C:469:LEU:CD1	0.79	2.39	5	1
1:C:563:LYS:HB2	1:C:564:PRO:HD3	0.78	1.55	5	4
1:A:297:LYS:HE2	1:C:476:PRO:HB2	0.78	1.56	4	2
1:A:392:GLU:O	1:A:396:LYS:HG3	0.77	1.80	6	1
1:C:465:GLU:O	1:C:469:LEU:CD1	0.77	2.32	7	3
1:A:393:TYR:HD1	1:A:396:LYS:HE3	0.77	1.40	6	1
1:A:391:GLU:O	1:A:395:LYS:CG	0.76	2.31	6	1
3:A:13:PCW:H73	4:A:34:17F:HN1	0.76	1.38	9	2
1:A:308:ARG:HD3	1:C:469:LEU:HD21	0.75	1.57	7	1
3:A:11:PCW:H62	3:A:25:PCW:H31	0.74	1.58	10	1
4:A:40:17F:H4	4:A:40:17F:HN1	0.74	1.41	3	2
1:A:393:TYR:HD1	1:A:396:LYS:CE	0.74	1.95	6	1
3:A:45:PCW:H40	3:A:57:PCW:H61	0.73	1.57	10	2
3:A:6:PCW:H39	3:A:7:PCW:H62	0.73	1.59	1	1
1:A:393:TYR:CD1	1:A:396:LYS:HE3	0.73	2.18	6	1
3:A:54:PCW:H321	3:A:72:PCW:H132	0.73	1.61	10	1
3:A:5:PCW:H2	3:A:5:PCW:H52	0.72	1.61	9	2
4:A:34:17F:HN1A	2:B:167:LYS:HD3	0.72	1.44	7	1
1:C:590:GLU:HA	1:C:593:LYS:HE3	0.71	1.62	8	2
2:B:79:LEU:HG	2:B:159:LEU:HD22	0.71	1.61	6	8
1:A:218:ARG:HE	3:A:15:PCW:H19	0.70	1.45	6	2
3:A:4:PCW:H31	3:A:4:PCW:H41	0.70	1.64	1	1
3:A:16:PCW:H351	4:A:39:17F:H8A	0.69	1.63	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:369:GLU:OE1	1:A:373:GLN:CD	0.69	2.34	2	1
3:A:45:PCW:H39	3:A:57:PCW:H71	0.69	1.65	9	1
3:A:26:PCW:H332	4:A:40:17F:H20A	0.69	1.63	4	1
1:A:279:LEU:HB3	1:C:495:LYS:HE3	0.69	1.65	10	4
1:C:458:ASP:HA	1:C:461:LYS:HE2	0.69	1.63	6	1
1:A:276:VAL:O	1:A:280:ARG:HB2	0.69	1.88	8	3
3:A:58:PCW:H332	3:A:61:PCW:H351	0.69	1.64	8	1
1:A:308:ARG:CG	1:C:469:LEU:HD21	0.68	2.14	10	2
3:A:18:PCW:H341	3:A:18:PCW:H131	0.68	1.66	9	1
4:A:34:17F:H20	4:A:34:17F:H8A	0.68	1.66	9	1
1:A:255:GLN:HB2	1:A:256:PRO:HD3	0.67	1.65	4	2
3:A:32:PCW:H62	4:A:38:17F:HN1	0.67	1.49	2	1
1:A:308:ARG:HD3	1:C:469:LEU:HD11	0.67	1.65	7	2
1:A:393:TYR:CD1	1:A:396:LYS:NZ	0.67	2.62	6	1
1:A:388:SER:HB2	1:C:594:LYS:HE2	0.67	1.66	3	1
3:A:53:PCW:H41	3:A:68:PCW:H321	0.66	1.66	7	1
3:A:66:PCW:H212	3:A:67:PCW:H82	0.66	1.66	8	1
1:A:308:ARG:HG2	1:C:469:LEU:HD11	0.66	0.70	5	1
3:A:25:PCW:H452	3:A:25:PCW:H182	0.66	1.66	1	1
3:A:42:PCW:H52	4:A:75:17F:H2	0.66	1.68	8	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.66	1.90	6	9
3:A:7:PCW:H11	3:A:16:PCW:H12	0.66	1.67	9	1
3:A:1:PCW:H52	4:A:35:17F:HN1A	0.65	1.50	3	1
3:A:46:PCW:H42	4:A:73:17F:HN1A	0.65	1.50	8	1
3:A:12:PCW:H52	4:A:37:17F:HN1	0.65	1.51	10	1
1:C:503:MET:HA	1:C:506:ARG:HD2	0.65	1.67	2	4
3:A:16:PCW:H121	4:A:39:17F:H9	0.65	1.68	6	1
1:A:376:LEU:HB2	1:A:377:PRO:HD3	0.65	1.68	10	1
4:A:39:17F:H18A	4:A:39:17F:H9A	0.65	1.69	9	1
3:A:46:PCW:H31	3:A:71:PCW:H362	0.64	1.68	8	1
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.64	1.67	7	3
3:A:9:PCW:H61	3:A:26:PCW:H61	0.64	1.68	10	1
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.64	1.68	4	2
1:A:301:LEU:HD22	1:C:473:LYS:HG2	0.64	1.69	8	2
3:A:28:PCW:H161	3:A:28:PCW:H39	0.64	1.68	8	1
3:A:26:PCW:H382	3:A:26:PCW:H152	0.64	1.70	9	1
1:A:308:ARG:CD	1:C:469:LEU:HD11	0.64	2.23	8	1
4:A:35:17F:HN1A	2:B:73:ARG:HH22	0.64	1.35	9	1
1:A:264:LYS:HE2	1:C:509:ALA:HB1	0.64	1.69	10	1
3:A:49:PCW:H62	4:A:80:17F:HN1	0.64	1.51	3	1
3:A:32:PCW:H81	4:A:38:17F:HN1A	0.64	1.52	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:392:GLU:OE2	1:A:395:LYS:NZ	0.63	2.24	6	1
3:A:13:PCW:H41	4:A:34:17F:N1	0.63	2.08	9	1
3:A:17:PCW:H172	3:A:21:PCW:H141	0.63	1.69	5	1
3:A:17:PCW:H332	3:A:17:PCW:H132	0.63	1.70	1	1
3:A:68:PCW:H121	3:A:69:PCW:H371	0.63	1.70	9	1
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.62	1.69	8	3
1:A:393:TYR:CD1	1:A:396:LYS:CE	0.62	2.80	6	1
3:A:5:PCW:H83	4:A:38:17F:H4A	0.62	1.70	8	1
1:C:505:ASP:HA	1:C:508:ARG:HD2	0.62	1.72	8	3
3:A:66:PCW:H432	4:A:79:17F:H57	0.62	1.71	9	1
4:A:74:17F:H9	4:A:74:17F:H20A	0.62	1.69	5	1
3:A:58:PCW:H12	3:A:61:PCW:H381	0.62	1.69	9	1
4:A:36:17F:HN1A	2:B:73:ARG:NH1	0.62	1.93	10	1
1:C:418:GLN:O	1:C:422:VAL:HB	0.62	1.95	10	2
3:A:60:PCW:H31	3:A:61:PCW:H382	0.62	1.72	5	1
3:A:9:PCW:H122	3:A:11:PCW:H2	0.62	1.70	7	1
3:A:13:PCW:H122	3:A:18:PCW:H122	0.62	1.71	8	1
3:A:30:PCW:H62	4:A:34:17F:H2	0.61	1.71	8	1
1:A:392:GLU:HA	1:A:395:LYS:HB2	0.61	1.71	6	1
4:A:33:17F:HN1	2:B:73:ARG:HH12	0.61	1.39	8	1
1:A:308:ARG:HG3	1:C:469:LEU:HD11	0.61	1.72	8	2
3:A:14:PCW:H31	4:A:34:17F:H57	0.61	1.72	7	1
3:A:19:PCW:H322	3:A:23:PCW:H352	0.61	1.70	5	1
3:A:14:PCW:H432	4:A:34:17F:H20A	0.61	1.72	10	1
2:B:32:TYR:HD1	5:B:201:GNP:H4'	0.61	1.56	1	1
2:B:30:ASP:HA	5:B:201:GNP:H3'	0.61	1.73	9	1
1:C:561:LYS:HA	1:C:565:ALA:HB3	0.61	1.73	7	2
1:A:334:ARG:HD2	1:C:440:GLU:OE1	0.60	1.96	7	2
1:A:231:ASN:HA	1:A:234:LYS:HE2	0.60	1.73	3	3
3:A:1:PCW:H41	4:A:35:17F:H1A	0.60	1.72	8	1
1:A:330:ARG:HH21	1:C:447:GLU:HB2	0.60	1.56	6	1
1:A:365:LYS:O	1:A:369:GLU:HB2	0.60	1.97	2	2
1:A:308:ARG:CB	1:C:469:LEU:CD1	0.60	2.76	5	1
2:B:12:GLY:HA3	2:B:61:GLN:HG3	0.60	1.73	1	1
2:B:84:ILE:HD12	2:B:123:ARG:HG3	0.60	1.72	1	1
2:B:25:GLN:HE21	2:B:25:GLN:HA	0.60	1.57	2	1
3:A:13:PCW:H41	4:A:34:17F:HN1	0.60	1.57	9	1
3:A:53:PCW:H83	3:A:68:PCW:H322	0.59	1.74	3	1
4:A:77:17F:HN1	4:A:77:17F:P1	0.59	2.20	4	1
3:A:3:PCW:H422	3:A:18:PCW:H132	0.59	1.73	1	1
3:A:63:PCW:H352	3:A:63:PCW:H122	0.59	1.74	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:74:17F:H46	4:A:75:17F:H35	0.59	1.74	6	1
3:A:41:PCW:H61	4:A:77:17F:H1A	0.59	1.73	7	1
1:A:250:VAL:O	1:A:254:VAL:HB	0.59	1.97	2	9
3:A:51:PCW:H41	3:A:71:PCW:H412	0.59	1.74	8	1
3:A:32:PCW:H83	4:A:35:17F:H4A	0.59	1.74	4	1
3:A:49:PCW:H121	3:A:57:PCW:H372	0.59	1.74	8	1
1:C:451:LYS:O	1:C:455:TYR:HB2	0.58	1.98	5	6
3:A:20:PCW:H322	3:A:31:PCW:H11	0.58	1.72	3	1
3:A:59:PCW:H451	4:A:77:17F:H46	0.58	1.74	9	1
1:C:466:GLU:HA	1:C:469:LEU:HD12	0.58	1.73	6	2
3:A:20:PCW:H81	3:A:31:PCW:O2P	0.58	1.98	2	1
3:A:42:PCW:H352	3:A:42:PCW:H151	0.58	1.76	3	1
1:A:345:ARG:HG2	1:C:429:ASN:OD1	0.58	1.97	1	1
3:A:68:PCW:H332	3:A:69:PCW:H322	0.58	1.76	10	1
2:B:22:GLN:O	2:B:26:ASN:HA	0.58	1.99	7	9
3:A:42:PCW:H20	3:A:61:PCW:H71	0.58	1.74	6	1
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.57	1.76	10	3
3:A:6:PCW:H471	3:A:28:PCW:H19	0.57	1.75	2	1
3:A:30:PCW:H121	4:A:40:17F:H6	0.57	1.76	10	1
2:B:109:VAL:HB	2:B:111:MET:HE3	0.57	1.75	10	4
3:A:9:PCW:H39	3:A:14:PCW:H52	0.57	1.76	9	1
1:A:369:GLU:O	1:A:373:GLN:CG	0.57	2.50	10	1
3:A:12:PCW:H83	4:A:37:17F:H1A	0.57	1.74	10	1
3:A:9:PCW:H73	3:A:30:PCW:O2P	0.57	2.00	3	1
3:A:62:PCW:O2P	3:A:63:PCW:H62	0.57	1.99	5	1
1:C:414:LYS:O	1:C:418:GLN:HG3	0.57	2.00	4	2
3:A:16:PCW:H242	4:A:39:17F:H4	0.57	1.76	5	1
1:C:478:ARG:O	1:C:482:GLN:HB2	0.57	1.99	1	3
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.57	1.76	4	9
1:A:308:ARG:HG2	1:C:469:LEU:CG	0.57	2.29	5	1
3:A:43:PCW:H411	3:A:71:PCW:H232	0.57	1.77	5	1
3:A:3:PCW:H61	3:A:19:PCW:H2	0.56	1.77	7	1
3:A:3:PCW:H361	3:A:18:PCW:H31	0.56	1.76	10	1
3:A:13:PCW:H73	4:A:34:17F:N1	0.56	2.14	9	2
3:A:68:PCW:H371	3:A:68:PCW:H131	0.56	1.77	1	1
3:A:63:PCW:P	4:A:75:17F:HN1A	0.56	2.22	2	2
3:A:30:PCW:H31	3:A:30:PCW:H51	0.56	1.75	3	1
4:A:35:17F:H43	3:A:55:PCW:H222	0.56	1.76	5	1
3:A:42:PCW:H19	3:A:42:PCW:H352	0.56	1.77	5	1
3:A:16:PCW:H322	4:A:39:17F:H8A	0.56	1.77	8	1
3:A:25:PCW:H131	3:A:31:PCW:H12	0.56	1.78	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:59:PCW:H121	4:A:77:17F:H19A	0.56	1.77	10	1
2:B:68:ARG:HA	2:B:71:TYR:CE2	0.56	2.36	9	2
1:A:242:GLU:HB3	1:C:532:ARG:HH21	0.56	1.61	8	1
1:C:447:GLU:OE1	1:C:451:LYS:HE2	0.56	2.01	10	2
4:A:36:17F:HN1A	2:B:41:ARG:HE	0.56	1.40	5	1
1:A:375:LEU:HA	1:A:378:VAL:HG12	0.56	1.75	6	2
3:A:32:PCW:H72	4:A:38:17F:N1	0.56	2.16	3	1
3:A:19:PCW:H42	3:A:29:PCW:O1P	0.56	2.00	4	1
3:A:9:PCW:H331	3:A:14:PCW:H321	0.56	1.78	3	1
1:A:371:LEU:HD22	4:A:38:17F:H54	0.56	1.77	6	1
3:A:45:PCW:H471	4:A:79:17F:H18	0.56	1.77	7	1
2:B:158:THR:HA	2:B:161:ARG:HD2	0.56	1.78	7	1
3:A:30:PCW:H72	4:A:40:17F:O5	0.56	2.00	5	1
2:B:101:LYS:HG2	2:B:107:GLU:HA	0.56	1.76	6	1
1:C:466:GLU:OE1	1:C:469:LEU:HD12	0.55	2.01	1	1
3:A:53:PCW:H141	3:A:68:PCW:H431	0.55	1.77	4	1
3:A:18:PCW:H252	3:A:49:PCW:H422	0.55	1.78	10	1
3:A:1:PCW:H42	3:A:26:PCW:H331	0.55	1.78	1	1
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.55	1.77	3	2
3:A:70:PCW:H351	3:A:71:PCW:H121	0.55	1.78	5	1
3:A:49:PCW:O2P	3:A:57:PCW:H71	0.55	2.01	7	1
1:A:327:LEU:HD23	1:A:330:ARG:HD2	0.55	1.77	6	1
3:A:25:PCW:H271	3:A:31:PCW:H451	0.55	1.78	10	1
1:A:392:GLU:CD	1:A:395:LYS:CD	0.55	2.76	6	1
3:A:1:PCW:O2P	3:A:17:PCW:H83	0.55	2.02	10	1
3:A:42:PCW:H231	3:A:52:PCW:H351	0.55	1.76	10	1
3:A:42:PCW:O31	3:A:42:PCW:H82	0.55	2.02	1	1
3:A:6:PCW:H232	3:A:24:PCW:H232	0.55	1.78	10	1
3:A:7:PCW:H32	3:A:16:PCW:H31	0.55	1.77	4	1
2:B:45:VAL:HA	2:B:50:THR:HA	0.55	1.78	7	2
3:A:11:PCW:H262	4:A:75:17F:H48	0.55	1.78	8	1
3:A:44:PCW:H172	4:A:77:17F:H6	0.55	1.79	2	1
1:A:243:MET:HA	1:A:246:ASP:HB2	0.55	1.79	8	1
3:A:13:PCW:H11	3:A:18:PCW:H41	0.55	1.77	9	1
3:A:71:PCW:H71	3:A:71:PCW:H19	0.55	1.79	9	1
3:A:7:PCW:H72	2:B:105:ASP:HB2	0.54	1.78	5	1
3:A:32:PCW:H81	4:A:38:17F:N1	0.54	2.16	5	1
3:A:50:PCW:H31	4:A:78:17F:H4	0.54	1.78	7	1
3:A:17:PCW:H152	3:A:17:PCW:H341	0.54	1.79	5	2
1:A:330:ARG:NH2	1:C:444:ASP:HA	0.54	2.17	6	1
3:A:4:PCW:H471	4:A:39:17F:H38	0.54	1.78	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:42:PCW:H81	3:A:63:PCW:O1P	0.54	2.01	3	1
1:C:465:GLU:O	1:C:469:LEU:HD12	0.54	2.02	7	1
4:A:74:17F:H11	4:A:74:17F:H20A	0.54	1.77	2	1
3:A:67:PCW:H2	4:A:74:17F:H63	0.54	1.79	7	1
1:C:401:LEU:O	1:C:405:TRP:HB2	0.54	2.03	6	1
1:A:239:LEU:HA	1:A:242:GLU:HB2	0.54	1.79	3	1
4:A:35:17F:HN1A	2:B:73:ARG:NH1	0.54	1.92	5	1
3:A:43:PCW:H31	3:A:43:PCW:H41	0.54	1.80	9	1
3:A:44:PCW:H221	3:A:59:PCW:H222	0.54	1.80	2	1
1:A:279:LEU:HB3	1:C:495:LYS:HD3	0.54	1.78	8	1
3:A:11:PCW:H39	3:A:28:PCW:H152	0.54	1.79	6	1
1:C:465:GLU:O	1:C:469:LEU:HB2	0.54	2.01	7	1
1:C:544:LEU:O	1:C:548:HIS:HB2	0.54	2.03	9	1
1:A:312:HIS:HE1	1:C:465:GLU:HB2	0.54	1.63	3	3
4:A:36:17F:H2	2:B:67:MET:HE1	0.54	1.79	3	1
4:A:39:17F:H58	4:A:39:17F:H11A	0.54	1.80	5	1
3:A:59:PCW:H19	4:A:77:17F:H33	0.53	1.79	3	1
3:A:51:PCW:H322	3:A:56:PCW:H32	0.53	1.79	8	1
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.53	1.79	1	2
4:A:40:17F:H51	3:A:68:PCW:H212	0.53	1.79	2	1
3:A:29:PCW:H122	3:A:31:PCW:H342	0.53	1.79	5	1
3:A:19:PCW:H331	3:A:29:PCW:H361	0.53	1.78	2	1
2:B:18:ALA:HB2	5:B:201:GNP:O1A	0.53	2.03	7	1
4:A:33:17F:H12A	4:A:35:17F:H9A	0.53	1.79	9	1
3:A:9:PCW:H71	3:A:30:PCW:O1P	0.53	2.04	1	1
1:C:589:GLU:HG2	1:C:593:LYS:HE2	0.53	1.80	3	1
1:A:288:ARG:O	1:A:292:HIS:HB2	0.53	2.03	4	1
3:A:66:PCW:H19	4:A:78:17F:H5	0.53	1.79	4	1
1:C:469:LEU:HD22	1:C:473:LYS:NZ	0.53	2.18	3	1
3:A:59:PCW:H321	4:A:77:17F:H9A	0.53	1.79	7	1
2:B:160:VAL:HG12	2:B:164:ARG:HD2	0.53	1.80	7	1
3:A:66:PCW:H121	4:A:79:17F:H18A	0.53	1.81	1	1
3:A:48:PCW:H63	3:A:61:PCW:H411	0.53	1.81	3	1
3:A:1:PCW:H51	3:A:26:PCW:H362	0.53	1.80	5	1
4:A:35:17F:HN1A	2:B:5:LYS:NZ	0.53	2.01	8	1
4:A:74:17F:H71	4:A:79:17F:H9	0.53	1.80	9	1
3:A:18:PCW:H20	4:A:37:17F:H12	0.53	1.81	4	1
3:A:23:PCW:H372	4:A:34:17F:H67	0.53	1.80	4	1
3:A:25:PCW:H422	3:A:31:PCW:H39	0.53	1.80	6	1
1:C:469:LEU:HD22	1:C:473:LYS:HZ2	0.53	1.62	3	1
1:C:567:GLU:O	1:C:571:GLN:CB	0.53	2.57	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:519:ALA:HB3	1:C:520:PRO:HD3	0.53	1.79	1	1
3:A:51:PCW:H142	3:A:56:PCW:H211	0.53	1.80	4	1
1:C:510:HIS:O	1:C:514:LEU:HG	0.53	2.04	8	1
1:C:417:GLU:O	1:C:421:PRO:HD2	0.53	2.04	9	4
1:C:491:GLU:O	1:C:495:LYS:HG3	0.53	2.03	7	2
2:B:68:ARG:HA	2:B:71:TYR:CZ	0.52	2.39	6	2
3:A:12:PCW:H71	4:A:37:17F:HN1A	0.52	1.63	6	1
3:A:9:PCW:H51	3:A:14:PCW:H322	0.52	1.82	7	1
3:A:27:PCW:H81	4:A:37:17F:H4A	0.52	1.80	7	1
3:A:48:PCW:H141	3:A:54:PCW:H141	0.52	1.80	2	1
3:A:6:PCW:H361	3:A:28:PCW:H2	0.52	1.79	7	1
3:A:20:PCW:H321	3:A:20:PCW:H41	0.52	1.82	9	1
3:A:25:PCW:H412	3:A:25:PCW:H162	0.52	1.81	9	1
4:A:35:17F:H47	3:A:55:PCW:H221	0.52	1.82	1	1
3:A:12:PCW:H352	4:A:36:17F:H5	0.52	1.82	2	1
1:A:202:LYS:HZ3	1:A:202:LYS:HB3	0.52	1.65	10	1
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.52	1.80	10	2
3:A:13:PCW:H42	4:A:34:17F:O1	0.52	2.04	1	1
3:A:20:PCW:H83	3:A:31:PCW:O2P	0.52	2.04	8	3
3:A:28:PCW:H181	4:A:39:17F:H52	0.52	1.80	6	1
3:A:30:PCW:H73	4:A:34:17F:O2	0.52	2.04	7	1
3:A:3:PCW:H71	3:A:19:PCW:H2	0.52	1.81	2	1
3:A:59:PCW:H231	4:A:77:17F:H12	0.52	1.81	5	1
3:A:59:PCW:O2P	3:A:61:PCW:H83	0.52	2.05	9	1
3:A:48:PCW:O31	3:A:48:PCW:H52	0.52	2.03	10	1
1:C:469:LEU:O	1:C:473:LYS:HB2	0.52	2.05	5	3
1:A:338:LEU:HA	1:A:341:ASN:HB3	0.52	1.82	10	1
3:A:24:PCW:H73	2:B:37:GLU:HB3	0.52	1.81	2	1
1:A:363:LYS:HE2	1:C:411:THR:HB	0.52	1.80	3	1
3:A:1:PCW:C6	4:A:35:17F:HN1A	0.52	2.18	4	1
3:A:48:PCW:H322	3:A:54:PCW:H181	0.52	1.80	6	1
3:A:6:PCW:H32	3:A:11:PCW:H322	0.52	1.80	10	1
3:A:10:PCW:H131	3:A:22:PCW:H331	0.52	1.81	10	2
3:A:1:PCW:H2	4:A:35:17F:H18A	0.52	1.80	2	1
1:C:474:VAL:O	1:C:478:ARG:HB2	0.52	2.04	2	2
4:A:40:17F:H4	4:A:40:17F:N1	0.52	2.18	3	1
3:A:65:PCW:O31	3:A:65:PCW:H73	0.52	2.05	3	1
1:A:301:LEU:HB3	1:C:473:LYS:HE3	0.52	1.81	4	1
1:C:568:ASP:OD1	1:C:571:GLN:OE1	0.52	2.28	10	1
3:A:1:PCW:H2	3:A:26:PCW:H372	0.51	1.81	1	1
3:A:2:PCW:H62	3:A:5:PCW:O2P	0.51	2.05	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:42:PCW:H442	3:A:52:PCW:H382	0.51	1.80	1	1
3:A:32:PCW:H71	4:A:38:17F:N1	0.51	2.19	5	1
3:A:13:PCW:H81	4:A:37:17F:H1A	0.51	1.80	4	1
3:A:2:PCW:H42	3:A:17:PCW:O2P	0.51	2.05	6	1
1:C:427:TRP:HA	1:C:427:TRP:CE3	0.51	2.40	7	1
1:C:559:SER:HA	1:C:562:ALA:HB3	0.51	1.82	10	1
4:A:37:17F:O1	2:B:5:LYS:HE2	0.51	2.05	7	1
3:A:63:PCW:P	4:A:75:17F:N1	0.51	2.82	2	1
1:A:275:LYS:O	1:A:279:LEU:HB2	0.51	2.06	3	1
3:A:9:PCW:H81	3:A:30:PCW:O2P	0.51	2.06	2	1
3:A:63:PCW:H422	3:A:63:PCW:H152	0.51	1.82	5	1
3:A:17:PCW:H73	4:A:38:17F:O1	0.51	2.06	2	1
3:A:13:PCW:H41	4:A:34:17F:O1	0.51	2.06	4	1
3:A:32:PCW:H61	4:A:38:17F:HN1A	0.51	1.65	5	1
3:A:26:PCW:H42	2:B:3:GLU:OE1	0.51	2.06	10	1
1:A:330:ARG:HH21	1:C:447:GLU:HB3	0.51	1.67	1	2
3:A:51:PCW:H2	3:A:71:PCW:H382	0.51	1.82	6	1
2:B:36:ILE:HA	2:B:59:ALA:HB2	0.50	1.83	5	2
3:A:47:PCW:H172	4:A:76:17F:H4	0.50	1.83	3	1
3:A:49:PCW:C6	4:A:80:17F:HN1	0.50	2.18	3	1
3:A:44:PCW:H321	3:A:55:PCW:H62	0.50	1.81	10	1
3:A:6:PCW:P	3:A:16:PCW:O1P	0.50	2.69	4	1
1:C:421:PRO:O	1:C:425:GLU:HG3	0.50	2.07	5	1
3:A:63:PCW:H412	3:A:72:PCW:H232	0.50	1.82	8	1
1:A:310:ARG:O	1:A:314:ASP:HB2	0.50	2.07	1	2
3:A:6:PCW:H381	3:A:16:PCW:H321	0.50	1.83	4	1
3:A:22:PCW:H32	4:A:37:17F:H1A	0.50	1.82	8	1
3:A:43:PCW:H451	3:A:69:PCW:H361	0.50	1.83	9	1
3:A:9:PCW:H71	3:A:30:PCW:O2P	0.50	2.06	10	1
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.50	2.37	1	2
3:A:60:PCW:H182	3:A:62:PCW:H222	0.50	1.81	4	1
3:A:41:PCW:H31	3:A:52:PCW:H372	0.50	1.84	6	1
3:A:4:PCW:H242	3:A:32:PCW:H221	0.50	1.84	7	1
3:A:10:PCW:H281	4:A:37:17F:H61	0.50	1.83	7	1
3:A:72:PCW:H382	4:A:78:17F:H38	0.50	1.84	7	1
3:A:32:PCW:H83	4:A:38:17F:HN1A	0.50	1.67	8	1
1:C:491:GLU:HB3	1:C:495:LYS:HE2	0.50	1.83	8	1
3:A:1:PCW:O11	3:A:17:PCW:H83	0.50	2.07	4	1
3:A:54:PCW:H31	3:A:54:PCW:H372	0.50	1.82	5	1
3:A:8:PCW:H72	3:A:22:PCW:O1P	0.50	2.07	7	1
4:A:74:17F:H5	4:A:74:17F:H20A	0.50	1.84	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:5:PCW:H381	3:A:17:PCW:H331	0.50	1.82	10	1
3:A:15:PCW:H81	4:A:39:17F:O2	0.50	2.07	10	1
1:C:455:TYR:O	1:C:459:PHE:HB2	0.50	2.07	10	3
4:A:36:17F:HN1A	2:B:41:ARG:NE	0.50	2.04	5	1
1:A:341:ASN:ND2	1:C:433:GLU:HA	0.50	2.22	8	2
1:A:221:LEU:HA	1:A:224:VAL:HG12	0.50	1.82	9	2
3:A:64:PCW:H442	3:A:68:PCW:H271	0.50	1.82	3	1
4:A:33:17F:C4	4:A:33:17F:H1	0.50	2.36	4	1
1:A:332:ALA:O	1:A:336:GLU:HG2	0.50	2.07	8	1
4:A:33:17F:HN1	2:B:73:ARG:NH1	0.50	2.05	8	1
3:A:62:PCW:H372	3:A:72:PCW:H152	0.50	1.84	8	1
3:A:60:PCW:H51	3:A:61:PCW:H321	0.50	1.82	10	1
3:A:49:PCW:H82	4:A:80:17F:O2	0.49	2.07	7	1
3:A:15:PCW:H71	4:A:39:17F:N1	0.49	2.22	2	1
1:A:325:ASP:HA	1:A:328:ARG:HD2	0.49	1.84	6	2
3:A:53:PCW:H331	3:A:68:PCW:H381	0.49	1.84	4	1
1:C:442:SER:O	1:C:446:GLU:HB2	0.49	2.07	4	1
1:C:443:LYS:O	1:C:447:GLU:HB2	0.49	2.06	10	2
3:A:9:PCW:H342	3:A:14:PCW:H61	0.49	1.83	3	1
3:A:26:PCW:O1P	3:A:30:PCW:H83	0.49	2.08	5	1
3:A:62:PCW:H351	3:A:72:PCW:H332	0.49	1.83	6	1
1:C:508:ARG:O	1:C:512:ASP:HB2	0.49	2.07	3	3
3:A:24:PCW:H322	3:A:25:PCW:H122	0.49	1.85	10	1
3:A:67:PCW:H232	4:A:75:17F:H11A	0.49	1.84	7	1
4:A:35:17F:HN1A	2:B:5:LYS:HZ3	0.49	1.48	8	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.49	1.84	10	1
1:A:224:VAL:O	1:A:228:PHE:HB2	0.49	2.08	2	2
1:A:334:ARG:HD2	1:C:440:GLU:OE2	0.49	2.07	8	1
1:A:392:GLU:O	1:A:396:LYS:HG2	0.49	2.07	10	2
3:A:47:PCW:H31	4:A:73:17F:O5	0.49	2.07	6	1
3:A:72:PCW:H41	3:A:72:PCW:O31	0.49	2.08	1	1
3:A:14:PCW:H232	4:A:37:17F:H11A	0.49	1.84	2	1
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.49	1.84	4	1
3:A:41:PCW:H73	3:A:44:PCW:O1P	0.49	2.08	5	1
1:A:327:LEU:HA	1:A:330:ARG:HG2	0.49	1.84	6	1
3:A:47:PCW:H242	4:A:76:17F:H33	0.49	1.83	10	1
2:B:126:ASP:HB3	2:B:129:GLN:HG3	0.49	1.84	3	1
3:A:6:PCW:O1P	3:A:16:PCW:H63	0.49	2.08	5	1
3:A:48:PCW:H39	3:A:54:PCW:H432	0.49	1.84	9	1
3:A:22:PCW:H132	4:A:37:17F:H6	0.49	1.84	1	1
1:A:298:LEU:O	1:A:302:GLY:HA3	0.49	2.07	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:116:ASN:HA	2:B:144:THR:O	0.49	2.08	6	2
3:A:49:PCW:H142	3:A:57:PCW:H331	0.48	1.85	3	1
3:A:57:PCW:H2	3:A:57:PCW:H52	0.48	1.84	6	1
1:A:253:LYS:O	1:A:257:TYR:HB2	0.48	2.07	8	1
3:A:3:PCW:H122	3:A:19:PCW:H121	0.48	1.84	10	1
2:B:32:TYR:HA	5:B:201:GNP:H5'1	0.48	1.84	8	1
1:C:411:THR:O	1:C:415:LEU:HG	0.48	2.09	10	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.48	1.85	7	2
3:A:44:PCW:H131	4:A:77:17F:H2	0.48	1.85	4	1
1:A:231:ASN:HA	1:A:234:LYS:CE	0.48	2.38	10	2
3:A:7:PCW:H11	3:A:16:PCW:O2P	0.48	2.08	1	1
3:A:9:PCW:H73	3:A:26:PCW:O2P	0.48	2.09	1	1
1:C:441:MET:HA	1:C:444:ASP:HB2	0.48	1.84	2	1
1:A:391:GLU:O	1:A:395:LYS:HB2	0.48	2.09	4	1
1:A:308:ARG:HD3	1:C:469:LEU:CD1	0.48	2.38	7	1
3:A:18:PCW:H42	2:B:41:ARG:HD3	0.48	1.85	7	1
3:A:47:PCW:H242	4:A:76:17F:H60	0.48	1.84	8	1
1:A:388:SER:HB2	1:C:594:LYS:CE	0.48	2.38	10	1
1:A:363:LYS:HA	1:A:367:ALA:HB3	0.48	1.84	1	1
3:A:12:PCW:H73	2:B:105:ASP:OD2	0.48	2.07	4	1
4:A:79:17F:H58	4:A:79:17F:H69	0.48	1.85	5	1
3:A:17:PCW:H32	2:B:172:LYS:HG2	0.48	1.86	1	1
3:A:32:PCW:H63	4:A:38:17F:N1	0.48	2.24	3	1
4:A:37:17F:N1	2:B:5:LYS:NZ	0.48	2.61	7	1
3:A:32:PCW:H83	4:A:38:17F:N1	0.48	2.23	8	1
3:A:13:PCW:H81	3:A:30:PCW:H321	0.48	1.86	1	1
1:C:546:GLU:O	1:C:550:LYS:HD2	0.48	2.08	6	3
3:A:42:PCW:H341	3:A:52:PCW:H341	0.48	1.84	10	1
1:A:322:PRO:O	1:A:326:GLU:HG3	0.48	2.09	2	1
3:A:4:PCW:H61	4:A:33:17F:H2	0.48	1.84	2	1
3:A:20:PCW:H31	3:A:31:PCW:H31	0.48	1.85	4	1
3:A:52:PCW:H122	3:A:60:PCW:H11	0.48	1.85	7	1
3:A:70:PCW:O31	3:A:70:PCW:H62	0.48	2.09	7	1
3:A:2:PCW:O1P	3:A:21:PCW:H31	0.48	2.08	8	1
3:A:49:PCW:H332	3:A:57:PCW:H371	0.48	1.86	8	1
3:A:49:PCW:H322	3:A:57:PCW:H2	0.48	1.86	9	1
1:C:495:LYS:O	1:C:499:LEU:HB2	0.48	2.09	6	7
3:A:42:PCW:H82	3:A:63:PCW:O1P	0.48	2.09	2	1
2:B:102:ARG:HH21	2:B:103:VAL:HG12	0.48	1.69	4	1
3:A:66:PCW:H151	4:A:78:17F:H19A	0.48	1.85	6	1
1:C:534:GLU:HA	1:C:537:LYS:HE3	0.48	1.85	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:8:PCW:H283	1:C:451:LYS:HB3	0.48	1.86	1	1
3:A:43:PCW:H122	3:A:43:PCW:H351	0.48	1.86	2	1
1:A:355:GLU:HA	1:A:355:GLU:OE1	0.48	2.08	4	1
2:B:144:THR:HA	2:B:150:GLN:O	0.48	2.09	7	2
1:A:358:SER:O	1:A:362:GLU:HG3	0.48	2.09	10	2
3:A:48:PCW:H39	3:A:54:PCW:H452	0.47	1.85	1	1
3:A:2:PCW:H81	2:B:105:ASP:OD1	0.47	2.08	6	1
1:C:502:GLU:HG2	1:C:506:ARG:HE	0.47	1.68	8	2
1:A:308:ARG:HD3	1:C:469:LEU:CD2	0.47	2.32	7	1
3:A:1:PCW:H422	4:A:36:17F:H43	0.47	1.86	9	1
3:A:41:PCW:H31	3:A:42:PCW:H211	0.47	1.86	2	1
3:A:13:PCW:H241	3:A:18:PCW:H372	0.47	1.84	3	1
3:A:49:PCW:H331	4:A:80:17F:H19	0.47	1.85	9	1
3:A:46:PCW:O2P	3:A:51:PCW:H83	0.47	2.09	10	1
4:A:76:17F:H18	4:A:76:17F:H9	0.47	1.86	1	1
1:C:421:PRO:O	1:C:425:GLU:HG2	0.47	2.10	1	1
3:A:22:PCW:N	4:A:37:17F:N1	0.47	2.62	4	2
3:A:6:PCW:H342	3:A:28:PCW:H62	0.47	1.86	7	1
3:A:62:PCW:H412	4:A:78:17F:H54	0.47	1.87	8	1
3:A:20:PCW:O2P	3:A:24:PCW:H83	0.47	2.09	10	1
1:A:387:LEU:O	1:A:391:GLU:HG3	0.47	2.09	1	2
3:A:57:PCW:H261	4:A:80:17F:H45	0.47	1.85	1	1
1:A:363:LYS:O	1:A:367:ALA:HB3	0.47	2.10	4	3
3:A:55:PCW:H411	3:A:64:PCW:H352	0.47	1.85	3	1
3:A:42:PCW:C20	3:A:61:PCW:H71	0.47	2.40	6	1
3:A:2:PCW:H62	3:A:17:PCW:H2	0.47	1.85	7	1
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.47	2.39	1	3
3:A:6:PCW:H40	3:A:7:PCW:H83	0.47	1.85	1	1
1:A:316:LEU:HG	1:C:462:LYS:HE3	0.47	1.86	7	2
1:C:479:ALA:O	1:C:483:GLU:HG2	0.47	2.09	2	1
3:A:16:PCW:O11	3:A:16:PCW:H82	0.47	2.10	3	1
3:A:18:PCW:H222	4:A:37:17F:H64	0.47	1.85	3	1
3:A:44:PCW:H131	4:A:77:17F:H4A	0.47	1.85	3	1
3:A:16:PCW:H322	4:A:39:17F:H11	0.47	1.87	4	1
3:A:25:PCW:O2P	3:A:31:PCW:H51	0.47	2.09	4	1
1:A:225:THR:O	1:A:229:TRP:HB2	0.47	2.09	6	3
3:A:3:PCW:H122	3:A:19:PCW:H141	0.47	1.85	6	1
3:A:9:PCW:H82	3:A:30:PCW:O2P	0.47	2.09	7	1
3:A:5:PCW:H83	3:A:5:PCW:O31	0.47	2.10	1	1
3:A:41:PCW:H141	3:A:61:PCW:H141	0.47	1.87	1	1
3:A:24:PCW:H361	3:A:25:PCW:H121	0.47	1.87	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:570:ARG:O	1:C:574:LEU:HG	0.47	2.09	3	1
1:A:247:LEU:HA	1:A:250:VAL:HG12	0.47	1.87	1	1
1:A:293:GLU:O	1:A:297:LYS:HB2	0.47	2.09	3	1
4:A:34:17F:H11A	4:A:40:17F:H59	0.47	1.87	6	1
3:A:53:PCW:O2P	3:A:55:PCW:H61	0.47	2.09	10	1
3:A:62:PCW:H41	3:A:62:PCW:O31	0.47	2.10	4	1
3:A:12:PCW:H321	3:A:30:PCW:H141	0.46	1.87	2	1
3:A:13:PCW:H31	4:A:37:17F:H12	0.46	1.86	2	1
4:A:77:17F:P1	4:A:77:17F:N1	0.46	2.88	4	1
1:A:392:GLU:OE1	1:A:395:LYS:HD3	0.46	2.08	6	1
3:A:20:PCW:O1P	3:A:31:PCW:H11	0.46	2.10	6	1
3:A:12:PCW:H82	4:A:37:17F:O4	0.46	2.10	8	1
3:A:6:PCW:P	3:A:24:PCW:O2P	0.46	2.74	1	1
4:A:38:17F:H8	4:A:38:17F:H20A	0.46	1.87	5	1
4:A:39:17F:H33	4:A:39:17F:H8	0.46	1.87	5	1
3:A:19:PCW:H362	3:A:19:PCW:H121	0.46	1.86	7	1
3:A:12:PCW:H63	4:A:37:17F:N1	0.46	2.26	9	1
3:A:12:PCW:H151	3:A:22:PCW:H122	0.46	1.86	1	1
3:A:42:PCW:H252	3:A:52:PCW:H212	0.46	1.87	1	1
1:A:203:LEU:O	1:A:207:TRP:HB2	0.46	2.10	7	2
1:A:299:SER:HB2	1:A:300:PRO:CD	0.46	2.39	4	1
2:B:16:LYS:HB3	2:B:57:ASP:OD1	0.46	2.10	4	1
1:C:561:LYS:O	1:C:565:ALA:HB3	0.46	2.10	6	1
3:A:26:PCW:H51	3:A:28:PCW:O1P	0.46	2.11	8	1
3:A:30:PCW:H83	4:A:34:17F:O2	0.46	2.10	2	1
3:A:43:PCW:H471	3:A:70:PCW:H351	0.46	1.87	3	1
3:A:54:PCW:H331	3:A:54:PCW:H131	0.46	1.87	4	1
3:A:50:PCW:H62	4:A:78:17F:HN1	0.46	1.70	5	1
3:A:26:PCW:H372	3:A:26:PCW:H131	0.46	1.86	6	1
2:B:58:THR:HG22	2:B:71:TYR:CE1	0.46	2.46	7	1
2:B:62:GLU:OE1	2:B:68:ARG:HD2	0.46	2.10	8	1
3:A:30:PCW:H81	2:B:39:SER:OG	0.46	2.10	10	1
3:A:6:PCW:O1P	3:A:7:PCW:H71	0.46	2.09	2	1
3:A:23:PCW:H212	3:A:49:PCW:H461	0.46	1.87	2	1
4:A:36:17F:H46	3:A:68:PCW:H271	0.46	1.86	2	1
1:C:456:LEU:O	1:C:460:GLN:HB2	0.46	2.10	3	1
3:A:6:PCW:H341	3:A:28:PCW:H121	0.46	1.87	5	1
4:A:40:17F:H43	3:A:43:PCW:H252	0.46	1.87	6	1
1:A:310:ARG:O	1:A:314:ASP:HB3	0.46	2.11	7	1
3:A:28:PCW:H261	3:A:42:PCW:H452	0.46	1.86	10	1
2:B:41:ARG:HD3	2:B:54:ASP:OD1	0.46	2.11	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:534:GLU:O	1:C:538:GLU:HG2	0.46	2.10	4	1
3:A:53:PCW:H341	3:A:68:PCW:H372	0.46	1.87	8	1
3:A:16:PCW:H212	3:A:24:PCW:H441	0.46	1.88	9	1
3:A:51:PCW:H362	3:A:56:PCW:H11	0.46	1.85	9	1
3:A:51:PCW:O1P	3:A:56:PCW:H32	0.46	2.11	3	1
3:A:53:PCW:H142	3:A:56:PCW:H382	0.46	1.87	3	1
3:A:68:PCW:H421	3:A:70:PCW:H231	0.46	1.87	5	1
1:C:563:LYS:HB2	1:C:564:PRO:CD	0.46	2.41	6	2
3:A:28:PCW:O4P	3:A:28:PCW:H2	0.46	2.10	1	1
3:A:53:PCW:O2P	3:A:55:PCW:H71	0.46	2.10	1	1
3:A:22:PCW:H132	3:A:22:PCW:H341	0.46	1.87	4	1
3:A:59:PCW:H2	4:A:77:17F:H9	0.46	1.87	4	1
1:C:460:GLN:O	1:C:464:GLN:HG3	0.46	2.11	4	1
3:A:53:PCW:H31	3:A:64:PCW:H32	0.46	1.88	7	1
3:A:41:PCW:O31	3:A:61:PCW:H81	0.46	2.10	1	1
2:B:79:LEU:HD23	2:B:112:VAL:HB	0.46	1.87	8	4
1:A:234:LYS:HE3	1:C:539:ASN:OD1	0.46	2.11	10	3
3:A:60:PCW:O2P	3:A:63:PCW:H81	0.46	2.10	3	1
1:C:563:LYS:CB	1:C:564:PRO:HD3	0.46	2.38	3	2
1:A:253:LYS:C	1:A:256:PRO:HD2	0.46	2.36	4	1
3:A:53:PCW:H132	3:A:64:PCW:H162	0.46	1.87	4	1
4:A:33:17F:P1	4:A:33:17F:HN1	0.46	2.34	5	2
3:A:24:PCW:N	4:A:39:17F:N1	0.45	2.64	1	1
3:A:10:PCW:H51	3:A:21:PCW:O2P	0.45	2.11	4	1
3:A:23:PCW:H451	3:A:29:PCW:H371	0.45	1.88	5	1
3:A:44:PCW:H42	3:A:53:PCW:H42	0.45	1.88	6	1
3:A:14:PCW:H42	3:A:25:PCW:H62	0.45	1.86	5	1
3:A:25:PCW:H381	3:A:29:PCW:H431	0.45	1.87	6	1
3:A:5:PCW:H12	3:A:17:PCW:H342	0.45	1.87	7	1
4:A:34:17F:HN1A	2:B:167:LYS:CD	0.45	2.20	7	1
3:A:1:PCW:H472	4:A:36:17F:H45	0.45	1.88	8	1
3:A:30:PCW:H31	3:A:30:PCW:H41	0.45	1.88	8	1
1:C:466:GLU:HA	1:C:469:LEU:HB2	0.45	1.87	10	1
1:C:585:LEU:O	1:C:589:GLU:HB2	0.45	2.12	1	1
3:A:32:PCW:H52	4:A:35:17F:H6	0.45	1.87	2	1
1:A:345:ARG:O	1:A:349:TYR:HB2	0.45	2.12	5	1
2:B:84:ILE:HG12	2:B:118:CYS:HA	0.45	1.88	6	1
3:A:22:PCW:O2P	3:A:27:PCW:H62	0.45	2.10	7	1
3:A:48:PCW:H81	3:A:60:PCW:O11	0.45	2.12	7	1
3:A:12:PCW:H72	3:A:22:PCW:O2P	0.45	2.10	2	1
3:A:11:PCW:H71	2:B:3:GLU:OE1	0.45	2.10	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:530:ALA:O	1:C:534:GLU:HG3	0.45	2.11	4	2
1:C:422:VAL:HA	1:C:425:GLU:OE2	0.45	2.11	5	1
3:A:4:PCW:H251	3:A:32:PCW:H182	0.45	1.87	7	1
3:A:4:PCW:H222	3:A:32:PCW:H262	0.45	1.87	10	1
3:A:57:PCW:H212	4:A:80:17F:H48	0.45	1.88	10	1
3:A:9:PCW:H62	3:A:9:PCW:O11	0.45	2.12	3	1
1:A:264:LYS:CE	1:C:509:ALA:HB1	0.45	2.42	5	1
3:A:22:PCW:H442	3:A:30:PCW:H261	0.45	1.88	5	1
2:B:100:ILE:HA	2:B:103:VAL:HG22	0.45	1.88	10	2
3:A:3:PCW:O2P	3:A:23:PCW:H62	0.45	2.11	7	1
3:A:68:PCW:H19	3:A:70:PCW:H262	0.45	1.89	7	1
3:A:12:PCW:H63	4:A:37:17F:HN1	0.45	1.72	9	1
3:A:26:PCW:H39	4:A:33:17F:H46	0.45	1.88	9	1
4:A:35:17F:HN1A	2:B:73:ARG:NH2	0.45	2.07	9	1
3:A:43:PCW:O11	3:A:43:PCW:H83	0.45	2.12	2	1
3:A:48:PCW:H41	3:A:48:PCW:O31	0.45	2.12	2	1
3:A:9:PCW:H412	3:A:29:PCW:H412	0.45	1.89	3	1
1:C:491:GLU:HB3	1:C:495:LYS:HZ2	0.45	1.72	3	1
1:A:268:GLU:OE1	1:C:506:ARG:HD3	0.45	2.12	4	3
3:A:57:PCW:H141	4:A:76:17F:H45	0.45	1.89	6	1
2:B:45:VAL:HG22	2:B:50:THR:HB	0.45	1.88	7	1
3:A:6:PCW:H342	3:A:16:PCW:H321	0.45	1.89	9	1
4:A:79:17F:H64	4:A:80:17F:H67	0.45	1.89	9	1
1:A:376:LEU:O	1:A:380:GLU:HG3	0.45	2.11	10	1
4:A:76:17F:H8A	4:A:76:17F:H20	0.45	1.88	10	1
1:C:550:LYS:O	1:C:554:HIS:HB2	0.45	2.12	2	1
1:A:337:ALA:O	1:A:341:ASN:HB2	0.45	2.12	4	1
3:A:43:PCW:H332	3:A:43:PCW:H132	0.45	1.87	5	1
2:B:46:ILE:HD11	2:B:53:LEU:HD11	0.45	1.88	7	1
1:A:363:LYS:HG2	1:C:411:THR:HG22	0.45	1.88	4	2
3:A:31:PCW:H52	3:A:31:PCW:O31	0.45	2.12	1	1
3:A:12:PCW:H342	3:A:30:PCW:H121	0.45	1.89	2	1
1:C:448:VAL:O	1:C:452:VAL:HB	0.45	2.12	4	1
1:C:415:LEU:HA	1:C:418:GLN:NE2	0.45	2.27	7	1
1:C:499:LEU:O	1:C:503:MET:HB2	0.45	2.11	10	1
3:A:17:PCW:H182	3:A:21:PCW:H122	0.45	1.88	2	1
3:A:54:PCW:H82	3:A:62:PCW:O2P	0.45	2.12	4	1
3:A:68:PCW:O2P	3:A:69:PCW:H41	0.45	2.12	6	1
3:A:54:PCW:O3P	3:A:60:PCW:H82	0.44	2.12	3	1
1:A:242:GLU:OE1	1:C:528:ARG:HB3	0.44	2.12	4	1
3:A:27:PCW:H372	3:A:27:PCW:H161	0.44	1.88	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:58:THR:HG22	2:B:71:TYR:HE1	0.44	1.72	7	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.44	2.37	3	5
2:B:80:CYS:HB2	2:B:113:LEU:HD12	0.44	1.88	4	1
1:A:308:ARG:HG3	1:C:465:GLU:HB3	0.44	1.88	5	1
1:A:308:ARG:CD	1:C:469:LEU:CD2	0.44	2.79	7	1
1:A:202:LYS:HE3	1:C:576:VAL:HG21	0.44	1.89	8	1
2:B:6:LEU:HD22	2:B:159:LEU:HD23	0.44	1.88	8	2
3:A:13:PCW:H152	3:A:18:PCW:H322	0.44	1.89	2	1
3:A:12:PCW:H51	2:B:39:SER:HB2	0.44	1.88	3	1
1:A:359:THR:O	1:A:363:LYS:HG3	0.44	2.12	7	2
1:A:330:ARG:O	1:A:334:ARG:HG2	0.44	2.11	7	2
1:C:464:GLN:O	1:C:468:GLU:HB2	0.44	2.13	8	1
2:B:73:ARG:HH21	2:B:103:VAL:HA	0.44	1.71	10	1
1:A:266:GLN:O	1:A:270:GLU:HG3	0.44	2.13	2	1
3:A:24:PCW:H271	3:A:25:PCW:H221	0.44	1.90	2	1
3:A:13:PCW:H161	3:A:18:PCW:H332	0.44	1.88	6	1
3:A:53:PCW:H181	3:A:64:PCW:H182	0.44	1.88	8	1
1:C:549:ALA:O	1:C:553:GLU:HG3	0.44	2.12	8	2
1:A:249:GLU:O	1:A:253:LYS:HB2	0.44	2.12	10	1
3:A:66:PCW:H471	4:A:79:17F:H59	0.44	1.88	1	1
3:A:44:PCW:H452	3:A:64:PCW:H461	0.44	1.90	2	1
3:A:11:PCW:H72	3:A:24:PCW:O2P	0.44	2.12	3	1
3:A:14:PCW:O2P	3:A:23:PCW:H41	0.44	2.12	3	1
1:A:214:PHE:HE1	3:A:15:PCW:H272	0.44	1.72	6	1
3:A:45:PCW:H241	3:A:57:PCW:H371	0.44	1.89	6	1
3:A:5:PCW:H142	4:A:38:17F:H8A	0.44	1.88	7	1
3:A:10:PCW:H341	3:A:21:PCW:H342	0.44	1.89	2	1
3:A:1:PCW:H232	4:A:38:17F:H58	0.44	1.89	3	1
3:A:11:PCW:H52	3:A:24:PCW:O2P	0.44	2.12	3	1
3:A:18:PCW:H371	3:A:19:PCW:H20	0.44	1.90	3	1
3:A:43:PCW:O1P	3:A:68:PCW:H73	0.44	2.12	3	1
4:A:36:17F:HN1A	2:B:41:ARG:HH21	0.44	1.54	5	1
1:C:517:HIS:O	1:C:521:TYR:HB2	0.44	2.13	6	2
1:A:229:TRP:O	1:A:233:GLU:HG3	0.44	2.13	7	1
1:A:292:HIS:O	1:A:296:GLU:HG2	0.44	2.13	7	1
3:A:20:PCW:H151	3:A:31:PCW:H422	0.44	1.89	7	1
3:A:26:PCW:H32	3:A:28:PCW:H331	0.44	1.88	8	1
3:A:32:PCW:O31	4:A:33:17F:H20A	0.44	2.12	9	1
3:A:43:PCW:O2P	3:A:45:PCW:H83	0.44	2.13	2	1
1:A:268:GLU:O	1:A:272:TYR:HB2	0.44	2.13	3	1
3:A:10:PCW:H332	3:A:21:PCW:H322	0.44	1.89	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:44:PCW:H141	4:A:77:17F:H4A	0.44	1.90	4	1
1:C:550:LYS:HA	1:C:553:GLU:OE1	0.44	2.13	5	1
3:A:21:PCW:H441	3:A:51:PCW:H262	0.44	1.90	5	1
1:A:202:LYS:O	1:A:206:ASN:HB2	0.44	2.13	9	1
3:A:6:PCW:H372	3:A:7:PCW:H331	0.44	1.88	9	1
3:A:70:PCW:H73	3:A:70:PCW:H19	0.44	1.90	9	1
1:C:473:LYS:O	1:C:477:LEU:HB2	0.44	2.12	9	1
3:A:62:PCW:H142	3:A:72:PCW:H172	0.44	1.88	10	1
1:A:335:LEU:O	1:A:339:LYS:HB2	0.44	2.12	1	1
1:C:533:LEU:O	1:C:537:LYS:HG3	0.44	2.13	6	2
3:A:47:PCW:H283	4:A:76:17F:H12	0.44	1.90	8	1
1:A:271:LEU:O	1:A:275:LYS:HG2	0.43	2.13	2	2
3:A:12:PCW:H62	2:B:37:GLU:OE1	0.43	2.13	6	1
3:A:6:PCW:H283	3:A:24:PCW:H182	0.43	1.89	10	1
3:A:23:PCW:H31	3:A:23:PCW:H41	0.43	1.90	10	1
3:A:44:PCW:H341	3:A:68:PCW:H332	0.43	1.90	3	1
3:A:15:PCW:H372	3:A:15:PCW:H211	0.43	1.89	5	1
2:B:5:LYS:N	2:B:5:LYS:HD3	0.43	2.28	7	1
3:A:9:PCW:H39	3:A:14:PCW:H82	0.43	1.89	9	1
1:A:224:VAL:HG22	1:C:550:LYS:HD3	0.43	1.90	1	1
1:A:273:ARG:HA	1:A:276:VAL:HG12	0.43	1.91	1	1
1:C:576:VAL:O	1:C:580:PHE:HB2	0.43	2.14	4	1
3:A:62:PCW:O1P	3:A:72:PCW:H63	0.43	2.13	6	1
3:A:58:PCW:H381	3:A:60:PCW:H151	0.43	1.90	8	1
3:A:26:PCW:H41	4:A:40:17F:O1	0.43	2.13	10	1
3:A:1:PCW:H212	4:A:35:17F:H32	0.43	1.91	1	1
3:A:20:PCW:O2P	3:A:24:PCW:H81	0.43	2.13	4	1
3:A:21:PCW:H172	3:A:21:PCW:H361	0.43	1.89	4	1
3:A:28:PCW:H452	3:A:63:PCW:H222	0.43	1.89	4	1
1:C:577:LEU:O	1:C:581:LYS:HB2	0.43	2.14	4	1
1:A:312:HIS:HA	1:C:462:LYS:HD3	0.43	1.91	7	1
3:A:42:PCW:H412	3:A:69:PCW:H141	0.43	1.89	9	1
3:A:48:PCW:H352	3:A:54:PCW:H152	0.43	1.90	1	1
3:A:3:PCW:H40	3:A:19:PCW:H242	0.43	1.89	3	1
2:B:126:ASP:OD2	2:B:128:LYS:HB3	0.43	2.13	4	1
3:A:6:PCW:H31	3:A:16:PCW:H332	0.43	1.89	2	1
1:C:508:ARG:O	1:C:512:ASP:HB3	0.43	2.14	4	1
1:A:362:GLU:HB3	1:C:414:LYS:HD3	0.43	1.90	5	1
3:A:1:PCW:H372	3:A:5:PCW:H431	0.43	1.91	6	1
3:A:20:PCW:H451	3:A:31:PCW:H242	0.43	1.91	6	1
3:A:27:PCW:H61	4:A:37:17F:O2	0.43	2.14	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:47:PCW:H331	3:A:71:PCW:H241	0.43	1.90	8	1
3:A:46:PCW:O2P	3:A:71:PCW:H352	0.43	2.13	9	1
1:A:357:LEU:HA	1:A:360:LEU:HB2	0.43	1.91	4	1
1:C:422:VAL:O	1:C:426:PHE:HB2	0.43	2.14	5	1
3:A:9:PCW:H73	2:B:3:GLU:OE1	0.43	2.13	9	1
4:A:37:17F:H55	3:A:57:PCW:H452	0.43	1.91	1	1
3:A:62:PCW:O1P	3:A:72:PCW:H51	0.43	2.14	1	1
3:A:62:PCW:H341	4:A:78:17F:H36	0.43	1.91	1	1
1:A:301:LEU:HD13	1:C:473:LYS:HG3	0.43	1.91	4	1
3:A:41:PCW:H182	3:A:58:PCW:H371	0.43	1.90	4	1
1:A:280:ARG:O	1:A:284:GLN:HB2	0.43	2.13	4	1
3:A:12:PCW:H71	4:A:37:17F:O3	0.43	2.14	5	1
3:A:23:PCW:H141	4:A:34:17F:H61	0.43	1.90	6	1
3:A:30:PCW:H142	4:A:40:17F:HN1A	0.43	1.74	3	1
3:A:41:PCW:H62	3:A:44:PCW:O11	0.43	2.14	3	1
1:C:522:SER:O	1:C:526:ARG:HG3	0.43	2.13	8	1
3:A:4:PCW:H82	3:A:7:PCW:O1P	0.42	2.14	1	1
2:B:69:ASP:O	2:B:73:ARG:HG3	0.42	2.14	5	1
3:A:43:PCW:O31	3:A:45:PCW:H82	0.42	2.14	7	1
3:A:30:PCW:H461	4:A:34:17F:H53	0.42	1.90	8	1
3:A:42:PCW:H442	3:A:52:PCW:H361	0.42	1.90	9	1
3:A:32:PCW:H421	4:A:35:17F:H49	0.42	1.91	10	1
3:A:56:PCW:O11	3:A:56:PCW:H83	0.42	2.14	3	1
3:A:14:PCW:H372	4:A:34:17F:H34	0.42	1.91	5	1
3:A:48:PCW:H332	3:A:54:PCW:H142	0.42	1.91	5	1
3:A:49:PCW:H362	3:A:57:PCW:H171	0.42	1.92	7	1
1:A:248:GLU:O	1:A:252:ALA:HB3	0.42	2.14	9	1
2:B:30:ASP:O	5:B:201:GNP:H3'	0.42	2.14	10	1
3:A:13:PCW:H342	3:A:18:PCW:H121	0.42	1.90	2	1
3:A:42:PCW:H51	4:A:75:17F:O1	0.42	2.14	2	1
3:A:62:PCW:H31	3:A:72:PCW:O11	0.42	2.14	4	1
3:A:68:PCW:H31	3:A:70:PCW:H232	0.42	1.90	4	1
3:A:41:PCW:H451	3:A:58:PCW:H451	0.42	1.90	5	1
3:A:72:PCW:O31	3:A:72:PCW:H42	0.42	2.14	7	1
1:C:581:LYS:O	1:C:585:LEU:HG	0.42	2.14	10	2
1:C:578:GLU:O	1:C:582:VAL:HG23	0.42	2.14	8	1
3:A:10:PCW:H73	3:A:21:PCW:O31	0.42	2.13	10	1
3:A:41:PCW:O2P	3:A:61:PCW:H72	0.42	2.14	10	1
3:A:62:PCW:H352	3:A:72:PCW:H122	0.42	1.92	3	1
3:A:48:PCW:H341	3:A:54:PCW:H351	0.42	1.92	6	1
1:C:413:SER:O	1:C:417:GLU:HG3	0.42	2.15	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:12:PCW:H331	3:A:12:PCW:H151	0.42	1.91	8	1
1:C:561:LYS:HE3	1:C:561:LYS:HA	0.42	1.90	8	1
2:B:97:ARG:HD2	2:B:111:MET:SD	0.42	2.54	10	1
3:A:1:PCW:H431	3:A:26:PCW:H221	0.42	1.90	1	1
3:A:14:PCW:H142	4:A:34:17F:H34	0.42	1.90	1	1
3:A:62:PCW:H362	3:A:72:PCW:H331	0.42	1.90	3	1
2:B:41:ARG:HD3	2:B:54:ASP:OD2	0.42	2.14	3	1
3:A:63:PCW:O2P	3:A:63:PCW:N	0.42	2.52	4	1
3:A:14:PCW:O2P	3:A:19:PCW:H81	0.42	2.15	5	1
1:A:308:ARG:HG3	1:C:469:LEU:CD1	0.42	2.42	8	1
1:A:348:GLU:O	1:A:352:LYS:HG3	0.42	2.13	5	1
3:A:43:PCW:H442	3:A:43:PCW:H162	0.42	1.91	5	1
3:A:10:PCW:H462	3:A:10:PCW:H172	0.42	1.91	9	1
1:C:587:ALA:O	1:C:591:TYR:HB2	0.42	2.14	9	1
2:B:9:VAL:HB	2:B:96:TYR:CE2	0.42	2.49	9	1
1:C:431:GLU:O	1:C:435:GLU:HG3	0.42	2.14	10	1
3:A:9:PCW:H321	3:A:14:PCW:H342	0.42	1.90	3	1
3:A:54:PCW:H332	3:A:72:PCW:H121	0.42	1.91	3	1
1:C:412:PHE:HA	1:C:415:LEU:HD12	0.42	1.90	6	1
2:B:20:THR:O	2:B:24:ILE:HG12	0.42	2.14	6	1
3:A:57:PCW:H63	4:A:80:17F:HN1A	0.42	1.74	1	1
2:B:34:PRO:HA	5:B:201:GNP:O3G	0.42	2.15	4	3
4:A:36:17F:HN1A	2:B:41:ARG:NH2	0.42	2.13	5	1
3:A:68:PCW:H32	3:A:70:PCW:H142	0.42	1.90	6	1
3:A:53:PCW:H212	3:A:64:PCW:H212	0.42	1.92	8	1
1:A:338:LEU:O	1:A:342:GLY:HA3	0.42	2.15	9	1
3:A:4:PCW:H161	3:A:7:PCW:H221	0.42	1.91	10	1
3:A:15:PCW:H61	4:A:39:17F:O2	0.42	2.15	10	1
3:A:11:PCW:H62	3:A:24:PCW:O2P	0.42	2.14	4	1
3:A:58:PCW:H362	3:A:61:PCW:H451	0.42	1.91	4	1
3:A:1:PCW:H20	3:A:32:PCW:H351	0.42	1.91	6	1
3:A:5:PCW:H31	3:A:17:PCW:H321	0.42	1.91	6	1
3:A:56:PCW:O2P	3:A:70:PCW:H41	0.42	2.15	7	1
3:A:3:PCW:H362	3:A:18:PCW:H12	0.42	1.92	9	1
3:A:43:PCW:H32	3:A:69:PCW:O3P	0.42	2.15	9	1
3:A:6:PCW:P	3:A:11:PCW:O2P	0.42	2.78	10	1
1:C:498:PRO:O	1:C:502:GLU:HB2	0.42	2.14	10	1
3:A:65:PCW:H2	3:A:65:PCW:O4P	0.42	2.15	1	1
4:A:75:17F:H2	4:A:75:17F:H4	0.42	1.92	1	1
1:A:268:GLU:OE2	1:C:510:HIS:NE2	0.42	2.53	4	1
3:A:11:PCW:H171	3:A:28:PCW:H411	0.42	1.92	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:57:PCW:H41	3:A:57:PCW:O31	0.42	2.15	8	1
3:A:25:PCW:H42	3:A:31:PCW:O1P	0.42	2.14	9	1
3:A:23:PCW:H40	3:A:29:PCW:H351	0.41	1.91	1	1
3:A:1:PCW:N	4:A:35:17F:N1	0.41	2.64	4	1
3:A:13:PCW:H73	4:A:37:17F:O4	0.41	2.15	5	1
3:A:21:PCW:H142	4:A:36:17F:H57	0.41	1.91	5	1
4:A:75:17F:H75	4:A:75:17F:H52	0.41	1.91	5	1
1:A:264:LYS:O	1:A:268:GLU:HG3	0.41	2.14	6	1
3:A:49:PCW:O2P	3:A:57:PCW:H61	0.41	2.14	7	1
3:A:1:PCW:H40	4:A:33:17F:H51	0.41	1.91	2	1
3:A:46:PCW:H39	3:A:47:PCW:H412	0.41	1.91	2	1
4:A:77:17F:H18A	4:A:77:17F:H9A	0.41	1.92	2	1
1:A:348:GLU:HB3	1:A:352:LYS:HE2	0.41	1.91	5	1
1:C:502:GLU:O	1:C:506:ARG:HG3	0.41	2.15	1	1
3:A:49:PCW:H82	4:A:80:17F:HN1	0.41	1.74	2	1
3:A:4:PCW:H461	4:A:39:17F:H70	0.41	1.91	3	1
2:B:72:MET:HE1	2:B:99:GLN:HG2	0.41	1.90	4	1
4:A:33:17F:H10	4:A:35:17F:H6A	0.41	1.92	5	1
3:A:16:PCW:O1P	3:A:16:PCW:H2	0.41	2.15	6	1
3:A:54:PCW:H132	3:A:54:PCW:H362	0.41	1.91	7	1
3:A:55:PCW:H411	3:A:64:PCW:H39	0.41	1.90	9	1
1:A:233:GLU:O	1:A:237:GLU:HB2	0.41	2.15	1	1
3:A:7:PCW:H231	3:A:61:PCW:H271	0.41	1.93	1	1
3:A:1:PCW:H422	3:A:68:PCW:H261	0.41	1.92	2	1
3:A:41:PCW:H231	3:A:58:PCW:H431	0.41	1.92	2	1
2:B:58:THR:HG21	2:B:71:TYR:CE1	0.41	2.50	2	1
2:B:80:CYS:HB3	2:B:93:ILE:HD12	0.41	1.91	2	1
3:A:19:PCW:H63	3:A:29:PCW:O1P	0.41	2.15	4	1
2:B:8:VAL:HG12	2:B:16:LYS:HD2	0.41	1.92	6	1
3:A:59:PCW:H181	4:A:77:17F:H8A	0.41	1.92	7	1
3:A:69:PCW:H372	3:A:69:PCW:H142	0.41	1.92	10	1
1:A:307:ASP:O	1:A:310:ARG:HB2	0.41	2.14	1	1
3:A:15:PCW:H431	3:A:20:PCW:H212	0.41	1.92	2	1
3:A:12:PCW:H432	3:A:30:PCW:H242	0.41	1.92	8	1
3:A:43:PCW:H11	3:A:70:PCW:H151	0.41	1.92	8	1
2:B:3:GLU:CD	2:B:5:LYS:HZ2	0.41	2.23	8	1
3:A:4:PCW:O2P	3:A:16:PCW:H82	0.41	2.16	2	1
3:A:1:PCW:H431	3:A:26:PCW:H241	0.41	1.91	5	1
3:A:28:PCW:H262	3:A:69:PCW:H211	0.41	1.93	5	1
1:A:330:ARG:HH22	1:C:448:VAL:HG23	0.41	1.76	9	1
3:A:42:PCW:H441	3:A:42:PCW:H221	0.41	1.92	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:15:PCW:H382	3:A:24:PCW:H462	0.41	1.93	1	1
3:A:2:PCW:H42	3:A:21:PCW:H11	0.41	1.92	2	1
1:A:375:LEU:O	1:A:379:LEU:HB2	0.41	2.16	3	1
3:A:19:PCW:H62	3:A:23:PCW:O2P	0.41	2.14	7	1
1:A:253:LYS:HE2	1:A:257:TYR:OH	0.41	2.15	10	1
3:A:15:PCW:H412	3:A:24:PCW:H461	0.41	1.93	10	1
3:A:2:PCW:H61	4:A:36:17F:O1	0.41	2.16	2	1
3:A:67:PCW:H241	3:A:69:PCW:H222	0.41	1.93	2	1
1:C:427:TRP:HA	1:C:427:TRP:HE3	0.41	1.74	7	1
1:C:465:GLU:C	1:C:469:LEU:HG	0.41	2.26	7	1
1:C:521:TYR:HA	1:C:524:GLU:OE1	0.41	2.16	7	1
3:A:44:PCW:H82	4:A:77:17F:O4	0.41	2.16	8	1
1:A:281:ALA:O	1:A:285:GLU:HG2	0.41	2.16	9	1
3:A:21:PCW:H432	3:A:51:PCW:H272	0.41	1.92	10	1
3:A:3:PCW:O2P	3:A:23:PCW:N	0.41	2.54	1	1
3:A:25:PCW:H351	3:A:25:PCW:H122	0.41	1.93	1	1
3:A:45:PCW:H73	3:A:71:PCW:H19	0.41	1.91	1	1
3:A:70:PCW:H2	3:A:70:PCW:O4P	0.41	2.16	1	1
3:A:64:PCW:H241	3:A:64:PCW:H351	0.41	1.92	2	1
3:A:8:PCW:H40	3:A:27:PCW:H261	0.41	1.92	4	1
3:A:43:PCW:H63	4:A:75:17F:H6	0.41	1.93	4	1
3:A:26:PCW:H11	3:A:28:PCW:O1P	0.41	2.16	5	1
1:A:330:ARG:NH2	1:C:447:GLU:HB2	0.41	2.27	6	1
3:A:9:PCW:H341	3:A:14:PCW:H372	0.41	1.92	6	1
3:A:57:PCW:H231	4:A:80:17F:H52	0.41	1.92	6	1
1:A:254:VAL:HA	1:A:257:TYR:HB2	0.41	1.92	7	1
3:A:3:PCW:H252	3:A:19:PCW:H241	0.41	1.93	7	1
3:A:3:PCW:H361	3:A:3:PCW:H121	0.41	1.93	7	1
1:A:228:PHE:O	1:A:232:LEU:HG	0.41	2.16	8	1
3:A:4:PCW:H432	3:A:7:PCW:H212	0.41	1.93	9	1
3:A:5:PCW:H39	3:A:17:PCW:H63	0.41	1.93	9	1
3:A:42:PCW:H283	3:A:52:PCW:H231	0.41	1.92	9	1
3:A:48:PCW:H452	3:A:54:PCW:H241	0.41	1.93	9	1
1:C:574:LEU:HB2	1:C:575:PRO:CD	0.41	2.46	9	1
3:A:5:PCW:H482	4:A:36:17F:H10A	0.41	1.92	10	1
3:A:16:PCW:H251	3:A:24:PCW:H361	0.41	1.91	10	1
3:A:32:PCW:H483	3:A:59:PCW:H271	0.41	1.91	10	1
2:B:24:ILE:HD11	2:B:55:ILE:HD12	0.41	1.92	10	1
2:B:31:GLU:O	5:B:201:GNP:H5'1	0.41	2.15	2	1
2:B:82:PHE:HE1	2:B:113:LEU:HG	0.41	1.76	2	1
1:A:376:LEU:HB2	1:A:377:PRO:CD	0.41	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:3:GLU:HG2	2:B:4:TYR:N	0.41	2.30	9	1
3:A:20:PCW:H73	3:A:31:PCW:O2P	0.41	2.16	10	1
3:A:41:PCW:H152	3:A:58:PCW:H361	0.40	1.92	1	1
3:A:12:PCW:H61	4:A:37:17F:O2	0.40	2.15	5	1
3:A:58:PCW:O31	3:A:58:PCW:H12	0.40	2.16	7	1
2:B:111:MET:HB2	2:B:139:ILE:HG21	0.40	1.93	8	1
1:A:334:ARG:HD3	1:C:440:GLU:OE1	0.40	2.15	1	1
3:A:2:PCW:H71	4:A:36:17F:O1	0.40	2.16	2	1
1:A:260:ASP:O	1:A:264:LYS:HD3	0.40	2.16	3	1
1:A:388:SER:O	1:A:392:GLU:HG2	0.40	2.16	3	1
3:A:7:PCW:H52	3:A:16:PCW:O2P	0.40	2.15	3	1
2:B:32:TYR:HD1	5:B:201:GNP:H5'1	0.40	1.75	5	1
1:A:332:ALA:O	1:A:336:GLU:HG3	0.40	2.17	7	1
1:C:561:LYS:HA	1:C:565:ALA:CB	0.40	2.45	7	1
3:A:28:PCW:H462	3:A:63:PCW:H241	0.40	1.94	8	1
3:A:30:PCW:H52	4:A:34:17F:O3	0.40	2.16	8	1
3:A:60:PCW:H82	3:A:61:PCW:H342	0.40	1.92	8	1
1:C:535:ALA:O	1:C:539:ASN:HB2	0.40	2.16	8	1
1:A:261:PHE:O	1:A:265:TRP:HB2	0.40	2.17	1	1
3:A:3:PCW:H361	3:A:18:PCW:H342	0.40	1.93	2	1
1:A:253:LYS:O	1:A:256:PRO:HD2	0.40	2.17	4	1
3:A:3:PCW:H81	3:A:19:PCW:O11	0.40	2.15	4	1
3:A:22:PCW:C7	4:A:37:17F:HN1	0.40	2.29	4	1
3:A:9:PCW:O2P	2:B:171:SER:HA	0.40	2.16	5	1
3:A:20:PCW:H271	4:A:78:17F:H44	0.40	1.92	7	1
1:A:246:ASP:O	1:A:250:VAL:HB	0.40	2.17	8	1
4:A:76:17F:H77	1:C:481:LEU:HD12	0.40	1.92	9	1
3:A:4:PCW:O2P	3:A:16:PCW:H83	0.40	2.16	10	1
3:A:16:PCW:H472	3:A:16:PCW:H272	0.40	1.93	10	1
3:A:42:PCW:H451	3:A:42:PCW:H231	0.40	1.92	3	1
1:A:264:LYS:HE3	1:C:509:ALA:HB1	0.40	1.92	5	1
3:A:48:PCW:H61	3:A:61:PCW:C40	0.40	2.47	5	1
3:A:42:PCW:O2P	3:A:69:PCW:H11	0.40	2.17	6	1
3:A:52:PCW:H131	3:A:60:PCW:O1P	0.40	2.17	6	1
3:A:45:PCW:H382	4:A:74:17F:H8	0.40	1.92	9	1
1:C:469:LEU:O	1:C:473:LYS:HE2	0.40	2.16	9	1
1:A:246:ASP:HA	1:C:528:ARG:NH1	0.40	2.32	1	1
1:A:279:LEU:HD22	1:C:495:LYS:HE3	0.40	1.93	1	1
3:A:9:PCW:H42	3:A:26:PCW:O2P	0.40	2.17	1	1
3:A:1:PCW:H181	3:A:5:PCW:H362	0.40	1.93	4	1
3:A:17:PCW:H41	3:A:17:PCW:O11	0.40	2.17	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:14:PCW:O1P	3:A:19:PCW:H73	0.40	2.17	9	1
2:B:168:GLU:HG2	2:B:172:LYS:HE2	0.40	1.93	9	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	195/200 (98%)	190±2 (98±1%)	4±1 (2±1%)	1±1 (0±0%)	26	74
1	C	195/200 (98%)	191±2 (98±1%)	4±2 (2±1%)	0±0 (0±0%)	37	78
2	B	170/187 (91%)	160±2 (94±1%)	10±2 (6±1%)	0±0 (0±0%)	44	80
All	All	5600/5870 (95%)	5416 (97%)	167 (3%)	17 (0%)	37	78

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	365	LYS	8
1	C	563	LYS	5
2	B	47	ASP	1
1	A	366	PRO	1
2	B	34	PRO	1
2	B	117	LYS	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	172/175 (98%)	154±3 (90±2%)	18±3 (10±2%)	9	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	171/175 (98%)	154±2 (90±1%)	16±2 (10±1%)	10	55
2	B	150/165 (91%)	134±3 (90±2%)	16±3 (10±2%)	9	53
All	All	4930/5150 (96%)	4431 (90%)	499 (10%)	9	54

All 196 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	235	GLU	10
1	A	254	VAL	10
1	C	516	THR	9
1	C	550	LYS	9
2	B	122	SER	9
1	A	272	TYR	8
2	B	16	LYS	8
2	B	74	THR	8
2	B	87	THR	8
1	A	220	GLN	8
1	C	480	GLU	7
2	B	17	SER	7
2	B	35	THR	7
2	B	39	SER	7
1	A	312	HIS	7
1	A	293	GLU	6
1	C	448	VAL	6
1	C	459	PHE	6
2	B	69	ASP	6
2	B	51	CYS	6
1	A	246	ASP	5
1	A	370	ASP	5
1	C	548	HIS	5
1	C	568	ASP	5
2	B	124	THR	5
1	A	394	THR	5
2	B	20	THR	5
2	B	148	THR	5
1	A	299	SER	5
1	A	228	PHE	4
1	A	289	GLN	4
1	A	325	ASP	4
1	C	405	TRP	4

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Mol	Chain	Res	Type	Models (Total)
1	C	487	GLN	4
1	C	561	LYS	4
2	B	43	GLN	4
2	B	92	ASP	4
2	B	107	GLU	4
2	B	127	THR	4
1	A	213	THR	4
1	A	318	THR	4
1	C	490	HIS	4
1	A	396	LYS	4
2	B	170	MET	4
1	A	229	TRP	3
1	A	381	SER	3
1	C	447	GLU	3
1	C	505	ASP	3
1	C	552	THR	3
1	C	583	SER	3
2	B	3	GLU	3
1	C	412	PHE	3
1	C	413	SER	3
1	C	444	ASP	3
2	B	50	THR	3
2	B	106	SER	3
1	A	215	SER	3
1	A	253	LYS	3
1	A	292	HIS	3
1	A	319	HIS	3
1	C	409	THR	3
1	A	212	SER	3
1	A	356	HIS	3
1	A	361	SER	3
1	C	407	SER	3
1	C	592	THR	3
2	B	71	TYR	3
1	C	463	TRP	3
1	A	385	SER	2
1	C	415	LEU	2
1	C	466	GLU	2
1	C	482	GLN	2
1	C	576	VAL	2
2	B	5	LYS	2
2	B	62	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	205	ASP	2
1	A	207	TRP	2
1	A	296	GLU	2
1	C	410	SER	2
1	C	427	TRP	2
1	C	554	HIS	2
1	A	209	SER	2
1	A	224	VAL	2
1	A	354	THR	2
1	A	360	LEU	2
1	C	455	TYR	2
1	C	467	MET	2
1	C	532	ARG	2
1	C	559	SER	2
2	B	65	SER	2
1	A	214	PHE	2
1	A	391	GLU	2
1	C	433	GLU	2
1	C	446	GLU	2
1	C	557	THR	2
2	B	102	ARG	2
1	A	392	GLU	2
1	C	425	GLU	2
1	C	473	LYS	2
1	C	594	LYS	2
2	B	85	ASN	2
2	B	132	ASP	2
2	B	168	GLU	2
1	A	378	VAL	2
1	C	418	GLN	2
1	C	556	SER	2
1	C	591	TYR	2
1	A	244	SER	2
1	A	202	LYS	2
1	C	494	GLU	2
1	A	265	TRP	1
1	C	483	GLU	1
2	B	29	VAL	1
2	B	63	GLU	1
2	B	80	CYS	1
1	A	211	THR	1
1	A	237	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	245	LYS	1
1	A	303	GLU	1
1	C	417	GLU	1
1	C	439	GLN	1
1	C	442	SER	1
1	C	523	ASP	1
2	B	25	GLN	1
2	B	26	ASN	1
2	B	33	ASP	1
2	B	45	VAL	1
2	B	154	ASP	1
1	A	279	LEU	1
1	A	379	LEU	1
1	A	393	TYR	1
1	A	395	LYS	1
1	C	401	LEU	1
2	B	70	GLN	1
2	B	89	SER	1
2	B	97	ARG	1
1	A	206	ASN	1
1	A	359	THR	1
1	C	411	THR	1
1	C	586	SER	1
1	C	589	GLU	1
1	A	308	ARG	1
1	C	478	ARG	1
1	C	495	LYS	1
1	C	527	GLN	1
2	B	31	GLU	1
2	B	37	GLU	1
2	B	47	ASP	1
2	B	108	ASP	1
2	B	135	ARG	1
2	B	172	LYS	1
1	A	242	GLU	1
1	A	275	LYS	1
1	C	406	ASP	1
1	C	497	SER	1
1	C	501	GLU	1
2	B	30	ASP	1
2	B	38	ASP	1
1	A	257	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	264	LYS	1
1	A	274	GLN	1
1	A	350	HIS	1
1	A	369	GLU	1
1	A	386	PHE	1
1	C	404	ASN	1
1	C	457	ASP	1
1	C	579	SER	1
2	B	101	LYS	1
1	A	261	PHE	1
1	A	349	TYR	1
1	C	434	THR	1
1	C	464	GLN	1
1	C	468	GLU	1
1	C	546	GLU	1
2	B	58	THR	1
2	B	76	GLU	1
2	B	105	ASP	1
2	B	126	ASP	1
1	A	233	GLU	1
1	A	276	VAL	1
1	A	297	LYS	1
1	C	488	LYS	1
1	C	521	TYR	1
1	C	569	LEU	1
2	B	91	GLU	1
2	B	164	ARG	1
2	B	166	HIS	1
1	A	225	THR	1
1	A	227	GLU	1
1	A	330	ARG	1
1	A	345	ARG	1
1	A	365	LYS	1
1	C	426	PHE	1
1	C	458	ASP	1
2	B	57	ASP	1
2	B	150	GLN	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 oligosaccharides 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	22	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	55	-	53,53,53	1.07±0.00	5±0 (9±0%)
3	PCW	A	68	-	53,53,53	1.05±0.01	4±0 (6±0%)
4	17F	A	76	-	52,53,53	1.03±0.00	3±0 (5±0%)
3	PCW	A	2	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	19	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	3	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	23	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	71	-	53,53,53	1.05±0.00	4±0 (7±0%)
4	17F	A	73	-	52,53,53	1.04±0.01	3±0 (5±0%)
3	PCW	A	58	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	48	-	53,53,53	1.04±0.00	4±0 (8±0%)
3	PCW	A	65	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	10	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	A	74	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	60	-	53,53,53	1.05±0.00	4±0 (7±0%)
5	GNP	B	201	-	34,34,34	1.31±0.02	4±0 (11±0%)
3	PCW	A	41	-	53,53,53	1.04±0.01	4±0 (6±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	A	12	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	30	-	53,53,53	1.05±0.00	5±0 (9±0%)
3	PCW	A	18	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	5	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	20	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	62	-	53,53,53	1.04±0.00	4±0 (7±0%)
3	PCW	A	16	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	17F	A	33	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	63	-	53,53,53	1.04±0.00	4±0 (7±0%)
4	17F	A	38	-	52,53,53	1.03±0.00	3±0 (5±0%)
3	PCW	A	43	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	A	44	-	53,53,53	1.05±0.00	4±0 (7±0%)
3	PCW	A	52	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	17F	A	34	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	17	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	54	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	32	-	53,53,53	1.04±0.01	5±0 (9±0%)
3	PCW	A	57	-	53,53,53	1.04±0.00	4±0 (7±0%)
3	PCW	A	29	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	56	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	67	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	31	-	53,53,53	1.04±0.00	4±0 (7±0%)
3	PCW	A	72	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	70	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	59	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	50	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	42	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	14	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	46	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	64	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	A	15	-	53,53,53	1.04±0.01	5±0 (9±0%)
3	PCW	A	47	-	53,53,53	1.05±0.01	5±0 (8±0%)
4	17F	A	80	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	17F	A	36	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	66	-	53,53,53	1.05±0.01	5±0 (9±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	17F	A	39	-	52,53,53	1.03±0.00	3±0 (5±0%)
3	PCW	A	49	-	53,53,53	1.05±0.00	4±0 (7±0%)
4	17F	A	77	-	52,53,53	1.04±0.01	3±0 (5±0%)
3	PCW	A	1	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	A	78	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	21	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	A	27	-	53,53,53	1.07±0.01	5±0 (9±0%)
3	PCW	A	24	-	53,53,53	1.05±0.01	3±0 (6±0%)
4	17F	A	79	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	6	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	11	-	53,53,53	1.05±0.00	5±0 (9±0%)
3	PCW	A	28	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	8	-	53,53,53	1.05±0.00	5±0 (9±0%)
4	17F	A	40	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	17F	A	37	-	52,53,53	1.04±0.01	3±0 (5±0%)
3	PCW	A	51	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	25	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	7	-	53,53,53	1.04±0.01	5±0 (8±0%)
3	PCW	A	9	-	53,53,53	1.05±0.01	5±0 (8±0%)
4	17F	A	75	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	69	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	53	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	61	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	13	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	A	35	-	52,53,53	1.03±0.01	3±0 (5±0%)
3	PCW	A	45	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	4	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	26	-	53,53,53	1.05±0.01	4±0 (6±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	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	A	22	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	55	-	59,61,61	0.83±0.01	1±0 (1±0%)
3	PCW	A	68	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	A	76	-	54,60,60	1.04±0.02	5±0 (9±0%)
3	PCW	A	2	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	19	-	59,61,61	0.84±0.00	1±0 (1±0%)
3	PCW	A	3	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	23	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	71	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	73	-	54,60,60	1.05±0.01	5±0 (9±0%)
3	PCW	A	58	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	48	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	65	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	10	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	74	-	54,60,60	1.05±0.03	5±0 (9±0%)
3	PCW	A	60	-	59,61,61	2.32±0.00	5±0 (8±0%)
5	GNP	B	201	-	47,54,54	0.97±0.01	3±0 (5±1%)
3	PCW	A	41	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	12	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	30	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	18	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	5	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	20	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	62	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	16	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	33	-	54,60,60	1.76±0.02	10±0 (17±0%)
3	PCW	A	63	-	59,61,61	2.76±0.00	9±0 (15±0%)
4	17F	A	38	-	54,60,60	1.05±0.02	5±0 (9±0%)
3	PCW	A	43	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	44	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	52	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	34	-	54,60,60	1.05±0.02	5±0 (9±0%)
3	PCW	A	17	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	54	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	32	-	59,61,61	0.84±0.01	1±0 (1±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	A	57	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	29	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	56	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	67	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	31	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	72	-	59,61,61	0.84±0.00	1±0 (1±0%)
3	PCW	A	70	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	59	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	50	-	59,61,61	0.84±0.00	1±0 (1±0%)
3	PCW	A	42	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	14	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	46	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	64	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	15	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	47	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	80	-	54,60,60	1.02±0.01	4±0 (7±0%)
4	17F	A	36	-	54,60,60	1.04±0.02	5±0 (9±0%)
3	PCW	A	66	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	39	-	54,60,60	1.06±0.02	5±0 (9±0%)
3	PCW	A	49	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	77	-	54,60,60	1.76±0.01	10±0 (18±0%)
3	PCW	A	1	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	78	-	54,60,60	1.04±0.02	5±0 (9±0%)
3	PCW	A	21	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	27	-	59,61,61	0.83±0.01	1±0 (1±0%)
3	PCW	A	24	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	A	79	-	54,60,60	1.04±0.01	5±0 (9±0%)
3	PCW	A	6	-	59,61,61	2.77±0.01	9±0 (15±0%)
3	PCW	A	11	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	28	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	8	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	40	-	54,60,60	1.04±0.02	5±0 (8±0%)
4	17F	A	37	-	54,60,60	1.05±0.02	5±0 (9±0%)
3	PCW	A	51	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	25	-	59,61,61	2.32±0.00	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	A	7	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	9	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	75	-	54,60,60	1.04±0.01	5±0 (9±0%)
3	PCW	A	69	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	53	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	61	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	13	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	35	-	54,60,60	1.04±0.01	5±0 (9±0%)
3	PCW	A	45	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	4	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	26	-	59,61,61	2.32±0.00	5±0 (8±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	74	-	-	0±0,59,59,59	-
3	PCW	A	12	-	-	0±0,57,57,57	-
3	PCW	A	71	-	-	0±0,57,57,57	-
3	PCW	A	48	-	-	0±0,57,57,57	-
3	PCW	A	17	-	-	0±0,57,57,57	-
3	PCW	A	56	-	-	0±0,57,57,57	-
3	PCW	A	60	-	-	0±0,57,57,57	-
4	17F	A	34	-	-	0±0,59,59,59	-
3	PCW	A	29	-	-	0±0,57,57,57	-
3	PCW	A	41	-	-	0±0,57,57,57	-
3	PCW	A	42	-	-	0±0,57,57,57	-
3	PCW	A	21	-	-	0±0,57,57,57	-
3	PCW	A	67	-	-	0±0,57,57,57	-
3	PCW	A	49	-	-	0±0,57,57,57	-
4	17F	A	77	-	-	0±0,59,59,59	-
3	PCW	A	72	-	-	0±0,57,57,57	-
5	GNP	B	201	-	-	0±0,18,38,38	0±0,3,3,3
3	PCW	A	1	-	-	0±0,57,57,57	-
3	PCW	A	55	-	-	0±0,57,57,57	-
3	PCW	A	22	-	-	0±0,57,57,57	-
4	17F	A	76	-	-	0±0,59,59,59	-
3	PCW	A	9	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	17F	A	36	-	-	0±0,59,59,59	-
3	PCW	A	13	-	-	0±0,57,57,57	-
3	PCW	A	65	-	-	0±0,57,57,57	-
3	PCW	A	8	-	-	0±0,57,57,57	-
4	17F	A	33	-	-	0±0,59,59,59	-
3	PCW	A	19	-	-	0±0,57,57,57	-
3	PCW	A	15	-	-	0±0,57,57,57	-
3	PCW	A	70	-	-	0±0,57,57,57	-
3	PCW	A	51	-	-	0±0,57,57,57	-
3	PCW	A	52	-	-	0±0,57,57,57	-
4	17F	A	80	-	-	0±0,59,59,59	-
3	PCW	A	61	-	-	0±0,57,57,57	-
4	17F	A	40	-	-	0±0,59,59,59	-
3	PCW	A	58	-	-	0±0,57,57,57	-
3	PCW	A	4	-	-	0±0,57,57,57	-
3	PCW	A	11	-	-	0±0,57,57,57	-
4	17F	A	35	-	-	0±0,59,59,59	-
3	PCW	A	47	-	-	0±0,57,57,57	-
3	PCW	A	7	-	-	0±0,57,57,57	-
4	17F	A	39	-	-	0±0,59,59,59	-
3	PCW	A	59	-	-	0±0,57,57,57	-
3	PCW	A	30	-	-	0±0,57,57,57	-
3	PCW	A	64	-	-	0±0,57,57,57	-
3	PCW	A	62	-	-	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	14	-	-	0±0,57,57,57	-
3	PCW	A	25	-	-	0±0,57,57,57	-
3	PCW	A	28	-	-	0±0,57,57,57	-
3	PCW	A	43	-	-	0±0,57,57,57	-
4	17F	A	78	-	-	0±0,59,59,59	-
3	PCW	A	2	-	-	0±0,57,57,57	-
3	PCW	A	63	-	-	0±0,57,57,57	-
4	17F	A	79	-	-	0±0,59,59,59	-
3	PCW	A	46	-	-	0±0,57,57,57	-
3	PCW	A	20	-	-	0±0,57,57,57	-
3	PCW	A	32	-	-	0±0,57,57,57	-
3	PCW	A	5	-	-	0±0,57,57,57	-
3	PCW	A	16	-	-	0±0,57,57,57	-
3	PCW	A	6	-	-	0±0,57,57,57	-
3	PCW	A	10	-	-	0±0,57,57,57	-
3	PCW	A	50	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	54	-	-	0±0,57,57,57	-
4	17F	A	73	-	-	0±0,59,59,59	-
3	PCW	A	27	-	-	0±0,57,57,57	-
3	PCW	A	66	-	-	0±0,57,57,57	-
4	17F	A	37	-	-	0±0,59,59,59	-
3	PCW	A	57	-	-	0±0,57,57,57	-
3	PCW	A	69	-	-	0±0,57,57,57	-
3	PCW	A	18	-	-	0±0,57,57,57	-
4	17F	A	75	-	-	0±0,59,59,59	-
3	PCW	A	31	-	-	0±0,57,57,57	-
3	PCW	A	44	-	-	0±0,57,57,57	-
4	17F	A	38	-	-	0±0,59,59,59	-
3	PCW	A	23	-	-	0±0,57,57,57	-
3	PCW	A	53	-	-	0±0,57,57,57	-
3	PCW	A	3	-	-	0±0,57,57,57	-
3	PCW	A	24	-	-	0±0,57,57,57	-
3	PCW	A	45	-	-	0±0,57,57,57	-

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
5	B	201	GNP	PB-O2B	4.04	1.46	1.56	10	10
5	B	201	GNP	PG-O3G	3.36	1.47	1.56	4	10
5	B	201	GNP	PB-O3A	3.00	1.55	1.59	3	10
3	A	6	PCW	C5-N	2.81	1.42	1.51	5	10
3	A	69	PCW	C5-N	2.81	1.42	1.51	8	10
3	A	22	PCW	C5-N	2.79	1.43	1.51	5	10
3	A	44	PCW	C5-N	2.77	1.43	1.51	2	10
3	A	5	PCW	C5-N	2.76	1.43	1.51	5	10
3	A	25	PCW	C5-N	2.76	1.43	1.51	6	10
3	A	45	PCW	C5-N	2.76	1.43	1.51	9	10
3	A	21	PCW	C5-N	2.75	1.43	1.51	10	10
3	A	49	PCW	C5-N	2.75	1.43	1.51	8	10
3	A	60	PCW	C5-N	2.75	1.43	1.51	9	10
3	A	64	PCW	C5-N	2.75	1.43	1.51	10	10
3	A	67	PCW	C5-N	2.75	1.43	1.51	8	10
3	A	26	PCW	C5-N	2.75	1.43	1.51	5	10
3	A	57	PCW	C5-N	2.75	1.43	1.51	8	10
3	A	61	PCW	C5-N	2.75	1.43	1.51	4	10
3	A	29	PCW	C5-N	2.74	1.43	1.51	4	10
3	A	53	PCW	C5-N	2.74	1.43	1.51	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	17	PCW	C5-N	2.74	1.43	1.51	10	10
3	A	24	PCW	C5-N	2.73	1.43	1.51	9	10
3	A	46	PCW	C5-N	2.73	1.43	1.51	7	10
3	A	58	PCW	C5-N	2.73	1.43	1.51	5	10
3	A	3	PCW	C5-N	2.73	1.43	1.51	9	10
3	A	18	PCW	C5-N	2.73	1.43	1.51	1	10
3	A	51	PCW	C5-N	2.73	1.43	1.51	7	10
3	A	31	PCW	C5-N	2.73	1.43	1.51	9	10
3	A	1	PCW	C5-N	2.72	1.43	1.51	8	10
3	A	68	PCW	C5-N	2.73	1.43	1.51	10	10
3	A	70	PCW	C5-N	2.72	1.43	1.51	4	10
3	A	28	PCW	C5-N	2.72	1.43	1.51	6	10
3	A	20	PCW	C5-N	2.72	1.43	1.51	1	10
3	A	10	PCW	C5-N	2.72	1.43	1.51	6	10
3	A	71	PCW	C5-N	2.72	1.43	1.51	10	10
3	A	4	PCW	C5-N	2.71	1.43	1.51	6	10
3	A	62	PCW	C5-N	2.71	1.43	1.51	3	10
3	A	52	PCW	C5-N	2.71	1.43	1.51	10	10
3	A	56	PCW	C5-N	2.71	1.43	1.51	10	10
3	A	63	PCW	C5-N	2.70	1.43	1.51	8	10
3	A	42	PCW	C5-N	2.70	1.43	1.51	3	10
3	A	59	PCW	C5-N	2.69	1.43	1.51	2	10
3	A	41	PCW	C5-N	2.68	1.43	1.51	7	10
3	A	2	PCW	C5-N	2.68	1.43	1.51	8	10
3	A	23	PCW	C5-N	2.68	1.43	1.51	6	10
3	A	54	PCW	C5-N	2.66	1.43	1.51	7	10
3	A	14	PCW	C5-N	2.66	1.43	1.51	1	10
3	A	13	PCW	C5-N	2.66	1.43	1.51	6	10
3	A	43	PCW	C5-N	2.66	1.43	1.51	4	10
3	A	18	PCW	C1-C2	2.66	1.59	1.50	8	10
3	A	55	PCW	C1-C2	2.66	1.59	1.50	4	10
3	A	58	PCW	C1-C2	2.63	1.59	1.50	8	10
3	A	6	PCW	C1-C2	2.63	1.59	1.50	1	10
3	A	46	PCW	C1-C2	2.61	1.59	1.50	8	10
3	A	12	PCW	C1-C2	2.61	1.59	1.50	9	10
3	A	27	PCW	C1-C2	2.61	1.59	1.50	4	10
3	A	11	PCW	C1-C2	2.61	1.59	1.50	9	10
3	A	70	PCW	C1-C2	2.61	1.59	1.50	5	10
3	A	9	PCW	C1-C2	2.60	1.58	1.50	10	10
3	A	68	PCW	C1-C2	2.60	1.58	1.50	8	10
3	A	15	PCW	C1-C2	2.60	1.58	1.50	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	71	PCW	C1-C2	2.60	1.58	1.50	3	10
4	A	37	17F	O4-C3	2.60	1.29	1.22	7	10
3	A	20	PCW	C1-C2	2.59	1.58	1.50	8	10
3	A	66	PCW	C1-C2	2.59	1.58	1.50	5	10
4	A	36	17F	O4-C3	2.58	1.29	1.22	1	10
3	A	60	PCW	C1-C2	2.58	1.58	1.50	7	10
3	A	43	PCW	C1-C2	2.57	1.58	1.50	9	10
4	A	39	17F	O4-C3	2.57	1.29	1.22	7	10
4	A	74	17F	O4-C3	2.57	1.29	1.22	9	10
3	A	3	PCW	C1-C2	2.57	1.58	1.50	10	10
4	A	75	17F	O4-C3	2.57	1.29	1.22	3	10
3	A	57	PCW	C1-C2	2.57	1.58	1.50	4	10
4	A	77	17F	O4-C3	2.57	1.29	1.22	10	10
3	A	9	PCW	C5-N	2.56	1.43	1.51	2	10
3	A	14	PCW	C1-C2	2.56	1.58	1.50	4	10
3	A	61	PCW	C1-C2	2.56	1.58	1.50	7	10
3	A	16	PCW	C1-C2	2.56	1.58	1.50	7	10
3	A	21	PCW	C1-C2	2.56	1.58	1.50	3	10
3	A	24	PCW	C1-C2	2.56	1.58	1.50	5	10
3	A	22	PCW	C1-C2	2.56	1.58	1.50	1	10
3	A	63	PCW	C1-C2	2.56	1.58	1.50	1	10
3	A	28	PCW	C1-C2	2.56	1.58	1.50	2	10
3	A	59	PCW	C1-C2	2.56	1.58	1.50	9	10
3	A	19	PCW	C1-C2	2.55	1.58	1.50	7	10
3	A	52	PCW	C1-C2	2.55	1.58	1.50	9	10
3	A	67	PCW	C1-C2	2.55	1.58	1.50	10	10
3	A	30	PCW	C1-C2	2.55	1.58	1.50	2	10
3	A	7	PCW	C1-C2	2.55	1.58	1.50	5	10
3	A	26	PCW	C1-C2	2.55	1.58	1.50	10	10
3	A	42	PCW	C1-C2	2.55	1.58	1.50	5	10
3	A	51	PCW	C1-C2	2.55	1.58	1.50	6	10
3	A	72	PCW	C1-C2	2.55	1.58	1.50	8	10
3	A	4	PCW	C1-C2	2.54	1.58	1.50	7	10
3	A	10	PCW	C1-C2	2.54	1.58	1.50	2	10
3	A	64	PCW	C1-C2	2.54	1.58	1.50	6	10
3	A	47	PCW	C1-C2	2.54	1.58	1.50	1	10
4	A	80	17F	O4-C3	2.54	1.29	1.22	9	10
4	A	40	17F	O4-C3	2.54	1.29	1.22	8	10
3	A	44	PCW	C1-C2	2.53	1.58	1.50	1	10
3	A	17	PCW	C1-C2	2.53	1.58	1.50	1	10
3	A	2	PCW	C1-C2	2.53	1.58	1.50	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	65	PCW	C1-C2	2.53	1.58	1.50	1	10
3	A	56	PCW	C1-C2	2.53	1.58	1.50	3	10
4	A	38	17F	O4-C3	2.53	1.29	1.22	7	10
3	A	69	PCW	C1-C2	2.53	1.58	1.50	5	10
3	A	8	PCW	C1-C2	2.52	1.58	1.50	8	10
3	A	13	PCW	C1-C2	2.52	1.58	1.50	7	10
4	A	35	17F	O4-C3	2.52	1.29	1.22	2	10
3	A	50	PCW	C1-C2	2.52	1.58	1.50	9	10
3	A	25	PCW	C1-C2	2.52	1.58	1.50	4	10
3	A	23	PCW	C1-C2	2.51	1.58	1.50	8	10
3	A	32	PCW	C1-C2	2.52	1.58	1.50	4	10
4	A	33	17F	O4-C3	2.51	1.29	1.22	5	10
3	A	1	PCW	C1-C2	2.51	1.58	1.50	10	10
3	A	65	PCW	C5-N	2.51	1.43	1.51	1	10
4	A	34	17F	O4-C3	2.51	1.29	1.22	1	10
3	A	54	PCW	C1-C2	2.50	1.58	1.50	4	10
4	A	73	17F	O4-C3	2.50	1.29	1.22	2	10
3	A	5	PCW	C1-C2	2.50	1.58	1.50	7	10
4	A	78	17F	O4-C3	2.50	1.29	1.22	9	10
3	A	29	PCW	C1-C2	2.50	1.58	1.50	7	10
3	A	49	PCW	C1-C2	2.50	1.58	1.50	10	10
3	A	31	PCW	C1-C2	2.49	1.58	1.50	5	10
4	A	76	17F	O4-C3	2.49	1.29	1.22	4	10
4	A	79	17F	O4-C3	2.49	1.29	1.22	8	10
3	A	53	PCW	C1-C2	2.48	1.58	1.50	2	10
3	A	62	PCW	C1-C2	2.48	1.58	1.50	7	10
3	A	12	PCW	C5-N	2.47	1.43	1.51	5	10
3	A	48	PCW	C1-C2	2.47	1.58	1.50	7	10
3	A	48	PCW	C5-N	2.47	1.43	1.51	2	10
3	A	41	PCW	C1-C2	2.47	1.58	1.50	9	10
3	A	19	PCW	C5-N	2.47	1.44	1.51	1	10
3	A	7	PCW	C5-N	2.46	1.44	1.51	3	10
3	A	72	PCW	C5-N	2.46	1.44	1.51	9	10
3	A	50	PCW	C5-N	2.46	1.44	1.51	8	10
3	A	45	PCW	C1-C2	2.46	1.58	1.50	5	10
3	A	5	PCW	C33-C32	2.45	1.61	1.52	9	10
3	A	16	PCW	C5-N	2.45	1.44	1.51	1	10
3	A	23	PCW	C33-C32	2.45	1.61	1.52	5	10
3	A	47	PCW	C5-N	2.44	1.44	1.51	8	10
3	A	11	PCW	C5-N	2.44	1.44	1.51	3	10
3	A	11	PCW	C33-C32	2.44	1.61	1.52	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	30	PCW	C5-N	2.44	1.44	1.51	3	10
3	A	15	PCW	C5-N	2.44	1.44	1.51	5	10
3	A	55	PCW	C33-C32	2.43	1.61	1.52	8	10
3	A	56	PCW	C33-C32	2.43	1.61	1.52	2	10
3	A	27	PCW	C5-N	2.42	1.44	1.51	3	10
4	A	37	17F	O5-C3	2.42	1.22	1.30	4	10
3	A	32	PCW	C5-N	2.42	1.44	1.51	6	10
3	A	45	PCW	C33-C32	2.42	1.61	1.52	7	10
3	A	66	PCW	C5-N	2.42	1.44	1.51	2	10
4	A	76	17F	O5-C3	2.42	1.22	1.30	6	10
3	A	1	PCW	C33-C32	2.41	1.61	1.52	1	10
4	A	78	17F	O5-C3	2.42	1.22	1.30	2	10
3	A	10	PCW	C33-C32	2.41	1.61	1.52	7	10
3	A	18	PCW	C33-C32	2.41	1.61	1.52	1	10
4	A	74	17F	O5-C3	2.41	1.23	1.30	10	10
4	A	38	17F	O5-C3	2.41	1.23	1.30	10	10
3	A	9	PCW	C33-C32	2.41	1.61	1.52	3	10
4	A	75	17F	O5-C3	2.41	1.23	1.30	9	10
3	A	52	PCW	C33-C32	2.40	1.61	1.52	9	10
4	A	79	17F	O5-C3	2.40	1.23	1.30	1	10
3	A	14	PCW	C33-C32	2.40	1.61	1.52	7	10
4	A	80	17F	O5-C3	2.40	1.23	1.30	5	10
3	A	51	PCW	C33-C32	2.40	1.61	1.52	7	10
4	A	73	17F	O5-C3	2.40	1.23	1.30	9	10
3	A	8	PCW	C33-C32	2.40	1.61	1.52	8	10
3	A	55	PCW	C5-N	2.40	1.44	1.51	6	10
3	A	69	PCW	C33-C32	2.40	1.61	1.52	5	10
3	A	30	PCW	C33-C32	2.40	1.61	1.52	10	10
3	A	8	PCW	C5-N	2.40	1.44	1.51	2	10
3	A	46	PCW	C33-C32	2.40	1.61	1.52	7	10
3	A	58	PCW	C33-C32	2.40	1.61	1.52	1	10
3	A	50	PCW	C33-C32	2.39	1.61	1.52	1	10
3	A	61	PCW	C33-C32	2.39	1.61	1.52	9	10
3	A	66	PCW	C33-C32	2.39	1.61	1.52	7	10
3	A	32	PCW	C33-C32	2.39	1.61	1.52	4	10
3	A	60	PCW	C33-C32	2.39	1.61	1.52	7	10
3	A	67	PCW	C33-C32	2.39	1.61	1.52	3	10
3	A	15	PCW	C33-C32	2.39	1.60	1.52	9	10
4	A	77	17F	O5-C3	2.39	1.23	1.30	1	10
5	B	201	GNP	PG-O1G	2.39	1.49	1.46	1	10
3	A	64	PCW	C33-C32	2.38	1.60	1.52	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	22	PCW	C33-C32	2.38	1.60	1.52	10	10
3	A	28	PCW	C33-C32	2.38	1.60	1.52	7	10
3	A	48	PCW	C33-C32	2.38	1.60	1.52	8	10
3	A	57	PCW	C33-C32	2.38	1.60	1.52	7	10
4	A	35	17F	O5-C3	2.38	1.23	1.30	5	10
4	A	39	17F	O5-C3	2.38	1.23	1.30	8	10
3	A	31	PCW	C33-C32	2.38	1.60	1.52	4	10
3	A	63	PCW	C33-C32	2.38	1.60	1.52	8	10
3	A	20	PCW	C33-C32	2.37	1.60	1.52	1	10
3	A	59	PCW	C33-C32	2.38	1.60	1.52	5	10
3	A	2	PCW	C33-C32	2.37	1.60	1.52	1	10
3	A	44	PCW	C33-C32	2.37	1.60	1.52	1	10
3	A	26	PCW	C33-C32	2.37	1.60	1.52	1	10
3	A	42	PCW	C33-C32	2.37	1.60	1.52	9	10
3	A	49	PCW	C33-C32	2.37	1.60	1.52	5	10
3	A	68	PCW	C33-C32	2.37	1.60	1.52	1	10
4	A	36	17F	O5-C3	2.37	1.23	1.30	7	10
3	A	7	PCW	C33-C32	2.37	1.60	1.52	10	10
3	A	6	PCW	C33-C32	2.36	1.60	1.52	1	10
3	A	3	PCW	C33-C32	2.36	1.60	1.52	4	10
3	A	43	PCW	C33-C32	2.36	1.60	1.52	4	10
3	A	13	PCW	C33-C32	2.36	1.60	1.52	7	10
3	A	21	PCW	C33-C32	2.36	1.60	1.52	3	10
3	A	27	PCW	C33-C32	2.36	1.60	1.52	4	10
4	A	40	17F	O5-C3	2.36	1.23	1.30	9	10
3	A	54	PCW	C33-C32	2.36	1.60	1.52	3	10
3	A	17	PCW	C33-C32	2.36	1.60	1.52	2	10
3	A	19	PCW	C33-C32	2.36	1.60	1.52	8	10
3	A	29	PCW	C33-C32	2.36	1.60	1.52	4	10
4	A	34	17F	O5-C3	2.36	1.23	1.30	10	10
3	A	71	PCW	C33-C32	2.36	1.60	1.52	6	10
3	A	25	PCW	C33-C32	2.35	1.60	1.52	8	10
3	A	65	PCW	C33-C32	2.35	1.60	1.52	5	10
3	A	53	PCW	C33-C32	2.35	1.60	1.52	1	10
3	A	70	PCW	C33-C32	2.35	1.60	1.52	2	10
3	A	16	PCW	C33-C32	2.35	1.60	1.52	3	10
3	A	24	PCW	C33-C32	2.35	1.60	1.52	1	10
3	A	41	PCW	C33-C32	2.35	1.60	1.52	3	10
3	A	47	PCW	C33-C32	2.35	1.60	1.52	6	10
3	A	4	PCW	C33-C32	2.35	1.60	1.52	5	10
3	A	72	PCW	C33-C32	2.34	1.60	1.52	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	12	PCW	C33-C32	2.34	1.60	1.52	8	10
3	A	62	PCW	C33-C32	2.34	1.60	1.52	3	10
4	A	33	17F	O5-C3	2.33	1.23	1.30	6	10
3	A	27	PCW	C7-N	2.28	1.43	1.50	1	10
3	A	9	PCW	C7-N	2.26	1.43	1.50	10	10
3	A	27	PCW	C3-C2	2.26	1.57	1.50	4	10
3	A	72	PCW	C7-N	2.26	1.43	1.50	7	10
3	A	32	PCW	C7-N	2.25	1.43	1.50	1	10
3	A	66	PCW	C7-N	2.25	1.43	1.50	3	10
3	A	55	PCW	C7-N	2.24	1.43	1.50	1	10
3	A	65	PCW	C7-N	2.24	1.43	1.50	7	10
3	A	12	PCW	C7-N	2.24	1.43	1.50	9	10
3	A	15	PCW	C7-N	2.24	1.43	1.50	3	10
3	A	47	PCW	C7-N	2.23	1.43	1.50	9	10
3	A	50	PCW	C7-N	2.23	1.43	1.50	7	10
3	A	16	PCW	C7-N	2.22	1.43	1.50	3	10
3	A	7	PCW	C7-N	2.22	1.43	1.50	7	10
3	A	58	PCW	C3-C2	2.20	1.57	1.50	5	10
3	A	8	PCW	C7-N	2.20	1.43	1.50	6	10
3	A	30	PCW	C7-N	2.19	1.43	1.50	8	10
3	A	11	PCW	C7-N	2.19	1.43	1.50	7	10
3	A	48	PCW	C7-N	2.19	1.43	1.50	5	10
3	A	55	PCW	C3-C2	2.19	1.57	1.50	5	10
3	A	7	PCW	C3-C2	2.17	1.57	1.50	5	6
3	A	8	PCW	C3-C2	2.17	1.57	1.50	9	9
3	A	19	PCW	C7-N	2.17	1.43	1.50	6	10
3	A	54	PCW	C3-C2	2.16	1.57	1.50	3	8
3	A	26	PCW	C3-C2	2.16	1.57	1.50	10	7
3	A	5	PCW	C3-C2	2.16	1.57	1.50	10	10
3	A	42	PCW	C3-C2	2.16	1.57	1.50	3	9
3	A	47	PCW	C3-C2	2.15	1.57	1.50	2	7
3	A	41	PCW	C3-C2	2.15	1.57	1.50	1	6
3	A	68	PCW	C3-C2	2.15	1.57	1.50	10	6
3	A	29	PCW	C3-C2	2.15	1.57	1.50	4	9
3	A	3	PCW	C3-C2	2.15	1.57	1.50	3	8
3	A	10	PCW	C3-C2	2.14	1.57	1.50	2	9
3	A	15	PCW	C3-C2	2.14	1.57	1.50	5	9
3	A	46	PCW	C3-C2	2.14	1.57	1.50	7	10
3	A	49	PCW	C3-C2	2.14	1.57	1.50	7	10
3	A	63	PCW	C3-C2	2.14	1.57	1.50	10	9
3	A	70	PCW	C3-C2	2.14	1.57	1.50	4	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	12	PCW	C3-C2	2.14	1.57	1.50	6	9
4	A	75	17F	C1X-C2X	2.14	1.61	1.52	8	9
3	A	11	PCW	C3-C2	2.13	1.57	1.50	2	9
3	A	16	PCW	C3-C2	2.13	1.57	1.50	7	10
3	A	30	PCW	C3-C2	2.13	1.57	1.50	9	8
3	A	50	PCW	C3-C2	2.13	1.57	1.50	5	9
3	A	51	PCW	C3-C2	2.13	1.57	1.50	7	8
3	A	18	PCW	C3-C2	2.13	1.57	1.50	3	6
3	A	32	PCW	C3-C2	2.13	1.57	1.50	1	10
3	A	65	PCW	C3-C2	2.13	1.57	1.50	7	10
3	A	71	PCW	C3-C2	2.13	1.57	1.50	10	9
4	A	77	17F	C1X-C2X	2.13	1.61	1.52	5	10
3	A	6	PCW	C3-C2	2.13	1.57	1.50	3	8
3	A	19	PCW	C3-C2	2.12	1.57	1.50	7	8
3	A	22	PCW	C3-C2	2.12	1.57	1.50	3	10
4	A	38	17F	C1X-C2X	2.12	1.61	1.52	10	9
3	A	61	PCW	C3-C2	2.12	1.57	1.50	4	8
4	A	36	17F	C1X-C2X	2.12	1.61	1.52	9	10
3	A	14	PCW	C3-C2	2.12	1.57	1.50	2	8
3	A	25	PCW	C3-C2	2.12	1.57	1.50	4	10
3	A	13	PCW	C3-C2	2.12	1.57	1.50	3	8
3	A	44	PCW	C3-C2	2.12	1.57	1.50	4	9
4	A	73	17F	C1X-C2X	2.12	1.61	1.52	6	10
3	A	4	PCW	C3-C2	2.12	1.57	1.50	4	9
3	A	43	PCW	C3-C2	2.11	1.57	1.50	7	7
4	A	78	17F	C1X-C2X	2.11	1.61	1.52	5	8
3	A	2	PCW	C3-C2	2.11	1.57	1.50	9	9
3	A	23	PCW	C3-C2	2.11	1.57	1.50	5	8
3	A	31	PCW	C3-C2	2.11	1.57	1.50	2	8
3	A	48	PCW	C3-C2	2.11	1.57	1.50	5	4
4	A	74	17F	C1X-C2X	2.11	1.61	1.52	9	8
3	A	9	PCW	C3-C2	2.11	1.57	1.50	2	7
3	A	56	PCW	C3-C2	2.11	1.57	1.50	5	10
3	A	59	PCW	C3-C2	2.10	1.57	1.50	10	8
3	A	60	PCW	C3-C2	2.10	1.57	1.50	9	9
4	A	34	17F	C1X-C2X	2.10	1.61	1.52	1	10
3	A	52	PCW	C3-C2	2.10	1.57	1.50	4	8
4	A	37	17F	C1X-C2X	2.10	1.61	1.52	5	10
4	A	76	17F	C1X-C2X	2.10	1.61	1.52	4	10
3	A	1	PCW	C3-C2	2.09	1.57	1.50	1	8
3	A	45	PCW	C3-C2	2.09	1.57	1.50	4	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	53	PCW	C3-C2	2.09	1.57	1.50	7	8
3	A	57	PCW	C3-C2	2.09	1.57	1.50	6	8
3	A	69	PCW	C3-C2	2.09	1.57	1.50	4	6
3	A	62	PCW	C3-C2	2.09	1.57	1.50	8	8
3	A	64	PCW	C3-C2	2.09	1.57	1.50	3	7
3	A	67	PCW	C3-C2	2.09	1.57	1.50	9	8
3	A	17	PCW	C3-C2	2.09	1.57	1.50	1	9
3	A	20	PCW	C3-C2	2.09	1.57	1.50	10	8
4	A	35	17F	C1X-C2X	2.09	1.61	1.52	6	9
4	A	40	17F	C1X-C2X	2.09	1.61	1.52	3	10
3	A	21	PCW	C3-C2	2.08	1.57	1.50	6	6
4	A	80	17F	C1X-C2X	2.08	1.61	1.52	4	10
3	A	66	PCW	C3-C2	2.08	1.57	1.50	6	9
3	A	72	PCW	C3-C2	2.08	1.57	1.50	8	10
4	A	39	17F	C1X-C2X	2.08	1.61	1.52	6	7
3	A	24	PCW	C3-C2	2.08	1.57	1.50	10	4
3	A	28	PCW	C3-C2	2.07	1.57	1.50	6	9
4	A	79	17F	C1X-C2X	2.07	1.61	1.52	3	9
4	A	33	17F	C1X-C2X	2.06	1.61	1.52	10	9

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	12.03	77.38	108.98	1	10
3	A	42	PCW	C8-N-C7	12.01	77.44	108.98	1	10
3	A	68	PCW	C8-N-C7	11.99	77.48	108.98	3	10
3	A	10	PCW	C8-N-C7	11.98	77.51	108.98	10	10
3	A	46	PCW	C8-N-C7	11.97	77.53	108.98	2	10
3	A	51	PCW	C8-N-C7	11.97	77.55	108.98	8	10
3	A	56	PCW	C8-N-C7	11.95	77.58	108.98	6	10
3	A	4	PCW	C8-N-C7	11.95	77.60	108.98	1	10
3	A	49	PCW	C8-N-C7	11.93	77.63	108.98	7	10
3	A	67	PCW	C8-N-C7	11.93	77.63	108.98	7	10
3	A	29	PCW	C8-N-C7	11.93	77.64	108.98	2	10
3	A	44	PCW	C8-N-C7	11.93	77.64	108.98	9	10
3	A	69	PCW	C8-N-C7	11.92	77.66	108.98	3	10
3	A	22	PCW	C8-N-C7	11.92	77.67	108.98	9	10
3	A	6	PCW	C8-N-C7	11.91	77.68	108.98	10	10
3	A	3	PCW	C8-N-C7	11.91	77.70	108.98	9	10
3	A	21	PCW	C8-N-C7	11.91	77.70	108.98	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	25	PCW	C8-N-C7	11.91	77.70	108.98	4	10
3	A	18	PCW	C8-N-C7	11.90	77.72	108.98	8	10
3	A	59	PCW	C8-N-C7	11.90	77.73	108.98	1	10
3	A	41	PCW	C8-N-C7	11.90	77.73	108.98	9	10
3	A	14	PCW	C8-N-C7	11.89	77.74	108.98	7	10
3	A	24	PCW	C8-N-C7	11.89	77.74	108.98	1	10
3	A	54	PCW	C8-N-C7	11.89	77.73	108.98	2	10
3	A	62	PCW	C8-N-C7	11.89	77.74	108.98	10	10
3	A	17	PCW	C8-N-C7	11.89	77.74	108.98	3	10
3	A	64	PCW	C8-N-C7	11.89	77.74	108.98	8	10
3	A	52	PCW	C8-N-C7	11.89	77.74	108.98	5	10
3	A	45	PCW	C8-N-C7	11.89	77.75	108.98	7	10
3	A	20	PCW	C8-N-C7	11.89	77.76	108.98	10	10
3	A	31	PCW	C8-N-C7	11.88	77.76	108.98	9	10
3	A	1	PCW	C8-N-C7	11.88	77.77	108.98	7	10
3	A	2	PCW	C8-N-C7	11.88	77.77	108.98	2	10
3	A	5	PCW	C8-N-C7	11.88	77.77	108.98	7	10
3	A	23	PCW	C8-N-C7	11.87	77.79	108.98	7	10
3	A	61	PCW	C8-N-C7	11.87	77.79	108.98	2	10
3	A	28	PCW	C8-N-C7	11.87	77.80	108.98	10	10
3	A	43	PCW	C8-N-C7	11.87	77.80	108.98	3	10
3	A	70	PCW	C8-N-C7	11.87	77.80	108.98	5	10
3	A	26	PCW	C8-N-C7	11.86	77.81	108.98	7	10
3	A	57	PCW	C8-N-C7	11.86	77.81	108.98	10	10
3	A	53	PCW	C8-N-C7	11.85	77.86	108.98	10	10
3	A	71	PCW	C8-N-C7	11.85	77.86	108.98	7	10
3	A	60	PCW	C8-N-C7	11.84	77.87	108.98	3	10
3	A	58	PCW	C8-N-C7	11.84	77.87	108.98	8	10
3	A	63	PCW	C8-N-C7	11.83	77.89	108.98	8	10
3	A	43	PCW	C8-N-C6	10.12	82.41	108.98	2	10
3	A	17	PCW	C8-N-C6	10.10	82.44	108.98	7	10
3	A	61	PCW	C8-N-C6	10.09	82.48	108.98	9	10
3	A	23	PCW	C8-N-C6	10.07	82.52	108.98	2	10
3	A	20	PCW	C8-N-C6	10.06	82.54	108.98	5	10
3	A	25	PCW	C8-N-C6	10.06	82.56	108.98	2	10
3	A	21	PCW	C8-N-C6	10.05	82.58	108.98	9	10
3	A	63	PCW	C8-N-C6	10.05	82.58	108.98	1	10
3	A	69	PCW	C8-N-C6	10.05	82.58	108.98	9	10
3	A	10	PCW	C8-N-C6	10.04	82.59	108.98	3	10
3	A	13	PCW	C8-N-C6	10.04	82.61	108.98	9	10
3	A	14	PCW	C8-N-C6	10.04	82.61	108.98	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	24	PCW	C8-N-C6	10.03	82.62	108.98	10	10
3	A	45	PCW	C8-N-C6	10.03	82.62	108.98	4	10
3	A	57	PCW	C8-N-C6	10.03	82.63	108.98	6	10
3	A	1	PCW	C8-N-C6	10.03	82.64	108.98	4	10
3	A	5	PCW	C8-N-C6	10.02	82.65	108.98	3	10
3	A	67	PCW	C8-N-C6	10.02	82.66	108.98	5	10
3	A	18	PCW	C8-N-C6	10.02	82.66	108.98	7	10
3	A	28	PCW	C8-N-C6	10.02	82.66	108.98	1	10
3	A	58	PCW	C8-N-C6	10.02	82.66	108.98	2	10
3	A	62	PCW	C8-N-C6	10.02	82.66	108.98	5	10
3	A	3	PCW	C8-N-C6	10.01	82.67	108.98	8	10
3	A	29	PCW	C8-N-C6	10.01	82.67	108.98	8	10
3	A	64	PCW	C8-N-C6	10.01	82.68	108.98	2	10
3	A	56	PCW	C8-N-C6	10.01	82.69	108.98	10	10
3	A	6	PCW	C8-N-C6	10.01	82.69	108.98	1	10
3	A	46	PCW	C8-N-C6	10.01	82.69	108.98	7	10
3	A	71	PCW	C8-N-C6	10.01	82.69	108.98	9	10
3	A	31	PCW	C8-N-C6	10.01	82.70	108.98	2	10
3	A	44	PCW	C8-N-C6	10.00	82.70	108.98	8	10
3	A	52	PCW	C8-N-C6	10.00	82.71	108.98	8	10
3	A	2	PCW	C8-N-C6	10.00	82.71	108.98	10	10
3	A	22	PCW	C8-N-C6	10.00	82.71	108.98	4	10
3	A	41	PCW	C8-N-C6	10.00	82.71	108.98	6	10
3	A	4	PCW	C8-N-C6	10.00	82.72	108.98	5	10
3	A	70	PCW	C8-N-C6	9.99	82.73	108.98	4	10
3	A	60	PCW	C8-N-C6	9.99	82.74	108.98	7	10
3	A	51	PCW	C8-N-C6	9.98	82.75	108.98	5	10
3	A	59	PCW	C8-N-C6	9.98	82.76	108.98	7	10
3	A	42	PCW	C8-N-C6	9.98	82.77	108.98	6	10
3	A	49	PCW	C8-N-C6	9.98	82.77	108.98	9	10
3	A	54	PCW	C8-N-C6	9.97	82.78	108.98	5	10
3	A	26	PCW	C8-N-C6	9.97	82.79	108.98	1	10
3	A	53	PCW	C8-N-C6	9.97	82.79	108.98	7	10
3	A	68	PCW	C8-N-C6	9.94	82.86	108.98	8	10
3	A	6	PCW	O4P-P-O2P	7.65	78.62	108.94	10	10
3	A	63	PCW	O4P-P-O2P	7.57	78.93	108.94	9	10
4	A	77	17F	O2-P1-O6	6.35	78.79	107.57	3	10
4	A	33	17F	O2-P1-O6	6.33	78.86	107.57	3	10
4	A	33	17F	O2-P1-O3	6.14	79.74	107.57	4	10
4	A	77	17F	O2-P1-O3	6.10	79.94	107.57	4	10
3	A	6	PCW	O1P-P-O2P	5.84	85.27	112.44	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	63	PCW	O3P-P-O2P	5.82	85.86	108.94	1	10
3	A	6	PCW	O3P-P-O2P	5.79	86.00	108.94	8	10
3	A	63	PCW	O1P-P-O2P	5.77	85.59	112.44	9	10
3	A	23	PCW	C8-N-C5	5.42	88.35	109.91	5	10
3	A	1	PCW	C8-N-C5	5.41	88.41	109.91	1	10
3	A	57	PCW	C8-N-C5	5.41	88.42	109.91	1	10
3	A	60	PCW	C8-N-C5	5.40	88.45	109.91	8	10
3	A	18	PCW	C8-N-C5	5.39	88.47	109.91	1	10
3	A	42	PCW	C8-N-C5	5.39	88.47	109.91	5	10
3	A	56	PCW	C8-N-C5	5.39	88.48	109.91	5	10
3	A	59	PCW	C8-N-C5	5.39	88.47	109.91	10	10
3	A	45	PCW	C8-N-C5	5.39	88.50	109.91	10	10
3	A	58	PCW	C8-N-C5	5.39	88.49	109.91	3	10
3	A	53	PCW	C8-N-C5	5.38	88.50	109.91	1	10
3	A	24	PCW	C8-N-C5	5.38	88.52	109.91	2	10
3	A	68	PCW	C8-N-C5	5.38	88.52	109.91	2	10
3	A	46	PCW	C8-N-C5	5.38	88.53	109.91	8	10
3	A	20	PCW	C8-N-C5	5.38	88.54	109.91	3	10
3	A	5	PCW	C8-N-C5	5.37	88.55	109.91	3	10
3	A	10	PCW	C8-N-C5	5.37	88.55	109.91	1	10
3	A	13	PCW	C8-N-C5	5.37	88.55	109.91	3	10
3	A	28	PCW	C8-N-C5	5.37	88.55	109.91	6	10
3	A	62	PCW	C8-N-C5	5.37	88.57	109.91	7	10
3	A	31	PCW	C8-N-C5	5.37	88.58	109.91	8	10
3	A	69	PCW	C8-N-C5	5.37	88.58	109.91	7	10
3	A	22	PCW	C8-N-C5	5.37	88.58	109.91	10	10
3	A	29	PCW	C8-N-C5	5.37	88.58	109.91	3	10
3	A	70	PCW	C8-N-C5	5.36	88.59	109.91	7	10
3	A	6	PCW	C8-N-C5	5.36	88.60	109.91	7	10
3	A	25	PCW	C8-N-C5	5.36	88.60	109.91	6	10
3	A	51	PCW	C8-N-C5	5.36	88.60	109.91	2	10
3	A	54	PCW	C8-N-C5	5.36	88.59	109.91	1	10
3	A	61	PCW	C8-N-C5	5.36	88.60	109.91	5	10
3	A	63	PCW	C8-N-C5	5.36	88.60	109.91	8	10
3	A	2	PCW	C8-N-C5	5.36	88.60	109.91	6	10
3	A	4	PCW	C8-N-C5	5.36	88.61	109.91	7	10
3	A	17	PCW	C8-N-C5	5.36	88.60	109.91	5	10
3	A	41	PCW	C8-N-C5	5.36	88.60	109.91	3	10
3	A	71	PCW	C8-N-C5	5.36	88.61	109.91	2	10
3	A	44	PCW	C8-N-C5	5.36	88.62	109.91	4	10
3	A	67	PCW	C8-N-C5	5.36	88.61	109.91	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	3	PCW	C8-N-C5	5.36	88.62	109.91	4	10
3	A	43	PCW	C8-N-C5	5.36	88.62	109.91	10	10
3	A	64	PCW	C8-N-C5	5.35	88.64	109.91	1	10
3	A	26	PCW	C8-N-C5	5.35	88.65	109.91	1	10
3	A	21	PCW	C8-N-C5	5.35	88.66	109.91	3	10
3	A	14	PCW	C8-N-C5	5.34	88.67	109.91	4	10
3	A	52	PCW	C8-N-C5	5.34	88.68	109.91	10	10
3	A	49	PCW	C8-N-C5	5.33	88.71	109.91	3	10
4	A	77	17F	O2-P1-O1	4.76	90.28	112.44	2	10
4	A	33	17F	O2-P1-O1	4.73	90.46	112.44	10	10
4	A	33	17F	O3-C1-C2	4.27	111.78	108.06	7	10
4	A	77	17F	O3-C1-C2	4.20	111.72	108.06	4	10
4	A	74	17F	O3-C1-C2	4.01	111.55	108.06	4	10
4	A	39	17F	O3-C1-C2	3.93	111.49	108.06	2	10
4	A	76	17F	O3-C1-C2	3.92	111.47	108.06	2	10
4	A	34	17F	O3-C1-C2	3.69	111.28	108.06	3	10
4	A	40	17F	O3-C1-C2	3.67	111.26	108.06	5	10
4	A	37	17F	O3-C1-C2	3.59	111.19	108.06	7	10
4	A	35	17F	O3-C1-C2	3.58	111.18	108.06	10	10
4	A	38	17F	O3-C1-C2	3.56	111.16	108.06	3	10
4	A	73	17F	O3-C1-C2	3.54	111.15	108.06	3	10
4	A	79	17F	O3-C1-C2	3.53	111.14	108.06	10	10
4	A	78	17F	O3-C1-C2	3.48	111.09	108.06	2	10
3	A	6	PCW	O1P-P-O4P	3.47	123.29	107.57	6	10
3	A	63	PCW	O1P-P-O4P	3.44	123.17	107.57	3	10
4	A	35	17F	O5-C3-O4	3.41	116.33	124.08	4	10
4	A	80	17F	O3-C1-C2	3.41	111.03	108.06	9	10
4	A	80	17F	O5-C3-O4	3.38	116.42	124.08	9	10
4	A	34	17F	O5-C3-O4	3.37	116.42	124.08	10	10
4	A	73	17F	O5-C3-O4	3.37	116.44	124.08	2	10
4	A	78	17F	O5-C3-O4	3.36	116.45	124.08	10	10
4	A	74	17F	O5-C3-O4	3.36	116.46	124.08	1	10
4	A	36	17F	O5-C3-O4	3.36	116.46	124.08	3	10
3	A	46	PCW	C6-N-C5	3.35	123.25	109.91	4	10
4	A	40	17F	O5-C3-O4	3.35	116.48	124.08	3	10
4	A	38	17F	O5-C3-O4	3.35	116.49	124.08	4	10
4	A	79	17F	O5-C3-O4	3.34	116.49	124.08	7	10
4	A	37	17F	O5-C3-O4	3.34	116.49	124.08	4	10
4	A	75	17F	O5-C3-O4	3.34	116.51	124.08	6	10
3	A	43	PCW	C6-N-C5	3.33	123.16	109.91	2	10
4	A	39	17F	O5-C3-O4	3.33	116.52	124.08	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	77	17F	O5-C3-O4	3.33	116.52	124.08	1	10
4	A	33	17F	O5-C3-O4	3.33	116.53	124.08	6	10
3	A	22	PCW	C6-N-C5	3.32	123.10	109.91	10	10
3	A	6	PCW	C6-N-C5	3.32	123.09	109.91	10	10
3	A	71	PCW	C6-N-C5	3.32	123.09	109.91	9	10
3	A	5	PCW	C6-N-C5	3.31	123.08	109.91	10	10
3	A	23	PCW	C6-N-C5	3.31	123.08	109.91	5	10
3	A	44	PCW	C6-N-C5	3.31	123.08	109.91	5	10
3	A	18	PCW	C6-N-C5	3.31	123.08	109.91	2	10
3	A	24	PCW	C6-N-C5	3.31	123.07	109.91	2	10
3	A	25	PCW	C6-N-C5	3.31	123.07	109.91	1	10
3	A	70	PCW	C6-N-C5	3.31	123.07	109.91	4	10
3	A	29	PCW	C6-N-C5	3.31	123.06	109.91	5	10
3	A	51	PCW	C6-N-C5	3.31	123.06	109.91	1	10
3	A	41	PCW	C6-N-C5	3.31	123.05	109.91	3	10
3	A	61	PCW	C6-N-C5	3.31	123.05	109.91	10	10
3	A	57	PCW	C6-N-C5	3.30	123.03	109.91	8	10
3	A	21	PCW	C6-N-C5	3.30	123.02	109.91	9	10
3	A	31	PCW	C6-N-C5	3.30	123.02	109.91	6	10
3	A	60	PCW	C6-N-C5	3.30	123.02	109.91	8	10
3	A	26	PCW	C6-N-C5	3.30	123.02	109.91	9	10
4	A	76	17F	O5-C3-O4	3.30	116.60	124.08	9	10
3	A	59	PCW	C6-N-C5	3.30	123.01	109.91	3	10
3	A	10	PCW	C6-N-C5	3.29	123.01	109.91	4	10
3	A	67	PCW	C6-N-C5	3.29	123.00	109.91	1	10
3	A	42	PCW	C6-N-C5	3.29	123.00	109.91	7	10
3	A	52	PCW	C6-N-C5	3.29	123.00	109.91	3	10
3	A	13	PCW	C6-N-C5	3.29	122.99	109.91	3	10
3	A	56	PCW	C6-N-C5	3.29	122.99	109.91	4	10
3	A	62	PCW	C6-N-C5	3.29	123.00	109.91	8	10
3	A	28	PCW	C6-N-C5	3.29	122.98	109.91	8	10
3	A	45	PCW	C6-N-C5	3.29	122.97	109.91	5	10
3	A	20	PCW	C6-N-C5	3.28	122.97	109.91	6	10
3	A	17	PCW	C6-N-C5	3.28	122.95	109.91	8	10
3	A	58	PCW	C6-N-C5	3.28	122.95	109.91	10	10
3	A	63	PCW	C6-N-C5	3.28	122.94	109.91	1	10
3	A	49	PCW	C6-N-C5	3.28	122.94	109.91	1	10
3	A	2	PCW	C6-N-C5	3.28	122.93	109.91	1	10
3	A	4	PCW	C6-N-C5	3.28	122.93	109.91	5	10
3	A	64	PCW	C6-N-C5	3.27	122.93	109.91	6	10
3	A	69	PCW	C6-N-C5	3.27	122.91	109.91	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	36	17F	O3-C1-C2	3.27	110.91	108.06	3	10
3	A	53	PCW	C6-N-C5	3.27	122.89	109.91	10	10
3	A	3	PCW	C6-N-C5	3.26	122.89	109.91	1	10
3	A	54	PCW	C6-N-C5	3.26	122.88	109.91	9	10
3	A	68	PCW	C6-N-C5	3.26	122.88	109.91	9	10
3	A	14	PCW	C6-N-C5	3.26	122.86	109.91	1	10
3	A	1	PCW	C6-N-C5	3.23	122.75	109.91	1	10
4	A	75	17F	O3-C1-C2	3.16	110.82	108.06	4	10
5	B	201	GNP	O3G-PG-O1G	3.08	105.72	113.45	10	10
5	B	201	GNP	O2G-PG-O3G	2.97	115.56	107.59	7	10
4	A	76	17F	O7-C7-O8	2.93	130.96	123.63	9	10
4	A	78	17F	O7-C7-O8	2.93	130.95	123.63	10	10
4	A	79	17F	O7-C7-O8	2.92	130.93	123.63	2	10
4	A	35	17F	O7-C7-O8	2.91	130.91	123.63	5	10
4	A	75	17F	O7-C7-O8	2.91	130.90	123.63	5	10
4	A	77	17F	O7-C7-O8	2.91	130.90	123.63	1	10
4	A	74	17F	O7-C7-O8	2.91	130.90	123.63	1	10
4	A	34	17F	O7-C7-O8	2.90	130.89	123.63	1	10
4	A	38	17F	O7-C7-O8	2.90	130.88	123.63	5	10
4	A	40	17F	O7-C7-O8	2.90	130.87	123.63	10	10
4	A	39	17F	O7-C7-O8	2.89	130.86	123.63	4	10
4	A	33	17F	O7-C7-O8	2.89	130.85	123.63	7	10
4	A	73	17F	O7-C7-O8	2.88	130.84	123.63	9	10
4	A	37	17F	O7-C7-O8	2.87	130.81	123.63	6	10
4	A	36	17F	O7-C7-O8	2.84	130.74	123.63	4	10
4	A	80	17F	O7-C7-O8	2.83	130.71	123.63	8	10
4	A	33	17F	O3-P1-O1	2.76	119.87	108.94	6	10
4	A	77	17F	O3-P1-O1	2.76	119.86	108.94	10	10
3	A	32	PCW	C8-N-C7	2.75	101.76	108.98	1	10
3	A	50	PCW	C8-N-C7	2.73	101.81	108.98	7	10
3	A	65	PCW	C8-N-C7	2.70	101.87	108.98	6	10
3	A	9	PCW	C8-N-C7	2.70	101.88	108.98	5	10
3	A	30	PCW	C8-N-C7	2.69	101.90	108.98	9	10
3	A	12	PCW	C8-N-C7	2.69	101.91	108.98	6	10
3	A	16	PCW	C8-N-C7	2.68	101.93	108.98	10	10
3	A	48	PCW	C8-N-C7	2.68	101.93	108.98	5	10
3	A	66	PCW	C8-N-C7	2.68	101.94	108.98	7	10
3	A	72	PCW	C8-N-C7	2.67	101.97	108.98	10	10
3	A	11	PCW	C8-N-C7	2.66	101.98	108.98	9	10
3	A	47	PCW	C8-N-C7	2.66	102.00	108.98	4	10
3	A	15	PCW	C8-N-C7	2.65	102.03	108.98	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	19	PCW	C8-N-C7	2.64	102.04	108.98	7	10
3	A	8	PCW	C8-N-C7	2.63	102.06	108.98	4	10
3	A	7	PCW	C8-N-C7	2.63	102.08	108.98	3	10
3	A	27	PCW	C8-N-C7	2.62	102.09	108.98	10	10
3	A	55	PCW	C8-N-C7	2.62	102.08	108.98	10	10
4	A	34	17F	C5-O9-C17	2.57	111.65	117.80	3	10
4	A	77	17F	C5-O9-C17	2.54	111.72	117.80	7	10
3	A	23	PCW	C7-N-C5	2.54	119.99	109.91	4	10
3	A	70	PCW	C7-N-C5	2.53	119.97	109.91	10	10
4	A	36	17F	C5-O9-C17	2.52	111.76	117.80	7	10
4	A	39	17F	C5-O9-C17	2.50	111.81	117.80	5	10
4	A	77	17F	O6-P1-O1	2.49	118.81	108.94	6	10
4	A	75	17F	C5-O9-C17	2.49	111.84	117.80	8	10
4	A	80	17F	O9-C17-O10	2.49	129.52	123.70	1	10
3	A	20	PCW	C7-N-C5	2.48	119.79	109.91	10	10
3	A	31	PCW	C7-N-C5	2.49	119.79	109.91	8	10
3	A	63	PCW	C7-N-C5	2.48	119.78	109.91	6	10
3	A	17	PCW	C7-N-C5	2.48	119.78	109.91	2	10
4	A	74	17F	C5-O9-C17	2.48	111.86	117.80	2	10
3	A	24	PCW	C7-N-C5	2.48	119.77	109.91	5	10
3	A	6	PCW	C7-N-C5	2.48	119.77	109.91	8	10
3	A	1	PCW	C7-N-C5	2.47	119.75	109.91	3	10
3	A	61	PCW	C7-N-C5	2.47	119.74	109.91	7	10
4	A	33	17F	O6-P1-O1	2.47	118.73	108.94	3	10
4	A	73	17F	C5-O9-C17	2.47	111.89	117.80	7	10
3	A	14	PCW	C7-N-C5	2.47	119.71	109.91	10	10
4	A	35	17F	C5-O9-C17	2.47	111.89	117.80	3	10
4	A	33	17F	C5-O9-C17	2.46	111.90	117.80	9	6
3	A	22	PCW	C7-N-C5	2.46	119.68	109.91	9	10
3	A	25	PCW	C7-N-C5	2.46	119.68	109.91	10	10
3	A	10	PCW	C7-N-C5	2.46	119.67	109.91	5	10
3	A	42	PCW	C7-N-C5	2.46	119.67	109.91	2	10
3	A	2	PCW	C7-N-C5	2.45	119.66	109.91	4	10
3	A	56	PCW	C7-N-C5	2.45	119.66	109.91	1	10
3	A	54	PCW	C7-N-C5	2.45	119.65	109.91	6	10
4	A	76	17F	C5-O9-C17	2.45	111.93	117.80	3	9
3	A	43	PCW	C7-N-C5	2.45	119.64	109.91	1	10
3	A	58	PCW	C7-N-C5	2.45	119.64	109.91	4	10
3	A	68	PCW	C7-N-C5	2.45	119.63	109.91	4	10
3	A	69	PCW	C7-N-C5	2.45	119.63	109.91	7	10
3	A	64	PCW	C7-N-C5	2.44	119.62	109.91	5	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	52	PCW	C7-N-C5	2.44	119.62	109.91	6	10
3	A	49	PCW	C7-N-C5	2.44	119.60	109.91	7	10
3	A	71	PCW	C7-N-C5	2.44	119.60	109.91	7	10
4	A	40	17F	C5-O9-C17	2.44	111.96	117.80	3	6
3	A	26	PCW	C7-N-C5	2.43	119.58	109.91	5	10
4	A	37	17F	C5-O9-C17	2.43	111.97	117.80	5	10
3	A	57	PCW	C7-N-C5	2.43	119.57	109.91	10	10
3	A	21	PCW	C7-N-C5	2.43	119.57	109.91	8	10
4	A	73	17F	O9-C17-O10	2.43	129.39	123.70	9	10
3	A	59	PCW	C7-N-C5	2.43	119.56	109.91	1	10
4	A	79	17F	O9-C17-O10	2.43	129.38	123.70	2	10
3	A	46	PCW	C7-N-C5	2.42	119.55	109.91	2	10
3	A	29	PCW	C7-N-C5	2.42	119.55	109.91	4	10
3	A	45	PCW	C7-N-C5	2.42	119.54	109.91	7	10
3	A	13	PCW	C7-N-C5	2.42	119.52	109.91	2	10
3	A	44	PCW	C7-N-C5	2.42	119.52	109.91	9	10
3	A	18	PCW	C7-N-C5	2.42	119.51	109.91	8	10
3	A	28	PCW	C7-N-C5	2.42	119.51	109.91	2	10
3	A	3	PCW	C7-N-C5	2.41	119.50	109.91	10	10
3	A	67	PCW	C7-N-C5	2.41	119.50	109.91	3	10
3	A	62	PCW	C7-N-C5	2.41	119.50	109.91	7	10
3	A	51	PCW	C7-N-C5	2.41	119.48	109.91	7	10
4	A	35	17F	O9-C17-O10	2.41	129.33	123.70	9	10
4	A	78	17F	O9-C17-O10	2.40	129.32	123.70	7	10
3	A	4	PCW	C7-N-C5	2.40	119.45	109.91	2	10
4	A	78	17F	C5-O9-C17	2.40	112.05	117.80	10	10
3	A	53	PCW	C7-N-C5	2.39	119.43	109.91	8	10
4	A	74	17F	O9-C17-O10	2.39	129.29	123.70	3	10
3	A	60	PCW	C7-N-C5	2.39	119.40	109.91	5	10
3	A	5	PCW	C7-N-C5	2.38	119.38	109.91	7	10
4	A	38	17F	C5-O9-C17	2.38	112.09	117.80	10	10
4	A	38	17F	O9-C17-O10	2.38	129.26	123.70	1	10
4	A	79	17F	C5-O9-C17	2.38	112.11	117.80	5	10
3	A	41	PCW	C7-N-C5	2.37	119.35	109.91	4	10
4	A	76	17F	O9-C17-O10	2.36	129.23	123.70	2	10
4	A	37	17F	O9-C17-O10	2.35	129.19	123.70	2	10
4	A	75	17F	O9-C17-O10	2.32	129.13	123.70	9	10
4	A	40	17F	O9-C17-O10	2.32	129.12	123.70	5	10
4	A	77	17F	O9-C17-O10	2.30	129.09	123.70	2	10
4	A	34	17F	O9-C17-O10	2.29	129.06	123.70	2	10
4	A	33	17F	O9-C17-O10	2.29	129.05	123.70	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	39	17F	O9-C17-O10	2.27	129.02	123.70	7	10
4	A	36	17F	O9-C17-O10	2.27	129.01	123.70	3	10
5	B	201	GNP	O2A-PA-O3A	2.06	112.84	107.27	4	6
3	A	13	PCW	C7-N-C6	2.01	114.25	108.98	2	1
3	A	6	PCW	O1P-P-O3P	2.00	116.64	107.57	5	1

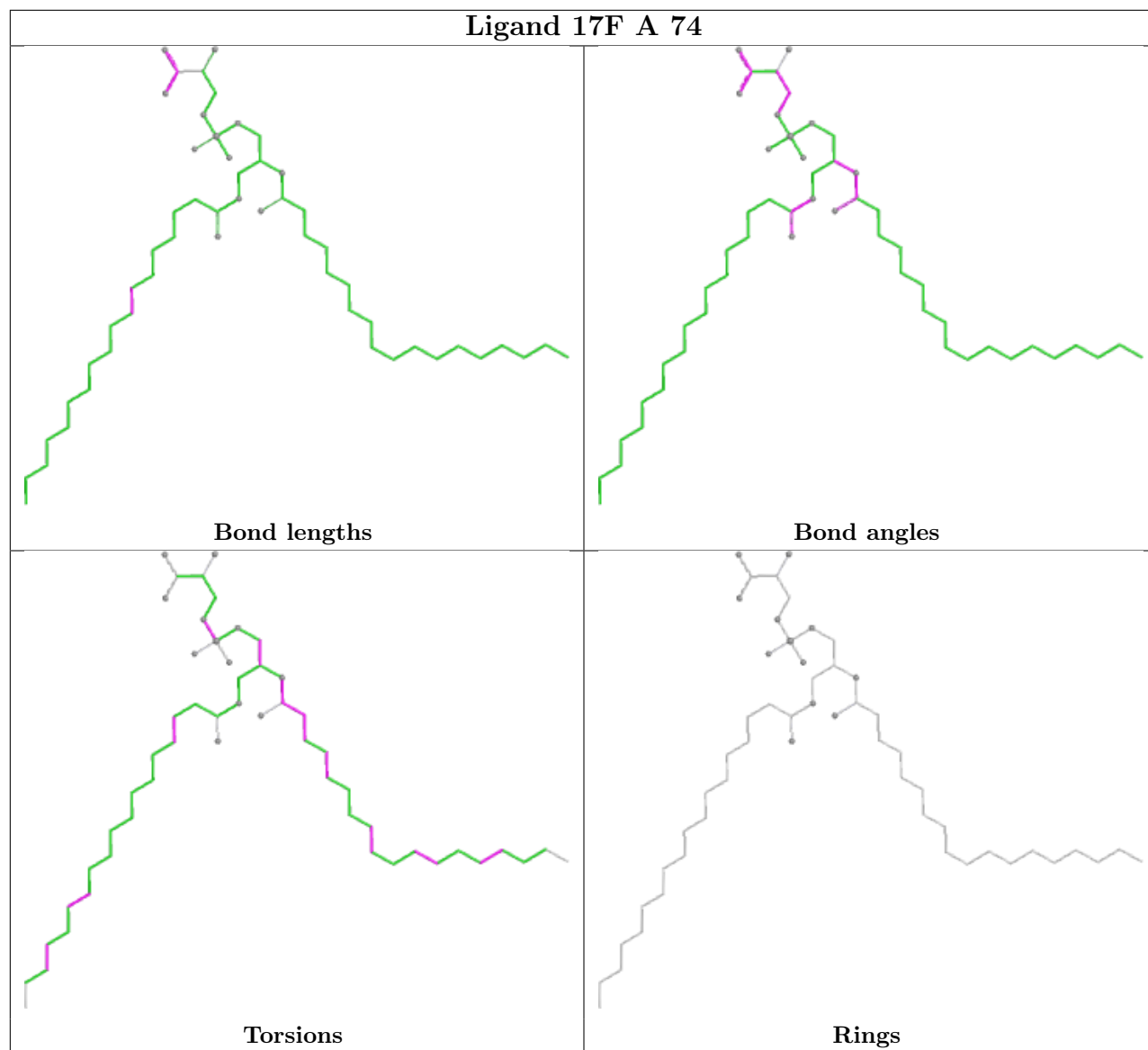
There are no chirality outliers.

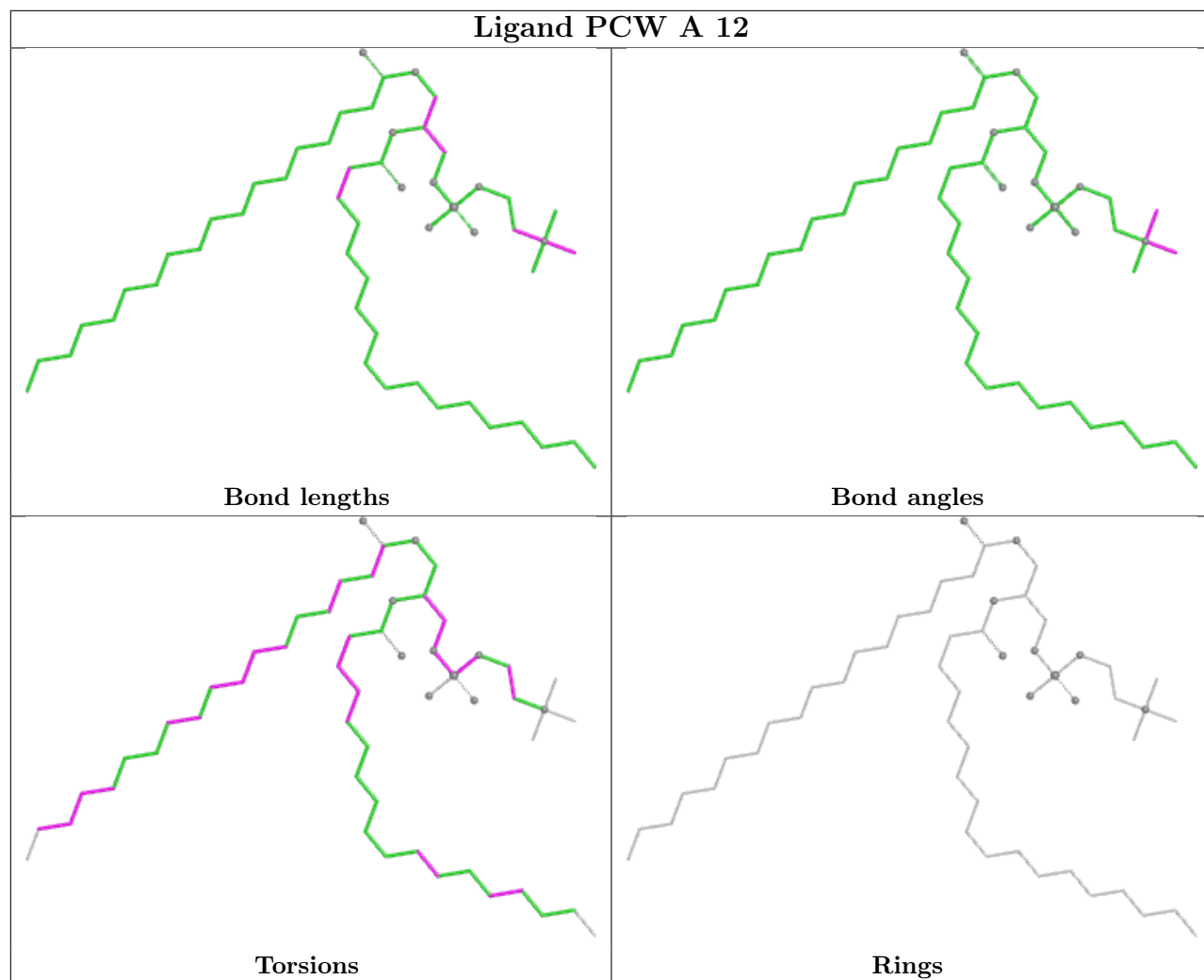
All unique torsion outliers are listed below.

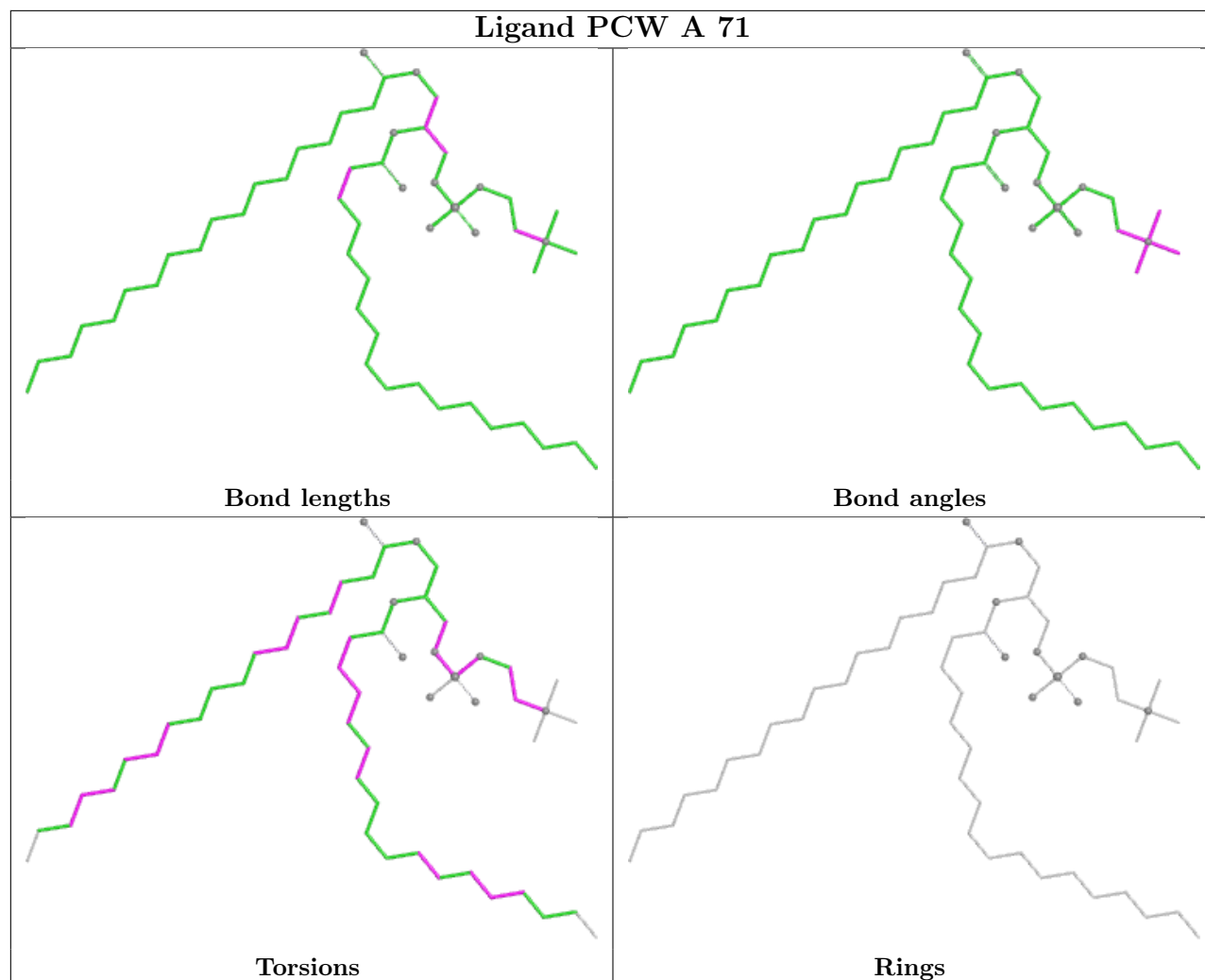
Mol	Chain	Res	Type	Atoms	Models (Total)
5	B	201	GNP	PB-N3B-PG-O1G	1

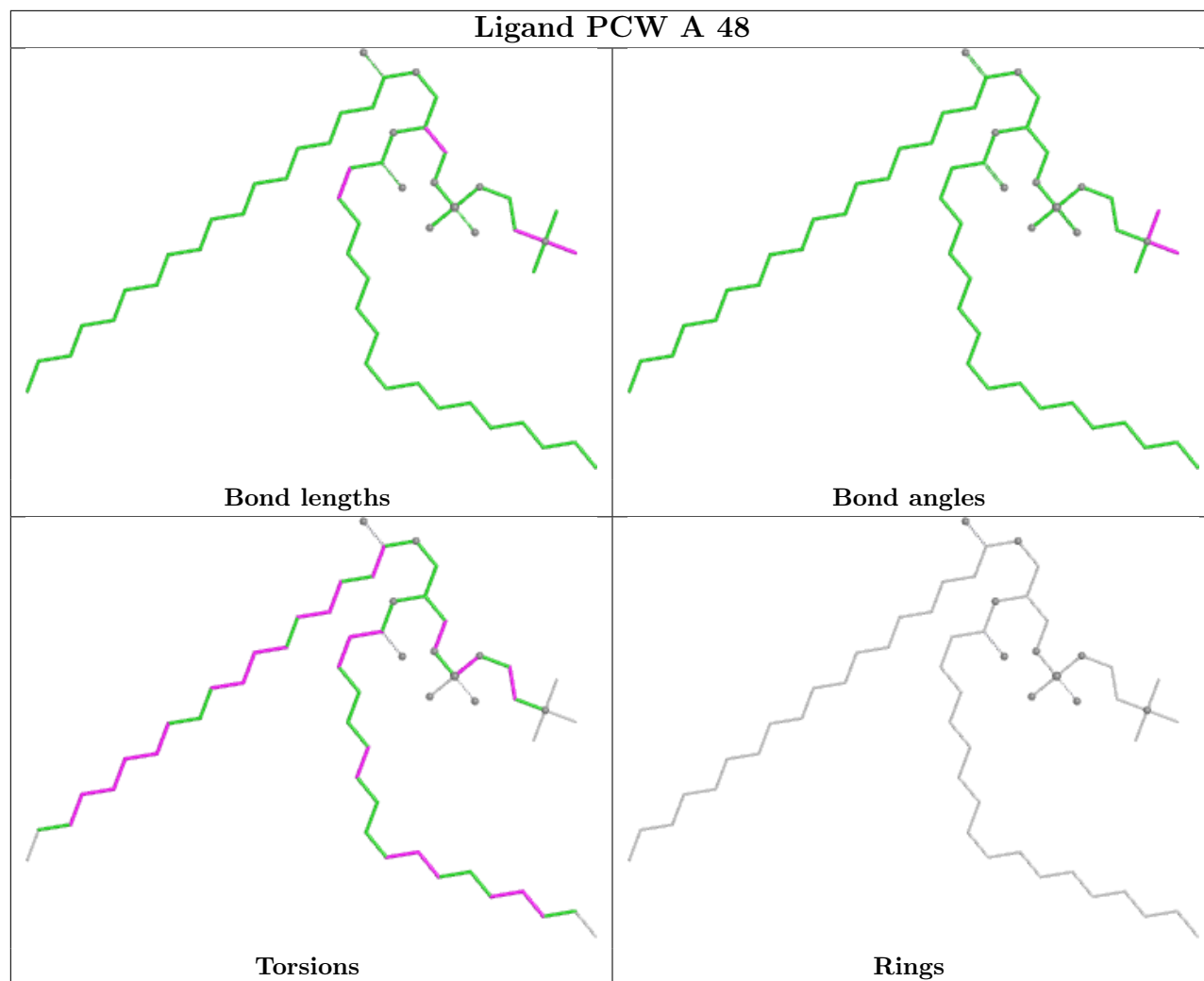
There are no ring outliers.

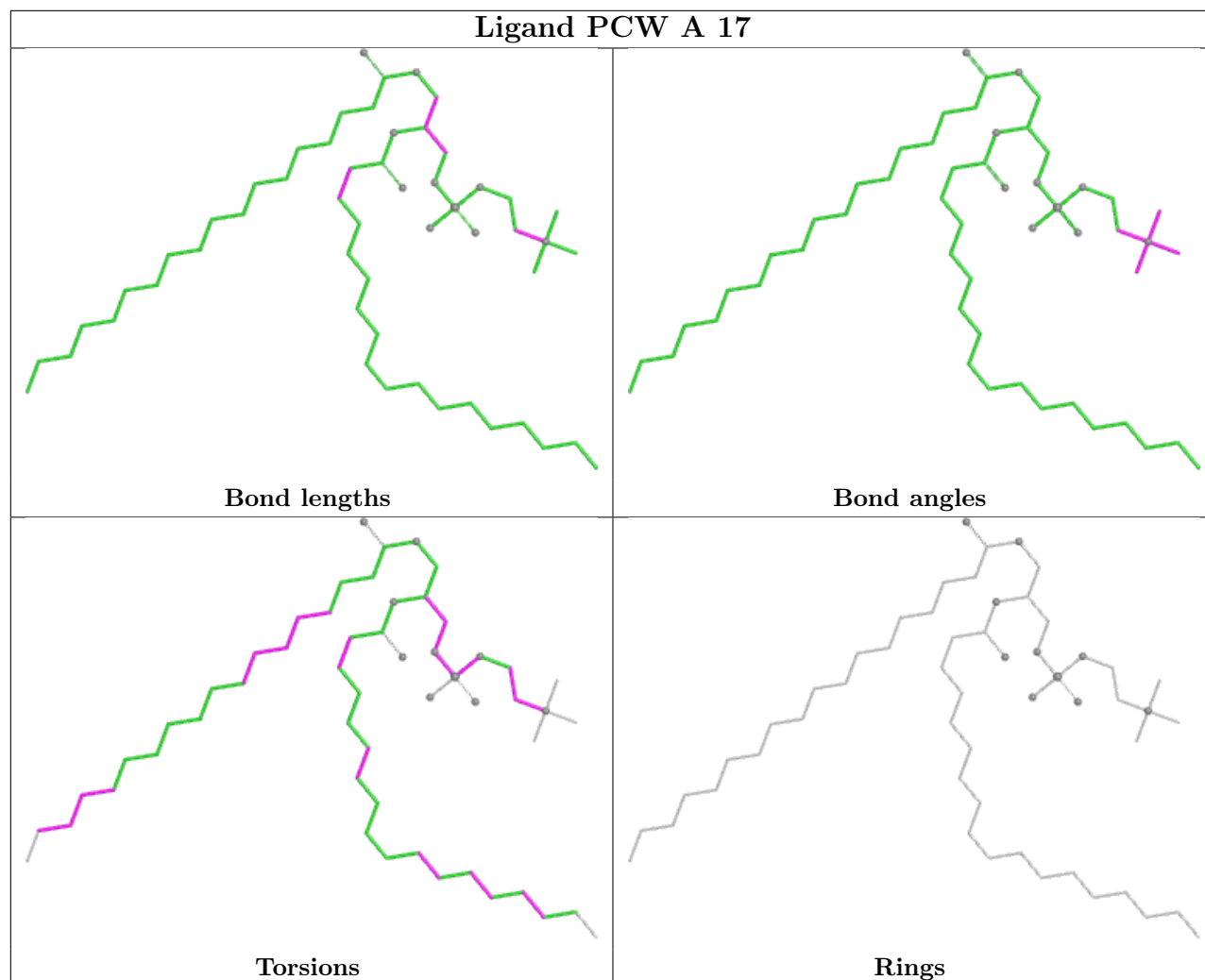
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

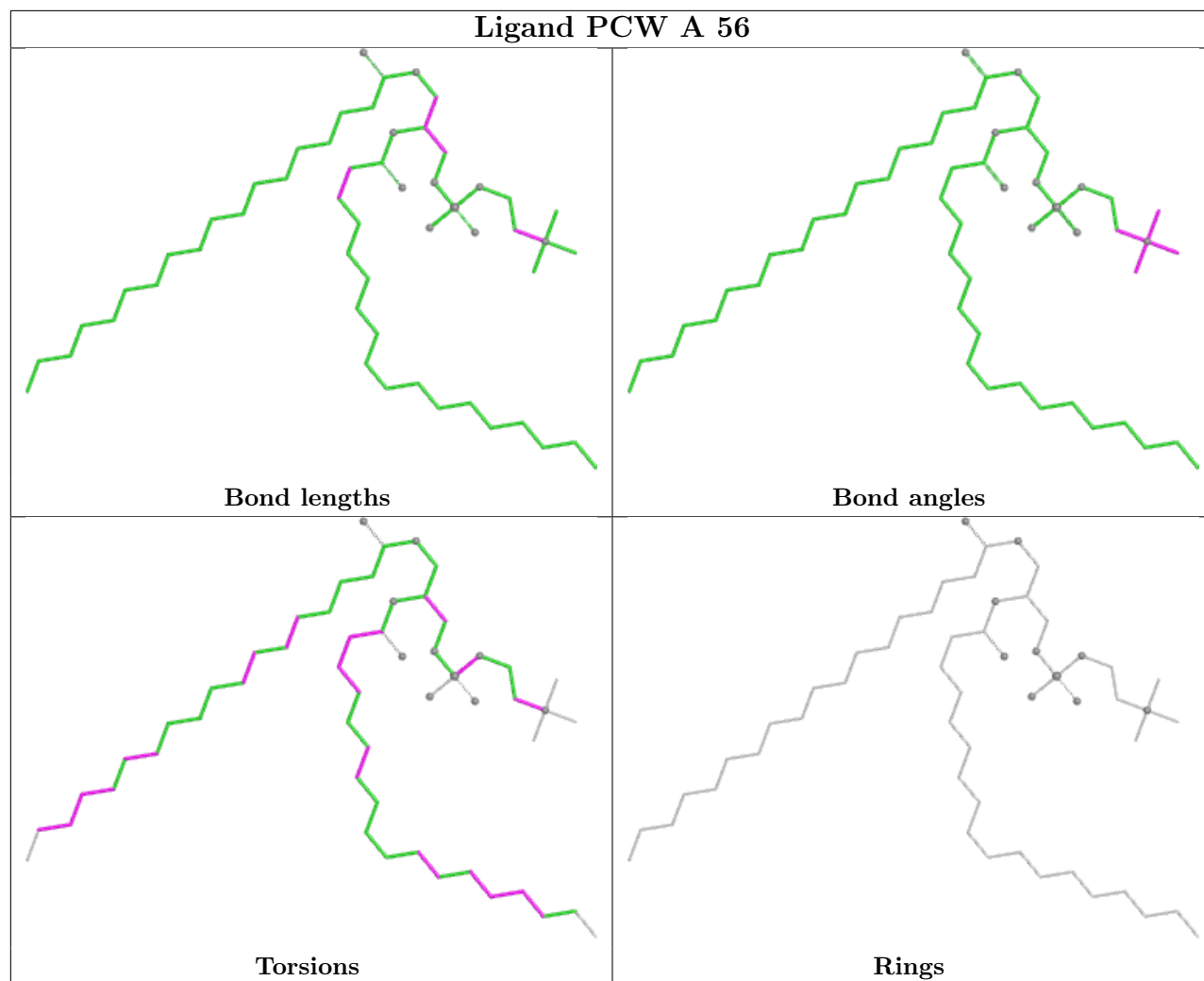


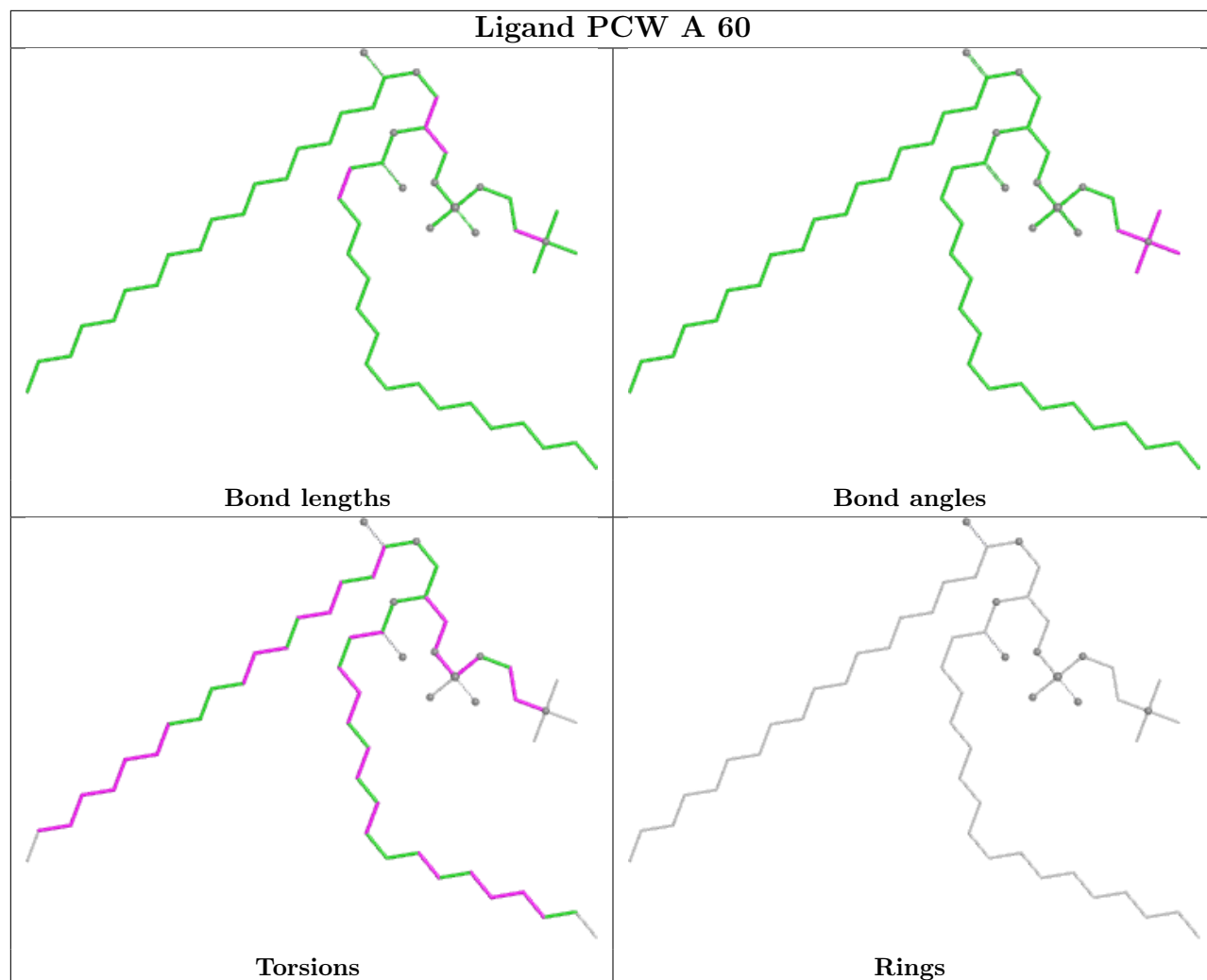


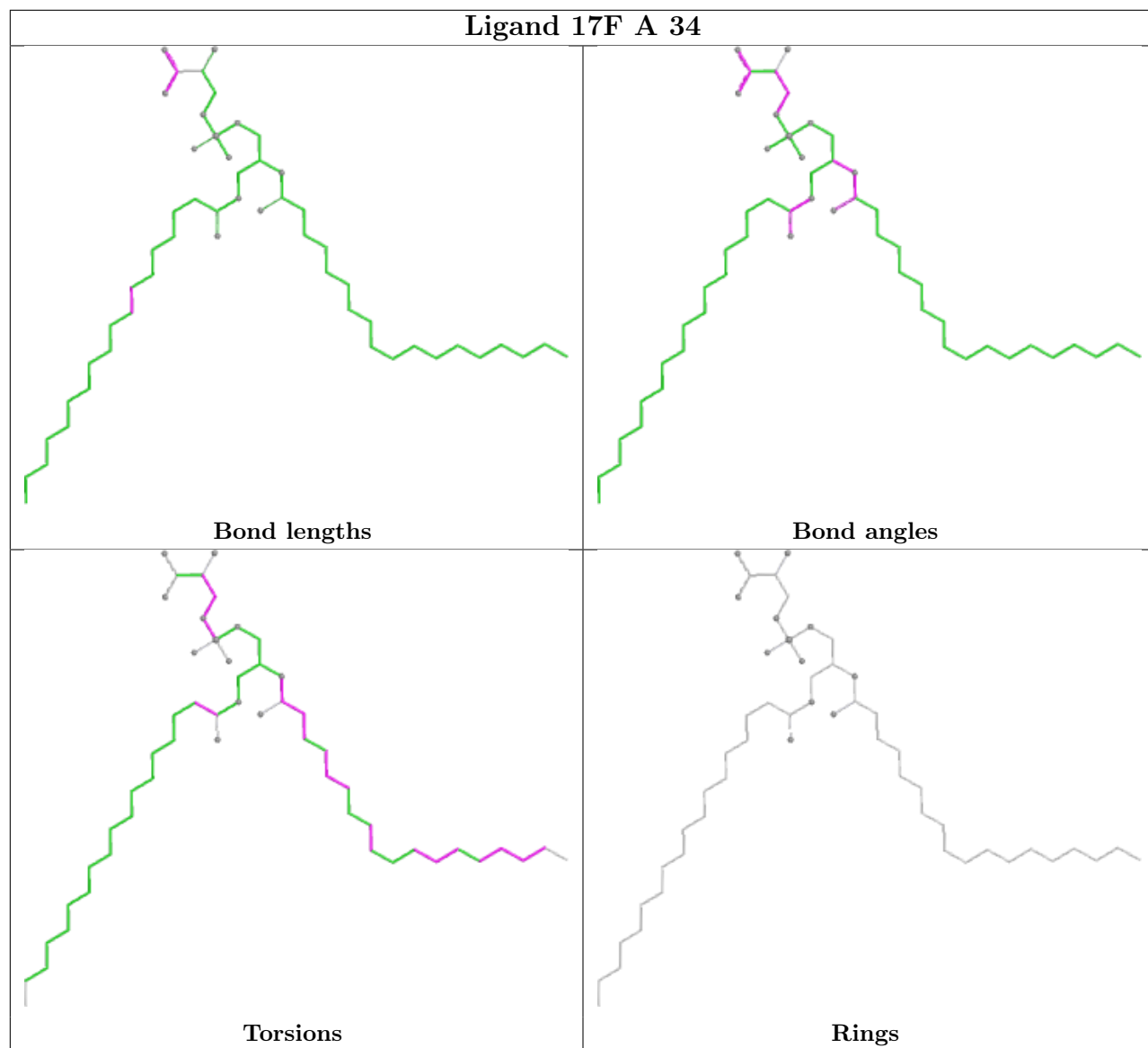


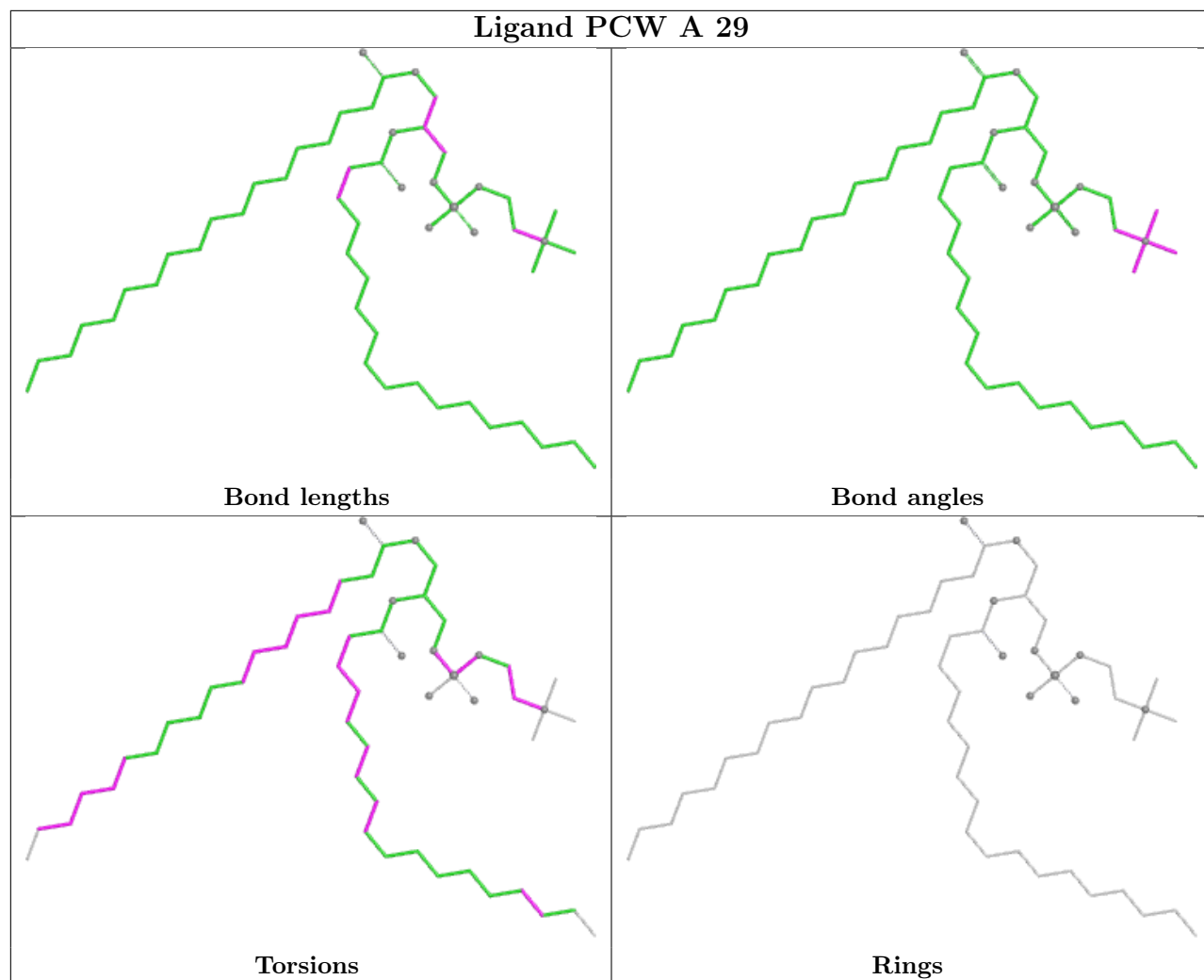


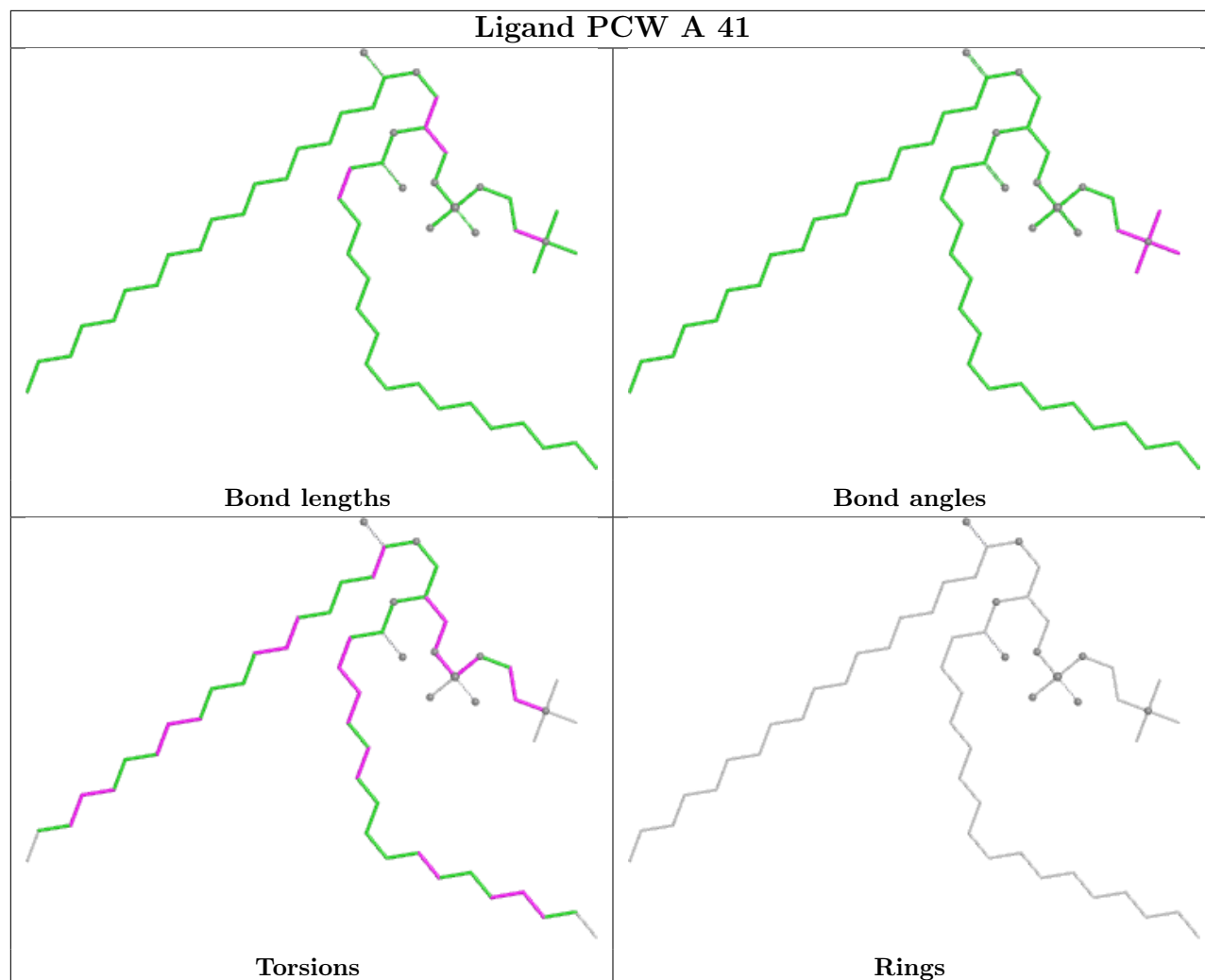


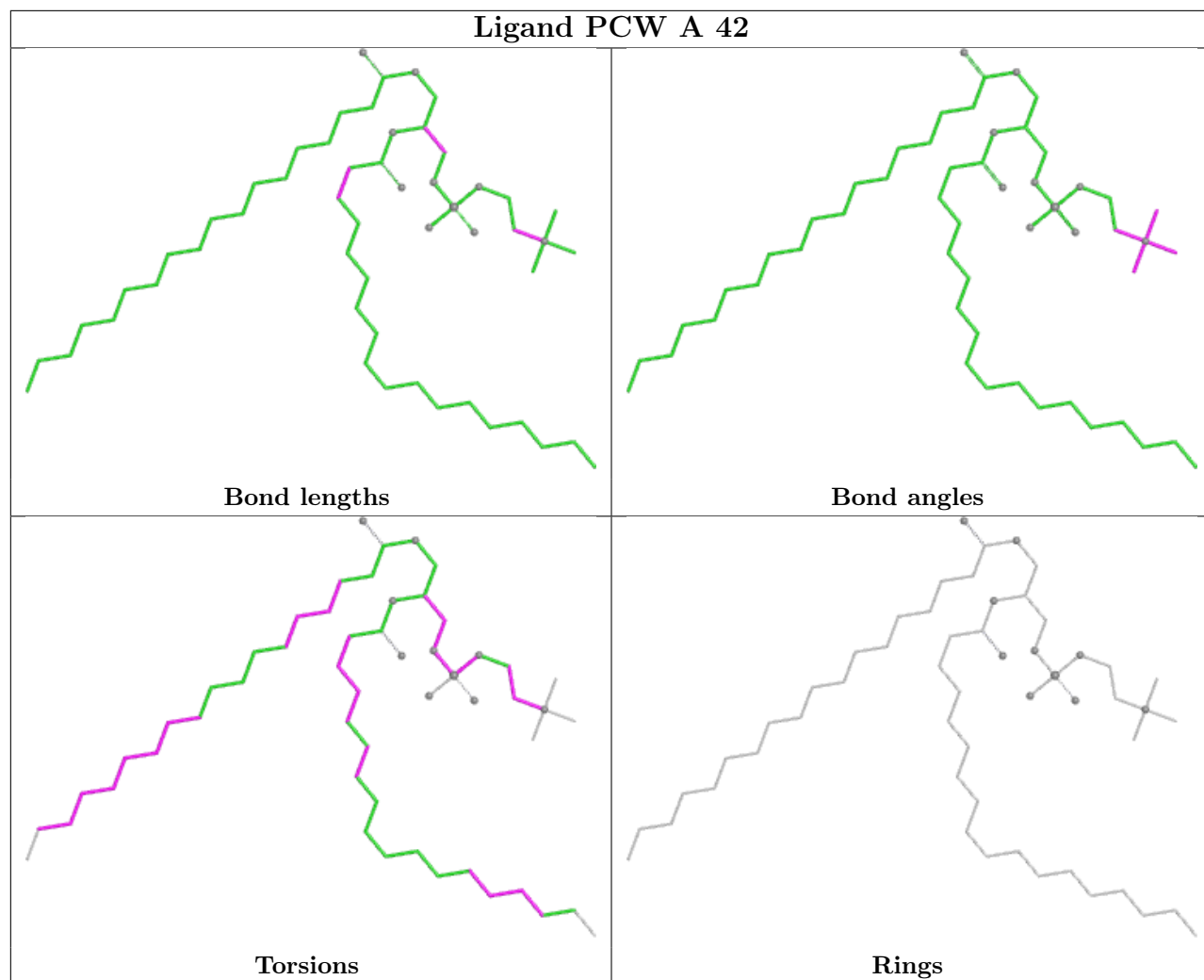


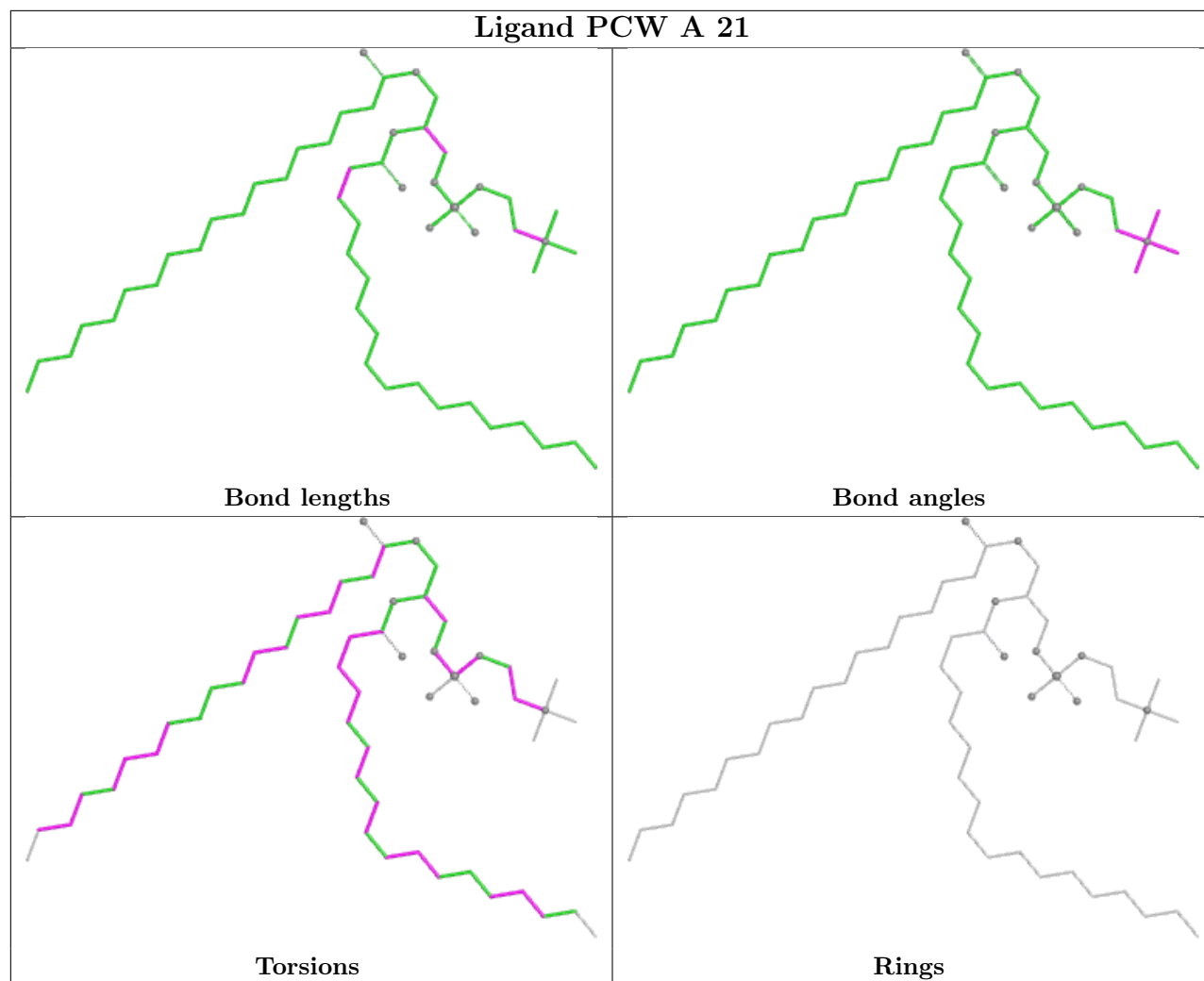


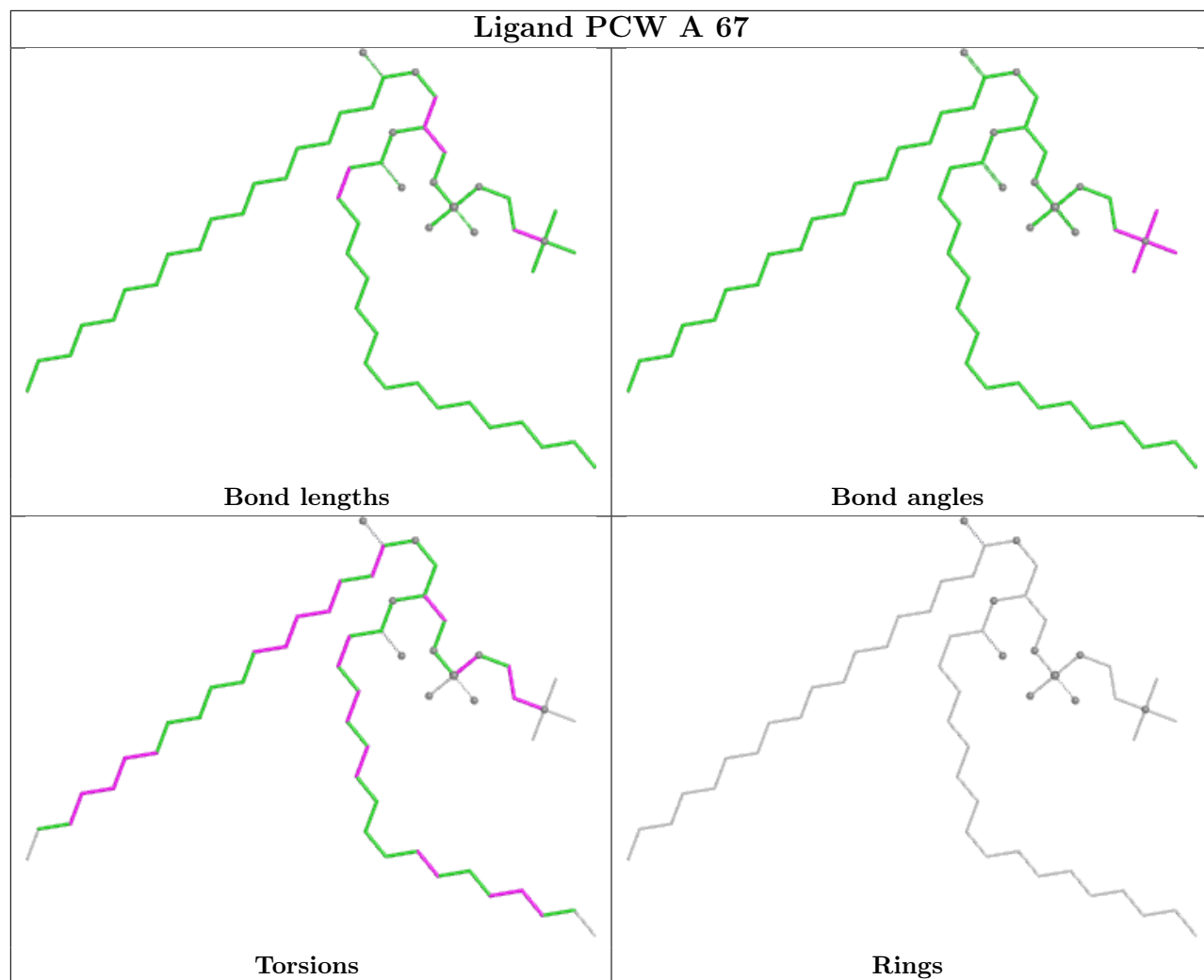


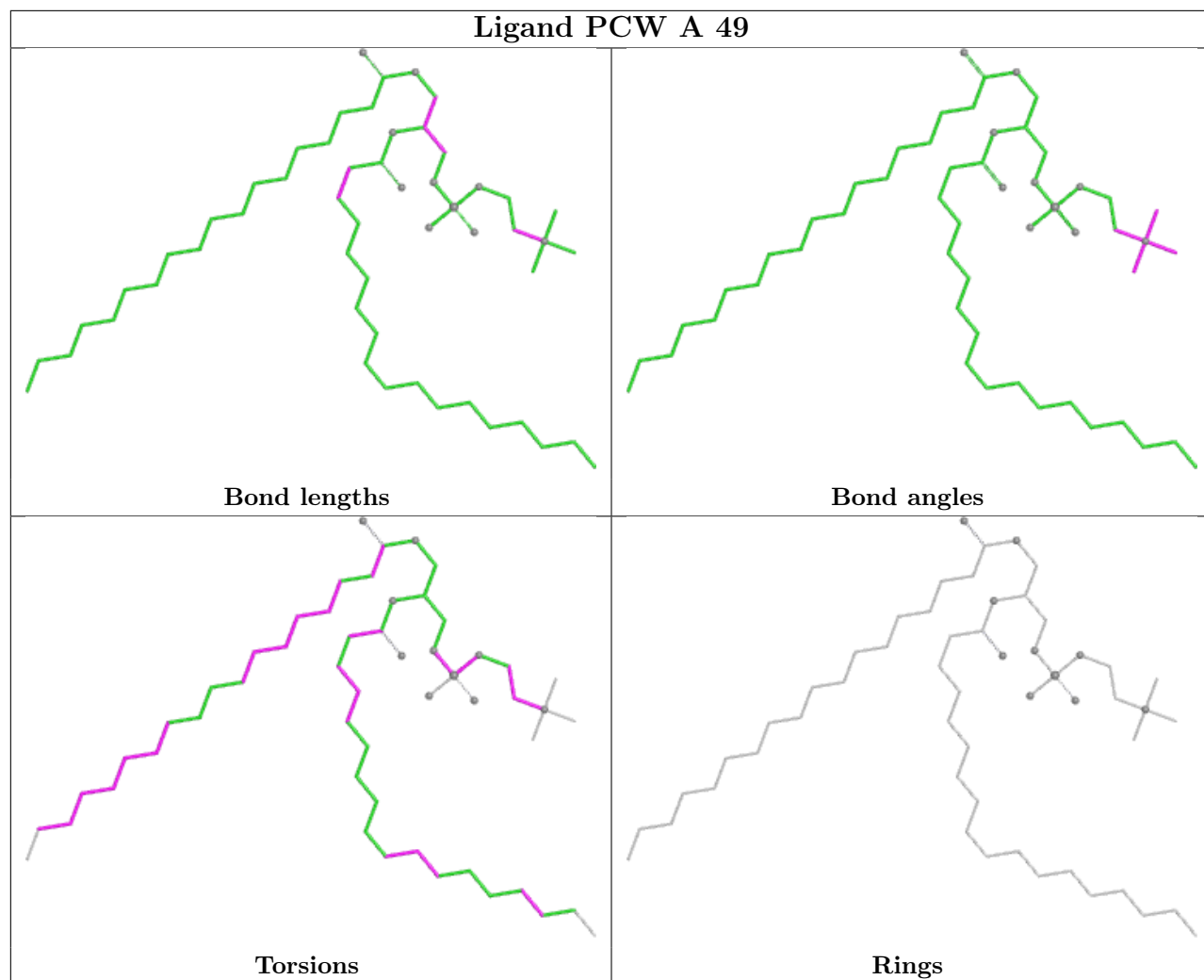


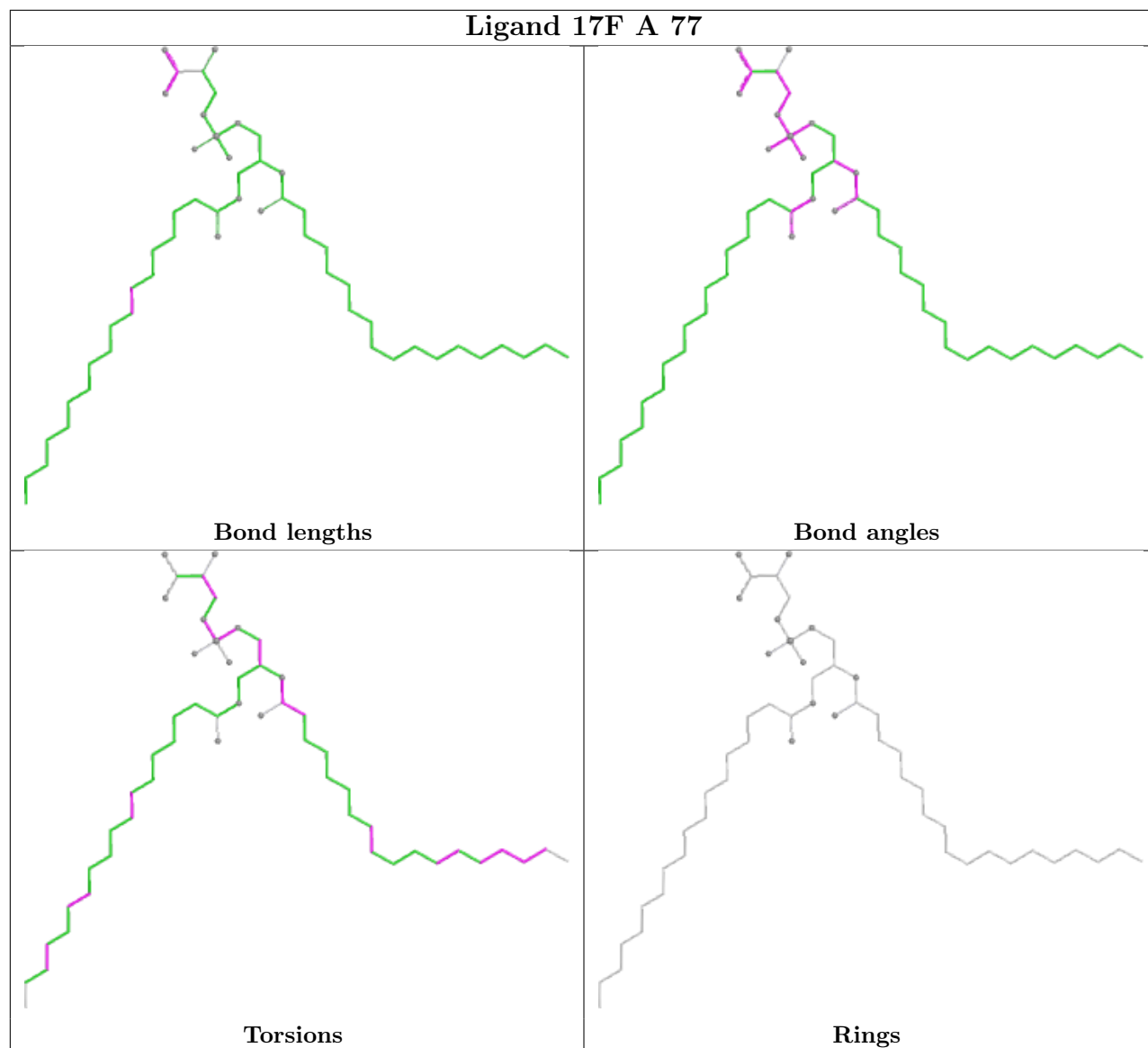


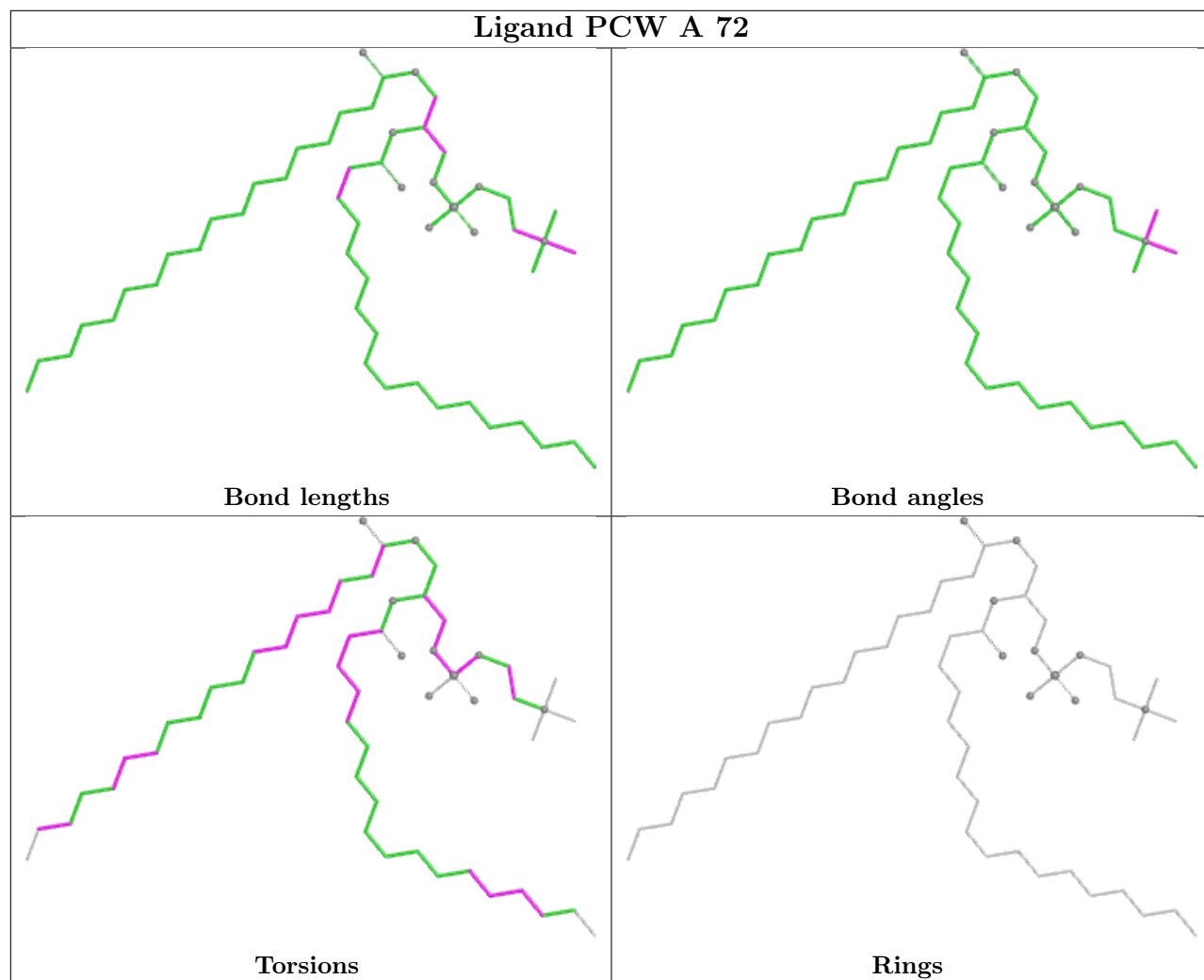


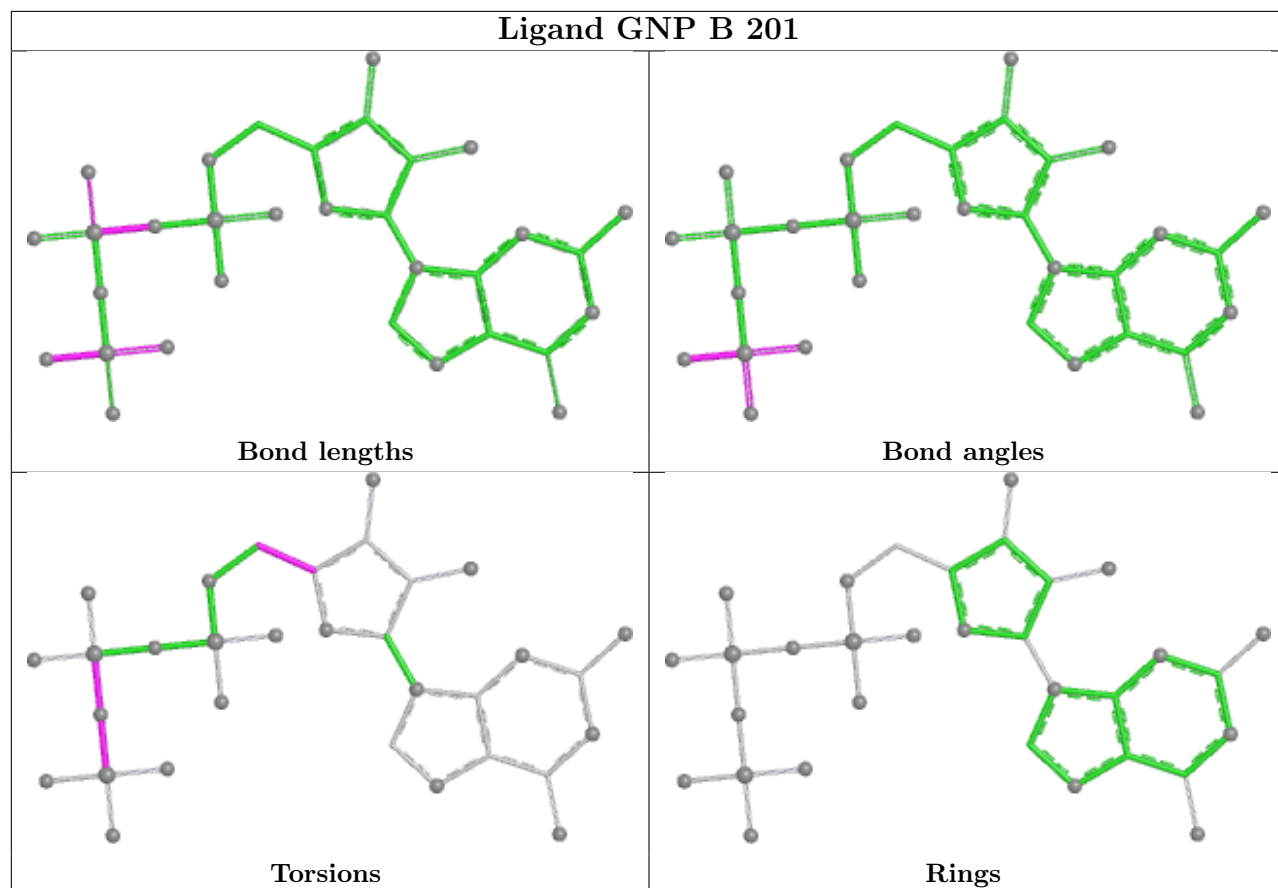


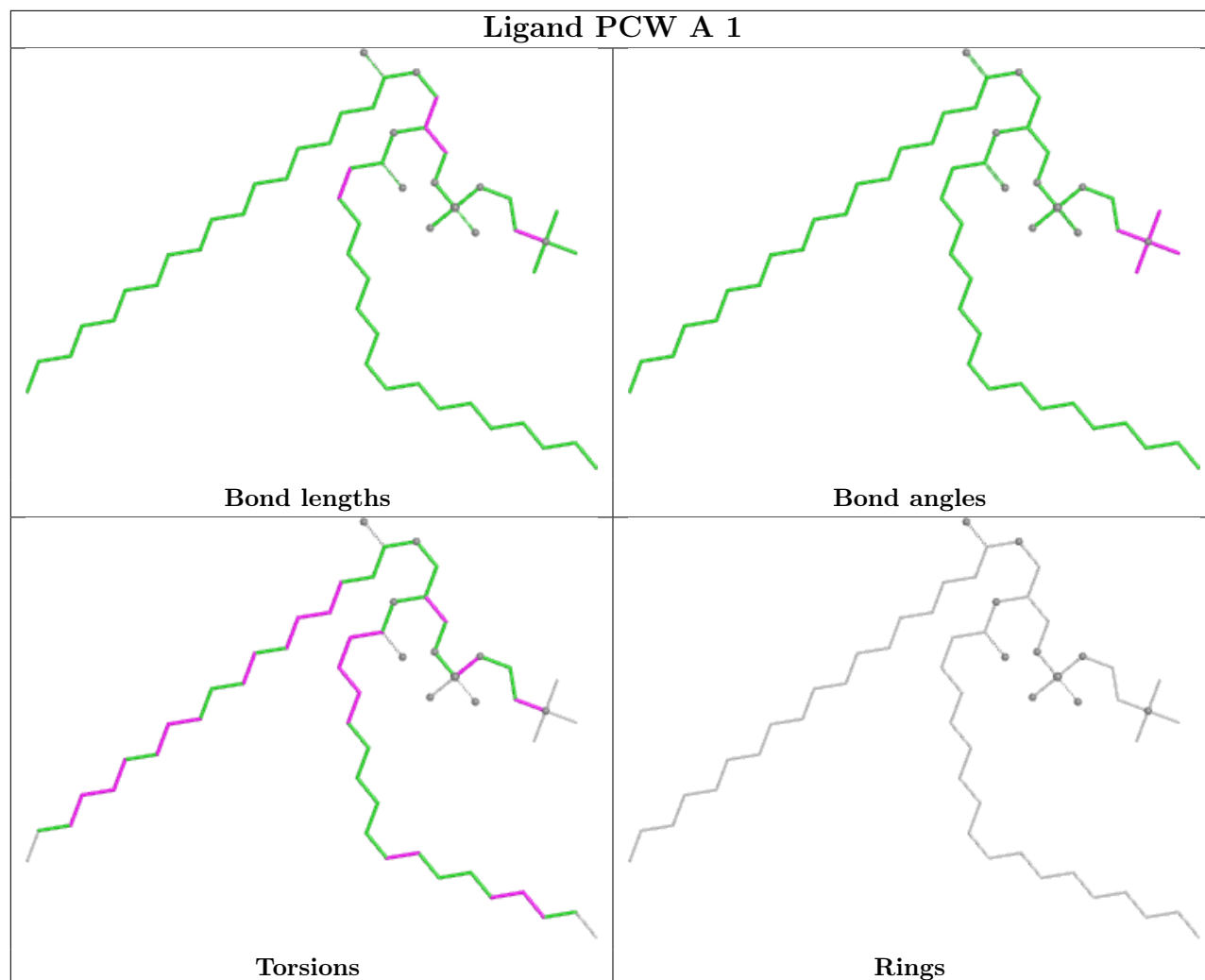


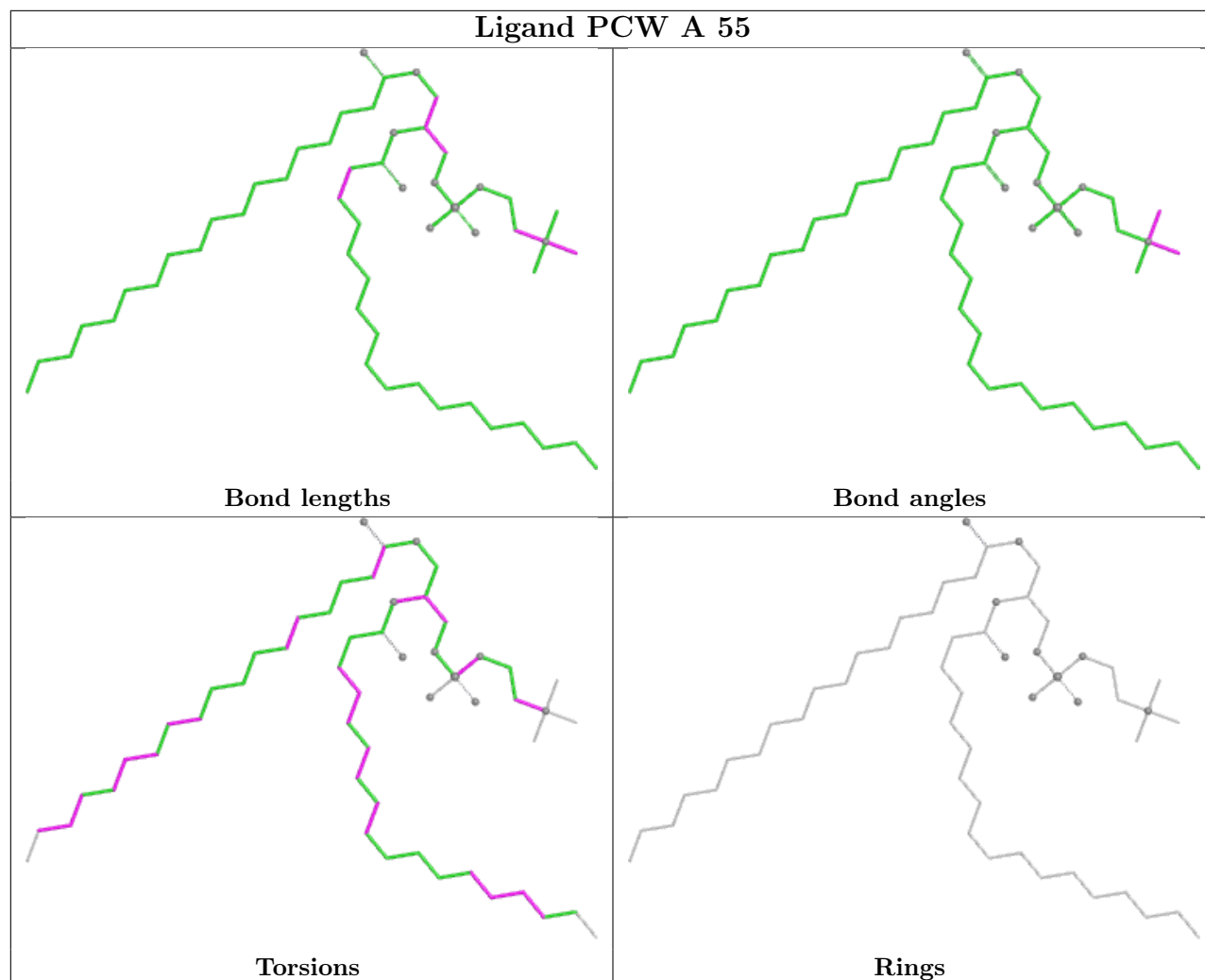


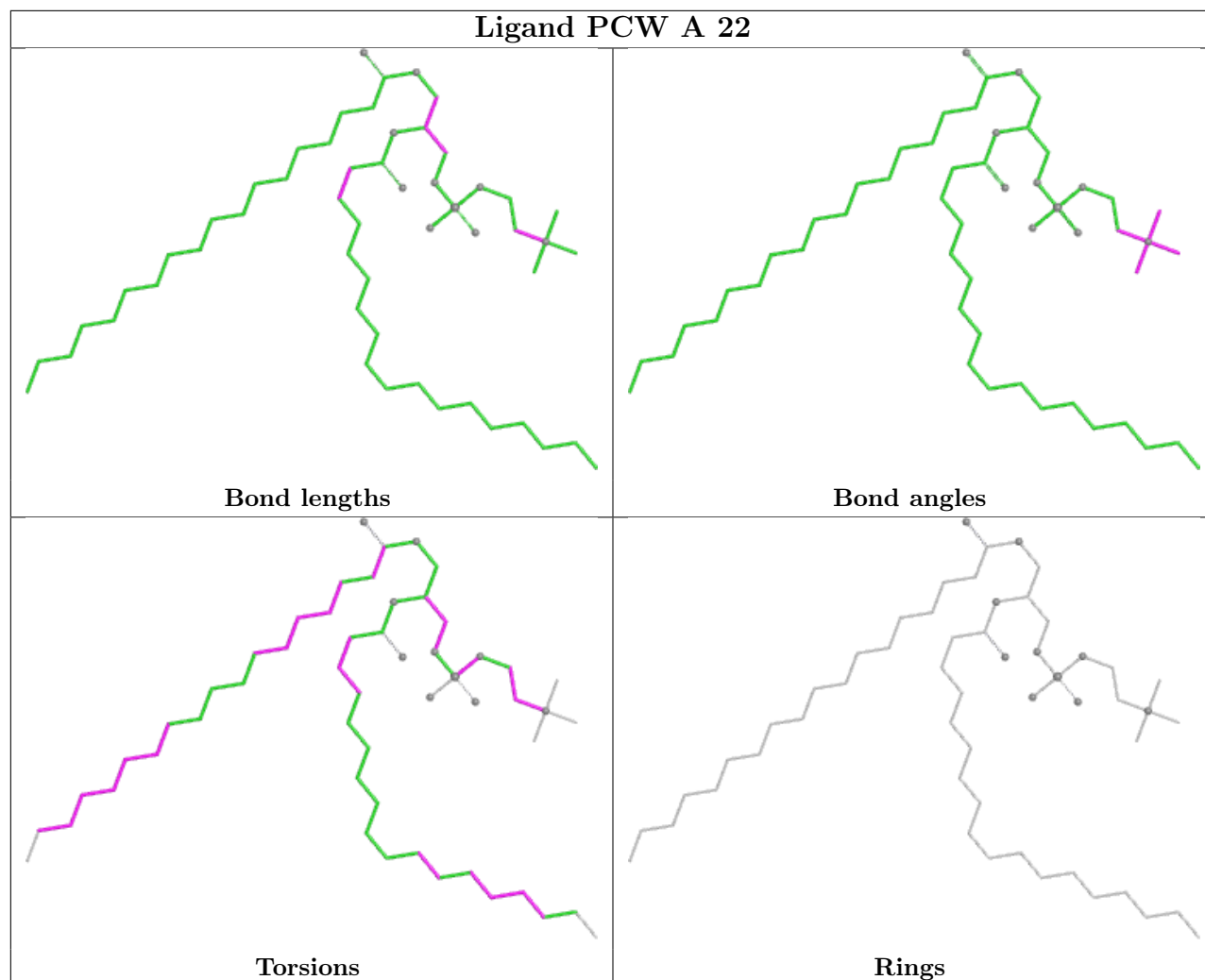


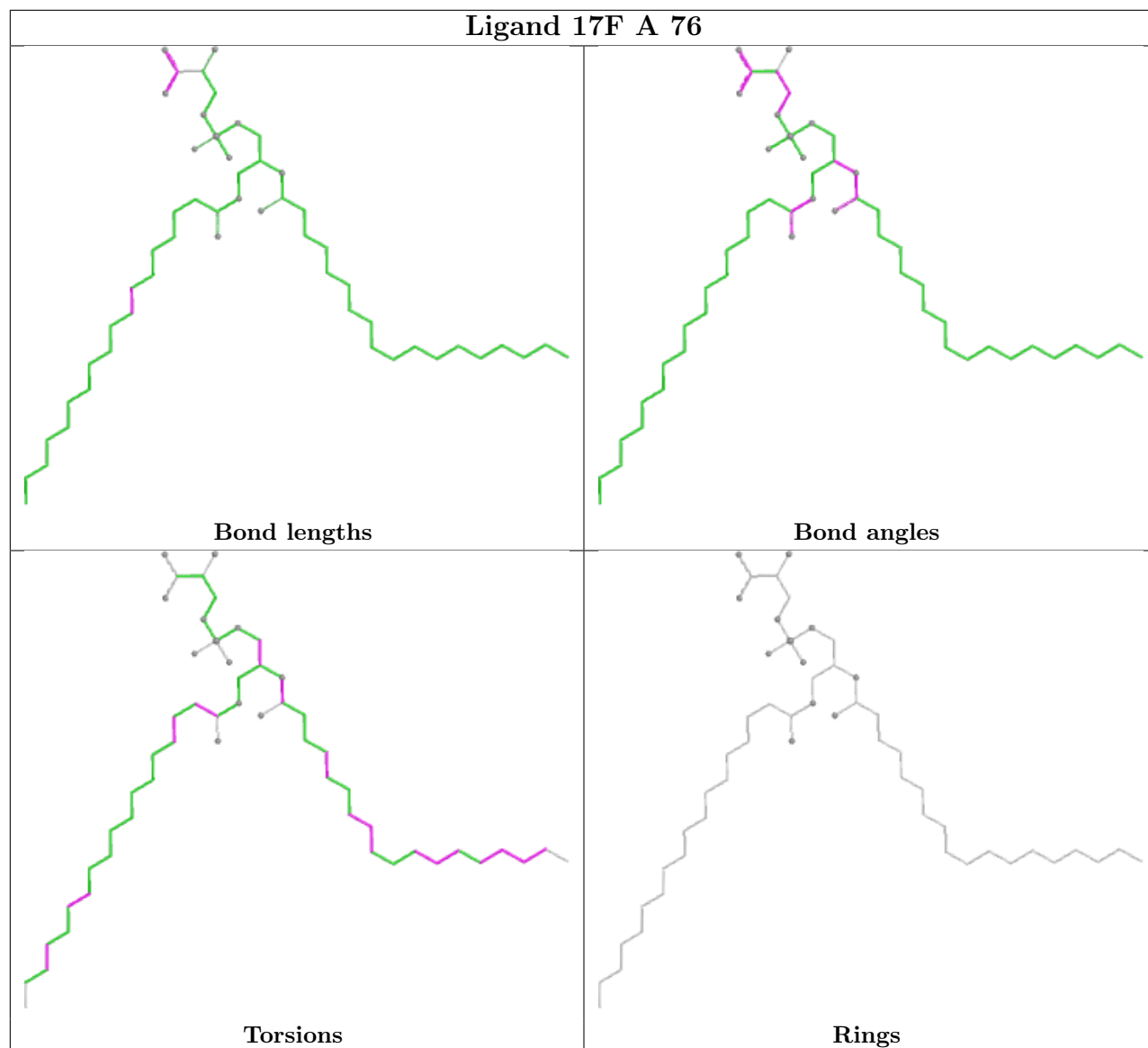


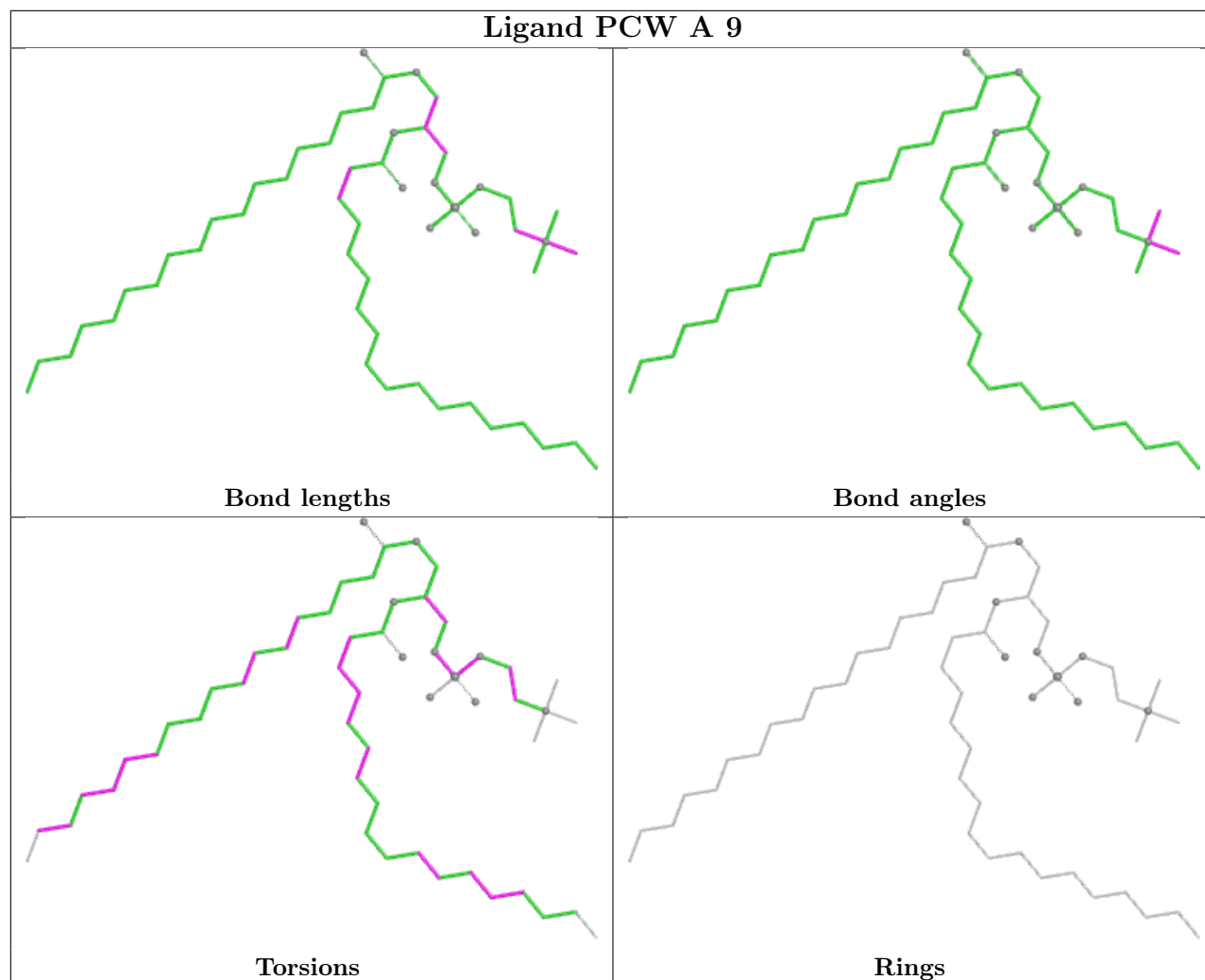


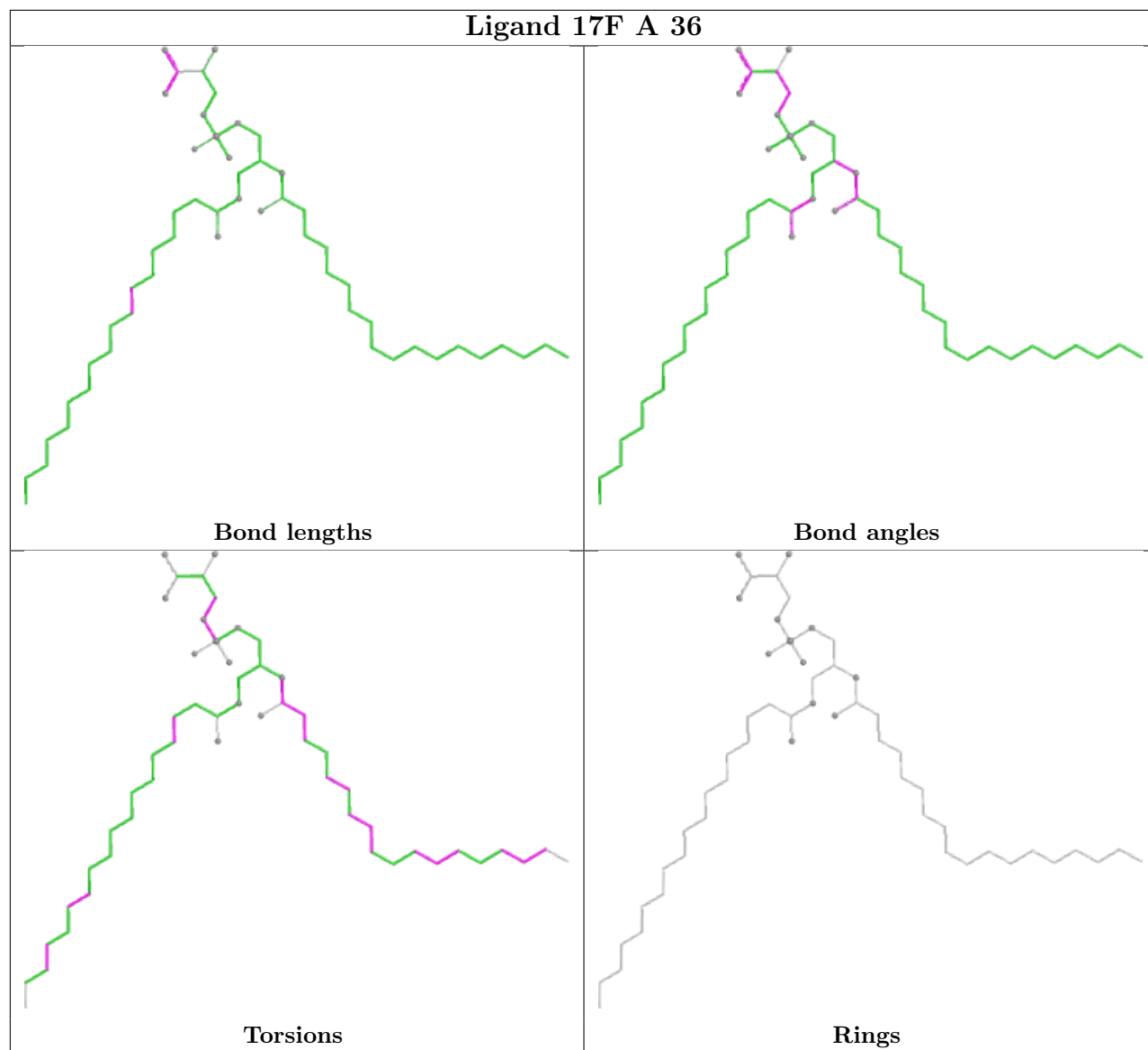


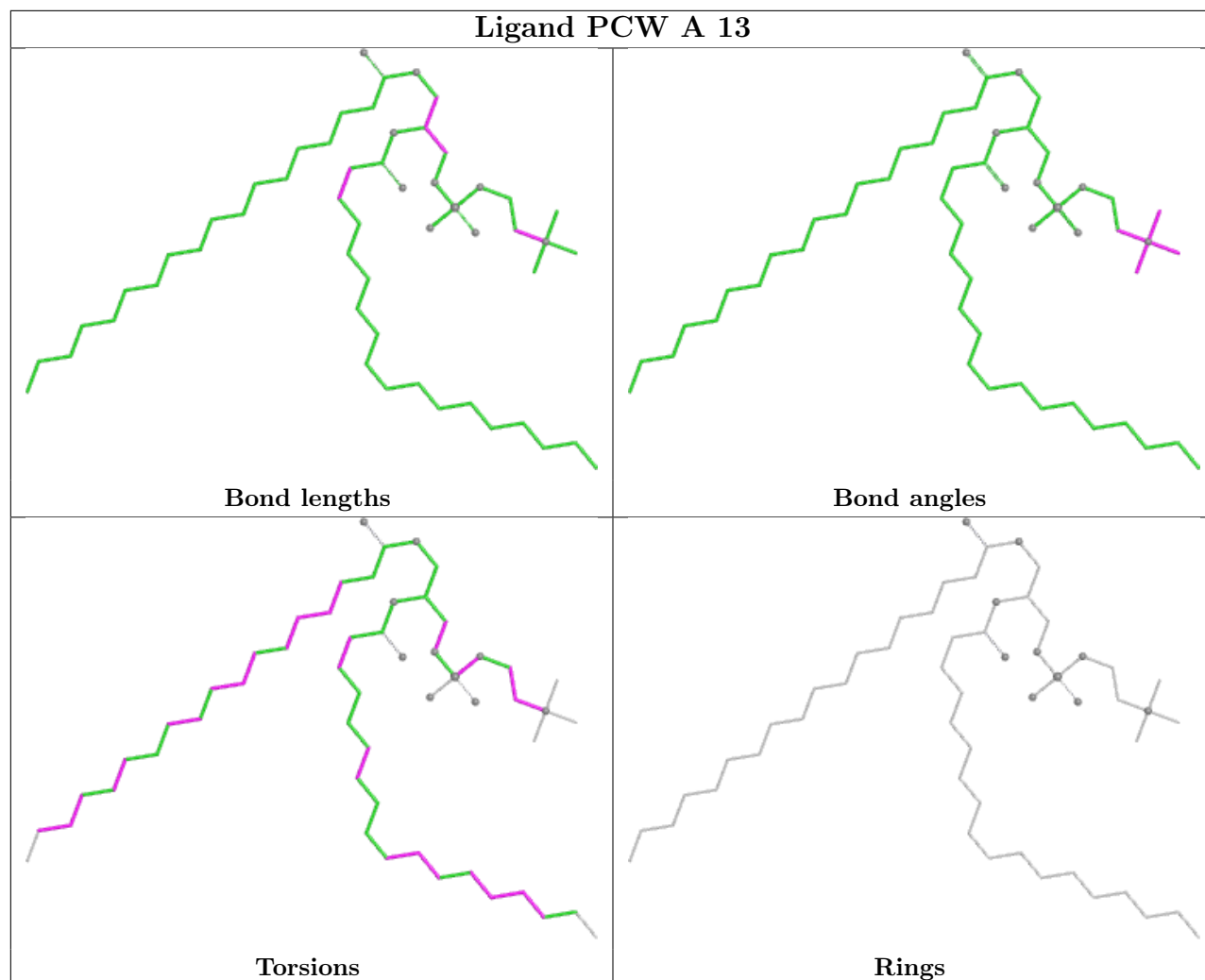


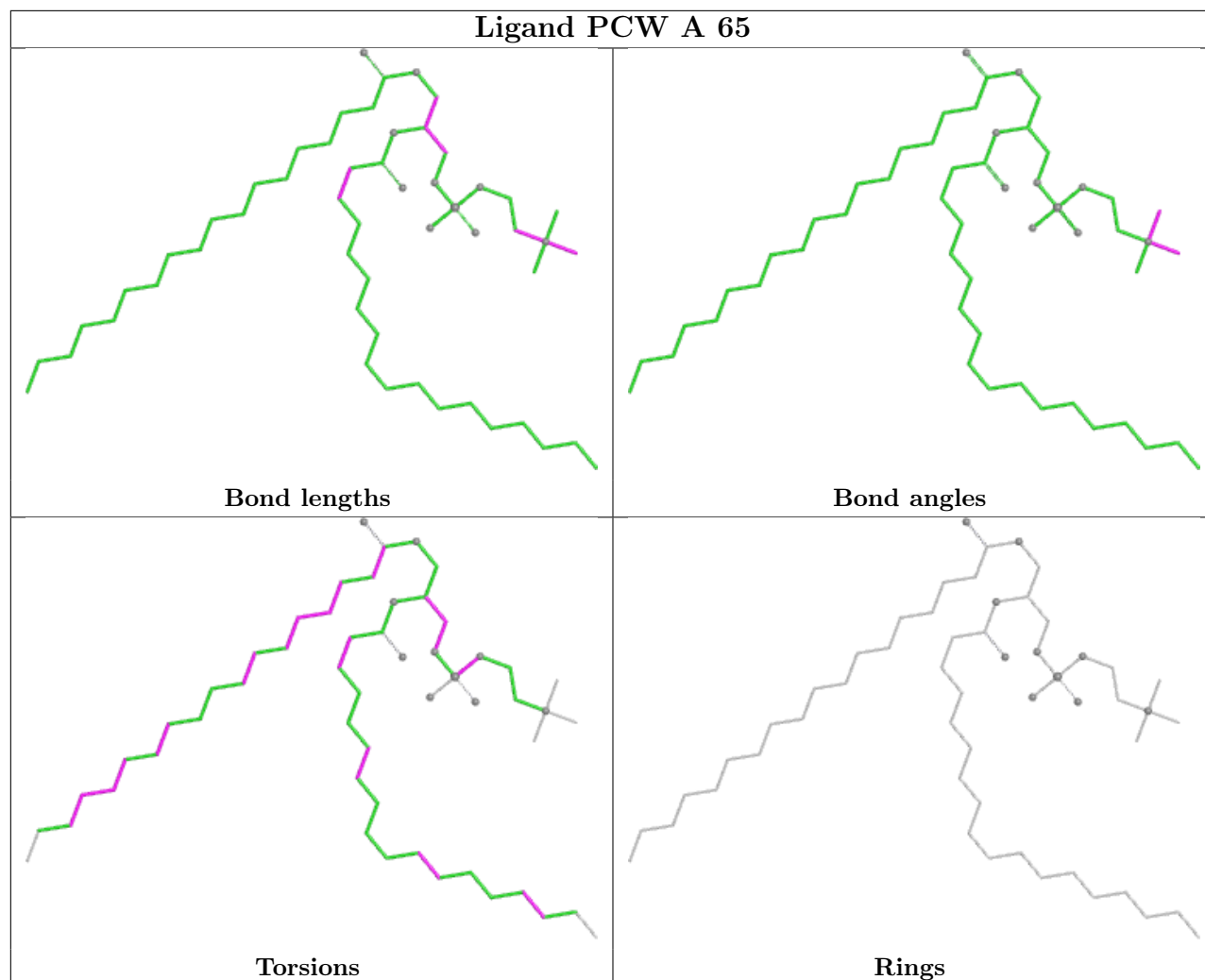


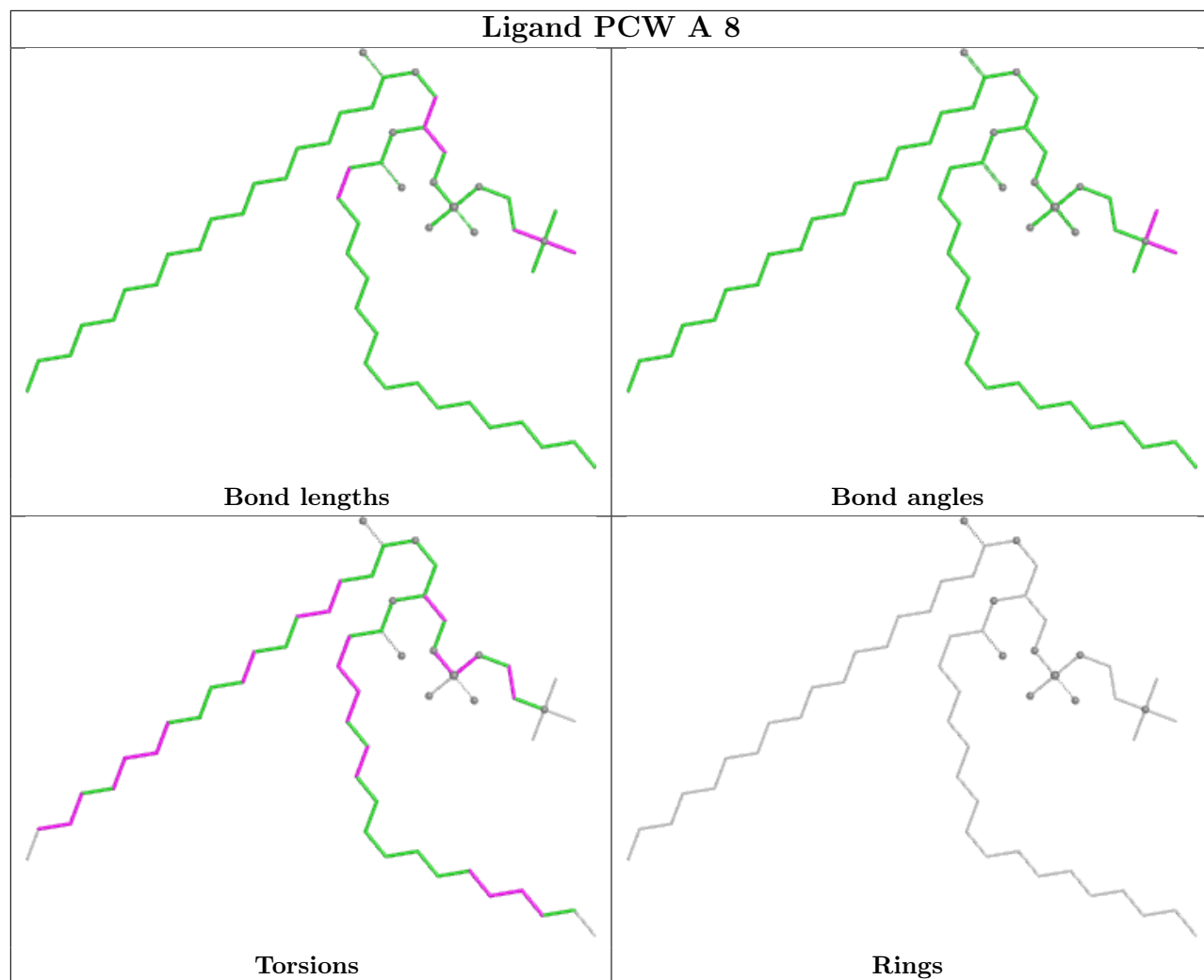


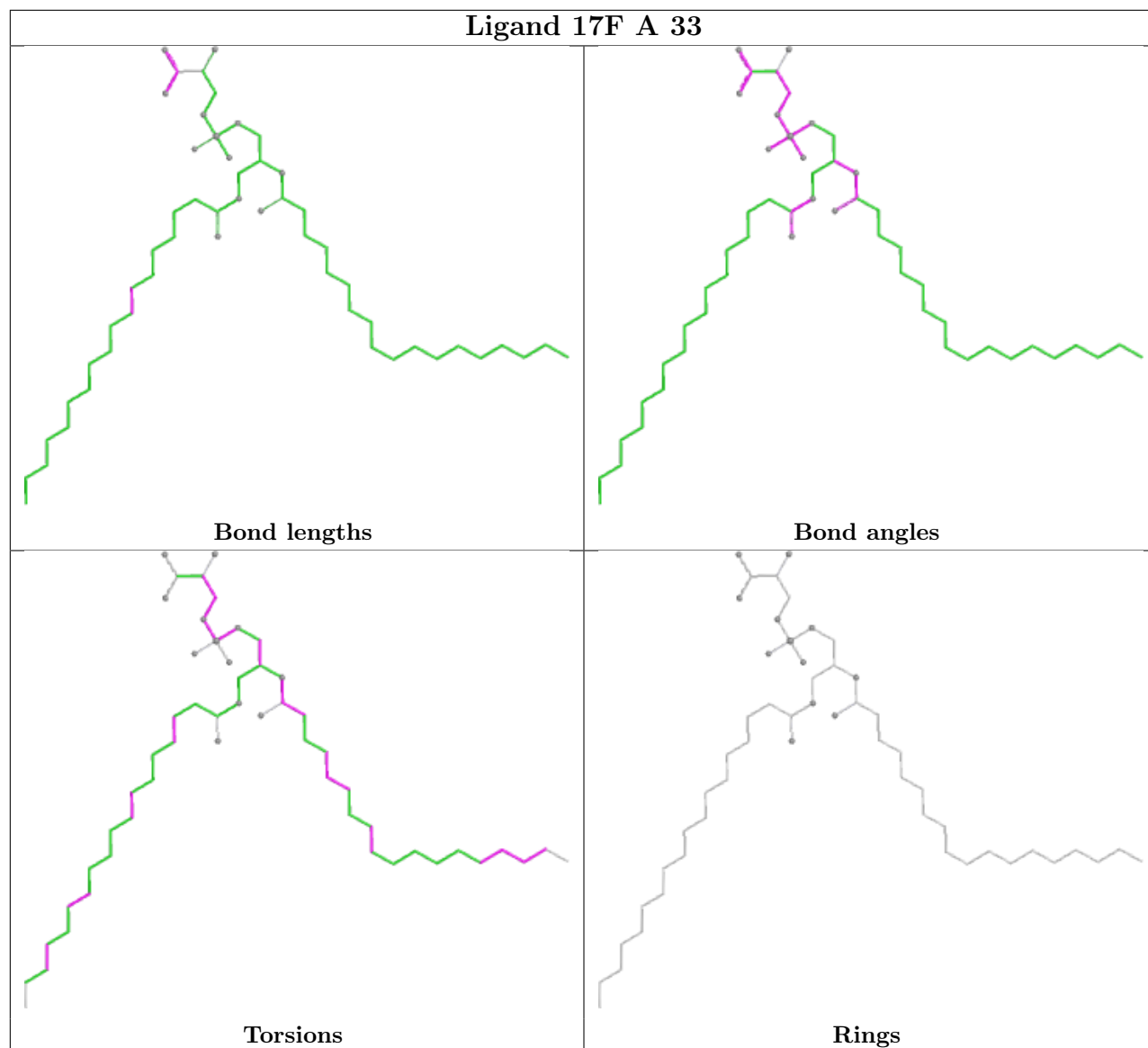


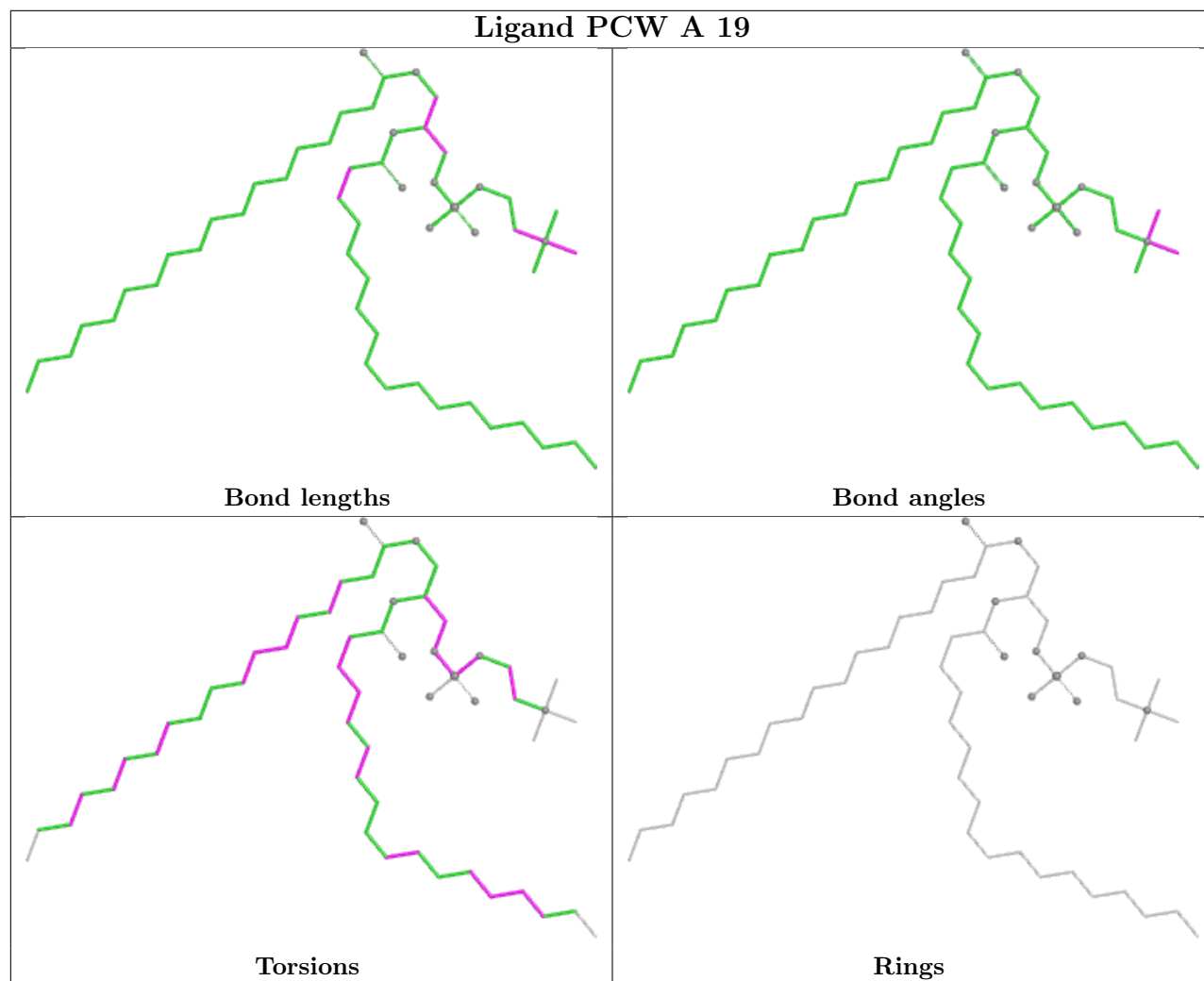


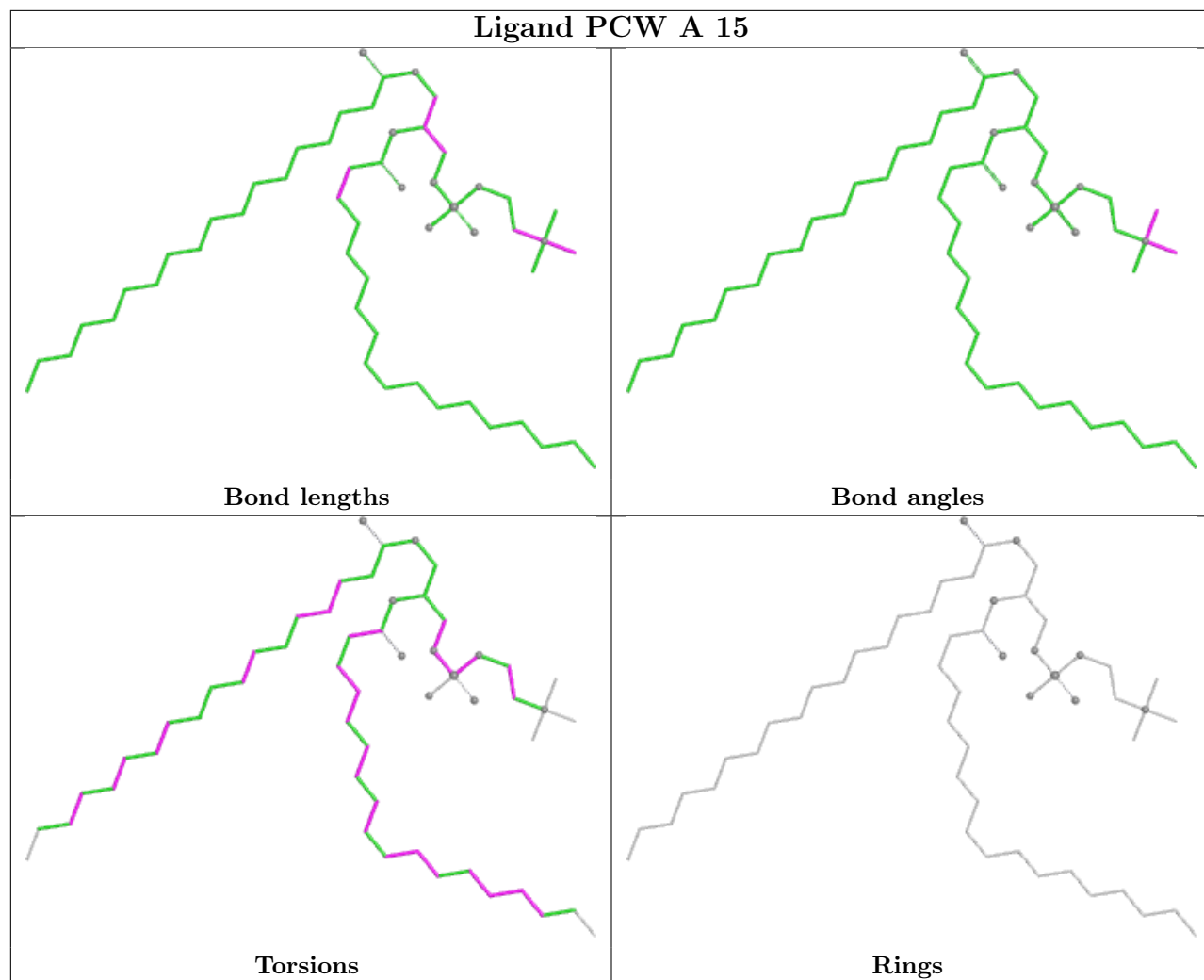


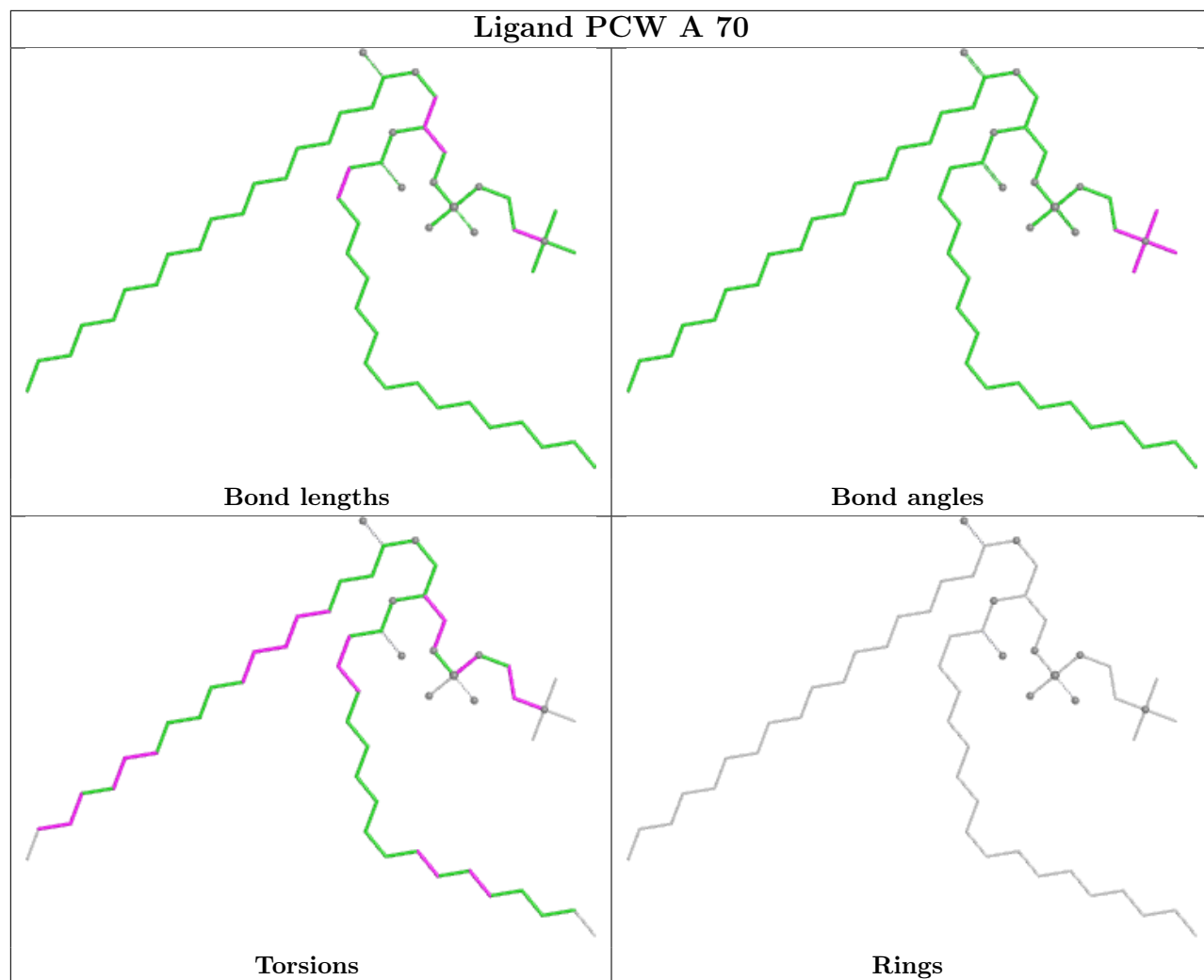


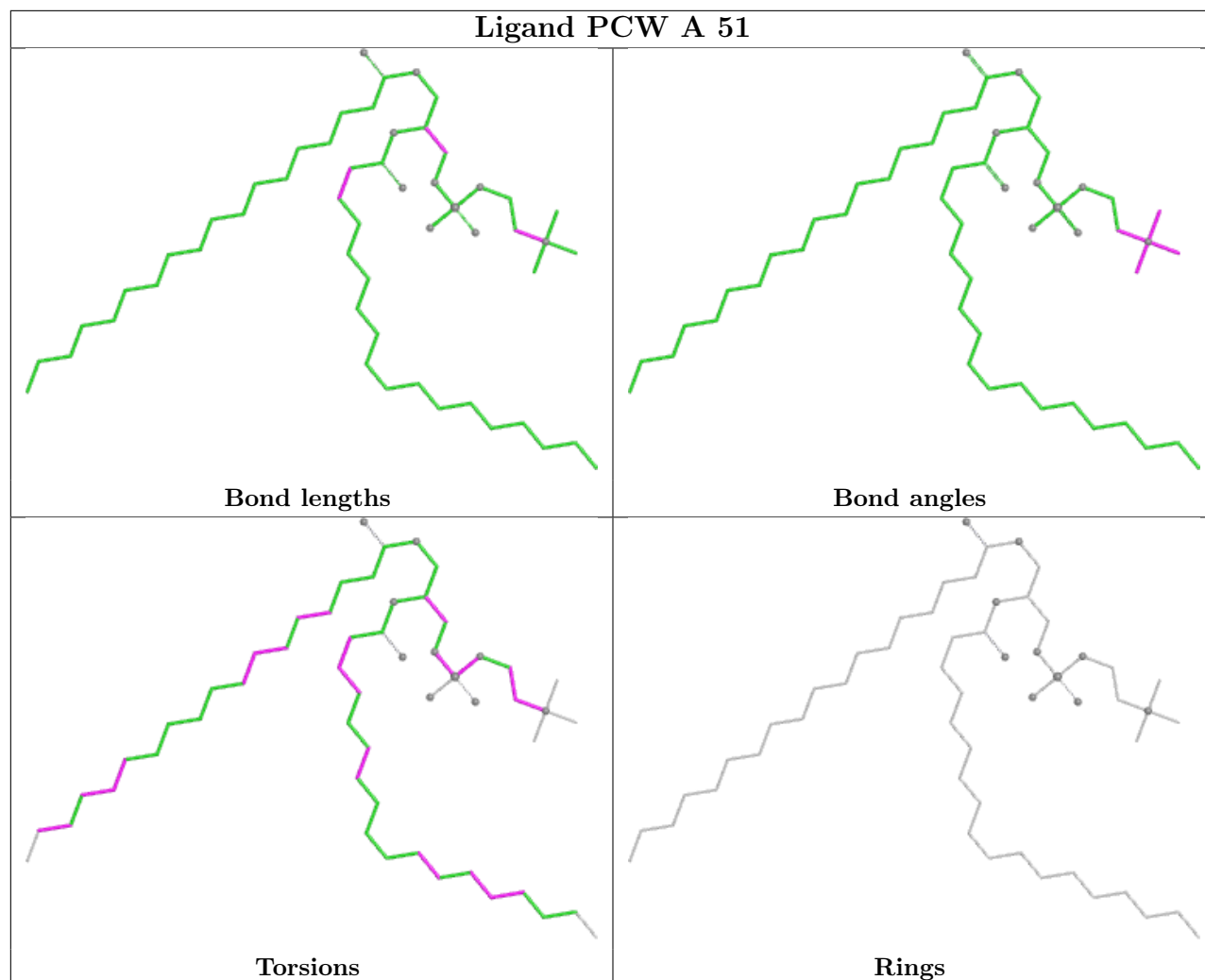


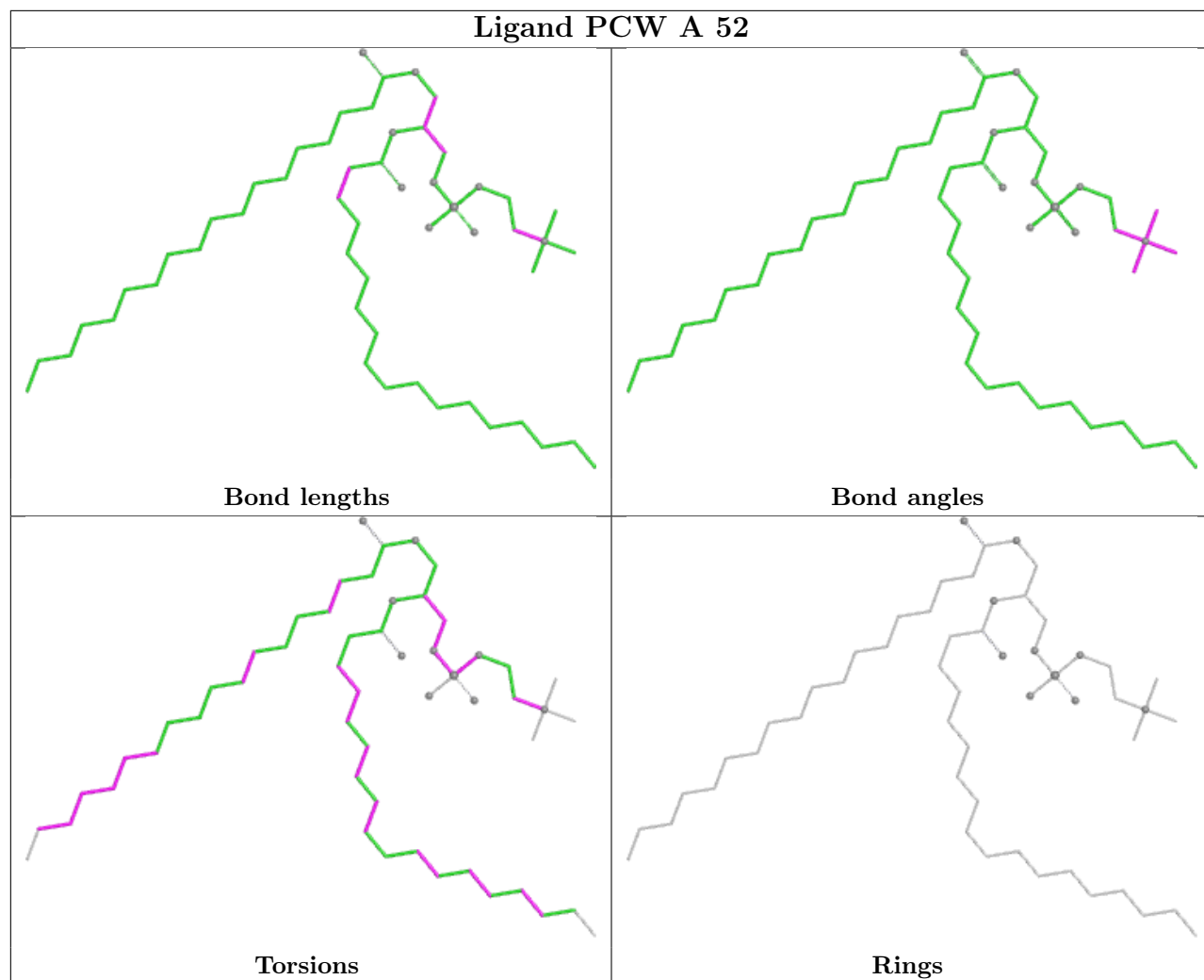


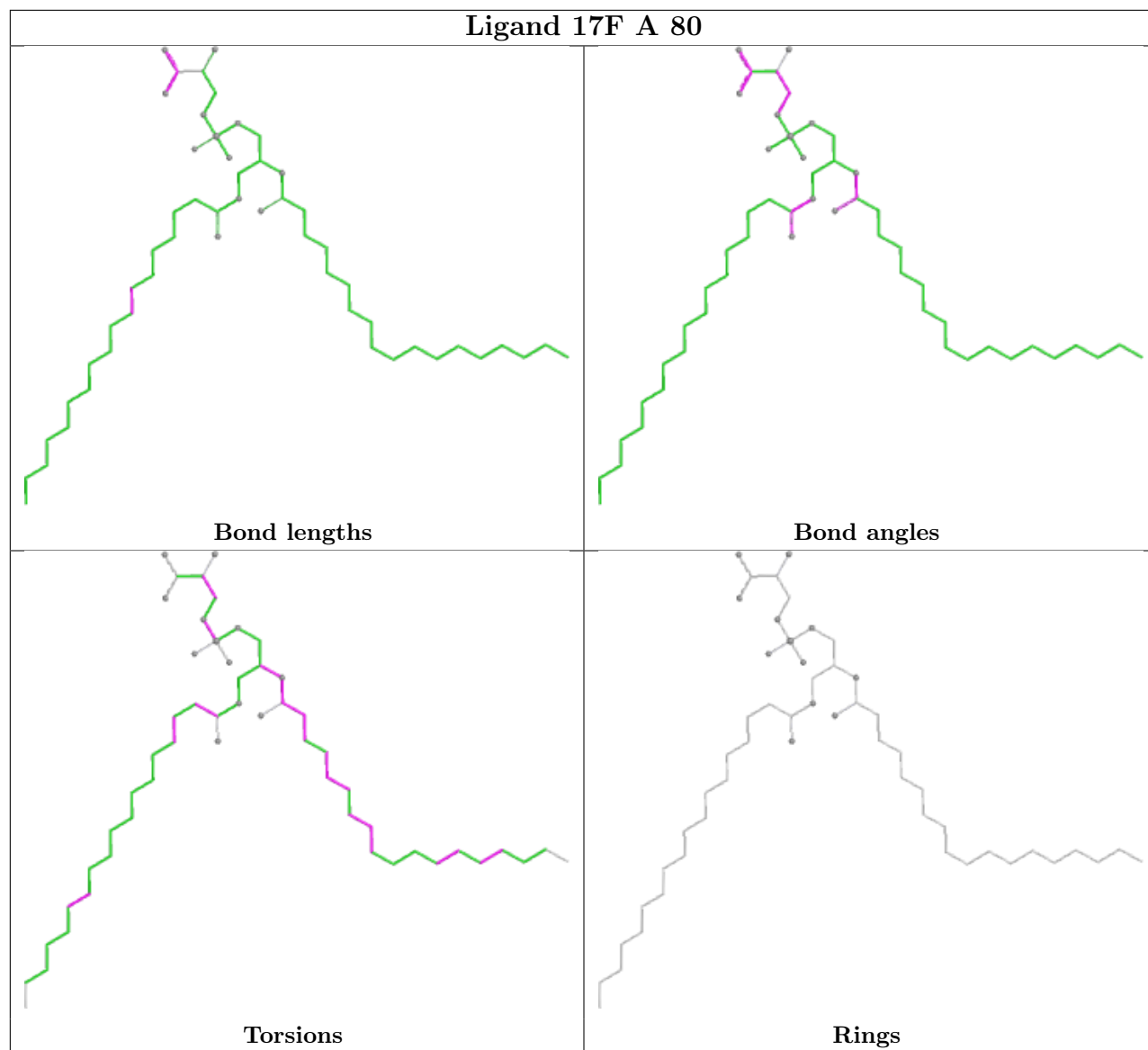


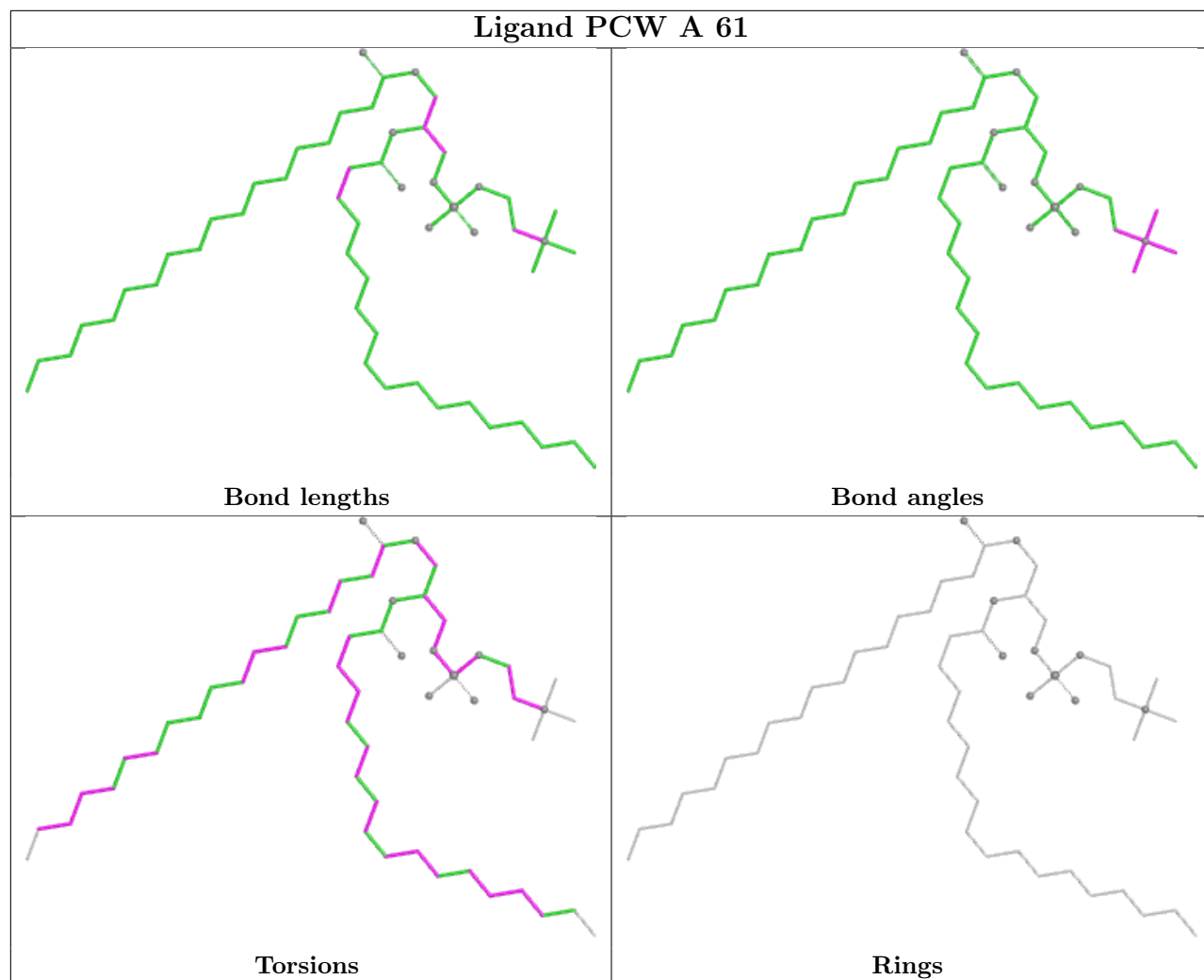


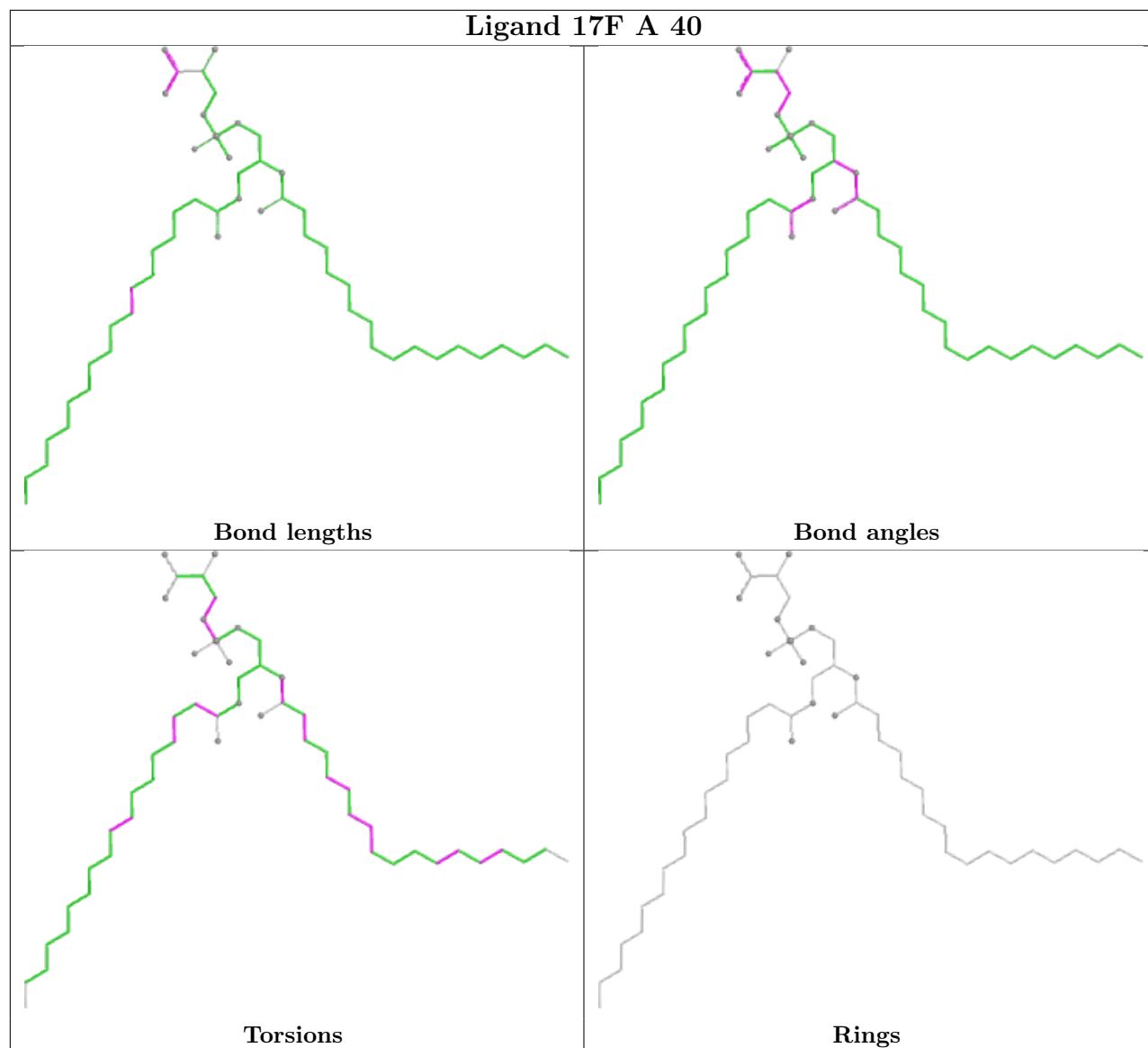


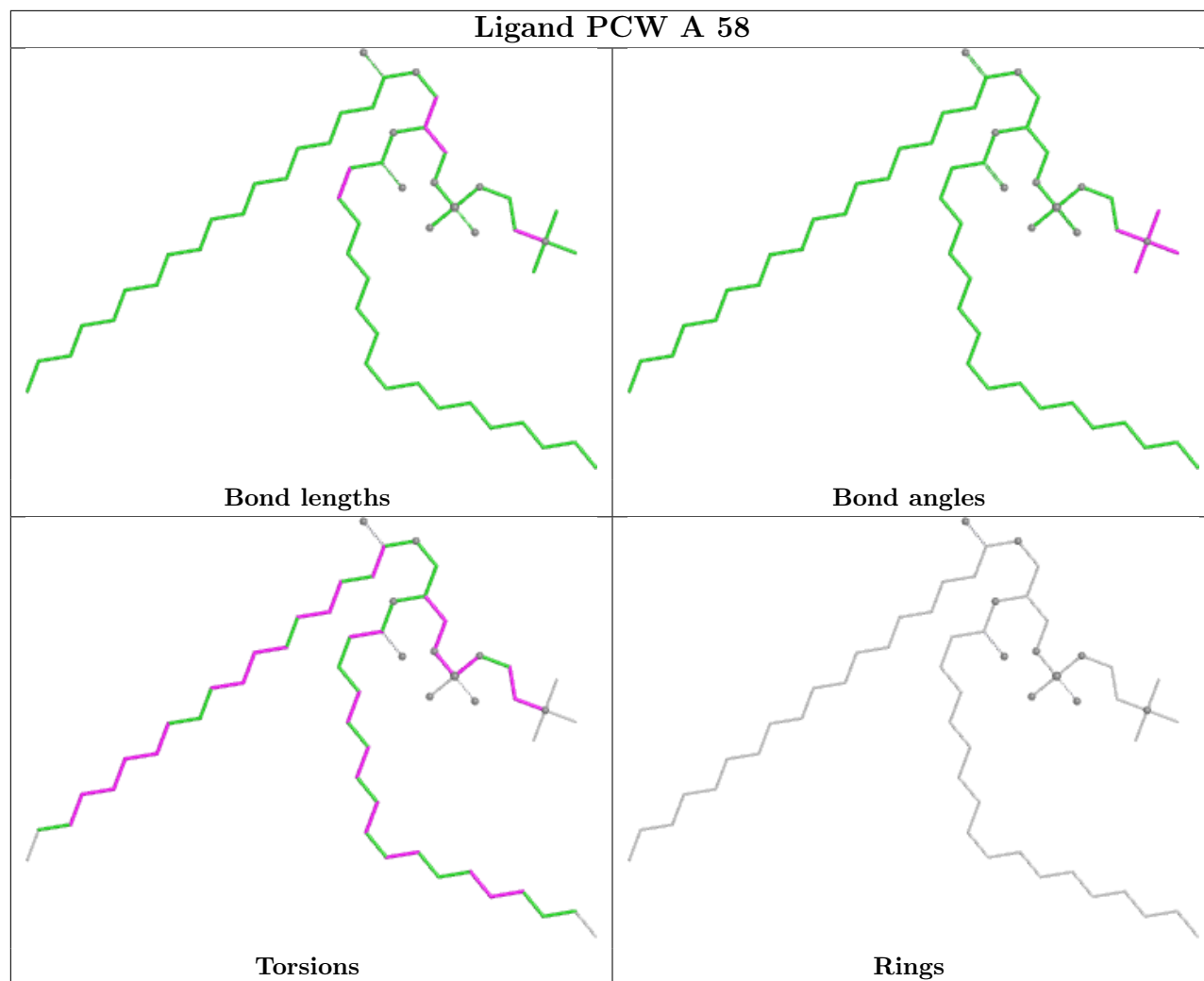


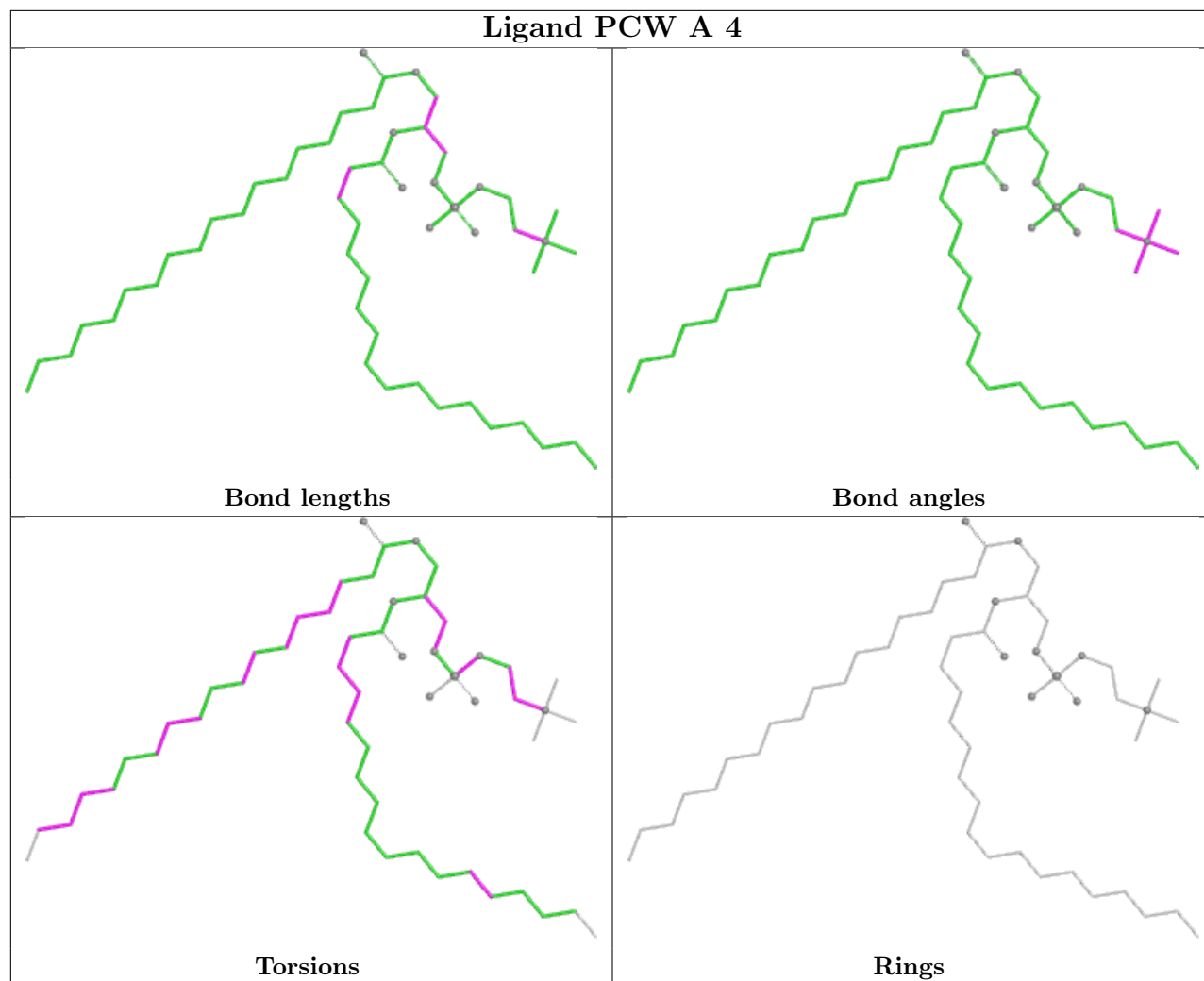


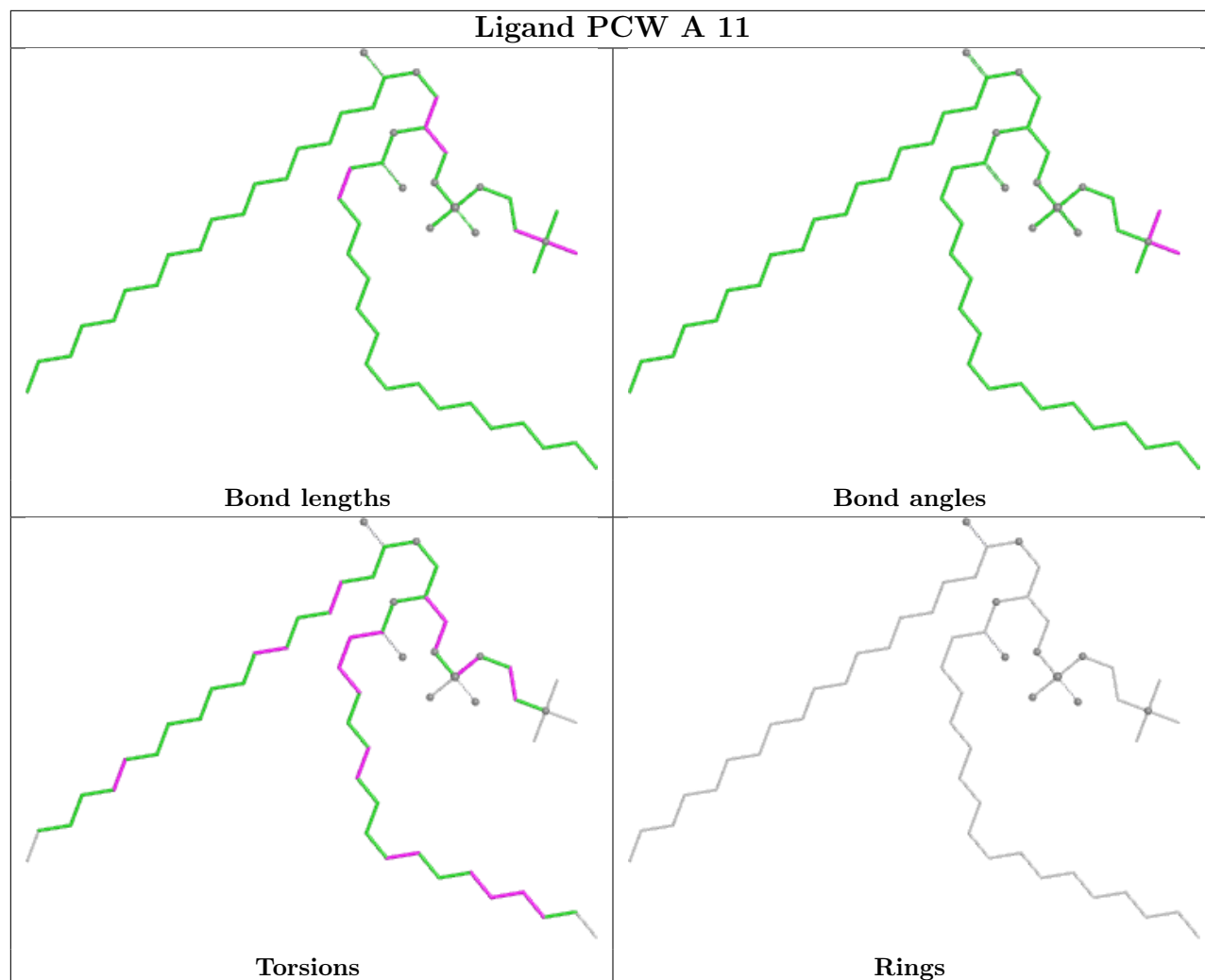


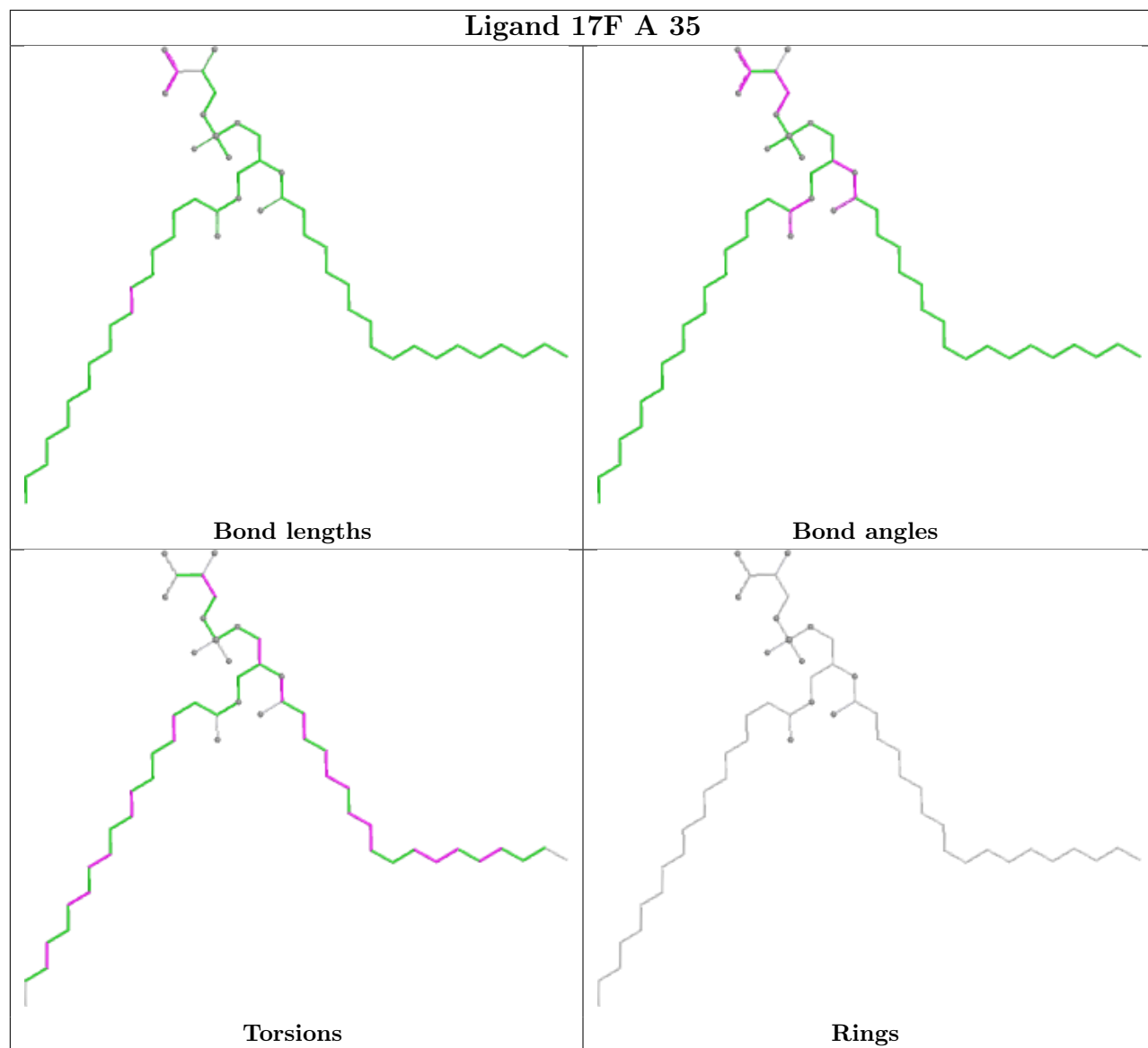


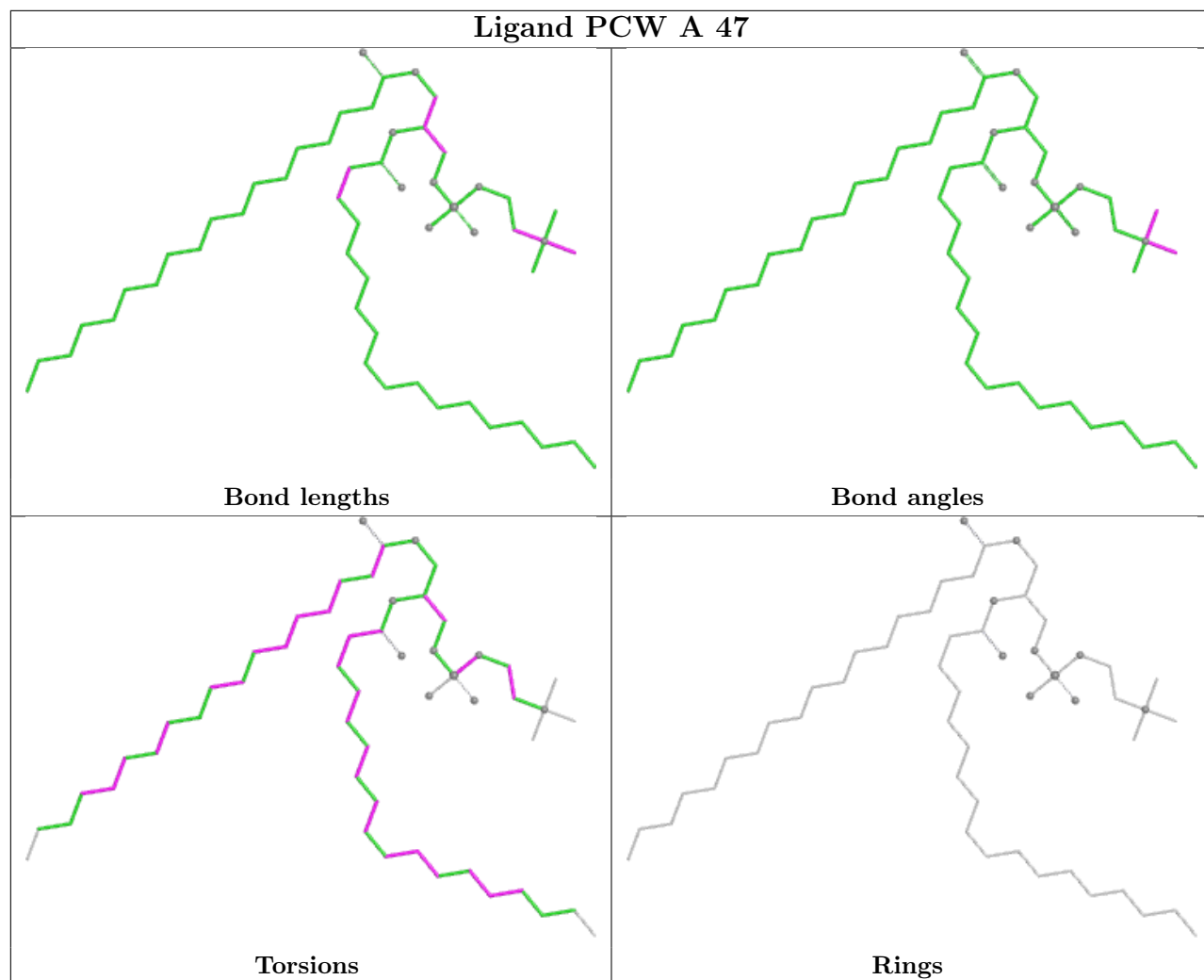


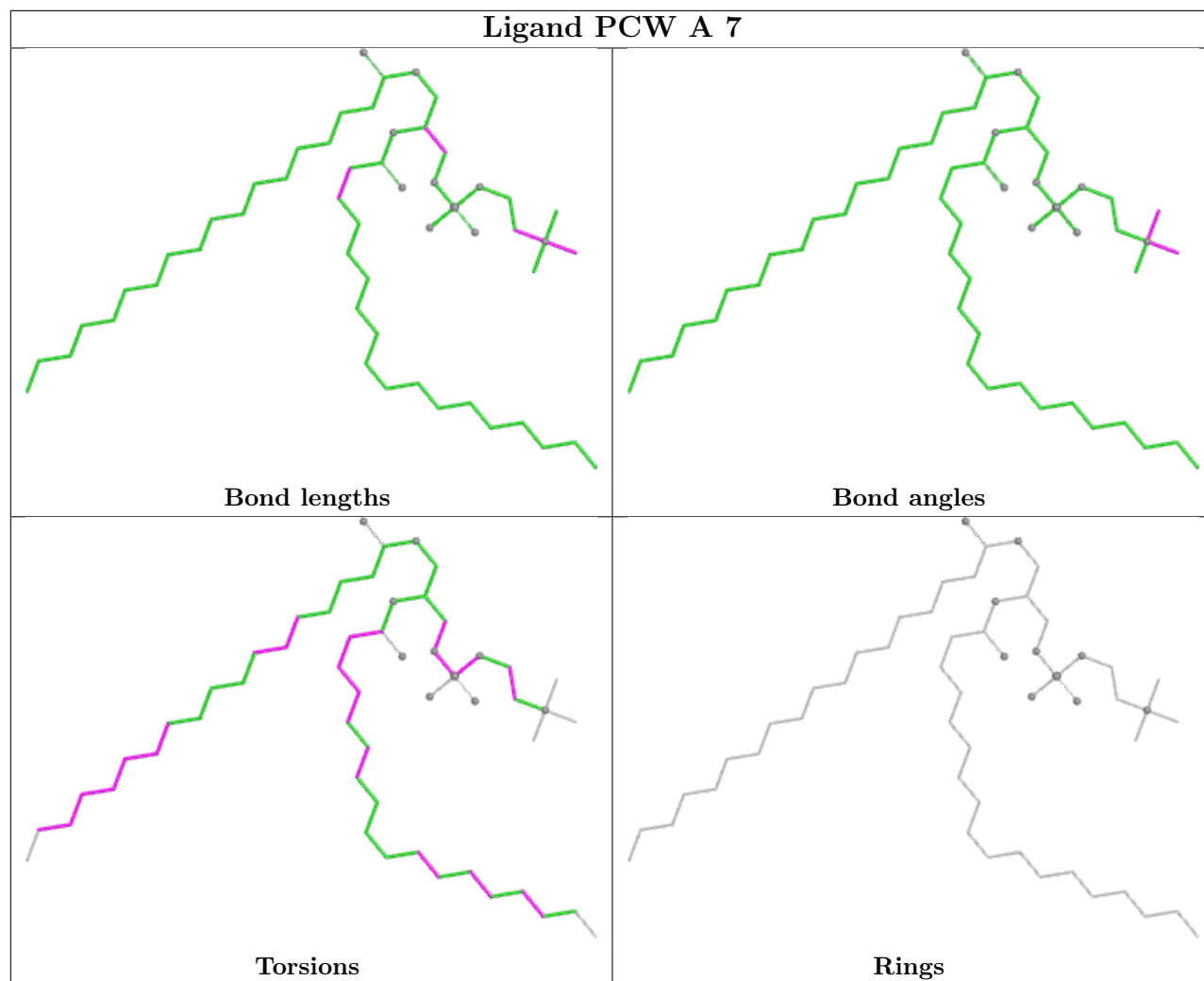


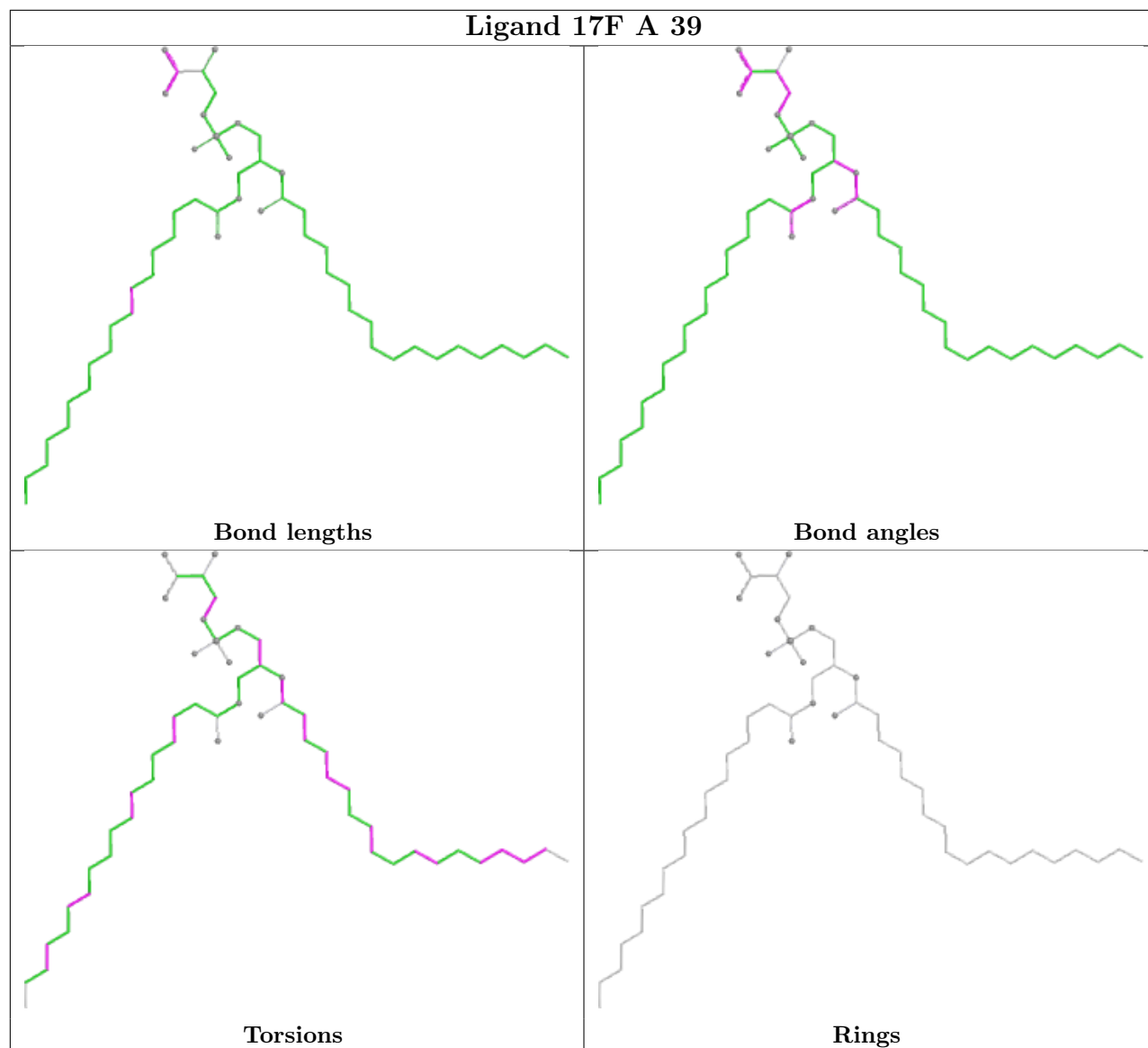


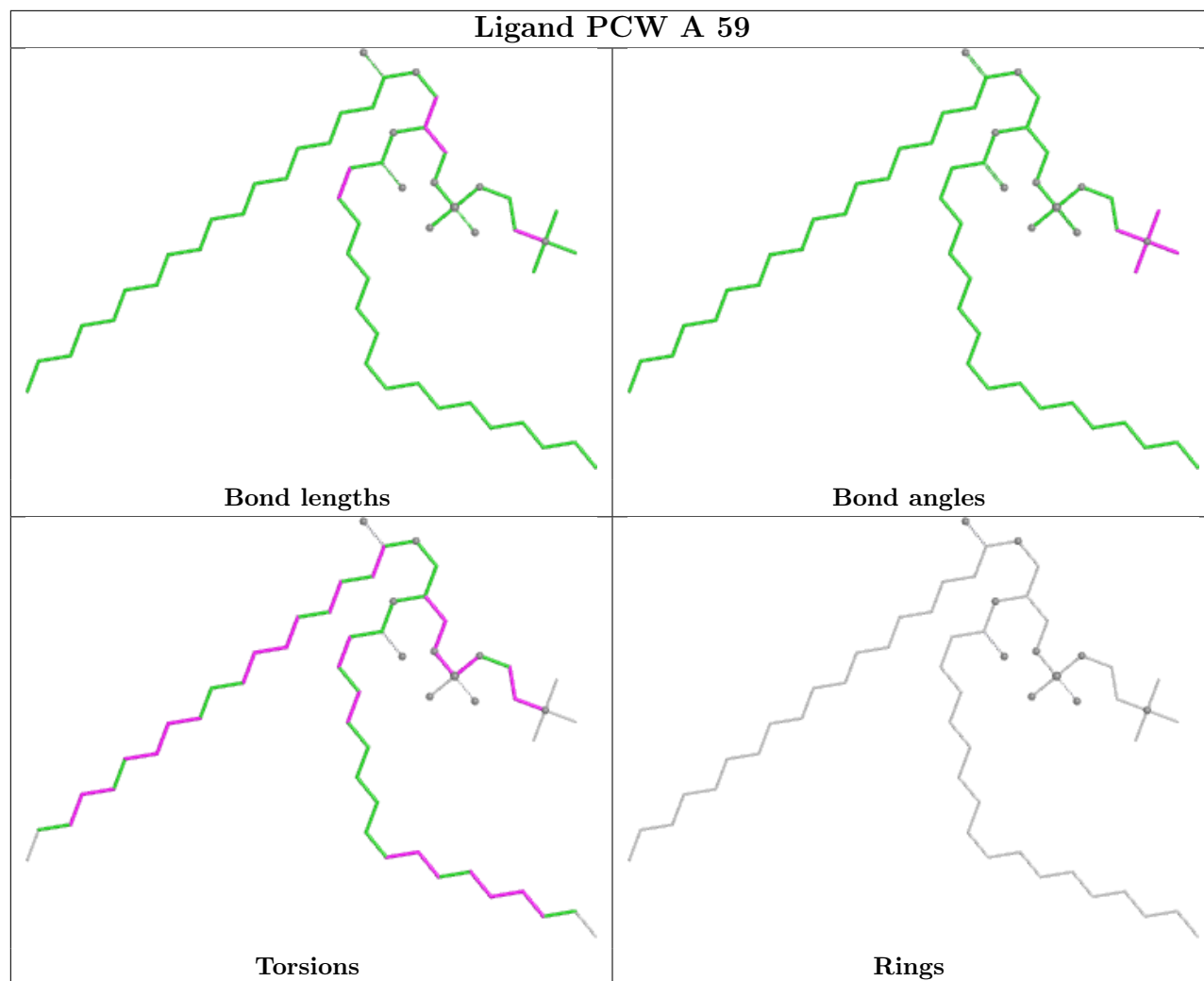


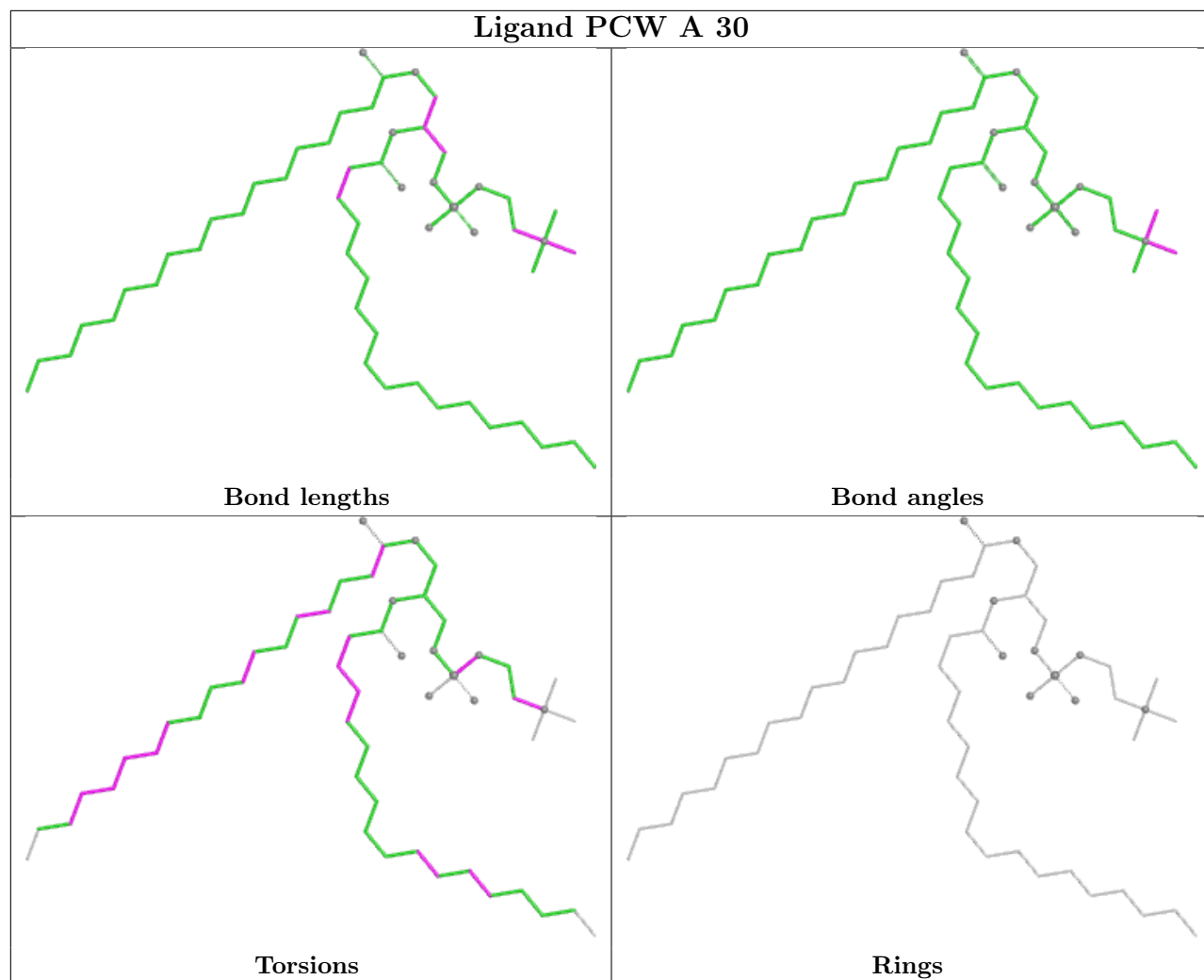


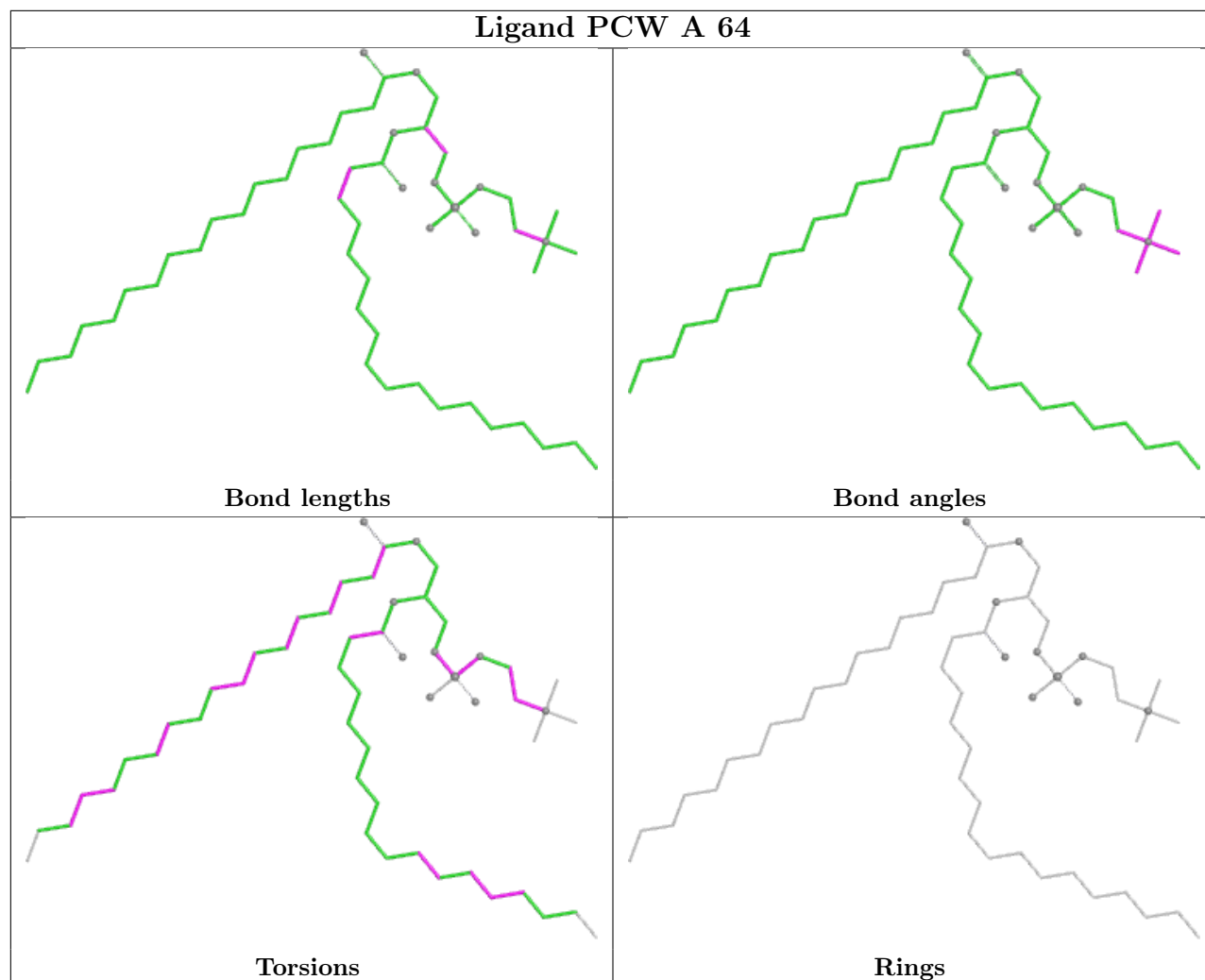


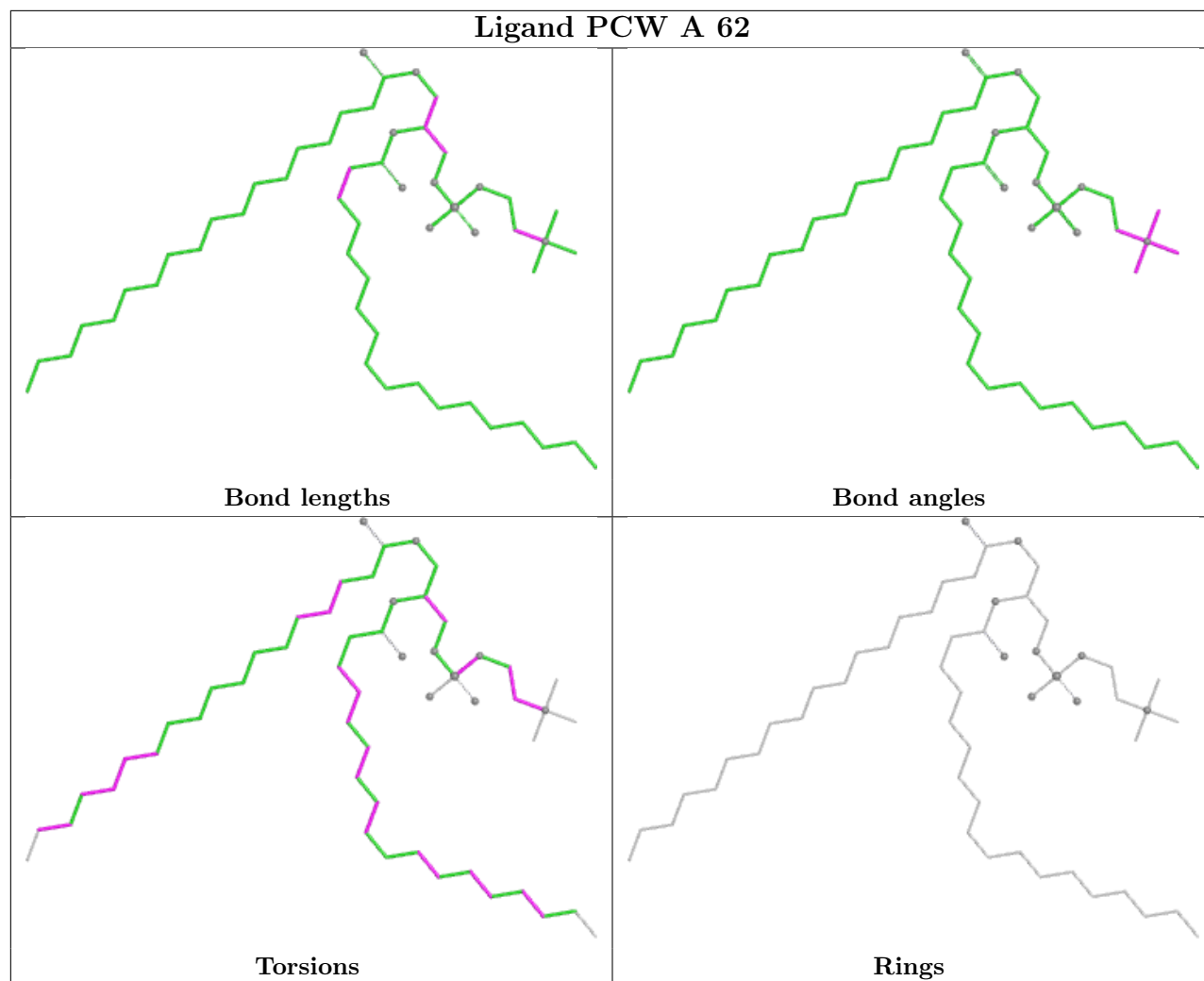


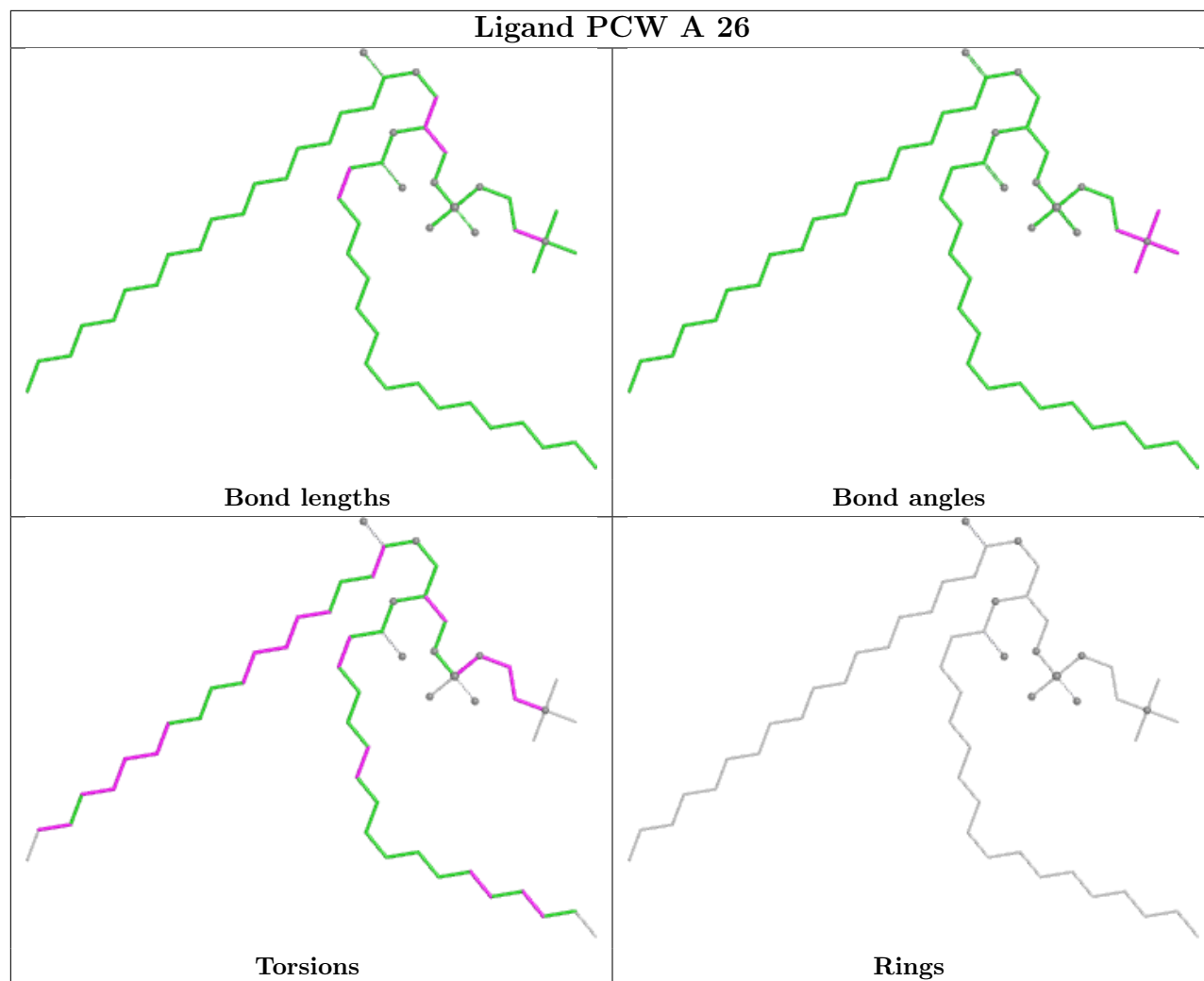


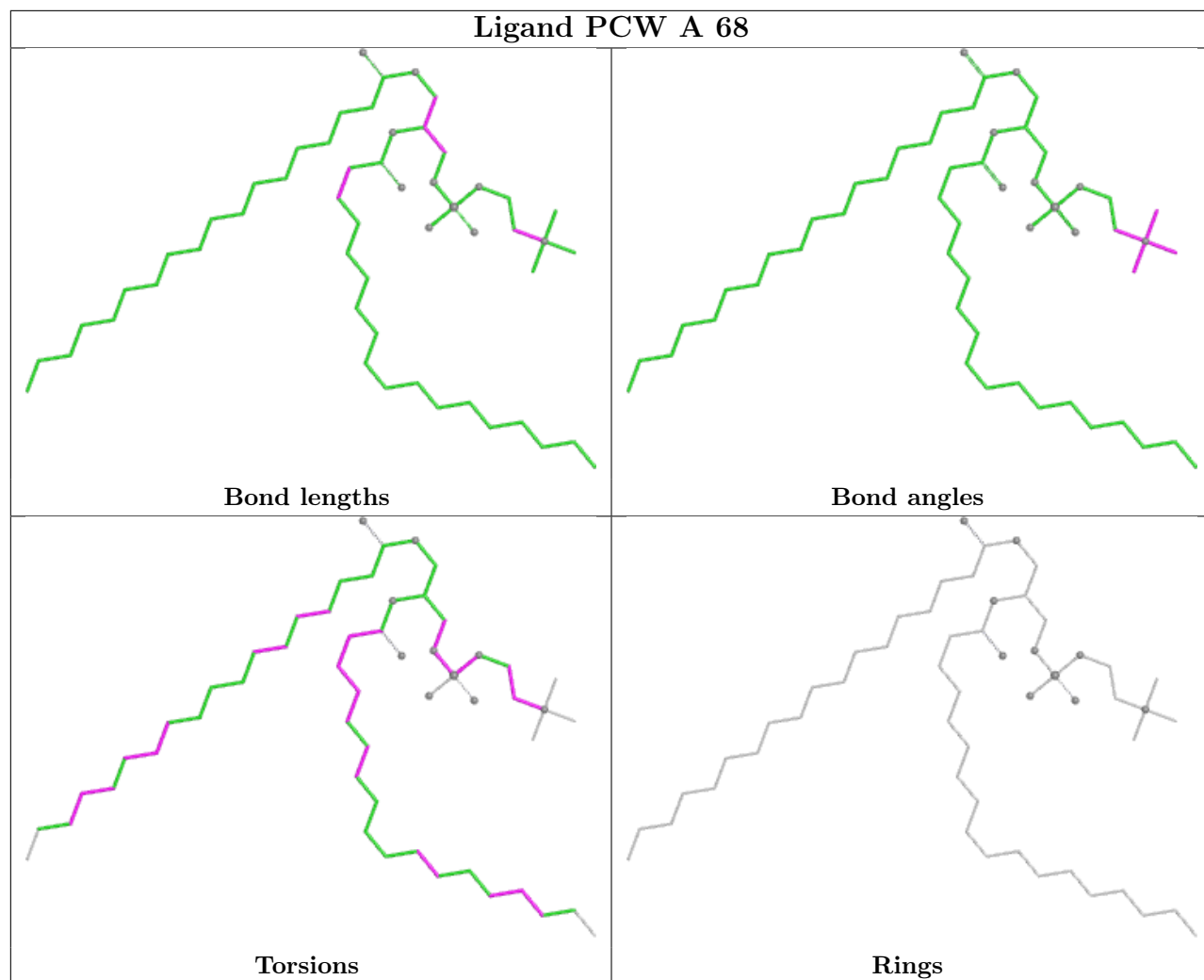


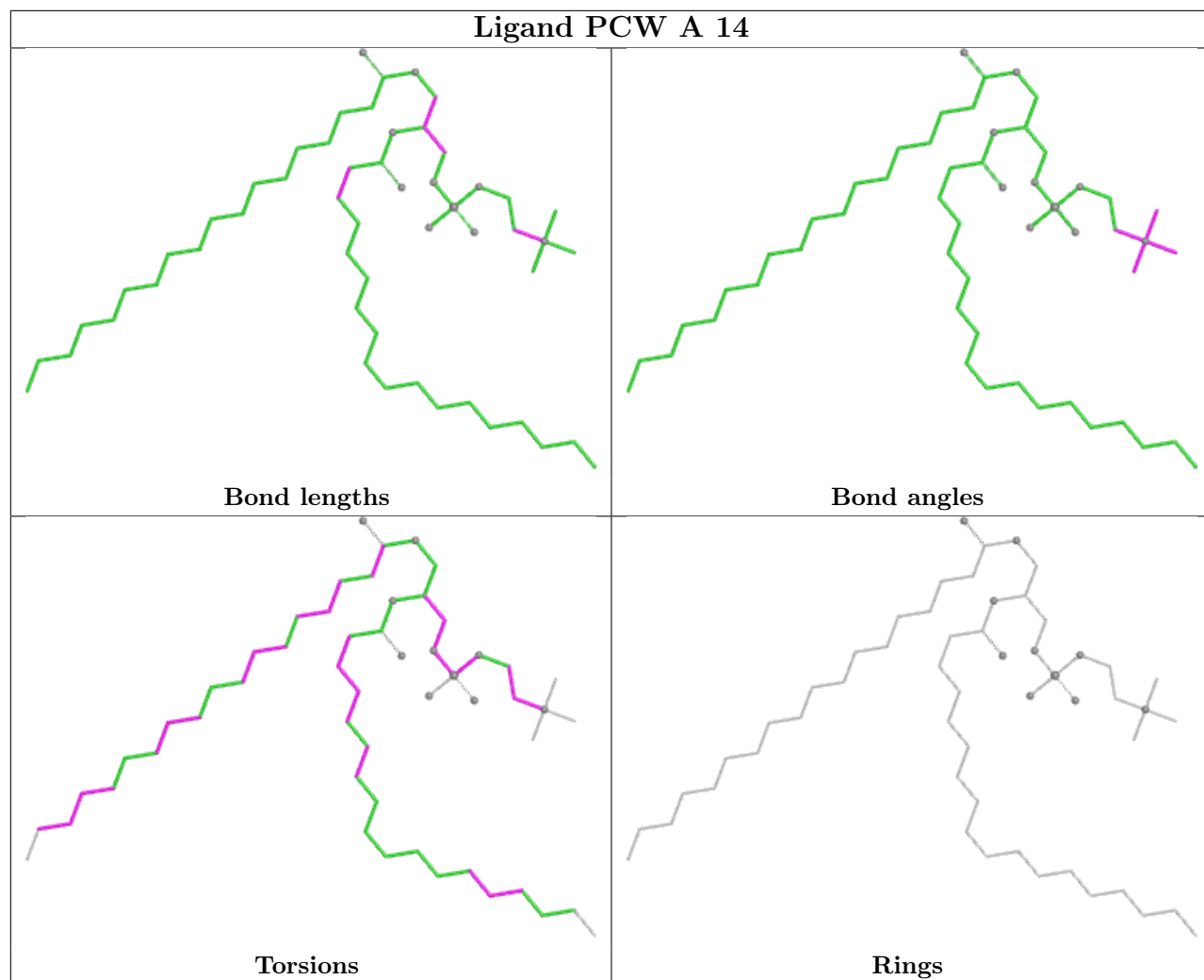


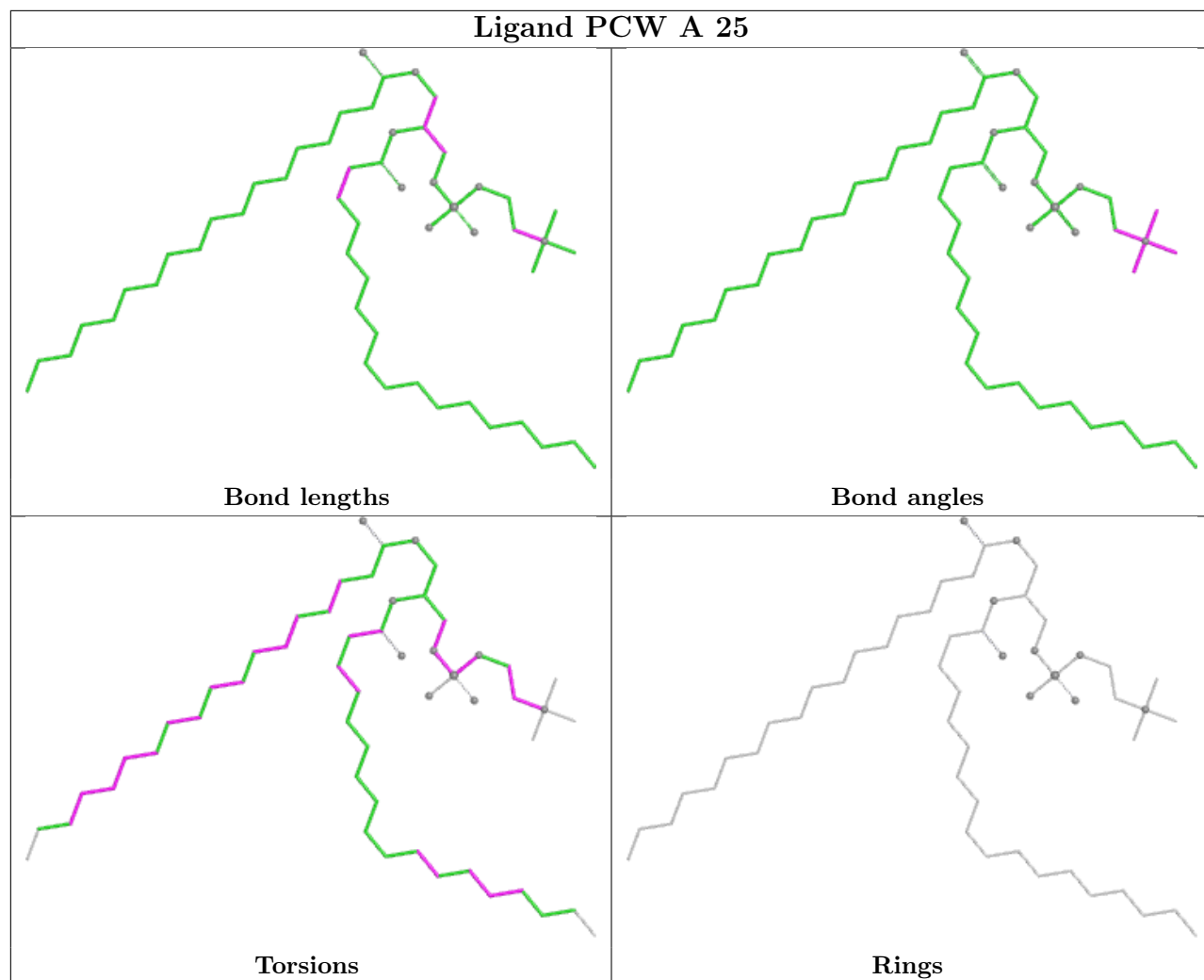


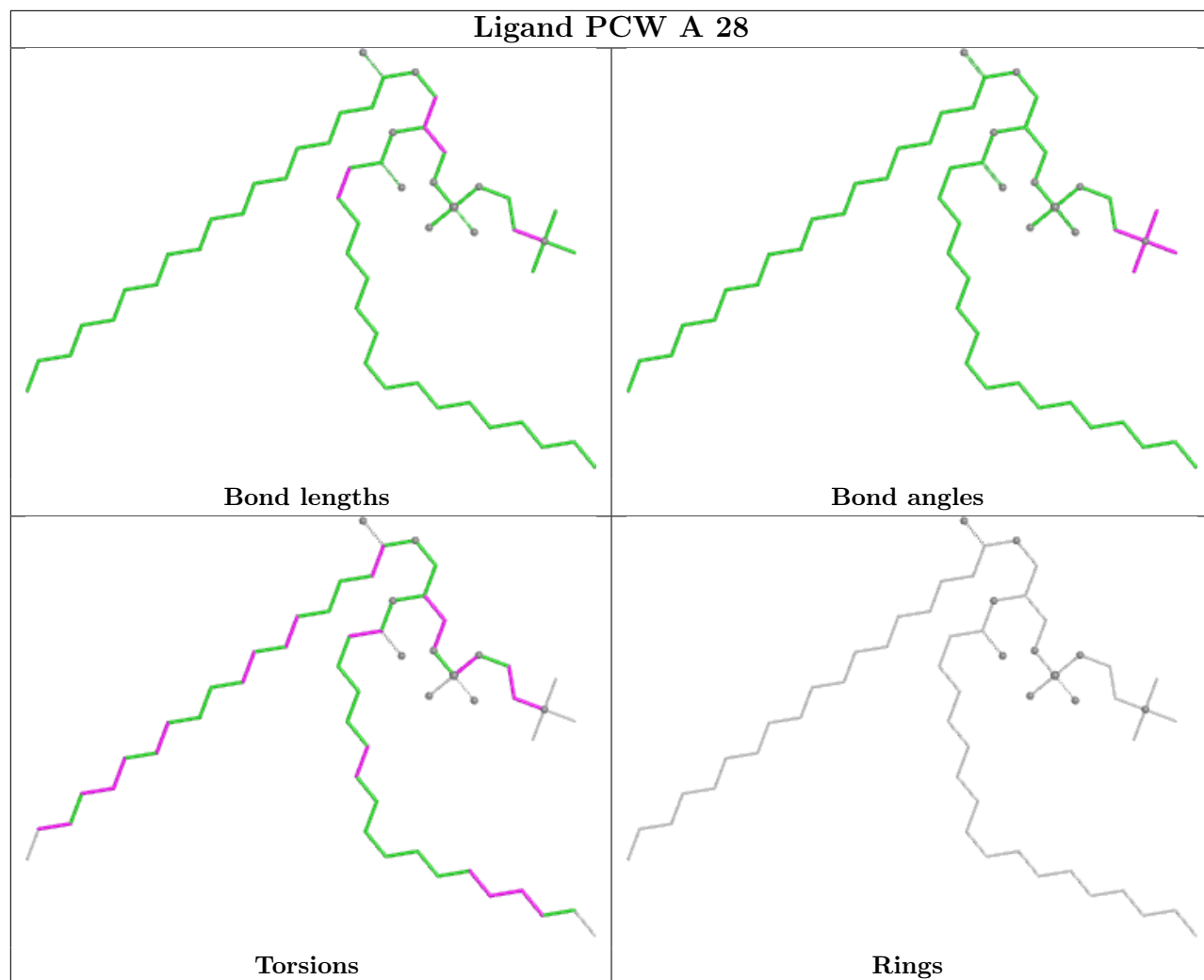


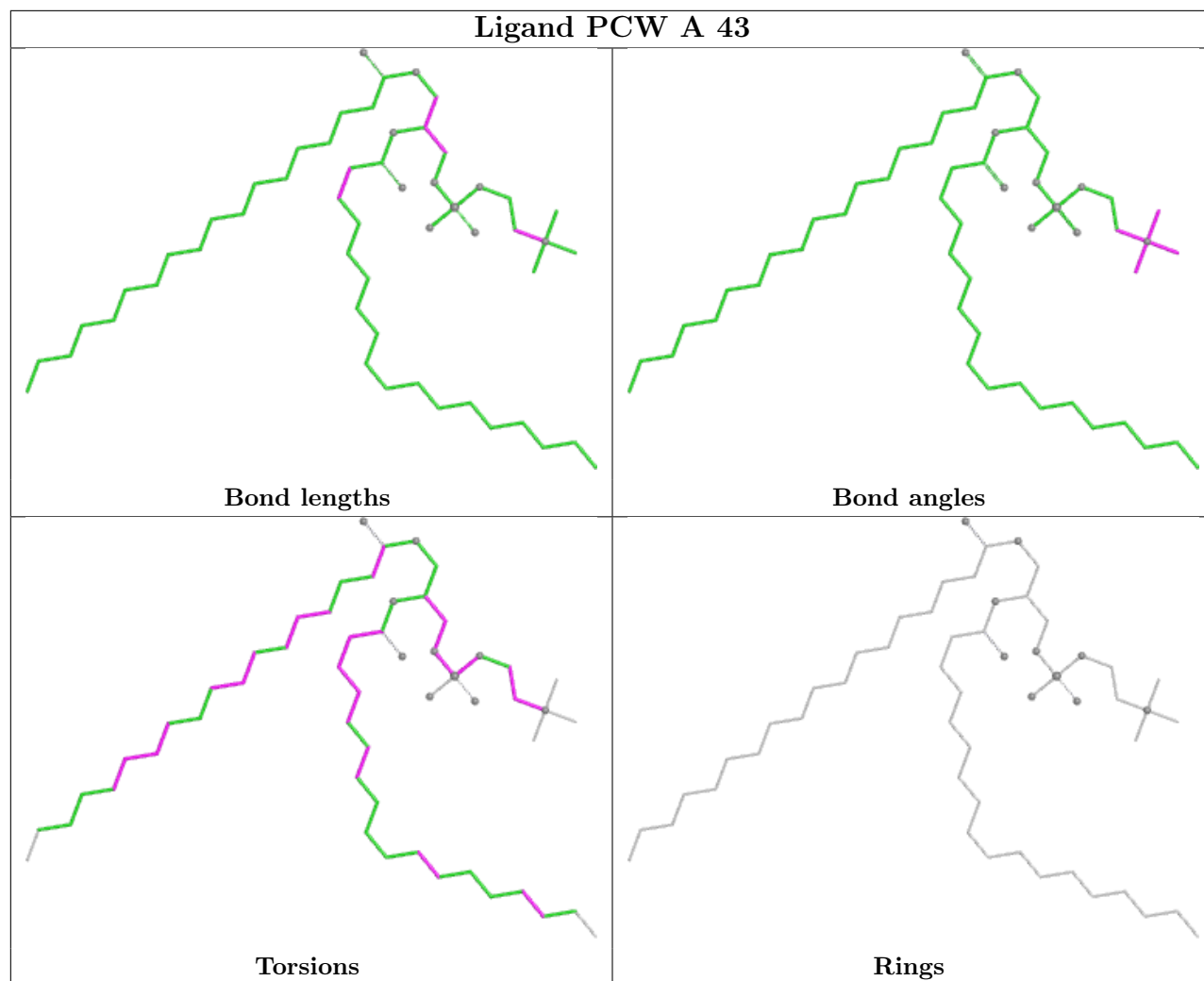


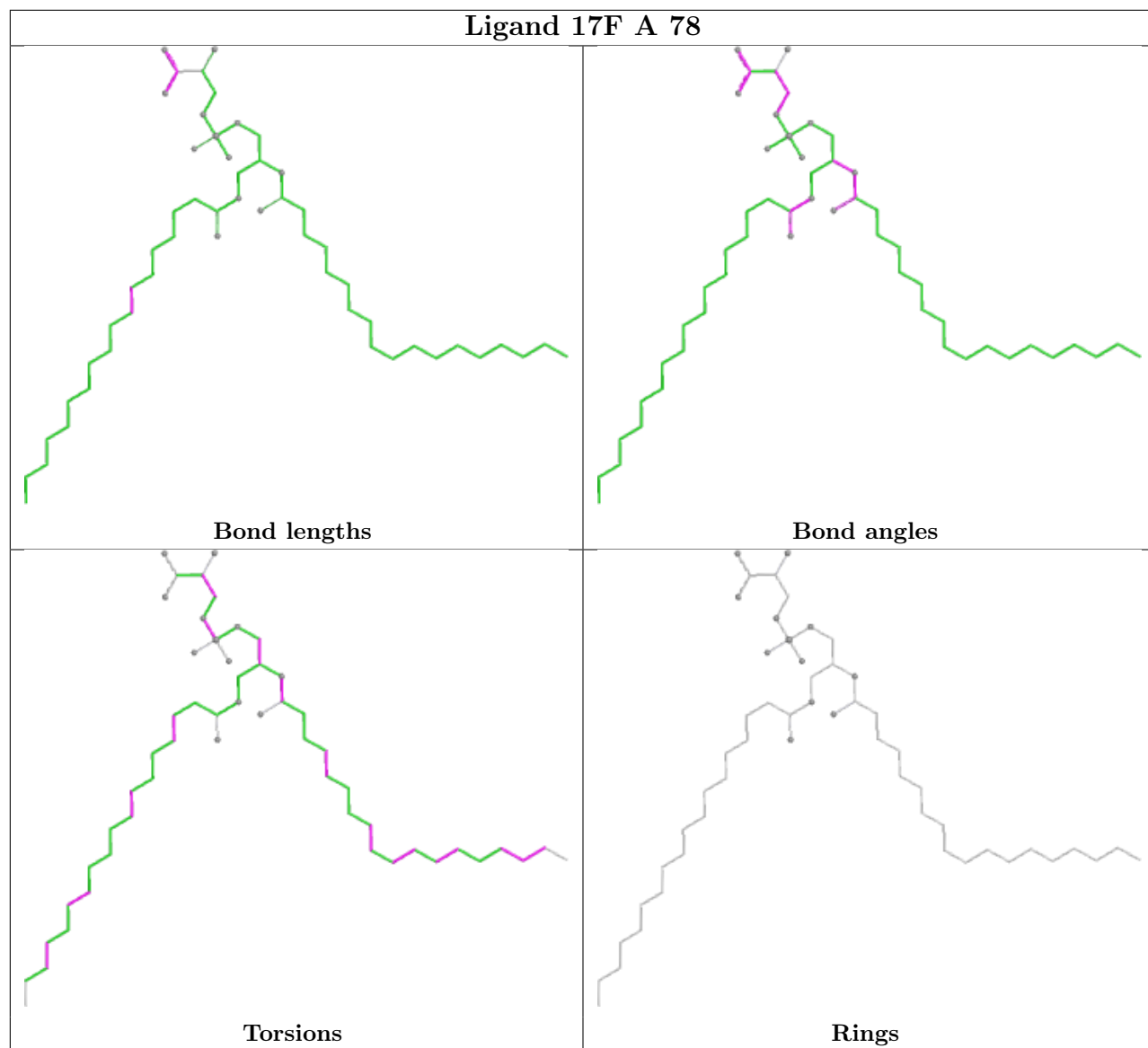


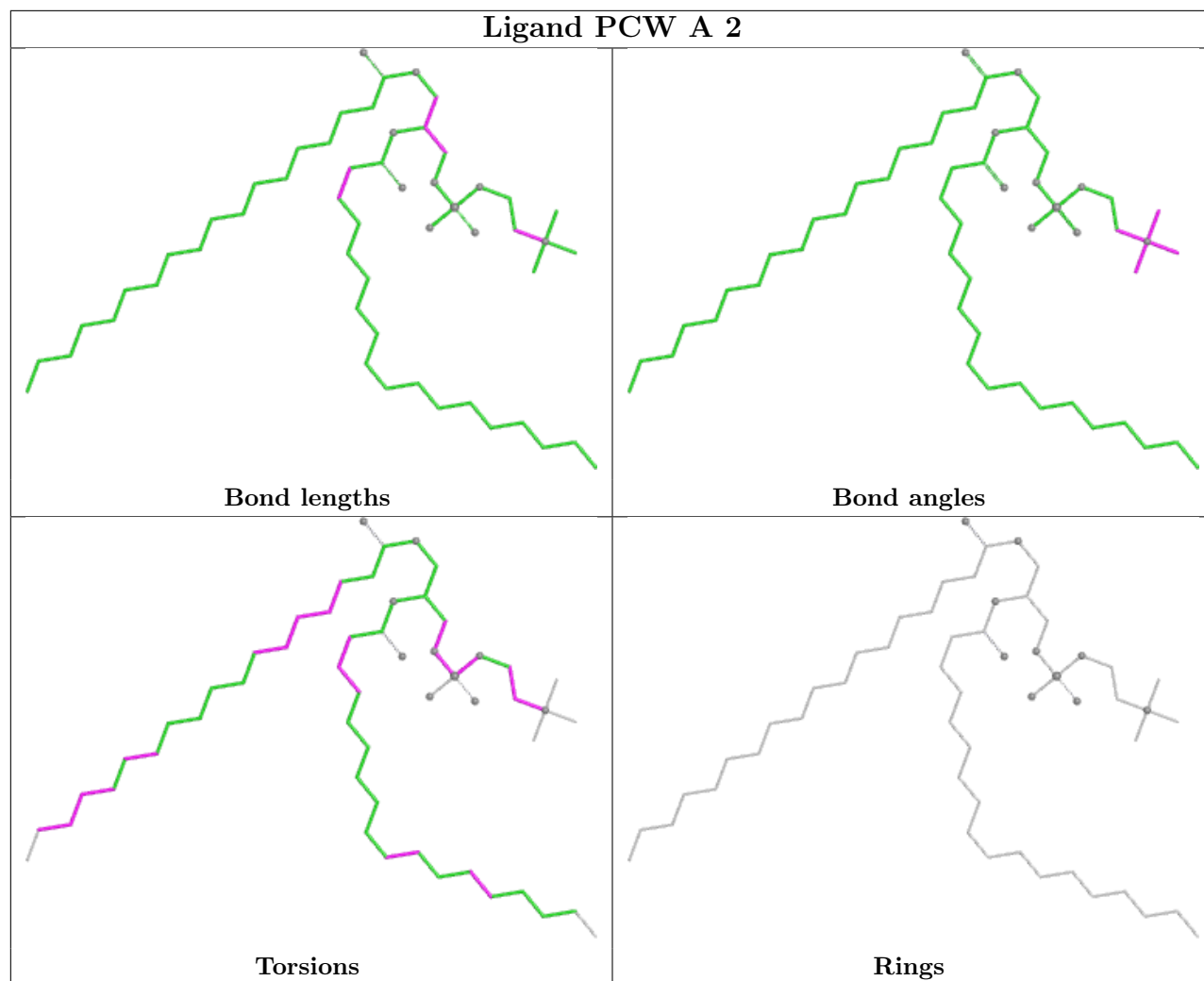


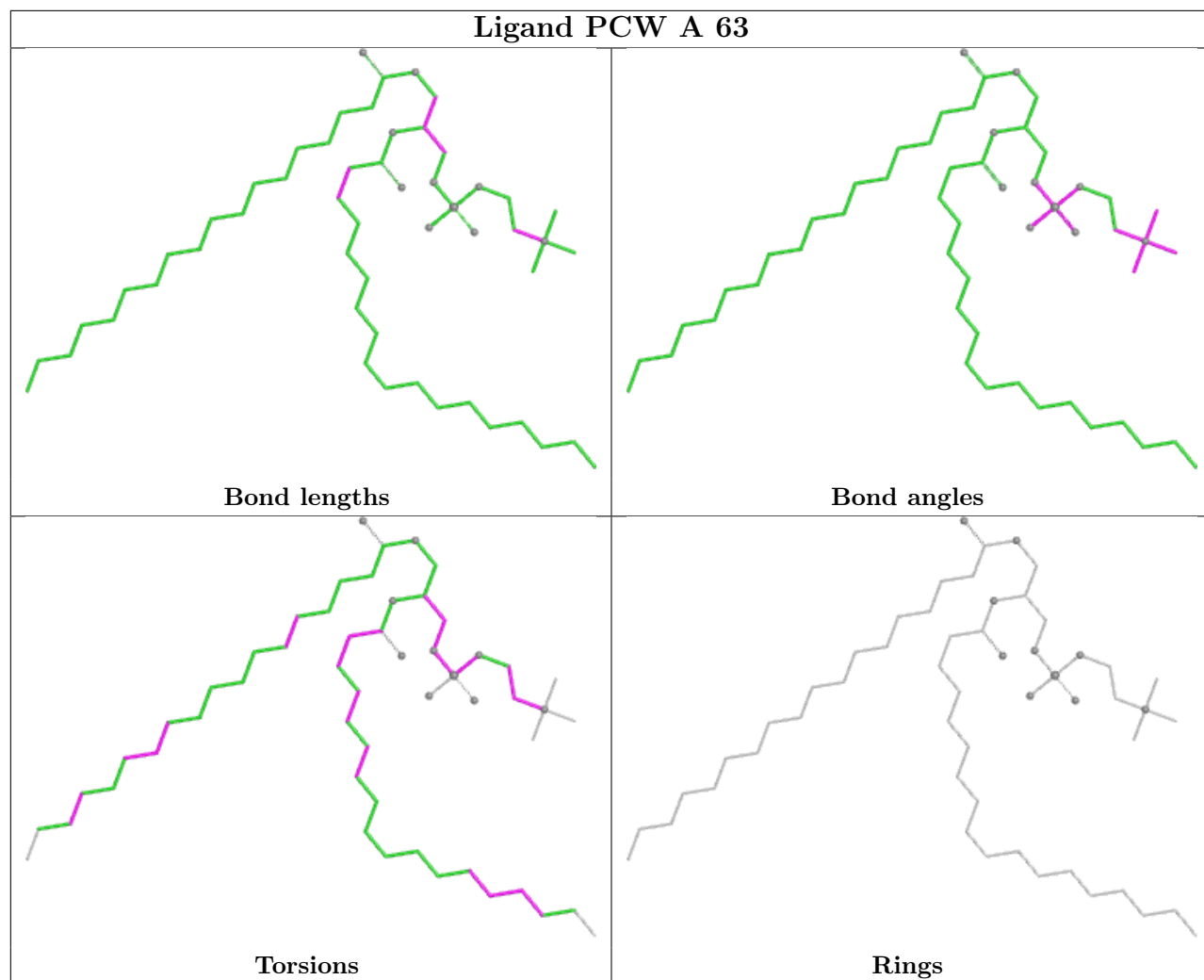


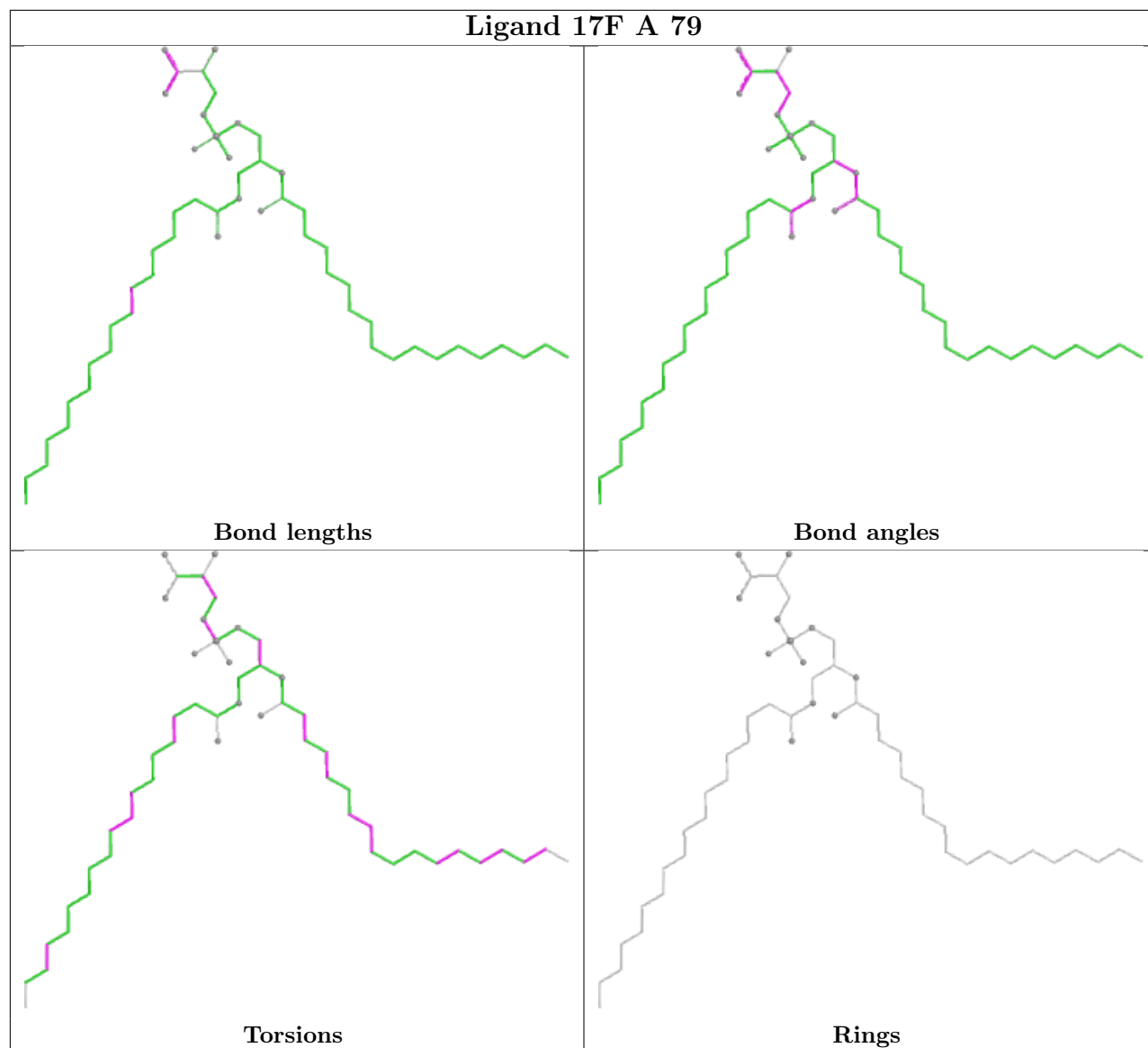


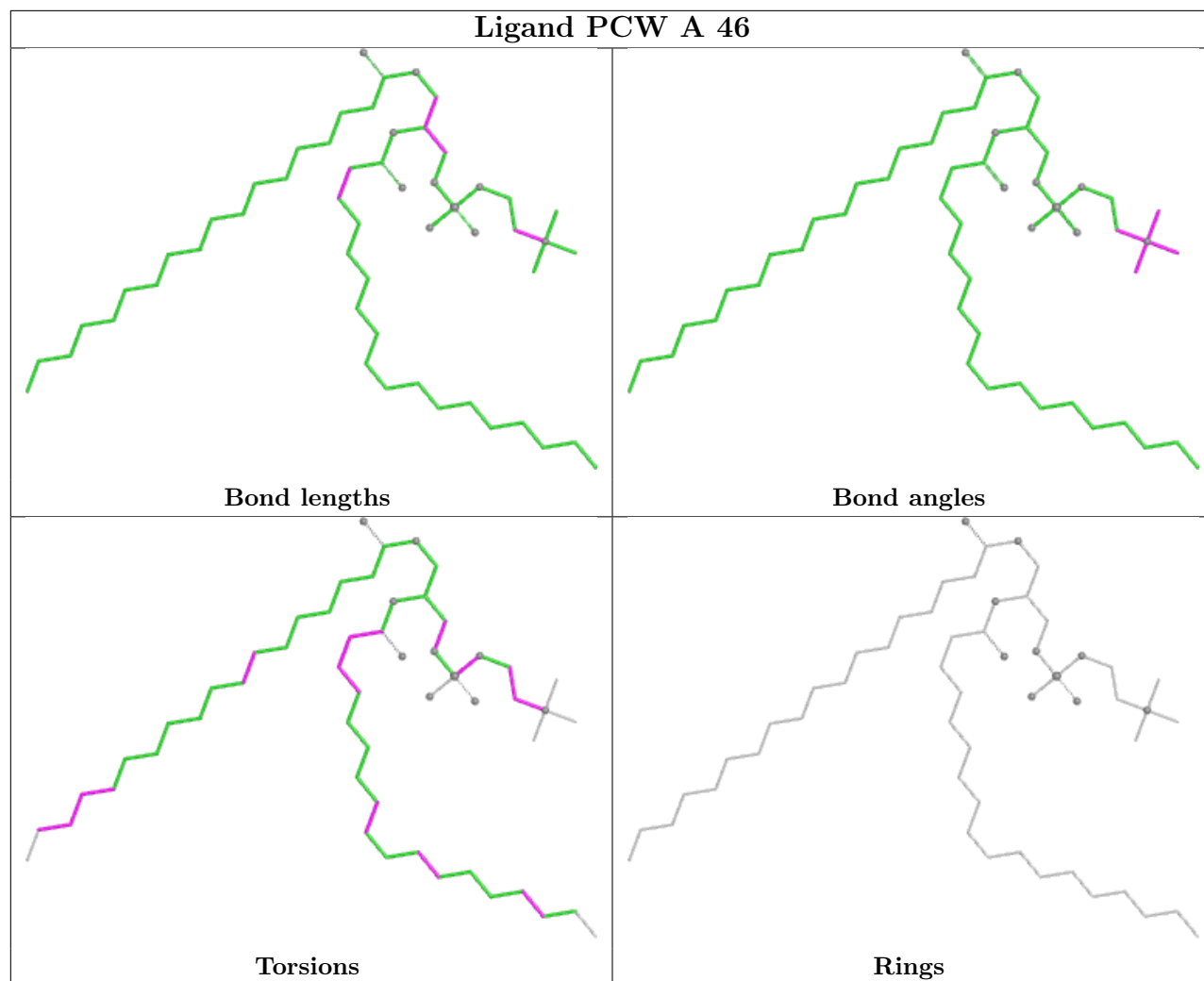


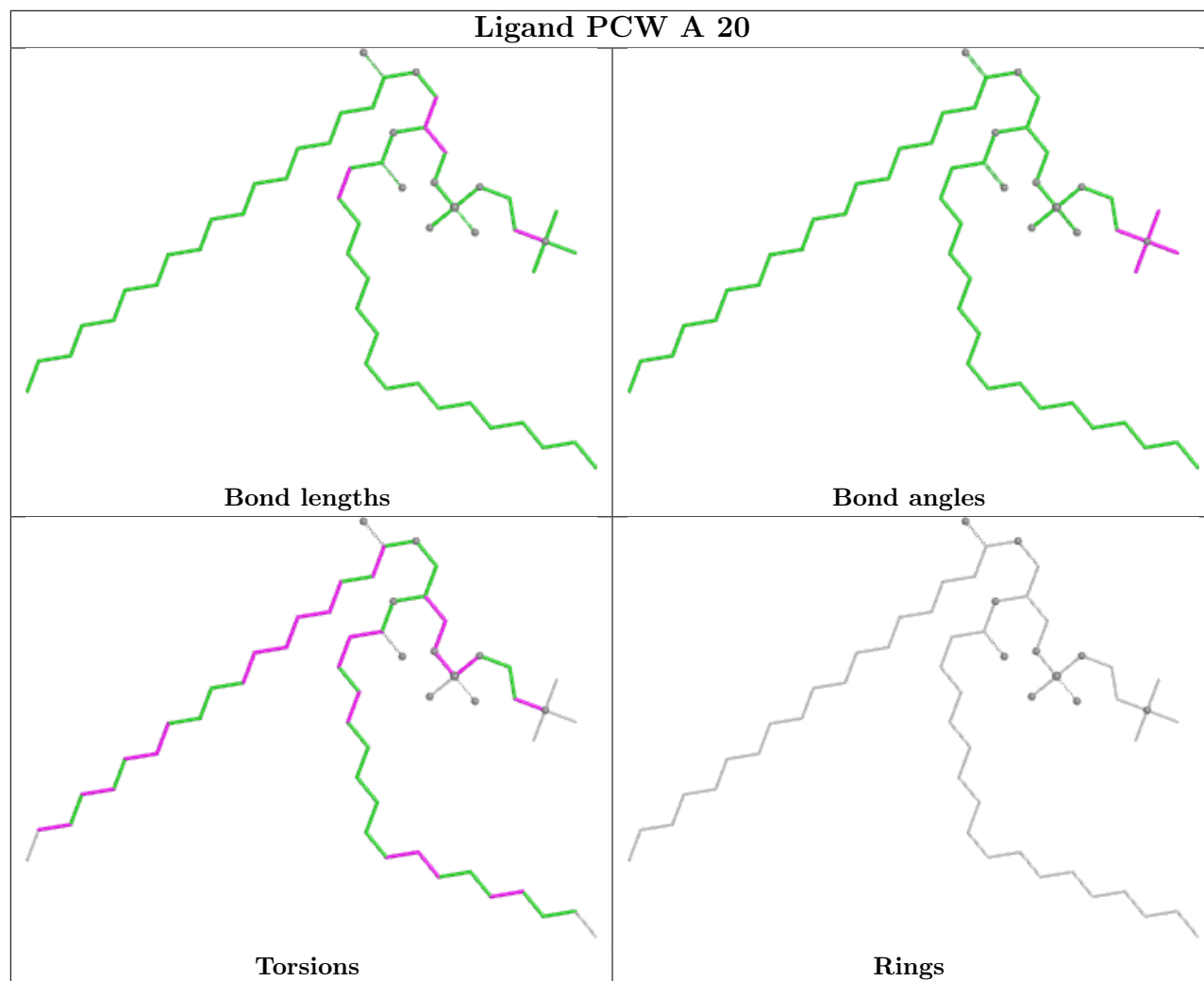


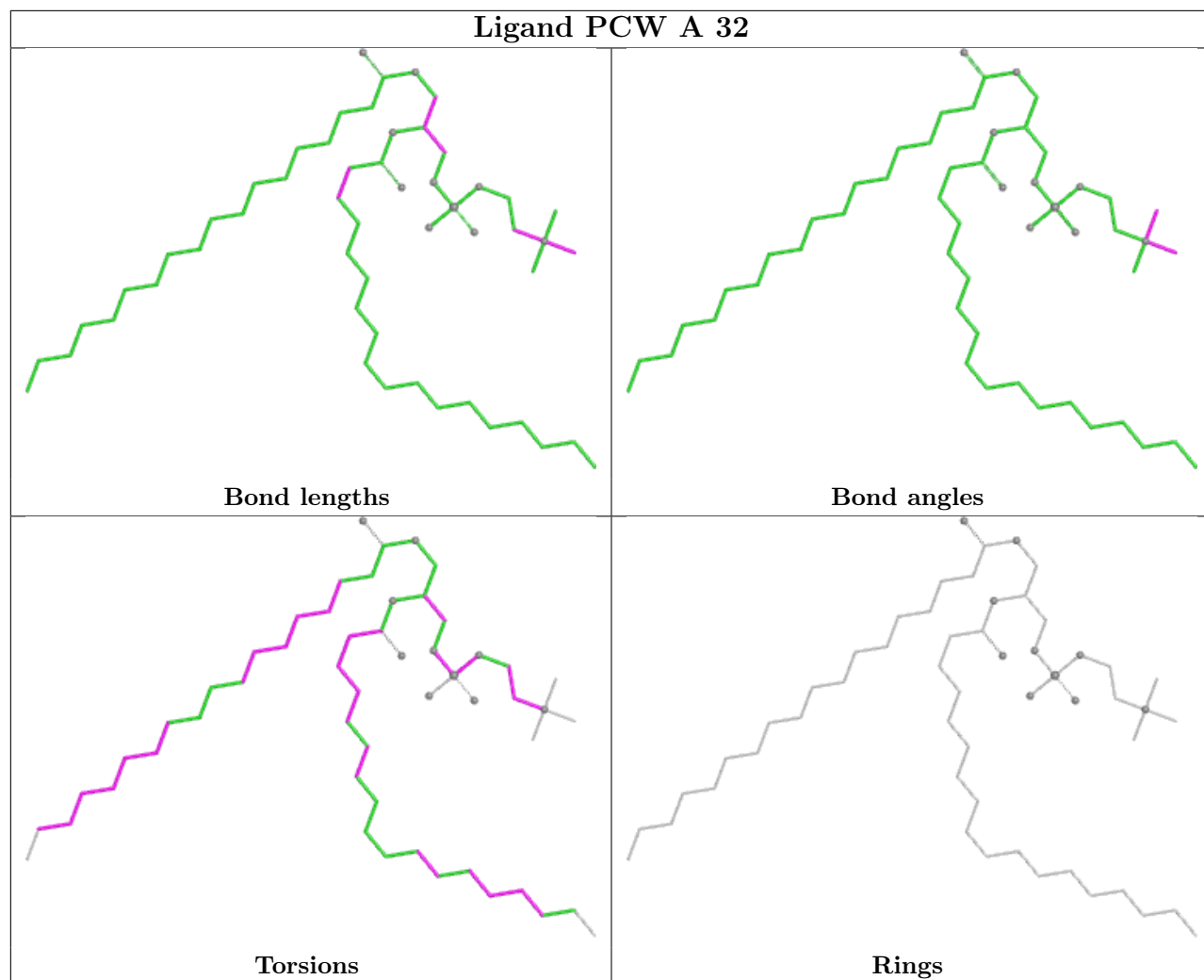


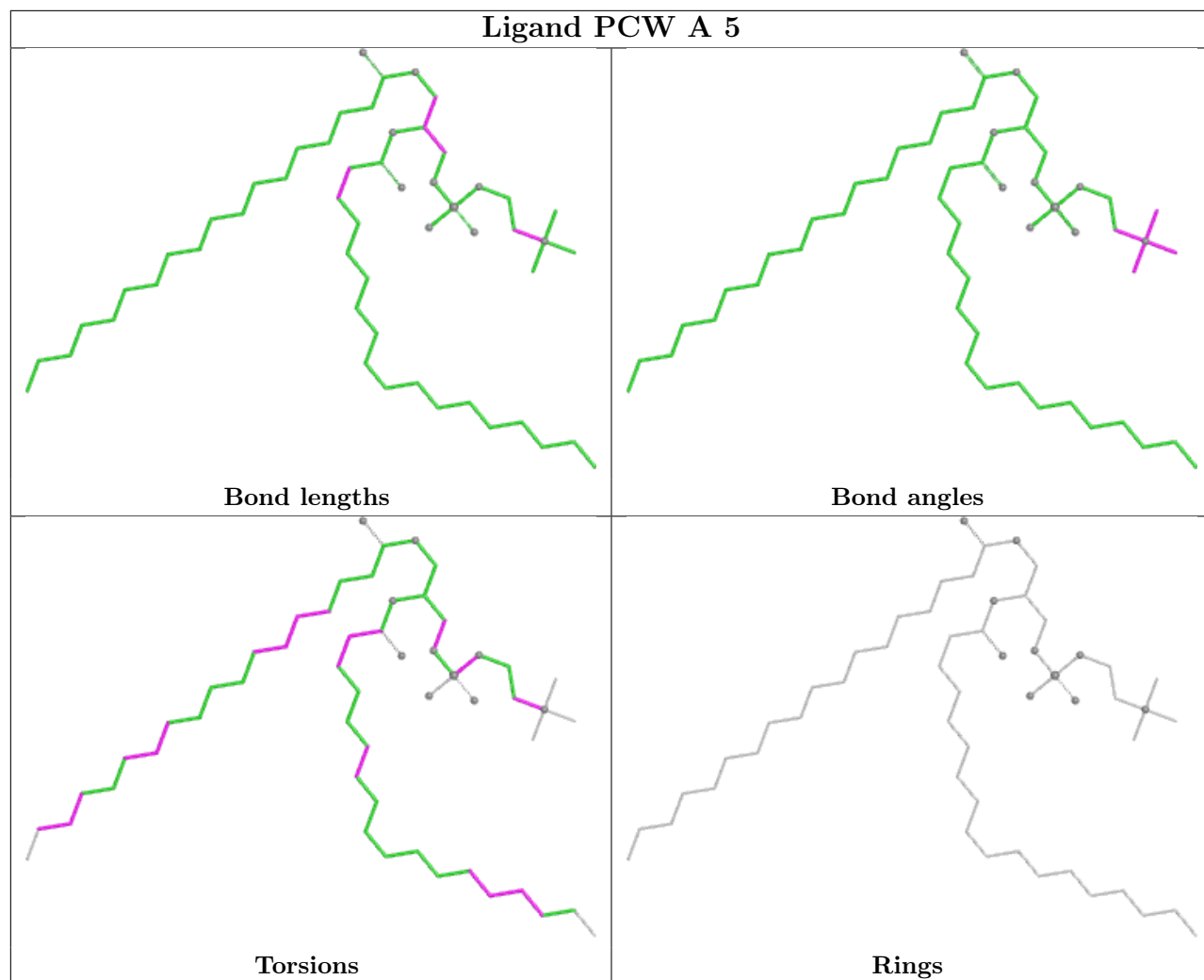


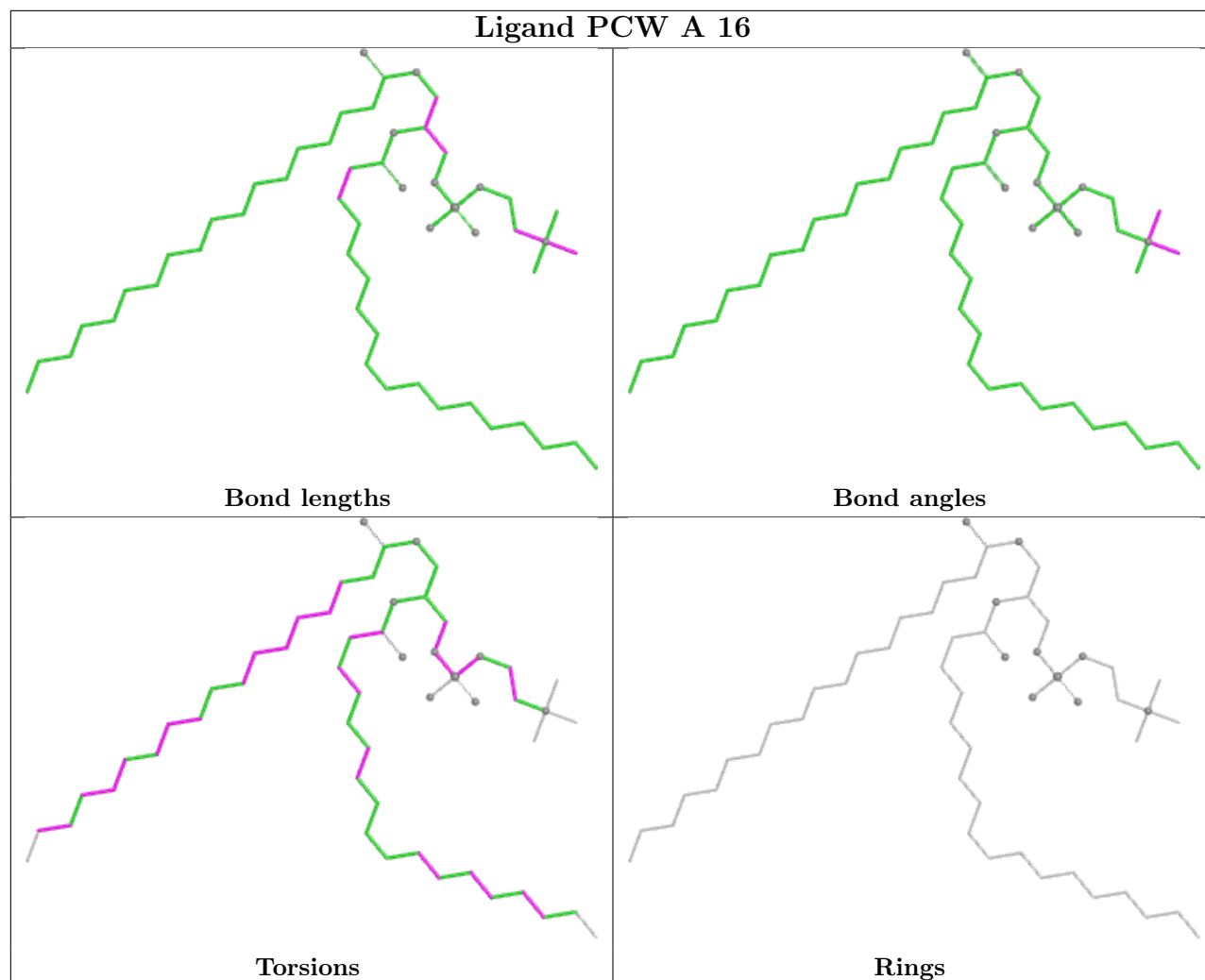


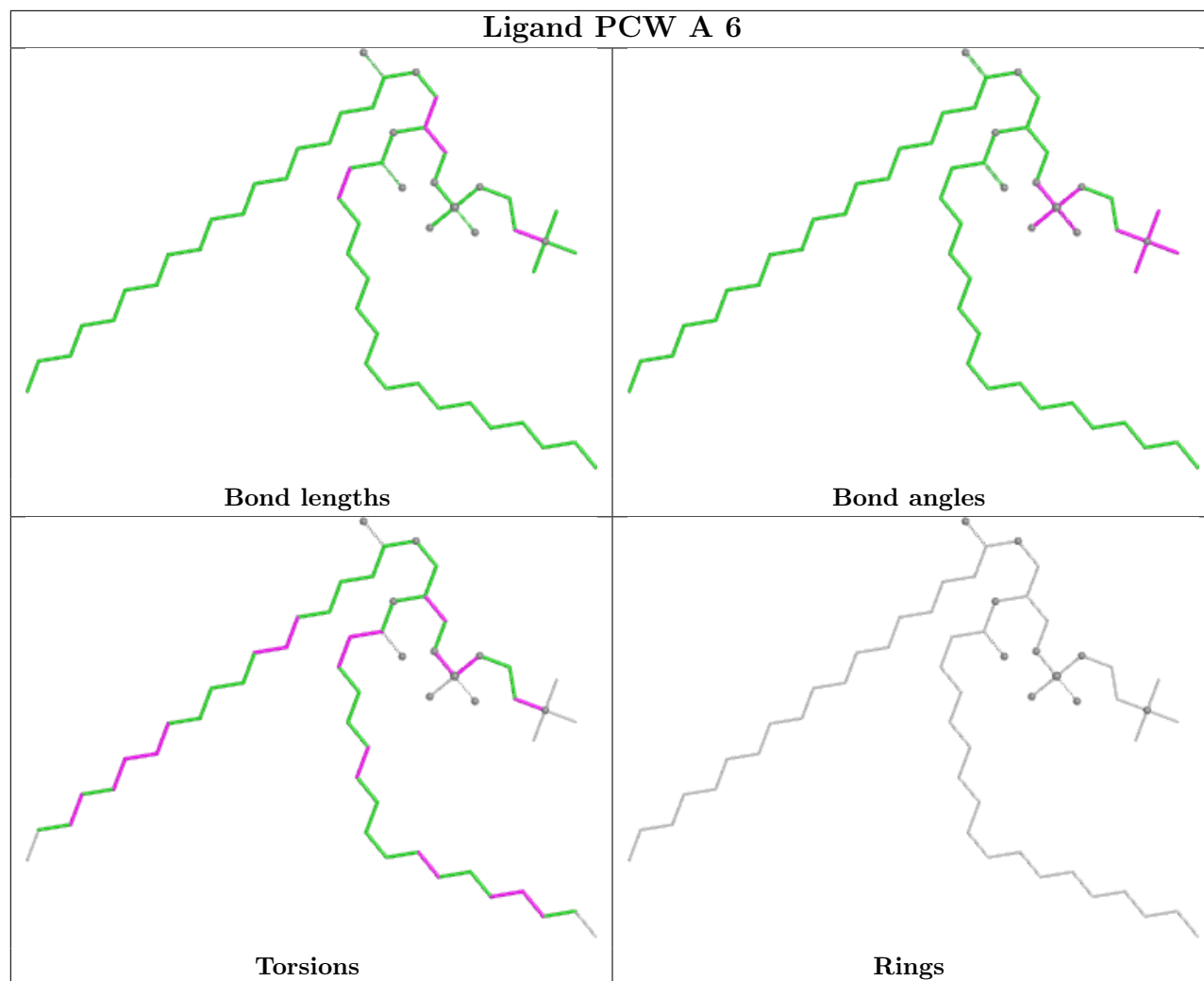


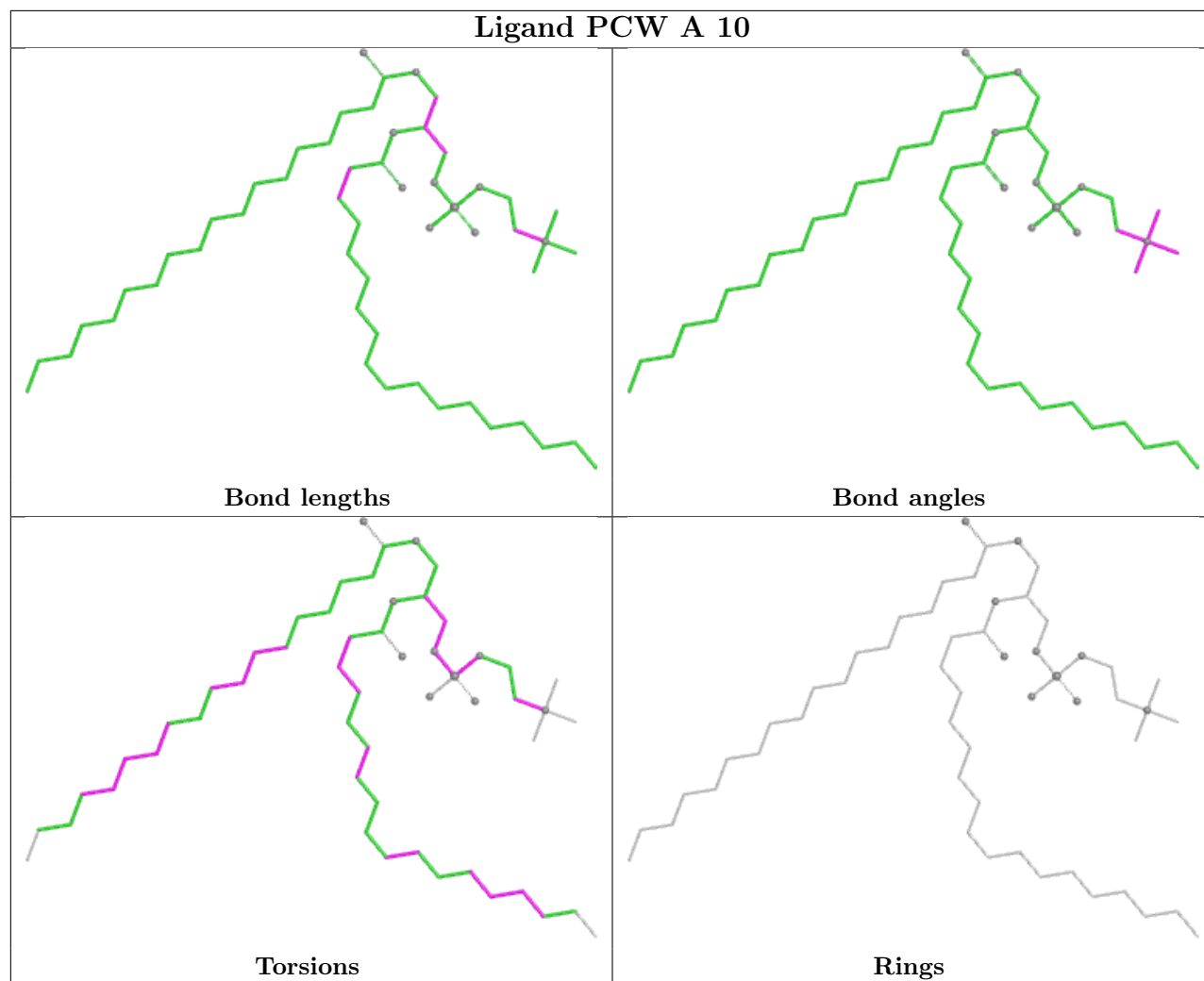


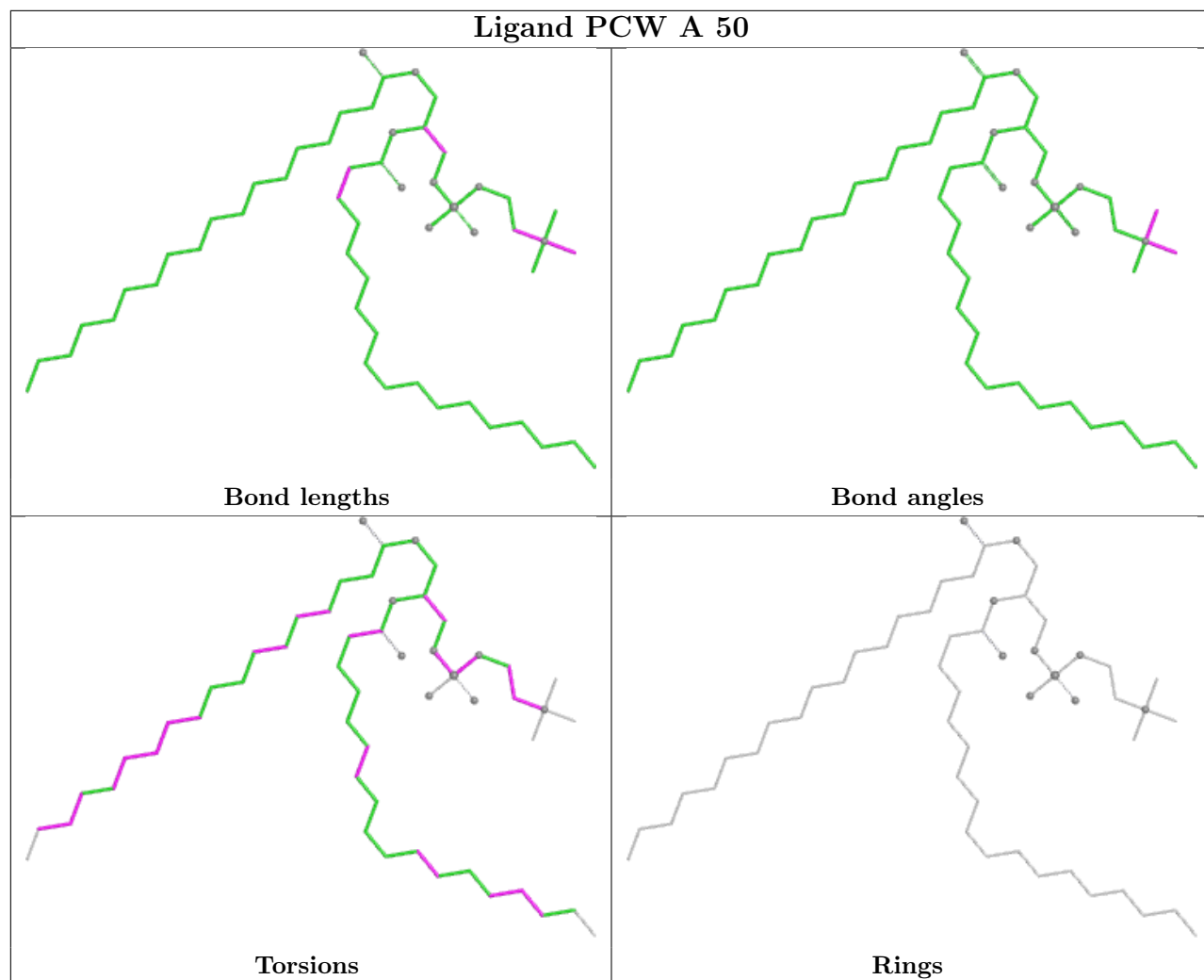


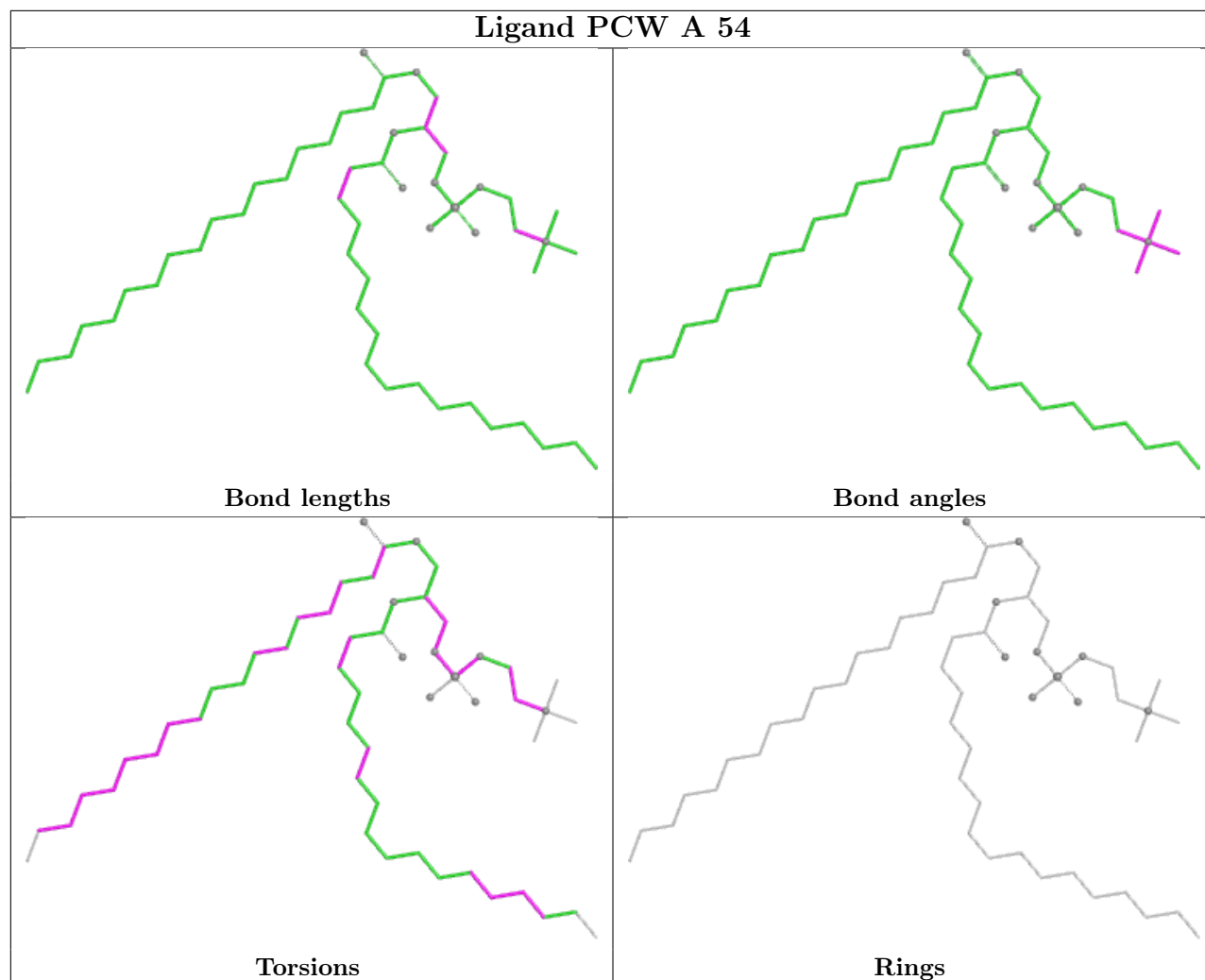


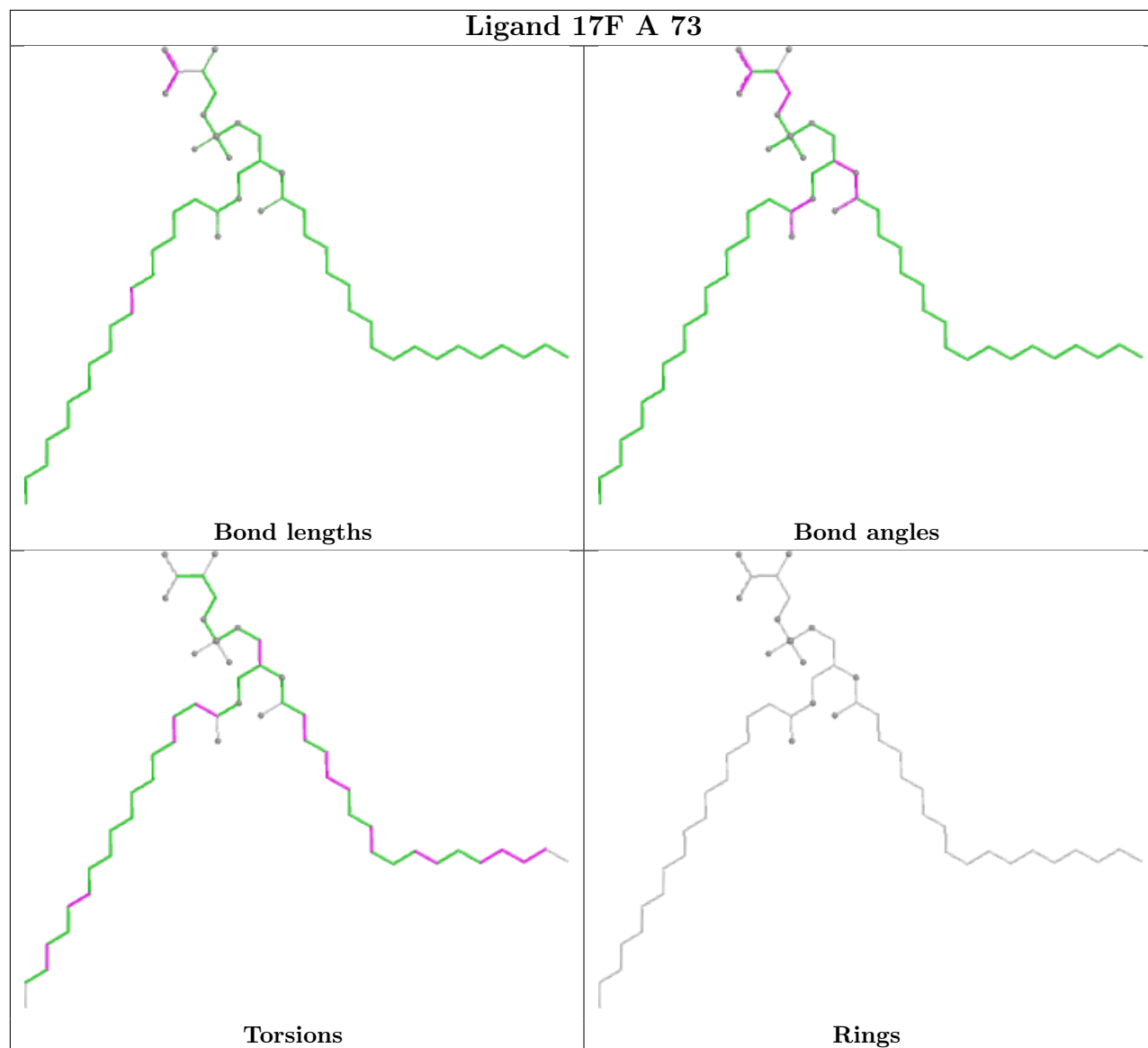


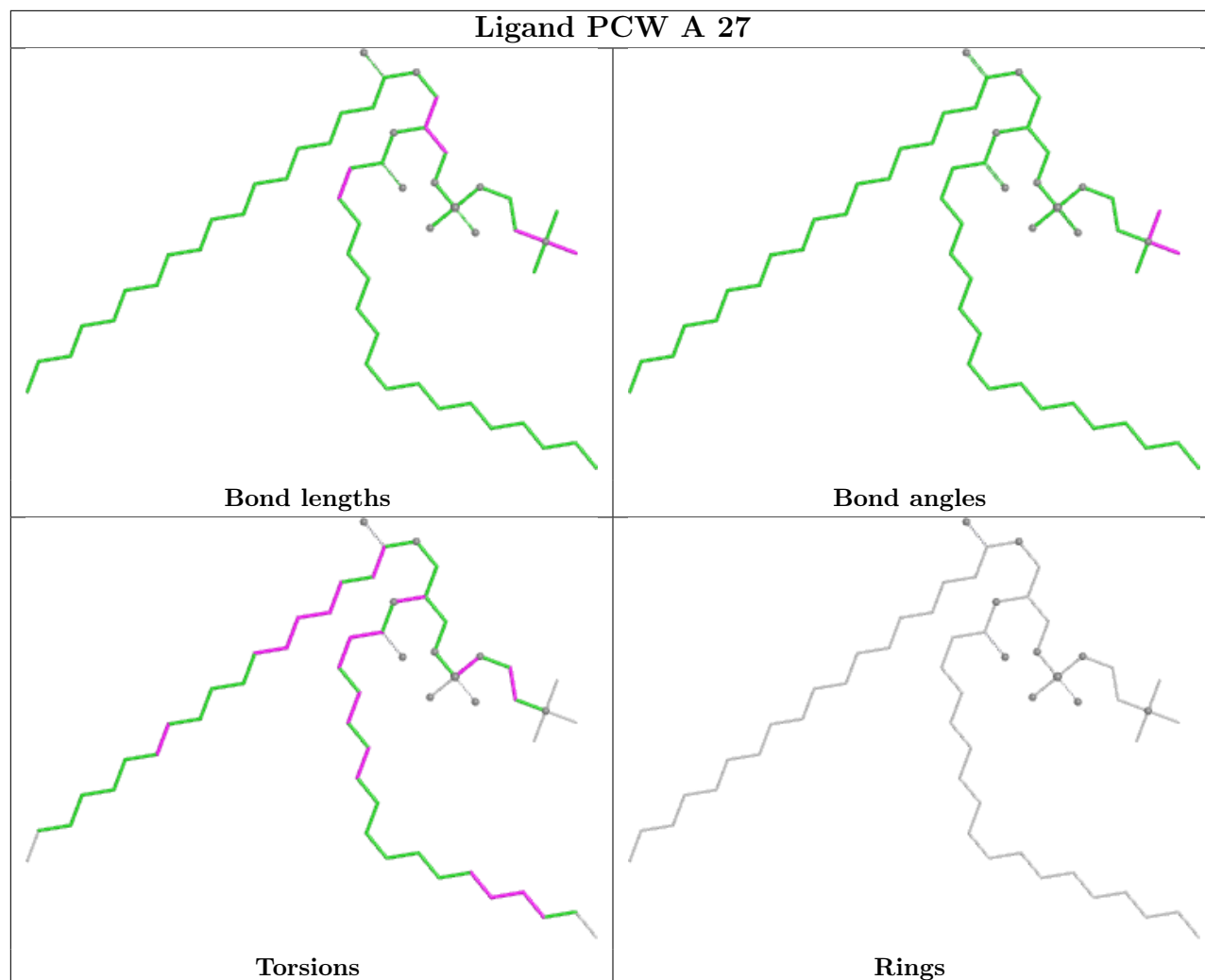


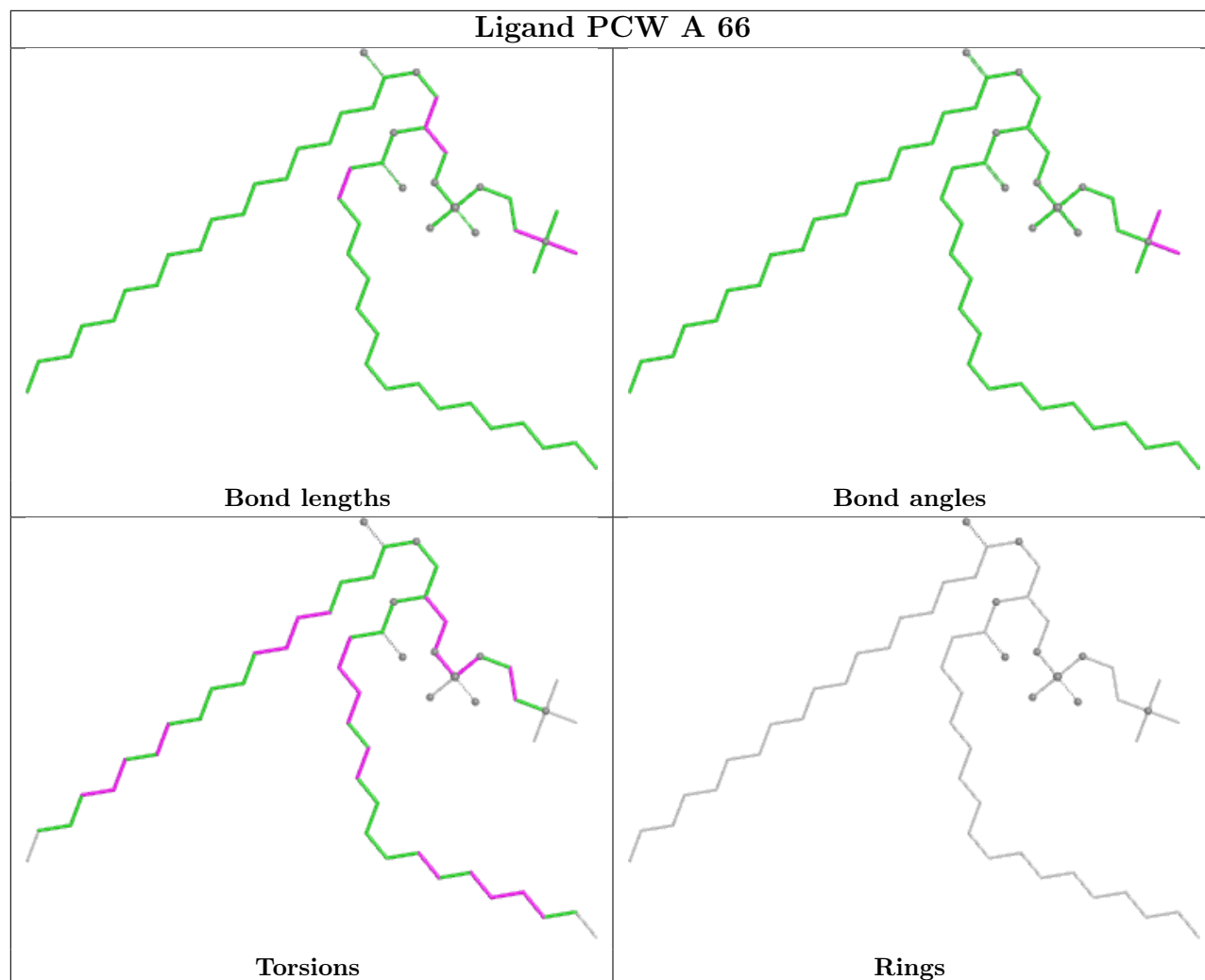


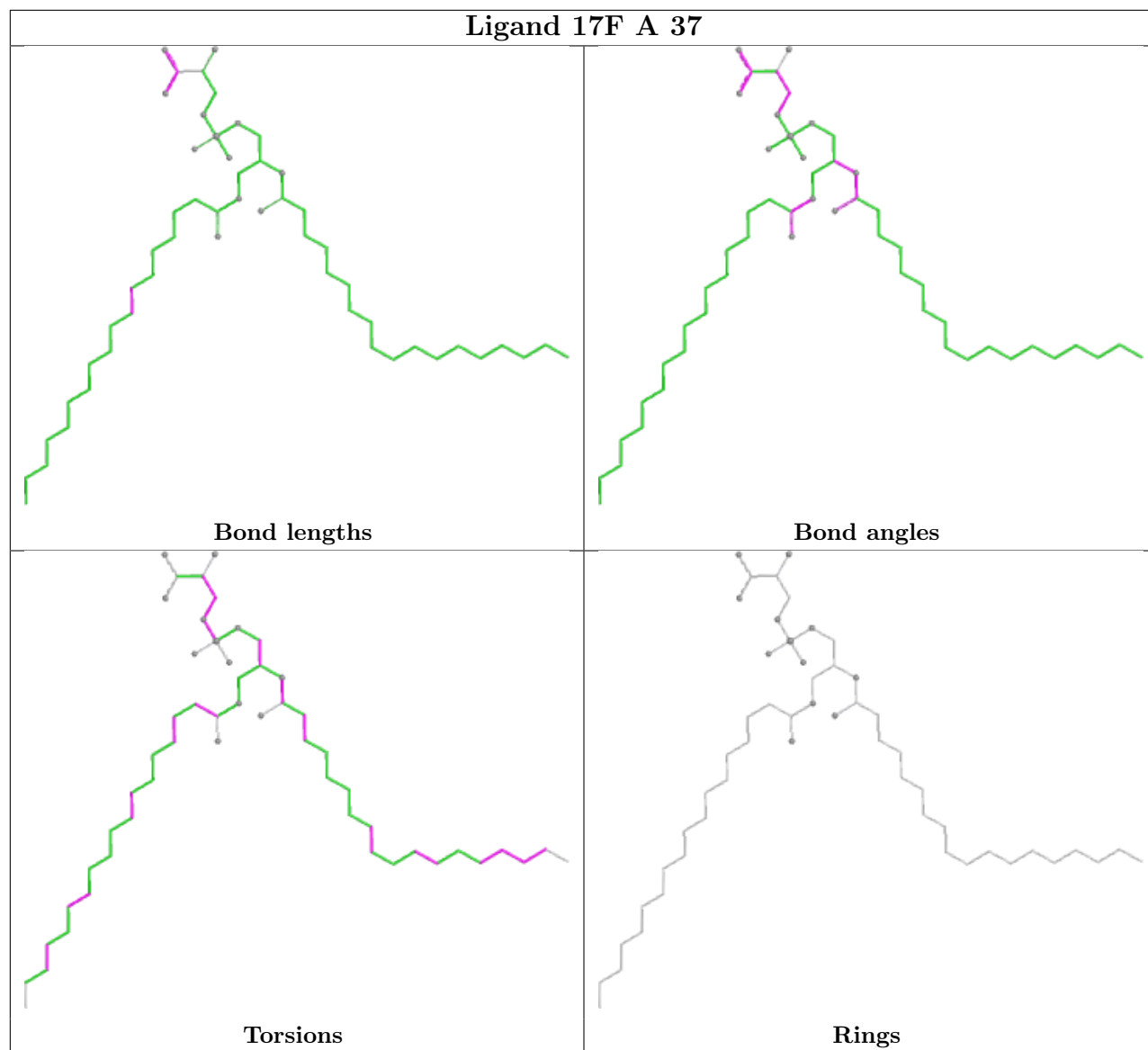


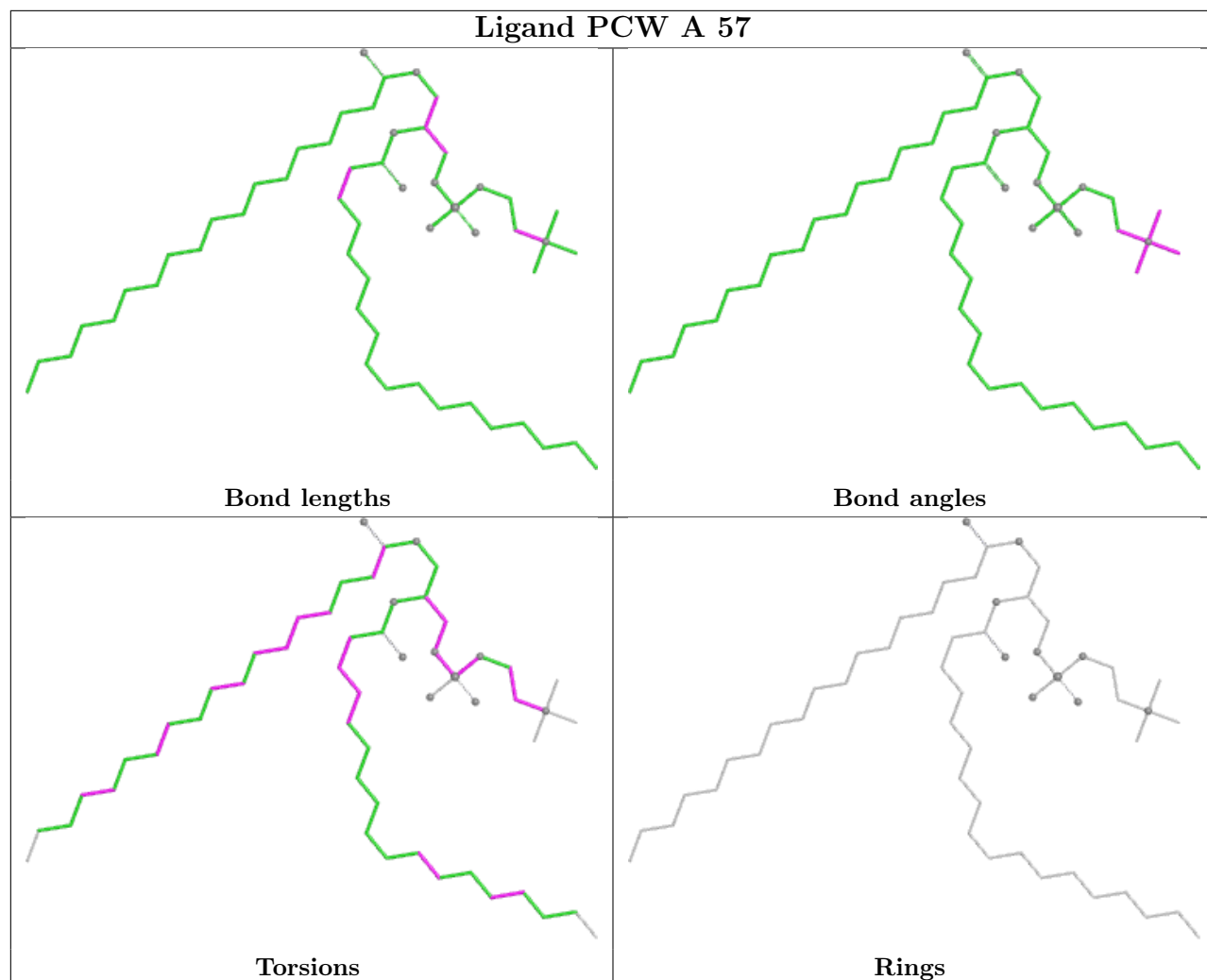


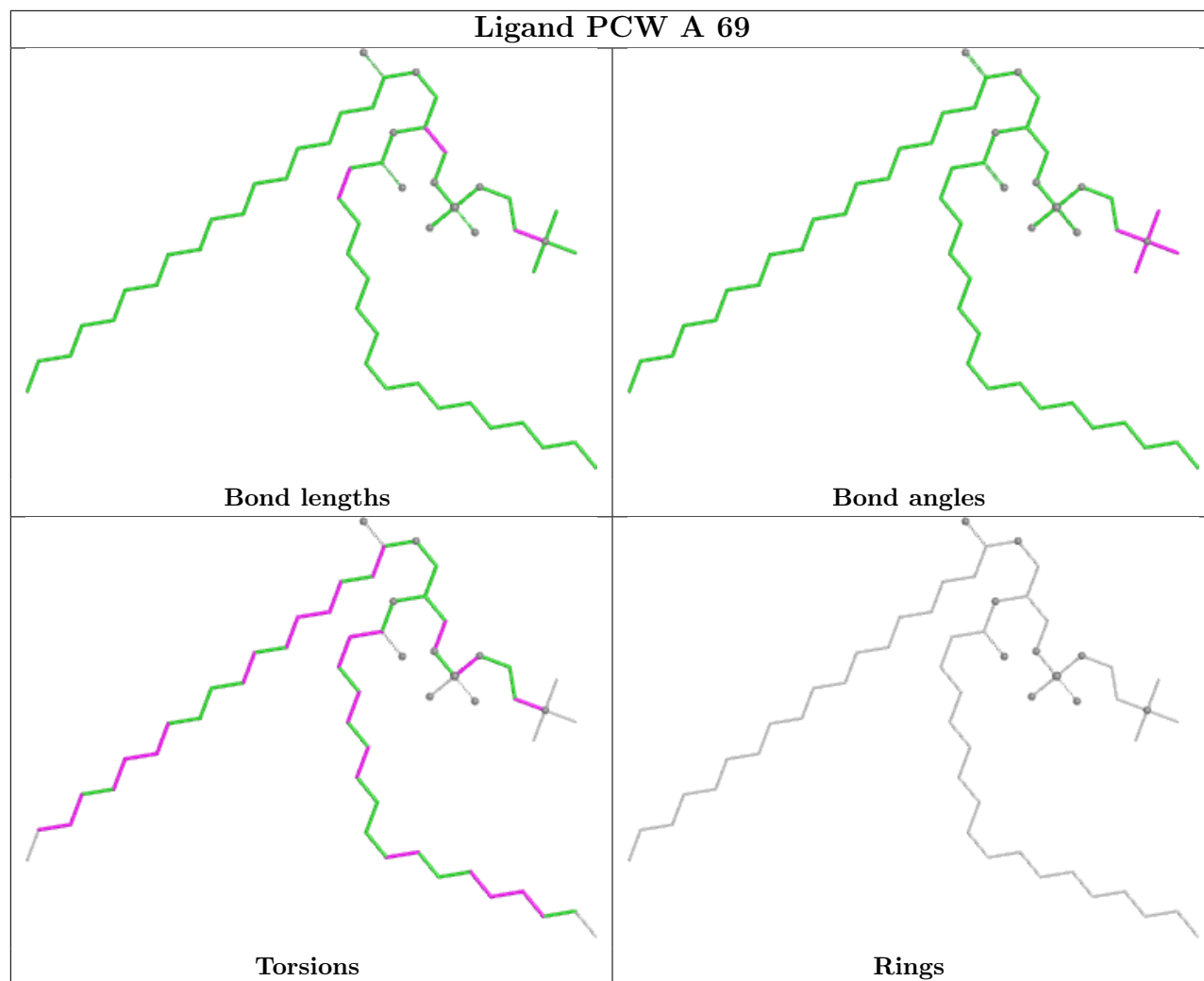


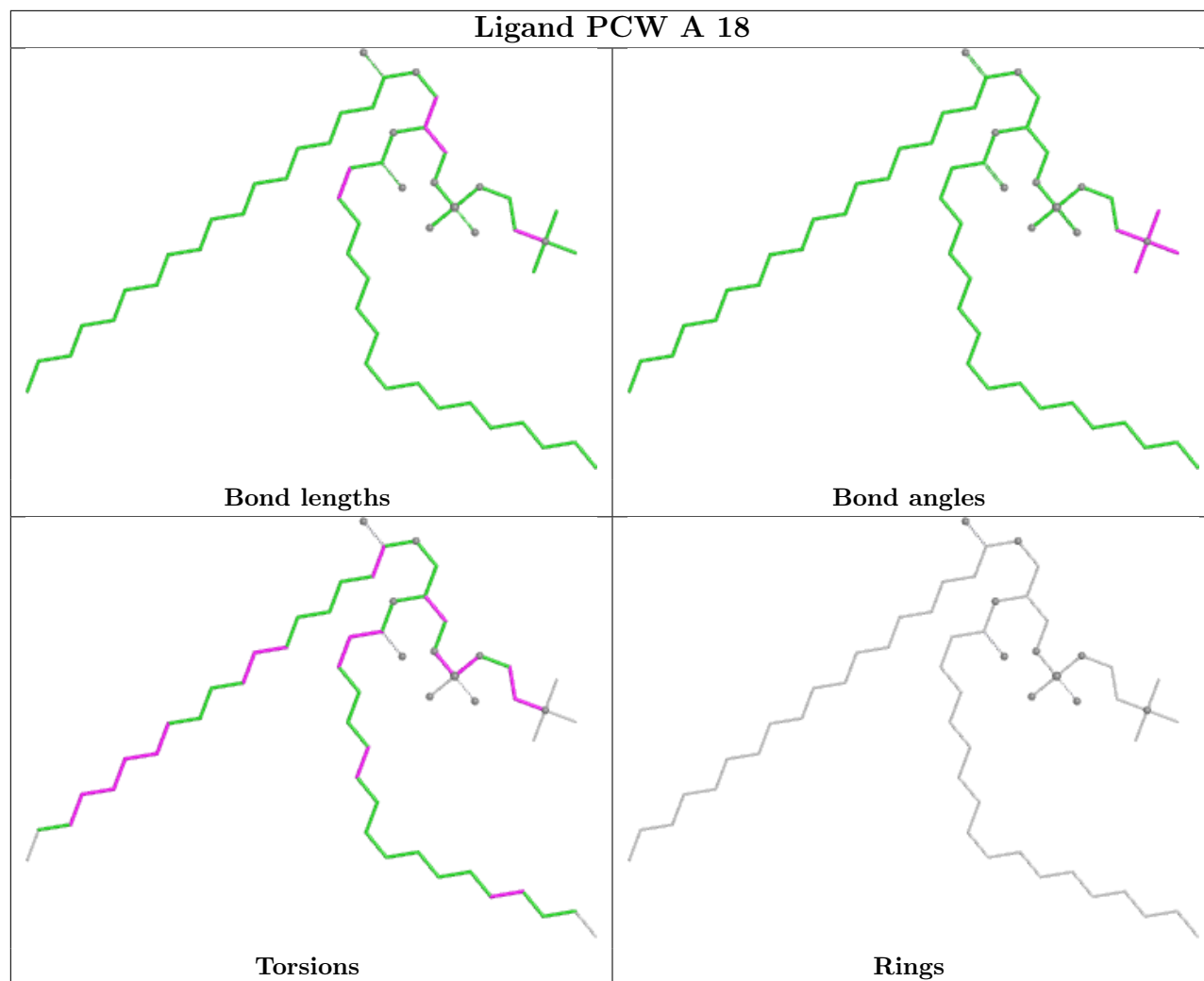


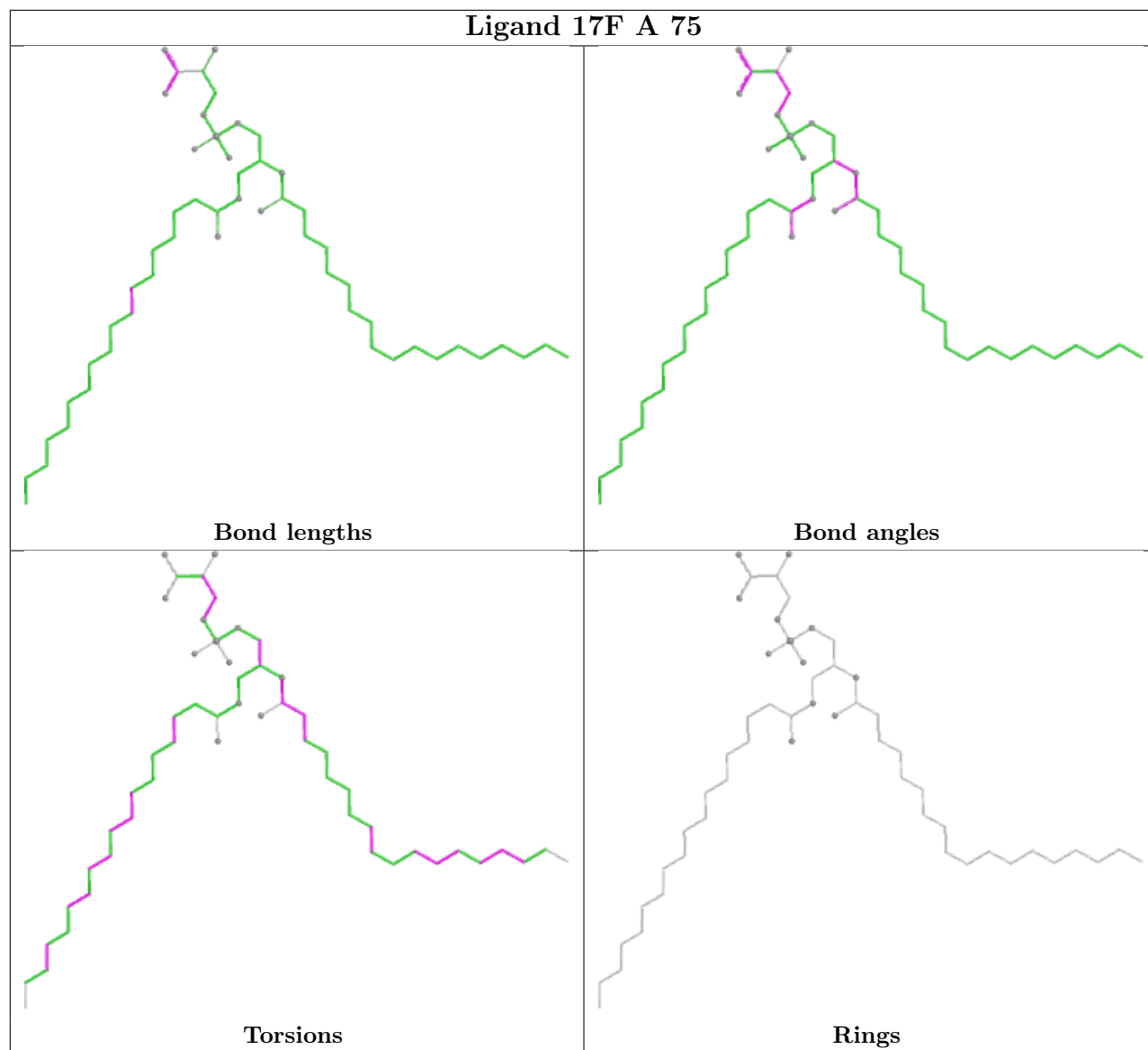


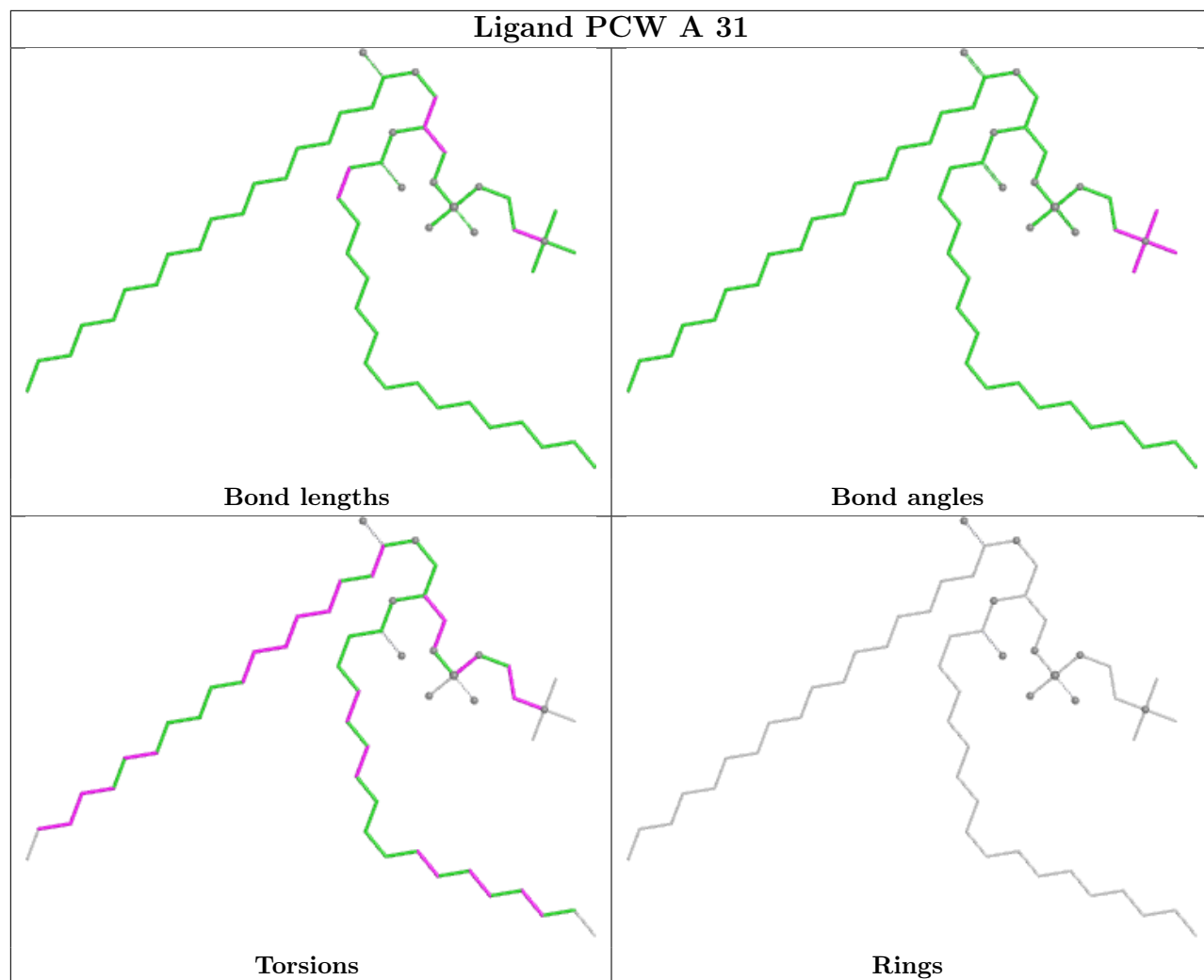


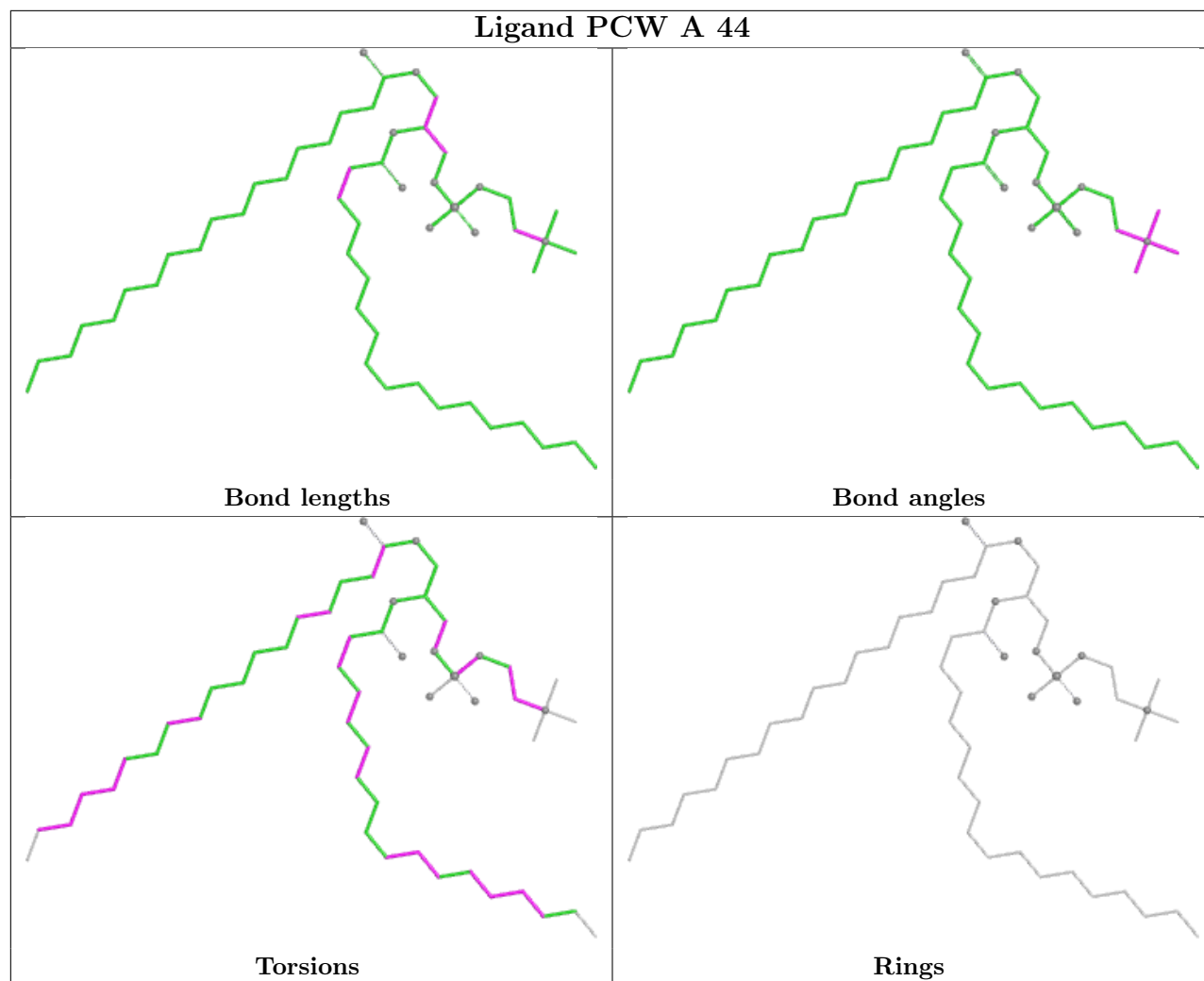


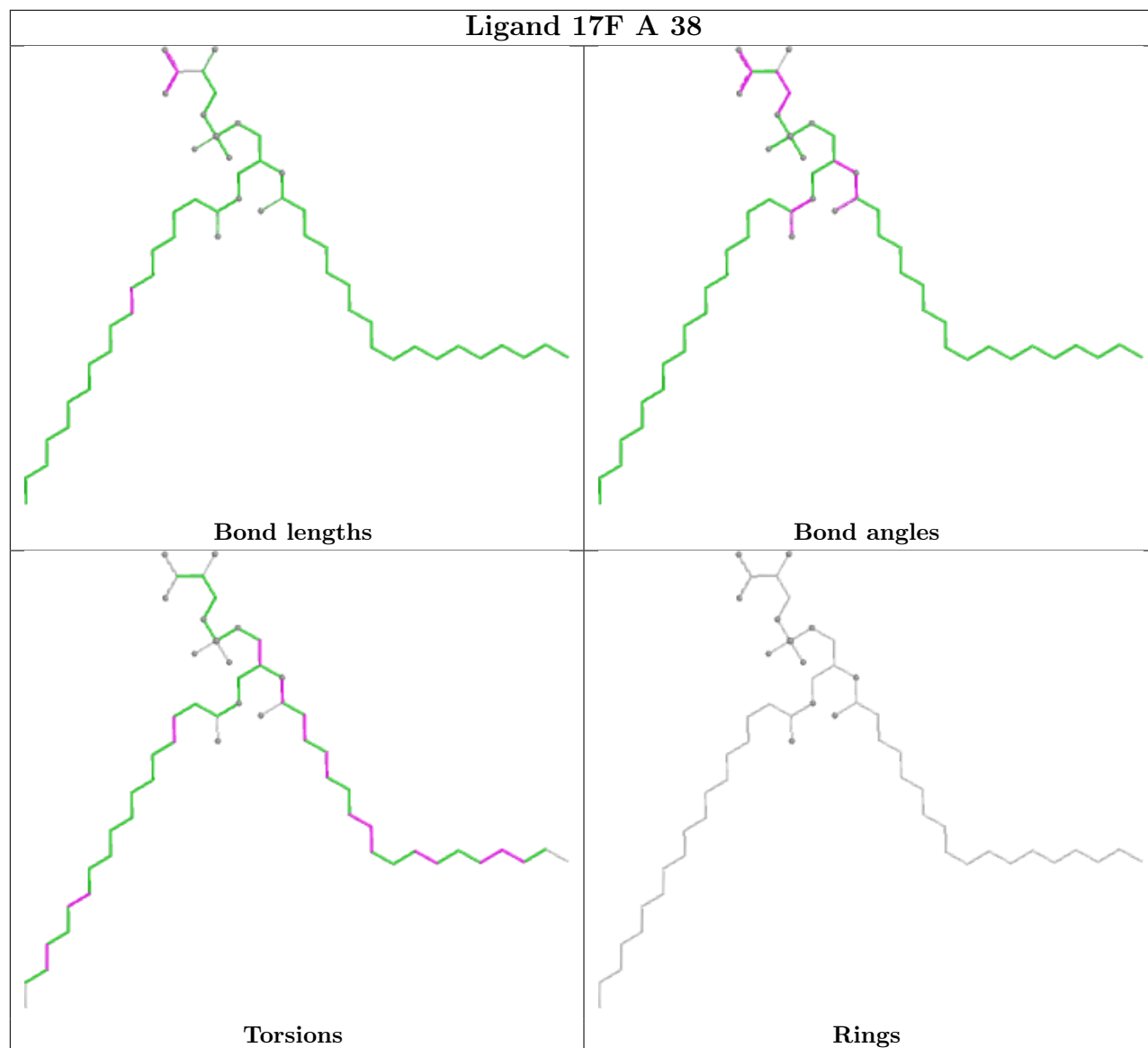


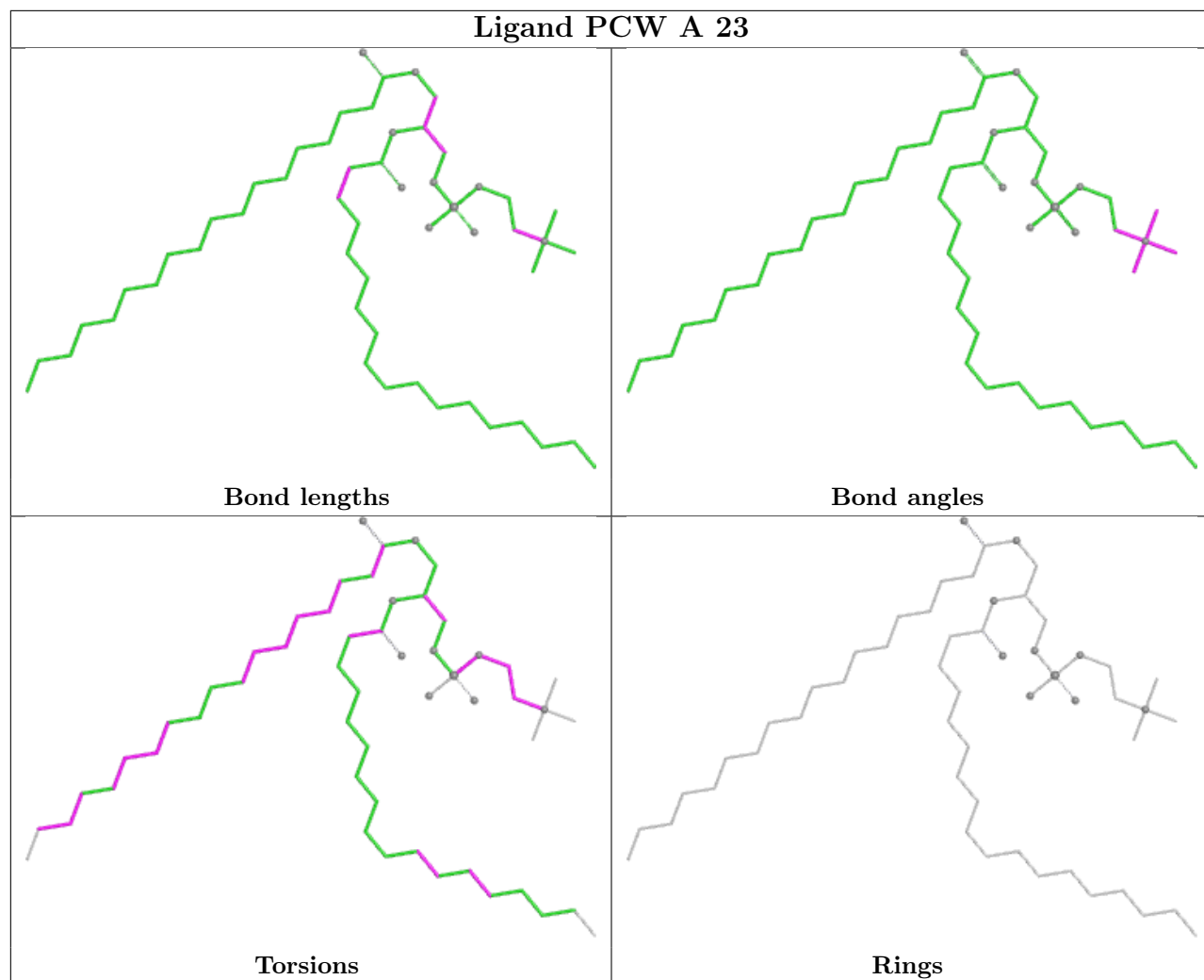


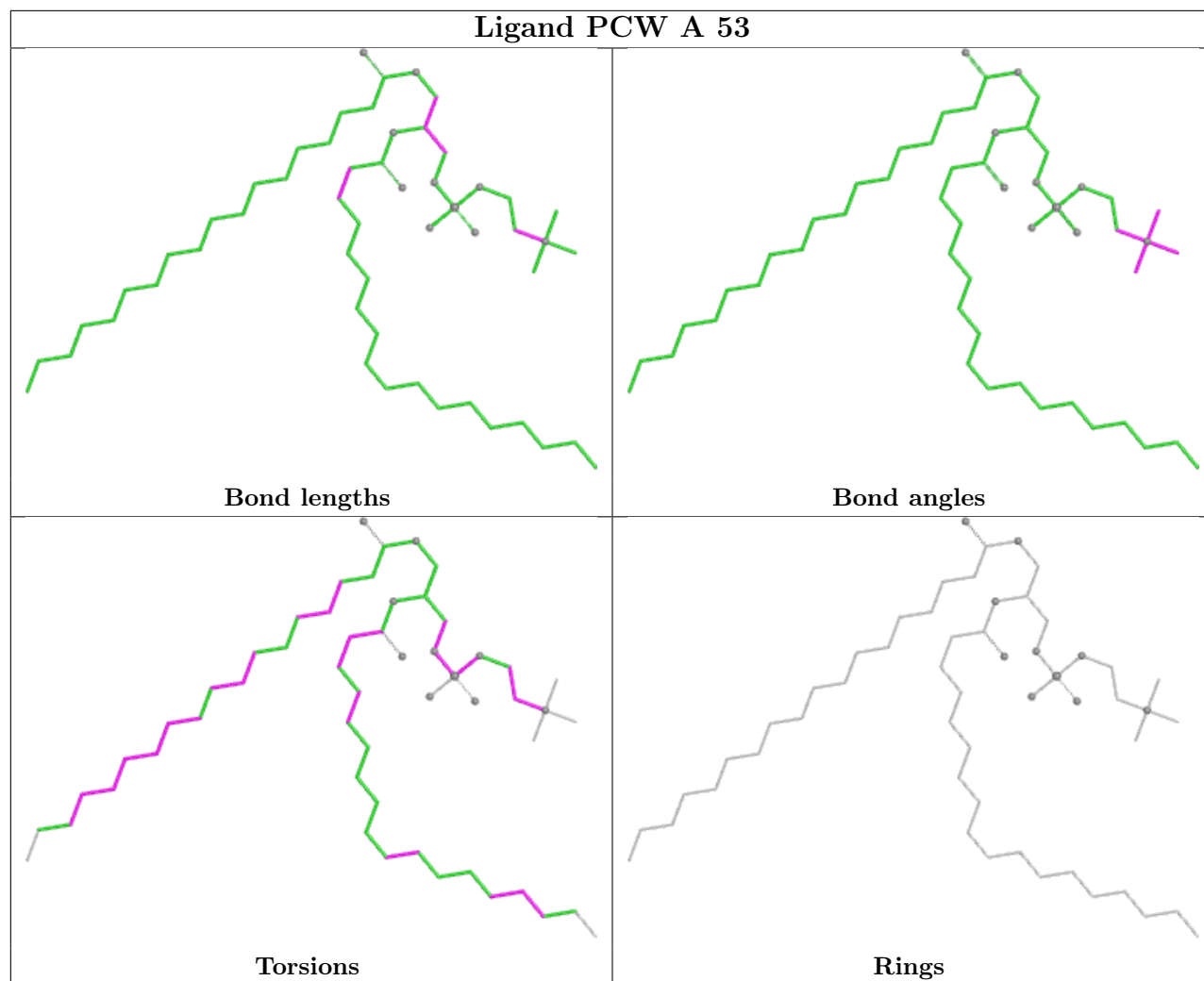


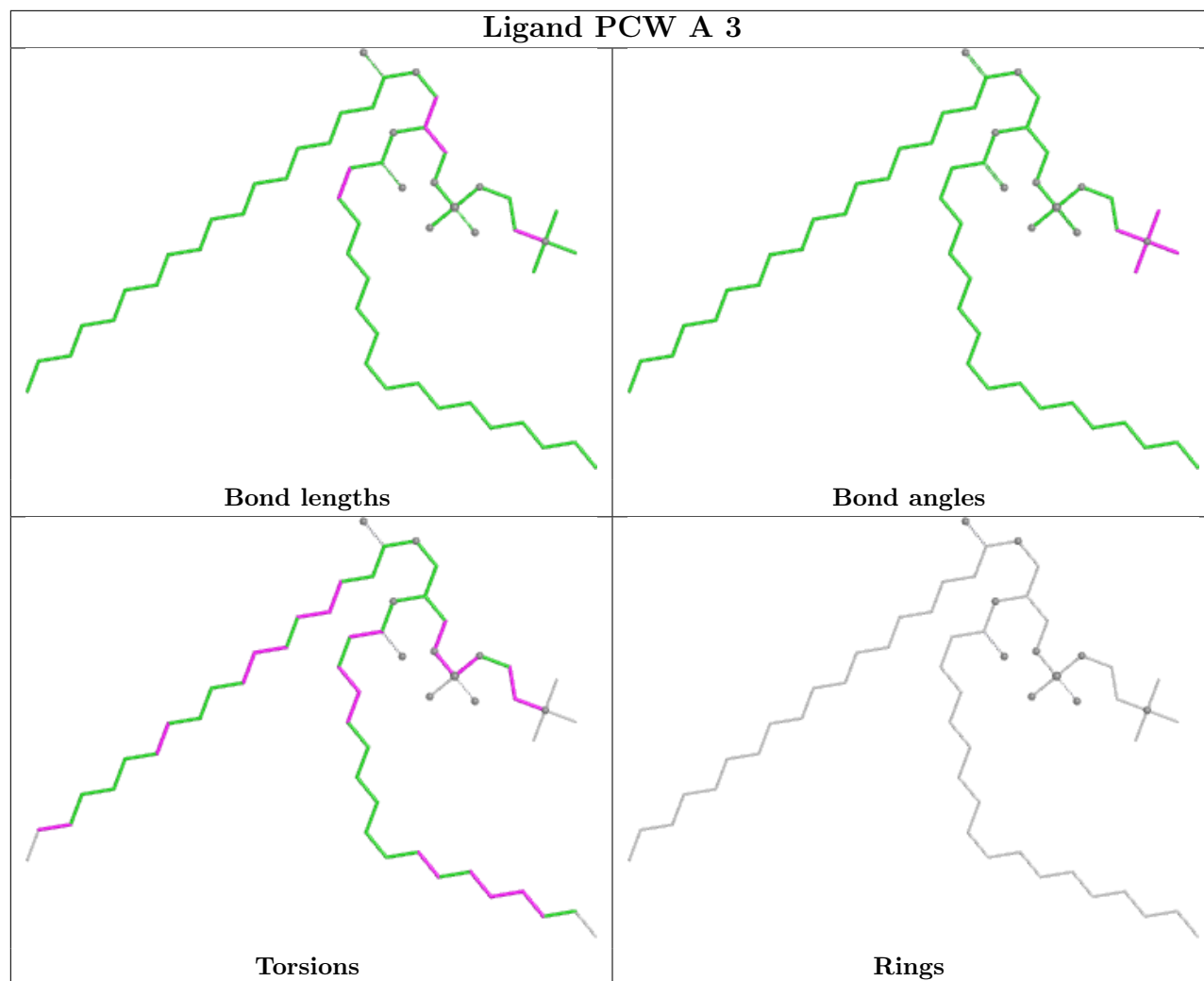


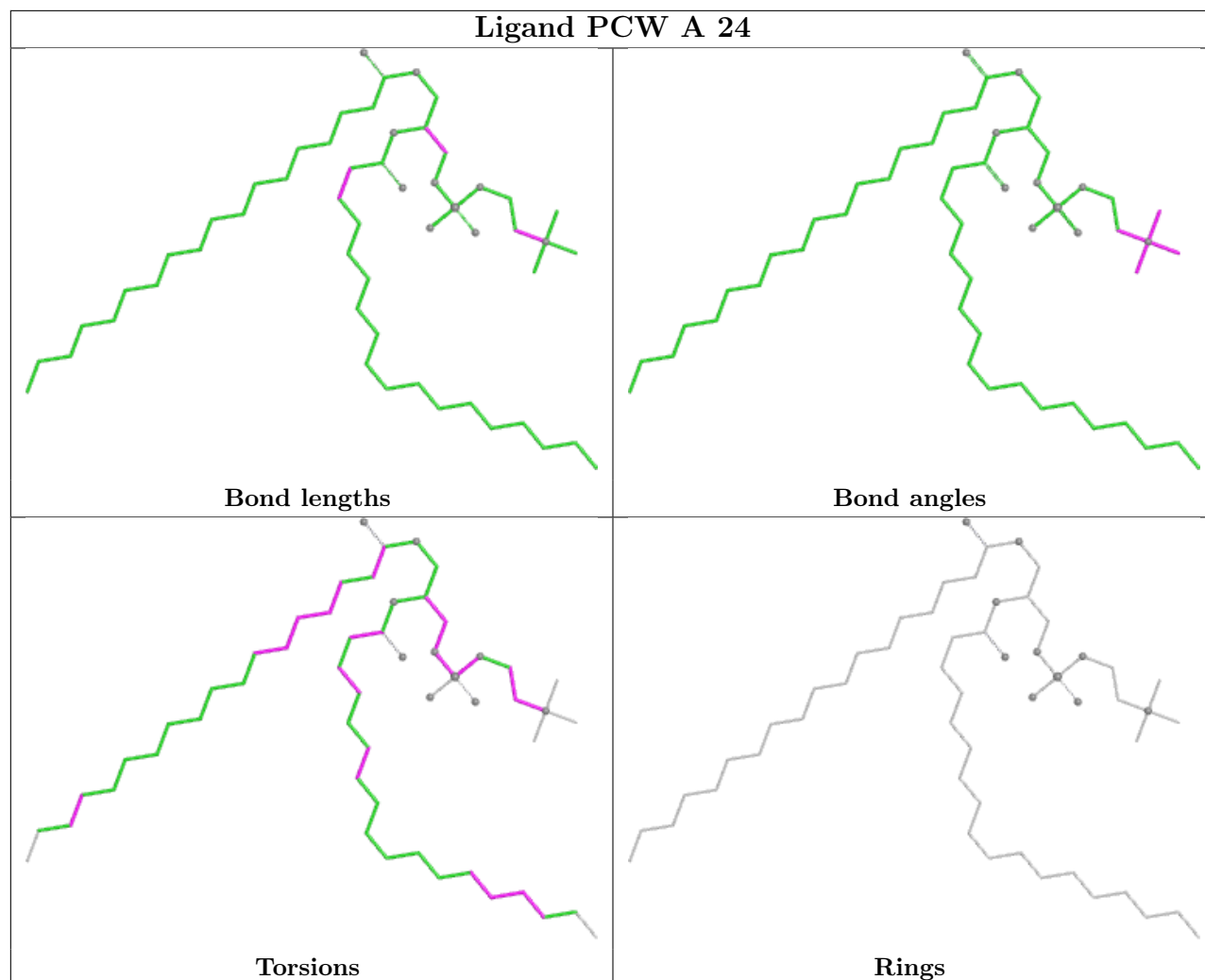


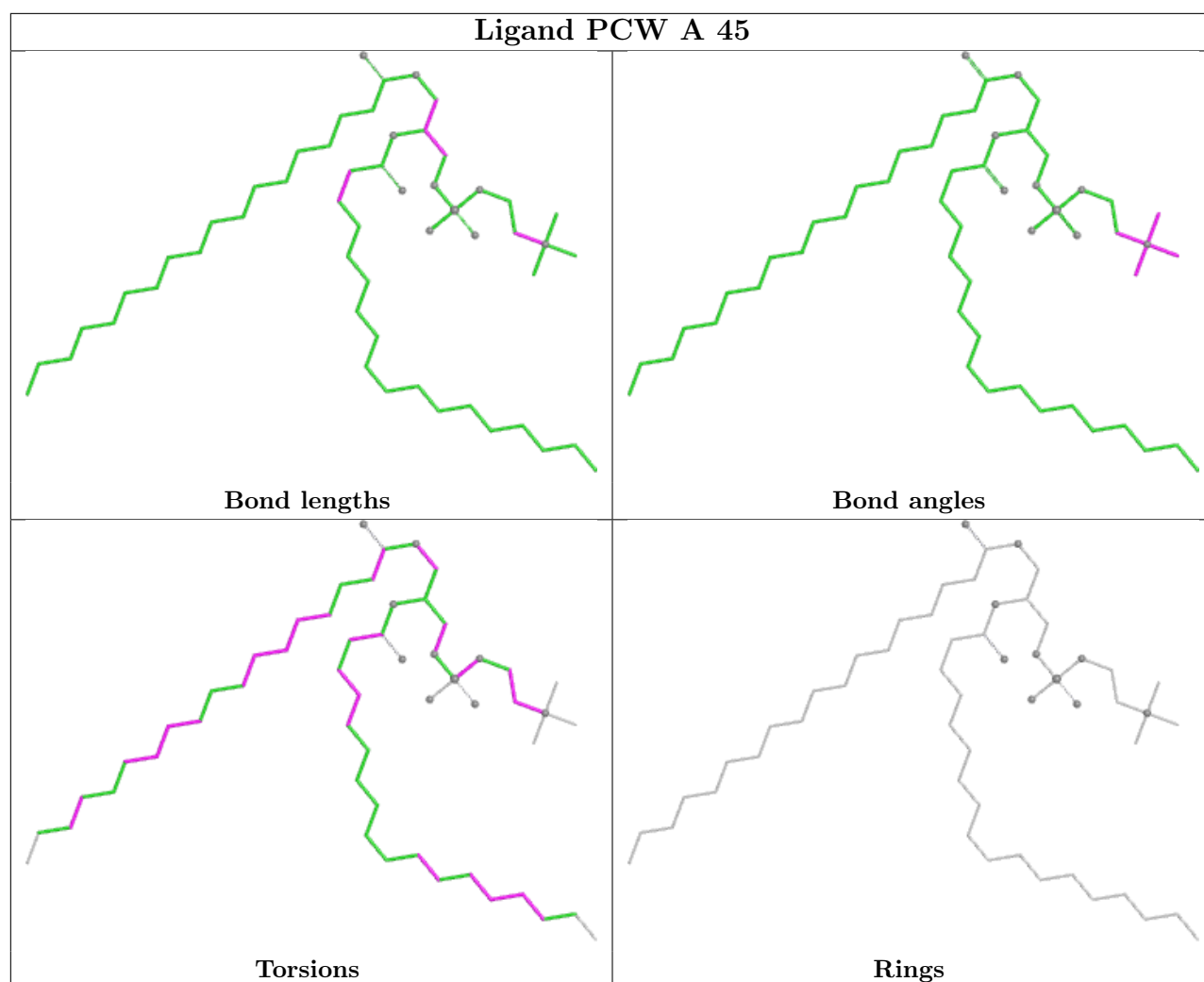












## 6.7 Other polymers [i](#)

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 1% for the well-defined parts and 1% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_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	11
Number of unparsed shifts	0
Number of shifts with mapping errors	33
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 33 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	21	ILE	HD11	0.511	?	1
1	B	21	ILE	HD12	0.511	?	1
1	B	21	ILE	HD13	0.511	?	1
1	B	24	ILE	HD11	0.398	?	1
1	B	24	ILE	HD12	0.398	?	1
1	B	24	ILE	HD13	0.398	?	1
1	B	36	ILE	HD11	0.708	?	1
1	B	36	ILE	HD12	0.708	?	1
1	B	36	ILE	HD13	0.708	?	1
1	B	46	ILE	HD11	0.374	?	1
1	B	46	ILE	HD12	0.374	?	1
1	B	46	ILE	HD13	0.374	?	1
1	B	55	ILE	HD11	0.458	?	1
1	B	55	ILE	HD12	0.458	?	1

*Continued on next page...*

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	55	ILE	HD13	0.458	?	1
1	B	84	ILE	HD11	0.707	?	1
1	B	84	ILE	HD12	0.707	?	1
1	B	84	ILE	HD13	0.707	?	1
1	B	93	ILE	HD11	0.727	?	1
1	B	93	ILE	HD12	0.727	?	1
1	B	93	ILE	HD13	0.727	?	1
1	B	100	ILE	HD11	0.238	?	1
1	B	100	ILE	HD12	0.238	?	1
1	B	100	ILE	HD13	0.238	?	1
1	B	139	ILE	HD11	0.82	?	1
1	B	139	ILE	HD12	0.82	?	1
1	B	139	ILE	HD13	0.82	?	1
1	B	142	ILE	HD11	0.624	?	1
1	B	142	ILE	HD12	0.624	?	1
1	B	142	ILE	HD13	0.624	?	1
1	B	163	ILE	HD11	0.629	?	1
1	B	163	ILE	HD12	0.629	?	1
1	B	163	ILE	HD13	0.629	?	1

### 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 1%, i.e. 44 atoms were assigned a chemical shift out of a possible 7885. 0 out of 106 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/2794 (0%)	0/1129 (0%)	0/1122 (0%)	0/543 (0%)
Sidechain	44/4619 (1%)	33/2968 (1%)	11/1446 (1%)	0/205 (0%)
Aromatic	0/472 (0%)	0/244 (0%)	0/228 (0%)	0/0 (—%)
Overall	44/7885 (1%)	33/4341 (1%)	11/2796 (0%)	0/748 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 44 atoms were assigned a chemical shift out of a possible 8175. 0 out of 108 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/2895 (0%)	0/1170 (0%)	0/1162 (0%)	0/563 (0%)
Sidechain	44/4808 (1%)	33/3087 (1%)	11/1505 (1%)	0/216 (0%)
Aromatic	0/472 (0%)	0/244 (0%)	0/228 (0%)	0/0 (—%)
Overall	44/8175 (1%)	33/4501 (1%)	11/2895 (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](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B:

