



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 01:47 PM UTC

PDB ID : 2MSE / pdb_00002mse
BMRB ID : 25116
Title : NMR data-driven model of GTPase KRas-GNP:ARafRBD complex 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

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>.

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

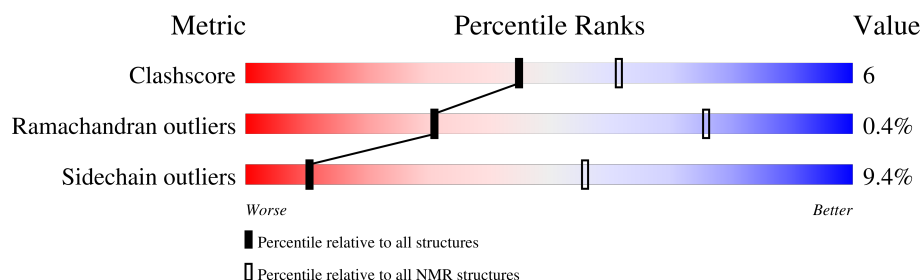
1 Overall quality at a glance

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 ≥ 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	68% 10% 20% .
1	C	200	86% 11% ..
2	B	187	77% 14% 8% .
3	D	73	79% 21%

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:239-A:395, C:401-C:596 (353)	0.44	3
2	B:2-B:171, D:808-D:880 (243)	0.95	5

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9709 atoms, of which 64 are hydrogens and 0 are deuteriums.

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

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

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
2	B	185	Total	C	H	N	O	S	0
			1492	923	16	257	287	9	

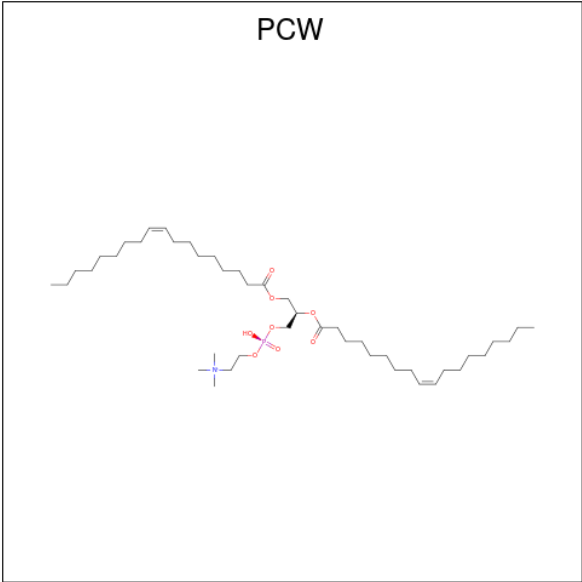
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Serine/threonine-protein kinase A-Raf.

Mol	Chain	Residues	Atoms						Trace
3	D	73	Total	C	H	N	O	S	0
			573	360	4	99	107	3	

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



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

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

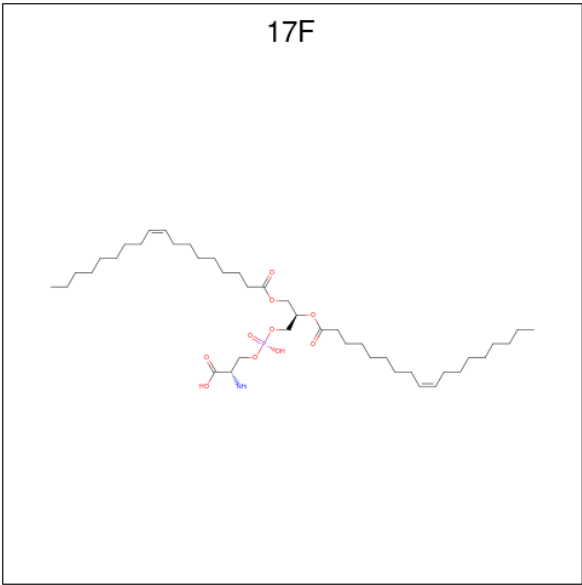
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphor
yl]-L-serine (CCD ID: 17F) (formula: C₄₂H₇₈NO₁₀P).



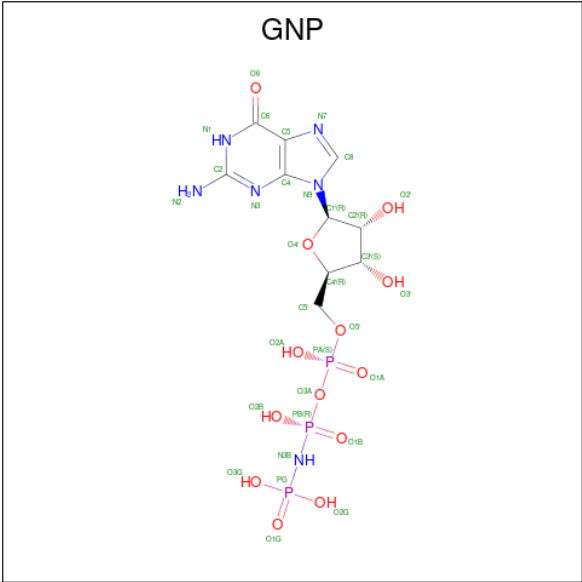
Mol	Chain	Residues	Atoms				
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1

Continued on next page...

Continued from previous page...

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

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
6	B	1	32	10	6	13	3

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
			Total	Mg
7	B	1	1	1

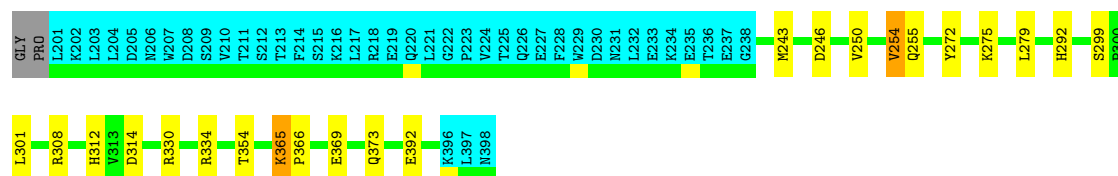
4 Residue-property plots

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

Chain A: 



- Molecule 1: Apolipoprotein A-I

Chain C: 



- Molecule 2: GTPase KRas

Chain B: 



- Molecule 3: Serine/threonine-protein kinase A-Raf

Chain D: 



4.2 Scores per residue for each member of the ensemble

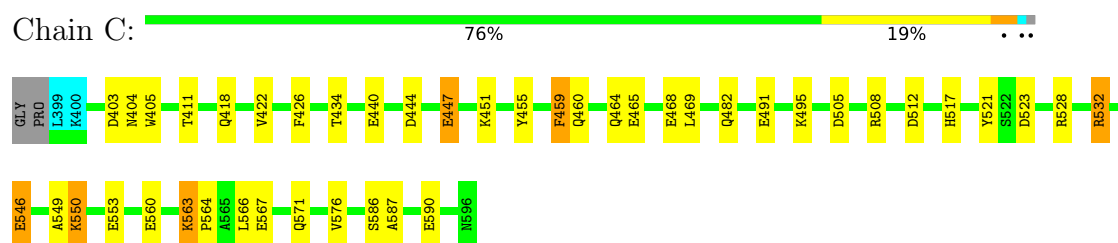
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

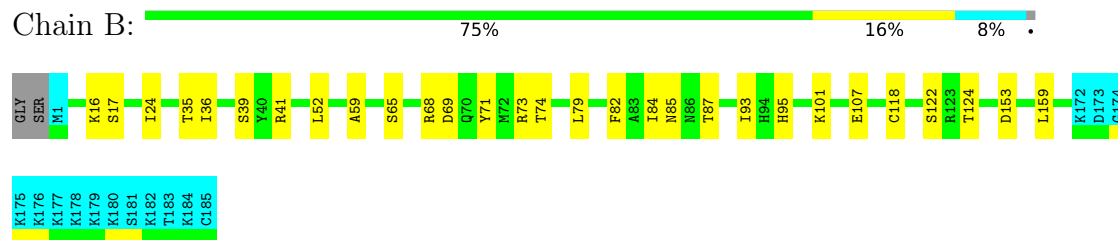
- Molecule 1: Apolipoprotein A-I



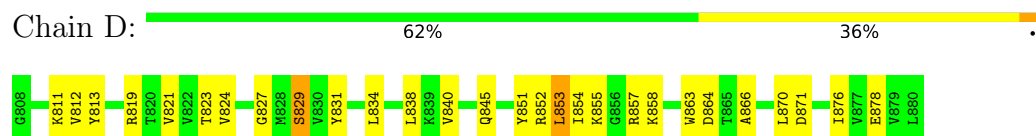
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



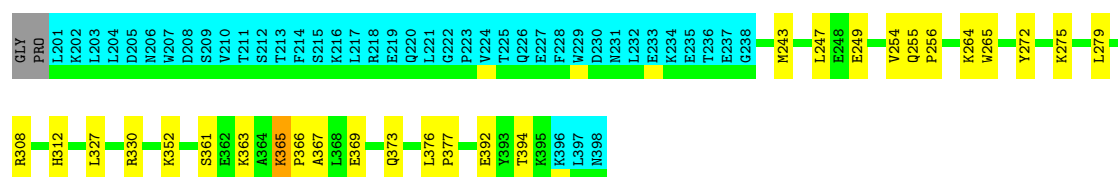
- Molecule 3: Serine/threonine-protein kinase A-Raf



4.2.2 Score per residue for model 2

- Molecule 1: Apolipoprotein A-I





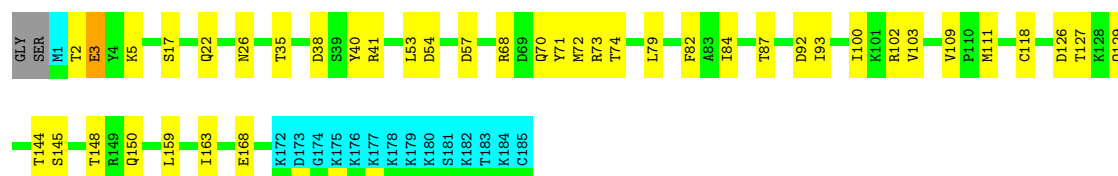
• Molecule 1: Apolipoprotein A-I

Chain C: 79% 18% ...



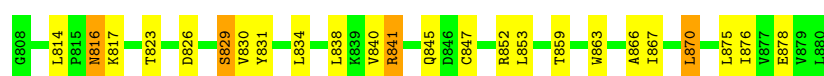
• Molecule 2: GTPase KRas

Chain B: 69% 21% 8%



• Molecule 3: Serine/threonine-protein kinase A-Raf

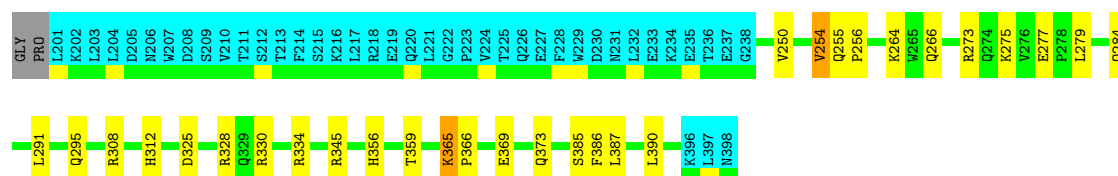
Chain D: 67% 27% 5%



4.2.3 Score per residue for model 3 (medoid)

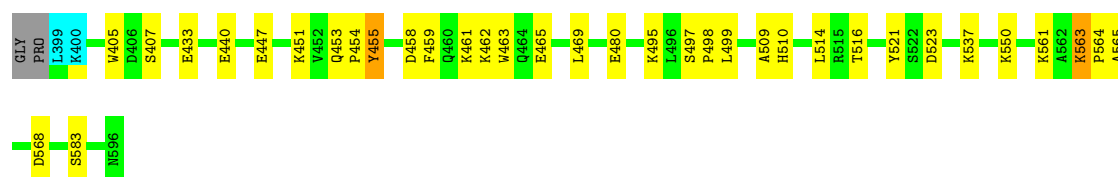
• Molecule 1: Apolipoprotein A-I

Chain A: 64% 14% 20%



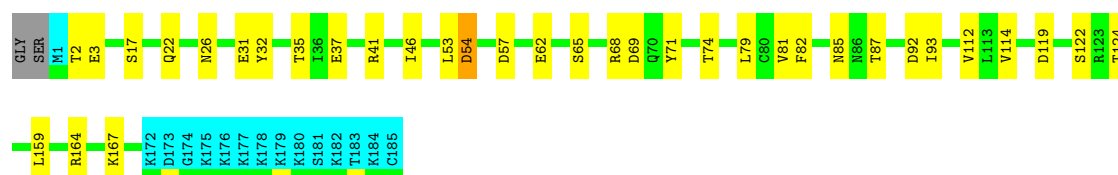
• Molecule 1: Apolipoprotein A-I

Chain C: 80% 16% ...



- Molecule 2: GTPase KRas

Chain B: 72% 18% 8%



- Molecule 3: Serine/threonine-protein kinase A-Raf

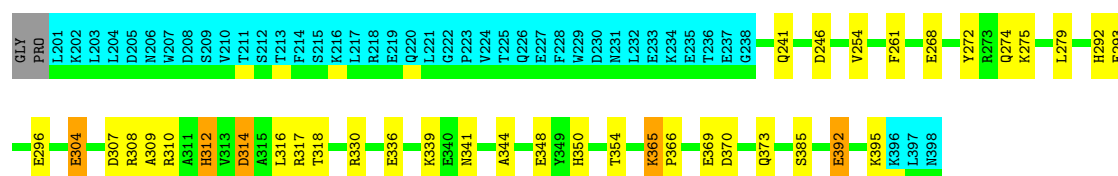
Chain D: 68% 29%



4.2.4 Score per residue for model 4

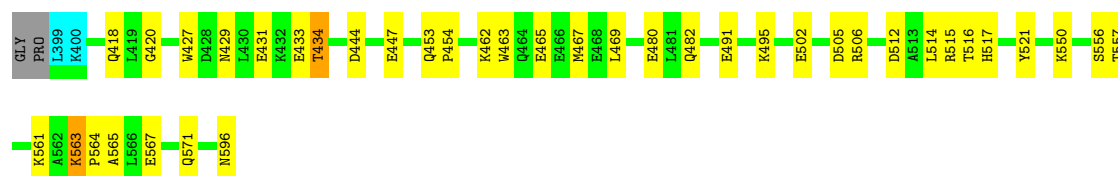
- Molecule 1: Apolipoprotein A-I

Chain A: 60% 16% 20%



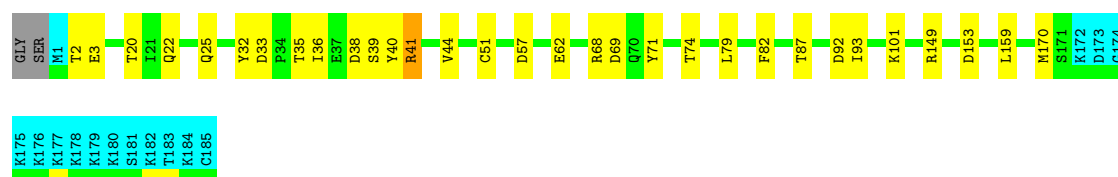
- Molecule 1: Apolipoprotein A-I

Chain C: 78% 18%



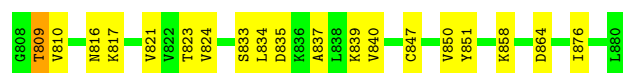
- Molecule 2: GTPase KRas

Chain B: 74% 16% 8%



- Molecule 3: Serine/threonine-protein kinase A-Raf

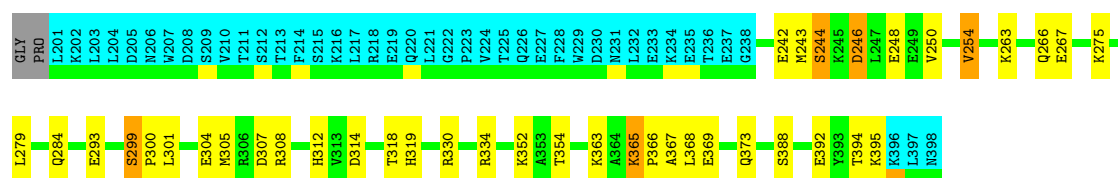
Chain D: 74% 25%



4.2.5 Score per residue for model 5

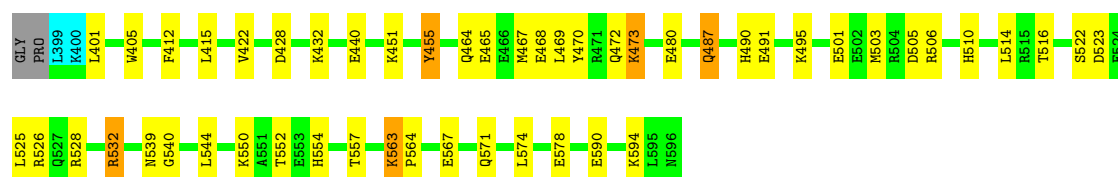
- Molecule 1: Apolipoprotein A-I

Chain A: 58% 18% 20%



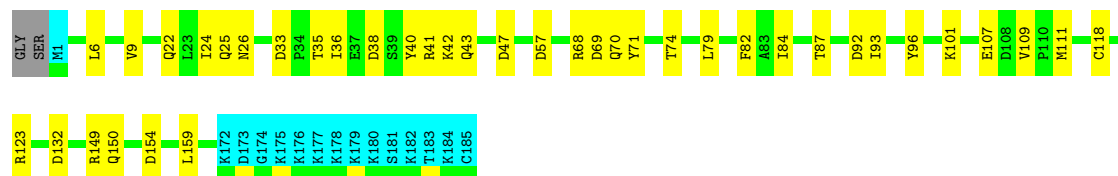
- Molecule 1: Apolipoprotein A-I

Chain C: 72% 23%



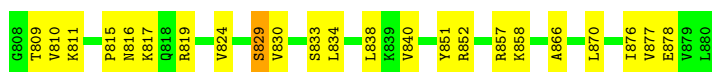
- Molecule 2: GTPase KRas

Chain B: 70% 21% 8%



- Molecule 3: Serine/threonine-protein kinase A-Raf

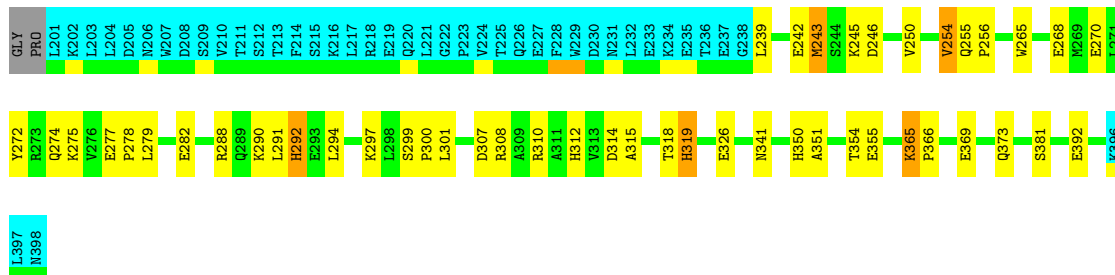
Chain D: 68% 30%



4.2.6 Score per residue for model 6

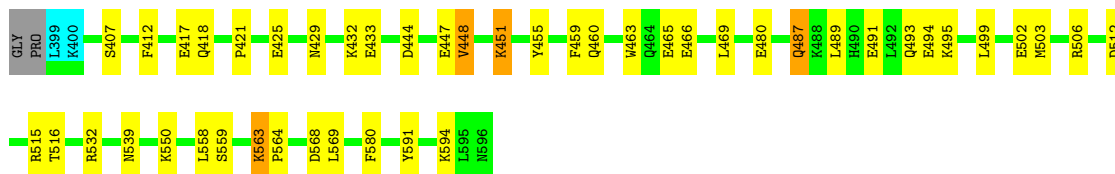
- Molecule 1: Apolipoprotein A-I

Chain A: 54% 22% 20%



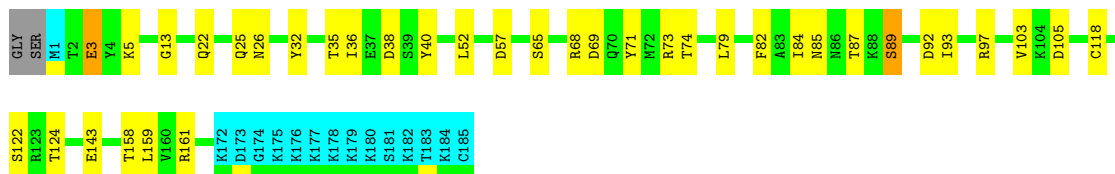
- Molecule 1: Apolipoprotein A-I

Chain C: 75% 21%



- Molecule 2: GTPase KRas

Chain B: 71% 19% 8%



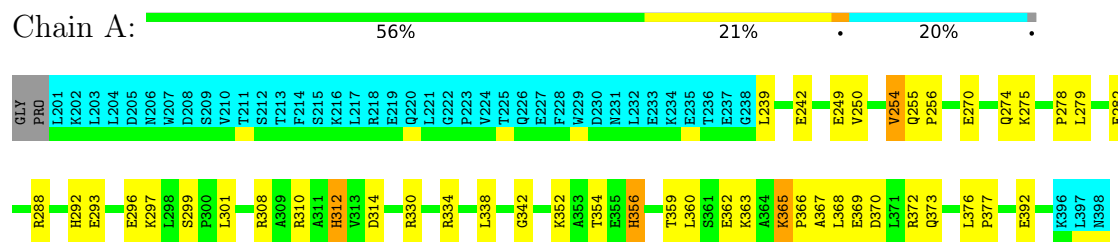
- Molecule 3: Serine/threonine-protein kinase A-Raf

Chain D: 78% 19%

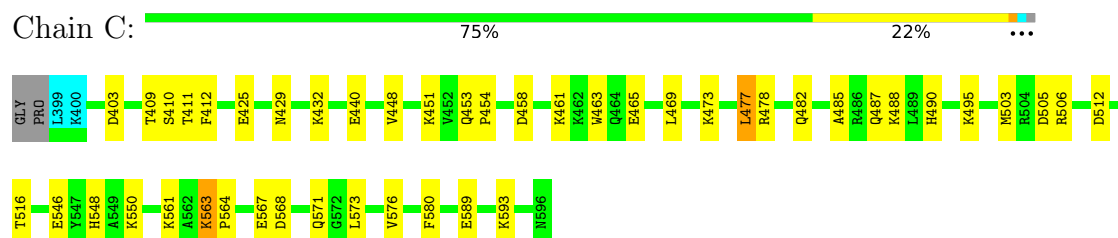


4.2.7 Score per residue for model 7

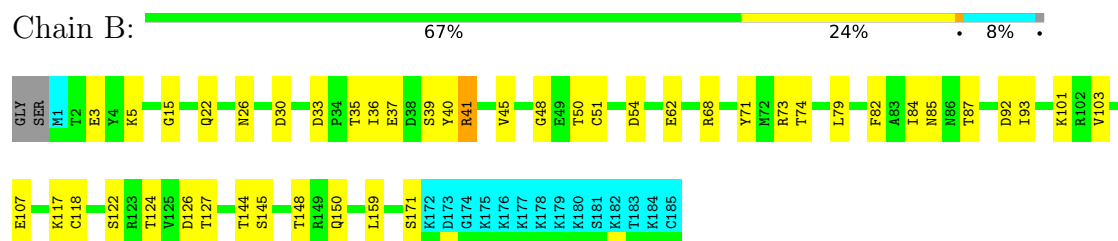
- Molecule 1: Apolipoprotein A-I



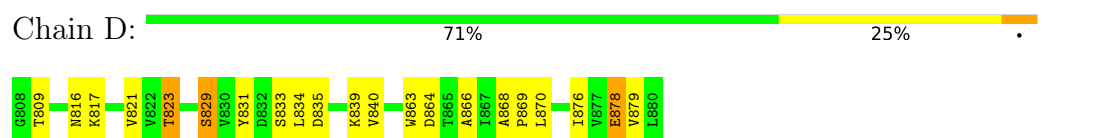
• Molecule 1: Apolipoprotein A-I



• Molecule 2: GTPase KRas

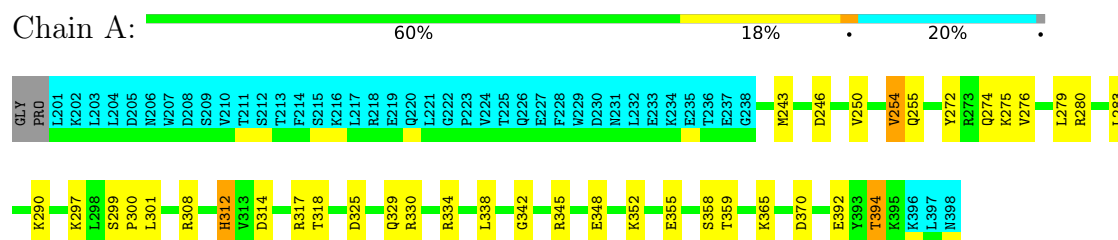


• Molecule 3: Serine/threonine-protein kinase A-Raf



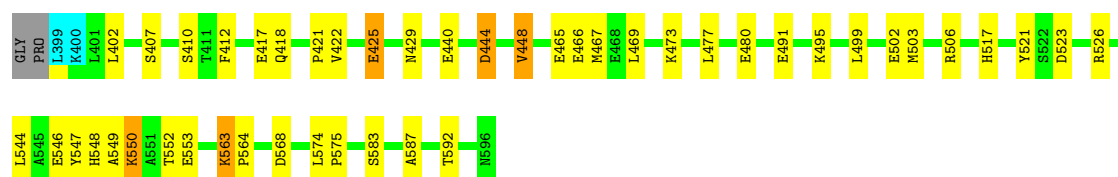
4.2.8 Score per residue for model 8

• Molecule 1: Apolipoprotein A-I



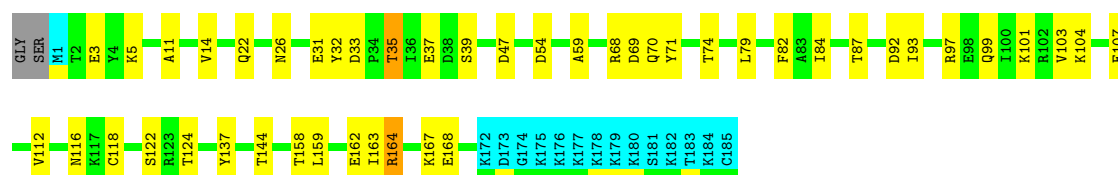
• Molecule 1: Apolipoprotein A-I





- Molecule 2: GTPase KRas

Chain B: 66% 24% 8%



- Molecule 3: Serine/threonine-protein kinase A-Raf

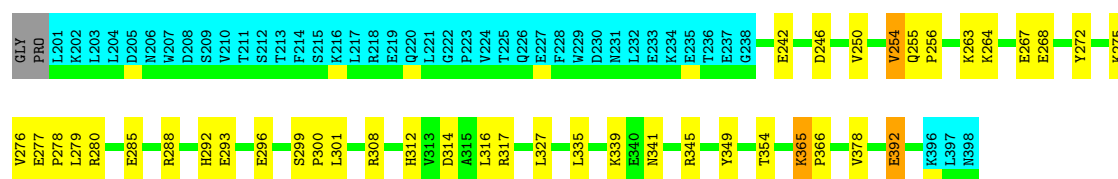
Chain D: 71% 29%



4.2.9 Score per residue for model 9

- Molecule 1: Apolipoprotein A-I

Chain A: 58% 19% 20%



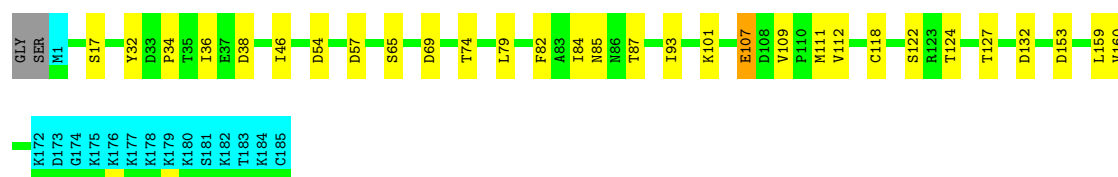
- Molecule 1: Apolipoprotein A-I

Chain C: 76% 20%



- Molecule 2: GTPase KRas

Chain B: 75% 16% 8%



- Molecule 3: Serine/threonine-protein kinase A-Raf

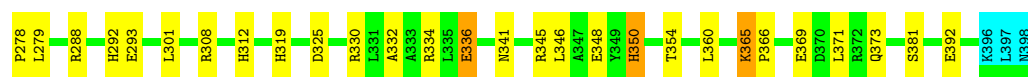
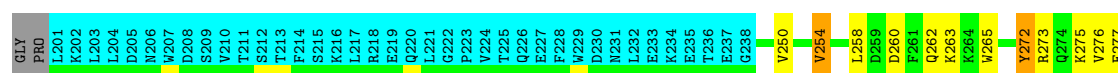
Chain D: 74% 23% .



4.2.10 Score per residue for model 10

- Molecule 1: Apolipoprotein A-I

Chain A: 58% 18% 20% .



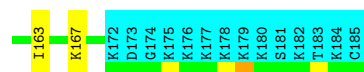
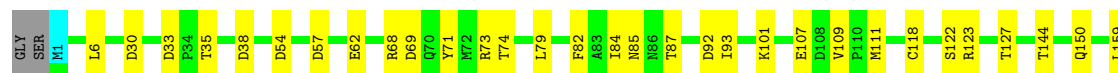
- Molecule 1: Apolipoprotein A-I

Chain C: 78% 18% . .



- Molecule 2: GTPase KRas

Chain B: 73% 18% 8% .



- Molecule 3: Serine/threonine-protein kinase A-Raf

Chain D: 79% 16% .

8808	8812	8819	8823	8824	8829	8834	8853	8857	8858	8859	8866	8871	8876	8877	8878	8879	8880
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

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	
CHARMM-GUI	structure solution	
HADDOCK	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	52
Number of shifts mapped to atoms	13
Number of unparsed shifts	0
Number of shifts with mapping errors	39
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, PCW, MG, 17F

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.41±0.01	0±0/1305 (0.0± 0.0%)	0.78±0.01	0±0/1752 (0.0± 0.0%)
1	C	0.40±0.01	0±0/1634 (0.0± 0.0%)	0.80±0.01	0±0/2196 (0.0± 0.0%)
2	B	0.33±0.00	0±0/1378 (0.0± 0.0%)	0.69±0.02	0±0/1859 (0.0± 0.0%)
3	D	0.36±0.02	0±0/575 (0.0± 0.0%)	0.66±0.02	0±0/778 (0.0± 0.0%)
All	All	0.38	0/48920 (0.0%)	0.75	1/65850 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	36	ILE	N-CA-C	-6.38	106.58	112.96	9	1

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	1284	18	1297	25±6
1	C	1607	22	1603	30±7
2	B	1356	16	1336	17±5
3	D	569	4	598	15±5
4	A	3456	0	5376	60±9

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes
5	A	864	0	1216	23±4
6	B	32	0	13	0±0
All	All	91690	600	114390	1295

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:CD	1:C:469:LEU:HD11	1.48	1.34	1	1
1:C:465:GLU:O	1:C:469:LEU:HG	1.32	1.19	2	9
1:C:465:GLU:O	1:C:469:LEU:CG	1.26	1.82	7	6
1:A:308:ARG:CG	1:C:469:LEU:HD11	1.21	1.63	1	3
1:A:308:ARG:CD	1:C:469:LEU:CD1	1.17	2.21	1	1
1:A:308:ARG:HG3	1:C:469:LEU:CD1	1.15	1.72	5	4
1:A:308:ARG:HD3	1:C:469:LEU:CD1	1.10	1.75	1	2
1:C:567:GLU:O	1:C:571:GLN:HG3	1.07	1.48	2	7
1:A:308:ARG:CG	1:C:469:LEU:CD1	1.05	2.34	1	2
1:A:308:ARG:CD	1:C:469:LEU:HD21	1.03	1.82	4	2
1:A:308:ARG:HG3	1:C:469:LEU:HD11	1.01	1.26	9	3
1:A:308:ARG:HG3	1:C:469:LEU:HD21	1.01	1.27	10	6
1:A:308:ARG:HD2	1:C:469:LEU:HD21	0.99	1.33	1	2
1:A:369:GLU:O	1:A:373:GLN:HG3	0.99	1.58	10	8
1:A:308:ARG:HD3	1:C:469:LEU:HD11	0.96	0.97	1	2
1:C:465:GLU:O	1:C:469:LEU:CB	0.94	2.16	7	2
5:A:38:17F:H1	5:A:38:17F:H4	0.90	1.43	1	1
1:A:297:LYS:HE2	1:C:477:LEU:HG	0.90	1.39	7	1
2:B:38:ASP:HB2	2:B:57:ASP:HB3	0.89	1.39	9	6
1:C:465:GLU:O	1:C:469:LEU:CD1	0.85	2.25	7	2
1:A:308:ARG:HD2	1:C:469:LEU:CD2	0.84	2.00	1	2
5:A:37:17F:HN1	3:D:857:ARG:HH21	0.83	1.16	1	1
5:A:74:17F:HN1	5:A:74:17F:H4	0.82	1.30	4	1
4:A:30:PCW:H73	5:A:40:17F:HN1	0.81	1.35	3	1
1:A:279:LEU:HD22	1:C:495:LYS:HG2	0.80	1.53	1	7
1:C:563:LYS:HB2	1:C:564:PRO:HD3	0.80	1.52	2	9
1:A:308:ARG:HD3	1:C:469:LEU:HD21	0.78	1.55	4	1
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.78	1.56	3	8
1:C:466:GLU:OE1	1:C:469:LEU:HD12	0.77	1.79	10	1
4:A:24:PCW:H41	3:D:853:LEU:HG	0.76	1.58	9	1
1:C:567:GLU:O	1:C:571:GLN:CG	0.75	2.34	2	3
5:A:74:17F:H4A	5:A:79:17F:HN1A	0.75	1.41	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:36:ILE:HD11	3:D:809:THR:HG21	0.75	1.59	4	4
4:A:7:PCW:H20	3:D:857:ARG:HH12	0.75	1.42	5	1
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.74	1.59	8	7
1:A:308:ARG:CD	1:C:469:LEU:CG	0.74	2.65	1	1
4:A:6:PCW:H341	4:A:28:PCW:H152	0.73	1.58	7	1
2:B:79:LEU:HG	2:B:159:LEU:HD22	0.73	1.60	9	10
4:A:7:PCW:H72	3:D:879:VAL:HB	0.72	1.60	9	1
4:A:9:PCW:H322	4:A:14:PCW:H351	0.71	1.62	8	1
4:A:12:PCW:H362	4:A:30:PCW:H152	0.71	1.62	4	1
4:A:7:PCW:H2	4:A:16:PCW:H11	0.71	1.62	8	1
1:A:260:ASP:HA	1:A:263:LYS:HE2	0.71	1.60	10	1
4:A:43:PCW:H82	5:A:74:17F:HN1A	0.71	1.45	9	1
1:C:453:GLN:HB2	1:C:454:PRO:HD3	0.71	1.61	4	5
3:D:829:SER:HA	3:D:866:ALA:HA	0.70	1.60	3	7
4:A:45:PCW:H132	4:A:45:PCW:H331	0.70	1.62	6	1
4:A:57:PCW:H42	5:A:80:17F:HN1A	0.70	1.46	3	1
4:A:45:PCW:H40	4:A:57:PCW:H61	0.70	1.61	8	1
4:A:9:PCW:H31	4:A:9:PCW:H41	0.70	1.64	2	2
1:A:341:ASN:HD21	1:C:433:GLU:HA	0.70	1.47	6	4
1:A:316:LEU:HG	1:C:462:LYS:HE3	0.69	1.63	4	2
4:A:6:PCW:H122	4:A:16:PCW:H352	0.69	1.64	10	1
4:A:56:PCW:H132	4:A:56:PCW:H331	0.69	1.63	2	1
1:C:465:GLU:O	1:C:469:LEU:HB2	0.69	1.86	7	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.69	1.88	1	9
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.69	1.63	1	2
1:A:308:ARG:CG	1:C:469:LEU:HD21	0.68	2.15	8	2
4:A:23:PCW:H32	5:A:34:17F:H63	0.68	1.65	5	1
4:A:15:PCW:H321	4:A:16:PCW:H19	0.68	1.64	10	1
4:A:10:PCW:H131	4:A:22:PCW:H351	0.68	1.65	4	1
1:A:308:ARG:CB	1:C:469:LEU:HD11	0.67	2.20	1	3
1:A:308:ARG:HD2	1:C:469:LEU:CG	0.67	2.17	1	1
4:A:12:PCW:H73	5:A:37:17F:HN1A	0.67	1.48	4	1
1:A:352:LYS:HG2	1:C:422:VAL:HG13	0.67	1.66	2	1
2:B:101:LYS:HD2	2:B:107:GLU:HG3	0.66	1.66	8	2
4:A:12:PCW:H72	5:A:40:17F:HN1	0.66	1.49	8	1
1:C:418:GLN:O	1:C:422:VAL:HB	0.66	1.89	2	3
4:A:67:PCW:H81	5:A:78:17F:H37	0.66	1.67	10	1
4:A:54:PCW:H331	4:A:54:PCW:H131	0.66	1.66	2	1
2:B:101:LYS:HG2	2:B:107:GLU:HA	0.66	1.67	9	2
4:A:15:PCW:H71	5:A:39:17F:H2	0.66	1.67	9	1
1:A:308:ARG:CD	1:C:469:LEU:CD2	0.66	2.73	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:101:LYS:HE3	2:B:107:GLU:HB3	0.66	1.67	9	1
4:A:31:PCW:H2	4:A:31:PCW:H52	0.65	1.68	3	1
3:D:851:TYR:HB3	3:D:858:LYS:HB3	0.65	1.67	1	1
2:B:36:ILE:CD1	3:D:809:THR:HG21	0.65	2.21	7	4
1:C:547:TYR:HA	1:C:550:LYS:HB2	0.65	1.69	8	1
1:A:369:GLU:O	1:A:373:GLN:CG	0.65	2.43	10	2
4:A:1:PCW:H41	5:A:35:17F:H1	0.65	1.67	4	1
4:A:13:PCW:H122	5:A:37:17F:H37	0.65	1.69	2	1
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.65	1.69	6	3
4:A:1:PCW:H152	5:A:38:17F:H33	0.65	1.69	9	1
5:A:38:17F:H1	5:A:38:17F:C4	0.64	2.22	1	1
1:A:308:ARG:HD3	1:C:469:LEU:CD2	0.64	2.21	4	1
4:A:23:PCW:H73	5:A:34:17F:HN1A	0.64	1.52	1	1
4:A:12:PCW:H72	5:A:40:17F:N1	0.64	2.07	8	1
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.64	1.69	3	2
4:A:31:PCW:H71	3:D:853:LEU:HG	0.64	1.67	10	1
2:B:82:PHE:HB2	2:B:89:SER:HB2	0.64	1.69	6	1
4:A:3:PCW:H322	4:A:3:PCW:H51	0.64	1.69	7	1
4:A:6:PCW:H152	4:A:24:PCW:H132	0.64	1.69	3	1
1:A:308:ARG:HG3	1:C:469:LEU:CD2	0.64	2.16	8	6
3:D:812:VAL:HG11	3:D:834:LEU:HD11	0.63	1.71	8	3
4:A:17:PCW:H81	5:A:38:17F:O1	0.63	1.93	3	2
4:A:43:PCW:H62	4:A:69:PCW:H11	0.63	1.71	1	1
1:C:465:GLU:O	1:C:469:LEU:HD12	0.63	1.92	7	2
4:A:42:PCW:H71	5:A:75:17F:HN1	0.63	1.53	2	1
4:A:60:PCW:H151	4:A:61:PCW:H442	0.63	1.70	9	1
2:B:68:ARG:HG2	2:B:72:MET:HE2	0.63	1.70	2	1
2:B:25:GLN:NE2	3:D:840:VAL:HA	0.63	2.09	4	3
2:B:36:ILE:HA	2:B:59:ALA:HB2	0.63	1.69	1	1
4:A:3:PCW:H11	4:A:18:PCW:H11	0.62	1.71	4	1
5:A:34:17F:H9	5:A:40:17F:H63	0.62	1.71	9	1
4:A:32:PCW:H61	5:A:38:17F:N1	0.62	2.09	3	1
4:A:30:PCW:H352	4:A:30:PCW:H122	0.62	1.72	2	1
4:A:62:PCW:H431	5:A:78:17F:H47	0.62	1.70	5	1
4:A:5:PCW:H73	3:D:853:LEU:HD22	0.62	1.71	6	1
1:C:574:LEU:HB2	1:C:575:PRO:HD3	0.62	1.72	8	2
4:A:71:PCW:H71	4:A:71:PCW:H19	0.62	1.72	1	1
4:A:54:PCW:H352	4:A:72:PCW:H11	0.61	1.71	10	1
4:A:9:PCW:H81	3:D:876:ILE:HG23	0.61	1.73	3	1
4:A:17:PCW:H12	2:B:70:GLN:HB2	0.61	1.72	8	1
2:B:103:VAL:HG23	2:B:104:LYS:HE2	0.61	1.72	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:34:17F:HN1A	3:D:858:LYS:H	0.61	1.35	3	1
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.61	1.72	7	2
3:D:840:VAL:HG13	3:D:841:ARG:HG3	0.61	1.73	2	2
4:A:27:PCW:H41	5:A:37:17F:O2	0.61	1.96	4	2
4:A:30:PCW:H52	4:A:30:PCW:H31	0.60	1.73	2	1
4:A:67:PCW:H83	5:A:78:17F:H37	0.60	1.71	4	1
4:A:13:PCW:H31	4:A:14:PCW:H151	0.60	1.72	6	1
4:A:20:PCW:H62	3:D:879:VAL:HB	0.60	1.73	10	1
1:A:301:LEU:HD22	1:C:473:LYS:HE2	0.60	1.72	5	1
4:A:21:PCW:H72	5:A:36:17F:H1	0.60	1.73	6	1
3:D:852:ARG:HD3	3:D:870:LEU:HD11	0.60	1.73	2	2
1:A:250:VAL:O	1:A:254:VAL:HB	0.60	1.97	6	8
2:B:40:TYR:CE2	3:D:840:VAL:HG22	0.60	2.31	7	5
3:D:813:TYR:HB2	3:D:876:ILE:HG12	0.60	1.72	6	1
2:B:35:THR:HG22	2:B:59:ALA:HA	0.60	1.73	8	1
4:A:14:PCW:H451	5:A:34:17F:H19A	0.60	1.74	10	1
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.60	1.73	3	10
4:A:43:PCW:O1P	4:A:68:PCW:H83	0.60	1.97	3	1
4:A:50:PCW:H31	5:A:78:17F:H4	0.60	1.73	9	2
5:A:73:17F:H57	5:A:73:17F:H30	0.60	1.73	6	1
4:A:1:PCW:H181	5:A:35:17F:H18	0.59	1.73	10	1
4:A:12:PCW:H42	5:A:37:17F:N1	0.59	2.12	2	1
2:B:32:TYR:HA	6:B:201:GNP:H5'1	0.59	1.73	8	3
5:A:40:17F:HN1	2:B:5:LYS:NZ	0.59	1.94	6	1
4:A:49:PCW:H32	4:A:57:PCW:H62	0.59	1.72	9	1
4:A:30:PCW:H73	5:A:40:17F:N1	0.59	2.10	3	1
4:A:49:PCW:H122	4:A:57:PCW:H361	0.59	1.71	5	1
3:D:811:LYS:HB3	3:D:821:VAL:HG22	0.59	1.73	1	1
4:A:9:PCW:H132	4:A:26:PCW:H12	0.59	1.73	3	1
4:A:17:PCW:H41	4:A:17:PCW:H322	0.59	1.75	6	1
4:A:46:PCW:H252	4:A:46:PCW:H182	0.59	1.74	10	1
1:C:503:MET:HA	1:C:506:ARG:HD2	0.59	1.74	5	5
4:A:59:PCW:H342	5:A:77:17F:H9A	0.59	1.74	3	1
4:A:67:PCW:H61	5:A:78:17F:H8	0.59	1.74	3	1
2:B:73:ARG:HD3	2:B:103:VAL:HB	0.59	1.75	6	1
4:A:46:PCW:H11	4:A:71:PCW:H381	0.59	1.73	2	1
4:A:57:PCW:H41	4:A:57:PCW:O31	0.59	1.98	9	1
1:C:561:LYS:HA	1:C:565:ALA:HB3	0.58	1.74	2	1
4:A:12:PCW:H11	4:A:30:PCW:H121	0.58	1.74	3	1
1:A:242:GLU:HB3	1:C:532:ARG:HH21	0.58	1.58	6	2
5:A:75:17F:HN1	5:A:75:17F:H4	0.58	1.57	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:3:PCW:H332	4:A:23:PCW:H31	0.58	1.76	8	1
4:A:60:PCW:H381	4:A:62:PCW:H152	0.58	1.74	5	1
4:A:12:PCW:H152	4:A:22:PCW:H352	0.58	1.75	10	1
4:A:10:PCW:H83	5:A:36:17F:HN1A	0.58	1.58	6	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.58	1.75	9	3
4:A:11:PCW:H322	4:A:28:PCW:H62	0.58	1.74	9	1
4:A:67:PCW:H141	5:A:75:17F:H60	0.58	1.74	10	1
1:C:491:GLU:HB3	1:C:495:LYS:HE2	0.58	1.76	4	5
4:A:10:PCW:H62	3:D:876:ILE:HG23	0.58	1.76	7	1
1:A:264:LYS:HE3	1:C:509:ALA:HB1	0.58	1.73	2	2
4:A:3:PCW:H61	4:A:19:PCW:H2	0.58	1.76	6	1
1:A:334:ARG:HD2	1:C:440:GLU:OE1	0.57	1.99	8	6
1:A:330:ARG:O	1:A:334:ARG:HG2	0.57	1.98	7	5
4:A:2:PCW:H341	4:A:5:PCW:H152	0.57	1.76	4	1
4:A:1:PCW:H122	5:A:35:17F:H20	0.57	1.76	8	1
1:C:451:LYS:O	1:C:455:TYR:HB2	0.57	1.99	3	6
4:A:42:PCW:H39	4:A:69:PCW:H451	0.57	1.76	5	1
1:A:288:ARG:O	1:A:292:HIS:HB2	0.57	1.98	6	3
3:D:815:PRO:HD3	3:D:877:VAL:HB	0.57	1.76	5	2
3:D:814:LEU:HD13	3:D:841:ARG:HD2	0.57	1.74	6	3
4:A:26:PCW:H321	5:A:40:17F:H19	0.57	1.76	4	1
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.57	1.77	6	2
1:C:491:GLU:HG2	1:C:495:LYS:HE3	0.57	1.75	8	1
2:B:68:ARG:HA	2:B:71:TYR:CE2	0.57	2.34	6	8
4:A:18:PCW:H232	4:A:49:PCW:H442	0.57	1.75	8	1
4:A:59:PCW:H40	4:A:61:PCW:H161	0.57	1.77	8	1
1:A:308:ARG:HD3	1:C:469:LEU:CG	0.57	2.30	4	1
4:A:71:PCW:H132	4:A:71:PCW:H181	0.57	1.75	4	1
5:A:36:17F:H18A	5:A:40:17F:H36	0.56	1.77	1	1
4:A:4:PCW:H332	4:A:7:PCW:H31	0.56	1.75	4	1
4:A:24:PCW:H39	3:D:857:ARG:HH12	0.56	1.60	9	1
4:A:59:PCW:H121	5:A:77:17F:H11	0.56	1.76	7	1
4:A:53:PCW:H361	4:A:64:PCW:H122	0.56	1.77	8	1
2:B:47:ASP:HB2	2:B:164:ARG:HH22	0.56	1.59	8	1
2:B:22:GLN:O	2:B:26:ASN:HA	0.56	2.00	7	6
4:A:6:PCW:H2	4:A:11:PCW:H322	0.56	1.76	3	1
1:A:352:LYS:NZ	1:C:425:GLU:HB2	0.56	2.15	8	1
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.56	1.77	9	1
5:A:74:17F:H4	5:A:74:17F:N1	0.56	2.11	4	1
4:A:44:PCW:H371	4:A:69:PCW:H431	0.56	1.77	8	1
5:A:38:17F:H1A	2:B:43:GLN:NE2	0.56	2.15	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:7:PCW:H122	4:A:16:PCW:H32	0.56	1.76	7	1
4:A:5:PCW:H122	5:A:38:17F:H18A	0.56	1.78	4	1
4:A:43:PCW:O2P	4:A:45:PCW:H61	0.56	2.01	3	1
3:D:809:THR:HG22	3:D:823:THR:HA	0.56	1.77	7	1
4:A:19:PCW:H241	4:A:19:PCW:H161	0.56	1.76	8	1
1:A:345:ARG:HA	1:C:429:ASN:HD21	0.56	1.61	8	2
4:A:3:PCW:H321	4:A:18:PCW:H322	0.56	1.78	5	1
4:A:20:PCW:H32	4:A:24:PCW:H331	0.55	1.76	10	1
4:A:10:PCW:H142	4:A:10:PCW:H381	0.55	1.76	8	1
2:B:46:ILE:HD11	2:B:53:LEU:HD11	0.55	1.78	3	1
4:A:9:PCW:H81	4:A:30:PCW:O2P	0.55	2.01	5	1
3:D:852:ARG:HD2	3:D:873:GLU:OE1	0.55	2.01	8	1
1:C:508:ARG:O	1:C:512:ASP:HB2	0.55	2.01	2	3
1:C:444:ASP:O	1:C:448:VAL:HB	0.55	2.02	8	2
1:C:528:ARG:HB3	1:C:532:ARG:NH2	0.55	2.16	1	2
2:B:41:ARG:NH1	3:D:817:LYS:HB2	0.55	2.16	7	3
4:A:19:PCW:H2	4:A:23:PCW:H11	0.55	1.77	3	1
2:B:101:LYS:HE2	2:B:107:GLU:HG3	0.55	1.79	10	1
3:D:851:TYR:HE1	3:D:878:GLU:HB3	0.55	1.62	5	1
3:D:838:LEU:HD12	3:D:845:GLN:HG3	0.55	1.78	1	2
1:A:352:LYS:NZ	1:C:425:GLU:HB3	0.55	2.17	7	1
4:A:44:PCW:H2	4:A:44:PCW:H41	0.55	1.78	6	1
4:A:66:PCW:H452	5:A:79:17F:H59	0.55	1.78	10	1
4:A:8:PCW:H321	4:A:22:PCW:H331	0.54	1.79	10	1
2:B:144:THR:HA	2:B:150:GLN:O	0.54	2.02	7	3
4:A:1:PCW:H82	5:A:35:17F:HN1A	0.54	1.61	6	1
4:A:48:PCW:H321	4:A:54:PCW:H131	0.54	1.78	5	1
1:C:544:LEU:O	1:C:548:HIS:HB2	0.54	2.03	8	1
1:A:308:ARG:CB	1:C:469:LEU:CD1	0.54	2.84	1	1
2:B:158:THR:HA	2:B:161:ARG:HD2	0.54	1.78	6	1
2:B:68:ARG:HA	2:B:71:TYR:CZ	0.54	2.37	7	2
4:A:67:PCW:H41	5:A:78:17F:H30	0.54	1.78	2	1
2:B:72:MET:HE3	2:B:103:VAL:HG11	0.54	1.78	2	1
1:C:502:GLU:HG2	1:C:506:ARG:HE	0.54	1.63	8	2
1:C:458:ASP:HA	1:C:461:LYS:HE3	0.54	1.78	7	1
1:C:473:LYS:O	1:C:477:LEU:HB2	0.54	2.03	7	2
4:A:53:PCW:H212	4:A:64:PCW:H151	0.54	1.80	2	1
4:A:9:PCW:H71	3:D:876:ILE:CG2	0.54	2.33	3	1
4:A:55:PCW:H63	4:A:64:PCW:H11	0.54	1.78	4	1
4:A:20:PCW:H332	4:A:20:PCW:H131	0.54	1.80	6	2
4:A:20:PCW:H122	4:A:20:PCW:H361	0.54	1.78	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:325:ASP:HA	1:A:328:ARG:HD2	0.54	1.79	3	2
4:A:30:PCW:H71	5:A:37:17F:O4	0.54	2.03	7	1
4:A:42:PCW:H162	4:A:52:PCW:H141	0.54	1.80	8	1
5:A:40:17F:H46	4:A:51:PCW:H432	0.54	1.80	4	1
4:A:32:PCW:H371	5:A:38:17F:H32	0.54	1.78	6	1
5:A:40:17F:HN1A	2:B:5:LYS:NZ	0.54	2.00	7	1
4:A:67:PCW:H142	4:A:67:PCW:H371	0.54	1.80	9	1
2:B:41:ARG:HB3	3:D:816:ASN:ND2	0.54	2.18	4	1
1:C:478:ARG:O	1:C:482:GLN:HB2	0.54	2.02	7	2
4:A:12:PCW:H41	3:D:855:LYS:HB2	0.53	1.79	1	1
4:A:5:PCW:H431	4:A:17:PCW:H352	0.53	1.80	3	1
3:D:870:LEU:HD12	3:D:873:GLU:HG2	0.53	1.80	3	1
1:C:469:LEU:O	1:C:473:LYS:HB2	0.53	2.03	5	1
4:A:13:PCW:H422	4:A:27:PCW:H371	0.53	1.80	6	1
2:B:73:ARG:HG2	2:B:103:VAL:HB	0.53	1.78	7	1
1:C:495:LYS:O	1:C:499:LEU:HB2	0.53	2.04	9	5
4:A:48:PCW:H81	4:A:58:PCW:O2P	0.53	2.03	5	1
4:A:30:PCW:H83	5:A:34:17F:O2	0.53	2.03	8	2
4:A:67:PCW:H341	4:A:72:PCW:H20	0.53	1.80	9	1
4:A:16:PCW:H451	5:A:39:17F:H60	0.53	1.78	2	1
1:A:308:ARG:HG3	1:C:469:LEU:HD13	0.53	1.76	1	1
1:C:546:GLU:O	1:C:550:LYS:HD2	0.53	2.03	1	2
4:A:42:PCW:H19	4:A:52:PCW:H121	0.53	1.80	2	1
4:A:19:PCW:H63	4:A:23:PCW:H2	0.53	1.79	3	1
1:A:244:SER:O	1:A:248:GLU:HB2	0.53	2.03	5	1
4:A:12:PCW:H342	4:A:30:PCW:H121	0.53	1.81	4	1
4:A:16:PCW:H152	5:A:39:17F:H19	0.53	1.80	9	1
4:A:51:PCW:H361	4:A:70:PCW:H341	0.53	1.79	10	1
4:A:29:PCW:H62	3:D:880:LEU:HB2	0.53	1.78	3	1
5:A:33:17F:O2	3:D:817:LYS:HA	0.53	2.03	5	1
4:A:8:PCW:H51	3:D:879:VAL:O	0.53	2.04	7	1
1:A:332:ALA:O	1:A:336:GLU:HB2	0.53	2.03	10	1
5:A:79:17F:H4	5:A:79:17F:H1	0.53	1.81	1	1
4:A:12:PCW:H352	5:A:36:17F:H5	0.53	1.81	4	1
3:D:811:LYS:HE3	3:D:819:ARG:HG3	0.53	1.79	5	1
4:A:30:PCW:H73	2:B:3:GLU:HB2	0.53	1.80	7	1
4:A:53:PCW:H61	4:A:68:PCW:O2P	0.53	2.04	9	1
4:A:62:PCW:H31	4:A:72:PCW:H2	0.53	1.80	9	1
4:A:12:PCW:H62	3:D:854:ILE:HB	0.53	1.79	1	1
4:A:17:PCW:H39	5:A:38:17F:H18	0.53	1.81	2	1
4:A:14:PCW:H131	4:A:23:PCW:H151	0.53	1.80	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:12:PCW:H142	4:A:22:PCW:H361	0.53	1.80	4	1
4:A:42:PCW:H2	4:A:42:PCW:O1P	0.53	2.04	7	1
4:A:13:PCW:H72	3:D:854:ILE:HB	0.53	1.80	3	1
4:A:6:PCW:O1P	4:A:7:PCW:H83	0.53	2.04	5	1
5:A:34:17F:H29	5:A:40:17F:H66	0.53	1.79	10	1
4:A:1:PCW:C6	5:A:35:17F:HN1A	0.52	2.17	3	1
4:A:5:PCW:H63	5:A:38:17F:H4A	0.52	1.81	4	1
4:A:44:PCW:H121	5:A:77:17F:H6	0.52	1.80	5	1
3:D:852:ARG:HD2	3:D:870:LEU:HD11	0.52	1.82	5	1
2:B:46:ILE:HD13	2:B:160:VAL:HG11	0.52	1.81	9	1
4:A:42:PCW:H40	4:A:52:PCW:H482	0.52	1.81	10	1
1:C:514:LEU:HA	1:C:517:HIS:HB2	0.52	1.81	4	1
4:A:26:PCW:H441	5:A:33:17F:H44	0.52	1.80	6	1
4:A:44:PCW:H12	4:A:69:PCW:H83	0.52	1.80	6	1
4:A:11:PCW:O31	4:A:26:PCW:H71	0.52	2.05	4	1
3:D:851:TYR:HB2	3:D:876:ILE:HG13	0.52	1.81	9	1
4:A:12:PCW:H63	5:A:37:17F:N1	0.52	2.18	2	1
4:A:15:PCW:H63	5:A:39:17F:O1	0.52	2.04	3	1
4:A:16:PCW:H352	5:A:39:17F:H8A	0.52	1.82	3	1
1:C:465:GLU:HB3	1:C:469:LEU:HD11	0.52	1.80	7	2
5:A:37:17F:O1	3:D:855:LYS:HD2	0.52	2.05	3	1
1:C:417:GLU:O	1:C:421:PRO:HD2	0.52	2.05	9	3
1:C:467:MET:HA	1:C:467:MET:HE2	0.52	1.81	8	1
3:D:858:LYS:HE2	3:D:876:ILE:HD13	0.52	1.80	5	3
4:A:13:PCW:H181	4:A:18:PCW:H162	0.52	1.81	9	1
4:A:42:PCW:H19	4:A:52:PCW:H322	0.52	1.81	10	1
4:A:13:PCW:H71	5:A:34:17F:O1	0.52	2.05	4	2
4:A:64:PCW:H352	4:A:64:PCW:H162	0.52	1.80	2	2
4:A:13:PCW:O1P	4:A:18:PCW:H82	0.52	2.05	3	1
4:A:9:PCW:H2	4:A:11:PCW:H32	0.52	1.81	7	1
5:A:33:17F:P1	5:A:33:17F:HN1	0.52	2.28	1	1
4:A:49:PCW:H122	4:A:57:PCW:H352	0.52	1.82	1	1
4:A:70:PCW:H63	4:A:70:PCW:H19	0.52	1.82	5	1
4:A:3:PCW:H321	4:A:18:PCW:O1P	0.52	2.05	7	1
4:A:7:PCW:O11	4:A:16:PCW:H73	0.52	2.05	1	1
1:A:310:ARG:O	1:A:314:ASP:HB2	0.52	2.05	4	2
4:A:54:PCW:H352	4:A:72:PCW:H122	0.52	1.81	4	1
4:A:6:PCW:P	4:A:11:PCW:O2P	0.52	2.68	6	1
4:A:10:PCW:H331	4:A:21:PCW:H322	0.52	1.82	6	1
2:B:3:GLU:HG2	2:B:52:LEU:HB2	0.52	1.82	6	1
4:A:27:PCW:H73	2:B:70:GLN:HB2	0.51	1.82	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:489:LEU:O	1:C:493:GLN:HB2	0.51	2.06	2	1
4:A:62:PCW:H361	4:A:72:PCW:H322	0.51	1.81	5	1
4:A:46:PCW:H61	5:A:73:17F:O1	0.51	2.05	9	1
4:A:10:PCW:H61	5:A:36:17F:H2	0.51	1.82	10	1
1:C:525:LEU:HD23	1:C:528:ARG:HD2	0.51	1.83	5	1
1:A:388:SER:HB3	1:C:594:LYS:HE2	0.51	1.81	5	1
4:A:42:PCW:H81	4:A:63:PCW:O2P	0.51	2.06	8	1
4:A:25:PCW:H421	4:A:29:PCW:H141	0.51	1.81	1	1
3:D:831:TYR:HB2	3:D:863:TRP:HB3	0.51	1.81	9	5
1:A:312:HIS:HE1	1:C:465:GLU:HB2	0.51	1.66	2	4
4:A:6:PCW:O2P	4:A:28:PCW:H81	0.51	2.06	7	1
4:A:66:PCW:H451	5:A:79:17F:H37	0.51	1.81	10	1
5:A:40:17F:N1	3:D:855:LYS:HA	0.51	2.20	1	1
4:A:22:PCW:H2	4:A:22:PCW:H52	0.51	1.83	3	1
4:A:56:PCW:H331	4:A:56:PCW:H131	0.51	1.81	8	2
4:A:70:PCW:O31	4:A:70:PCW:H41	0.51	2.04	6	1
4:A:62:PCW:H122	4:A:72:PCW:H152	0.51	1.82	8	1
4:A:1:PCW:H342	4:A:26:PCW:H351	0.51	1.81	1	1
4:A:70:PCW:H51	4:A:70:PCW:H2	0.51	1.83	1	1
1:A:341:ASN:ND2	1:C:433:GLU:HA	0.51	2.17	6	1
4:A:41:PCW:H351	4:A:52:PCW:H39	0.51	1.82	7	1
3:D:809:THR:HB	3:D:821:VAL:HG12	0.51	1.83	7	1
1:A:314:ASP:HA	1:A:317:ARG:HD2	0.51	1.82	9	3
4:A:65:PCW:H142	5:A:80:17F:H18A	0.51	1.83	5	1
1:A:352:LYS:HZ2	1:C:425:GLU:HB3	0.51	1.66	7	1
4:A:4:PCW:H71	2:B:167:LYS:HB3	0.51	1.82	3	1
4:A:43:PCW:H221	4:A:51:PCW:H462	0.51	1.83	3	1
4:A:67:PCW:H352	4:A:72:PCW:H241	0.51	1.82	3	1
4:A:17:PCW:O2P	3:D:876:ILE:HD11	0.51	2.06	6	1
4:A:62:PCW:H351	4:A:72:PCW:H332	0.51	1.83	8	1
2:B:79:LEU:HD23	2:B:112:VAL:HB	0.51	1.82	9	3
1:C:447:GLU:O	1:C:451:LYS:HB2	0.51	2.06	6	2
4:A:13:PCW:H73	5:A:34:17F:N1	0.51	2.21	8	1
3:D:853:LEU:HD21	3:D:858:LYS:HE3	0.50	1.84	6	1
4:A:24:PCW:H322	4:A:24:PCW:H41	0.50	1.83	10	1
4:A:51:PCW:H442	4:A:70:PCW:H442	0.50	1.82	1	1
4:A:30:PCW:H361	5:A:40:17F:H61	0.50	1.83	2	1
1:C:414:LYS:HA	1:C:417:GLU:HG3	0.50	1.82	2	1
4:A:17:PCW:H132	4:A:17:PCW:H62	0.50	1.82	5	1
2:B:45:VAL:HG22	2:B:50:THR:HB	0.50	1.84	7	1
4:A:3:PCW:H212	4:A:19:PCW:H181	0.50	1.82	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:279:LEU:HB3	1:C:495:LYS:HE3	0.50	1.83	9	1
5:A:75:17F:H4	5:A:75:17F:N1	0.50	2.20	1	1
4:A:13:PCW:H31	5:A:37:17F:H10	0.50	1.82	9	1
1:C:491:GLU:O	1:C:495:LYS:HG3	0.50	2.06	6	5
4:A:5:PCW:H12	4:A:17:PCW:H321	0.50	1.82	6	3
4:A:16:PCW:H63	2:B:3:GLU:HB2	0.50	1.83	4	1
1:A:239:LEU:O	1:A:243:MET:HB2	0.50	2.06	6	1
1:C:465:GLU:C	1:C:469:LEU:HD12	0.50	2.30	7	1
4:A:44:PCW:H82	4:A:44:PCW:H11	0.50	1.84	8	1
2:B:32:TYR:O	2:B:34:PRO:HD3	0.50	2.07	9	1
4:A:25:PCW:H122	4:A:31:PCW:H12	0.50	1.84	2	1
3:D:835:ASP:O	3:D:839:LYS:HG2	0.50	2.05	7	2
1:A:276:VAL:O	1:A:280:ARG:HB2	0.50	2.07	9	2
2:B:41:ARG:HH11	2:B:52:LEU:HD21	0.50	1.65	1	1
4:A:4:PCW:H332	4:A:7:PCW:H132	0.50	1.84	9	1
1:A:365:LYS:O	1:A:369:GLU:HB2	0.50	2.07	3	1
4:A:42:PCW:H82	4:A:42:PCW:O11	0.50	2.06	10	2
1:C:421:PRO:O	1:C:425:GLU:HG2	0.50	2.06	6	1
1:A:279:LEU:HD22	1:C:495:LYS:HE2	0.50	1.83	8	1
4:A:5:PCW:H39	4:A:17:PCW:H83	0.50	1.82	9	1
4:A:14:PCW:H141	5:A:34:17F:H19	0.50	1.83	10	1
4:A:43:PCW:O1P	4:A:68:PCW:H42	0.49	2.07	1	1
4:A:12:PCW:H11	4:A:30:PCW:H132	0.49	1.83	4	1
3:D:851:TYR:CD2	3:D:858:LYS:HB3	0.49	2.42	4	1
1:A:301:LEU:HB3	1:C:473:LYS:HE2	0.49	1.84	10	1
4:A:5:PCW:H382	5:A:38:17F:H18	0.49	1.83	10	1
1:A:363:LYS:HD3	1:C:411:THR:HG23	0.49	1.84	2	2
4:A:16:PCW:H362	5:A:39:17F:H10A	0.49	1.83	1	1
4:A:47:PCW:H122	4:A:49:PCW:H181	0.49	1.82	7	1
4:A:18:PCW:H171	5:A:37:17F:H12	0.49	1.84	1	1
3:D:824:VAL:HG11	3:D:871:ASP:HB2	0.49	1.84	10	2
1:A:275:LYS:O	1:A:279:LEU:HB2	0.49	2.07	2	1
2:B:41:ARG:HB3	3:D:816:ASN:OD1	0.49	2.08	2	1
4:A:10:PCW:H83	5:A:36:17F:HN1	0.49	1.66	4	1
2:B:45:VAL:HA	2:B:50:THR:HA	0.49	1.83	7	1
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.49	2.38	9	3
4:A:44:PCW:H62	5:A:77:17F:N1	0.49	2.22	4	1
1:A:308:ARG:HD2	1:C:465:GLU:OE1	0.49	2.08	5	1
4:A:61:PCW:H41	4:A:61:PCW:O31	0.49	2.06	6	1
4:A:43:PCW:H31	4:A:69:PCW:H12	0.49	1.85	8	1
4:A:58:PCW:H12	4:A:61:PCW:H431	0.49	1.85	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:9:PCW:H332	4:A:14:PCW:H341	0.49	1.83	10	1
4:A:42:PCW:O2P	4:A:43:PCW:H81	0.49	2.08	2	1
4:A:2:PCW:H331	4:A:17:PCW:H421	0.49	1.83	5	1
5:A:40:17F:HN1	2:B:5:LYS:HZ1	0.49	1.50	6	1
4:A:24:PCW:H42	4:A:25:PCW:H131	0.49	1.84	10	1
1:A:268:GLU:O	1:A:272:TYR:HB2	0.49	2.08	9	3
4:A:41:PCW:H322	4:A:52:PCW:H372	0.49	1.85	6	1
4:A:13:PCW:H82	3:D:857:ARG:HB2	0.49	1.83	3	1
3:D:838:LEU:HD21	3:D:877:VAL:HG11	0.49	1.85	8	2
1:A:297:LYS:O	1:A:301:LEU:HB2	0.49	2.08	8	2
1:C:479:ALA:O	1:C:483:GLU:HG2	0.49	2.08	9	1
1:A:273:ARG:HA	1:A:276:VAL:HG12	0.49	1.85	10	1
4:A:1:PCW:H352	5:A:35:17F:H32	0.49	1.85	2	1
5:A:35:17F:N1	2:B:170:MET:HE3	0.49	2.23	4	1
4:A:68:PCW:H39	4:A:68:PCW:H141	0.49	1.85	9	1
4:A:26:PCW:H11	4:A:28:PCW:O2P	0.49	2.08	10	1
4:A:15:PCW:H71	5:A:39:17F:O2	0.49	2.08	7	1
1:C:465:GLU:C	1:C:469:LEU:HG	0.49	2.23	7	1
4:A:43:PCW:H122	4:A:43:PCW:H372	0.49	1.83	8	1
1:C:489:LEU:O	1:C:493:GLN:HG3	0.48	2.07	6	1
4:A:3:PCW:H331	4:A:3:PCW:H82	0.48	1.85	7	1
4:A:8:PCW:H63	3:D:880:LEU:OXT	0.48	2.08	8	1
4:A:20:PCW:O2P	3:D:857:ARG:HG2	0.48	2.08	9	1
4:A:48:PCW:H332	4:A:54:PCW:H181	0.48	1.84	8	1
4:A:16:PCW:H341	4:A:28:PCW:H19	0.48	1.84	9	1
1:C:517:HIS:O	1:C:521:TYR:HB2	0.48	2.07	4	3
1:A:291:LEU:O	1:A:295:GLN:HG3	0.48	2.07	3	1
4:A:62:PCW:H472	4:A:72:PCW:H151	0.48	1.83	3	1
4:A:49:PCW:H322	4:A:57:PCW:H352	0.48	1.85	5	1
1:C:574:LEU:O	1:C:578:GLU:HG3	0.48	2.07	5	1
4:A:19:PCW:H321	4:A:23:PCW:H361	0.48	1.85	6	1
1:A:338:LEU:O	1:A:342:GLY:HA3	0.48	2.08	8	2
4:A:16:PCW:H61	5:A:39:17F:HN1	0.48	1.68	9	1
4:A:6:PCW:H121	4:A:16:PCW:H371	0.48	1.85	1	1
4:A:44:PCW:O31	4:A:55:PCW:H62	0.48	2.08	1	1
3:D:852:ARG:O	3:D:858:LYS:HA	0.48	2.08	1	1
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.48	2.39	9	5
4:A:49:PCW:O1P	4:A:57:PCW:H61	0.48	2.08	2	1
4:A:5:PCW:H73	5:A:38:17F:H4A	0.48	1.84	3	1
4:A:58:PCW:H121	4:A:61:PCW:H382	0.48	1.86	3	1
4:A:46:PCW:H321	4:A:71:PCW:H372	0.48	1.85	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:26:PCW:H472	4:A:68:PCW:H261	0.48	1.84	9	1
4:A:46:PCW:H71	5:A:73:17F:O1	0.48	2.08	9	1
4:A:52:PCW:H152	4:A:60:PCW:H331	0.48	1.86	1	1
2:B:22:GLN:HG3	2:B:149:ARG:HG3	0.48	1.85	5	2
4:A:2:PCW:H321	4:A:17:PCW:H351	0.48	1.85	7	1
1:C:465:GLU:C	1:C:469:LEU:CD1	0.48	2.86	7	1
4:A:11:PCW:H321	4:A:28:PCW:H2	0.48	1.83	9	1
4:A:25:PCW:H42	3:D:879:VAL:O	0.48	2.07	3	1
4:A:45:PCW:H152	5:A:74:17F:H19	0.48	1.84	3	1
4:A:1:PCW:H61	4:A:28:PCW:O2P	0.48	2.09	4	1
4:A:13:PCW:H73	5:A:37:17F:N1	0.48	2.23	4	1
5:A:38:17F:H1A	2:B:43:GLN:HE22	0.48	1.67	5	1
4:A:11:PCW:H351	4:A:28:PCW:H40	0.48	1.84	6	1
4:A:13:PCW:H332	4:A:18:PCW:H142	0.48	1.86	8	1
4:A:59:PCW:H39	4:A:61:PCW:H132	0.48	1.85	8	1
4:A:26:PCW:H19	5:A:40:17F:H72	0.48	1.85	2	1
4:A:59:PCW:H231	5:A:77:17F:H44	0.48	1.86	5	1
4:A:71:PCW:H19	4:A:71:PCW:H321	0.48	1.86	8	1
4:A:7:PCW:H52	4:A:16:PCW:O2P	0.48	2.09	1	1
4:A:9:PCW:H73	4:A:14:PCW:O31	0.48	2.09	1	1
5:A:40:17F:HN1	3:D:855:LYS:HA	0.48	1.68	1	1
4:A:49:PCW:O11	4:A:57:PCW:H73	0.48	2.08	2	1
4:A:11:PCW:H442	4:A:63:PCW:H241	0.48	1.84	5	1
4:A:44:PCW:H481	4:A:55:PCW:H212	0.48	1.85	1	1
4:A:49:PCW:O1P	4:A:57:PCW:H71	0.48	2.09	2	1
4:A:45:PCW:H371	4:A:49:PCW:H32	0.48	1.85	5	1
4:A:60:PCW:H461	4:A:63:PCW:H40	0.48	1.85	7	1
4:A:13:PCW:H382	4:A:18:PCW:H141	0.48	1.86	9	1
4:A:60:PCW:H483	4:A:63:PCW:H462	0.48	1.86	9	1
5:A:79:17F:H1	5:A:79:17F:C4	0.48	2.38	1	1
2:B:40:TYR:CE2	3:D:840:VAL:CG2	0.48	2.97	6	4
1:C:429:ASN:HA	1:C:432:LYS:HD2	0.48	1.86	6	2
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.48	1.86	7	2
4:A:12:PCW:H131	4:A:22:PCW:H122	0.47	1.85	1	1
4:A:12:PCW:H471	4:A:70:PCW:H471	0.47	1.85	1	1
1:A:336:GLU:HA	1:A:339:LYS:HE3	0.47	1.85	4	1
4:A:30:PCW:H41	5:A:34:17F:O2	0.47	2.09	5	1
3:D:850:VAL:HG12	3:D:877:VAL:HG22	0.47	1.86	8	1
5:A:33:17F:H11A	5:A:35:17F:H11A	0.47	1.86	9	1
4:A:66:PCW:H451	5:A:79:17F:H29	0.47	1.86	9	1
4:A:41:PCW:H71	4:A:59:PCW:O1P	0.47	2.09	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:56:PCW:O1P	4:A:70:PCW:H41	0.47	2.09	3	2
3:D:837:ALA:O	3:D:840:VAL:HG12	0.47	2.10	4	1
1:C:559:SER:HB2	1:C:563:LYS:HE2	0.47	1.85	6	1
1:A:359:THR:HA	1:A:362:GLU:OE1	0.47	2.08	7	1
4:A:50:PCW:H61	4:A:67:PCW:O2P	0.47	2.09	9	1
5:A:74:17F:H12	5:A:79:17F:H44	0.47	1.86	10	1
1:A:242:GLU:HB3	1:C:532:ARG:NH2	0.47	2.24	1	1
4:A:41:PCW:H412	4:A:59:PCW:H421	0.47	1.85	1	1
1:A:363:LYS:O	1:A:367:ALA:HB3	0.47	2.10	7	3
3:D:810:VAL:HG23	3:D:824:VAL:HG22	0.47	1.86	4	2
4:A:45:PCW:H261	5:A:79:17F:H49	0.47	1.85	6	1
1:C:466:GLU:OE1	1:C:469:LEU:CD1	0.47	2.58	10	1
4:A:3:PCW:H32	3:D:876:ILE:HG21	0.47	1.86	2	1
4:A:23:PCW:H441	4:A:29:PCW:H371	0.47	1.87	8	1
1:C:440:GLU:O	1:C:444:ASP:HB2	0.47	2.10	10	1
4:A:13:PCW:H42	5:A:34:17F:H2	0.47	1.87	1	1
4:A:63:PCW:H212	4:A:63:PCW:H481	0.47	1.85	5	1
3:D:841:ARG:HH11	3:D:841:ARG:HB3	0.47	1.68	6	1
4:A:11:PCW:H431	4:A:28:PCW:H231	0.47	1.86	7	1
1:C:430:LEU:HA	1:C:433:GLU:HB2	0.47	1.86	10	1
4:A:30:PCW:H461	4:A:30:PCW:H251	0.47	1.85	2	1
3:D:851:TYR:HD2	3:D:858:LYS:HB3	0.47	1.67	4	1
4:A:23:PCW:H172	4:A:23:PCW:H341	0.47	1.84	8	1
5:A:74:17F:H65	5:A:75:17F:H63	0.47	1.85	10	1
1:A:308:ARG:CG	1:C:469:LEU:CD2	0.47	2.91	1	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.47	1.86	4	1
4:A:66:PCW:H20	4:A:67:PCW:H62	0.47	1.86	4	1
3:D:834:LEU:HG	3:D:850:VAL:HG21	0.47	1.85	4	1
4:A:58:PCW:H151	4:A:61:PCW:H472	0.47	1.87	5	1
4:A:21:PCW:H152	4:A:51:PCW:H272	0.47	1.87	9	1
4:A:54:PCW:H321	4:A:72:PCW:H32	0.47	1.87	10	1
1:C:563:LYS:HB2	1:C:564:PRO:CD	0.47	2.39	1	4
1:C:561:LYS:O	1:C:565:ALA:HB3	0.47	2.10	3	2
4:A:6:PCW:H381	4:A:16:PCW:H11	0.47	1.87	7	1
4:A:13:PCW:H141	4:A:18:PCW:H171	0.47	1.86	8	1
4:A:71:PCW:H19	4:A:71:PCW:H81	0.47	1.85	9	1
1:C:549:ALA:O	1:C:553:GLU:HG3	0.47	2.09	8	2
4:A:14:PCW:H382	5:A:34:17F:H8	0.47	1.87	3	1
2:B:22:GLN:CG	2:B:149:ARG:HG3	0.47	2.40	5	1
4:A:8:PCW:H152	4:A:10:PCW:H141	0.47	1.86	8	1
1:A:376:LEU:HB2	1:A:377:PRO:CD	0.47	2.40	2	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:392:GLU:HA	1:A:395:LYS:HG2	0.47	1.87	1	1
4:A:42:PCW:H81	4:A:63:PCW:O3P	0.47	2.10	3	1
2:B:101:LYS:HE3	2:B:107:GLU:HG2	0.47	1.86	7	1
4:A:66:PCW:H20	4:A:67:PCW:H321	0.47	1.86	8	1
1:A:272:TYR:HD2	1:C:506:ARG:HH22	0.47	1.53	10	1
4:A:3:PCW:H362	4:A:18:PCW:H321	0.47	1.86	10	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.46	2.38	5	5
4:A:28:PCW:H461	4:A:63:PCW:H482	0.46	1.88	2	1
4:A:25:PCW:H61	4:A:29:PCW:O2P	0.46	2.10	3	1
4:A:67:PCW:H39	5:A:74:17F:H66	0.46	1.87	6	1
2:B:32:TYR:CD2	6:B:201:GNP:H5'1	0.46	2.45	6	1
4:A:23:PCW:O2P	2:B:73:ARG:HD2	0.46	2.10	10	1
5:A:34:17F:HN1A	5:A:37:17F:H2	0.46	1.70	4	1
4:A:53:PCW:H421	4:A:64:PCW:H481	0.46	1.88	5	1
4:A:44:PCW:H62	5:A:77:17F:HN1A	0.46	1.70	2	1
2:B:109:VAL:HB	2:B:111:MET:HE3	0.46	1.87	2	4
2:B:126:ASP:HB3	2:B:129:GLN:HG3	0.46	1.87	2	1
4:A:64:PCW:H431	4:A:64:PCW:H141	0.46	1.85	4	1
4:A:13:PCW:H73	5:A:34:17F:HN1	0.46	1.69	8	1
2:B:97:ARG:NH1	2:B:137:TYR:HB3	0.46	2.26	8	1
4:A:48:PCW:H442	4:A:54:PCW:H172	0.46	1.87	1	1
4:A:22:PCW:H73	4:A:22:PCW:O31	0.46	2.11	3	1
4:A:13:PCW:H283	4:A:18:PCW:H352	0.46	1.86	4	1
1:A:315:ALA:O	1:A:319:HIS:HB2	0.46	2.11	6	1
4:A:45:PCW:H39	4:A:57:PCW:H71	0.46	1.87	8	1
4:A:6:PCW:H331	4:A:28:PCW:H81	0.46	1.86	1	1
1:C:586:SER:O	1:C:590:GLU:HG3	0.46	2.10	1	2
4:A:13:PCW:H83	3:D:854:ILE:HB	0.46	1.87	3	1
4:A:22:PCW:O31	4:A:22:PCW:H52	0.46	2.11	4	1
2:B:84:ILE:HD12	2:B:123:ARG:HG3	0.46	1.88	10	2
1:A:351:ALA:O	1:A:355:GLU:HG2	0.46	2.10	6	1
1:A:372:ARG:O	1:A:376:LEU:HG	0.46	2.10	7	1
4:A:10:PCW:H41	3:D:876:ILE:CD1	0.46	2.41	7	1
2:B:41:ARG:HH12	3:D:817:LYS:HB2	0.46	1.71	7	1
4:A:43:PCW:H452	4:A:43:PCW:H121	0.46	1.88	8	1
4:A:31:PCW:H352	4:A:31:PCW:H172	0.46	1.87	9	1
4:A:12:PCW:H61	5:A:37:17F:HN1A	0.46	1.69	10	1
4:A:3:PCW:O2P	4:A:23:PCW:H63	0.46	2.11	3	1
4:A:72:PCW:H221	5:A:78:17F:H50	0.46	1.87	4	1
1:C:466:GLU:HA	1:C:469:LEU:HD12	0.46	1.87	6	1
4:A:11:PCW:H372	4:A:63:PCW:H281	0.46	1.86	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:33:17F:P1	5:A:33:17F:N1	0.46	2.89	1	1
4:A:6:PCW:O1P	4:A:28:PCW:H321	0.46	2.11	3	1
4:A:21:PCW:H221	4:A:51:PCW:H271	0.46	1.87	5	1
4:A:28:PCW:H412	4:A:28:PCW:H172	0.46	1.88	6	1
4:A:6:PCW:H332	4:A:16:PCW:H12	0.46	1.88	7	1
4:A:30:PCW:H42	5:A:34:17F:O2	0.46	2.10	7	1
4:A:30:PCW:H72	2:B:3:GLU:OE2	0.46	2.10	8	1
4:A:13:PCW:H12	5:A:37:17F:H8A	0.46	1.87	9	1
4:A:60:PCW:H131	4:A:61:PCW:H421	0.46	1.88	9	1
1:A:346:LEU:O	1:A:350:HIS:HB2	0.46	2.11	10	1
4:A:22:PCW:H2	4:A:22:PCW:O4P	0.46	2.11	10	1
4:A:12:PCW:H182	4:A:22:PCW:H262	0.46	1.87	1	1
1:A:307:ASP:HA	1:A:310:ARG:CD	0.46	2.41	6	1
3:D:858:LYS:HG2	3:D:876:ILE:HD12	0.46	1.88	6	1
1:A:355:GLU:HA	1:A:355:GLU:OE1	0.46	2.11	8	1
4:A:18:PCW:H20	5:A:37:17F:H12A	0.46	1.88	9	1
4:A:47:PCW:H241	5:A:76:17F:H11A	0.45	1.86	4	1
1:A:352:LYS:HG2	1:C:422:VAL:HG22	0.45	1.88	5	1
4:A:1:PCW:H2	5:A:35:17F:H18A	0.45	1.87	5	1
4:A:69:PCW:H331	4:A:69:PCW:H131	0.45	1.88	5	1
1:A:326:GLU:CD	1:C:451:LYS:HZ1	0.45	2.18	6	1
4:A:47:PCW:H31	5:A:73:17F:H4A	0.45	1.86	10	1
4:A:6:PCW:H39	4:A:16:PCW:H11	0.45	1.88	1	1
4:A:32:PCW:H321	5:A:33:17F:H20A	0.45	1.86	1	1
4:A:67:PCW:H73	5:A:78:17F:H37	0.45	1.87	2	1
1:C:461:LYS:O	1:C:465:GLU:HG3	0.45	2.11	10	2
4:A:9:PCW:H73	4:A:30:PCW:O2P	0.45	2.12	4	1
4:A:10:PCW:H81	4:A:12:PCW:H322	0.45	1.88	4	1
4:A:7:PCW:H42	5:A:35:17F:O5	0.45	2.12	6	1
4:A:8:PCW:H62	3:D:878:GLU:OE2	0.45	2.11	7	1
4:A:13:PCW:C7	5:A:34:17F:HN1	0.45	2.24	7	1
4:A:4:PCW:H51	4:A:7:PCW:O2P	0.45	2.11	9	1
1:A:327:LEU:HD23	1:A:330:ARG:HD3	0.45	1.88	2	1
4:A:14:PCW:H421	5:A:34:17F:H12	0.45	1.89	2	1
4:A:23:PCW:H42	2:B:3:GLU:OE2	0.45	2.11	2	1
4:A:25:PCW:H40	4:A:29:PCW:H231	0.45	1.88	7	1
4:A:42:PCW:H61	4:A:63:PCW:O2P	0.45	2.12	3	1
2:B:6:LEU:HD22	2:B:159:LEU:HD23	0.45	1.88	10	2
1:A:291:LEU:HD23	1:A:294:LEU:HD12	0.45	1.88	6	1
4:A:13:PCW:N	5:A:34:17F:N1	0.45	2.63	7	1
4:A:30:PCW:H32	5:A:40:17F:HN1	0.45	1.71	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:44:PCW:O2P	4:A:53:PCW:H62	0.45	2.10	10	1
2:B:62:GLU:OE1	2:B:68:ARG:HD2	0.45	2.12	10	1
4:A:12:PCW:H63	5:A:37:17F:HN1	0.45	1.71	2	1
1:C:563:LYS:CB	1:C:564:PRO:HD3	0.45	2.36	9	3
4:A:13:PCW:H42	5:A:34:17F:H1A	0.45	1.88	6	1
4:A:50:PCW:H451	5:A:78:17F:H65	0.45	1.89	9	1
4:A:20:PCW:H42	4:A:24:PCW:H61	0.45	1.88	10	1
4:A:32:PCW:H331	5:A:35:17F:H11	0.45	1.88	10	1
4:A:28:PCW:H81	2:B:3:GLU:OE2	0.45	2.11	3	1
4:A:43:PCW:O11	4:A:43:PCW:H62	0.45	2.11	3	1
2:B:85:ASN:HB3	2:B:122:SER:O	0.45	2.11	3	1
4:A:9:PCW:H452	4:A:25:PCW:H221	0.45	1.89	7	1
4:A:8:PCW:C32	4:A:22:PCW:H331	0.45	2.42	10	1
4:A:71:PCW:H332	4:A:71:PCW:H52	0.45	1.89	10	1
4:A:17:PCW:H261	5:A:36:17F:H61	0.45	1.88	1	1
4:A:42:PCW:H71	5:A:75:17F:N1	0.45	2.26	2	1
4:A:15:PCW:H42	5:A:39:17F:O1	0.45	2.10	3	1
1:A:392:GLU:HA	1:A:395:LYS:HD2	0.45	1.89	4	1
4:A:8:PCW:H72	4:A:27:PCW:O2P	0.45	2.11	4	1
1:A:278:PRO:O	1:A:282:GLU:HG3	0.45	2.12	6	2
4:A:48:PCW:H61	4:A:61:PCW:H422	0.45	1.88	9	1
4:A:22:PCW:C7	5:A:37:17F:HN1	0.45	2.25	10	1
4:A:41:PCW:H361	4:A:42:PCW:H272	0.45	1.89	1	1
4:A:47:PCW:H472	5:A:73:17F:H12A	0.45	1.88	1	1
4:A:54:PCW:H73	4:A:72:PCW:O11	0.45	2.12	1	1
4:A:62:PCW:H142	4:A:72:PCW:H152	0.45	1.88	3	1
3:D:834:LEU:HD11	3:D:877:VAL:HG21	0.45	1.87	3	1
1:A:242:GLU:OE1	1:C:528:ARG:HA	0.45	2.11	5	1
3:D:868:ALA:HB3	3:D:869:PRO:HD3	0.45	1.88	7	1
4:A:50:PCW:C4	5:A:78:17F:HN1	0.45	2.25	8	1
4:A:44:PCW:O11	4:A:44:PCW:H82	0.45	2.12	9	1
5:A:33:17F:H54	4:A:52:PCW:H461	0.45	1.88	1	1
4:A:32:PCW:H71	5:A:38:17F:HN1A	0.45	1.72	3	1
4:A:21:PCW:H442	4:A:51:PCW:H251	0.45	1.88	5	1
5:A:34:17F:H37	5:A:40:17F:H71	0.45	1.87	5	1
5:A:39:17F:H33	5:A:39:17F:H8	0.45	1.89	7	1
2:B:116:ASN:HA	2:B:144:THR:O	0.45	2.12	8	1
5:A:37:17F:H1	3:D:858:LYS:HD3	0.45	1.89	1	1
4:A:32:PCW:H482	4:A:55:PCW:H221	0.45	1.89	6	1
4:A:48:PCW:H332	4:A:54:PCW:H152	0.45	1.88	6	1
4:A:41:PCW:H81	4:A:59:PCW:O1P	0.45	2.12	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:23:PCW:H61	2:B:54:ASP:CG	0.44	2.37	2	1
4:A:53:PCW:H341	4:A:68:PCW:H151	0.44	1.89	2	1
4:A:24:PCW:H61	4:A:31:PCW:O1P	0.44	2.12	3	1
3:D:831:TYR:O	3:D:835:ASP:HB2	0.44	2.12	3	1
4:A:10:PCW:H81	4:A:22:PCW:O3P	0.44	2.12	7	1
5:A:40:17F:N1	2:B:5:LYS:NZ	0.44	2.65	7	1
4:A:8:PCW:H82	4:A:22:PCW:H362	0.44	1.88	10	1
4:A:1:PCW:H121	5:A:35:17F:H32	0.44	1.87	7	1
4:A:42:PCW:H262	4:A:52:PCW:H241	0.44	1.89	7	1
4:A:10:PCW:H71	5:A:36:17F:O2	0.44	2.11	1	1
1:C:455:TYR:O	1:C:459:PHE:HB2	0.44	2.12	1	1
2:B:41:ARG:HA	2:B:53:LEU:O	0.44	2.12	2	1
4:A:29:PCW:H71	3:D:847:CYS:HA	0.44	1.90	3	1
4:A:43:PCW:H371	5:A:75:17F:H10	0.44	1.89	6	1
1:A:363:LYS:HG2	1:C:411:THR:HG22	0.44	1.87	7	1
4:A:55:PCW:H382	4:A:64:PCW:H362	0.44	1.88	8	1
4:A:5:PCW:H211	4:A:5:PCW:H152	0.44	1.90	5	1
4:A:42:PCW:H12	4:A:69:PCW:H121	0.44	1.88	5	1
4:A:16:PCW:O31	4:A:16:PCW:H73	0.44	2.12	7	1
4:A:22:PCW:O2P	4:A:27:PCW:H83	0.44	2.13	3	1
4:A:48:PCW:H341	4:A:54:PCW:H121	0.44	1.89	3	1
4:A:49:PCW:H421	5:A:80:17F:H58	0.44	1.89	4	1
4:A:71:PCW:H41	5:A:73:17F:O4	0.44	2.12	8	1
4:A:45:PCW:H362	4:A:49:PCW:H152	0.44	1.88	9	1
2:B:73:ARG:HH21	2:B:103:VAL:HA	0.44	1.72	2	1
4:A:52:PCW:O2P	4:A:60:PCW:H71	0.44	2.13	4	1
1:C:458:ASP:HA	1:C:461:LYS:HD2	0.44	1.90	2	1
1:C:431:GLU:HA	1:C:434:THR:OG1	0.44	2.12	4	1
4:A:27:PCW:H82	5:A:37:17F:O2	0.44	2.13	5	2
4:A:10:PCW:H452	4:A:12:PCW:H232	0.44	1.89	6	1
1:A:356:HIS:HA	1:C:418:GLN:OE1	0.44	2.13	1	1
4:A:22:PCW:H11	5:A:37:17F:O2	0.44	2.12	3	1
4:A:32:PCW:H11	5:A:33:17F:H4	0.44	1.90	3	1
1:C:464:GLN:O	1:C:468:GLU:HG3	0.44	2.12	5	1
1:C:487:GLN:O	1:C:491:GLU:HG3	0.44	2.12	5	1
4:A:10:PCW:H262	5:A:73:17F:H53	0.44	1.88	8	1
4:A:17:PCW:O1P	4:A:17:PCW:H31	0.44	2.12	8	1
1:C:530:ALA:O	1:C:534:GLU:HG2	0.44	2.12	9	1
4:A:25:PCW:H132	4:A:31:PCW:H31	0.44	1.88	10	1
1:A:299:SER:HB2	1:A:300:PRO:CD	0.44	2.42	1	2
3:D:853:LEU:HD12	3:D:874:GLU:HB2	0.44	1.88	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:2:PCW:H19	3:D:857:ARG:HE	0.44	1.73	6	1
4:A:57:PCW:H122	4:A:57:PCW:H351	0.44	1.90	8	1
4:A:62:PCW:H71	4:A:67:PCW:O2P	0.44	2.13	8	1
2:B:11:ALA:O	2:B:14:VAL:HG22	0.44	2.13	8	1
4:A:3:PCW:H161	4:A:3:PCW:H39	0.43	1.90	1	1
4:A:1:PCW:H432	4:A:26:PCW:H182	0.43	1.89	6	1
4:A:42:PCW:H211	4:A:52:PCW:H342	0.43	1.88	6	1
4:A:14:PCW:H32	5:A:34:17F:H1	0.43	1.90	8	1
1:A:335:LEU:O	1:A:339:LYS:HG3	0.43	2.13	9	1
4:A:1:PCW:H212	5:A:38:17F:H19	0.43	1.90	1	1
4:A:44:PCW:O1P	4:A:55:PCW:H82	0.43	2.13	2	1
4:A:5:PCW:H39	4:A:17:PCW:H63	0.43	1.89	5	1
4:A:27:PCW:H73	5:A:37:17F:O2	0.43	2.13	5	1
4:A:66:PCW:H20	4:A:67:PCW:H82	0.43	1.88	5	1
1:C:428:ASP:O	1:C:432:LYS:HG3	0.43	2.12	5	1
4:A:26:PCW:O3P	5:A:40:17F:H19	0.43	2.13	6	1
4:A:62:PCW:H422	4:A:72:PCW:H172	0.43	1.89	6	1
1:C:458:ASP:O	1:C:462:LYS:HG3	0.43	2.13	9	1
4:A:17:PCW:H271	5:A:36:17F:H71	0.43	1.91	3	1
5:A:34:17F:HN1A	3:D:857:ARG:HA	0.43	1.73	3	1
1:A:330:ARG:HD3	1:C:444:ASP:OD2	0.43	2.14	4	1
4:A:44:PCW:C5	5:A:77:17F:HN1A	0.43	2.26	4	1
4:A:8:PCW:H411	4:A:27:PCW:H251	0.43	1.89	5	1
4:A:31:PCW:C7	3:D:876:ILE:HD11	0.43	2.43	10	1
4:A:42:PCW:H332	4:A:69:PCW:H132	0.43	1.89	10	1
4:A:44:PCW:H262	4:A:55:PCW:H19	0.43	1.89	10	1
4:A:60:PCW:H461	4:A:63:PCW:H432	0.43	1.90	10	1
4:A:23:PCW:H241	4:A:49:PCW:H40	0.43	1.90	1	1
4:A:14:PCW:H12	4:A:23:PCW:O31	0.43	2.13	9	1
4:A:4:PCW:O2P	4:A:16:PCW:H82	0.43	2.13	10	1
4:A:46:PCW:H361	4:A:71:PCW:H212	0.43	1.90	10	1
1:C:567:GLU:HG2	1:C:571:GLN:NE2	0.43	2.27	2	1
1:A:279:LEU:HB3	1:C:495:LYS:HD3	0.43	1.90	4	1
5:A:76:17F:H70	1:C:470:TYR:HB3	0.43	1.90	5	1
4:A:32:PCW:H483	5:A:38:17F:H55	0.43	1.90	6	1
4:A:59:PCW:H162	5:A:77:17F:H34	0.43	1.90	6	1
1:A:239:LEU:HD22	4:A:20:PCW:H462	0.43	1.91	1	1
1:A:365:LYS:HB2	1:A:366:PRO:CD	0.43	2.43	2	3
1:A:345:ARG:HD3	1:C:433:GLU:OE2	0.43	2.13	3	1
1:A:386:PHE:O	1:A:390:LEU:HG	0.43	2.14	3	1
4:A:53:PCW:H31	4:A:64:PCW:C3	0.43	2.44	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:510:HIS:O	1:C:514:LEU:HG	0.43	2.14	3	2
4:A:41:PCW:H212	4:A:61:PCW:H152	0.43	1.91	7	1
4:A:14:PCW:H471	4:A:30:PCW:H442	0.43	1.89	8	1
4:A:43:PCW:O2P	4:A:45:PCW:H71	0.43	2.14	3	1
1:C:485:ALA:HA	1:C:488:LYS:HG2	0.43	1.90	7	1
4:A:55:PCW:H62	5:A:77:17F:HN1A	0.43	1.72	8	1
1:A:277:GLU:HB3	1:A:278:PRO:CD	0.43	2.43	10	1
1:C:458:ASP:HA	1:C:461:LYS:HE2	0.43	1.91	10	1
1:C:512:ASP:O	1:C:515:ARG:HB2	0.43	2.13	10	2
2:B:9:VAL:HB	2:B:96:TYR:CE1	0.43	2.49	5	1
4:A:48:PCW:H372	4:A:54:PCW:H252	0.43	1.90	6	1
4:A:17:PCW:C1	2:B:70:GLN:HB2	0.43	2.41	8	1
4:A:3:PCW:H221	4:A:19:PCW:H182	0.43	1.90	9	1
3:D:811:LYS:HG2	3:D:821:VAL:HG22	0.43	1.90	9	1
3:D:858:LYS:HE3	3:D:876:ILE:HB	0.43	1.89	1	1
1:A:344:ALA:O	1:A:348:GLU:HG2	0.43	2.14	4	1
4:A:52:PCW:H31	4:A:52:PCW:H41	0.43	1.90	8	1
4:A:20:PCW:H462	4:A:31:PCW:H411	0.43	1.90	9	1
4:A:31:PCW:H331	4:A:31:PCW:H73	0.43	1.90	1	1
5:A:40:17F:H69	5:A:40:17F:H37	0.43	1.91	2	1
4:A:56:PCW:H332	4:A:56:PCW:H131	0.43	1.90	5	1
4:A:7:PCW:H321	5:A:33:17F:H9	0.42	1.89	4	1
1:A:263:LYS:O	1:A:267:GLU:HG3	0.42	2.14	9	2
4:A:53:PCW:H362	4:A:53:PCW:H151	0.42	1.90	6	1
4:A:30:PCW:H361	5:A:34:17F:H18	0.42	1.90	8	1
4:A:47:PCW:H20	5:A:76:17F:H20	0.42	1.91	8	1
2:B:163:ILE:O	2:B:167:LYS:HG2	0.42	2.14	8	2
1:A:243:MET:HA	1:A:246:ASP:HB2	0.42	1.90	5	1
5:A:37:17F:N1	3:D:817:LYS:NZ	0.42	2.67	7	1
1:C:589:GLU:O	1:C:593:LYS:HG3	0.42	2.14	7	1
1:A:376:LEU:HB2	1:A:377:PRO:HD3	0.42	1.91	2	2
4:A:23:PCW:H71	2:B:54:ASP:OD2	0.42	2.13	2	1
4:A:10:PCW:H352	4:A:21:PCW:H341	0.42	1.91	4	1
2:B:24:ILE:HA	2:B:42:LYS:HD2	0.42	1.90	5	1
4:A:68:PCW:O31	4:A:69:PCW:H73	0.42	2.15	6	1
2:B:40:TYR:C	3:D:818:GLN:HE22	0.42	2.22	6	1
4:A:7:PCW:H42	3:D:879:VAL:O	0.42	2.14	9	1
4:A:53:PCW:H152	4:A:64:PCW:H171	0.42	1.90	10	1
1:A:330:ARG:HD3	1:C:444:ASP:CG	0.42	2.39	1	1
5:A:38:17F:H2	5:A:38:17F:O2	0.42	2.13	1	1
2:B:69:ASP:O	2:B:73:ARG:HG3	0.42	2.14	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:830:VAL:O	3:D:834:LEU:HB2	0.42	2.14	2	2
4:A:9:PCW:H142	4:A:11:PCW:H132	0.42	1.90	5	1
4:A:44:PCW:O31	4:A:55:PCW:H83	0.42	2.13	5	1
2:B:118:CYS:HB3	2:B:143:GLU:HG2	0.42	1.91	6	1
4:A:20:PCW:H432	4:A:31:PCW:H122	0.42	1.90	7	1
4:A:8:PCW:O31	4:A:22:PCW:H71	0.42	2.14	8	1
4:A:9:PCW:H261	4:A:63:PCW:H241	0.42	1.91	3	1
4:A:12:PCW:O1P	3:D:855:LYS:HD3	0.42	2.14	3	1
5:A:33:17F:H8A	5:A:35:17F:H11A	0.42	1.92	1	1
4:A:10:PCW:C7	5:A:37:17F:HN1A	0.42	2.27	3	1
4:A:20:PCW:P	3:D:876:ILE:HG12	0.42	2.55	4	1
4:A:17:PCW:H121	5:A:36:17F:H6	0.42	1.90	6	1
4:A:5:PCW:H12	4:A:17:PCW:H361	0.42	1.91	8	1
1:C:502:GLU:O	1:C:506:ARG:HG3	0.42	2.15	2	4
1:A:270:GLU:O	1:A:274:GLN:HB2	0.42	2.14	6	1
4:A:14:PCW:H432	5:A:34:17F:H12	0.42	1.92	6	1
4:A:70:PCW:H351	4:A:71:PCW:H141	0.42	1.91	6	1
1:A:352:LYS:HZ2	1:C:425:GLU:CB	0.42	2.27	7	1
5:A:33:17F:C4	5:A:33:17F:H1	0.42	2.44	7	1
4:A:16:PCW:C8	5:A:39:17F:H6	0.42	2.44	8	1
1:C:576:VAL:O	1:C:580:PHE:HB2	0.42	2.15	9	1
1:A:258:LEU:O	1:A:262:GLN:HB2	0.42	2.14	10	1
4:A:23:PCW:H62	2:B:5:LYS:HG2	0.42	1.92	2	1
4:A:32:PCW:H342	5:A:35:17F:H12A	0.42	1.91	4	1
4:A:15:PCW:H42	5:A:39:17F:H1	0.42	1.91	8	1
4:A:16:PCW:O1P	4:A:16:PCW:H2	0.42	2.15	8	1
4:A:60:PCW:H322	4:A:63:PCW:H62	0.42	1.91	8	1
4:A:53:PCW:H371	4:A:68:PCW:H411	0.42	1.91	9	1
4:A:58:PCW:H351	4:A:61:PCW:H441	0.42	1.91	9	1
4:A:59:PCW:O11	4:A:59:PCW:H83	0.42	2.14	2	1
2:B:159:LEU:O	2:B:163:ILE:HG13	0.42	2.15	2	1
4:A:8:PCW:H73	4:A:22:PCW:O1P	0.42	2.14	3	1
4:A:12:PCW:H71	3:D:874:GLU:OE1	0.42	2.15	3	1
1:A:304:GLU:O	1:A:308:ARG:HG2	0.42	2.14	5	1
4:A:5:PCW:H461	4:A:17:PCW:H171	0.42	1.92	6	1
1:A:243:MET:HA	1:A:246:ASP:HB3	0.42	1.92	8	1
4:A:1:PCW:H471	4:A:26:PCW:H461	0.42	1.92	8	1
4:A:9:PCW:H81	4:A:26:PCW:O2P	0.42	2.14	8	1
1:A:345:ARG:O	1:A:349:TYR:HB2	0.42	2.15	9	1
4:A:42:PCW:H31	4:A:69:PCW:H151	0.42	1.92	9	1
1:C:427:TRP:O	1:C:431:GLU:HG2	0.42	2.15	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:12:PCW:O1P	3:D:857:ARG:HD3	0.42	2.14	1	1
4:A:2:PCW:N	4:A:5:PCW:O2P	0.42	2.53	4	1
4:A:7:PCW:H382	5:A:33:17F:H9A	0.42	1.91	5	1
1:A:356:HIS:O	1:A:360:LEU:HB2	0.42	2.14	7	1
4:A:6:PCW:H331	4:A:7:PCW:H81	0.42	1.91	7	1
4:A:11:PCW:H83	2:B:171:SER:HB3	0.42	1.92	7	1
4:A:48:PCW:H62	4:A:61:PCW:H39	0.42	1.91	7	1
4:A:68:PCW:H31	4:A:70:PCW:H171	0.42	1.91	8	1
4:A:26:PCW:H62	4:A:28:PCW:O1P	0.42	2.15	10	1
4:A:59:PCW:H51	5:A:77:17F:H8A	0.41	1.90	2	1
1:C:491:GLU:HB3	1:C:495:LYS:CE	0.41	2.44	5	3
4:A:30:PCW:H73	4:A:30:PCW:O11	0.41	2.15	6	1
4:A:48:PCW:H371	4:A:54:PCW:H431	0.41	1.91	7	1
4:A:59:PCW:H221	5:A:77:17F:H11A	0.41	1.91	7	1
2:B:15:GLY:HA2	6:B:201:GNP:O1A	0.41	2.16	7	1
5:A:74:17F:H56	5:A:79:17F:H4	0.41	1.92	9	1
4:A:31:PCW:O2P	3:D:876:ILE:HG21	0.41	2.15	10	1
4:A:44:PCW:H32	5:A:77:17F:HN1A	0.41	1.76	10	1
4:A:8:PCW:H41	4:A:22:PCW:O1P	0.41	2.15	3	1
1:C:458:ASP:HA	1:C:461:LYS:NZ	0.41	2.30	3	1
4:A:44:PCW:H82	5:A:77:17F:C3	0.41	2.46	5	1
4:A:44:PCW:H42	4:A:53:PCW:O1P	0.41	2.14	6	1
2:B:158:THR:O	2:B:162:GLU:HG2	0.41	2.15	8	1
4:A:13:PCW:H61	5:A:34:17F:O1	0.41	2.15	10	1
4:A:26:PCW:H152	4:A:26:PCW:H471	0.41	1.92	10	1
1:A:330:ARG:NH2	1:C:447:GLU:HB3	0.41	2.31	1	1
4:A:14:PCW:H352	5:A:34:17F:H59	0.41	1.92	7	1
1:C:451:LYS:C	1:C:454:PRO:HD2	0.41	2.40	7	1
5:A:34:17F:H42	5:A:75:17F:H52	0.41	1.91	8	1
4:A:48:PCW:H82	4:A:61:PCW:H411	0.41	1.91	10	1
4:A:1:PCW:H181	5:A:35:17F:H56	0.41	1.92	2	1
5:A:34:17F:HN1A	3:D:858:LYS:N	0.41	2.10	3	1
4:A:42:PCW:H231	4:A:42:PCW:H432	0.41	1.91	3	1
1:A:304:GLU:O	1:A:308:ARG:HG3	0.41	2.14	4	1
4:A:30:PCW:H82	5:A:34:17F:O3	0.41	2.16	4	1
4:A:13:PCW:H442	5:A:37:17F:H73	0.41	1.92	7	1
2:B:41:ARG:HD3	2:B:54:ASP:OD2	0.41	2.16	3	1
4:A:5:PCW:H42	3:D:853:LEU:HD13	0.41	1.92	6	1
4:A:13:PCW:H411	4:A:27:PCW:H351	0.41	1.91	6	1
4:A:14:PCW:H131	4:A:23:PCW:H2	0.41	1.92	2	1
4:A:4:PCW:H63	5:A:33:17F:P1	0.41	2.56	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:6:PCW:P	5:A:39:17F:O1	0.41	2.79	7	1
2:B:37:GLU:O	3:D:821:VAL:HG23	0.41	2.16	7	1
4:A:17:PCW:H181	5:A:36:17F:H19	0.41	1.92	8	1
4:A:62:PCW:H332	4:A:72:PCW:H19	0.41	1.90	8	1
1:A:330:ARG:HH12	1:C:448:VAL:HG23	0.41	1.76	10	1
4:A:43:PCW:H211	4:A:51:PCW:H431	0.41	1.92	10	1
4:A:51:PCW:H82	4:A:71:PCW:O31	0.41	2.16	10	1
4:A:56:PCW:H31	4:A:56:PCW:H51	0.41	1.92	1	1
4:A:67:PCW:H141	5:A:74:17F:H70	0.41	1.93	2	1
4:A:1:PCW:N	5:A:35:17F:N1	0.41	2.68	3	1
4:A:14:PCW:H151	4:A:23:PCW:H172	0.41	1.91	3	1
4:A:8:PCW:H63	4:A:27:PCW:O2P	0.41	2.15	4	1
4:A:50:PCW:H441	5:A:78:17F:H59	0.41	1.93	4	1
5:A:37:17F:HN1	3:D:817:LYS:NZ	0.41	2.13	7	1
5:A:37:17F:HN1	3:D:817:LYS:HZ2	0.41	1.58	7	1
1:A:285:GLU:HA	1:A:288:ARG:HD2	0.41	1.92	9	1
4:A:6:PCW:P	3:D:878:GLU:OE2	0.41	2.79	9	1
4:A:30:PCW:H39	5:A:40:17F:H74	0.41	1.93	9	1
4:A:5:PCW:H442	5:A:36:17F:H36	0.41	1.92	10	1
5:A:79:17F:H4	5:A:79:17F:C1	0.41	2.45	1	1
4:A:9:PCW:H52	4:A:14:PCW:O31	0.41	2.16	2	1
4:A:41:PCW:H231	4:A:61:PCW:H232	0.41	1.93	4	1
1:A:277:GLU:HB2	1:A:278:PRO:CD	0.41	2.45	6	1
4:A:42:PCW:H341	4:A:42:PCW:H19	0.41	1.93	8	1
4:A:6:PCW:H272	4:A:24:PCW:H481	0.41	1.93	9	1
4:A:11:PCW:H62	4:A:24:PCW:O11	0.41	2.15	9	1
4:A:42:PCW:H382	4:A:69:PCW:H152	0.41	1.92	10	1
4:A:53:PCW:H40	4:A:68:PCW:H462	0.41	1.93	10	1
1:C:508:ARG:O	1:C:512:ASP:HB3	0.41	2.16	10	1
4:A:30:PCW:H61	3:D:853:LEU:HD11	0.41	1.93	1	1
1:A:243:MET:O	1:A:247:LEU:HB2	0.41	2.16	2	1
4:A:8:PCW:H83	4:A:22:PCW:O1P	0.41	2.15	2	1
4:A:43:PCW:H12	4:A:68:PCW:O1P	0.41	2.16	2	1
4:A:62:PCW:H41	4:A:67:PCW:O2P	0.41	2.16	2	1
2:B:100:ILE:HA	2:B:103:VAL:HG22	0.41	1.92	2	1
2:B:81:VAL:HA	2:B:114:VAL:HB	0.41	1.92	3	1
4:A:5:PCW:H161	5:A:38:17F:H10A	0.41	1.91	4	1
4:A:44:PCW:H432	4:A:64:PCW:H40	0.41	1.93	4	1
4:A:46:PCW:O3P	4:A:71:PCW:H372	0.41	2.16	5	1
1:C:412:PHE:O	1:C:415:LEU:HB2	0.41	2.16	5	1
1:C:540:GLY:O	1:C:544:LEU:HG	0.41	2.16	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:14:PCW:H72	4:A:25:PCW:H31	0.41	1.92	6	1
4:A:48:PCW:H63	4:A:58:PCW:O11	0.41	2.16	6	1
4:A:25:PCW:O31	4:A:31:PCW:H62	0.41	2.16	7	1
1:A:325:ASP:O	1:A:329:GLN:HG3	0.41	2.15	8	1
5:A:40:17F:O4	2:B:5:LYS:HE2	0.41	2.16	8	1
1:A:264:LYS:O	1:A:268:GLU:HG3	0.41	2.15	9	1
4:A:14:PCW:H42	4:A:23:PCW:H371	0.41	1.92	9	1
4:A:28:PCW:H242	4:A:42:PCW:H481	0.41	1.92	10	1
1:C:578:GLU:O	1:C:582:VAL:HG23	0.41	2.16	10	1
4:A:25:PCW:H40	4:A:29:PCW:H321	0.41	1.92	1	1
4:A:30:PCW:H71	3:D:853:LEU:HD21	0.41	1.93	1	1
4:A:60:PCW:H411	4:A:72:PCW:H162	0.41	1.93	4	1
4:A:6:PCW:H82	5:A:39:17F:H2	0.41	1.91	5	1
4:A:9:PCW:O11	4:A:9:PCW:H51	0.41	2.15	5	1
4:A:9:PCW:H121	4:A:11:PCW:H122	0.41	1.91	6	1
4:A:52:PCW:H42	4:A:60:PCW:O1P	0.41	2.16	6	1
4:A:13:PCW:H141	5:A:37:17F:H37	0.41	1.93	7	1
4:A:41:PCW:O31	4:A:61:PCW:H81	0.41	2.16	8	1
1:C:490:HIS:HA	1:C:493:GLN:OE1	0.41	2.15	10	1
4:A:5:PCW:O4P	4:A:5:PCW:H2	0.40	2.16	1	1
3:D:867:ILE:HD11	3:D:875:LEU:HD11	0.40	1.93	2	1
1:A:290:LYS:HE3	1:C:487:GLN:OE1	0.40	2.16	6	1
4:A:8:PCW:H83	4:A:27:PCW:O2P	0.40	2.16	6	1
4:A:28:PCW:H451	4:A:63:PCW:H272	0.40	1.91	6	1
4:A:42:PCW:H73	4:A:42:PCW:O31	0.40	2.16	6	1
4:A:13:PCW:O1P	4:A:18:PCW:H62	0.40	2.16	8	1
4:A:12:PCW:H411	5:A:36:17F:H12A	0.40	1.92	9	1
4:A:12:PCW:H362	4:A:30:PCW:H181	0.40	1.93	10	1
4:A:48:PCW:H61	4:A:60:PCW:O11	0.40	2.15	10	1
1:C:574:LEU:HB2	1:C:575:PRO:CD	0.40	2.45	10	1
4:A:41:PCW:H351	4:A:59:PCW:H362	0.40	1.93	1	1
4:A:9:PCW:H172	4:A:26:PCW:H131	0.40	1.92	2	1
4:A:16:PCW:H122	5:A:39:17F:H69	0.40	1.93	2	1
4:A:12:PCW:H372	5:A:36:17F:H18A	0.40	1.93	4	1
4:A:43:PCW:O2P	4:A:45:PCW:H51	0.40	2.16	4	1
5:A:33:17F:N1	3:D:858:LYS:NZ	0.40	2.70	5	1
4:A:2:PCW:H61	3:D:815:PRO:HA	0.40	1.93	6	1
4:A:13:PCW:H42	5:A:34:17F:O5	0.40	2.16	6	1
4:A:54:PCW:O31	4:A:62:PCW:H131	0.40	2.17	7	1
1:A:272:TYR:O	1:A:276:VAL:HG23	0.40	2.17	9	1
1:A:260:ASP:HA	1:A:263:LYS:CE	0.40	2.38	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:18:PCW:H261	4:A:49:PCW:H442	0.40	1.91	10	1
4:A:5:PCW:H151	4:A:17:PCW:H382	0.40	1.93	1	1
4:A:48:PCW:H61	4:A:58:PCW:O11	0.40	2.16	2	1
1:C:561:LYS:HA	1:C:565:ALA:CB	0.40	2.46	2	1
4:A:41:PCW:H32	4:A:52:PCW:H122	0.40	1.92	3	1
4:A:16:PCW:H62	2:B:105:ASP:OD1	0.40	2.16	6	1
2:B:85:ASN:OD1	2:B:117:LYS:HD2	0.40	2.17	7	1
4:A:8:PCW:H341	4:A:10:PCW:H172	0.40	1.91	8	1
4:A:41:PCW:H261	4:A:58:PCW:H452	0.40	1.92	8	1
4:A:70:PCW:H62	4:A:70:PCW:O31	0.40	2.15	8	1
4:A:26:PCW:O31	5:A:40:17F:H19A	0.40	2.17	9	1
5:A:34:17F:H40	5:A:40:17F:H73	0.40	1.93	9	1
4:A:53:PCW:O2P	4:A:64:PCW:H81	0.40	2.17	9	1
4:A:17:PCW:H72	5:A:38:17F:O1	0.40	2.16	10	1
4:A:45:PCW:H141	5:A:74:17F:HN1	0.40	1.76	10	1
4:A:14:PCW:H252	4:A:14:PCW:H442	0.40	1.94	1	1
4:A:23:PCW:H73	5:A:34:17F:N1	0.40	2.29	1	1
4:A:58:PCW:O2P	4:A:60:PCW:H81	0.40	2.16	2	1
4:A:12:PCW:H131	5:A:37:17F:H6	0.40	1.93	3	1
4:A:65:PCW:H82	4:A:65:PCW:O11	0.40	2.17	3	1
2:B:36:ILE:HB	3:D:821:VAL:HB	0.40	1.92	4	1
4:A:58:PCW:H132	4:A:61:PCW:H451	0.40	1.91	5	1
1:A:239:LEU:HA	1:A:242:GLU:HB2	0.40	1.91	7	1
1:A:341:ASN:O	1:A:345:ARG:HG3	0.40	2.16	9	1
4:A:26:PCW:H432	4:A:26:PCW:H121	0.40	1.93	10	1
5:A:38:17F:H9	5:A:38:17F:H18A	0.40	1.92	1	1
4:A:46:PCW:H83	5:A:73:17F:O2	0.40	2.17	1	1
4:A:55:PCW:O2P	4:A:64:PCW:H12	0.40	2.16	2	1
5:A:34:17F:O4	3:D:857:ARG:HD3	0.40	2.17	3	1
1:A:246:ASP:CG	1:C:528:ARG:HD3	0.40	2.42	5	1
4:A:8:PCW:H82	4:A:22:PCW:O1P	0.40	2.16	5	1
4:A:1:PCW:H162	5:A:35:17F:H33	0.40	1.91	7	1
4:A:46:PCW:O2P	4:A:71:PCW:H332	0.40	2.15	9	1
4:A:62:PCW:H11	4:A:72:PCW:O3P	0.40	2.16	9	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	157/200 (78%)	153±1 (98±1%)	3±1 (2±1%)	1±0 (1±0%)	23	72
1	C	195/200 (98%)	190±1 (98±1%)	4±2 (2±1%)	1±0 (1±0%)	26	74
2	B	170/187 (91%)	161±3 (95±2%)	9±3 (5±1%)	0±0 (0±0%)	44	80
3	D	71/73 (97%)	66±2 (93±2%)	5±2 (7±2%)	0±0 (0±0%)	49	83
All	All	5930/6600 (90%)	5702 (96%)	204 (3%)	24 (0%)	31	76

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

Mol	Chain	Res	Type	Models (Total)
1	A	365	LYS	10
1	C	563	LYS	9
2	B	24	ILE	1
3	D	827	GLY	1
1	C	420	GLY	1
2	B	13	GLY	1
2	B	48	GLY	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	135/175 (77%)	122±3 (91±2%)	13±3 (9±2%)	10	55
1	C	172/175 (98%)	157±2 (91±1%)	15±2 (9±1%)	11	57
2	B	150/165 (91%)	136±2 (91±1%)	14±2 (9±1%)	11	57
3	D	64/64 (100%)	57±2 (89±3%)	7±2 (11±3%)	8	50
All	All	5210/5790 (90%)	4719 (91%)	491 (9%)	10	56

All 191 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	254	VAL	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	74	THR	10
2	B	87	THR	10
2	B	35	THR	9
1	A	312	HIS	8
1	C	550	LYS	8
3	D	823	THR	8
1	A	392	GLU	8
1	C	516	THR	8
2	B	92	ASP	8
3	D	829	SER	7
1	C	480	GLU	7
2	B	69	ASP	7
2	B	122	SER	6
2	B	124	THR	6
3	D	853	LEU	6
1	A	354	THR	6
1	A	318	THR	5
3	D	819	ARG	5
3	D	816	ASN	5
2	B	54	ASP	5
1	A	293	GLU	5
2	B	33	ASP	5
1	C	405	TRP	4
1	C	447	GLU	4
1	C	505	ASP	4
2	B	17	SER	4
2	B	39	SER	4
2	B	65	SER	4
2	B	85	ASN	4
3	D	864	ASP	4
3	D	878	GLU	4
1	C	487	GLN	4
2	B	127	THR	4
1	C	407	SER	4
1	C	455	TYR	4
1	C	463	TRP	4
1	C	568	ASP	4
3	D	834	LEU	4
1	A	246	ASP	4
1	C	448	VAL	4
1	A	385	SER	3
1	C	403	ASP	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	C	459	PHE	3
1	C	482	GLN	3
2	B	153	ASP	3
1	A	265	TRP	3
1	A	272	TYR	3
1	A	394	THR	3
1	C	444	ASP	3
1	C	466	GLU	3
1	C	552	THR	3
1	C	594	LYS	3
2	B	2	THR	3
3	D	841	ARG	3
3	D	847	CYS	3
3	D	859	THR	3
2	B	62	GLU	3
3	D	860	VAL	3
1	A	274	GLN	3
1	A	292	HIS	3
1	A	296	GLU	3
1	A	314	ASP	3
1	A	350	HIS	3
1	A	370	ASP	3
1	C	467	MET	3
2	B	41	ARG	3
3	D	809	THR	3
3	D	833	SER	3
1	A	319	HIS	3
1	C	412	PHE	3
1	C	451	LYS	3
1	A	243	MET	2
1	A	255	GLN	2
1	A	304	GLU	2
1	A	327	LEU	2
1	A	361	SER	2
1	A	371	LEU	2
1	C	404	ASN	2
1	C	434	THR	2
1	C	460	GLN	2
1	C	523	ASP	2
1	C	532	ARG	2
1	C	546	GLU	2
1	A	249	GLU	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	C	501	GLU	2
1	C	556	SER	2
1	C	557	THR	2
1	C	561	LYS	2
2	B	3	GLU	2
2	B	145	SER	2
2	B	148	THR	2
2	B	168	GLU	2
3	D	870	LEU	2
1	A	266	GLN	2
1	A	284	GLN	2
1	A	356	HIS	2
1	A	359	THR	2
1	C	583	SER	2
2	B	31	GLU	2
2	B	37	GLU	2
2	B	164	ARG	2
3	D	865	THR	2
1	C	418	GLN	2
2	B	51	CYS	2
1	A	299	SER	2
1	A	368	LEU	2
1	C	490	HIS	2
2	B	132	ASP	2
1	A	381	SER	2
1	C	580	PHE	2
1	C	410	SER	2
1	C	512	ASP	2
1	C	548	HIS	2
2	B	30	ASP	2
1	A	348	GLU	2
1	C	592	THR	2
1	A	276	VAL	1
1	A	297	LYS	1
1	C	426	PHE	1
1	C	464	GLN	1
1	C	468	GLU	1
1	C	560	GLU	1
1	C	566	LEU	1
2	B	16	LYS	1
2	B	95	HIS	1
3	D	813	TYR	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
3	D	840	VAL	1
1	C	457	ASP	1
2	B	71	TYR	1
2	B	102	ARG	1
3	D	826	ASP	1
1	A	273	ARG	1
1	A	277	GLU	1
1	A	387	LEU	1
1	C	462	LYS	1
1	C	521	TYR	1
1	C	537	LYS	1
2	B	57	ASP	1
2	B	119	ASP	1
1	A	241	GLN	1
1	A	261	PHE	1
1	C	427	TRP	1
1	C	429	ASN	1
1	C	596	ASN	1
2	B	20	THR	1
2	B	32	TYR	1
2	B	44	VAL	1
2	B	101	LYS	1
1	A	244	SER	1
1	A	305	MET	1
1	A	307	ASP	1
1	C	401	LEU	1
1	C	472	GLN	1
1	C	473	LYS	1
1	C	522	SER	1
1	C	554	HIS	1
1	C	590	GLU	1
2	B	47	ASP	1
2	B	70	GLN	1
2	B	150	GLN	1
2	B	154	ASP	1
1	A	245	LYS	1
1	C	494	GLU	1
1	C	558	LEU	1
2	B	89	SER	1
2	B	97	ARG	1
1	A	270	GLU	1
1	C	409	THR	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	C	477	LEU	1
2	B	126	ASP	1
1	A	283	LEU	1
1	A	290	LYS	1
1	A	358	SER	1
1	C	402	LEU	1
1	C	425	GLU	1
2	B	99	GLN	1
3	D	811	LYS	1
3	D	844	ASN	1
1	A	378	VAL	1
1	C	559	SER	1
1	C	576	VAL	1
1	C	584	PHE	1
2	B	107	GLU	1
3	D	861	THR	1
3	D	876	ILE	1
1	A	325	ASP	1
1	A	336	GLU	1
1	A	360	LEU	1
1	C	433	GLU	1
3	D	857	ARG	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
4	PCW	A	15	-	53,53,53	1.04±0.01	5±0 (8±0%)
4	PCW	A	68	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	26	-	53,53,53	1.05±0.01	4±0 (6±0%)
4	PCW	A	54	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	PCW	A	64	-	53,53,53	1.05±0.00	4±0 (7±0%)
4	PCW	A	62	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	PCW	A	5	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	PCW	A	11	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	PCW	A	48	-	53,53,53	1.04±0.01	5±0 (8±0%)
4	PCW	A	67	-	53,53,53	1.05±0.01	4±0 (6±0%)
4	PCW	A	22	-	53,53,53	1.04±0.01	4±0 (7±0%)
5	17F	A	39	-	52,53,53	1.03±0.00	3±0 (5±0%)
4	PCW	A	52	-	53,53,53	1.04±0.01	4±0 (6±0%)
4	PCW	A	10	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	17	-	53,53,53	1.05±0.01	4±0 (7±0%)
5	17F	A	34	-	52,53,53	1.03±0.00	3±0 (5±0%)
4	PCW	A	14	-	53,53,53	1.04±0.01	4±0 (7±0%)
6	GNP	B	201	-	34,34,34	1.30±0.02	4±0 (11±0%)
4	PCW	A	43	-	53,53,53	1.04±0.01	4±0 (6±0%)
4	PCW	A	21	-	53,53,53	1.05±0.01	4±0 (7±0%)
5	17F	A	35	-	52,53,53	1.03±0.01	3±0 (5±0%)
5	17F	A	76	-	52,53,53	1.03±0.01	3±0 (5±0%)
5	17F	A	79	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	PCW	A	1	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	71	-	53,53,53	1.04±0.01	4±0 (6±0%)
5	17F	A	78	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	PCW	A	60	-	53,53,53	1.05±0.00	4±0 (7±0%)
4	PCW	A	4	-	53,53,53	1.05±0.01	4±0 (7±0%)
5	17F	A	74	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	PCW	A	49	-	53,53,53	1.05±0.01	4±0 (6±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	17F	A	77	-	52,53,53	1.04±0.00	3±0 (5±0%)
4	PCW	A	32	-	53,53,53	1.04±0.01	5±0 (8±0%)
4	PCW	A	6	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	PCW	A	46	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	16	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	PCW	A	65	-	53,53,53	1.05±0.01	5±0 (9±0%)
5	17F	A	36	-	52,53,53	1.03±0.01	3±0 (5±0%)
5	17F	A	73	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	PCW	A	63	-	53,53,53	1.04±0.00	4±0 (7±0%)
4	PCW	A	20	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	18	-	53,53,53	1.04±0.01	4±0 (6±0%)
4	PCW	A	45	-	53,53,53	1.05±0.00	4±0 (7±0%)
5	17F	A	40	-	52,53,53	1.03±0.01	3±0 (5±0%)
5	17F	A	80	-	52,53,53	1.03±0.00	3±0 (5±0%)
4	PCW	A	9	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	PCW	A	30	-	53,53,53	1.05±0.01	5±0 (8±0%)
4	PCW	A	31	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	PCW	A	7	-	53,53,53	1.05±0.01	5±0 (8±0%)
4	PCW	A	27	-	53,53,53	1.07±0.01	5±0 (9±0%)
4	PCW	A	51	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	PCW	A	61	-	53,53,53	1.05±0.00	4±0 (7±0%)
4	PCW	A	12	-	53,53,53	1.05±0.00	5±0 (9±0%)
4	PCW	A	41	-	53,53,53	1.04±0.00	4±0 (7±0%)
4	PCW	A	56	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	57	-	53,53,53	1.05±0.01	4±0 (6±0%)
5	17F	A	33	-	52,53,53	1.04±0.01	3±0 (5±0%)
4	PCW	A	44	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	59	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	72	-	53,53,53	1.04±0.01	5±0 (9±0%)
4	PCW	A	53	-	53,53,53	1.04±0.00	4±0 (6±0%)
4	PCW	A	8	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	PCW	A	66	-	53,53,53	1.05±0.01	5±0 (8±0%)
4	PCW	A	42	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	70	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	29	-	53,53,53	1.05±0.00	4±0 (7±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PCW	A	13	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	58	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	2	-	53,53,53	1.04±0.00	4±0 (6±0%)
4	PCW	A	3	-	53,53,53	1.05±0.01	4±0 (6±0%)
4	PCW	A	25	-	53,53,53	1.05±0.01	4±0 (6±0%)
4	PCW	A	28	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	50	-	53,53,53	1.04±0.01	5±0 (8±0%)
4	PCW	A	69	-	53,53,53	1.05±0.00	4±0 (7±0%)
5	17F	A	38	-	52,53,53	1.02±0.00	3±0 (5±0%)
4	PCW	A	23	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	PCW	A	19	-	53,53,53	1.04±0.01	5±0 (8±0%)
5	17F	A	75	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	PCW	A	24	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	PCW	A	47	-	53,53,53	1.04±0.00	5±0 (9±0%)
5	17F	A	37	-	52,53,53	1.03±0.01	3±0 (5±0%)
4	PCW	A	55	-	53,53,53	1.07±0.01	5±0 (9±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PCW	A	15	-	59,61,61	0.85±0.01	1±0 (1±0%)
4	PCW	A	68	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	26	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	PCW	A	54	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	64	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	62	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	PCW	A	5	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	PCW	A	11	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	PCW	A	48	-	59,61,61	0.85±0.01	1±0 (1±0%)
4	PCW	A	67	-	59,61,61	2.32±0.00	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PCW	A	22	-	59,61,61	2.32±0.01	5±0 (8±0%)
5	17F	A	39	-	54,60,60	1.05±0.01	5±0 (9±0%)
4	PCW	A	52	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	10	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	PCW	A	17	-	59,61,61	2.32±0.00	5±0 (8±0%)
5	17F	A	34	-	54,60,60	1.05±0.02	5±0 (9±0%)
4	PCW	A	14	-	59,61,61	2.32±0.00	5±0 (8±0%)
6	GNP	B	201	-	47,54,54	0.97±0.01	2±0 (5±1%)
4	PCW	A	43	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	PCW	A	21	-	59,61,61	2.32±0.00	5±0 (8±0%)
5	17F	A	35	-	54,60,60	1.05±0.01	5±0 (9±0%)
5	17F	A	76	-	54,60,60	1.03±0.01	5±0 (9±0%)
5	17F	A	79	-	54,60,60	1.06±0.01	5±0 (9±0%)
4	PCW	A	1	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	PCW	A	71	-	59,61,61	2.32±0.00	5±0 (8±0%)
5	17F	A	78	-	54,60,60	1.04±0.02	5±0 (9±0%)
4	PCW	A	60	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	4	-	59,61,61	2.32±0.00	5±0 (8±0%)
5	17F	A	74	-	54,60,60	1.04±0.02	5±0 (9±0%)
4	PCW	A	49	-	59,61,61	2.32±0.00	5±0 (8±0%)
5	17F	A	77	-	54,60,60	1.76±0.01	10±0 (18±0%)
4	PCW	A	32	-	59,61,61	0.84±0.00	1±0 (1±0%)
4	PCW	A	6	-	59,61,61	2.76±0.00	9±0 (15±0%)
4	PCW	A	46	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	16	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	PCW	A	65	-	59,61,61	0.85±0.00	1±0 (1±0%)
5	17F	A	36	-	54,60,60	1.05±0.01	5±0 (9±0%)
5	17F	A	73	-	54,60,60	1.05±0.03	5±0 (9±0%)
4	PCW	A	63	-	59,61,61	2.76±0.00	9±0 (15±0%)
4	PCW	A	20	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	PCW	A	18	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	45	-	59,61,61	2.32±0.00	5±0 (8±0%)
5	17F	A	40	-	54,60,60	1.05±0.02	5±0 (8±0%)
5	17F	A	80	-	54,60,60	1.02±0.01	4±0 (7±0%)
4	PCW	A	9	-	59,61,61	0.84±0.01	1±0 (1±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
4	PCW	A	30	-	59,61,61	0.85±0.01	1±0 (1±0%)
4	PCW	A	31	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	7	-	59,61,61	0.85±0.01	1±0 (1±0%)
4	PCW	A	27	-	59,61,61	0.83±0.01	1±0 (1±0%)
4	PCW	A	51	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	61	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	PCW	A	12	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	PCW	A	41	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	56	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	57	-	59,61,61	2.32±0.00	5±0 (8±0%)
5	17F	A	33	-	54,60,60	1.77±0.02	10±0 (18±0%)
4	PCW	A	44	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	59	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	72	-	59,61,61	0.84±0.00	1±0 (1±0%)
4	PCW	A	53	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	8	-	59,61,61	0.85±0.01	1±0 (1±0%)
4	PCW	A	66	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	PCW	A	42	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	PCW	A	70	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	29	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	13	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	PCW	A	58	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	2	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	3	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	25	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	28	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	50	-	59,61,61	0.84±0.00	1±0 (1±0%)
4	PCW	A	69	-	59,61,61	2.32±0.00	5±0 (8±0%)
5	17F	A	38	-	54,60,60	1.05±0.02	5±0 (9±0%)
4	PCW	A	23	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	19	-	59,61,61	0.84±0.01	1±0 (1±0%)
5	17F	A	75	-	54,60,60	1.05±0.02	5±0 (9±0%)
4	PCW	A	24	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	PCW	A	47	-	59,61,61	0.84±0.01	1±0 (1±0%)
5	17F	A	37	-	54,60,60	1.04±0.01	5±0 (9±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PCW	A	55	-	59,61,61	0.83±0.01	1±0 (1±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	PCW	A	11	-	-	0±0,57,57,57	-
4	PCW	A	65	-	-	0±0,57,57,57	-
5	17F	A	36	-	-	0±0,59,59,59	-
4	PCW	A	15	-	-	0±0,57,57,57	-
5	17F	A	73	-	-	0±0,59,59,59	-
4	PCW	A	16	-	-	0±0,57,57,57	-
5	17F	A	35	-	-	0±0,59,59,59	-
5	17F	A	39	-	-	0±0,59,59,59	-
4	PCW	A	72	-	-	0±0,57,57,57	-
4	PCW	A	46	-	-	0±0,57,57,57	-
4	PCW	A	64	-	-	0±0,57,57,57	-
4	PCW	A	10	-	-	0±0,57,57,57	-
4	PCW	A	63	-	-	0±0,57,57,57	-
4	PCW	A	21	-	-	0±0,57,57,57	-
4	PCW	A	7	-	-	0±0,57,57,57	-
4	PCW	A	5	-	-	0±0,57,57,57	-
4	PCW	A	18	-	-	0±0,57,57,57	-
4	PCW	A	19	-	-	0±0,57,57,57	-
4	PCW	A	1	-	-	0±0,57,57,57	-
4	PCW	A	25	-	-	0±0,57,57,57	-
4	PCW	A	67	-	-	0±0,57,57,57	-
4	PCW	A	28	-	-	0±0,57,57,57	-
4	PCW	A	45	-	-	0±0,57,57,57	-
4	PCW	A	55	-	-	0±0,57,57,57	-
4	PCW	A	24	-	-	0±0,57,57,57	-
4	PCW	A	29	-	-	0±0,57,57,57	-
4	PCW	A	20	-	-	0±0,57,57,57	-
4	PCW	A	26	-	-	0±0,57,57,57	-
5	17F	A	40	-	-	0±0,59,59,59	-
4	PCW	A	6	-	-	0±0,57,57,57	-
4	PCW	A	23	-	-	0±0,57,57,57	-
4	PCW	A	30	-	-	0±0,57,57,57	-
4	PCW	A	61	-	-	0±0,57,57,57	-
4	PCW	A	44	-	-	0±0,57,57,57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	A	3	-	-	0±0,57,57,57	-
5	17F	A	78	-	-	0±0,59,59,59	-
4	PCW	A	48	-	-	0±0,57,57,57	-
4	PCW	A	52	-	-	0±0,57,57,57	-
4	PCW	A	70	-	-	0±0,57,57,57	-
5	17F	A	77	-	-	0±0,59,59,59	-
4	PCW	A	32	-	-	0±0,57,57,57	-
4	PCW	A	50	-	-	0±0,57,57,57	-
4	PCW	A	12	-	-	0±0,57,57,57	-
4	PCW	A	17	-	-	0±0,57,57,57	-
5	17F	A	33	-	-	0±0,59,59,59	-
4	PCW	A	49	-	-	0±0,57,57,57	-
4	PCW	A	56	-	-	0±0,57,57,57	-
4	PCW	A	68	-	-	0±0,57,57,57	-
4	PCW	A	8	-	-	0±0,57,57,57	-
4	PCW	A	51	-	-	0±0,57,57,57	-
5	17F	A	34	-	-	0±0,59,59,59	-
5	17F	A	79	-	-	0±0,59,59,59	-
4	PCW	A	54	-	-	0±0,57,57,57	-
5	17F	A	74	-	-	0±0,59,59,59	-
5	17F	A	76	-	-	0±0,59,59,59	-
4	PCW	A	22	-	-	0±0,57,57,57	-
4	PCW	A	47	-	-	0±0,57,57,57	-
4	PCW	A	62	-	-	0±0,57,57,57	-
4	PCW	A	43	-	-	0±0,57,57,57	-
4	PCW	A	31	-	-	0±0,57,57,57	-
4	PCW	A	59	-	-	0±0,57,57,57	-
5	17F	A	37	-	-	0±0,59,59,59	-
6	GNP	B	201	-	-	0±0,18,38,38	0±0,3,3,3
4	PCW	A	9	-	-	0±0,57,57,57	-
5	17F	A	38	-	-	0±0,59,59,59	-
4	PCW	A	14	-	-	0±0,57,57,57	-
4	PCW	A	2	-	-	0±0,57,57,57	-
5	17F	A	80	-	-	0±0,59,59,59	-
4	PCW	A	27	-	-	0±0,57,57,57	-
4	PCW	A	13	-	-	0±0,57,57,57	-
4	PCW	A	69	-	-	0±0,57,57,57	-
4	PCW	A	60	-	-	0±0,57,57,57	-
4	PCW	A	58	-	-	0±0,57,57,57	-
4	PCW	A	66	-	-	0±0,57,57,57	-
4	PCW	A	53	-	-	0±0,57,57,57	-
4	PCW	A	57	-	-	0±0,57,57,57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	A	42	-	-	0±0,57,57,57	-
5	17F	A	75	-	-	0±0,59,59,59	-
4	PCW	A	71	-	-	0±0,57,57,57	-
4	PCW	A	4	-	-	0±0,57,57,57	-
4	PCW	A	41	-	-	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
6	B	201	GNP	PB-O2B	4.05	1.46	1.56	4	10
6	B	201	GNP	PG-O3G	3.40	1.47	1.56	3	10
6	B	201	GNP	PB-O3A	2.98	1.55	1.59	4	10
4	A	56	PCW	C5-N	2.85	1.42	1.51	8	10
4	A	46	PCW	C5-N	2.83	1.42	1.51	9	10
4	A	42	PCW	C5-N	2.82	1.42	1.51	2	10
4	A	13	PCW	C5-N	2.81	1.42	1.51	6	10
4	A	14	PCW	C5-N	2.80	1.42	1.51	6	10
4	A	60	PCW	C5-N	2.79	1.43	1.51	10	10
4	A	6	PCW	C5-N	2.79	1.43	1.51	5	10
4	A	57	PCW	C5-N	2.78	1.43	1.51	8	10
4	A	71	PCW	C5-N	2.78	1.43	1.51	4	10
4	A	26	PCW	C5-N	2.77	1.43	1.51	5	10
4	A	49	PCW	C5-N	2.77	1.43	1.51	4	10
4	A	54	PCW	C5-N	2.77	1.43	1.51	8	10
4	A	70	PCW	C5-N	2.77	1.43	1.51	2	10
4	A	31	PCW	C5-N	2.76	1.43	1.51	5	10
4	A	45	PCW	C5-N	2.76	1.43	1.51	1	10
4	A	59	PCW	C5-N	2.76	1.43	1.51	8	10
4	A	5	PCW	C5-N	2.75	1.43	1.51	9	10
4	A	4	PCW	C5-N	2.75	1.43	1.51	7	10
4	A	62	PCW	C5-N	2.74	1.43	1.51	2	10
4	A	51	PCW	C5-N	2.74	1.43	1.51	8	10
4	A	21	PCW	C5-N	2.74	1.43	1.51	10	10
4	A	22	PCW	C5-N	2.74	1.43	1.51	4	10
4	A	64	PCW	C5-N	2.74	1.43	1.51	1	10
4	A	28	PCW	C5-N	2.73	1.43	1.51	8	10
4	A	24	PCW	C5-N	2.73	1.43	1.51	4	10
4	A	29	PCW	C5-N	2.73	1.43	1.51	6	10
4	A	67	PCW	C5-N	2.73	1.43	1.51	10	10
4	A	68	PCW	C5-N	2.72	1.43	1.51	6	10
4	A	25	PCW	C5-N	2.72	1.43	1.51	10	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	A	53	PCW	C5-N	2.72	1.43	1.51	10	10
4	A	10	PCW	C5-N	2.72	1.43	1.51	4	10
4	A	18	PCW	C5-N	2.72	1.43	1.51	7	10
4	A	58	PCW	C5-N	2.72	1.43	1.51	10	10
4	A	44	PCW	C5-N	2.71	1.43	1.51	6	10
4	A	69	PCW	C5-N	2.71	1.43	1.51	10	10
4	A	1	PCW	C5-N	2.71	1.43	1.51	6	10
4	A	17	PCW	C5-N	2.71	1.43	1.51	1	10
4	A	58	PCW	C1-C2	2.70	1.59	1.50	1	10
4	A	61	PCW	C5-N	2.70	1.43	1.51	2	10
4	A	23	PCW	C5-N	2.69	1.43	1.51	2	10
4	A	52	PCW	C5-N	2.69	1.43	1.51	6	10
4	A	3	PCW	C5-N	2.69	1.43	1.51	7	10
4	A	41	PCW	C5-N	2.69	1.43	1.51	4	10
4	A	20	PCW	C5-N	2.68	1.43	1.51	2	10
4	A	57	PCW	C1-C2	2.67	1.59	1.50	3	10
4	A	63	PCW	C5-N	2.67	1.43	1.51	6	10
4	A	2	PCW	C5-N	2.67	1.43	1.51	9	10
4	A	14	PCW	C1-C2	2.66	1.59	1.50	2	10
4	A	3	PCW	C1-C2	2.66	1.59	1.50	8	10
4	A	43	PCW	C5-N	2.65	1.43	1.51	2	10
4	A	16	PCW	C1-C2	2.64	1.59	1.50	1	10
4	A	27	PCW	C1-C2	2.64	1.59	1.50	1	10
4	A	4	PCW	C1-C2	2.63	1.59	1.50	4	10
4	A	10	PCW	C1-C2	2.62	1.59	1.50	8	10
4	A	55	PCW	C1-C2	2.61	1.59	1.50	7	10
4	A	11	PCW	C1-C2	2.61	1.59	1.50	3	10
4	A	23	PCW	C1-C2	2.60	1.58	1.50	8	10
4	A	63	PCW	C1-C2	2.60	1.58	1.50	2	10
4	A	59	PCW	C1-C2	2.60	1.58	1.50	10	10
4	A	1	PCW	C1-C2	2.59	1.58	1.50	5	10
5	A	37	17F	O4-C3	2.59	1.29	1.22	10	10
4	A	41	PCW	C1-C2	2.58	1.58	1.50	7	10
5	A	77	17F	O4-C3	2.58	1.29	1.22	2	10
5	A	33	17F	O4-C3	2.57	1.29	1.22	3	10
4	A	65	PCW	C1-C2	2.57	1.58	1.50	1	10
4	A	68	PCW	C1-C2	2.56	1.58	1.50	6	10
4	A	25	PCW	C1-C2	2.56	1.58	1.50	3	10
4	A	60	PCW	C1-C2	2.55	1.58	1.50	7	10
4	A	6	PCW	C1-C2	2.55	1.58	1.50	7	10
4	A	70	PCW	C1-C2	2.55	1.58	1.50	1	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
5	A	79	17F	O4-C3	2.55	1.29	1.22	4	10
5	A	34	17F	O4-C3	2.55	1.29	1.22	6	10
4	A	19	PCW	C1-C2	2.55	1.58	1.50	3	10
5	A	36	17F	O4-C3	2.55	1.29	1.22	9	10
4	A	30	PCW	C1-C2	2.55	1.58	1.50	7	10
4	A	20	PCW	C1-C2	2.55	1.58	1.50	6	10
4	A	9	PCW	C1-C2	2.54	1.58	1.50	4	10
4	A	12	PCW	C1-C2	2.54	1.58	1.50	6	10
4	A	28	PCW	C1-C2	2.54	1.58	1.50	6	10
4	A	53	PCW	C1-C2	2.54	1.58	1.50	6	10
4	A	24	PCW	C1-C2	2.54	1.58	1.50	1	10
4	A	43	PCW	C1-C2	2.54	1.58	1.50	4	10
4	A	13	PCW	C1-C2	2.54	1.58	1.50	7	10
4	A	17	PCW	C1-C2	2.53	1.58	1.50	8	10
4	A	66	PCW	C1-C2	2.54	1.58	1.50	9	10
4	A	21	PCW	C1-C2	2.53	1.58	1.50	10	10
5	A	35	17F	O4-C3	2.53	1.29	1.22	6	10
4	A	7	PCW	C1-C2	2.53	1.58	1.50	5	10
4	A	67	PCW	C1-C2	2.53	1.58	1.50	4	10
5	A	76	17F	O4-C3	2.53	1.29	1.22	9	10
4	A	5	PCW	C1-C2	2.53	1.58	1.50	3	10
5	A	39	17F	O4-C3	2.53	1.29	1.22	3	10
4	A	52	PCW	C1-C2	2.53	1.58	1.50	4	10
4	A	56	PCW	C1-C2	2.53	1.58	1.50	5	10
4	A	71	PCW	C1-C2	2.53	1.58	1.50	2	10
4	A	42	PCW	C1-C2	2.53	1.58	1.50	10	10
4	A	47	PCW	C1-C2	2.53	1.58	1.50	8	10
4	A	64	PCW	C1-C2	2.52	1.58	1.50	4	10
4	A	69	PCW	C1-C2	2.52	1.58	1.50	2	10
5	A	73	17F	O4-C3	2.53	1.29	1.22	3	10
4	A	18	PCW	C1-C2	2.52	1.58	1.50	7	10
4	A	8	PCW	C1-C2	2.52	1.58	1.50	4	10
4	A	49	PCW	C1-C2	2.52	1.58	1.50	4	10
5	A	75	17F	O4-C3	2.52	1.29	1.22	3	10
4	A	31	PCW	C1-C2	2.51	1.58	1.50	5	10
4	A	46	PCW	C1-C2	2.52	1.58	1.50	7	10
4	A	62	PCW	C1-C2	2.52	1.58	1.50	8	10
5	A	78	17F	O4-C3	2.51	1.29	1.22	10	10
4	A	44	PCW	C1-C2	2.51	1.58	1.50	3	10
4	A	45	PCW	C1-C2	2.51	1.58	1.50	10	10
5	A	80	17F	O4-C3	2.51	1.29	1.22	5	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
5	A	40	17F	O4-C3	2.51	1.29	1.22	1	10
4	A	2	PCW	C1-C2	2.50	1.58	1.50	7	10
4	A	50	PCW	C1-C2	2.50	1.58	1.50	5	10
4	A	26	PCW	C1-C2	2.50	1.58	1.50	6	10
4	A	61	PCW	C1-C2	2.50	1.58	1.50	2	10
4	A	48	PCW	C1-C2	2.49	1.58	1.50	7	10
5	A	74	17F	O4-C3	2.49	1.29	1.22	4	10
4	A	32	PCW	C1-C2	2.49	1.58	1.50	2	10
5	A	76	17F	O5-C3	2.49	1.22	1.30	8	10
4	A	51	PCW	C1-C2	2.48	1.58	1.50	10	10
4	A	15	PCW	C1-C2	2.48	1.58	1.50	9	10
4	A	29	PCW	C1-C2	2.48	1.58	1.50	1	10
4	A	72	PCW	C1-C2	2.48	1.58	1.50	2	10
5	A	38	17F	O4-C3	2.48	1.29	1.22	4	10
4	A	55	PCW	C5-N	2.47	1.43	1.51	7	10
4	A	20	PCW	C33-C32	2.47	1.61	1.52	7	10
4	A	30	PCW	C5-N	2.46	1.44	1.51	5	10
4	A	19	PCW	C5-N	2.46	1.44	1.51	2	10
4	A	9	PCW	C5-N	2.45	1.44	1.51	2	10
4	A	48	PCW	C5-N	2.45	1.44	1.51	1	10
4	A	54	PCW	C1-C2	2.45	1.58	1.50	1	10
4	A	22	PCW	C1-C2	2.44	1.58	1.50	1	10
4	A	9	PCW	C33-C32	2.44	1.61	1.52	9	10
4	A	16	PCW	C5-N	2.44	1.44	1.51	4	10
4	A	7	PCW	C33-C32	2.44	1.61	1.52	1	10
6	B	201	GNP	PG-O1G	2.44	1.49	1.46	7	10
4	A	65	PCW	C5-N	2.44	1.44	1.51	7	10
4	A	8	PCW	C5-N	2.43	1.44	1.51	4	10
5	A	36	17F	O5-C3	2.44	1.22	1.30	4	10
4	A	67	PCW	C33-C32	2.43	1.61	1.52	10	10
4	A	32	PCW	C5-N	2.43	1.44	1.51	8	10
4	A	11	PCW	C5-N	2.43	1.44	1.51	8	10
5	A	35	17F	O5-C3	2.43	1.22	1.30	7	10
4	A	66	PCW	C5-N	2.42	1.44	1.51	5	10
4	A	15	PCW	C5-N	2.42	1.44	1.51	6	10
4	A	24	PCW	C33-C32	2.41	1.61	1.52	2	10
4	A	12	PCW	C5-N	2.41	1.44	1.51	4	10
4	A	4	PCW	C33-C32	2.41	1.61	1.52	7	10
4	A	72	PCW	C33-C32	2.41	1.61	1.52	3	10
4	A	2	PCW	C33-C32	2.41	1.61	1.52	3	10
4	A	69	PCW	C33-C32	2.41	1.61	1.52	2	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
5	A	39	17F	O5-C3	2.41	1.23	1.30	4	10
4	A	10	PCW	C33-C32	2.41	1.61	1.52	2	10
4	A	17	PCW	C33-C32	2.41	1.61	1.52	10	10
4	A	23	PCW	C33-C32	2.41	1.61	1.52	1	10
5	A	75	17F	O5-C3	2.41	1.23	1.30	7	10
4	A	47	PCW	C5-N	2.40	1.44	1.51	3	10
4	A	45	PCW	C33-C32	2.40	1.61	1.52	2	10
4	A	50	PCW	C5-N	2.40	1.44	1.51	10	10
4	A	72	PCW	C5-N	2.40	1.44	1.51	5	10
5	A	79	17F	O5-C3	2.40	1.23	1.30	5	10
4	A	42	PCW	C33-C32	2.40	1.61	1.52	8	10
4	A	58	PCW	C33-C32	2.40	1.61	1.52	8	10
5	A	78	17F	O5-C3	2.40	1.23	1.30	3	10
4	A	31	PCW	C33-C32	2.40	1.61	1.52	8	10
4	A	60	PCW	C33-C32	2.40	1.61	1.52	8	10
4	A	11	PCW	C33-C32	2.39	1.61	1.52	7	10
4	A	27	PCW	C5-N	2.39	1.44	1.51	4	10
4	A	49	PCW	C33-C32	2.39	1.61	1.52	4	10
5	A	74	17F	O5-C3	2.39	1.23	1.30	3	10
4	A	55	PCW	C33-C32	2.39	1.61	1.52	1	10
4	A	7	PCW	C5-N	2.39	1.44	1.51	6	10
4	A	57	PCW	C33-C32	2.39	1.60	1.52	7	10
4	A	1	PCW	C33-C32	2.39	1.60	1.52	2	10
5	A	40	17F	O5-C3	2.39	1.23	1.30	5	10
4	A	62	PCW	C33-C32	2.39	1.60	1.52	1	10
4	A	41	PCW	C33-C32	2.39	1.60	1.52	7	10
4	A	8	PCW	C33-C32	2.38	1.60	1.52	2	10
4	A	19	PCW	C33-C32	2.38	1.60	1.52	4	10
4	A	29	PCW	C33-C32	2.38	1.60	1.52	8	10
4	A	52	PCW	C33-C32	2.39	1.60	1.52	5	10
4	A	28	PCW	C33-C32	2.38	1.60	1.52	10	10
4	A	30	PCW	C33-C32	2.38	1.60	1.52	4	10
4	A	47	PCW	C33-C32	2.38	1.60	1.52	4	10
4	A	3	PCW	C33-C32	2.38	1.60	1.52	6	10
4	A	5	PCW	C33-C32	2.38	1.60	1.52	8	10
4	A	13	PCW	C33-C32	2.38	1.60	1.52	6	10
4	A	63	PCW	C33-C32	2.38	1.60	1.52	4	10
4	A	21	PCW	C33-C32	2.38	1.60	1.52	10	10
5	A	80	17F	O5-C3	2.38	1.23	1.30	4	10
4	A	6	PCW	C33-C32	2.38	1.60	1.52	9	10
4	A	25	PCW	C33-C32	2.38	1.60	1.52	5	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	A	18	PCW	C33-C32	2.38	1.60	1.52	3	10
4	A	16	PCW	C33-C32	2.37	1.60	1.52	3	10
4	A	50	PCW	C33-C32	2.37	1.60	1.52	7	10
4	A	61	PCW	C33-C32	2.37	1.60	1.52	9	10
4	A	70	PCW	C33-C32	2.37	1.60	1.52	2	10
5	A	73	17F	O5-C3	2.37	1.23	1.30	8	10
4	A	14	PCW	C33-C32	2.37	1.60	1.52	7	10
4	A	15	PCW	C33-C32	2.37	1.60	1.52	4	10
4	A	26	PCW	C33-C32	2.37	1.60	1.52	4	10
4	A	43	PCW	C33-C32	2.37	1.60	1.52	3	10
4	A	44	PCW	C33-C32	2.37	1.60	1.52	2	10
4	A	46	PCW	C33-C32	2.37	1.60	1.52	1	10
4	A	48	PCW	C33-C32	2.37	1.60	1.52	10	10
4	A	64	PCW	C33-C32	2.37	1.60	1.52	10	10
4	A	54	PCW	C33-C32	2.37	1.60	1.52	8	10
4	A	68	PCW	C33-C32	2.37	1.60	1.52	1	10
4	A	53	PCW	C33-C32	2.36	1.60	1.52	1	10
5	A	34	17F	O5-C3	2.36	1.23	1.30	5	10
5	A	37	17F	O5-C3	2.36	1.23	1.30	7	10
4	A	66	PCW	C33-C32	2.36	1.60	1.52	10	10
5	A	77	17F	O5-C3	2.36	1.23	1.30	4	10
4	A	12	PCW	C33-C32	2.35	1.60	1.52	8	10
4	A	71	PCW	C33-C32	2.35	1.60	1.52	7	10
5	A	33	17F	O5-C3	2.35	1.23	1.30	5	10
4	A	27	PCW	C33-C32	2.35	1.60	1.52	5	10
4	A	32	PCW	C33-C32	2.35	1.60	1.52	1	10
4	A	22	PCW	C33-C32	2.34	1.60	1.52	6	10
4	A	59	PCW	C33-C32	2.34	1.60	1.52	2	10
4	A	51	PCW	C33-C32	2.34	1.60	1.52	1	10
5	A	38	17F	O5-C3	2.34	1.23	1.30	5	10
4	A	56	PCW	C33-C32	2.33	1.60	1.52	7	10
4	A	65	PCW	C33-C32	2.32	1.60	1.52	6	10
4	A	30	PCW	C7-N	2.31	1.43	1.50	3	10
4	A	16	PCW	C7-N	2.29	1.43	1.50	9	10
4	A	50	PCW	C7-N	2.27	1.43	1.50	10	10
4	A	66	PCW	C7-N	2.25	1.43	1.50	7	10
4	A	27	PCW	C7-N	2.24	1.43	1.50	9	10
4	A	55	PCW	C3-C2	2.24	1.57	1.50	7	10
4	A	32	PCW	C7-N	2.24	1.43	1.50	5	10
4	A	8	PCW	C7-N	2.23	1.43	1.50	2	10
4	A	48	PCW	C7-N	2.23	1.43	1.50	5	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	A	47	PCW	C7-N	2.23	1.43	1.50	3	10
4	A	72	PCW	C7-N	2.23	1.43	1.50	9	10
4	A	7	PCW	C7-N	2.23	1.43	1.50	9	10
4	A	12	PCW	C7-N	2.22	1.43	1.50	10	10
4	A	15	PCW	C7-N	2.22	1.43	1.50	8	10
4	A	27	PCW	C3-C2	2.22	1.57	1.50	4	10
4	A	65	PCW	C7-N	2.22	1.43	1.50	8	10
4	A	9	PCW	C7-N	2.21	1.43	1.50	4	10
4	A	55	PCW	C7-N	2.21	1.43	1.50	2	10
4	A	58	PCW	C3-C2	2.21	1.57	1.50	1	9
4	A	3	PCW	C3-C2	2.20	1.57	1.50	2	7
4	A	11	PCW	C7-N	2.18	1.43	1.50	7	10
4	A	67	PCW	C3-C2	2.18	1.57	1.50	5	7
4	A	6	PCW	C3-C2	2.18	1.57	1.50	8	10
4	A	59	PCW	C3-C2	2.17	1.57	1.50	3	8
4	A	19	PCW	C7-N	2.17	1.43	1.50	3	10
4	A	56	PCW	C3-C2	2.16	1.57	1.50	2	10
4	A	22	PCW	C3-C2	2.16	1.57	1.50	5	9
4	A	8	PCW	C3-C2	2.15	1.57	1.50	1	8
4	A	25	PCW	C3-C2	2.15	1.57	1.50	6	7
4	A	47	PCW	C3-C2	2.15	1.57	1.50	7	10
4	A	5	PCW	C3-C2	2.15	1.57	1.50	3	9
4	A	23	PCW	C3-C2	2.14	1.57	1.50	8	8
4	A	26	PCW	C3-C2	2.15	1.57	1.50	7	7
4	A	30	PCW	C3-C2	2.14	1.57	1.50	4	7
4	A	66	PCW	C3-C2	2.14	1.57	1.50	5	7
4	A	62	PCW	C3-C2	2.14	1.57	1.50	10	10
4	A	28	PCW	C3-C2	2.14	1.57	1.50	6	9
4	A	70	PCW	C3-C2	2.14	1.57	1.50	3	9
5	A	73	17F	C1X-C2X	2.14	1.61	1.52	5	9
4	A	12	PCW	C3-C2	2.14	1.57	1.50	8	8
4	A	64	PCW	C3-C2	2.13	1.57	1.50	1	9
5	A	78	17F	C1X-C2X	2.13	1.61	1.52	3	9
4	A	32	PCW	C3-C2	2.13	1.57	1.50	6	7
4	A	4	PCW	C3-C2	2.13	1.57	1.50	3	10
4	A	16	PCW	C3-C2	2.13	1.57	1.50	1	8
4	A	48	PCW	C3-C2	2.13	1.57	1.50	6	7
4	A	49	PCW	C3-C2	2.13	1.57	1.50	7	7
4	A	20	PCW	C3-C2	2.13	1.57	1.50	3	10
5	A	40	17F	C1X-C2X	2.13	1.61	1.52	6	10
4	A	53	PCW	C3-C2	2.12	1.57	1.50	7	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	A	63	PCW	C3-C2	2.12	1.57	1.50	9	10
4	A	71	PCW	C3-C2	2.12	1.57	1.50	10	7
4	A	65	PCW	C3-C2	2.12	1.57	1.50	8	9
5	A	77	17F	C1X-C2X	2.12	1.61	1.52	7	10
5	A	80	17F	C1X-C2X	2.12	1.61	1.52	3	10
4	A	29	PCW	C3-C2	2.12	1.57	1.50	10	9
5	A	37	17F	C1X-C2X	2.12	1.61	1.52	1	10
4	A	1	PCW	C3-C2	2.12	1.57	1.50	5	9
4	A	19	PCW	C3-C2	2.12	1.57	1.50	4	6
4	A	24	PCW	C3-C2	2.12	1.57	1.50	10	9
4	A	31	PCW	C3-C2	2.12	1.57	1.50	7	10
4	A	61	PCW	C3-C2	2.12	1.57	1.50	8	9
5	A	76	17F	C1X-C2X	2.12	1.61	1.52	1	9
4	A	50	PCW	C3-C2	2.12	1.57	1.50	3	7
4	A	2	PCW	C3-C2	2.11	1.57	1.50	1	7
4	A	43	PCW	C3-C2	2.11	1.57	1.50	6	5
4	A	13	PCW	C3-C2	2.11	1.57	1.50	7	8
4	A	18	PCW	C3-C2	2.11	1.57	1.50	10	7
5	A	79	17F	C1X-C2X	2.11	1.61	1.52	6	10
4	A	41	PCW	C3-C2	2.11	1.57	1.50	7	8
4	A	45	PCW	C3-C2	2.11	1.57	1.50	4	9
4	A	52	PCW	C3-C2	2.11	1.57	1.50	10	5
4	A	54	PCW	C3-C2	2.11	1.57	1.50	4	9
4	A	69	PCW	C3-C2	2.11	1.57	1.50	1	9
4	A	42	PCW	C3-C2	2.10	1.57	1.50	5	8
4	A	57	PCW	C3-C2	2.10	1.57	1.50	7	7
5	A	35	17F	C1X-C2X	2.10	1.61	1.52	2	9
5	A	36	17F	C1X-C2X	2.10	1.61	1.52	8	10
4	A	15	PCW	C3-C2	2.10	1.57	1.50	2	7
4	A	7	PCW	C3-C2	2.10	1.57	1.50	5	7
4	A	17	PCW	C3-C2	2.10	1.57	1.50	5	8
4	A	51	PCW	C3-C2	2.10	1.57	1.50	10	8
5	A	75	17F	C1X-C2X	2.10	1.61	1.52	9	9
4	A	14	PCW	C3-C2	2.09	1.57	1.50	1	8
5	A	33	17F	C1X-C2X	2.09	1.61	1.52	1	10
4	A	21	PCW	C3-C2	2.09	1.57	1.50	8	10
4	A	10	PCW	C3-C2	2.09	1.57	1.50	8	9
4	A	46	PCW	C3-C2	2.08	1.57	1.50	1	9
5	A	34	17F	C1X-C2X	2.08	1.61	1.52	2	9
4	A	11	PCW	C3-C2	2.08	1.57	1.50	7	8
5	A	39	17F	C1X-C2X	2.08	1.61	1.52	9	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
5	A	74	17F	C1X-C2X	2.08	1.61	1.52	9	8
4	A	44	PCW	C3-C2	2.08	1.57	1.50	2	10
5	A	38	17F	C1X-C2X	2.08	1.61	1.52	1	9
4	A	72	PCW	C3-C2	2.07	1.57	1.50	10	8
4	A	68	PCW	C3-C2	2.07	1.57	1.50	2	9
4	A	60	PCW	C3-C2	2.07	1.57	1.50	3	8
4	A	9	PCW	C3-C2	2.07	1.57	1.50	10	8

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
4	A	28	PCW	C8-N-C7	12.04	77.35	108.98	3	10
4	A	56	PCW	C8-N-C7	11.99	77.49	108.98	2	10
4	A	10	PCW	C8-N-C7	11.97	77.54	108.98	10	10
4	A	13	PCW	C8-N-C7	11.96	77.57	108.98	10	10
4	A	64	PCW	C8-N-C7	11.96	77.57	108.98	9	10
4	A	45	PCW	C8-N-C7	11.96	77.57	108.98	3	10
4	A	69	PCW	C8-N-C7	11.94	77.60	108.98	9	10
4	A	42	PCW	C8-N-C7	11.94	77.61	108.98	2	10
4	A	1	PCW	C8-N-C7	11.94	77.61	108.98	9	10
4	A	5	PCW	C8-N-C7	11.93	77.64	108.98	3	10
4	A	25	PCW	C8-N-C7	11.93	77.65	108.98	3	10
4	A	44	PCW	C8-N-C7	11.92	77.66	108.98	5	10
4	A	2	PCW	C8-N-C7	11.92	77.67	108.98	7	10
4	A	23	PCW	C8-N-C7	11.92	77.68	108.98	2	10
4	A	31	PCW	C8-N-C7	11.91	77.68	108.98	3	10
4	A	62	PCW	C8-N-C7	11.91	77.69	108.98	4	10
4	A	18	PCW	C8-N-C7	11.91	77.69	108.98	10	10
4	A	54	PCW	C8-N-C7	11.91	77.69	108.98	6	10
4	A	53	PCW	C8-N-C7	11.91	77.69	108.98	9	10
4	A	24	PCW	C8-N-C7	11.91	77.70	108.98	9	10
4	A	14	PCW	C8-N-C7	11.90	77.72	108.98	8	10
4	A	3	PCW	C8-N-C7	11.90	77.72	108.98	6	10
4	A	29	PCW	C8-N-C7	11.90	77.73	108.98	9	10
4	A	41	PCW	C8-N-C7	11.90	77.72	108.98	6	10
4	A	49	PCW	C8-N-C7	11.90	77.73	108.98	5	10
4	A	68	PCW	C8-N-C7	11.90	77.72	108.98	2	10
4	A	17	PCW	C8-N-C7	11.89	77.74	108.98	6	10
4	A	6	PCW	C8-N-C7	11.89	77.75	108.98	5	10
4	A	61	PCW	C8-N-C7	11.89	77.75	108.98	5	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	4	PCW	C8-N-C7	11.88	77.76	108.98	8	10
4	A	51	PCW	C8-N-C7	11.89	77.76	108.98	3	10
4	A	60	PCW	C8-N-C7	11.88	77.76	108.98	3	10
4	A	21	PCW	C8-N-C7	11.88	77.77	108.98	1	10
4	A	71	PCW	C8-N-C7	11.88	77.77	108.98	8	10
4	A	57	PCW	C8-N-C7	11.88	77.77	108.98	7	10
4	A	70	PCW	C8-N-C7	11.88	77.77	108.98	4	10
4	A	46	PCW	C8-N-C7	11.88	77.78	108.98	10	10
4	A	67	PCW	C8-N-C7	11.88	77.78	108.98	8	10
4	A	63	PCW	C8-N-C7	11.87	77.80	108.98	7	10
4	A	43	PCW	C8-N-C7	11.87	77.81	108.98	3	10
4	A	22	PCW	C8-N-C7	11.86	77.81	108.98	7	10
4	A	26	PCW	C8-N-C7	11.86	77.82	108.98	4	10
4	A	20	PCW	C8-N-C7	11.85	77.85	108.98	10	10
4	A	59	PCW	C8-N-C7	11.84	77.87	108.98	4	10
4	A	52	PCW	C8-N-C7	11.83	77.89	108.98	1	10
4	A	58	PCW	C8-N-C7	11.83	77.90	108.98	7	10
4	A	63	PCW	C8-N-C6	10.10	82.45	108.98	4	10
4	A	68	PCW	C8-N-C6	10.09	82.48	108.98	3	10
4	A	23	PCW	C8-N-C6	10.08	82.49	108.98	4	10
4	A	3	PCW	C8-N-C6	10.08	82.50	108.98	8	10
4	A	69	PCW	C8-N-C6	10.06	82.54	108.98	7	10
4	A	31	PCW	C8-N-C6	10.06	82.55	108.98	1	10
4	A	1	PCW	C8-N-C6	10.05	82.57	108.98	5	10
4	A	18	PCW	C8-N-C6	10.05	82.57	108.98	8	10
4	A	22	PCW	C8-N-C6	10.05	82.57	108.98	6	10
4	A	4	PCW	C8-N-C6	10.05	82.59	108.98	9	10
4	A	71	PCW	C8-N-C6	10.05	82.59	108.98	3	10
4	A	58	PCW	C8-N-C6	10.04	82.59	108.98	2	10
4	A	59	PCW	C8-N-C6	10.04	82.60	108.98	8	10
4	A	46	PCW	C8-N-C6	10.04	82.60	108.98	6	10
4	A	6	PCW	C8-N-C6	10.04	82.61	108.98	1	10
4	A	13	PCW	C8-N-C6	10.04	82.61	108.98	2	10
4	A	10	PCW	C8-N-C6	10.04	82.62	108.98	8	10
4	A	57	PCW	C8-N-C6	10.03	82.62	108.98	6	10
4	A	42	PCW	C8-N-C6	10.03	82.62	108.98	8	10
4	A	49	PCW	C8-N-C6	10.03	82.62	108.98	3	10
4	A	67	PCW	C8-N-C6	10.03	82.63	108.98	4	10
4	A	14	PCW	C8-N-C6	10.03	82.64	108.98	2	10
4	A	54	PCW	C8-N-C6	10.03	82.63	108.98	5	10
4	A	61	PCW	C8-N-C6	10.03	82.64	108.98	7	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	2	PCW	C8-N-C6	10.03	82.64	108.98	10	10
4	A	20	PCW	C8-N-C6	10.02	82.65	108.98	6	10
4	A	17	PCW	C8-N-C6	10.02	82.66	108.98	10	10
4	A	43	PCW	C8-N-C6	10.02	82.66	108.98	9	10
4	A	70	PCW	C8-N-C6	10.02	82.66	108.98	1	10
4	A	25	PCW	C8-N-C6	10.02	82.66	108.98	6	10
4	A	51	PCW	C8-N-C6	10.02	82.66	108.98	1	10
4	A	24	PCW	C8-N-C6	10.02	82.66	108.98	3	10
4	A	41	PCW	C8-N-C6	10.02	82.66	108.98	10	10
4	A	44	PCW	C8-N-C6	10.01	82.67	108.98	6	10
4	A	28	PCW	C8-N-C6	10.01	82.68	108.98	5	10
4	A	64	PCW	C8-N-C6	10.01	82.68	108.98	5	10
4	A	26	PCW	C8-N-C6	10.01	82.69	108.98	2	10
4	A	5	PCW	C8-N-C6	10.00	82.70	108.98	4	10
4	A	52	PCW	C8-N-C6	10.00	82.70	108.98	3	10
4	A	45	PCW	C8-N-C6	10.00	82.71	108.98	8	10
4	A	21	PCW	C8-N-C6	10.00	82.72	108.98	7	10
4	A	60	PCW	C8-N-C6	10.00	82.72	108.98	5	10
4	A	56	PCW	C8-N-C6	9.99	82.74	108.98	5	10
4	A	53	PCW	C8-N-C6	9.98	82.75	108.98	10	10
4	A	62	PCW	C8-N-C6	9.97	82.80	108.98	2	10
4	A	29	PCW	C8-N-C6	9.96	82.81	108.98	6	10
4	A	6	PCW	O4P-P-O2P	7.65	78.63	108.94	6	10
4	A	63	PCW	O4P-P-O2P	7.59	78.86	108.94	6	10
5	A	77	17F	O2-P1-O6	6.33	78.86	107.57	1	10
5	A	33	17F	O2-P1-O6	6.32	78.92	107.57	7	10
5	A	77	17F	O2-P1-O3	6.11	79.88	107.57	4	10
5	A	33	17F	O2-P1-O3	6.08	80.02	107.57	8	10
4	A	6	PCW	O3P-P-O2P	5.89	85.58	108.94	9	10
4	A	63	PCW	O1P-P-O2P	5.78	85.58	112.44	2	10
4	A	6	PCW	O1P-P-O2P	5.74	85.73	112.44	8	10
4	A	63	PCW	O3P-P-O2P	5.70	86.34	108.94	6	10
4	A	1	PCW	C8-N-C5	5.46	88.19	109.91	2	10
4	A	5	PCW	C8-N-C5	5.46	88.20	109.91	6	10
4	A	58	PCW	C8-N-C5	5.42	88.38	109.91	10	10
4	A	26	PCW	C8-N-C5	5.41	88.42	109.91	3	10
4	A	41	PCW	C8-N-C5	5.40	88.44	109.91	8	10
4	A	51	PCW	C8-N-C5	5.40	88.44	109.91	1	10
4	A	18	PCW	C8-N-C5	5.39	88.47	109.91	2	10
4	A	56	PCW	C8-N-C5	5.39	88.47	109.91	7	10
4	A	70	PCW	C8-N-C5	5.39	88.47	109.91	1	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	17	PCW	C8-N-C5	5.39	88.48	109.91	2	10
4	A	22	PCW	C8-N-C5	5.38	88.51	109.91	10	10
4	A	44	PCW	C8-N-C5	5.38	88.51	109.91	4	10
4	A	14	PCW	C8-N-C5	5.38	88.52	109.91	6	10
4	A	52	PCW	C8-N-C5	5.38	88.52	109.91	5	10
4	A	49	PCW	C8-N-C5	5.38	88.53	109.91	2	10
4	A	43	PCW	C8-N-C5	5.38	88.54	109.91	2	10
4	A	6	PCW	C8-N-C5	5.37	88.55	109.91	2	10
4	A	23	PCW	C8-N-C5	5.38	88.54	109.91	2	10
4	A	13	PCW	C8-N-C5	5.37	88.55	109.91	7	10
4	A	62	PCW	C8-N-C5	5.37	88.55	109.91	10	10
4	A	53	PCW	C8-N-C5	5.37	88.55	109.91	6	10
4	A	3	PCW	C8-N-C5	5.37	88.56	109.91	9	10
4	A	4	PCW	C8-N-C5	5.37	88.56	109.91	4	10
4	A	20	PCW	C8-N-C5	5.37	88.56	109.91	4	10
4	A	60	PCW	C8-N-C5	5.37	88.56	109.91	6	10
4	A	54	PCW	C8-N-C5	5.37	88.56	109.91	7	10
4	A	29	PCW	C8-N-C5	5.37	88.57	109.91	7	10
4	A	10	PCW	C8-N-C5	5.36	88.58	109.91	9	10
4	A	25	PCW	C8-N-C5	5.37	88.58	109.91	9	10
4	A	57	PCW	C8-N-C5	5.37	88.58	109.91	5	10
4	A	71	PCW	C8-N-C5	5.36	88.60	109.91	4	10
4	A	61	PCW	C8-N-C5	5.36	88.61	109.91	1	10
4	A	67	PCW	C8-N-C5	5.36	88.61	109.91	1	10
4	A	21	PCW	C8-N-C5	5.36	88.62	109.91	10	10
4	A	68	PCW	C8-N-C5	5.35	88.63	109.91	8	10
4	A	24	PCW	C8-N-C5	5.35	88.64	109.91	10	10
4	A	69	PCW	C8-N-C5	5.35	88.64	109.91	10	10
4	A	31	PCW	C8-N-C5	5.35	88.64	109.91	8	10
4	A	28	PCW	C8-N-C5	5.35	88.65	109.91	1	10
4	A	42	PCW	C8-N-C5	5.34	88.66	109.91	5	10
4	A	46	PCW	C8-N-C5	5.34	88.67	109.91	3	10
4	A	64	PCW	C8-N-C5	5.34	88.68	109.91	3	10
4	A	45	PCW	C8-N-C5	5.33	88.71	109.91	8	10
4	A	63	PCW	C8-N-C5	5.33	88.71	109.91	9	10
4	A	59	PCW	C8-N-C5	5.33	88.71	109.91	10	10
4	A	2	PCW	C8-N-C5	5.32	88.77	109.91	6	10
5	A	77	17F	O2-P1-O1	4.73	90.46	112.44	5	10
5	A	33	17F	O2-P1-O1	4.69	90.62	112.44	9	10
5	A	33	17F	O3-C1-C2	4.13	111.66	108.06	7	10
5	A	73	17F	O3-C1-C2	4.06	111.60	108.06	9	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	34	17F	O3-C1-C2	3.87	111.44	108.06	6	10
5	A	38	17F	O3-C1-C2	3.81	111.38	108.06	1	10
5	A	77	17F	O3-C1-C2	3.80	111.37	108.06	1	10
5	A	40	17F	O3-C1-C2	3.74	111.32	108.06	4	10
5	A	75	17F	O3-C1-C2	3.71	111.29	108.06	5	10
5	A	78	17F	O3-C1-C2	3.68	111.27	108.06	1	10
5	A	79	17F	O3-C1-C2	3.62	111.22	108.06	1	10
5	A	39	17F	O3-C1-C2	3.52	111.13	108.06	6	10
5	A	34	17F	O5-C3-O4	3.49	116.15	124.08	1	10
5	A	36	17F	O3-C1-C2	3.49	111.10	108.06	9	10
4	A	63	PCW	O1P-P-O4P	3.47	123.30	107.57	1	10
5	A	35	17F	O3-C1-C2	3.47	111.08	108.06	6	10
4	A	6	PCW	O1P-P-O4P	3.45	123.19	107.57	2	10
5	A	40	17F	O5-C3-O4	3.40	116.37	124.08	2	10
5	A	35	17F	O5-C3-O4	3.40	116.37	124.08	3	10
5	A	39	17F	O5-C3-O4	3.39	116.38	124.08	10	10
5	A	75	17F	O5-C3-O4	3.39	116.40	124.08	5	10
5	A	36	17F	O5-C3-O4	3.38	116.41	124.08	3	10
5	A	33	17F	O5-C3-O4	3.36	116.45	124.08	7	10
4	A	46	PCW	C6-N-C5	3.36	123.26	109.91	7	10
5	A	78	17F	O5-C3-O4	3.35	116.47	124.08	1	10
5	A	80	17F	O5-C3-O4	3.36	116.47	124.08	4	10
5	A	77	17F	O5-C3-O4	3.35	116.48	124.08	5	10
4	A	17	PCW	C6-N-C5	3.35	123.21	109.91	2	10
4	A	45	PCW	C6-N-C5	3.35	123.21	109.91	4	10
5	A	38	17F	O5-C3-O4	3.34	116.50	124.08	2	10
5	A	74	17F	O5-C3-O4	3.34	116.50	124.08	1	10
4	A	51	PCW	C6-N-C5	3.34	123.19	109.91	9	10
5	A	79	17F	O5-C3-O4	3.34	116.50	124.08	6	10
5	A	73	17F	O5-C3-O4	3.34	116.50	124.08	10	10
5	A	37	17F	O5-C3-O4	3.34	116.51	124.08	8	10
4	A	31	PCW	C6-N-C5	3.33	123.16	109.91	1	10
4	A	63	PCW	C6-N-C5	3.33	123.16	109.91	3	10
4	A	4	PCW	C6-N-C5	3.33	123.14	109.91	5	10
4	A	25	PCW	C6-N-C5	3.33	123.13	109.91	6	10
5	A	74	17F	O3-C1-C2	3.33	110.96	108.06	10	10
5	A	76	17F	O5-C3-O4	3.33	116.53	124.08	7	10
4	A	67	PCW	C6-N-C5	3.32	123.12	109.91	3	10
4	A	20	PCW	C6-N-C5	3.32	123.12	109.91	9	10
4	A	18	PCW	C6-N-C5	3.32	123.11	109.91	8	10
4	A	21	PCW	C6-N-C5	3.32	123.10	109.91	7	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	29	PCW	C6-N-C5	3.32	123.09	109.91	3	10
4	A	42	PCW	C6-N-C5	3.32	123.09	109.91	1	10
4	A	23	PCW	C6-N-C5	3.31	123.08	109.91	6	10
4	A	26	PCW	C6-N-C5	3.31	123.08	109.91	3	10
4	A	43	PCW	C6-N-C5	3.31	123.08	109.91	8	10
4	A	1	PCW	C6-N-C5	3.31	123.06	109.91	2	10
4	A	56	PCW	C6-N-C5	3.31	123.06	109.91	1	10
4	A	14	PCW	C6-N-C5	3.31	123.05	109.91	9	10
4	A	52	PCW	C6-N-C5	3.30	123.05	109.91	3	10
4	A	70	PCW	C6-N-C5	3.30	123.04	109.91	5	10
4	A	3	PCW	C6-N-C5	3.30	123.03	109.91	5	10
4	A	22	PCW	C6-N-C5	3.30	123.03	109.91	8	10
4	A	59	PCW	C6-N-C5	3.30	123.03	109.91	8	10
4	A	49	PCW	C6-N-C5	3.30	123.02	109.91	7	10
4	A	58	PCW	C6-N-C5	3.30	123.02	109.91	8	10
4	A	44	PCW	C6-N-C5	3.30	123.01	109.91	4	10
4	A	68	PCW	C6-N-C5	3.30	123.01	109.91	3	10
4	A	6	PCW	C6-N-C5	3.29	122.99	109.91	2	10
4	A	53	PCW	C6-N-C5	3.29	122.98	109.91	8	10
4	A	41	PCW	C6-N-C5	3.29	122.97	109.91	2	10
4	A	54	PCW	C6-N-C5	3.29	122.97	109.91	1	10
4	A	61	PCW	C6-N-C5	3.29	122.97	109.91	1	10
4	A	28	PCW	C6-N-C5	3.28	122.96	109.91	1	10
4	A	5	PCW	C6-N-C5	3.28	122.95	109.91	3	10
4	A	57	PCW	C6-N-C5	3.28	122.94	109.91	4	10
4	A	60	PCW	C6-N-C5	3.28	122.94	109.91	5	10
4	A	71	PCW	C6-N-C5	3.28	122.94	109.91	10	10
4	A	2	PCW	C6-N-C5	3.27	122.93	109.91	2	10
4	A	62	PCW	C6-N-C5	3.27	122.91	109.91	10	10
4	A	69	PCW	C6-N-C5	3.27	122.90	109.91	2	10
4	A	64	PCW	C6-N-C5	3.26	122.88	109.91	9	10
4	A	10	PCW	C6-N-C5	3.26	122.86	109.91	3	10
4	A	24	PCW	C6-N-C5	3.26	122.86	109.91	4	10
4	A	13	PCW	C6-N-C5	3.25	122.82	109.91	5	10
5	A	37	17F	O3-C1-C2	3.17	110.82	108.06	10	10
6	B	201	GNP	O3G-PG-O1G	3.10	105.67	113.45	6	10
5	A	76	17F	O3-C1-C2	3.05	110.72	108.06	7	10
5	A	80	17F	O3-C1-C2	3.02	110.69	108.06	8	10
5	A	74	17F	O7-C7-O8	2.97	131.06	123.63	1	10
5	A	76	17F	O7-C7-O8	2.93	130.95	123.63	6	10
5	A	80	17F	O7-C7-O8	2.92	130.93	123.63	10	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	77	17F	O7-C7-O8	2.91	130.90	123.63	7	10
6	B	201	GNP	O2G-PG-O3G	2.90	115.39	107.59	7	10
5	A	37	17F	O7-C7-O8	2.90	130.88	123.63	10	10
5	A	73	17F	O7-C7-O8	2.89	130.87	123.63	4	10
5	A	38	17F	O7-C7-O8	2.89	130.86	123.63	5	10
5	A	34	17F	O7-C7-O8	2.89	130.86	123.63	2	10
5	A	40	17F	O7-C7-O8	2.89	130.84	123.63	6	10
5	A	79	17F	O7-C7-O8	2.89	130.85	123.63	3	10
5	A	35	17F	O7-C7-O8	2.88	130.82	123.63	1	10
5	A	75	17F	O7-C7-O8	2.88	130.82	123.63	9	10
5	A	39	17F	O7-C7-O8	2.87	130.80	123.63	4	10
5	A	33	17F	O7-C7-O8	2.86	130.79	123.63	3	10
5	A	78	17F	O7-C7-O8	2.84	130.74	123.63	5	10
5	A	36	17F	O7-C7-O8	2.83	130.71	123.63	8	10
4	A	30	PCW	C8-N-C7	2.79	101.64	108.98	8	10
5	A	33	17F	O3-P1-O1	2.78	119.97	108.94	5	10
5	A	77	17F	O3-P1-O1	2.76	119.86	108.94	9	10
4	A	16	PCW	C8-N-C7	2.74	101.79	108.98	6	10
4	A	7	PCW	C8-N-C7	2.73	101.81	108.98	5	10
4	A	8	PCW	C8-N-C7	2.73	101.82	108.98	2	10
4	A	66	PCW	C8-N-C7	2.71	101.86	108.98	6	10
4	A	72	PCW	C8-N-C7	2.70	101.89	108.98	8	10
4	A	48	PCW	C8-N-C7	2.69	101.90	108.98	10	10
4	A	65	PCW	C8-N-C7	2.69	101.91	108.98	4	10
4	A	12	PCW	C8-N-C7	2.69	101.92	108.98	9	10
4	A	19	PCW	C8-N-C7	2.68	101.93	108.98	4	10
4	A	27	PCW	C8-N-C7	2.68	101.95	108.98	3	10
4	A	15	PCW	C8-N-C7	2.67	101.96	108.98	5	10
4	A	32	PCW	C8-N-C7	2.66	101.99	108.98	1	10
4	A	50	PCW	C8-N-C7	2.66	101.99	108.98	9	10
4	A	11	PCW	C8-N-C7	2.66	102.00	108.98	1	10
4	A	55	PCW	C8-N-C7	2.65	102.02	108.98	6	10
4	A	47	PCW	C8-N-C7	2.63	102.07	108.98	2	10
4	A	9	PCW	C8-N-C7	2.62	102.09	108.98	7	10
5	A	34	17F	C5-O9-C17	2.53	111.73	117.80	6	10
5	A	73	17F	C5-O9-C17	2.53	111.74	117.80	6	10
5	A	37	17F	C5-O9-C17	2.53	111.75	117.80	7	10
5	A	74	17F	C5-O9-C17	2.52	111.76	117.80	9	10
4	A	63	PCW	C7-N-C5	2.50	119.85	109.91	10	10
5	A	79	17F	C5-O9-C17	2.50	111.81	117.80	1	10
4	A	13	PCW	C7-N-C5	2.50	119.84	109.91	9	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	42	PCW	C7-N-C5	2.50	119.83	109.91	10	10
4	A	2	PCW	C7-N-C5	2.49	119.81	109.91	1	10
5	A	75	17F	C5-O9-C17	2.49	111.83	117.80	1	10
4	A	3	PCW	C7-N-C5	2.49	119.81	109.91	6	10
4	A	68	PCW	C7-N-C5	2.49	119.80	109.91	8	10
5	A	77	17F	C5-O9-C17	2.49	111.85	117.80	7	10
4	A	10	PCW	C7-N-C5	2.48	119.78	109.91	9	10
4	A	14	PCW	C7-N-C5	2.48	119.78	109.91	7	10
5	A	33	17F	C5-O9-C17	2.48	111.86	117.80	6	10
5	A	35	17F	C5-O9-C17	2.48	111.87	117.80	1	10
5	A	36	17F	C5-O9-C17	2.48	111.87	117.80	4	10
4	A	17	PCW	C7-N-C5	2.48	119.75	109.91	4	10
5	A	33	17F	O6-P1-O1	2.47	118.74	108.94	8	10
4	A	6	PCW	C7-N-C5	2.47	119.74	109.91	5	10
4	A	64	PCW	C7-N-C5	2.47	119.73	109.91	4	10
4	A	58	PCW	C7-N-C5	2.46	119.69	109.91	7	10
4	A	44	PCW	C7-N-C5	2.46	119.69	109.91	10	10
4	A	51	PCW	C7-N-C5	2.46	119.69	109.91	5	10
4	A	59	PCW	C7-N-C5	2.46	119.68	109.91	5	10
4	A	1	PCW	C7-N-C5	2.45	119.67	109.91	3	10
4	A	26	PCW	C7-N-C5	2.45	119.66	109.91	6	10
4	A	56	PCW	C7-N-C5	2.45	119.66	109.91	10	10
4	A	69	PCW	C7-N-C5	2.45	119.66	109.91	5	10
4	A	20	PCW	C7-N-C5	2.45	119.66	109.91	5	10
4	A	52	PCW	C7-N-C5	2.45	119.65	109.91	4	10
4	A	67	PCW	C7-N-C5	2.45	119.66	109.91	1	10
5	A	77	17F	O6-P1-O1	2.45	118.65	108.94	7	10
4	A	54	PCW	C7-N-C5	2.45	119.64	109.91	6	10
5	A	76	17F	C5-O9-C17	2.45	111.94	117.80	10	10
5	A	80	17F	O9-C17-O10	2.45	129.43	123.70	4	10
4	A	49	PCW	C7-N-C5	2.44	119.63	109.91	6	10
4	A	62	PCW	C7-N-C5	2.44	119.62	109.91	6	10
4	A	24	PCW	C7-N-C5	2.44	119.61	109.91	9	10
4	A	57	PCW	C7-N-C5	2.44	119.61	109.91	10	10
4	A	22	PCW	C7-N-C5	2.44	119.60	109.91	4	10
5	A	38	17F	O9-C17-O10	2.44	129.40	123.70	7	10
4	A	29	PCW	C7-N-C5	2.43	119.59	109.91	9	10
4	A	25	PCW	C7-N-C5	2.43	119.58	109.91	10	10
4	A	31	PCW	C7-N-C5	2.43	119.58	109.91	6	10
4	A	4	PCW	C7-N-C5	2.43	119.57	109.91	2	10
4	A	45	PCW	C7-N-C5	2.43	119.56	109.91	1	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	76	17F	O9-C17-O10	2.43	129.38	123.70	2	10
4	A	23	PCW	C7-N-C5	2.43	119.55	109.91	1	10
4	A	28	PCW	C7-N-C5	2.42	119.55	109.91	2	10
4	A	53	PCW	C7-N-C5	2.42	119.54	109.91	5	10
4	A	41	PCW	C7-N-C5	2.42	119.54	109.91	1	10
4	A	70	PCW	C7-N-C5	2.42	119.53	109.91	3	10
4	A	46	PCW	C7-N-C5	2.42	119.53	109.91	3	10
4	A	21	PCW	C7-N-C5	2.42	119.52	109.91	1	10
5	A	39	17F	C5-O9-C17	2.42	112.01	117.80	8	10
4	A	60	PCW	C7-N-C5	2.41	119.51	109.91	6	10
4	A	18	PCW	C7-N-C5	2.41	119.50	109.91	5	10
5	A	78	17F	C5-O9-C17	2.41	112.02	117.80	5	9
4	A	5	PCW	C7-N-C5	2.41	119.48	109.91	1	10
4	A	43	PCW	C7-N-C5	2.41	119.48	109.91	2	10
4	A	61	PCW	C7-N-C5	2.41	119.48	109.91	8	10
5	A	33	17F	O9-C17-O10	2.39	129.29	123.70	5	10
4	A	71	PCW	C7-N-C5	2.39	119.40	109.91	10	10
5	A	40	17F	O9-C17-O10	2.39	129.28	123.70	8	10
5	A	38	17F	C5-O9-C17	2.38	112.10	117.80	1	10
5	A	35	17F	O9-C17-O10	2.38	129.26	123.70	8	10
5	A	73	17F	O9-C17-O10	2.37	129.25	123.70	3	10
5	A	40	17F	C5-O9-C17	2.37	112.13	117.80	3	8
5	A	79	17F	O9-C17-O10	2.37	129.24	123.70	9	10
5	A	78	17F	O9-C17-O10	2.36	129.22	123.70	7	10
5	A	37	17F	O9-C17-O10	2.35	129.20	123.70	6	10
5	A	77	17F	O9-C17-O10	2.32	129.12	123.70	2	10
5	A	39	17F	O9-C17-O10	2.31	129.10	123.70	5	10
5	A	75	17F	O9-C17-O10	2.29	129.06	123.70	10	10
5	A	34	17F	O9-C17-O10	2.23	128.92	123.70	10	10
5	A	74	17F	O9-C17-O10	2.22	128.90	123.70	10	10
5	A	36	17F	O9-C17-O10	2.22	128.89	123.70	7	10
6	B	201	GNP	O2A-PA-O3A	2.07	112.88	107.27	10	5
4	A	54	PCW	C7-N-C6	2.06	114.40	108.98	8	1
4	A	45	PCW	C7-N-C6	2.06	114.38	108.98	3	1
4	A	6	PCW	O1P-P-O3P	2.03	116.78	107.57	7	2
4	A	13	PCW	C7-N-C6	2.02	114.29	108.98	4	1
4	A	49	PCW	C7-N-C6	2.02	114.29	108.98	1	1
4	A	63	PCW	O1P-P-O3P	2.02	116.73	107.57	4	2
4	A	62	PCW	C7-N-C6	2.01	114.25	108.98	4	1
4	A	44	PCW	C7-N-C6	2.00	114.23	108.98	6	1
4	A	17	PCW	C7-N-C6	2.00	114.23	108.98	7	1

Continued on next page...

Continued from previous page...

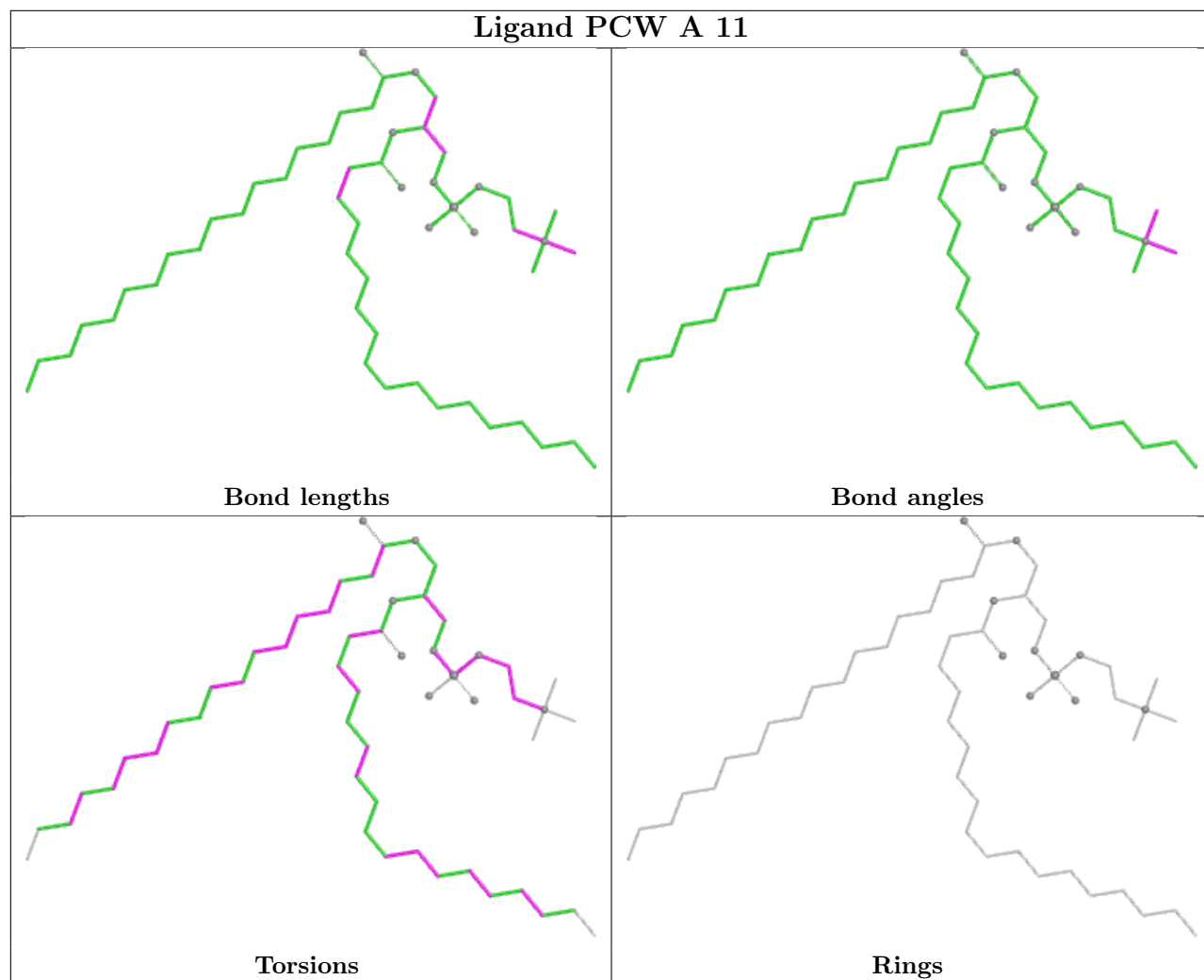
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	57	PCW	C7-N-C6	2.00	114.23	108.98	1	1

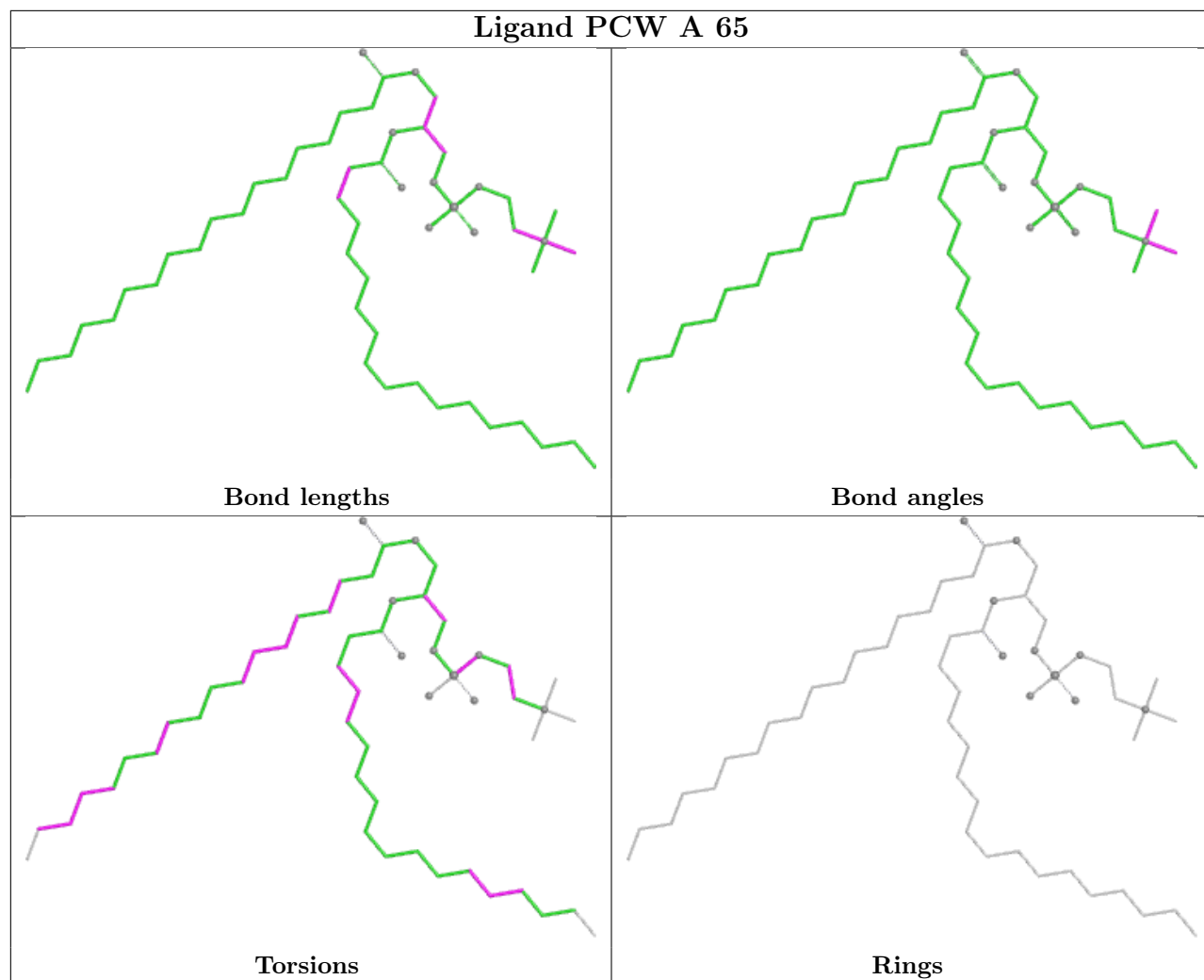
There are no chirality outliers.

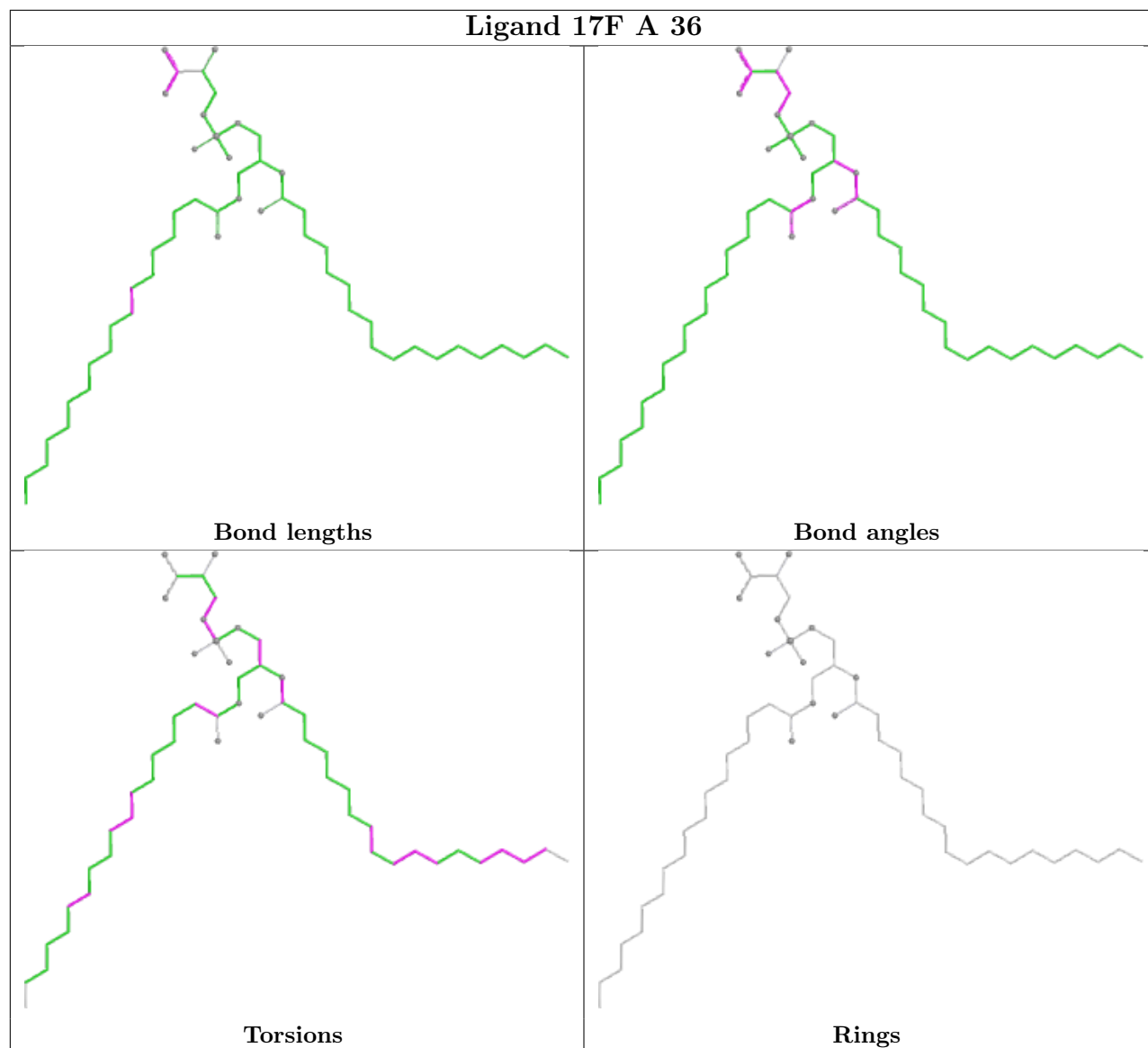
There are no torsion outliers.

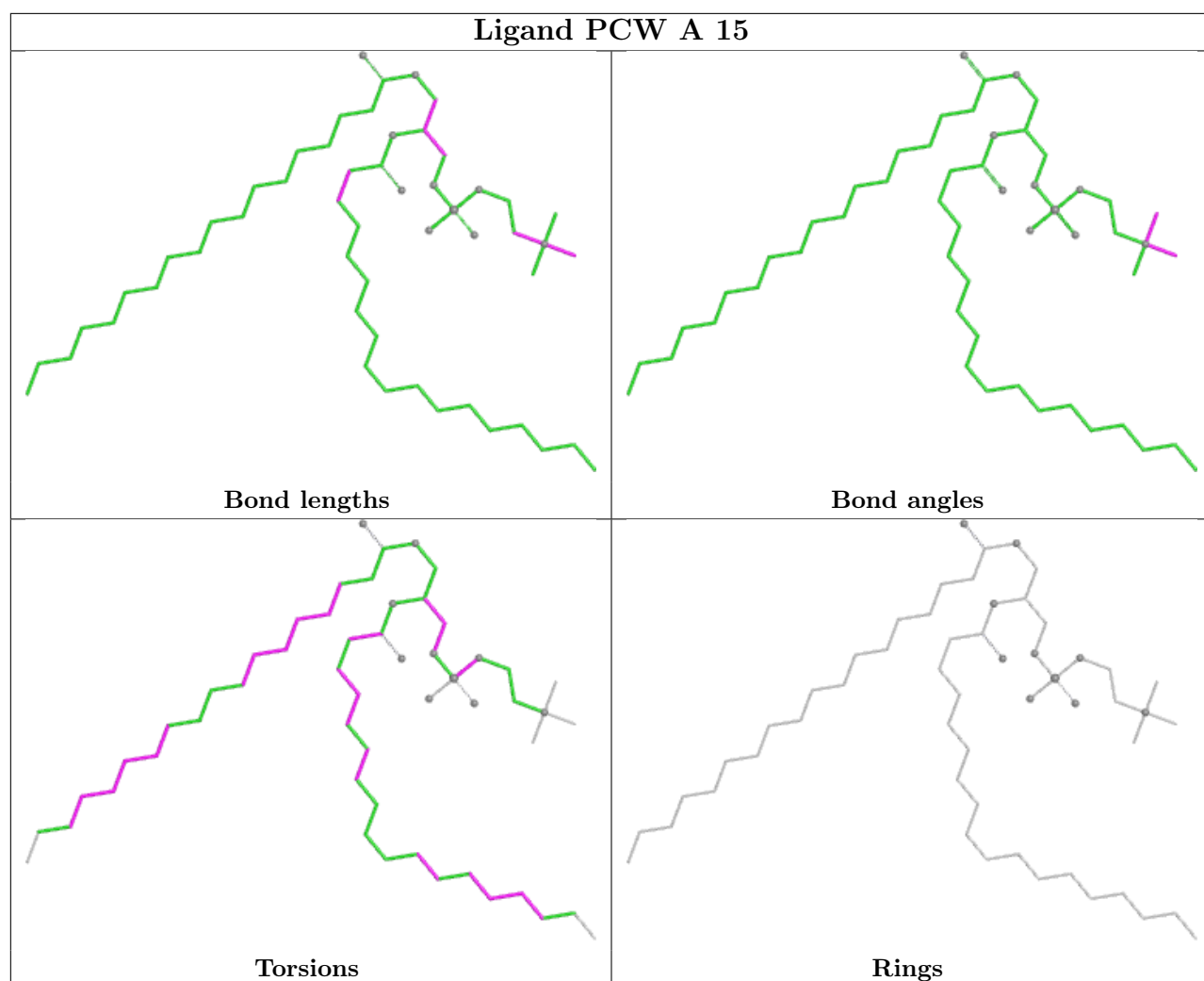
There are no ring outliers.

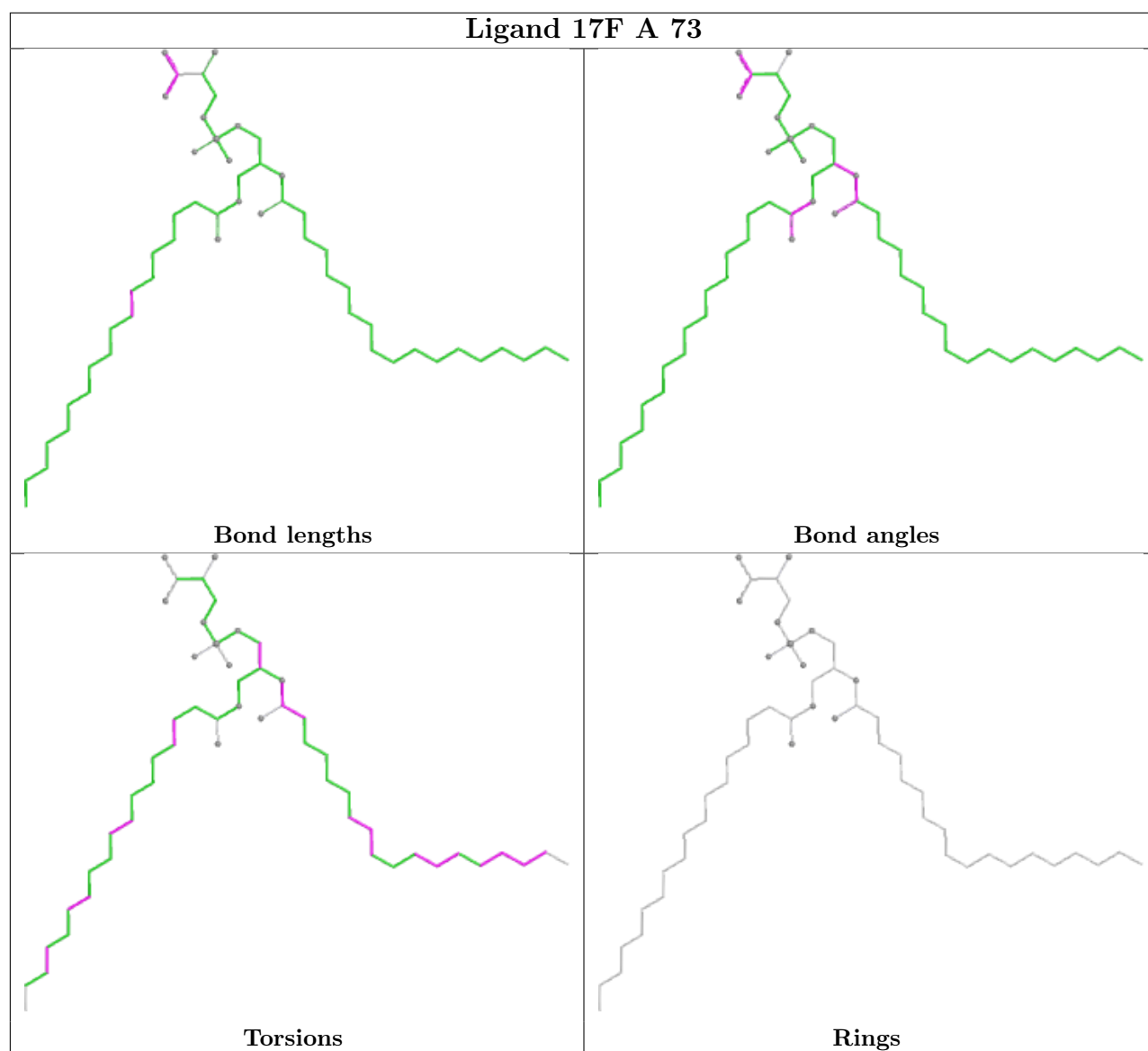
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

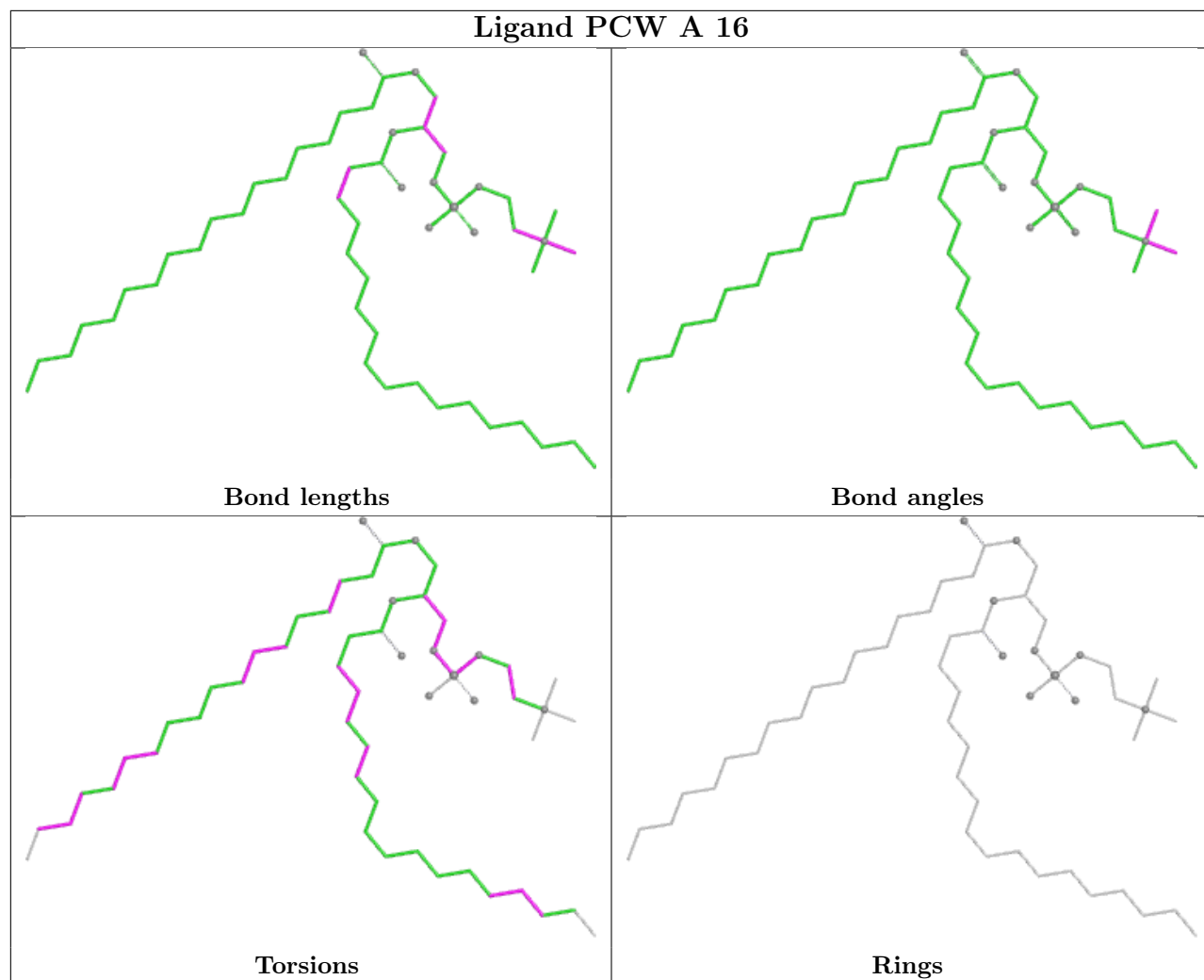


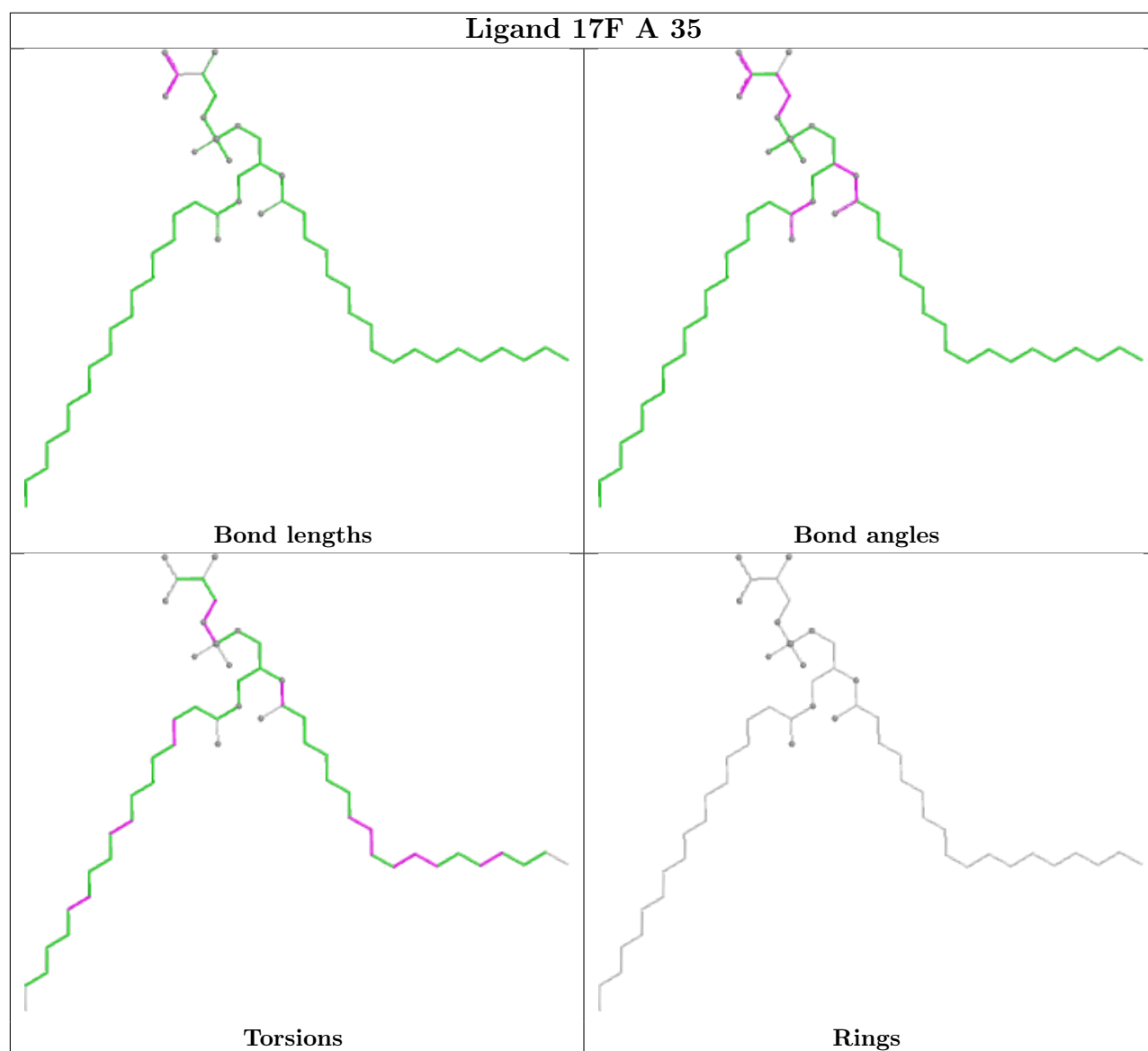


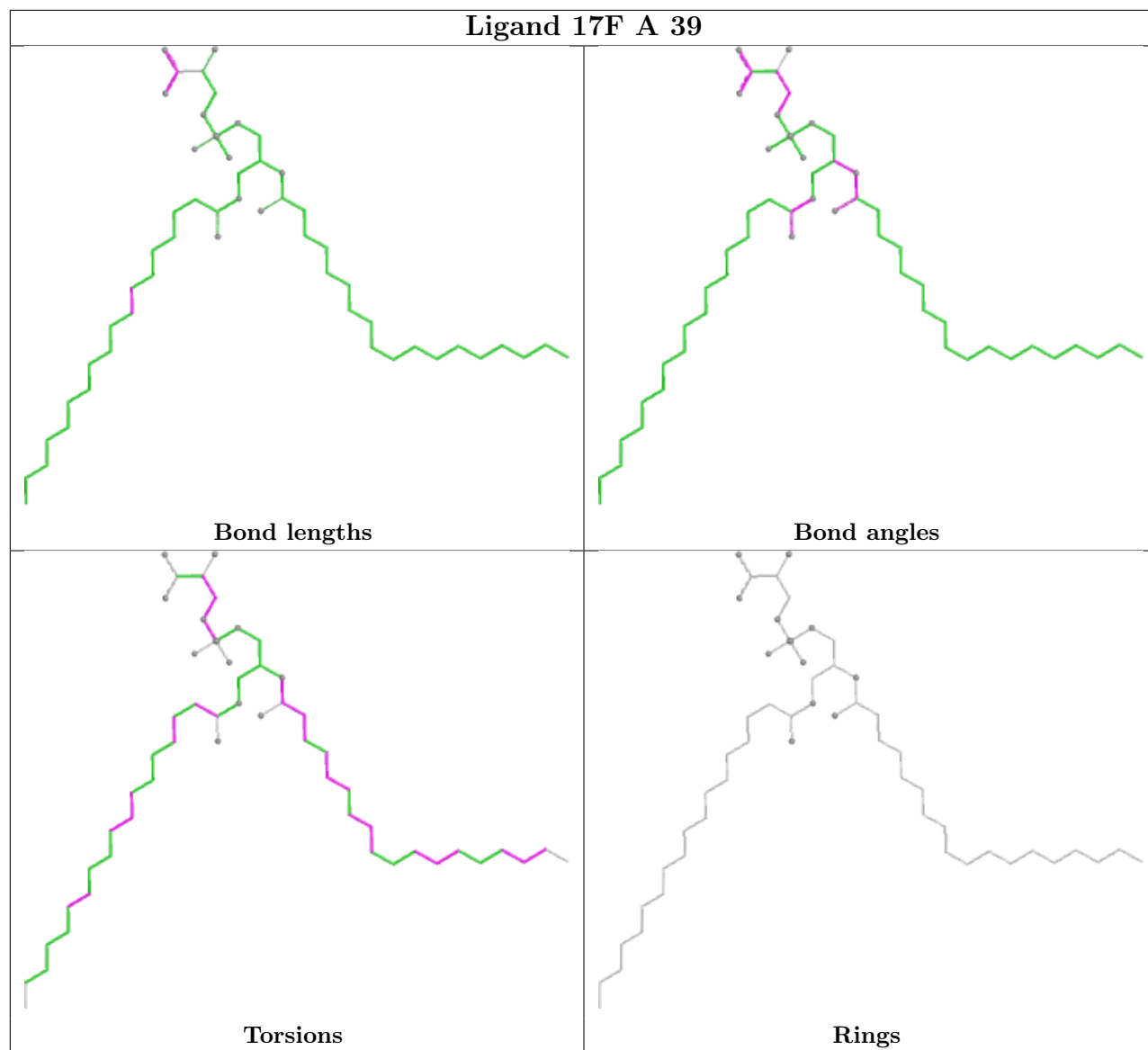


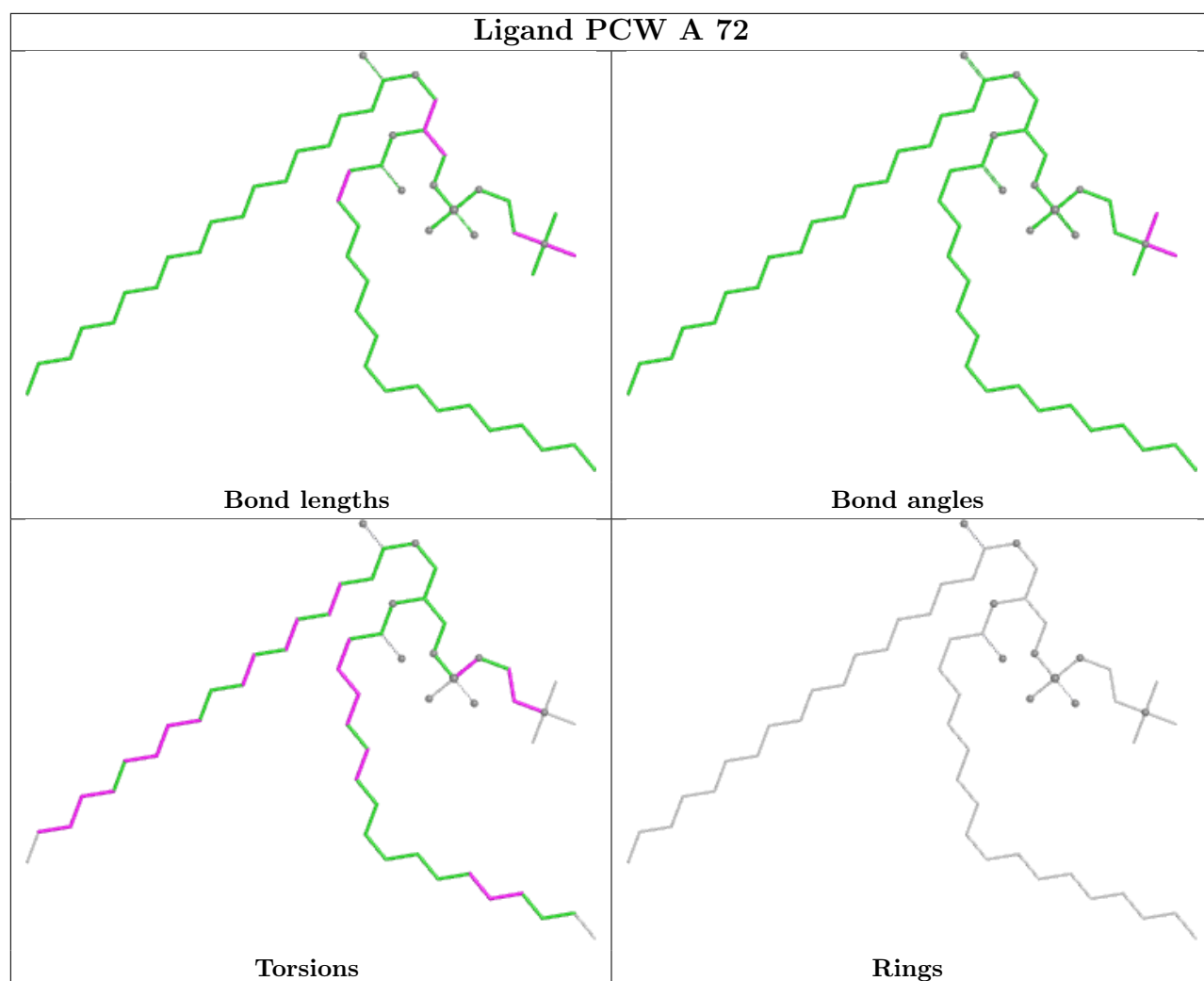


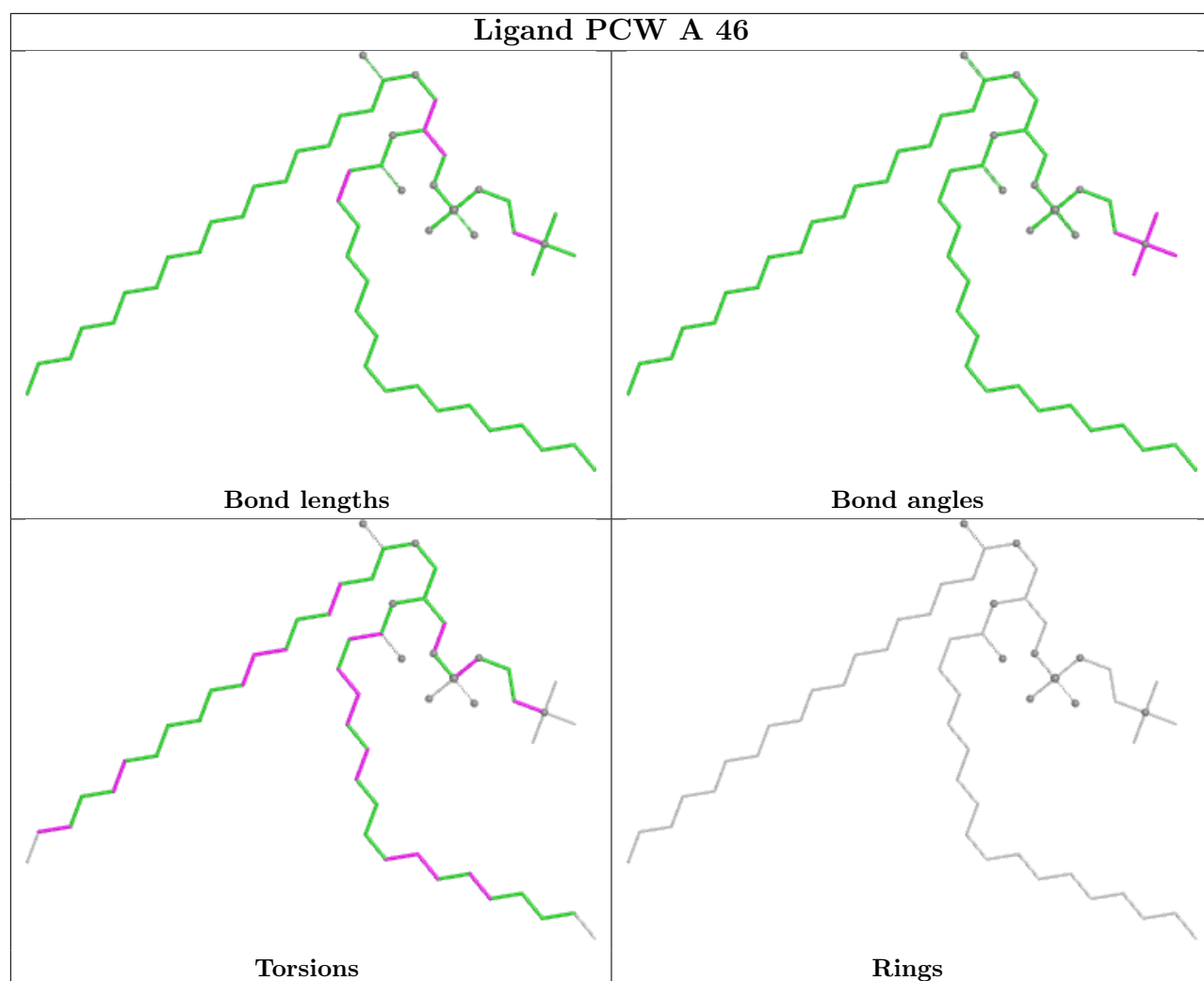


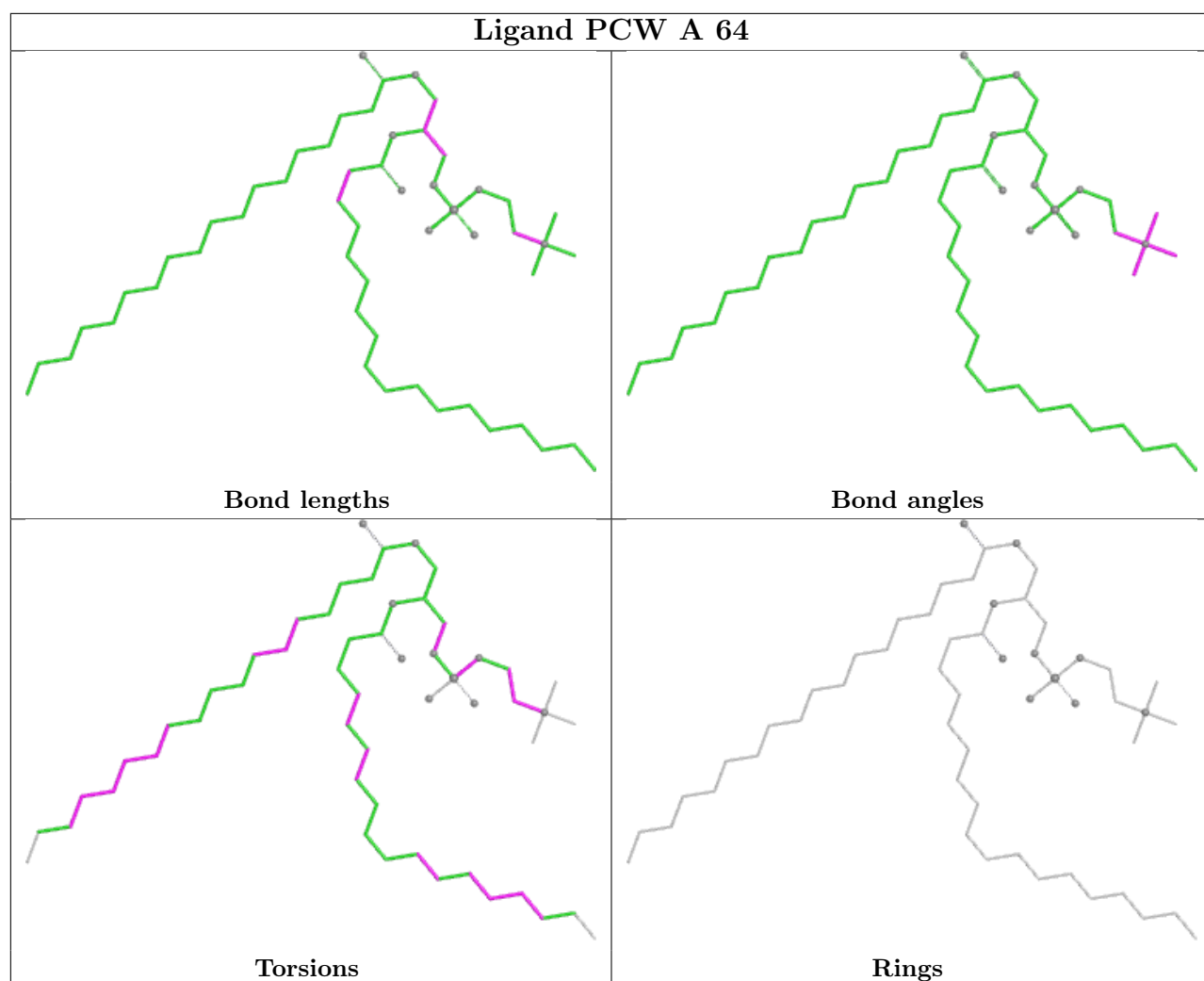


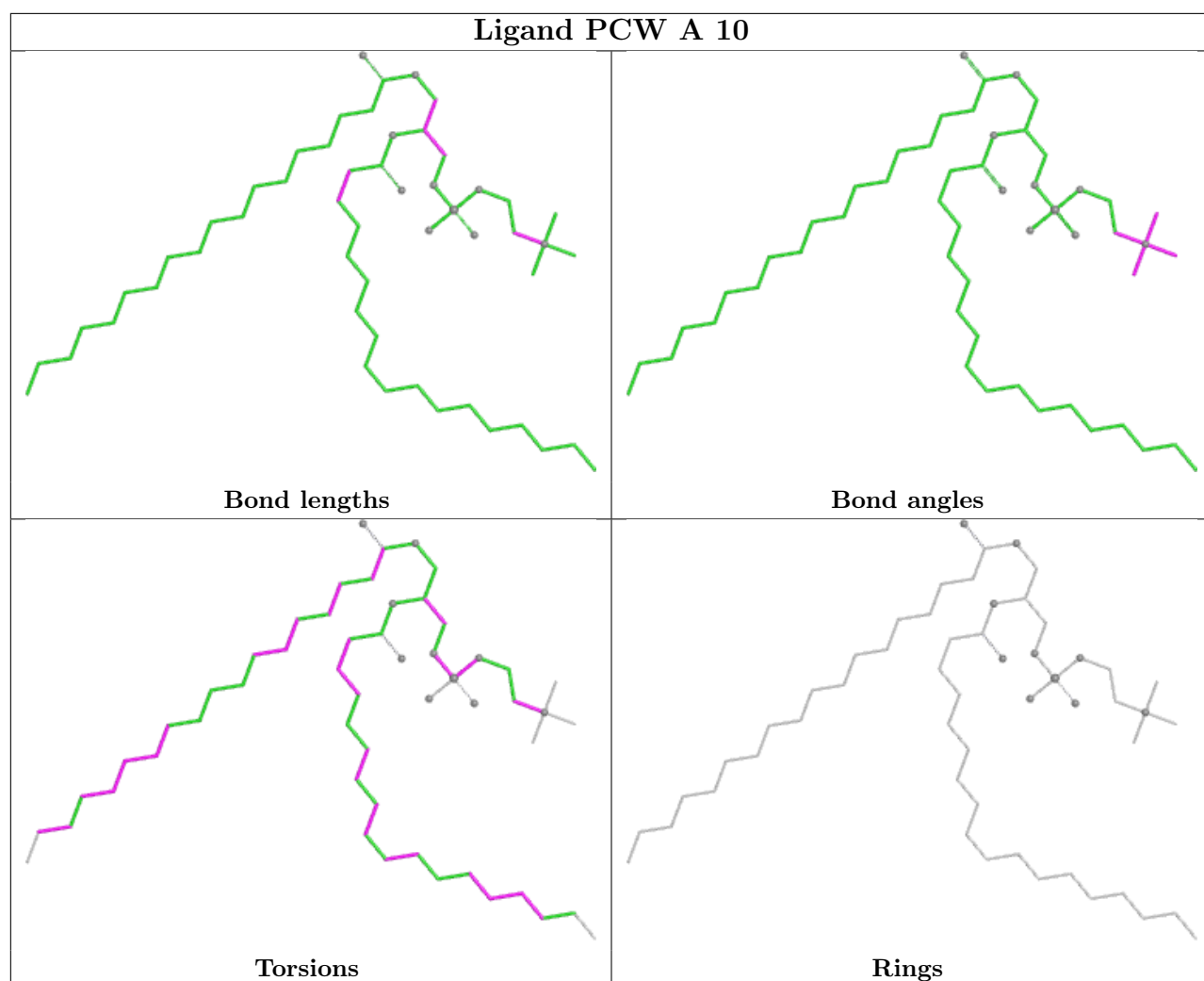


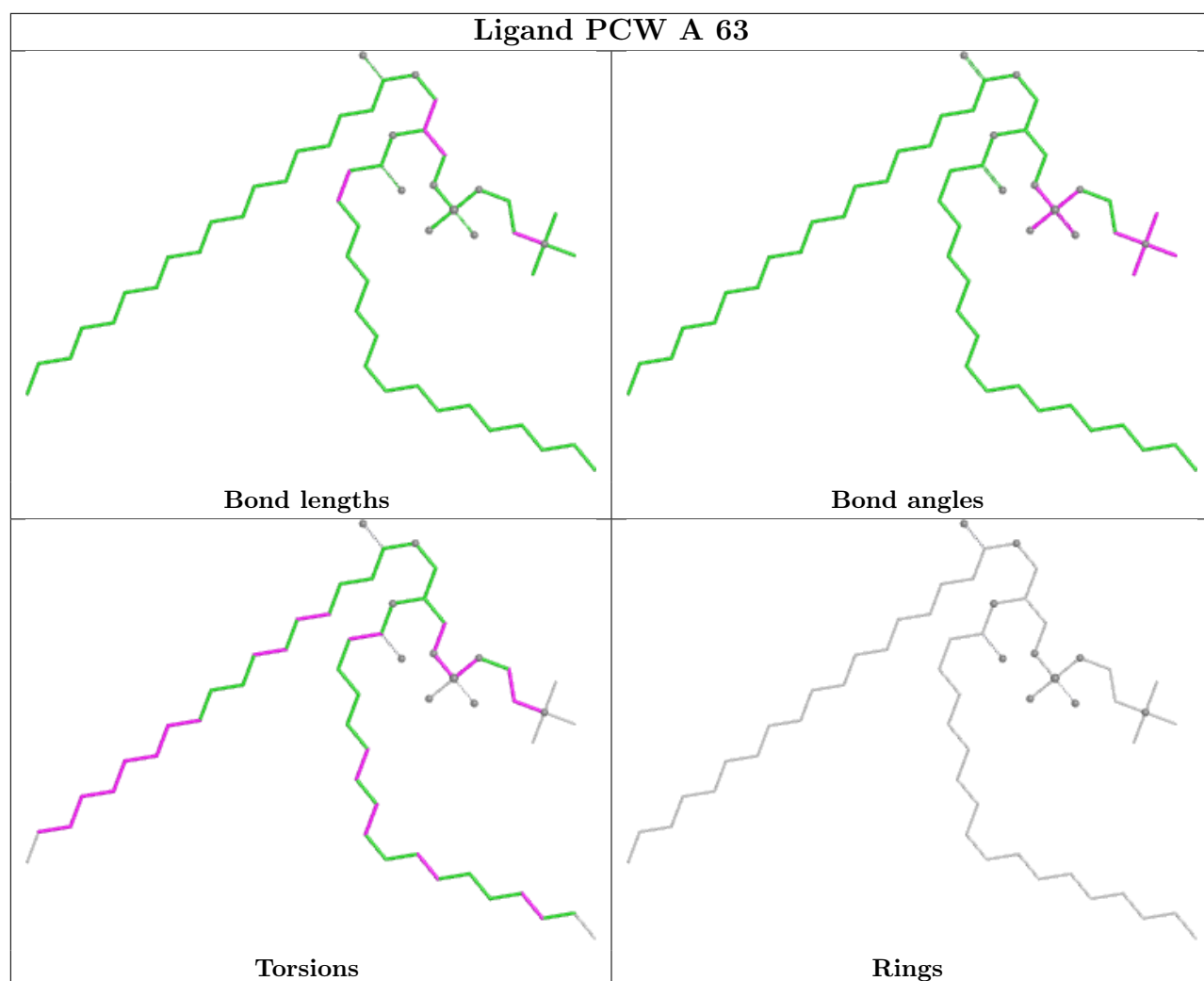


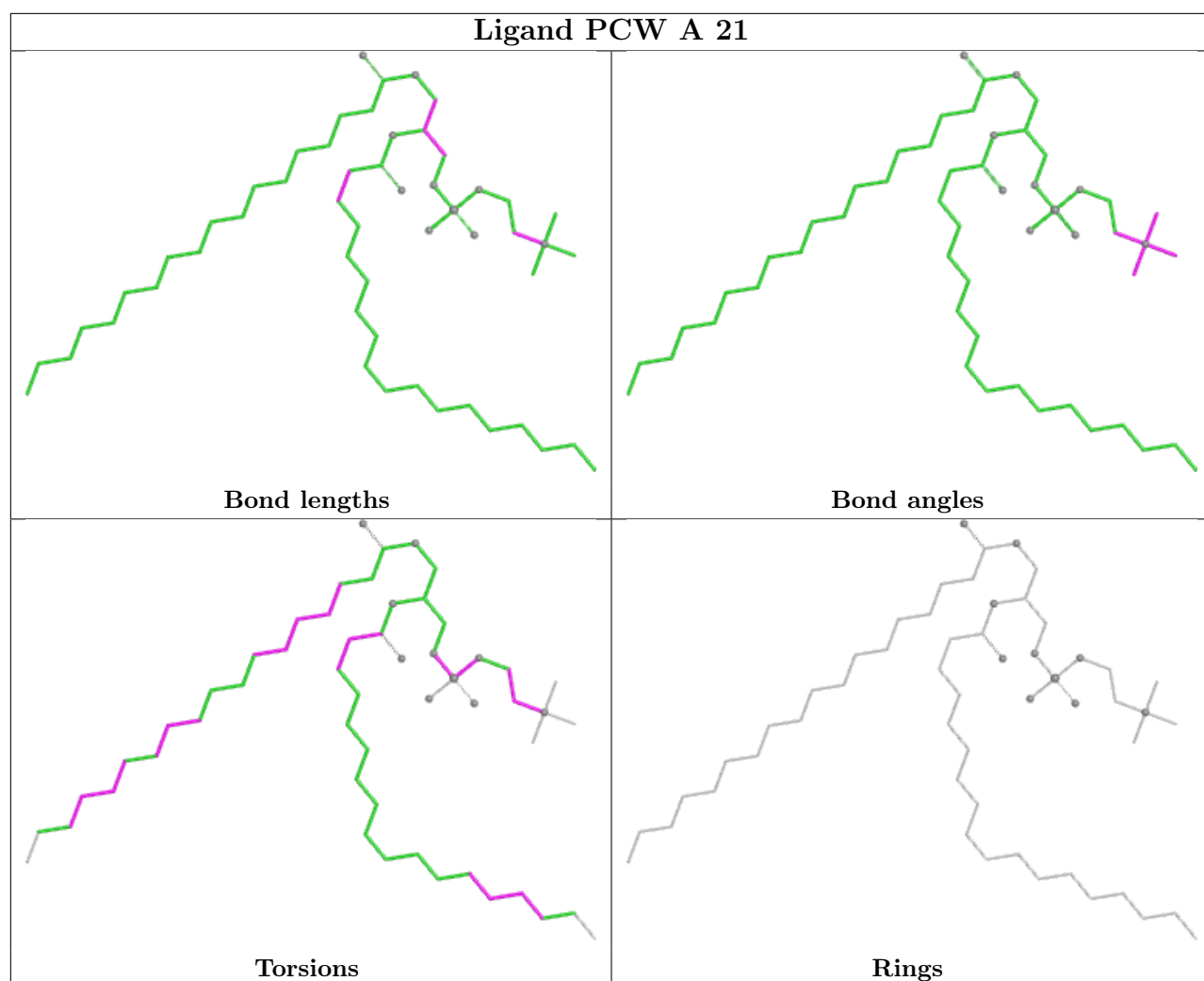


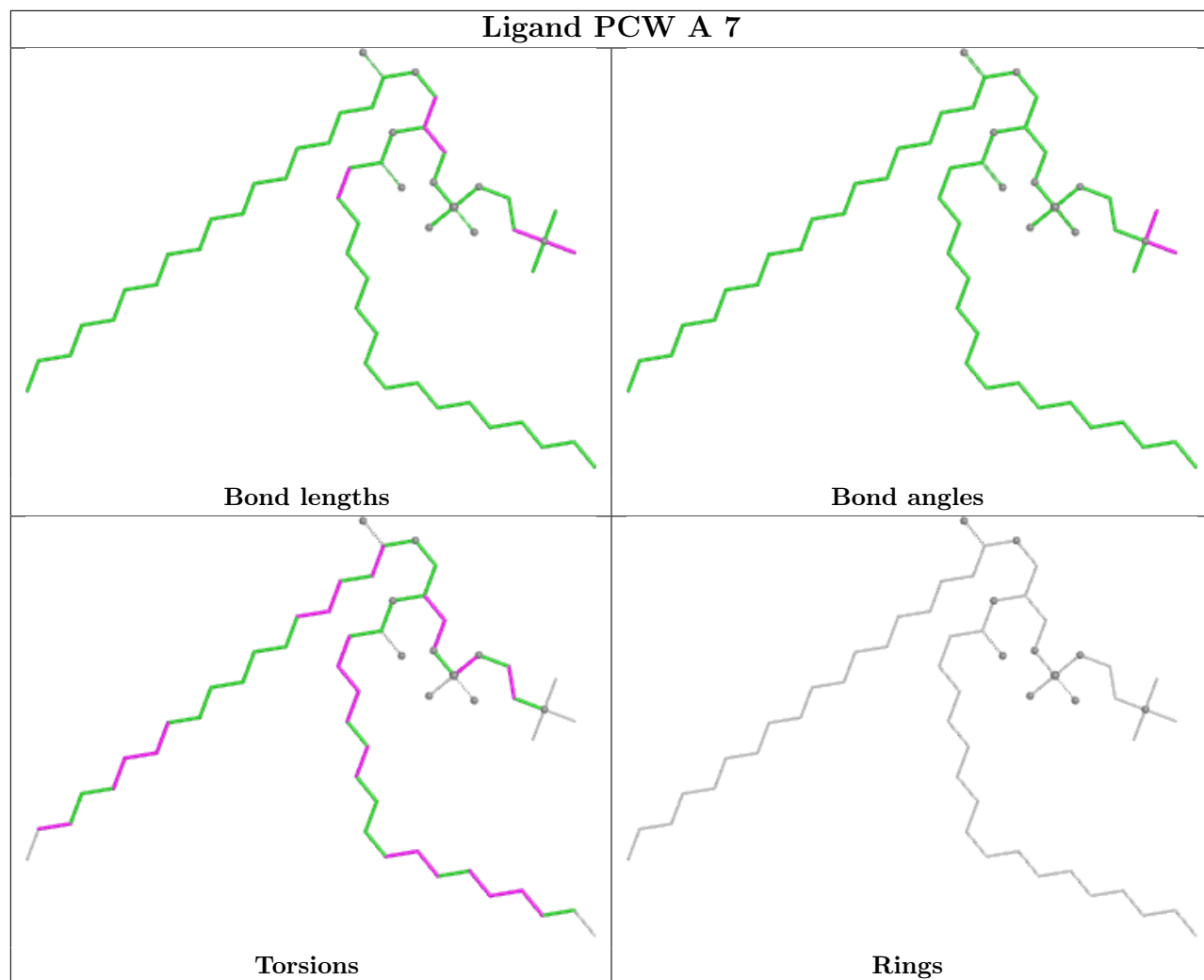


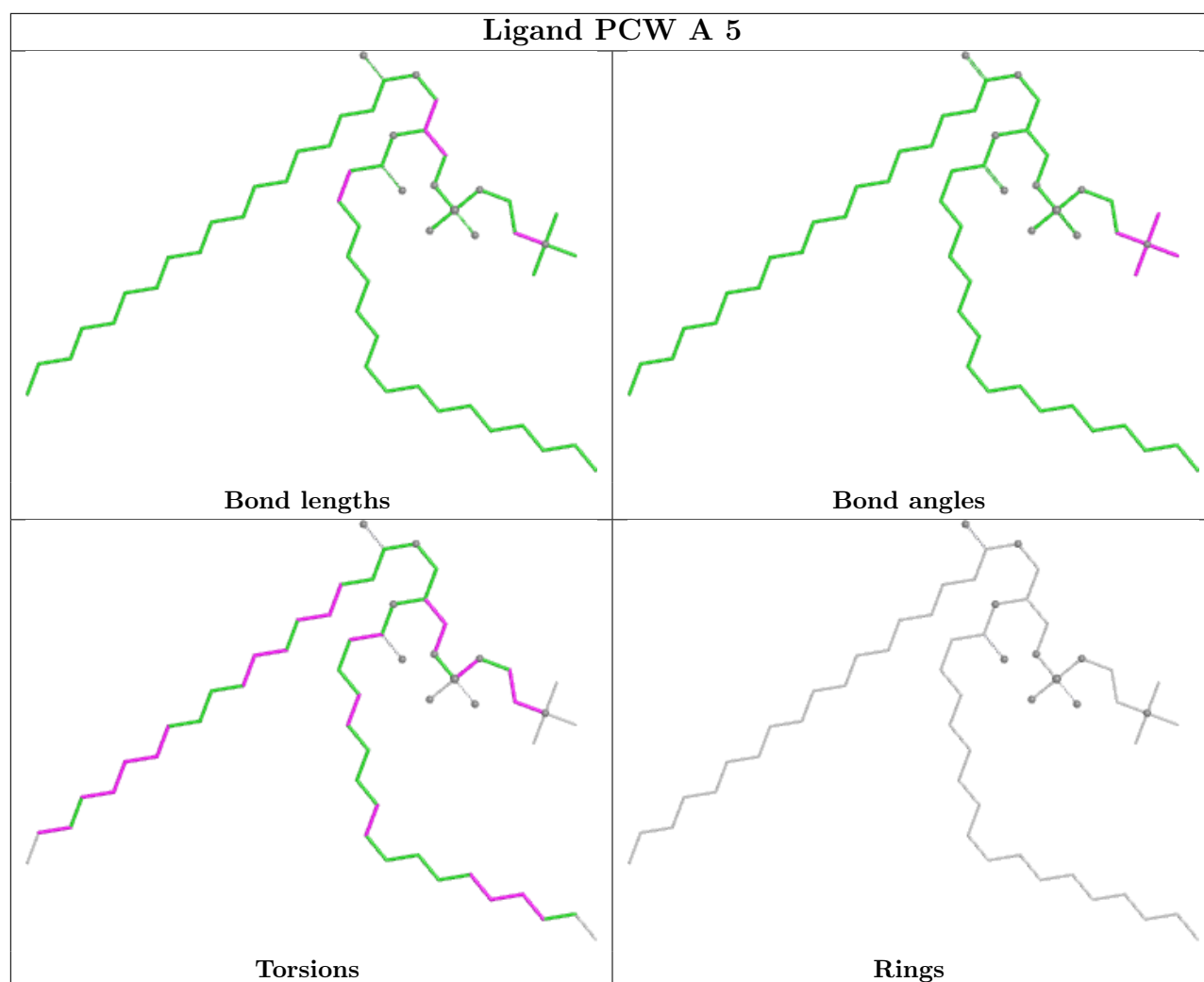


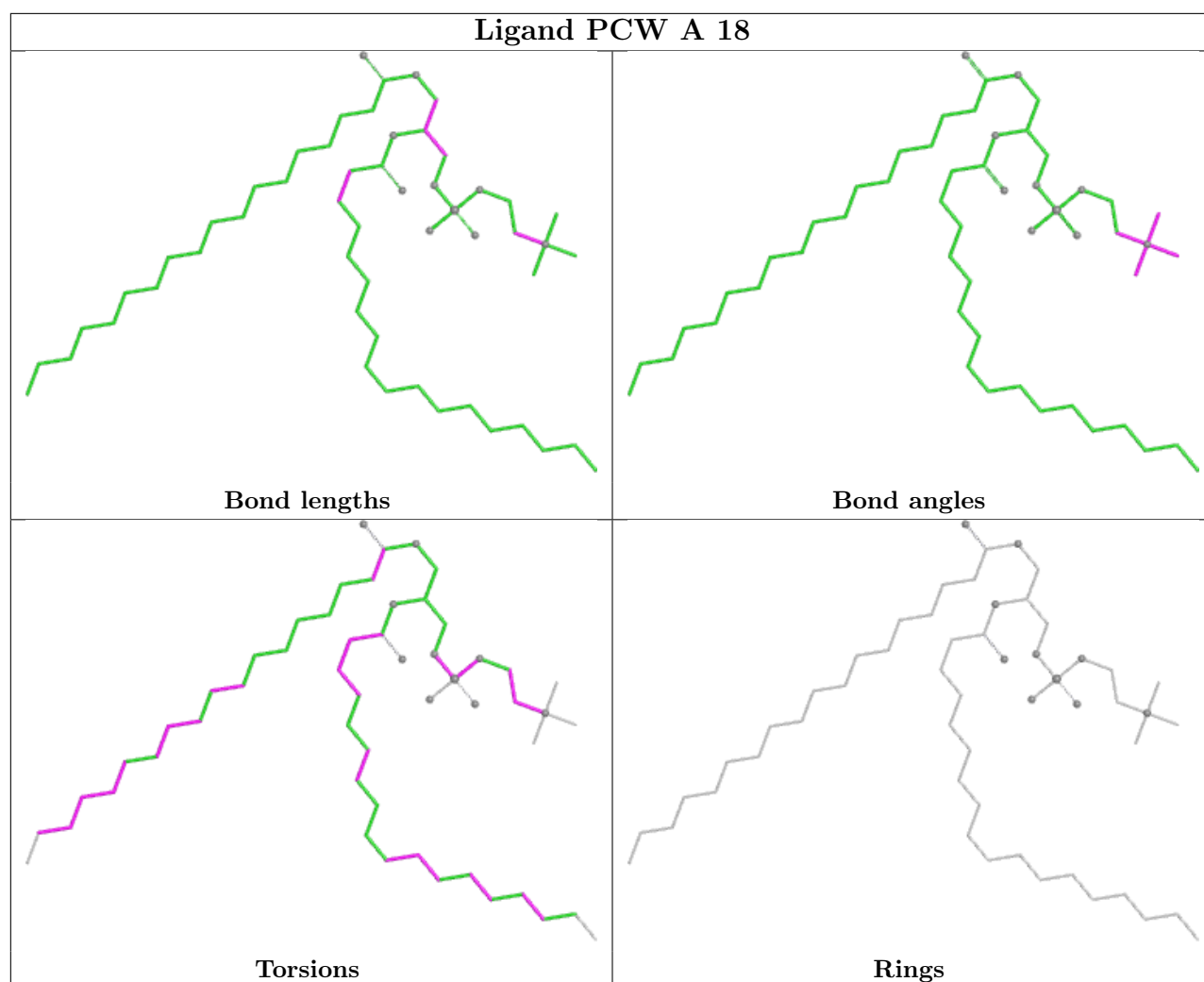


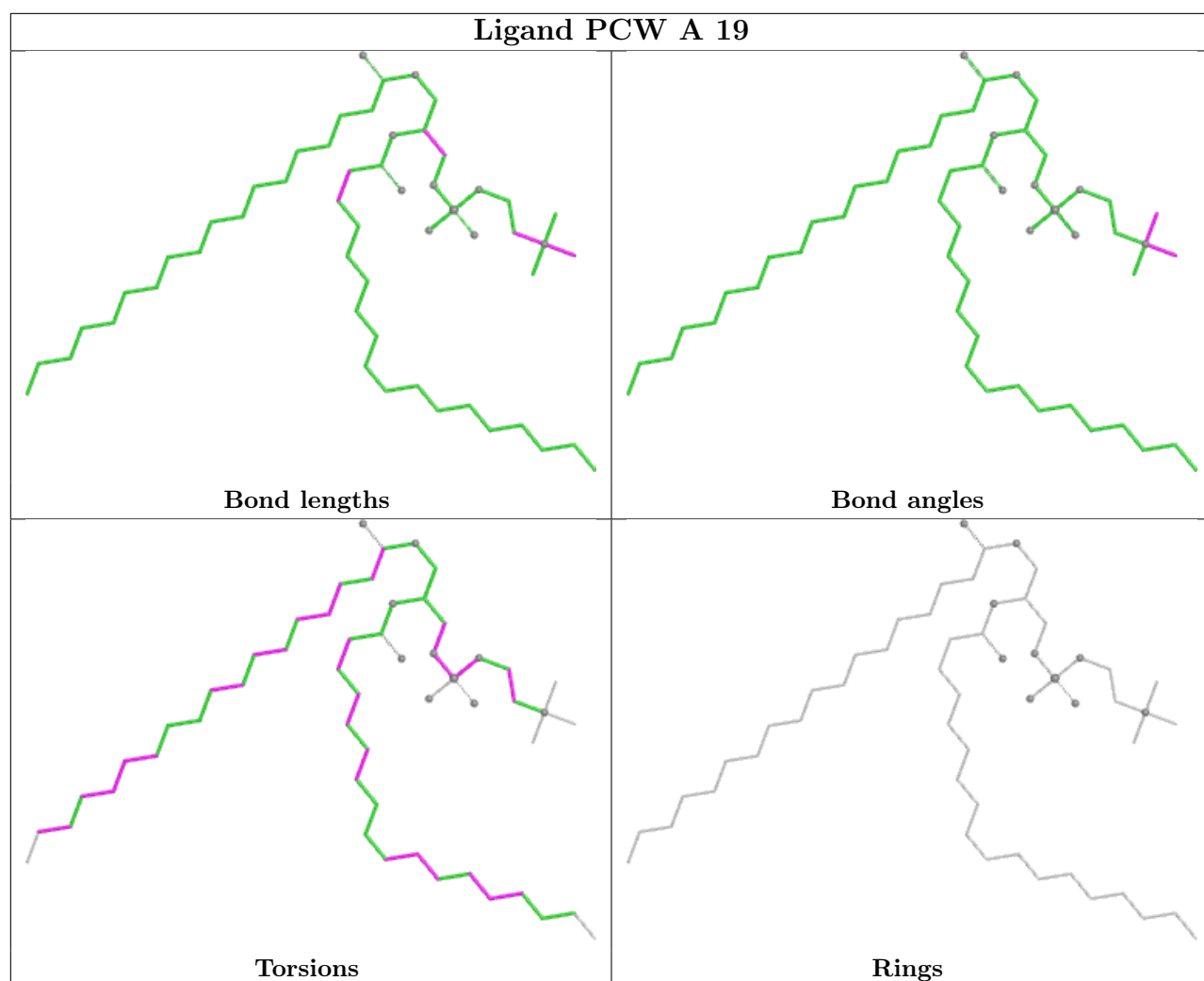


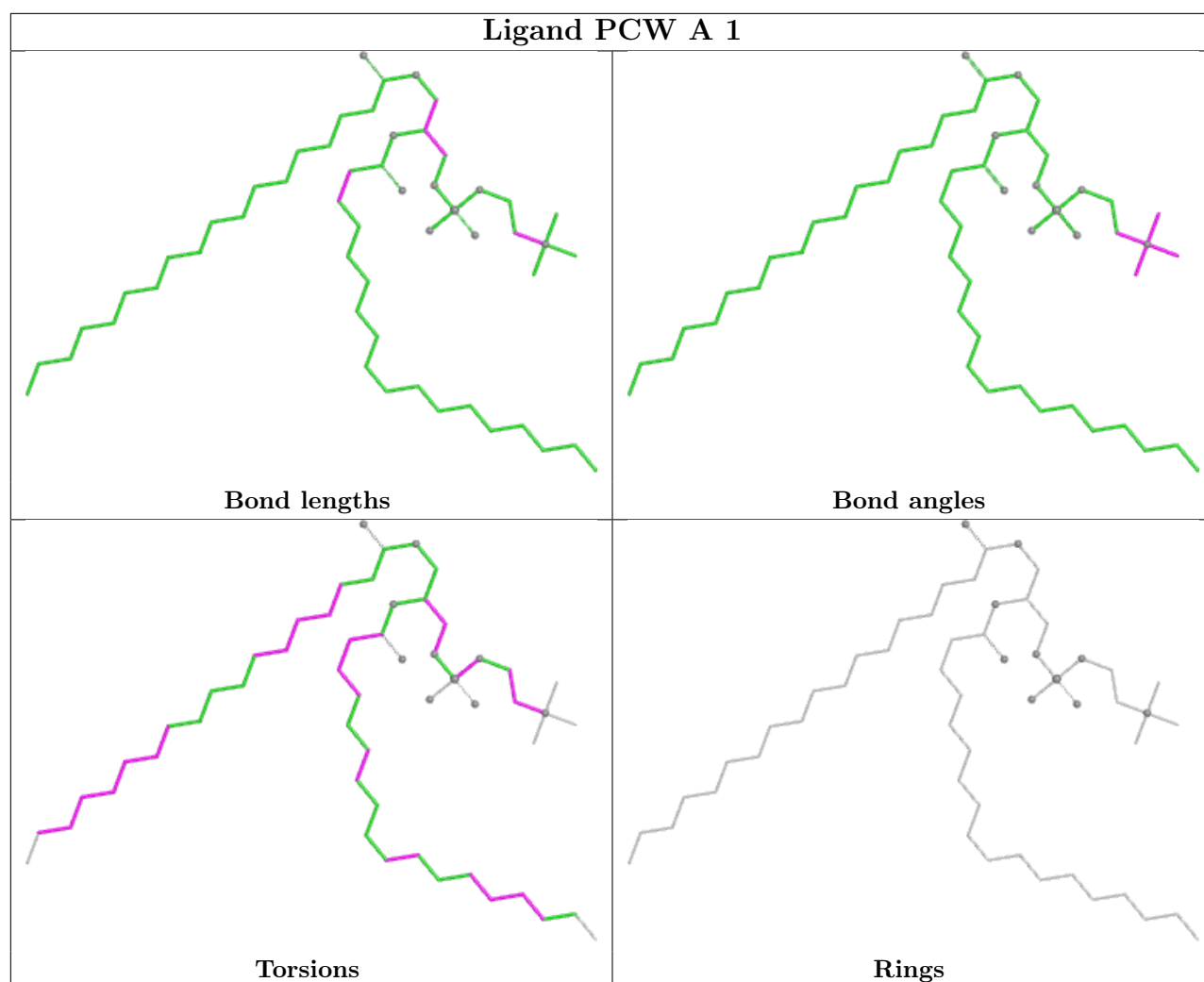


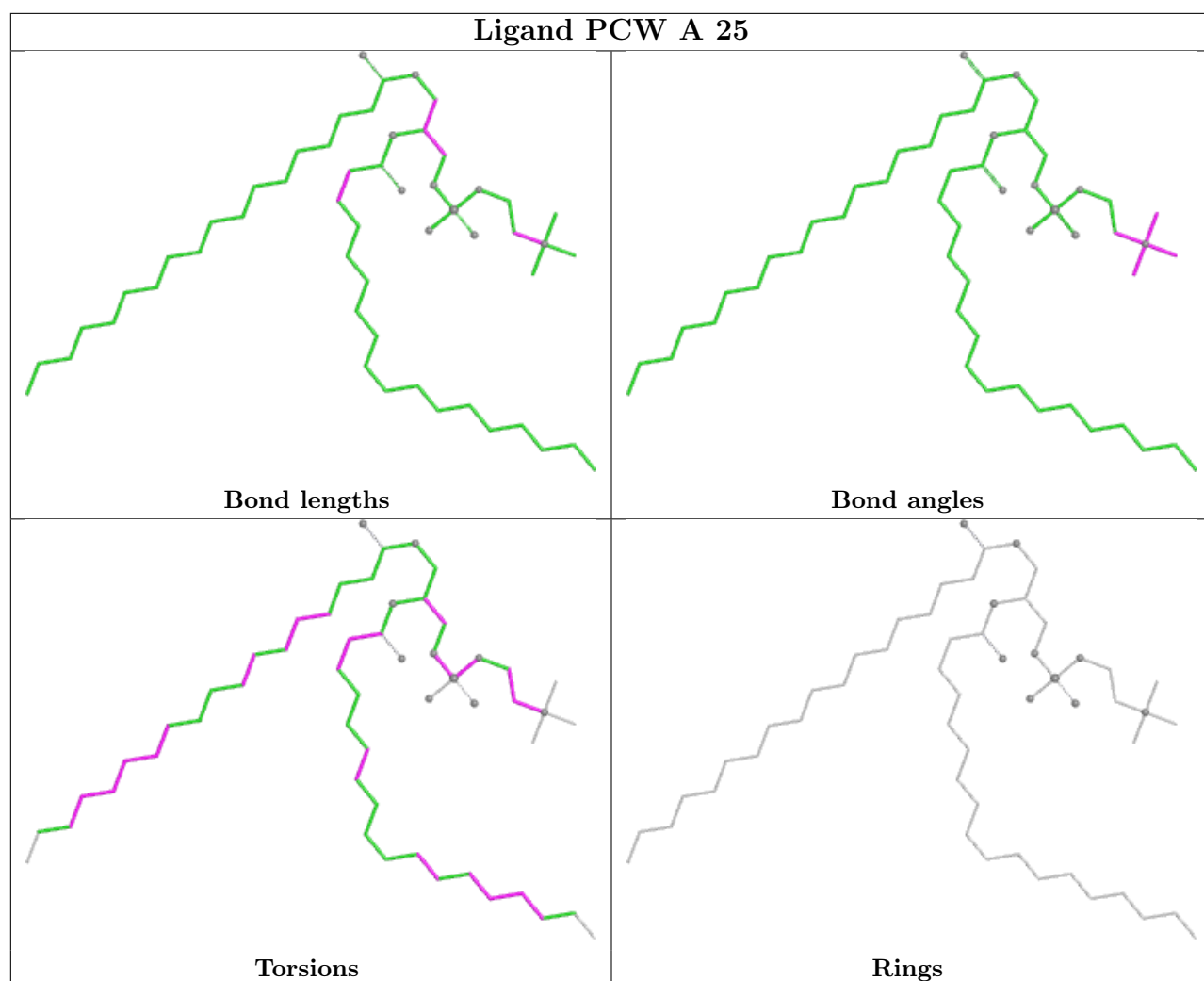


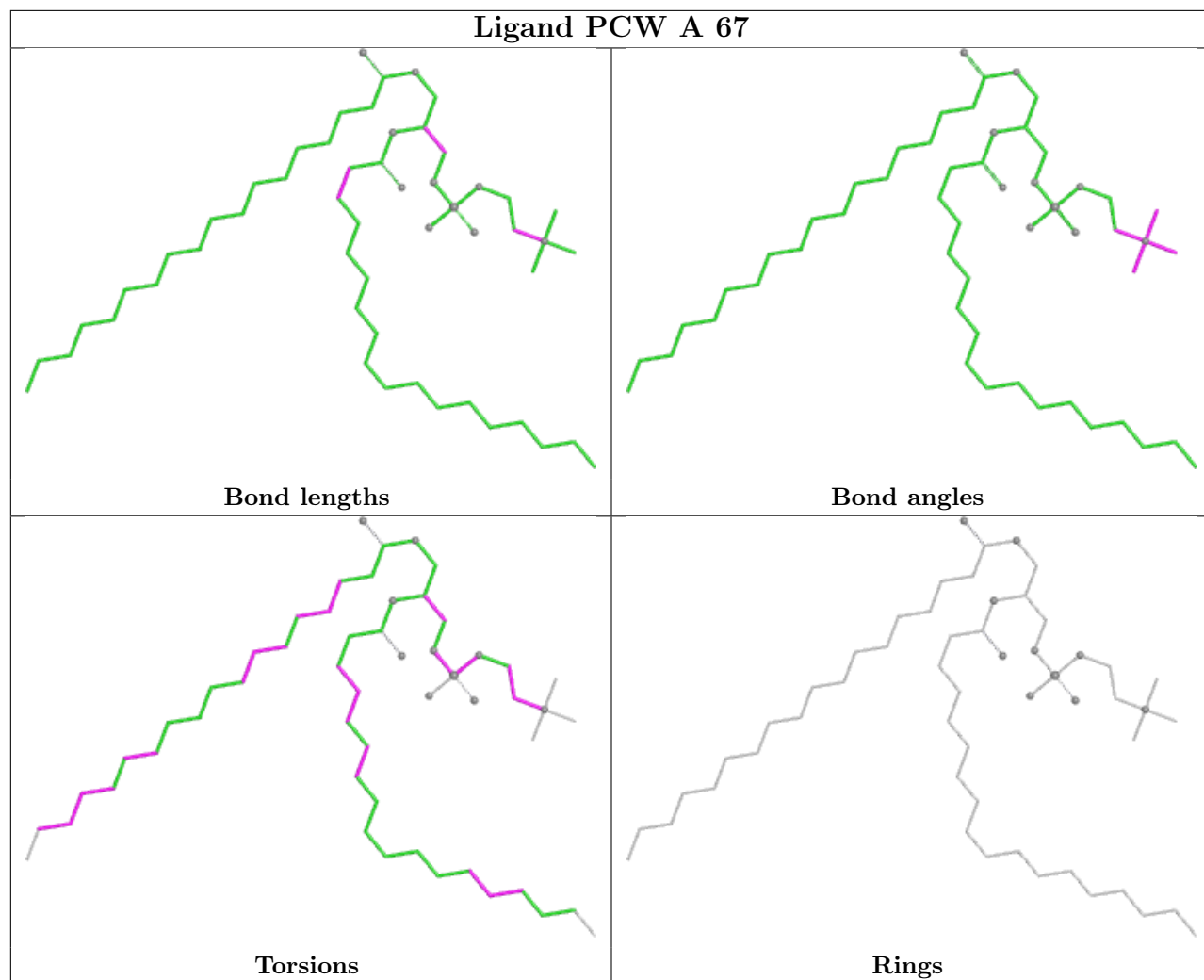


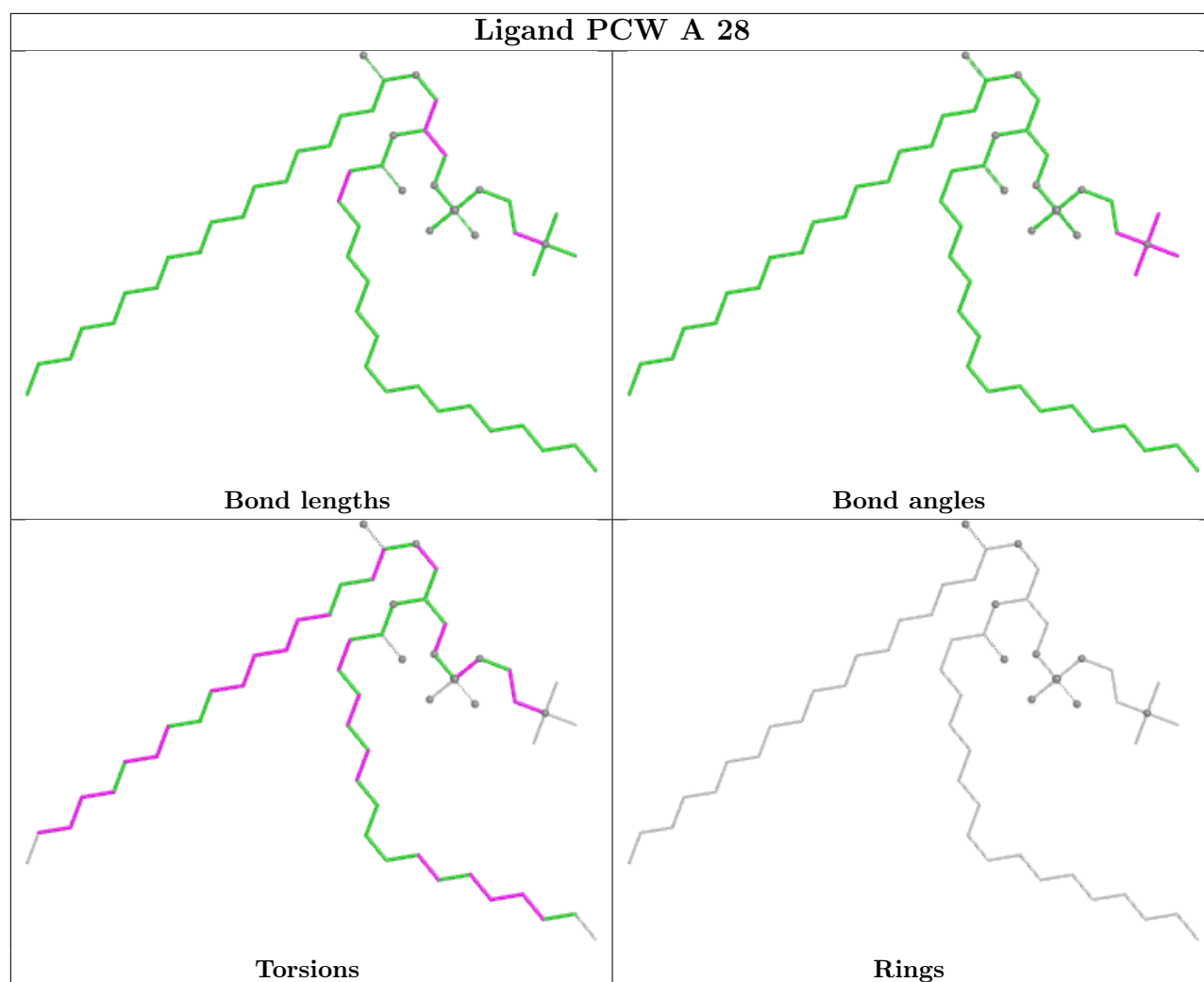


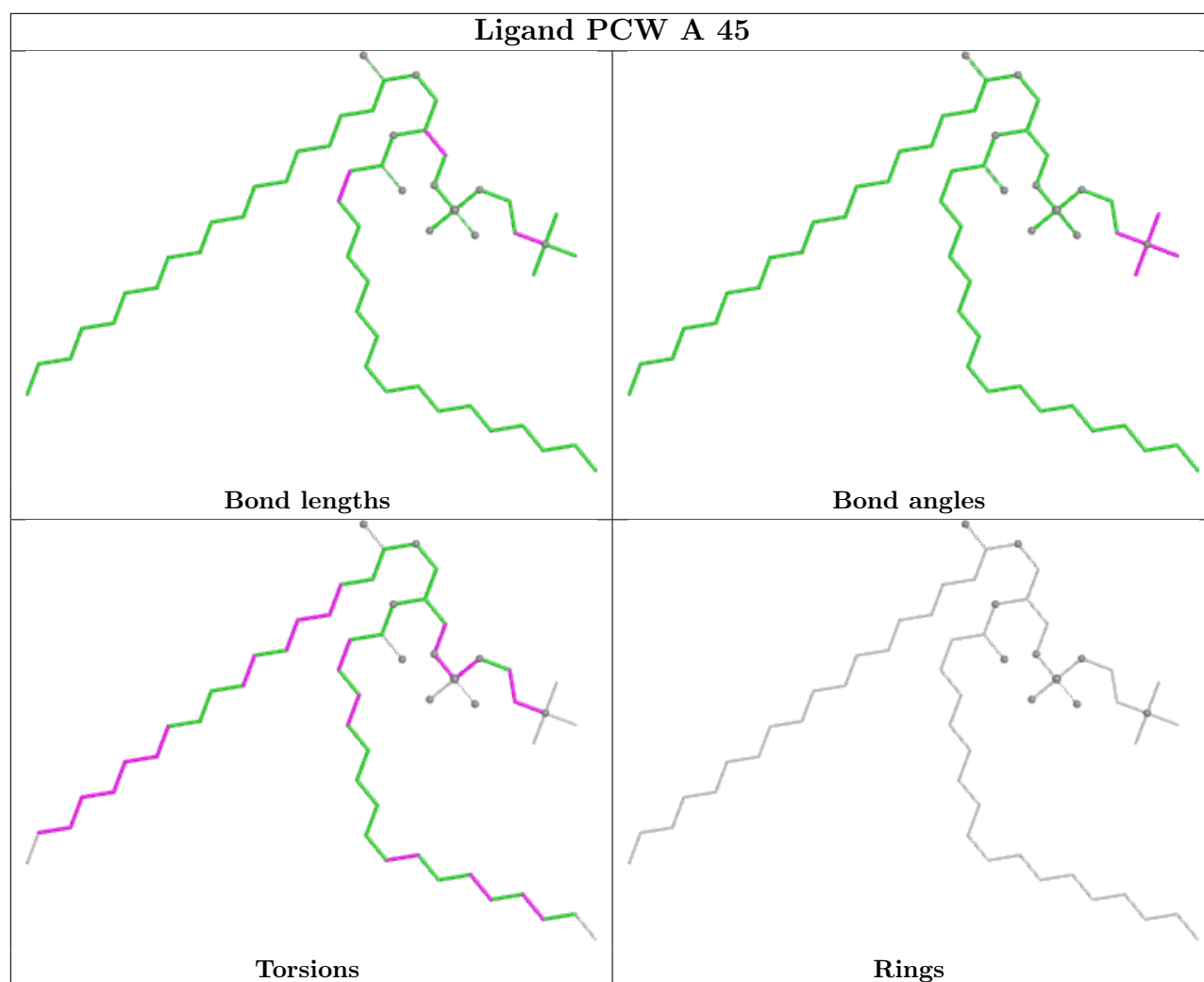


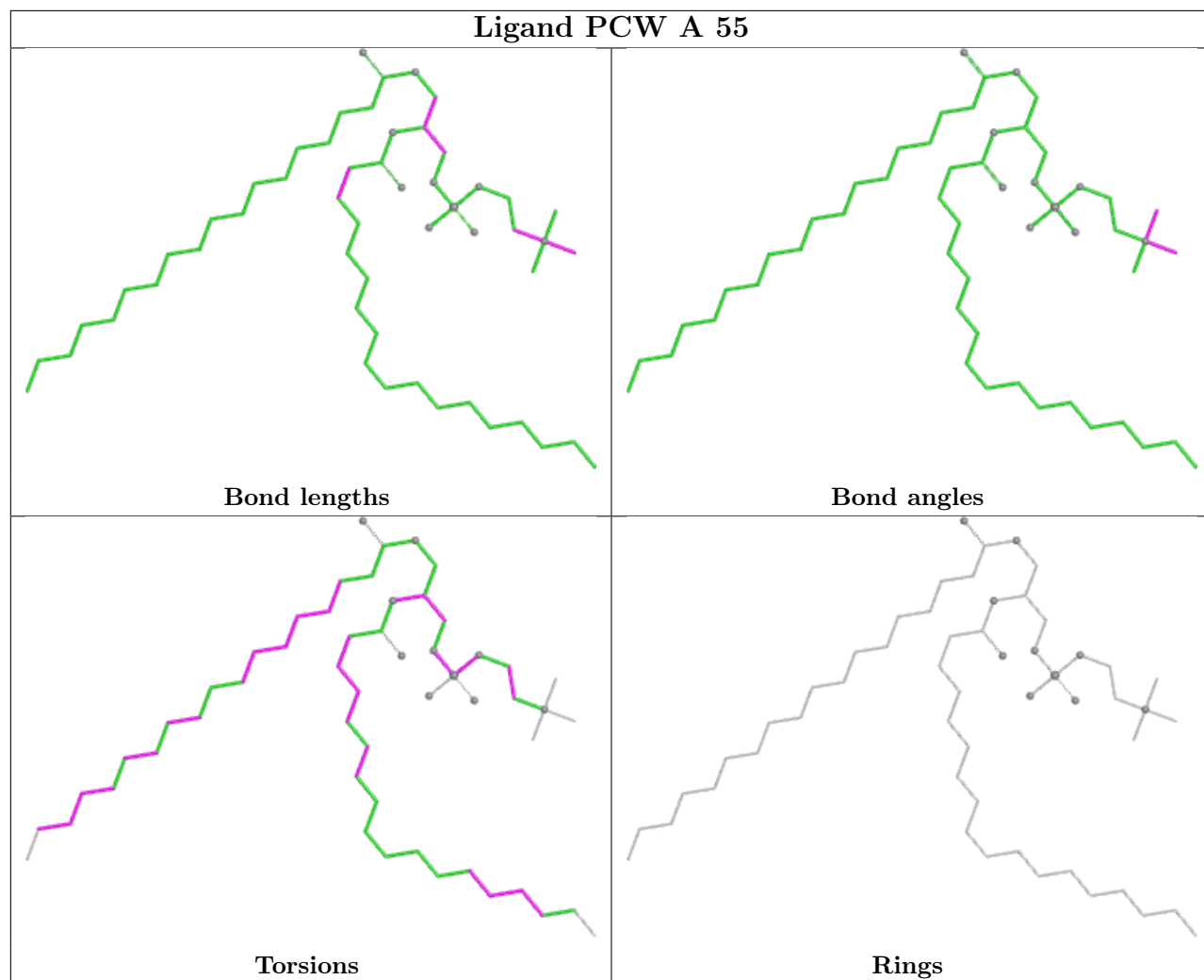


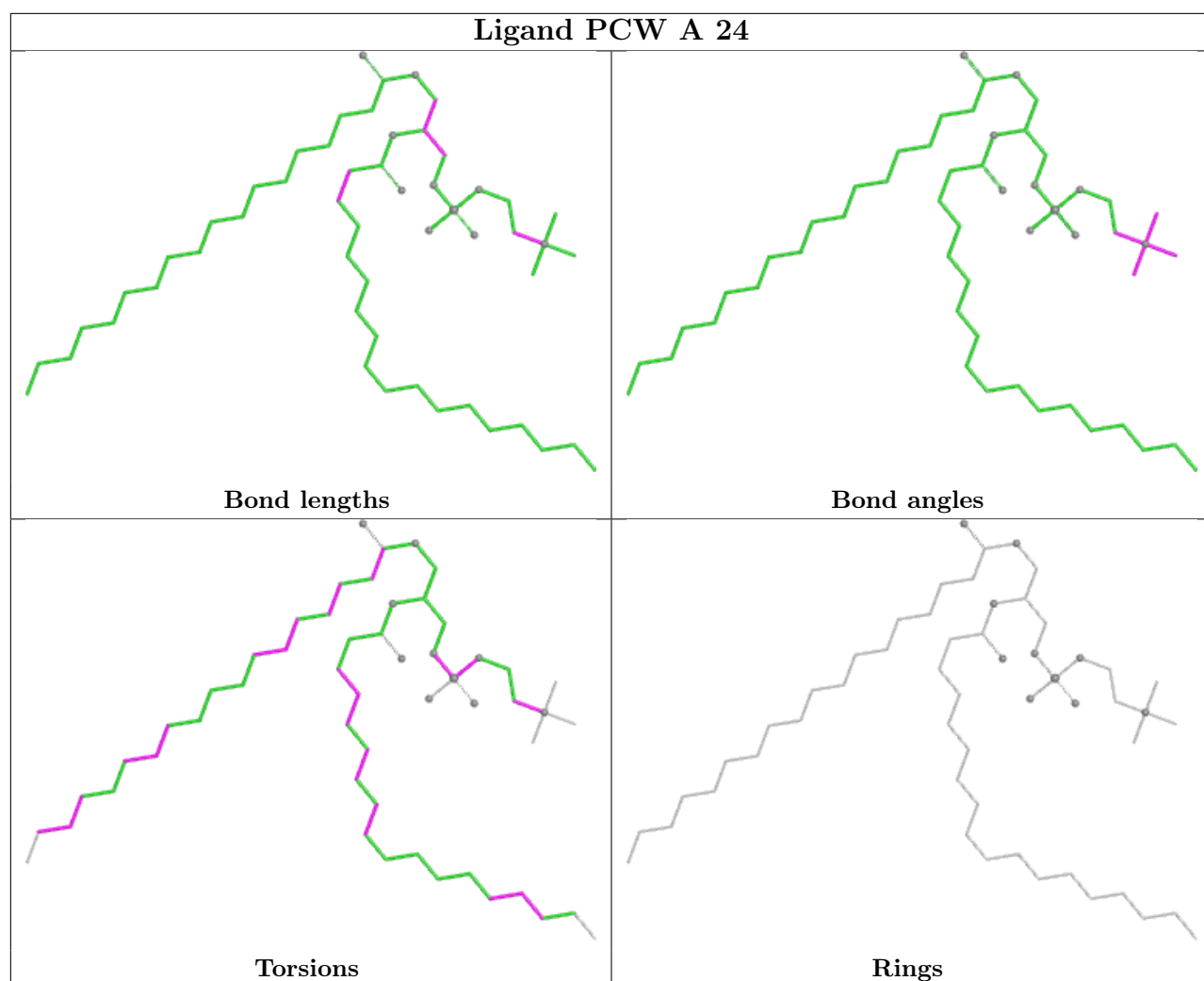


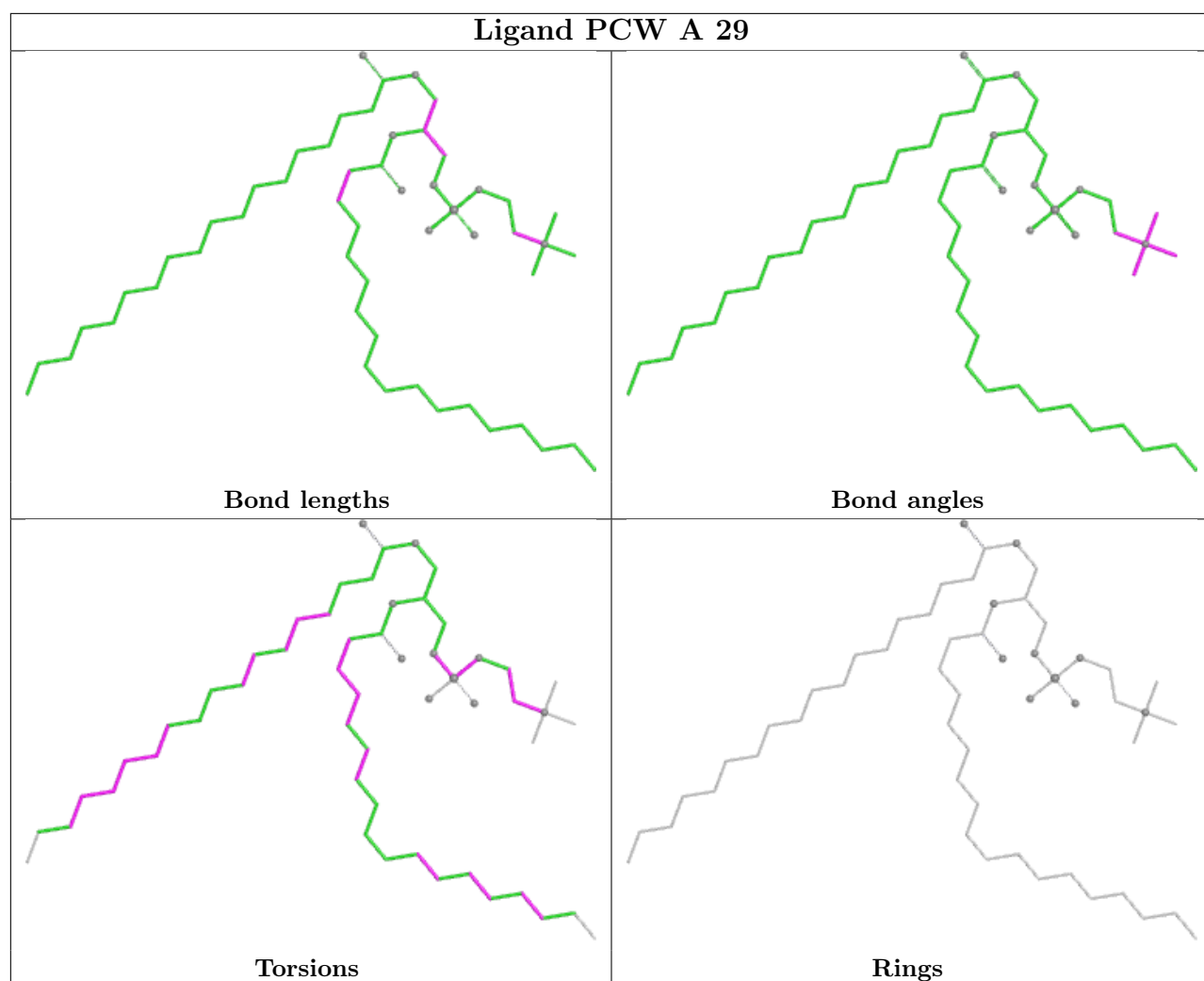


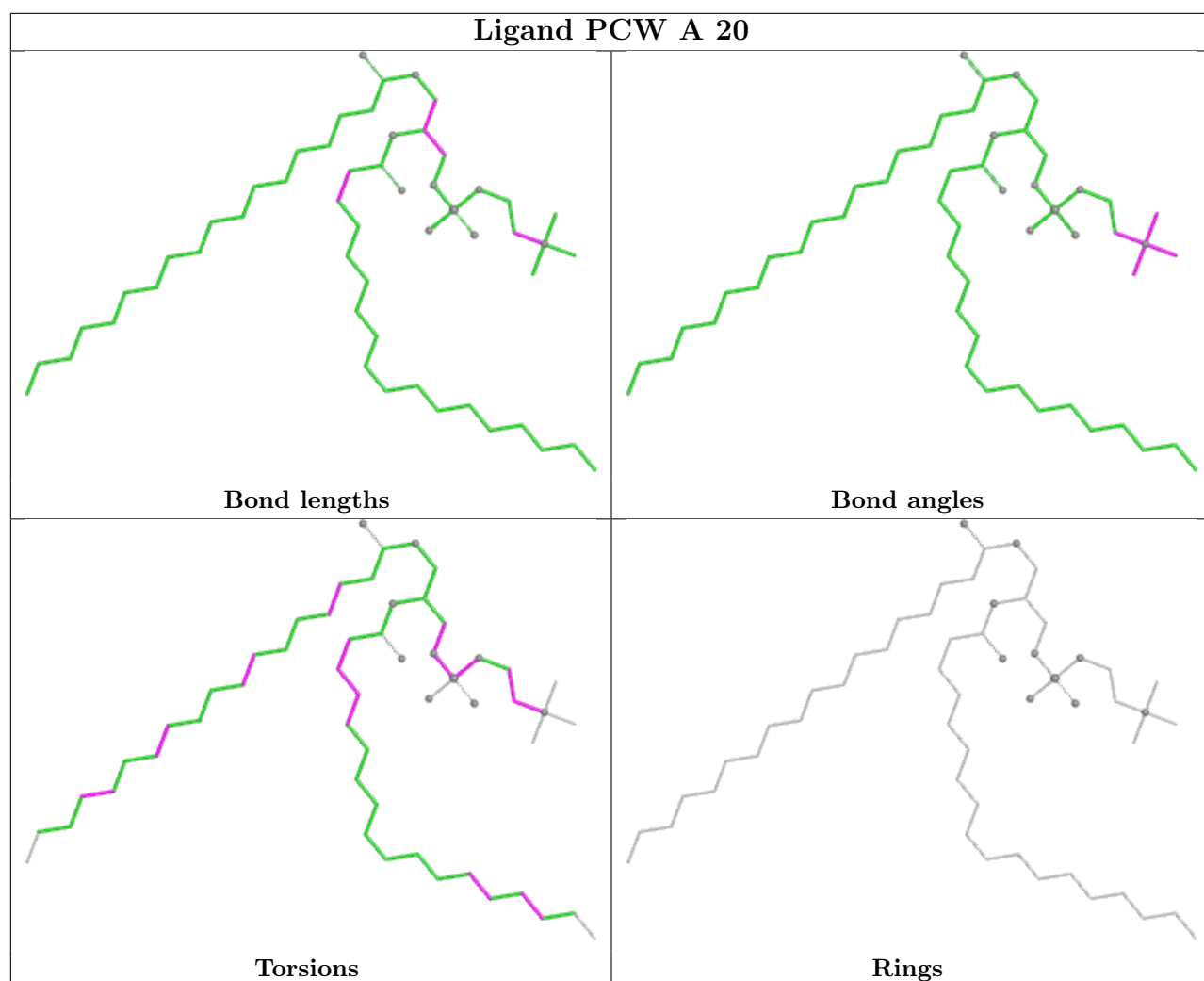


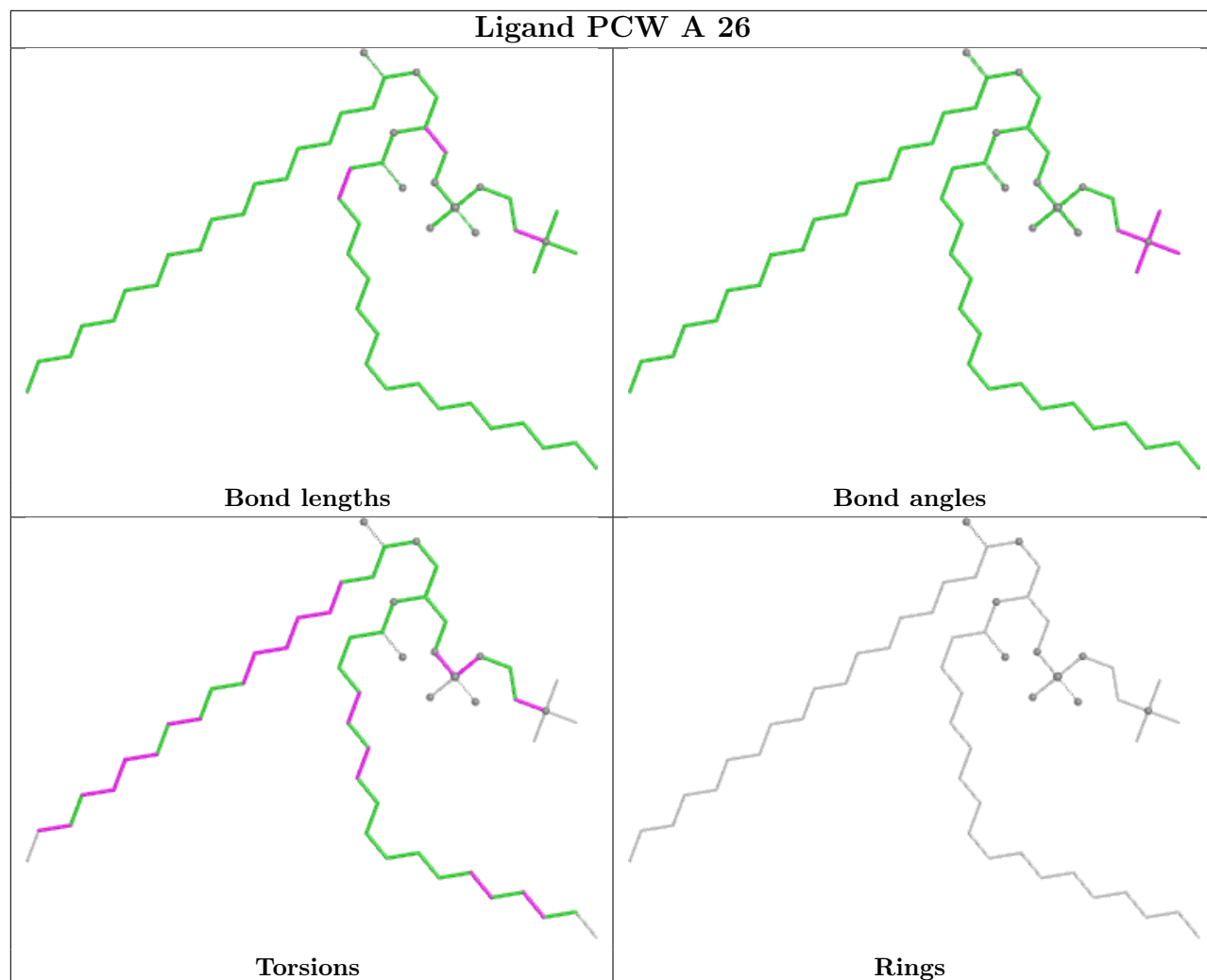


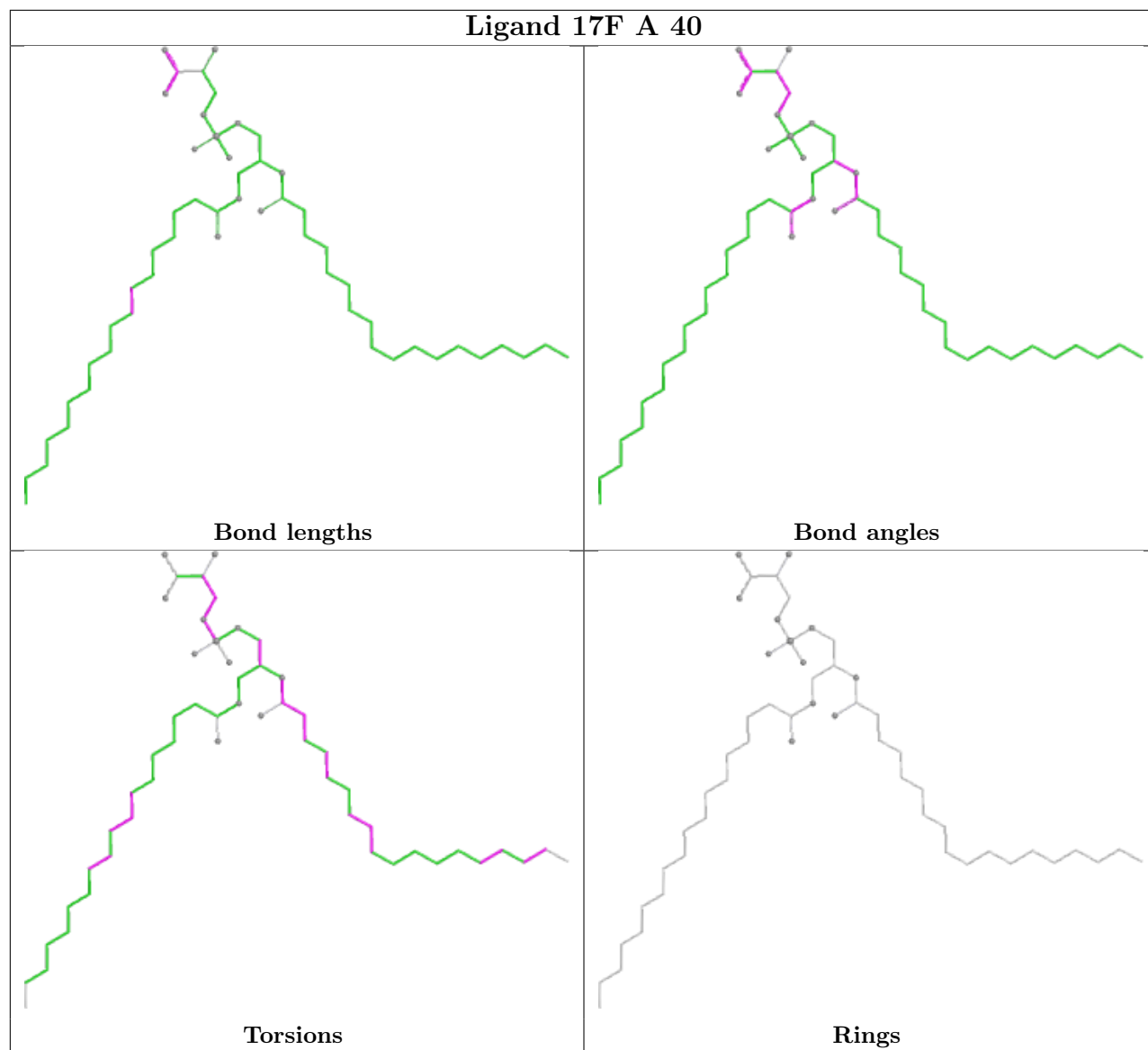


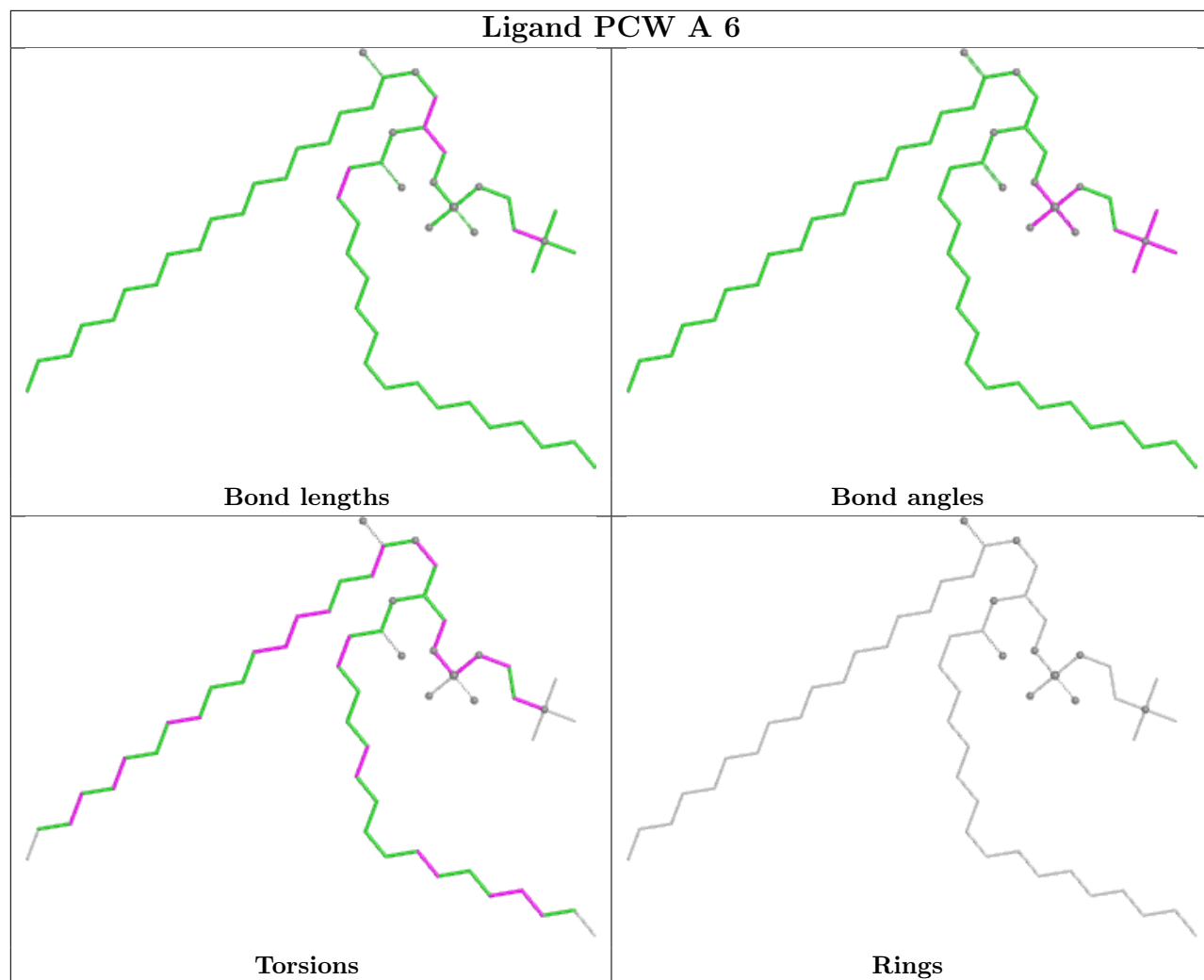


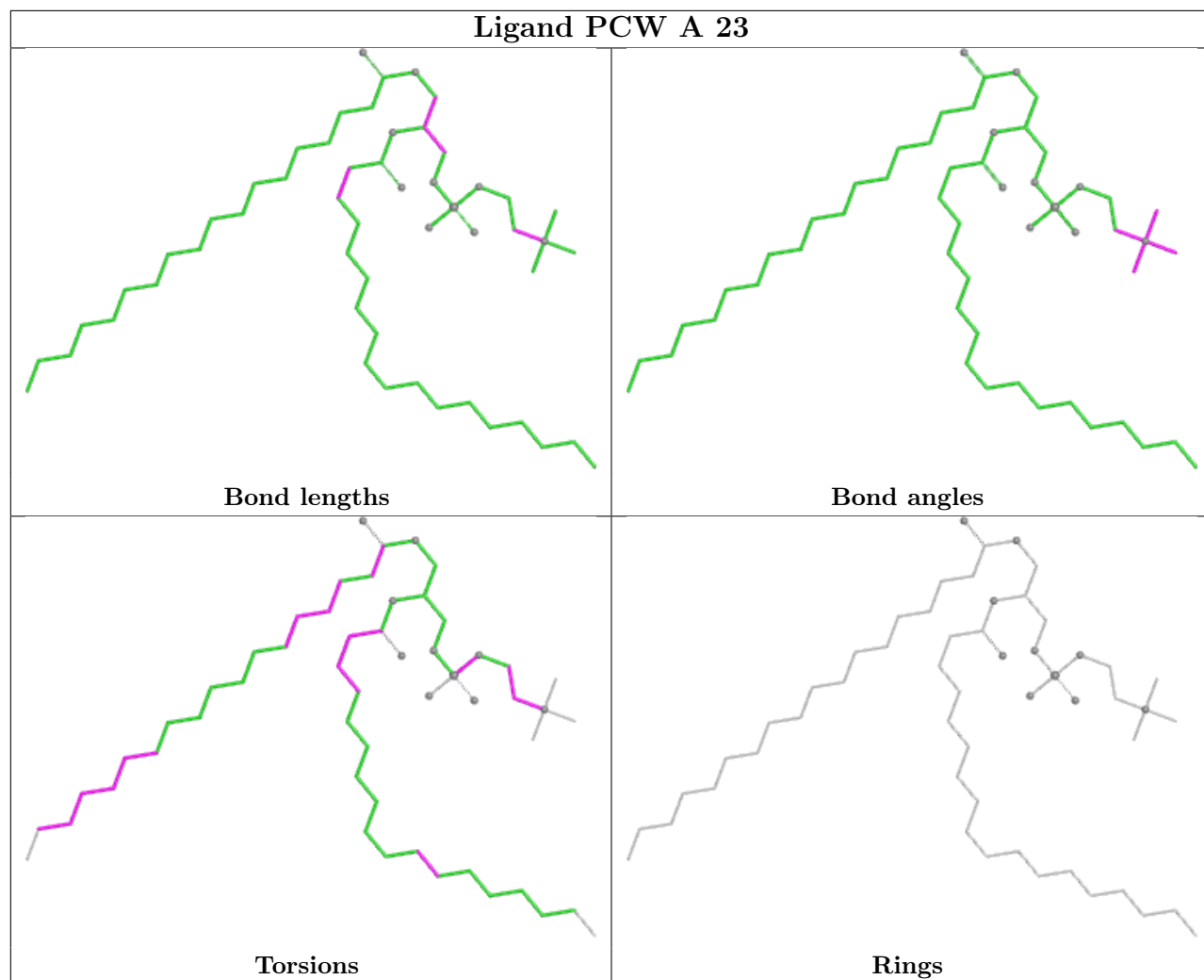


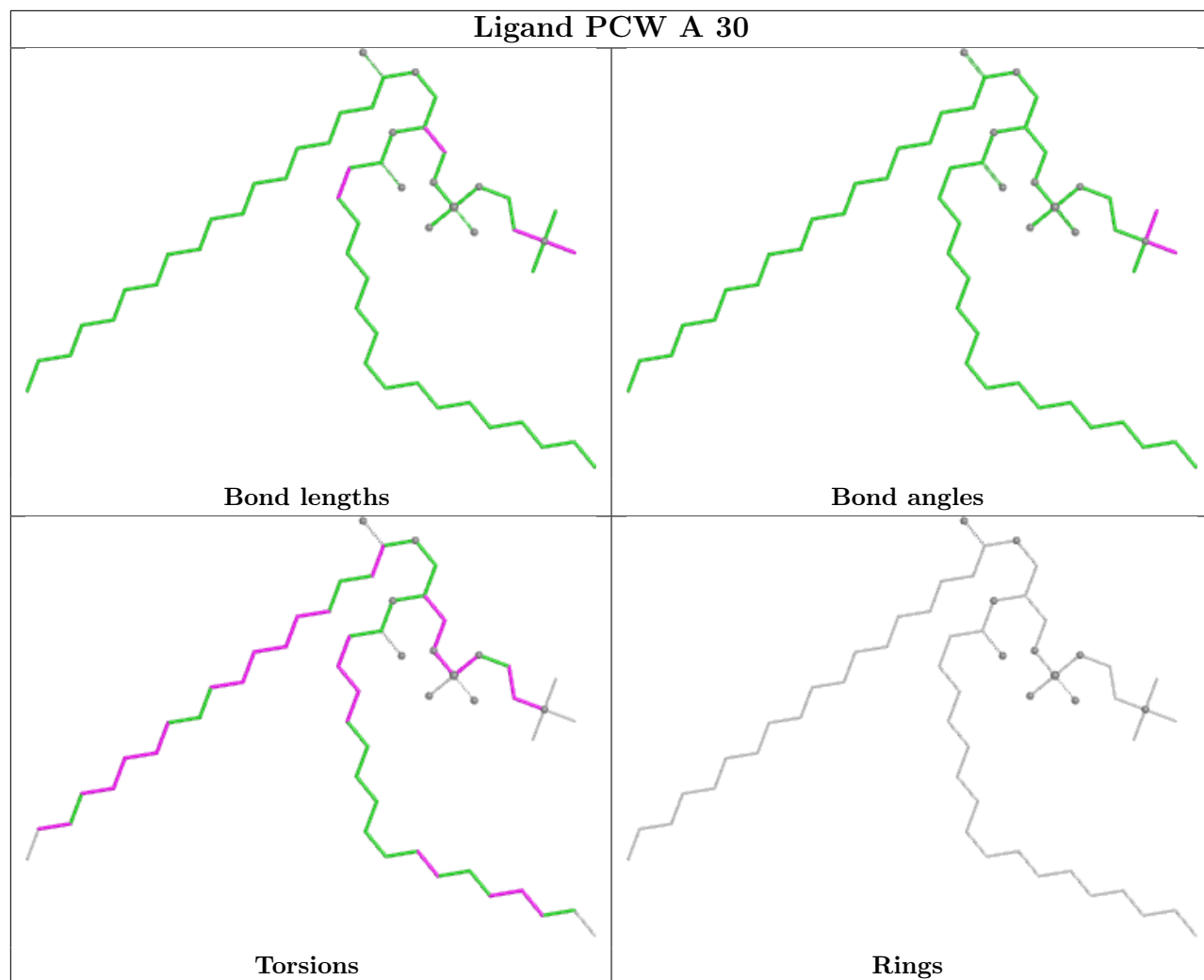


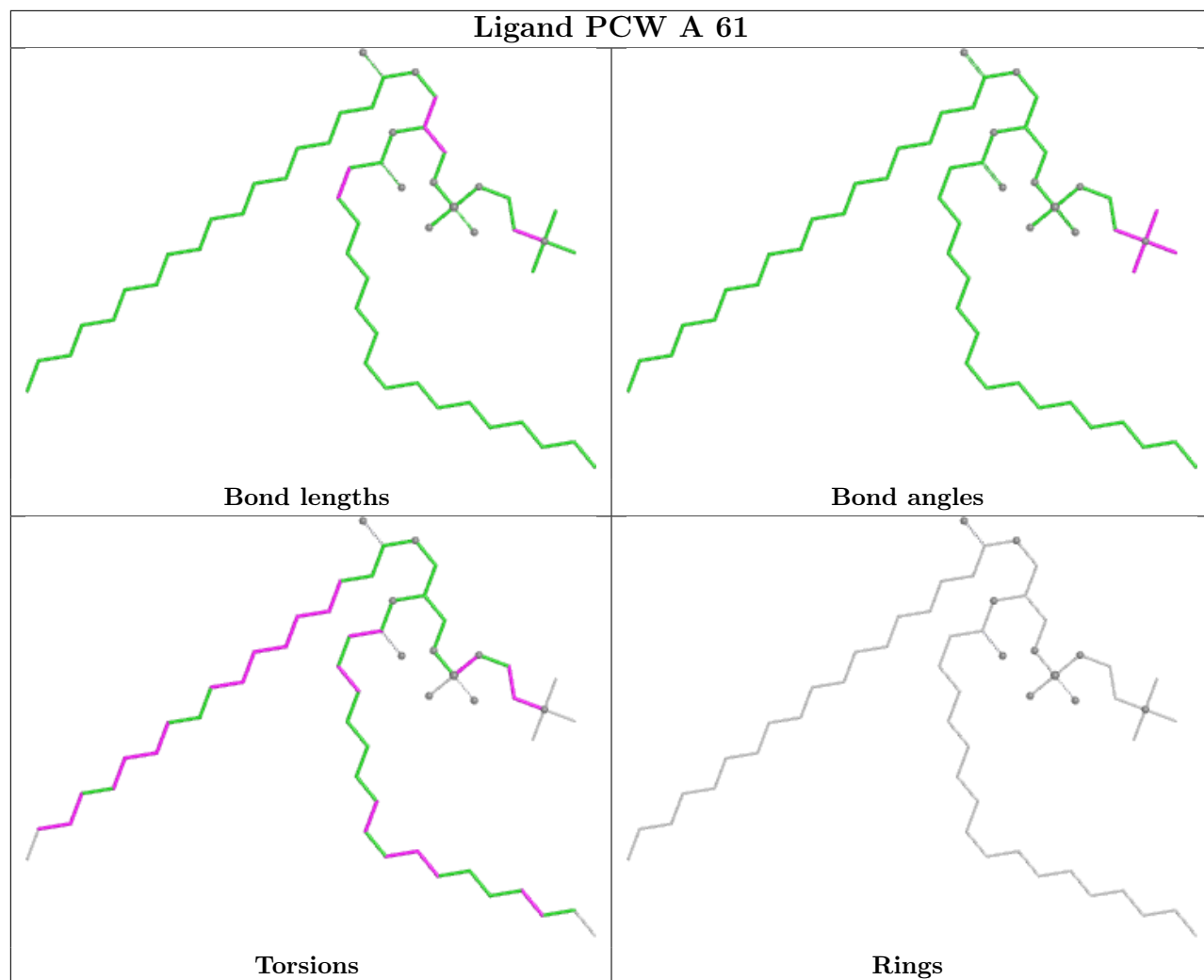


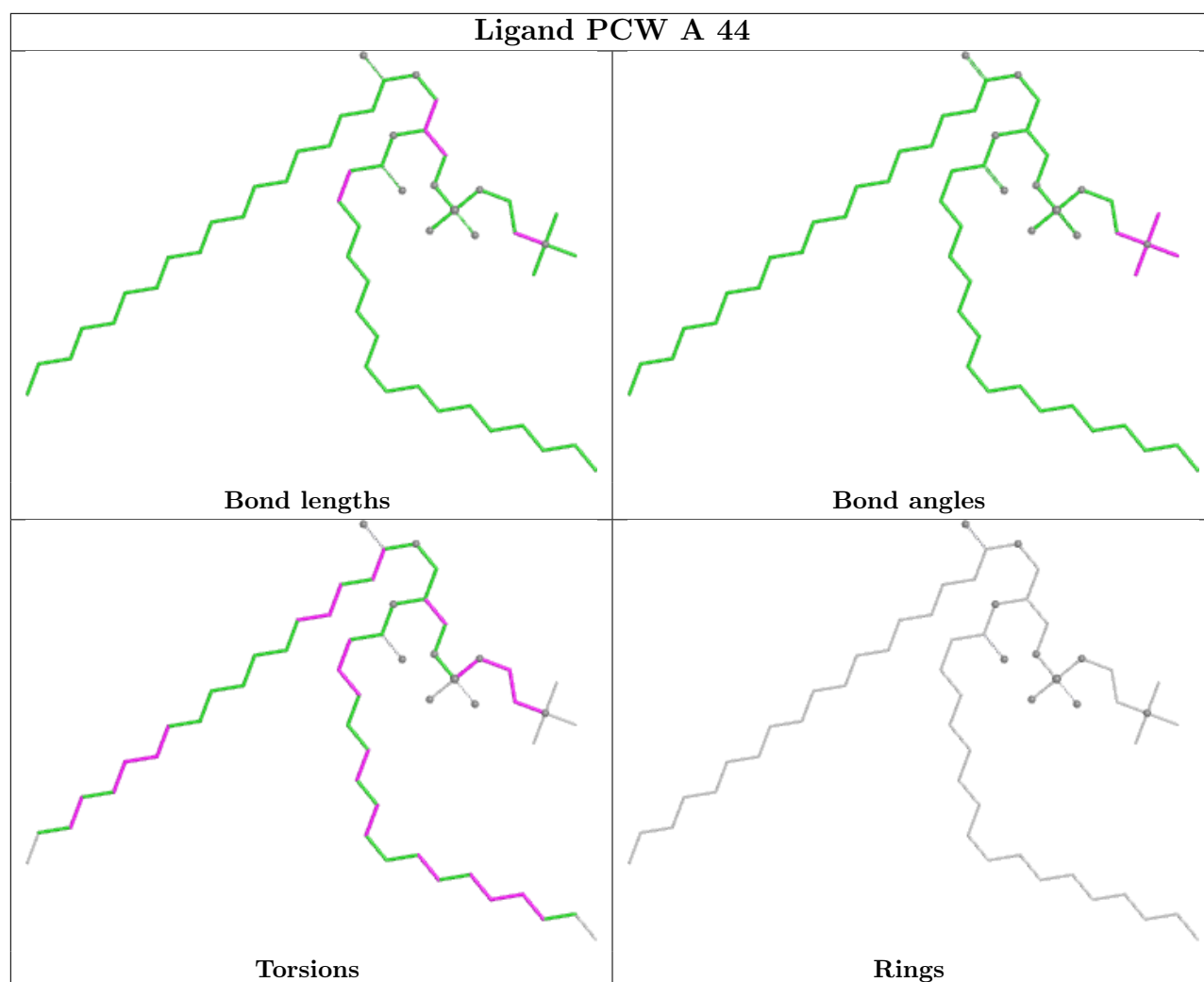


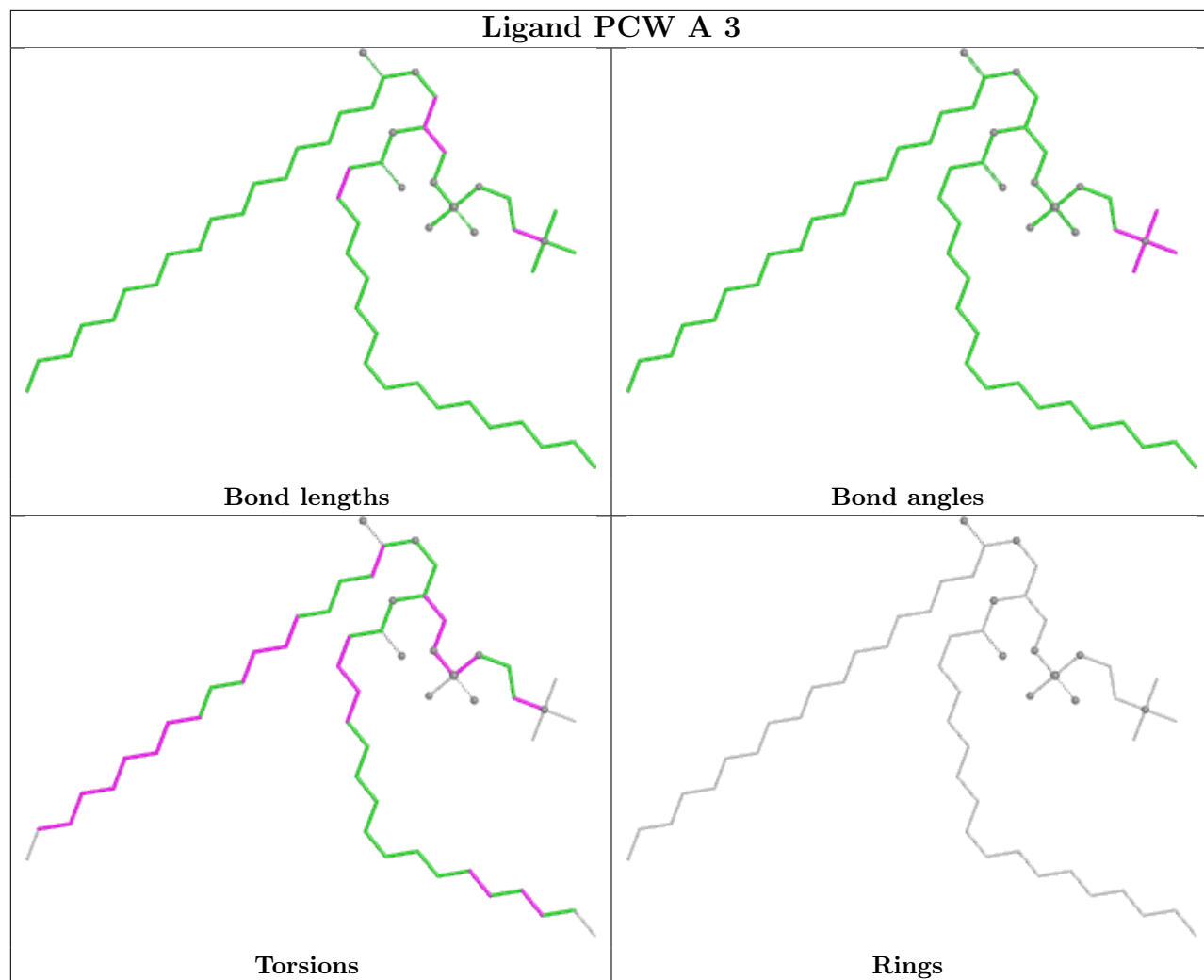




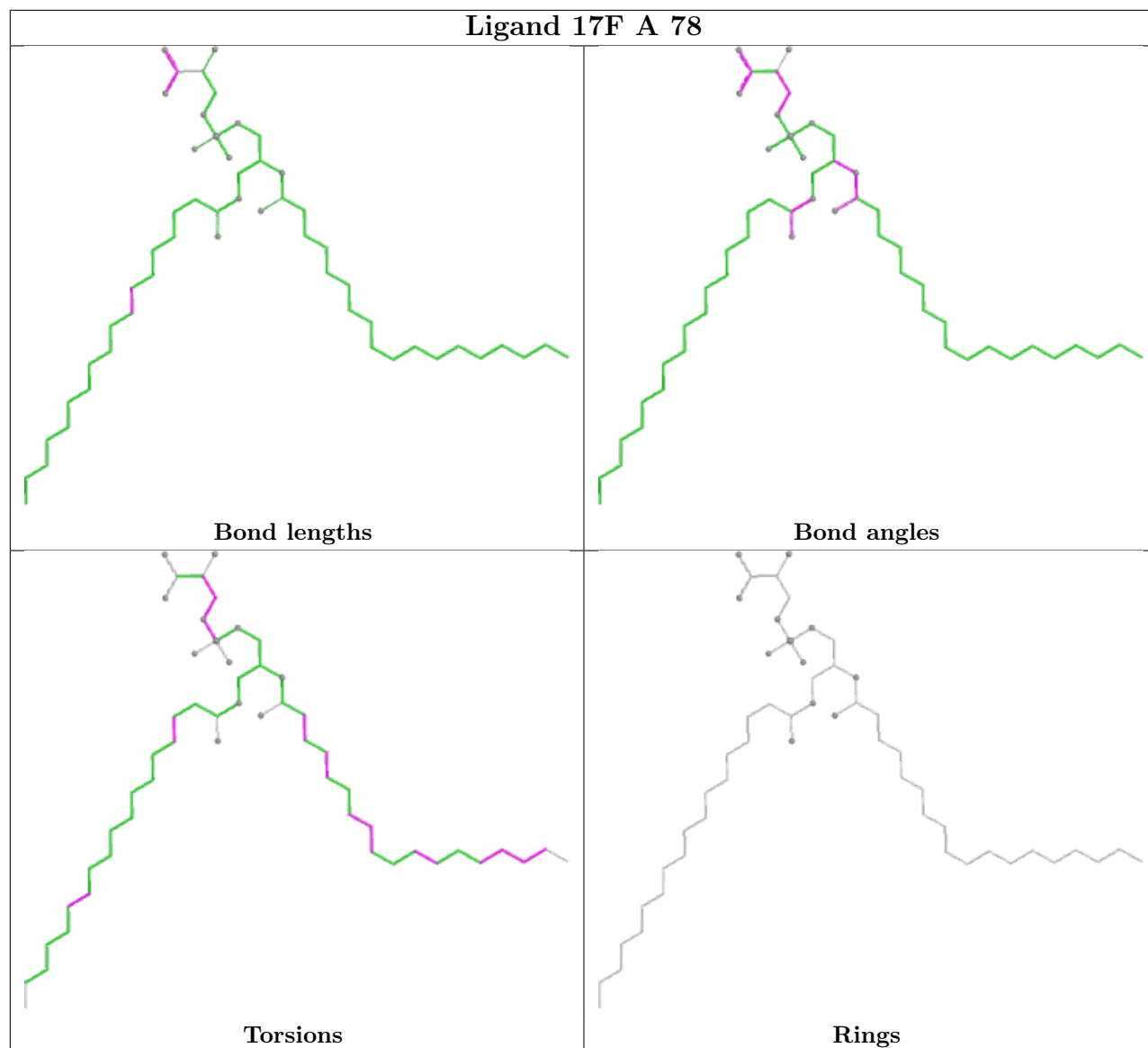


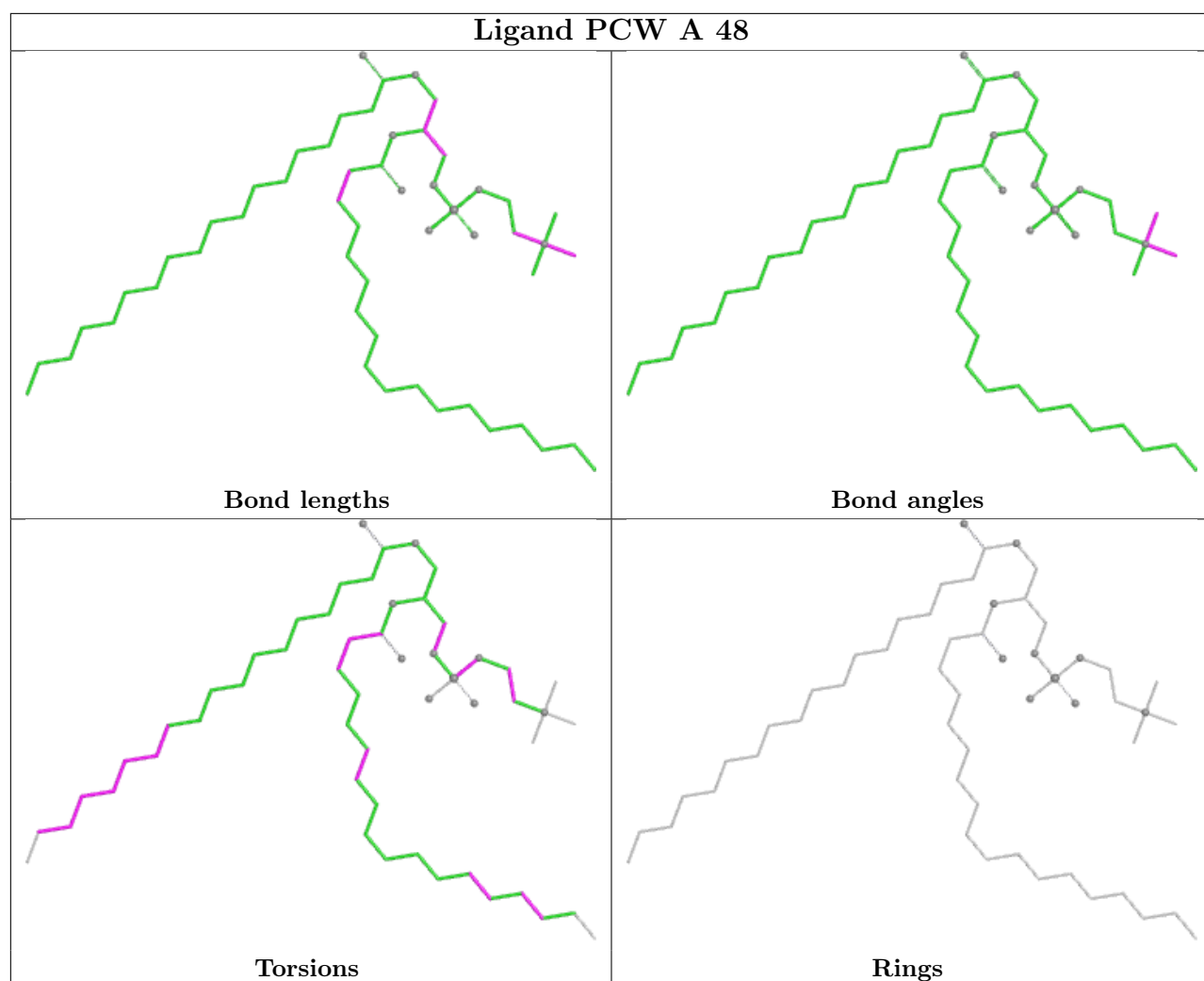


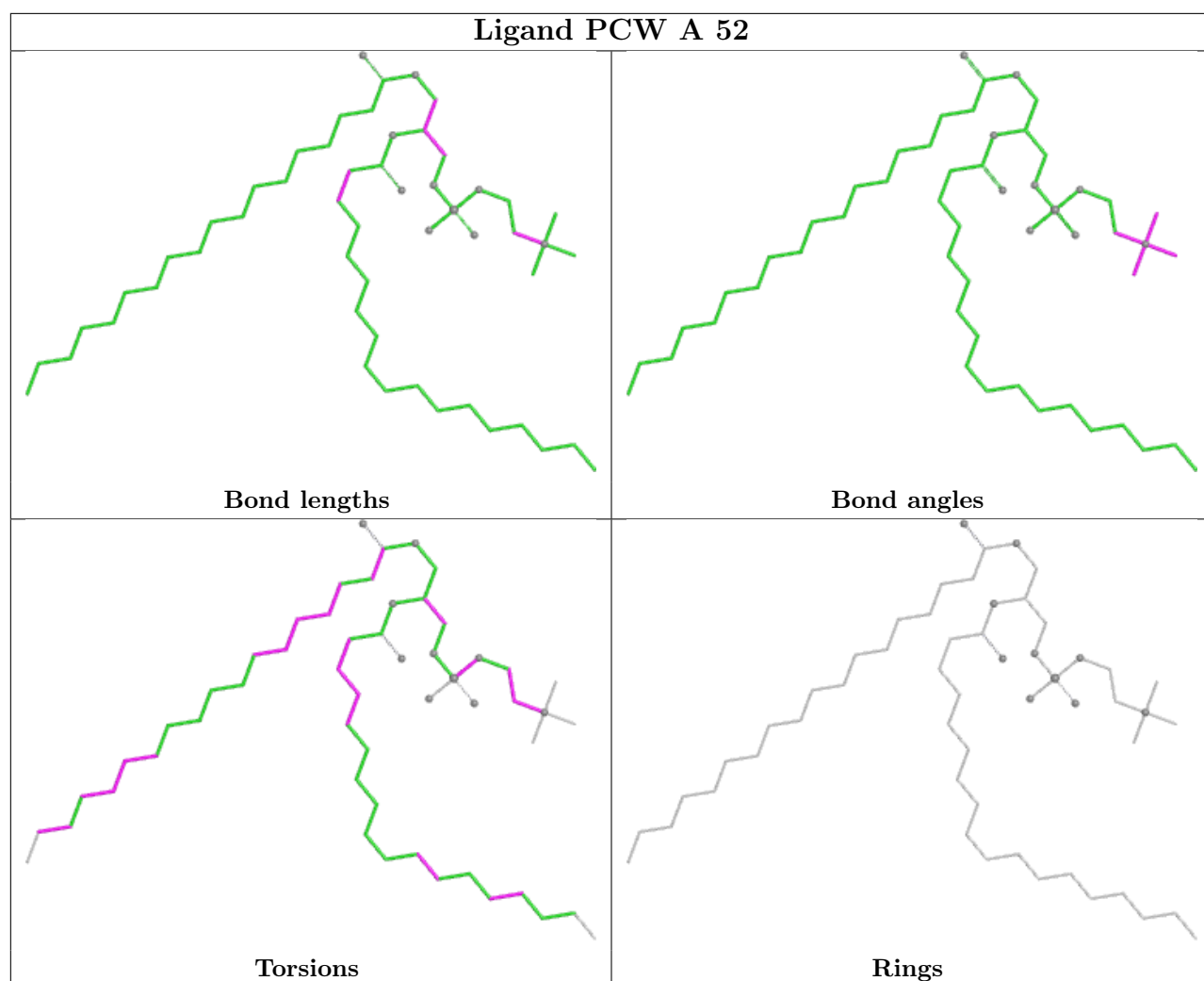


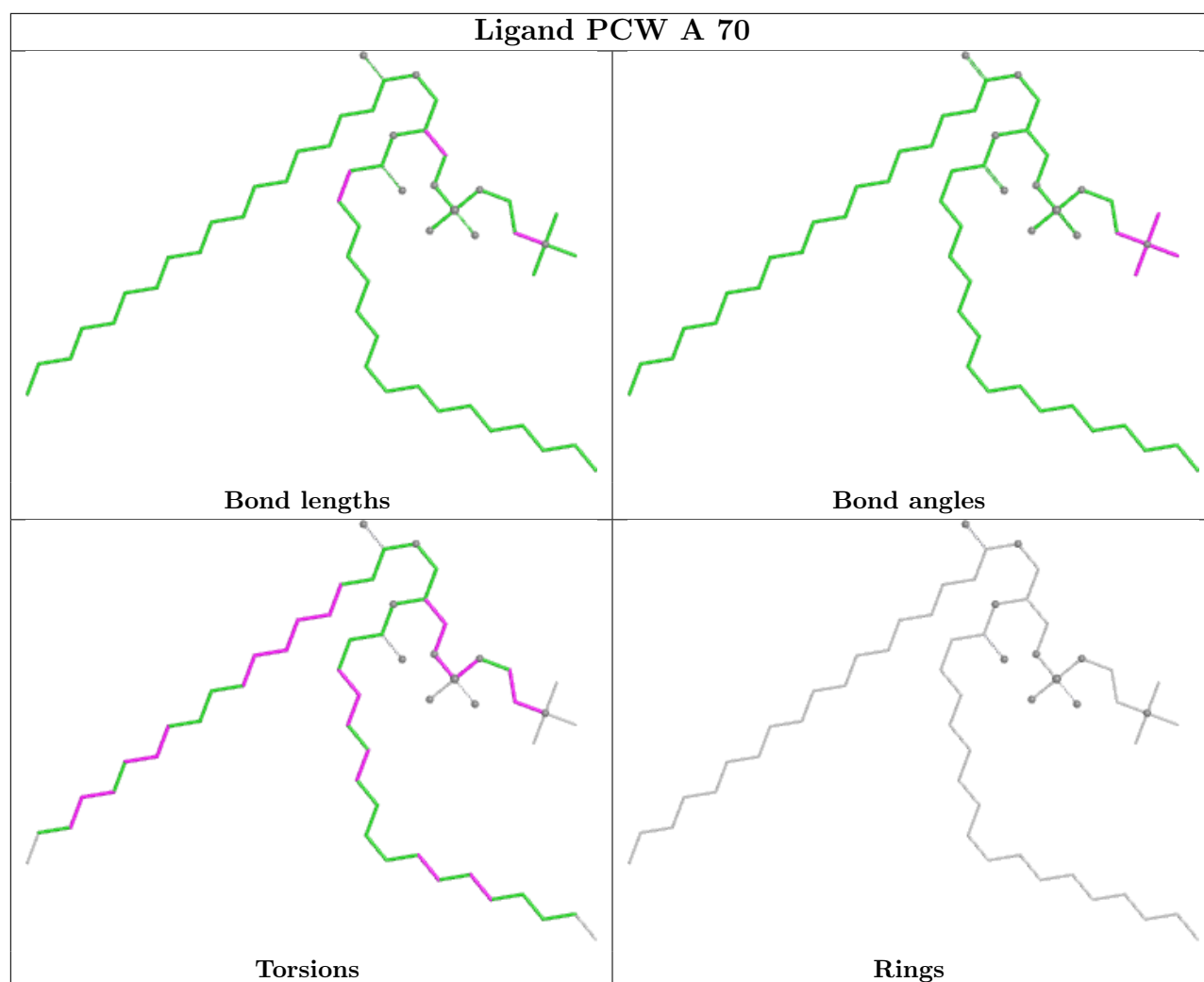


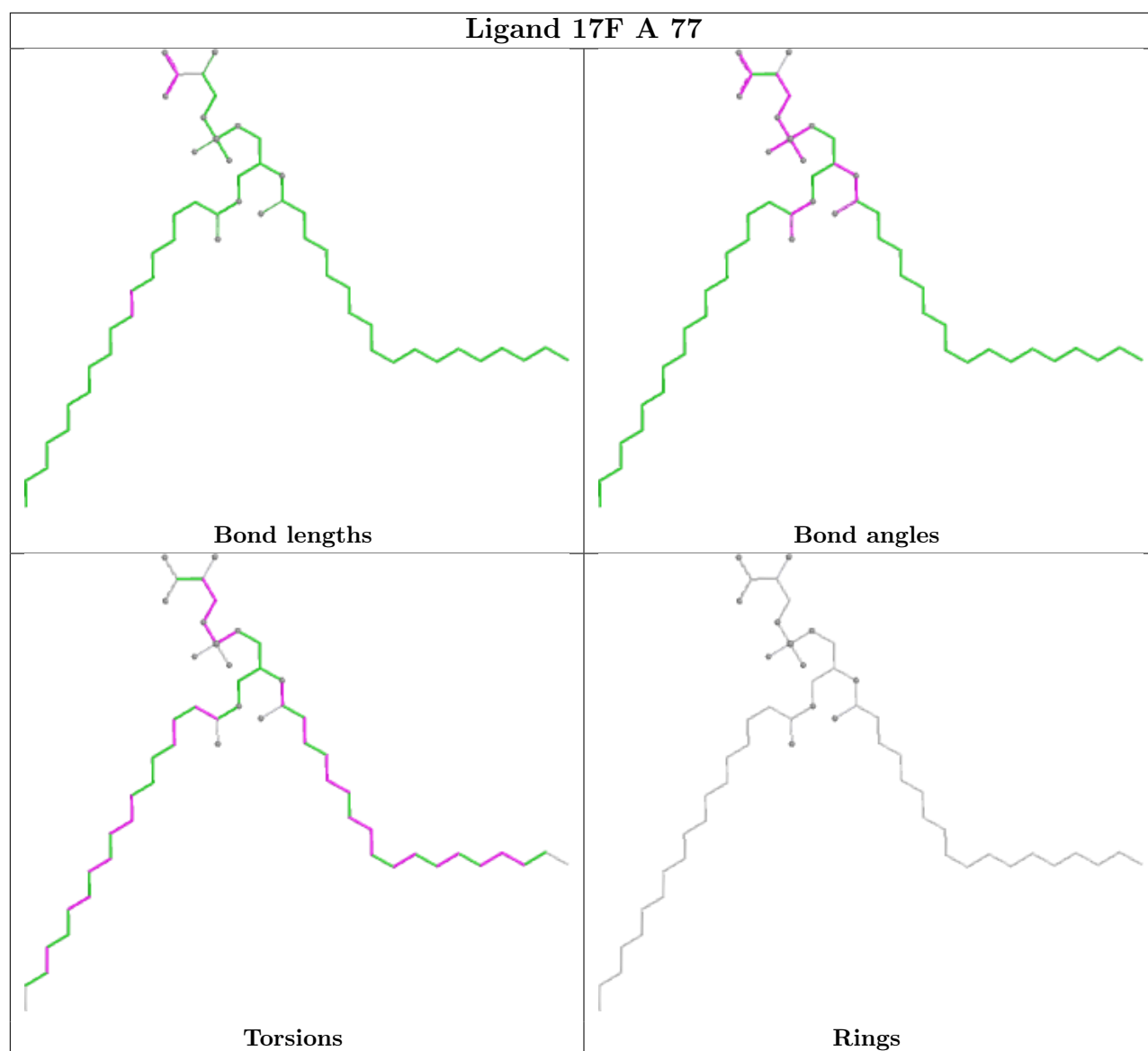
Ligand 17F A 78

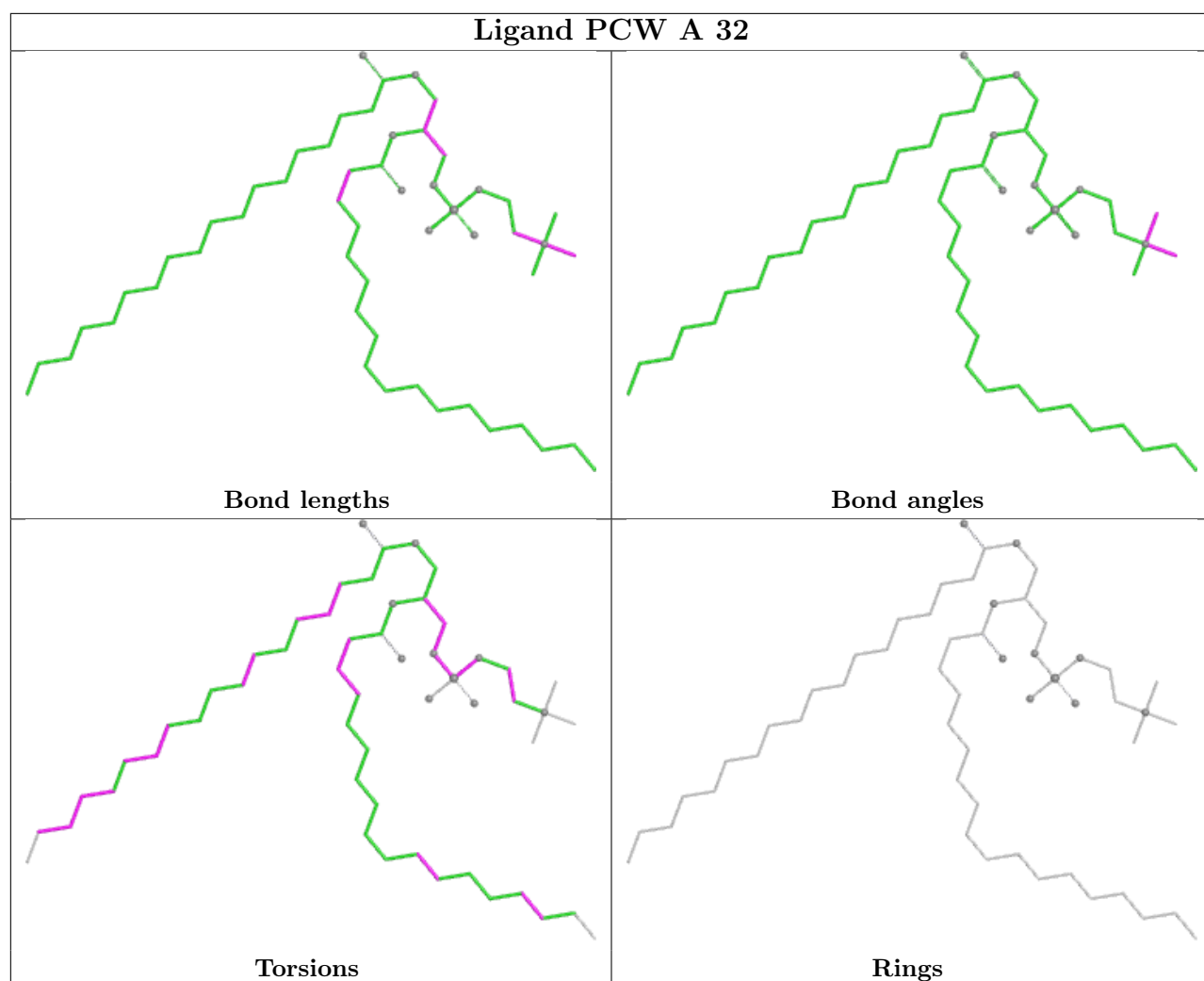


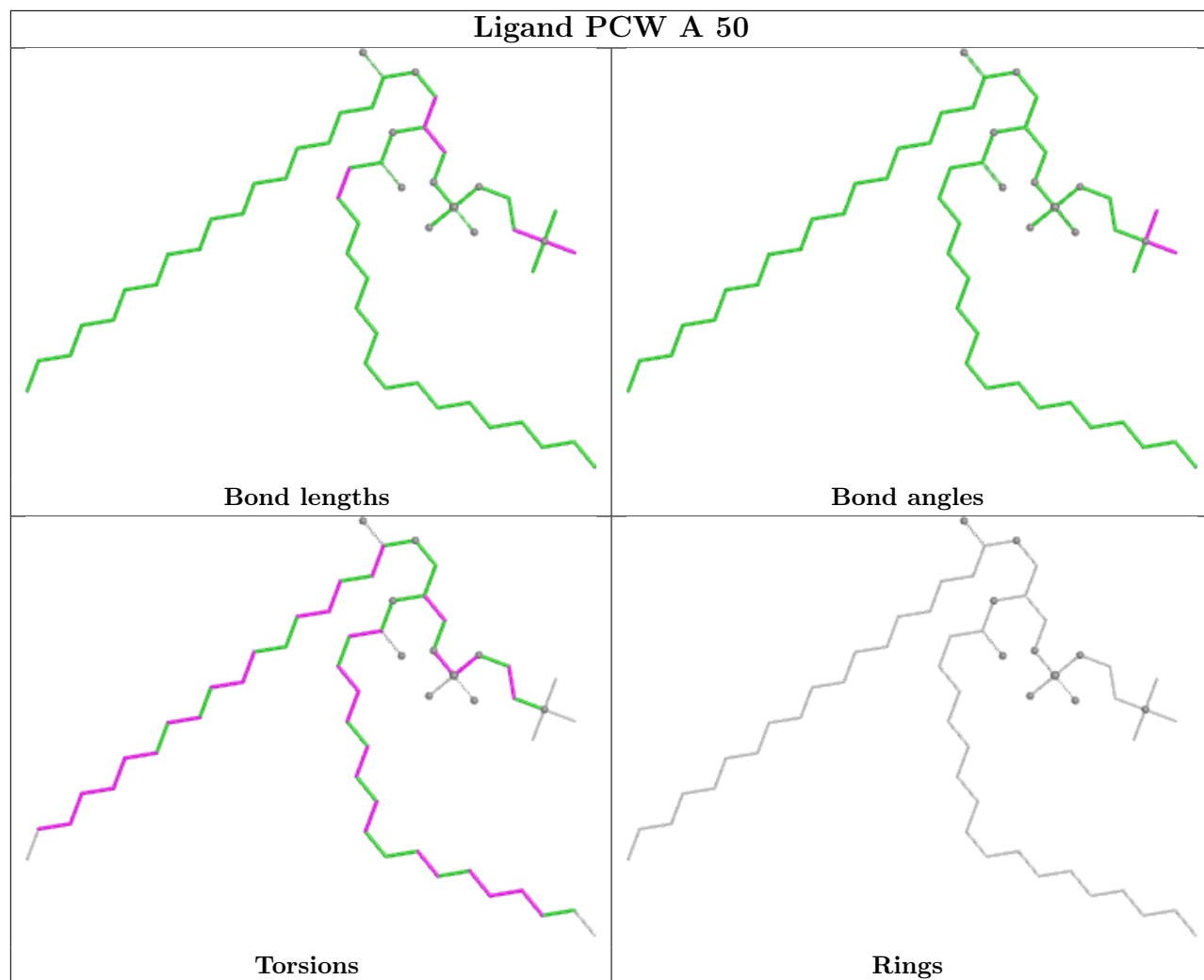


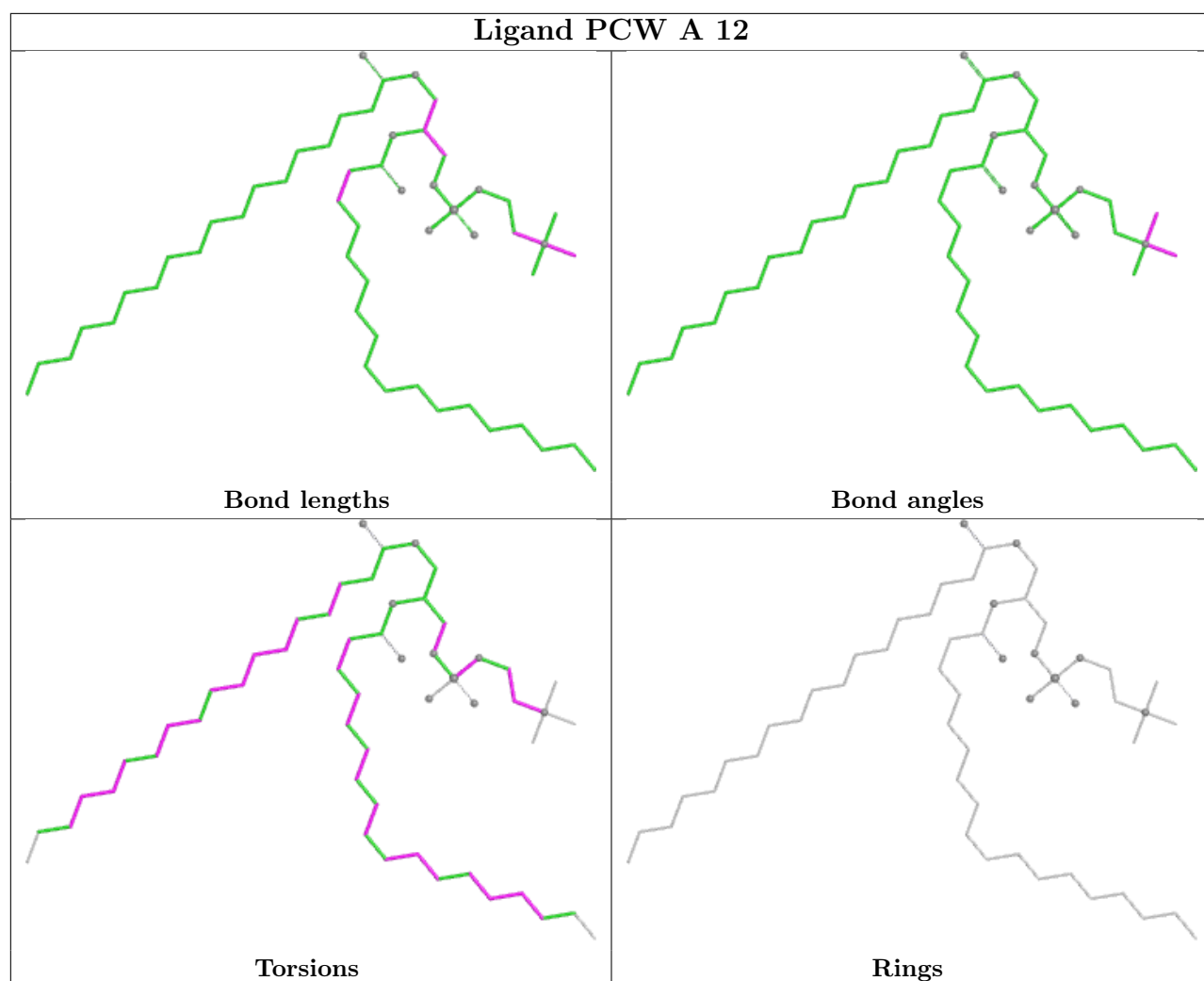


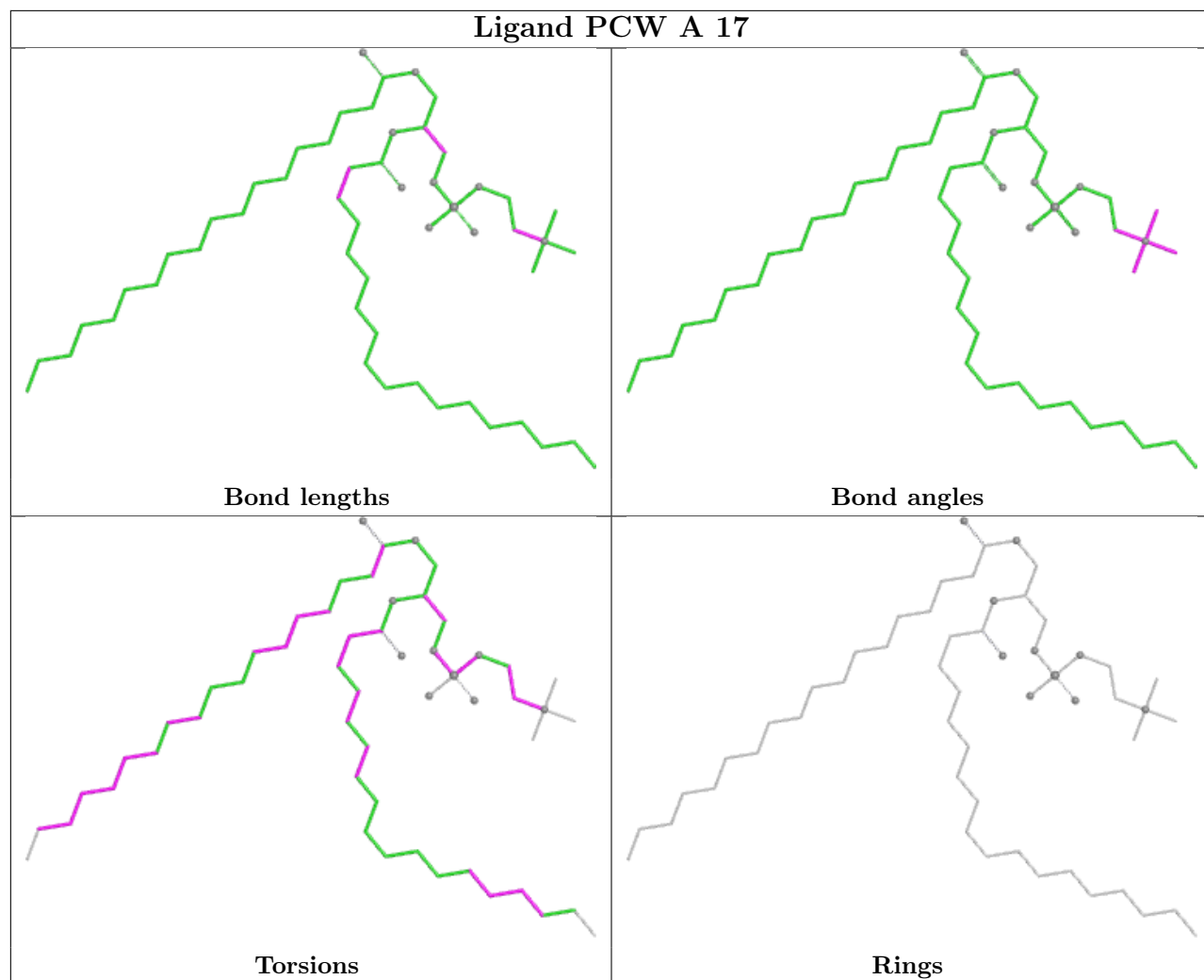


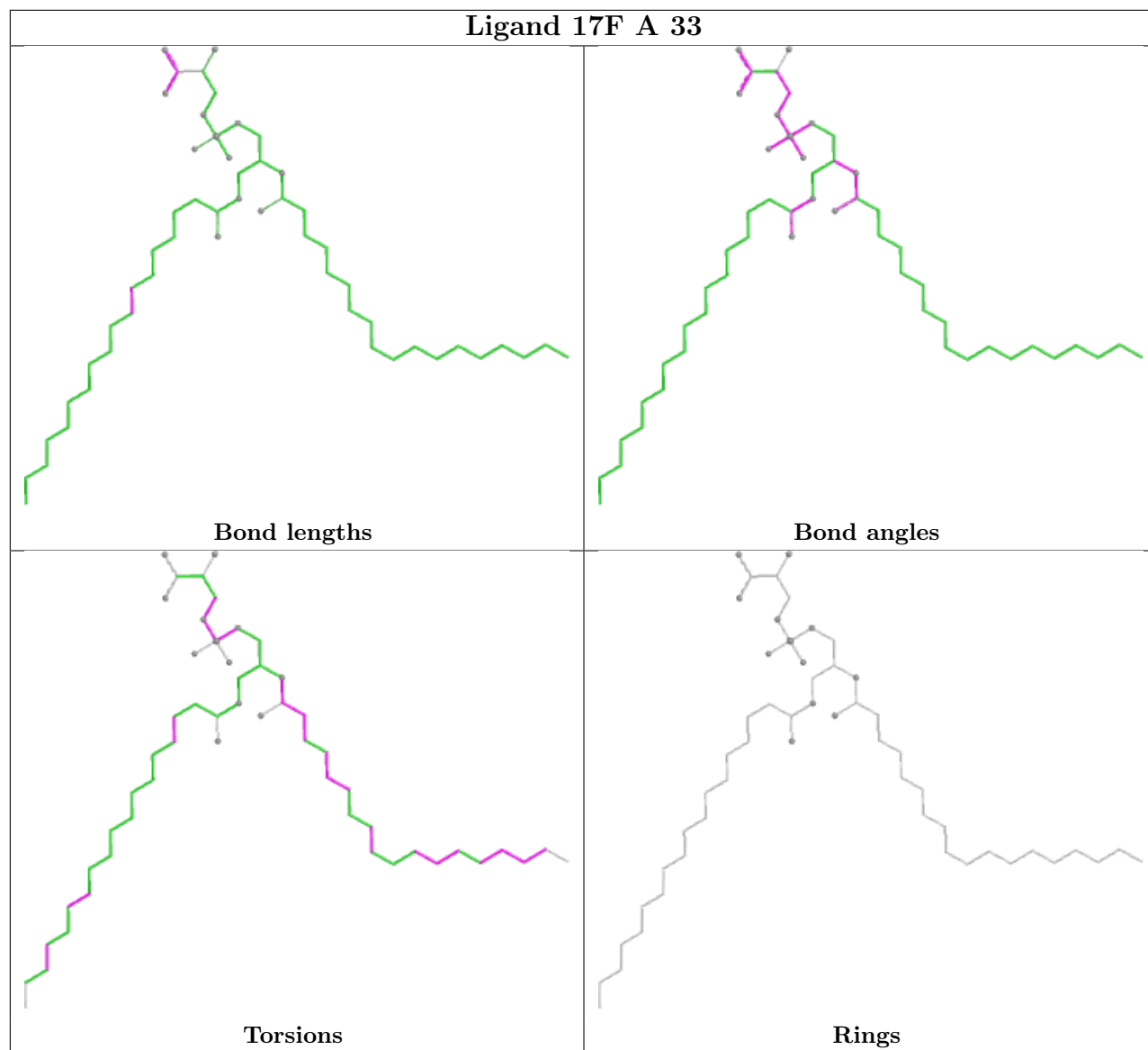


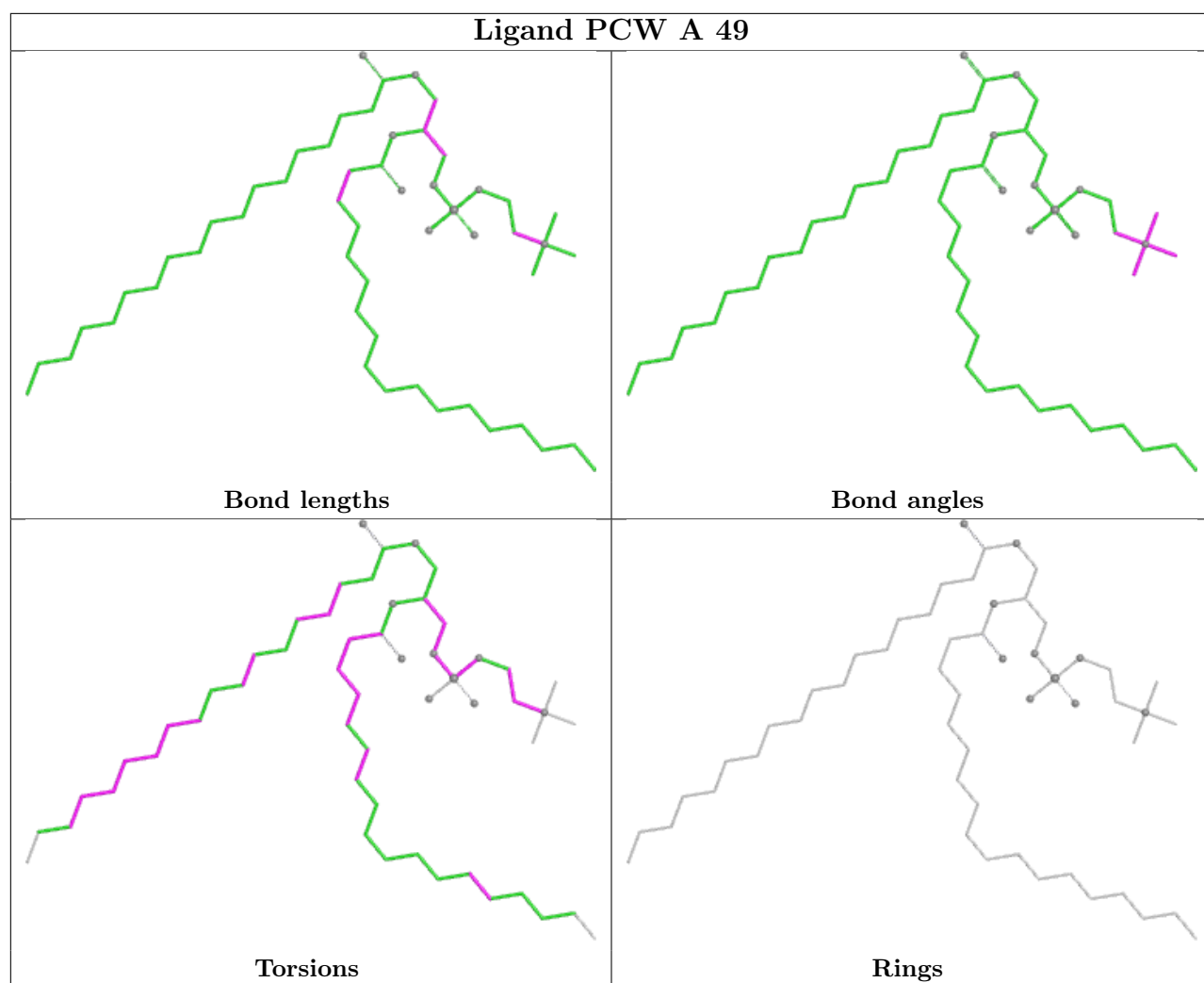


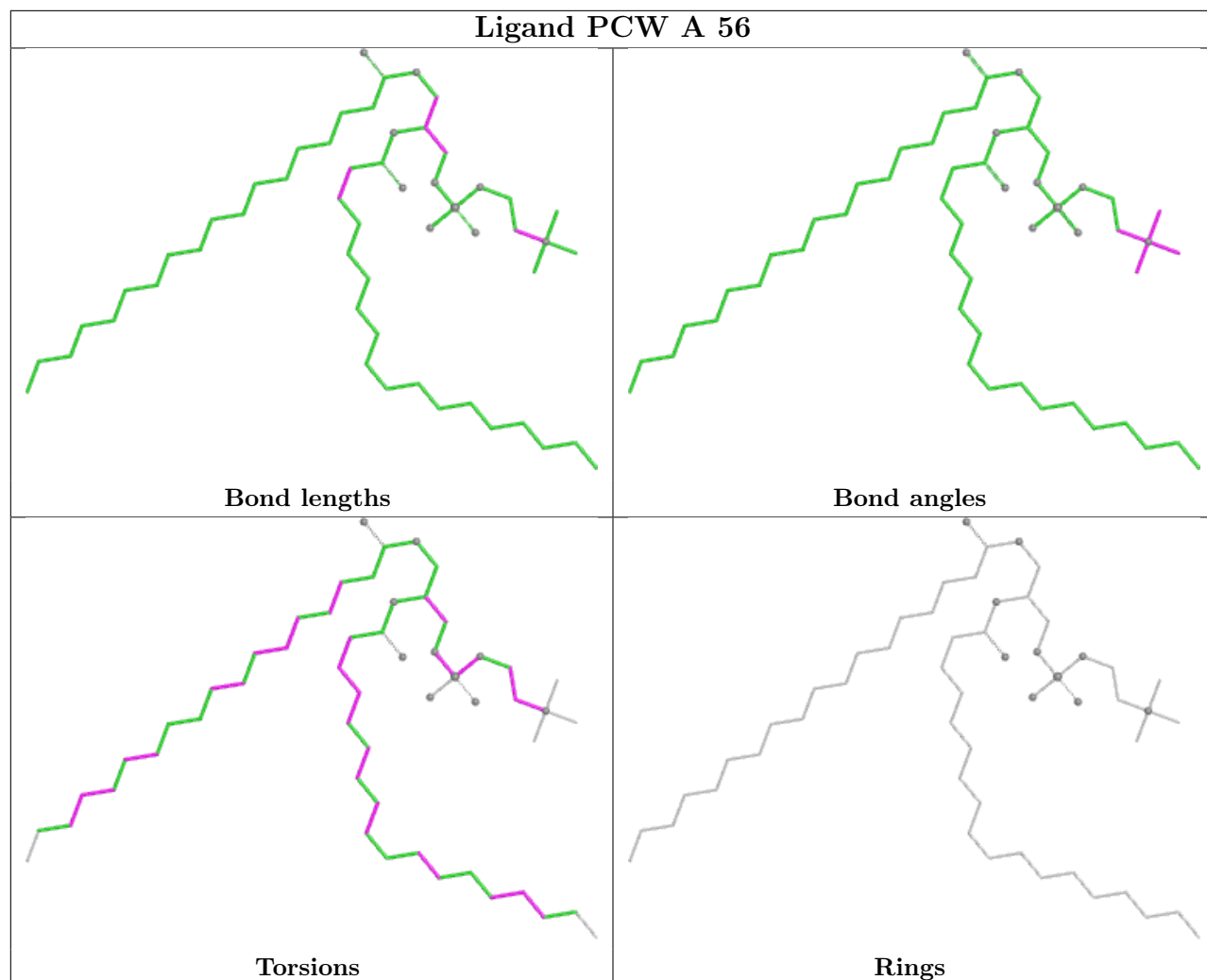


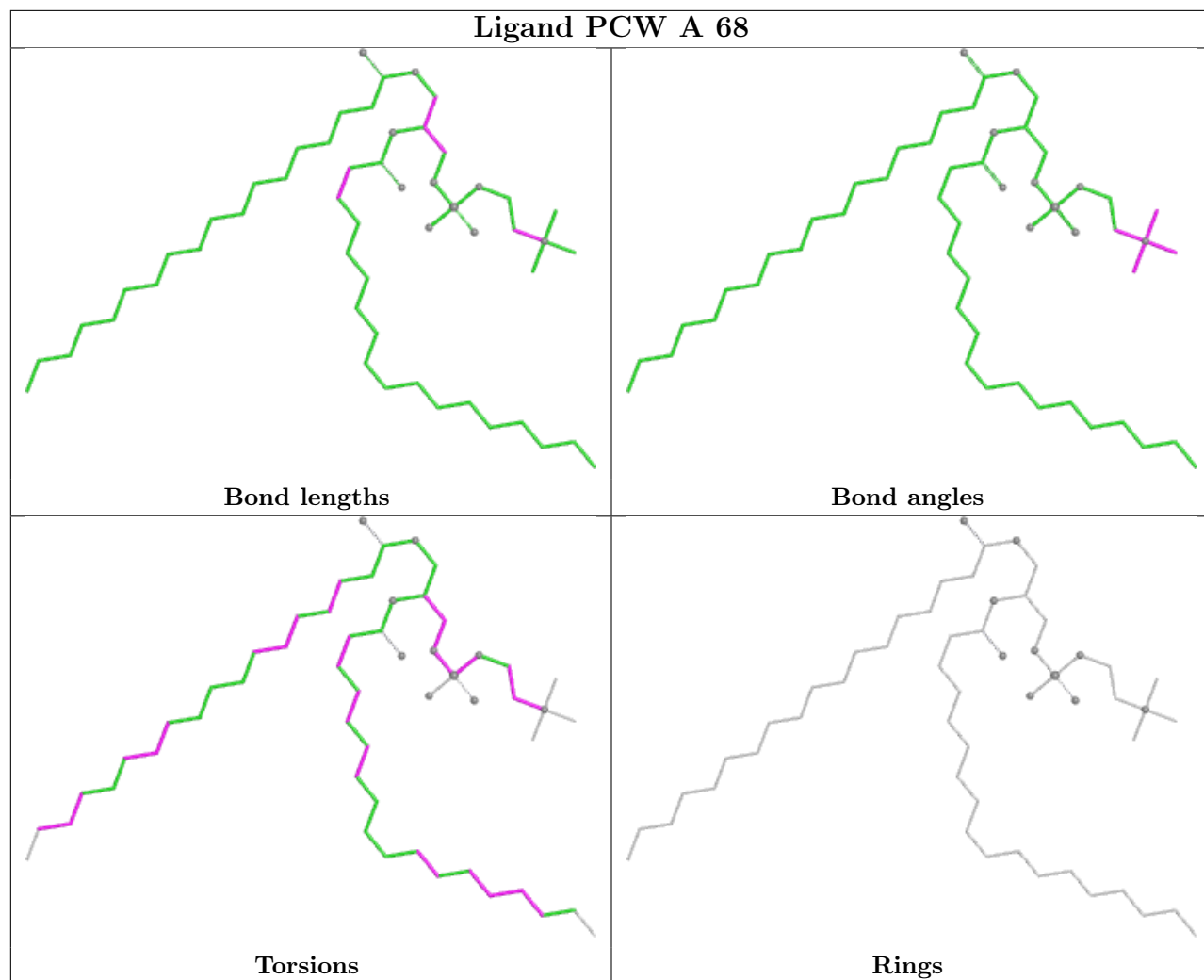


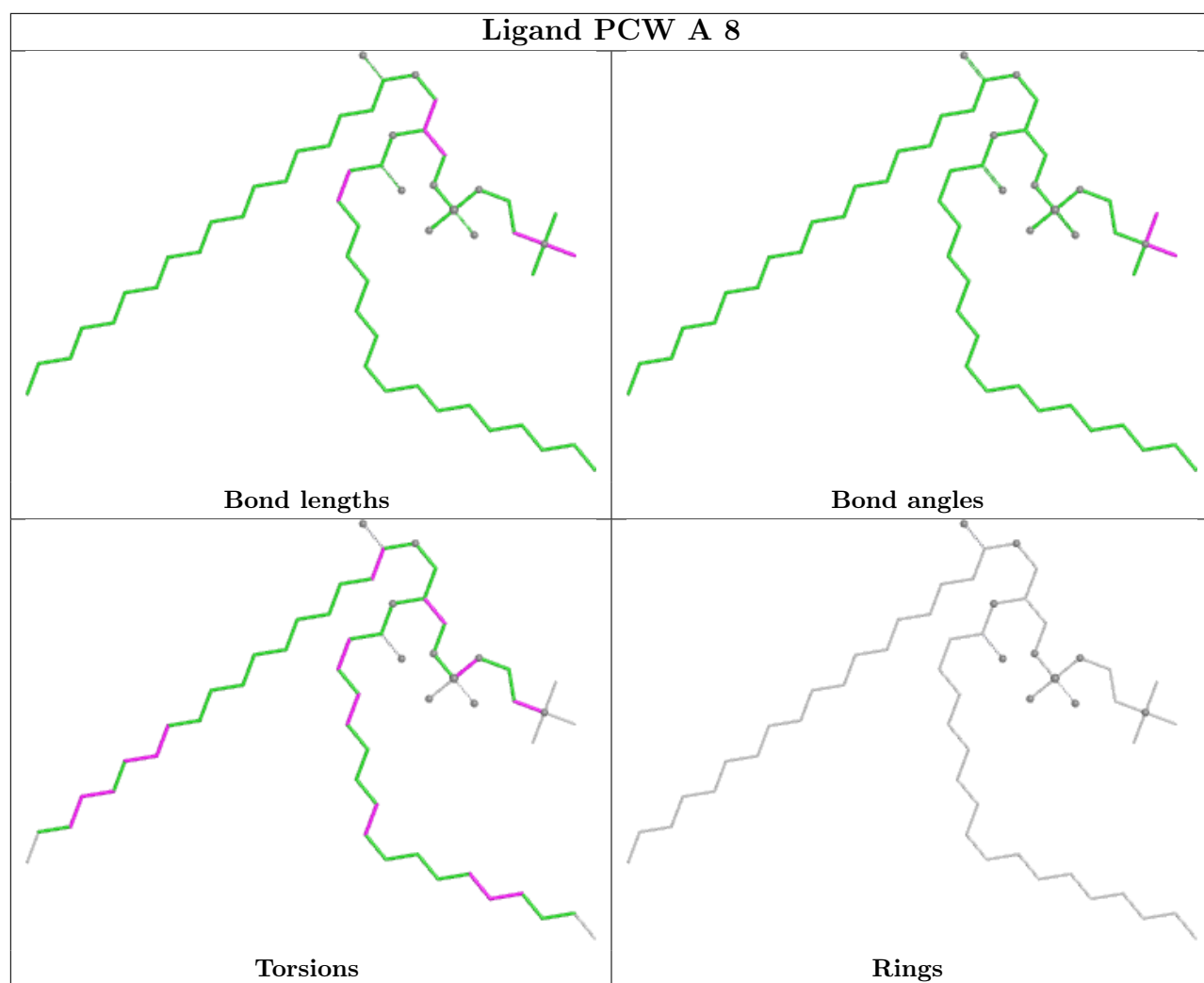


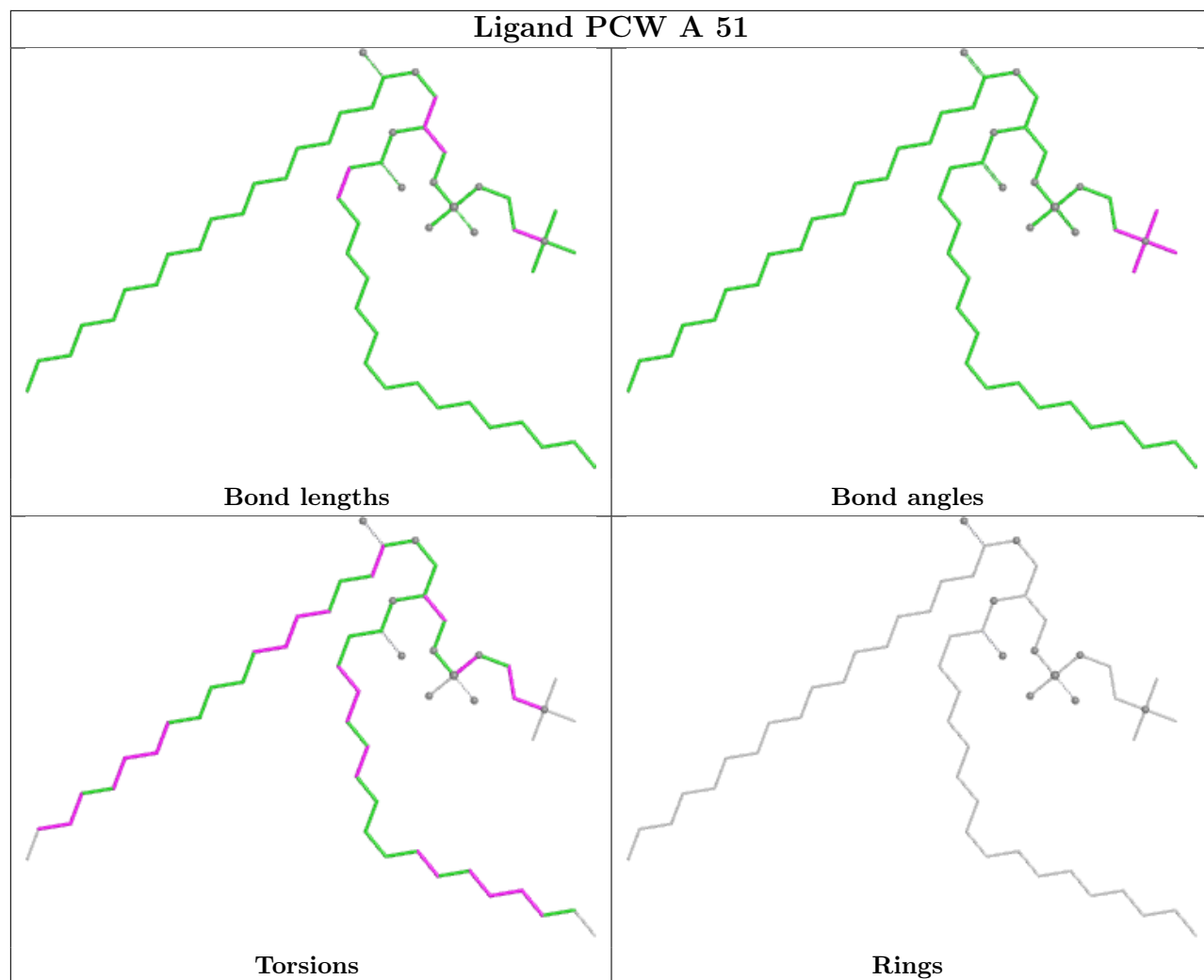




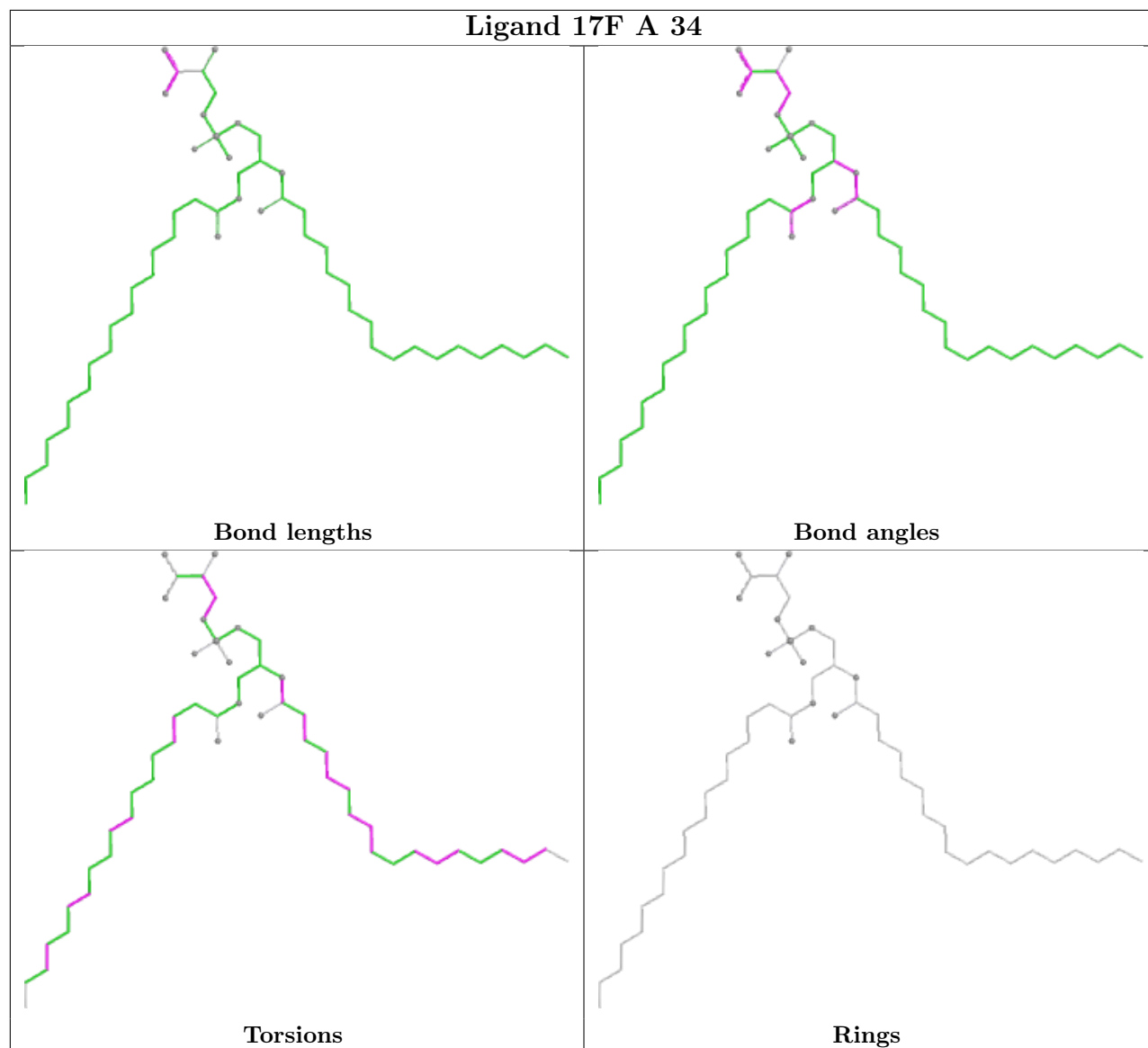


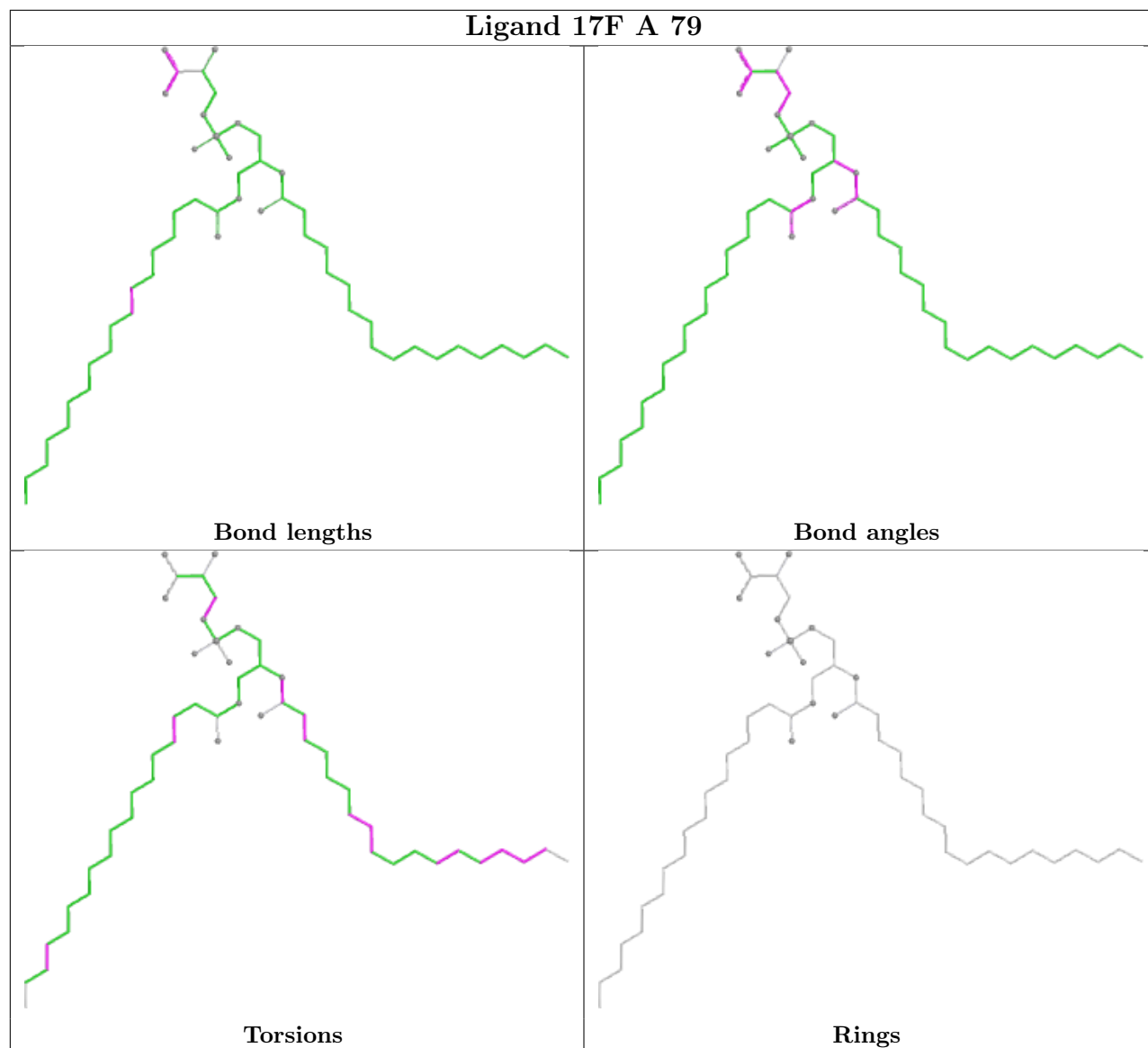


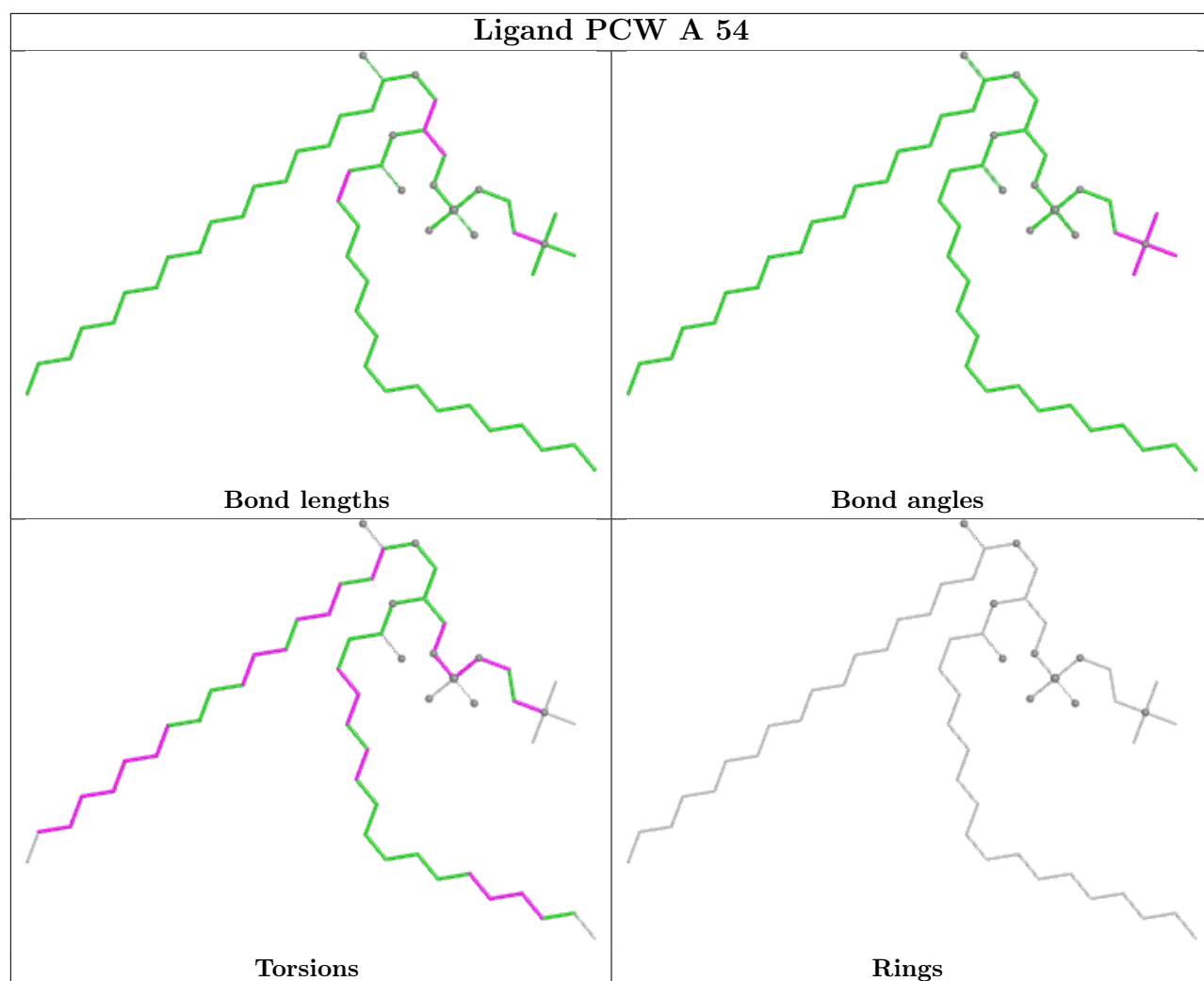


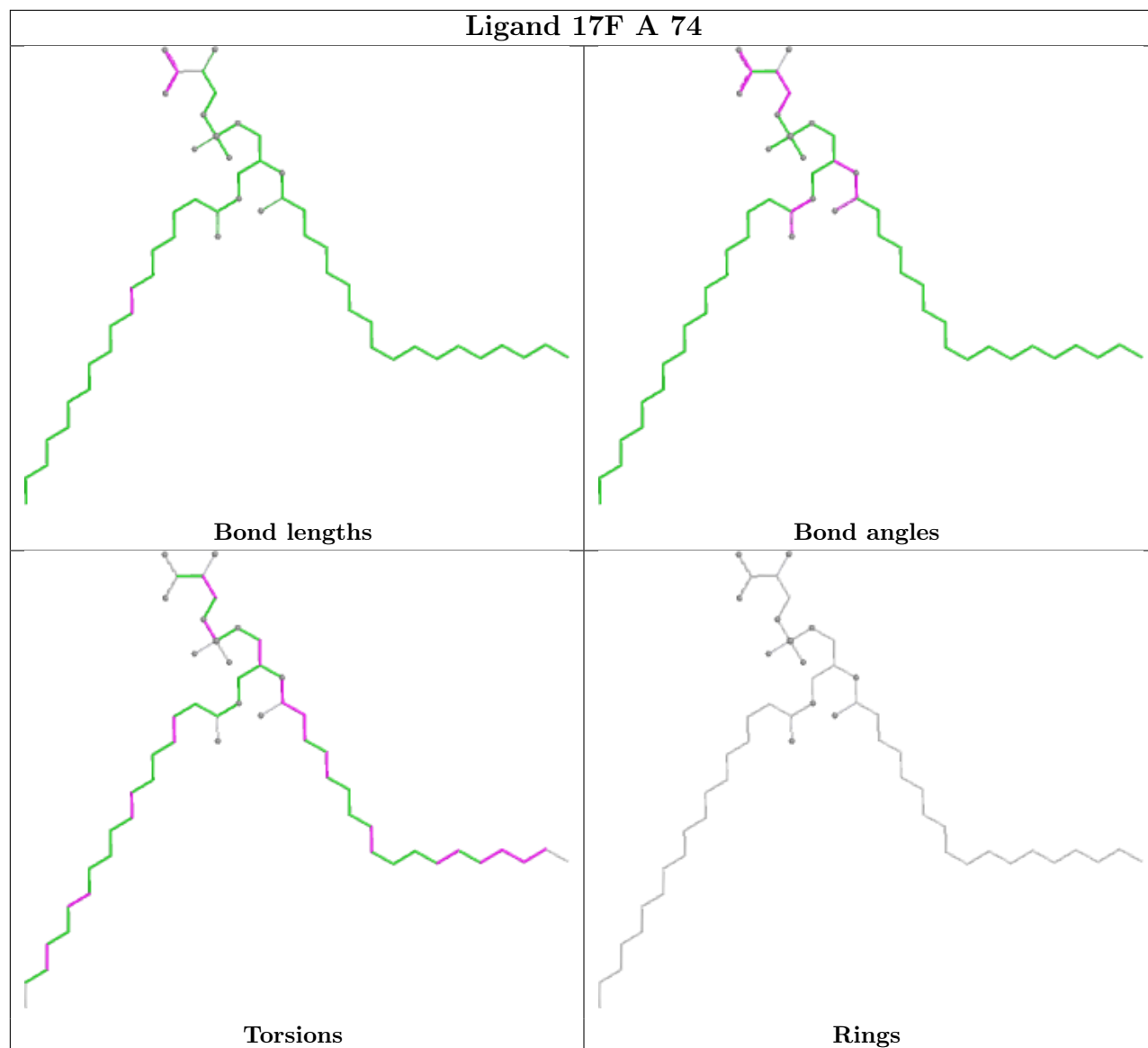


Ligand 17F A 34

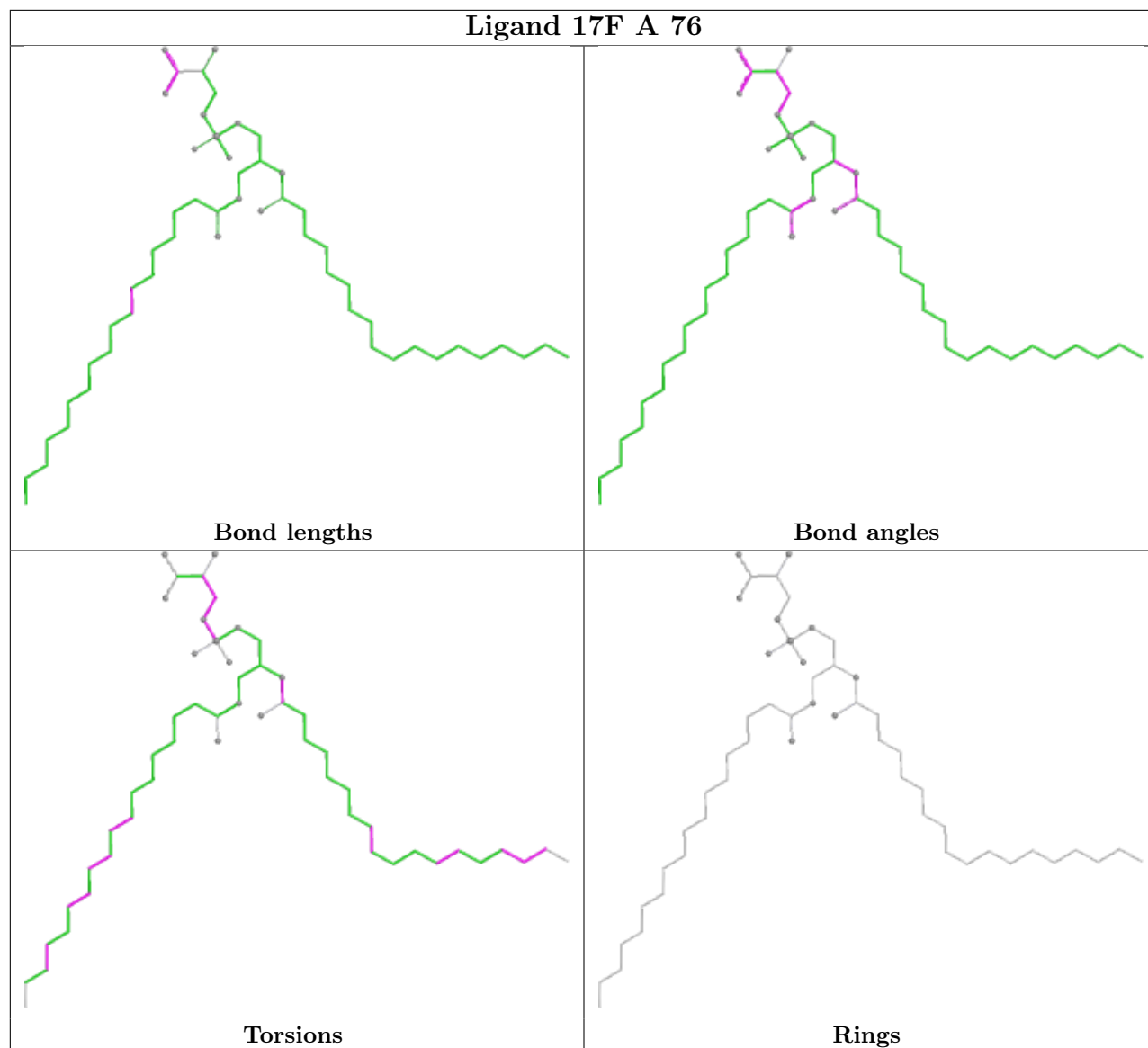


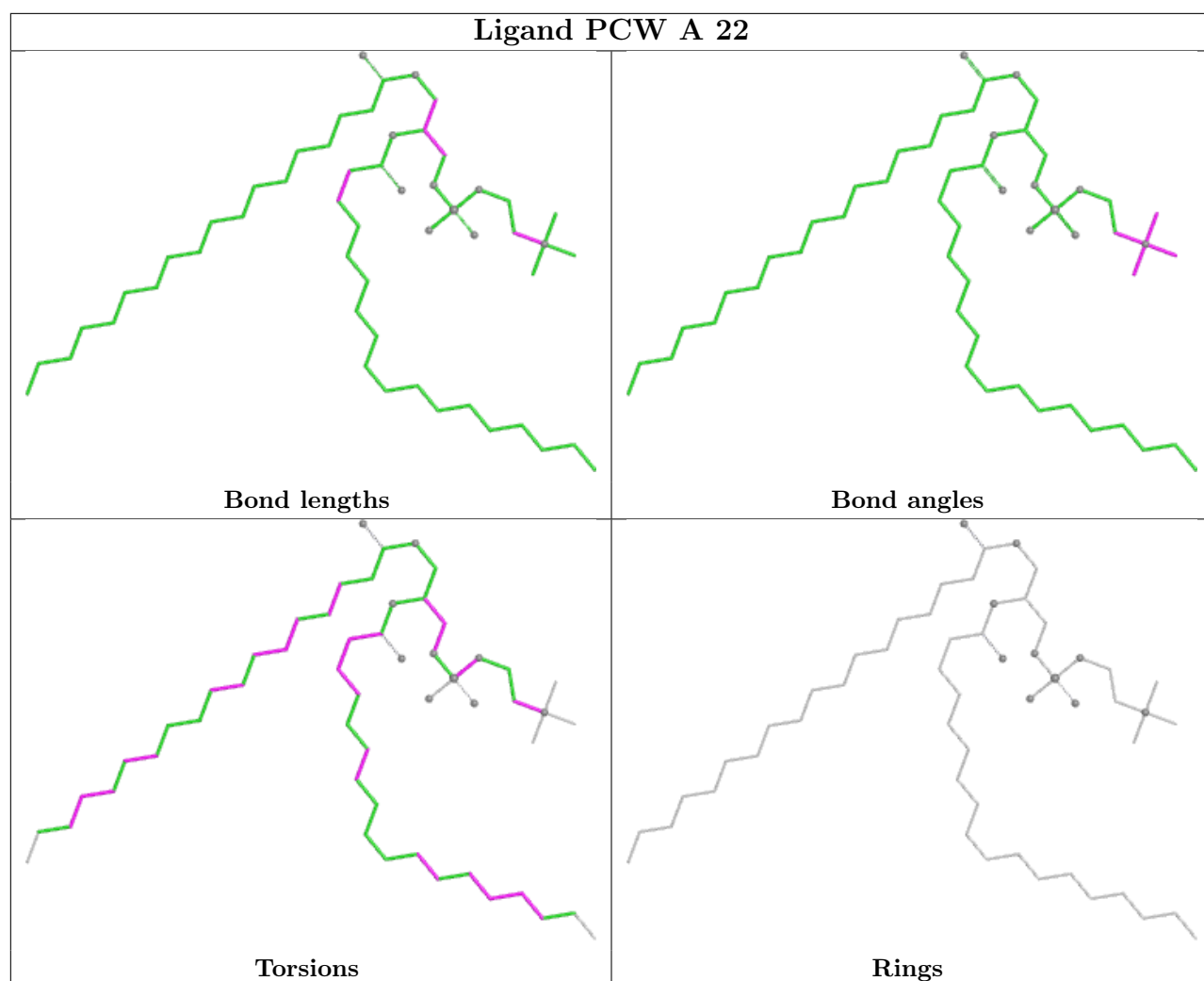


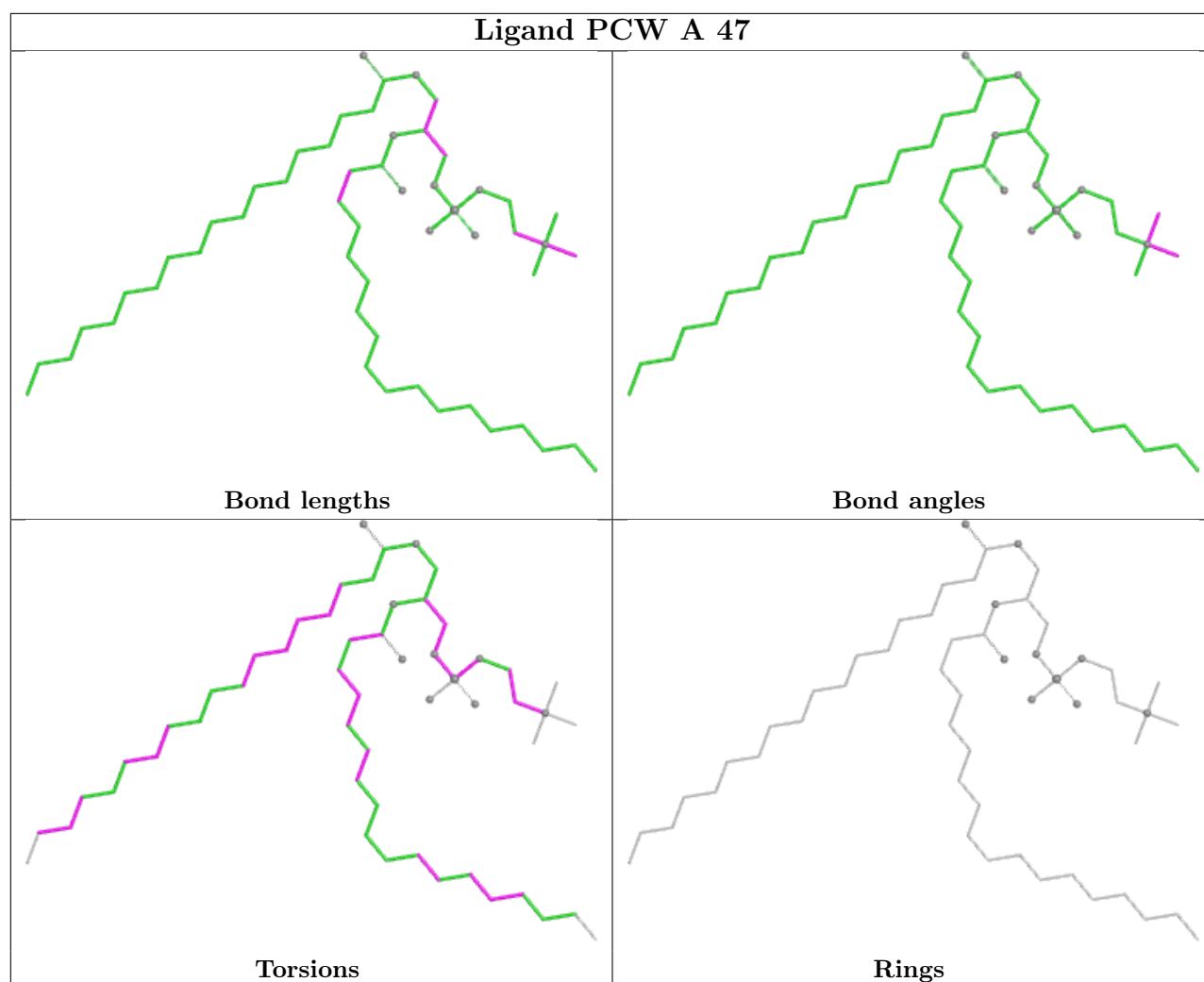


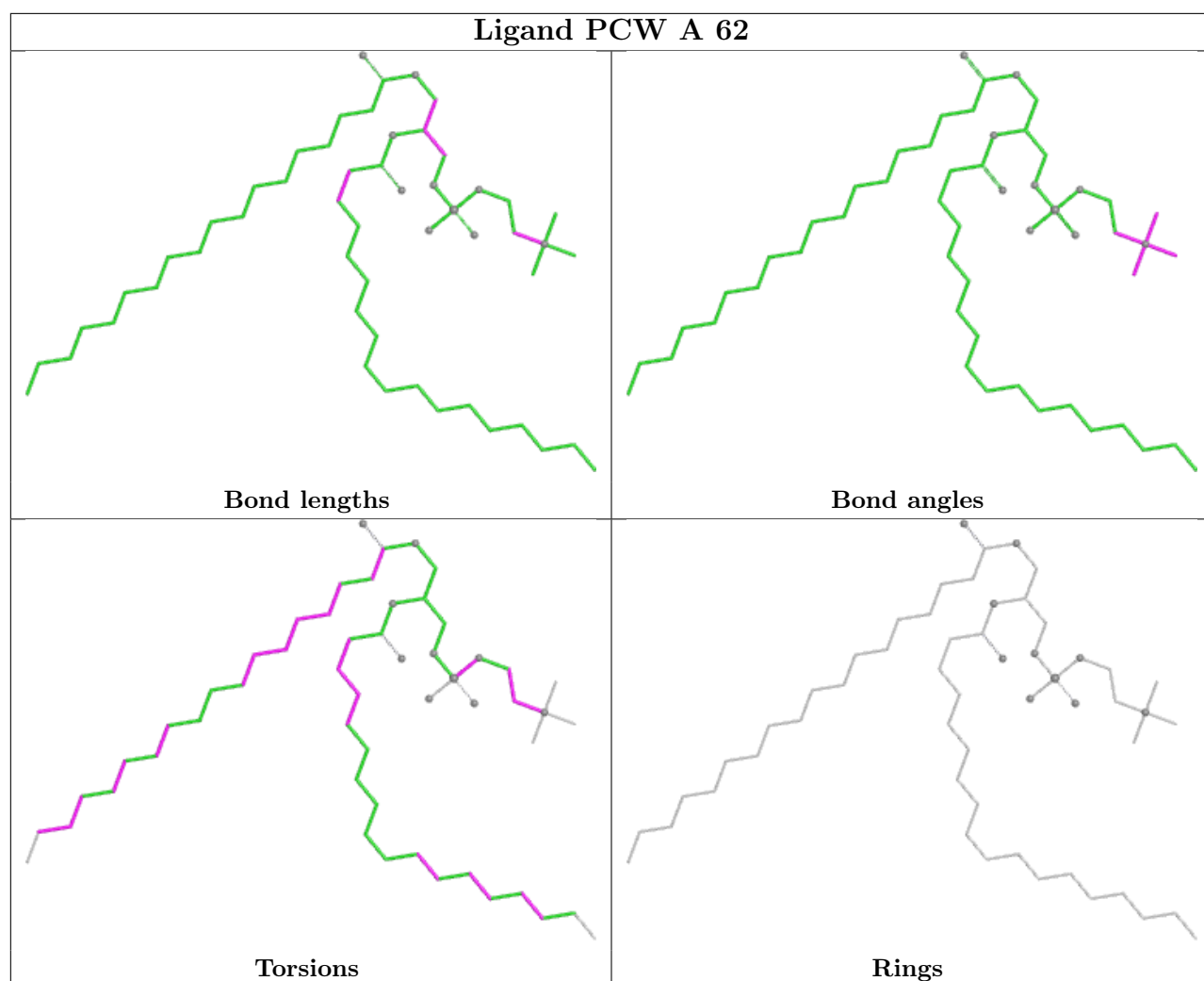


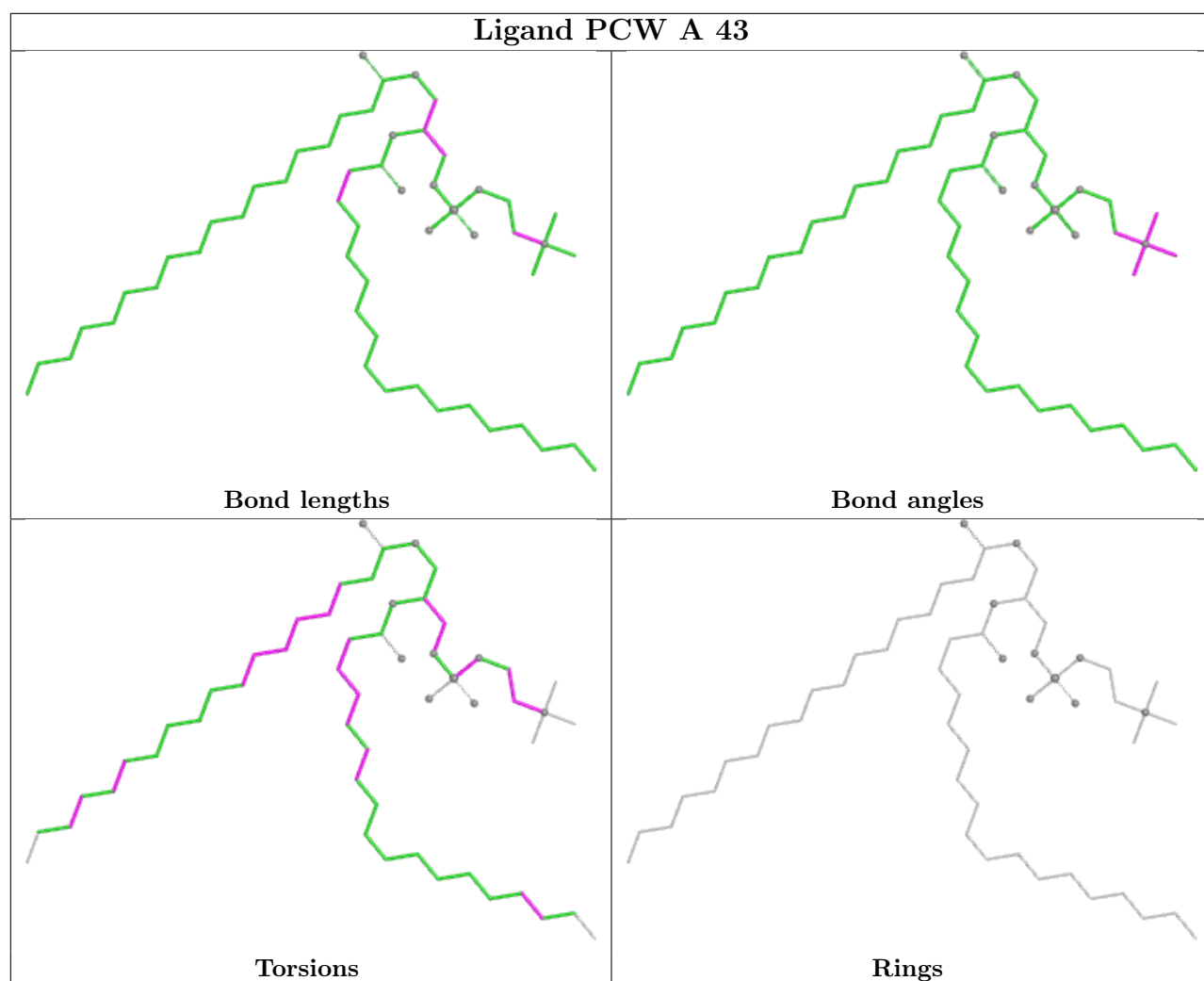
Ligand 17F A 76

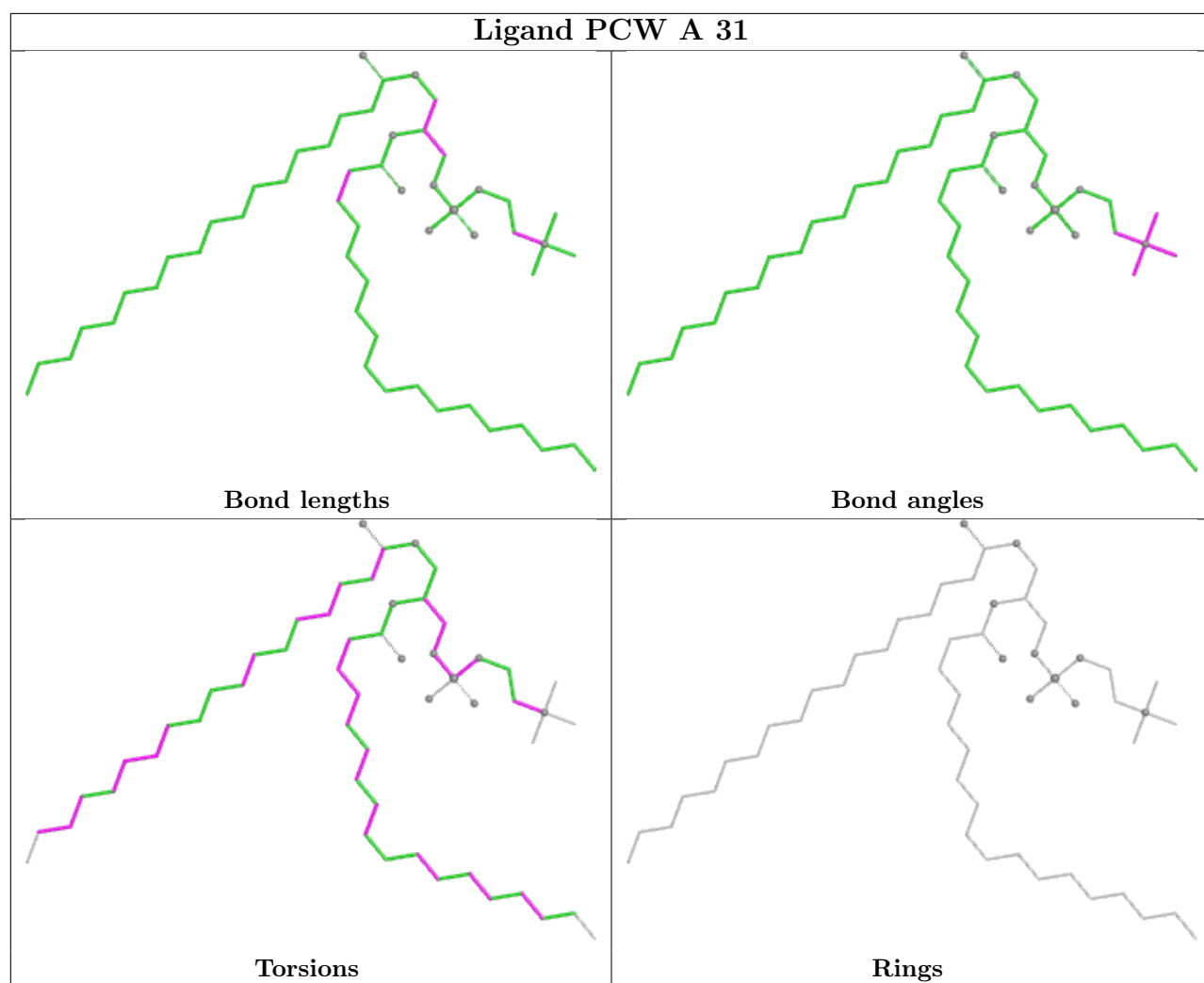


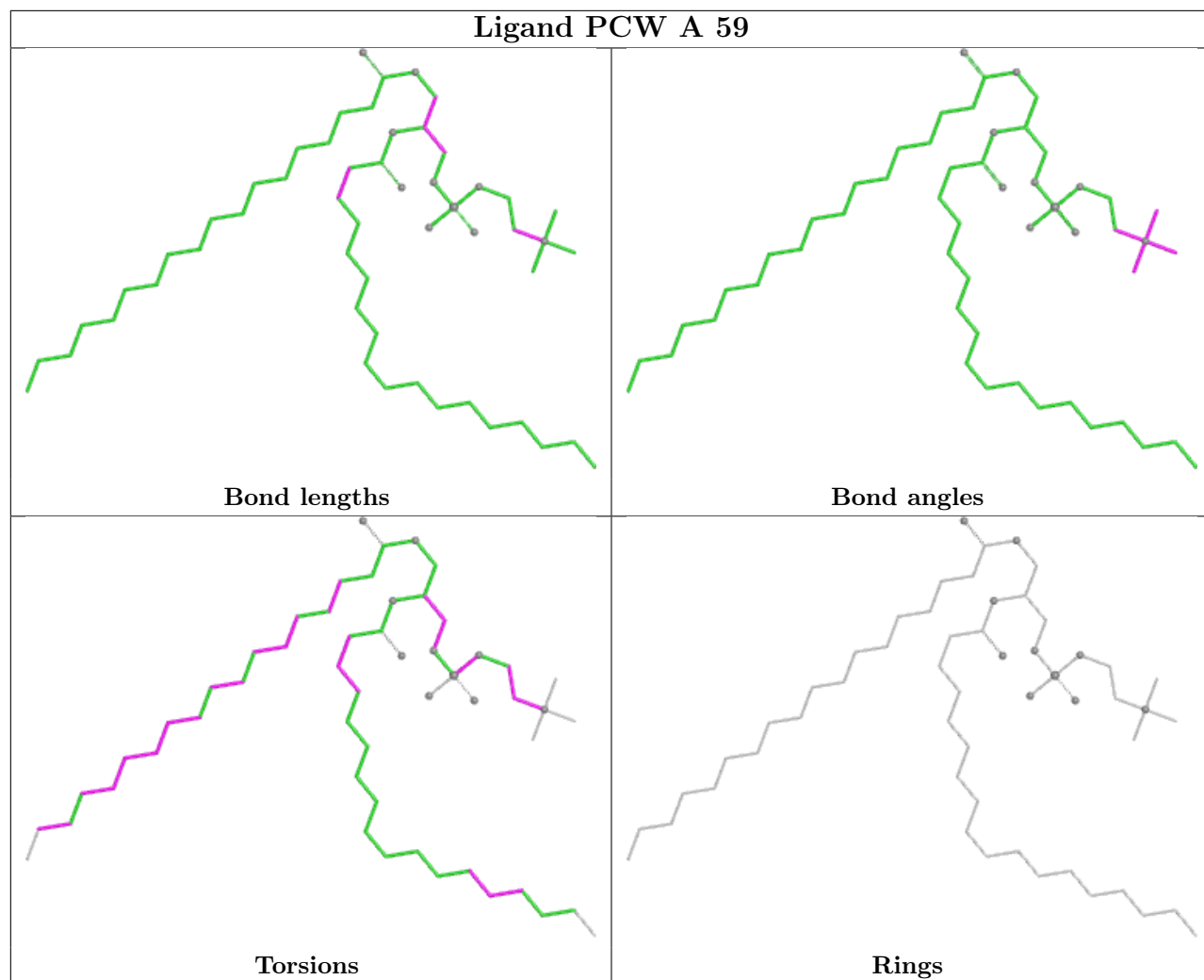


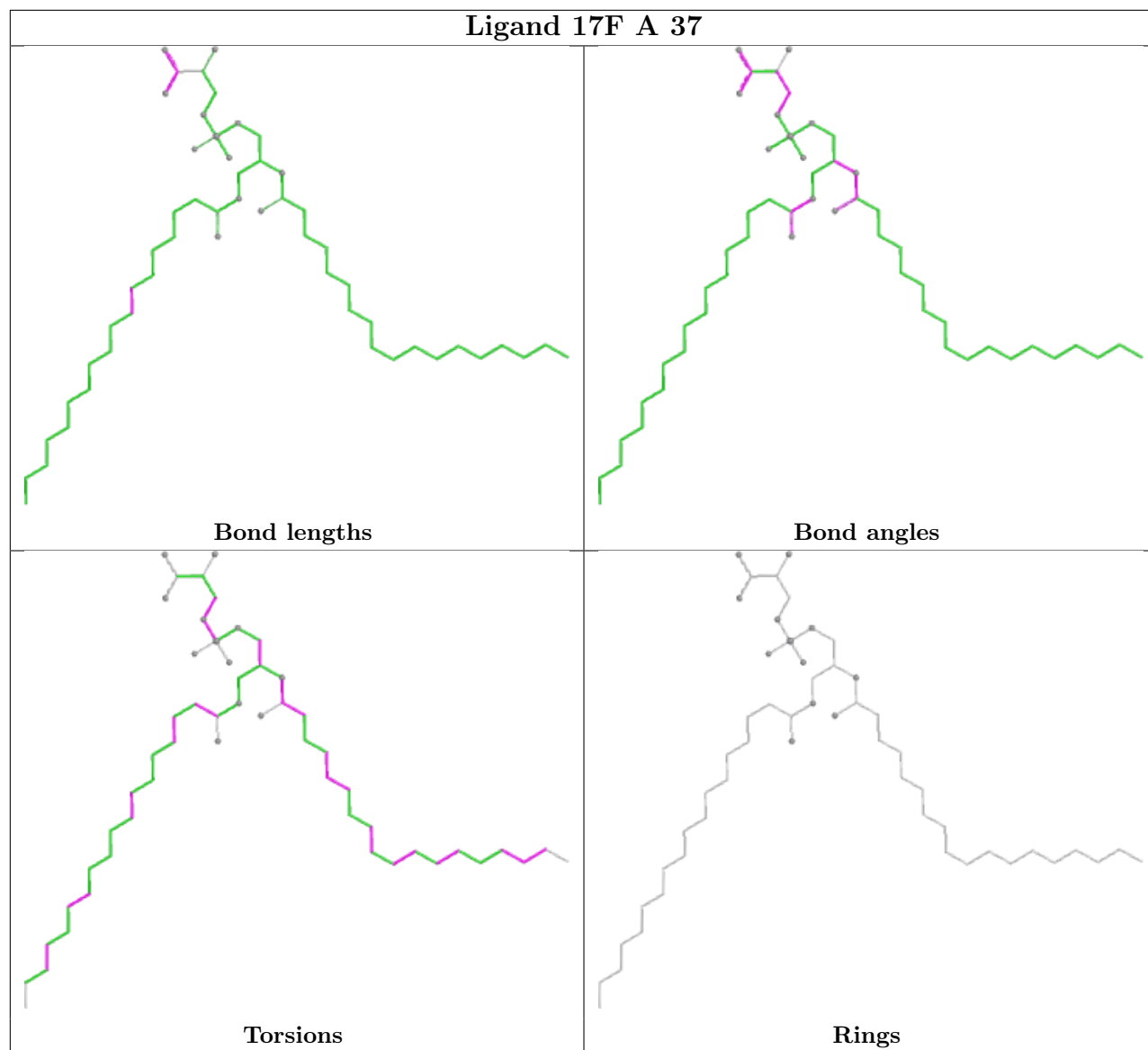


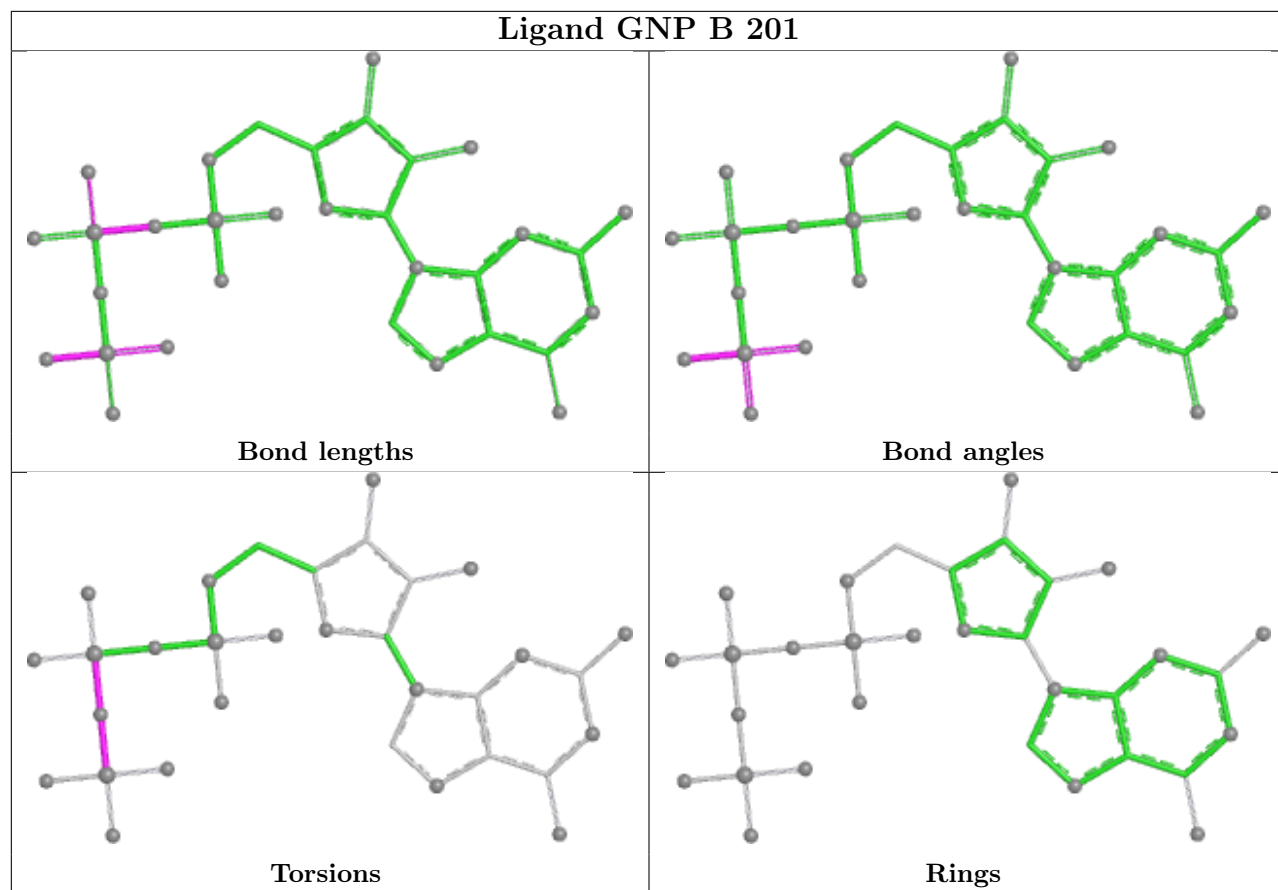


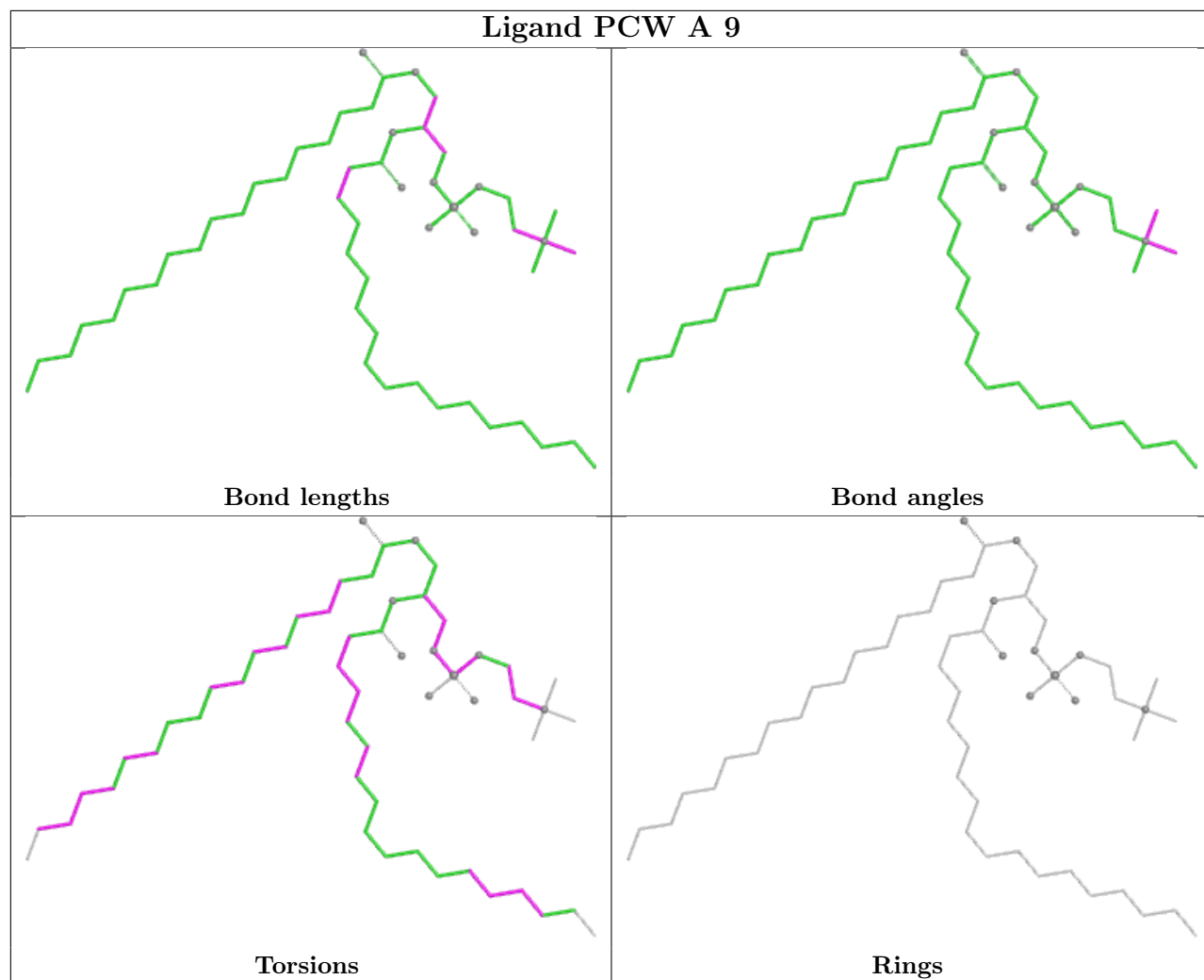


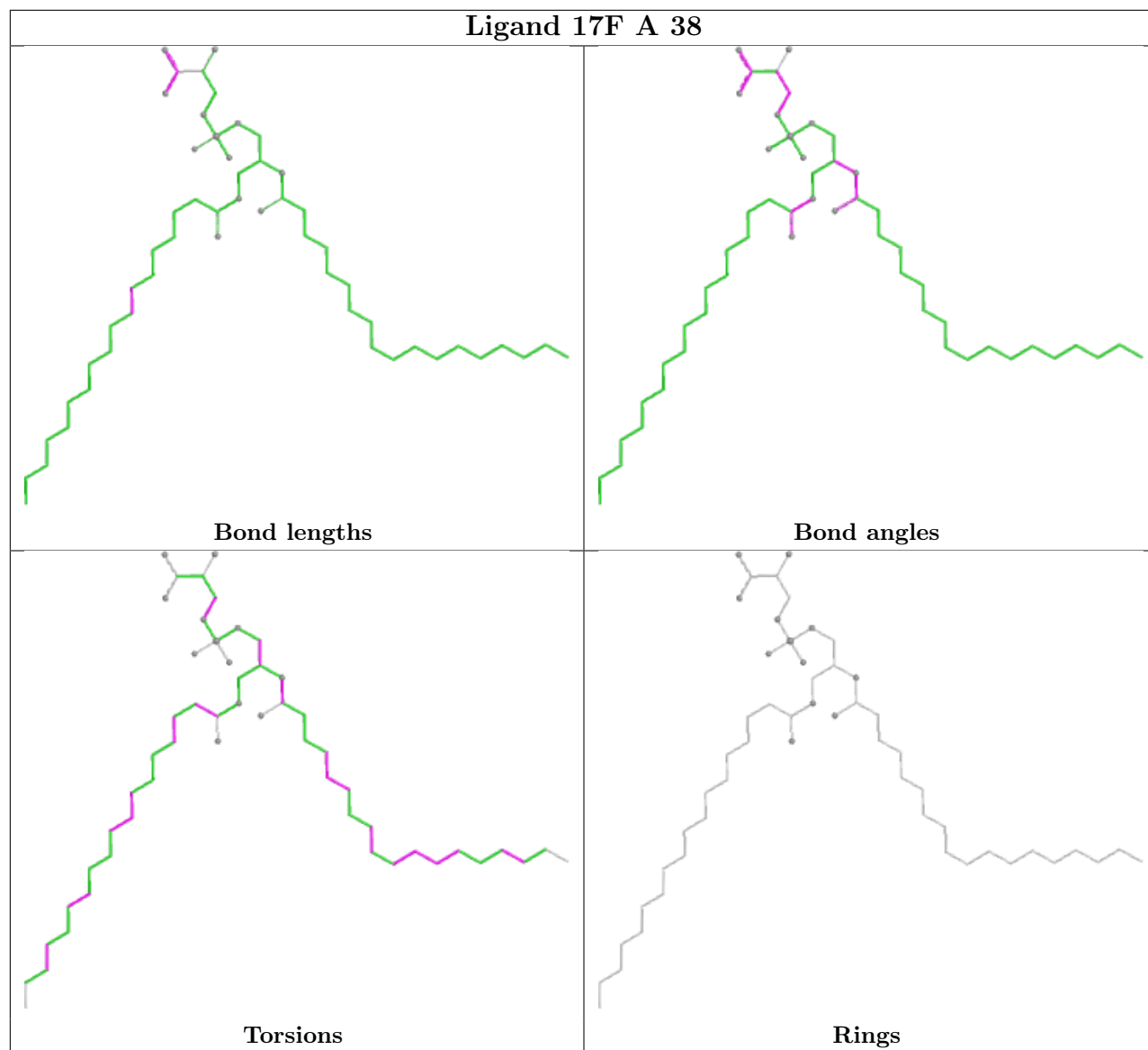


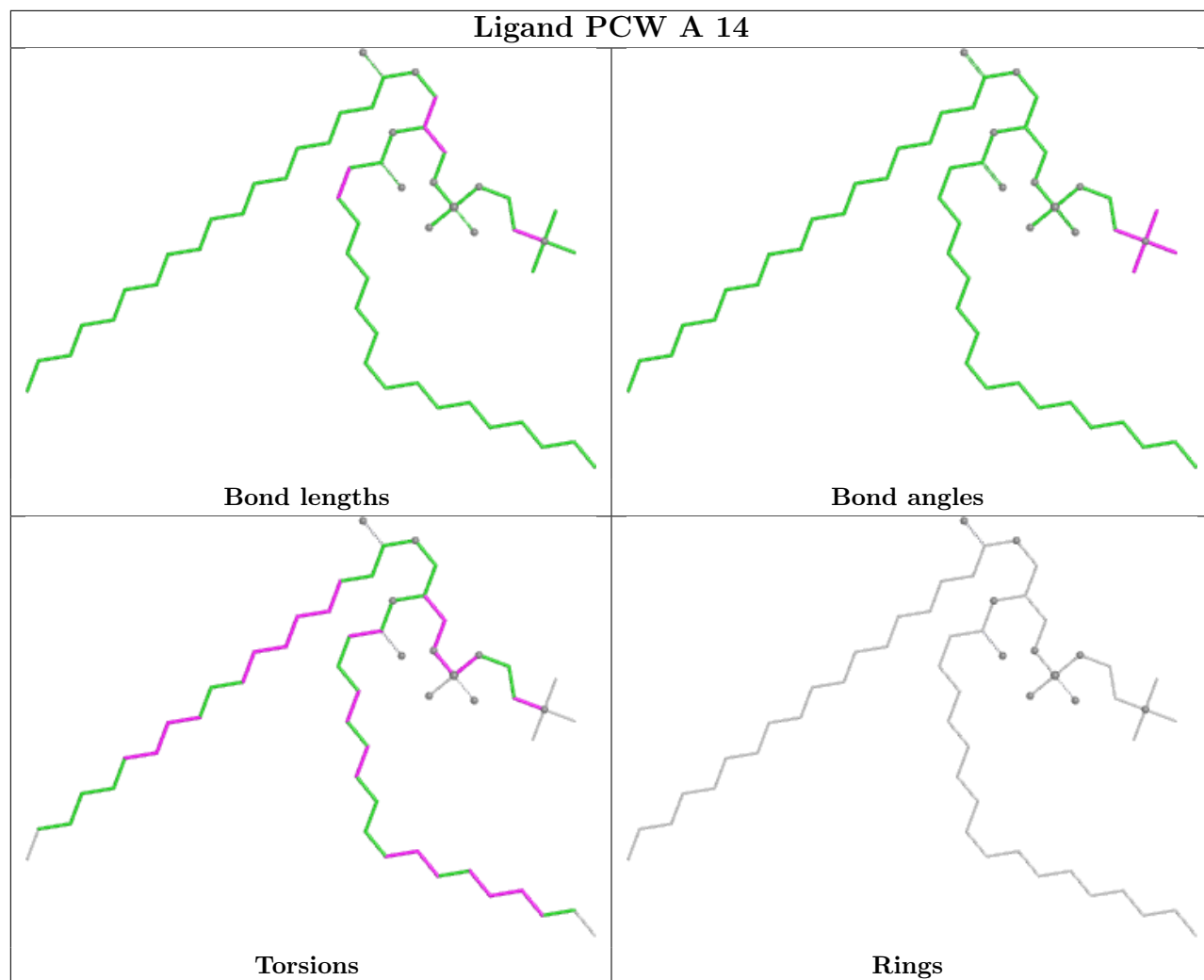


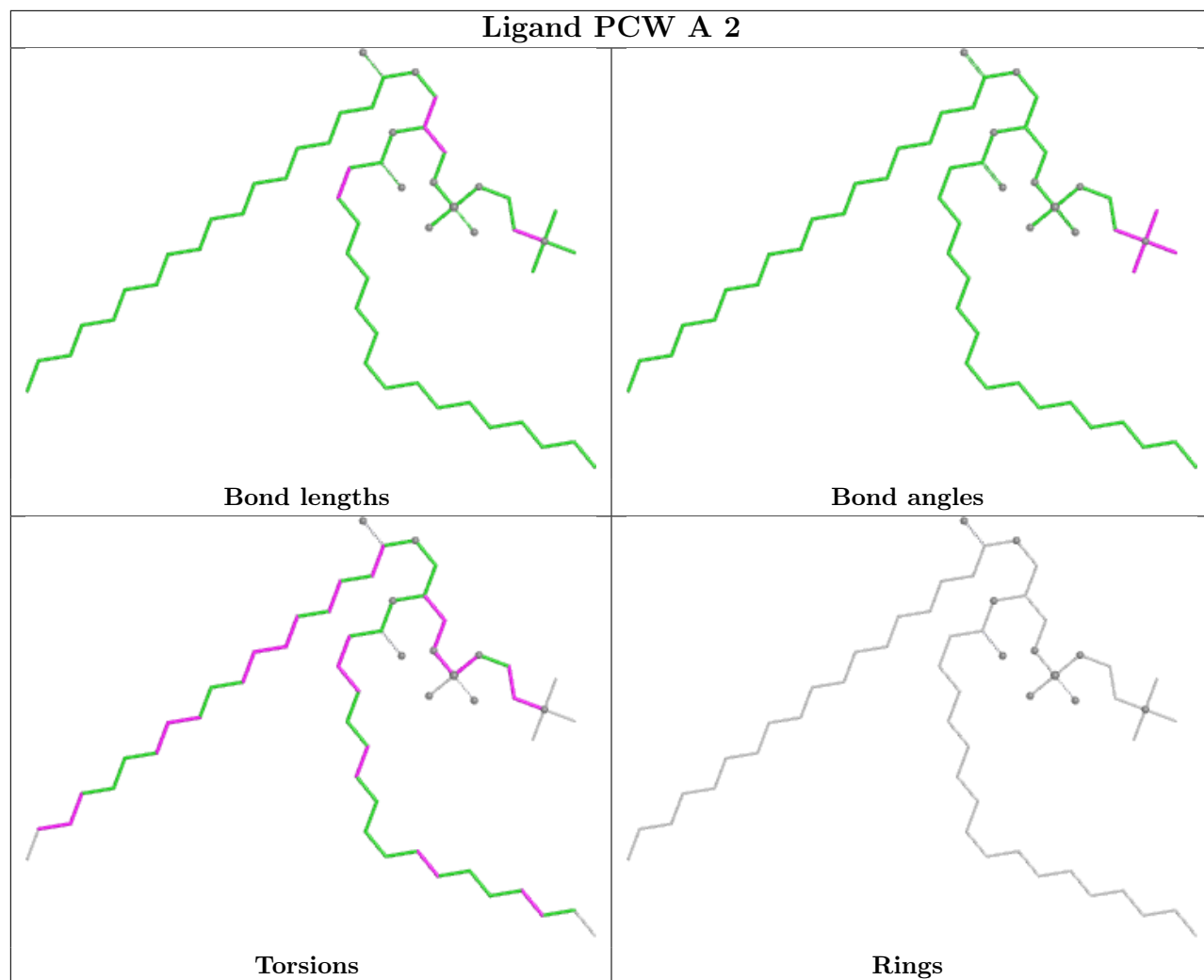




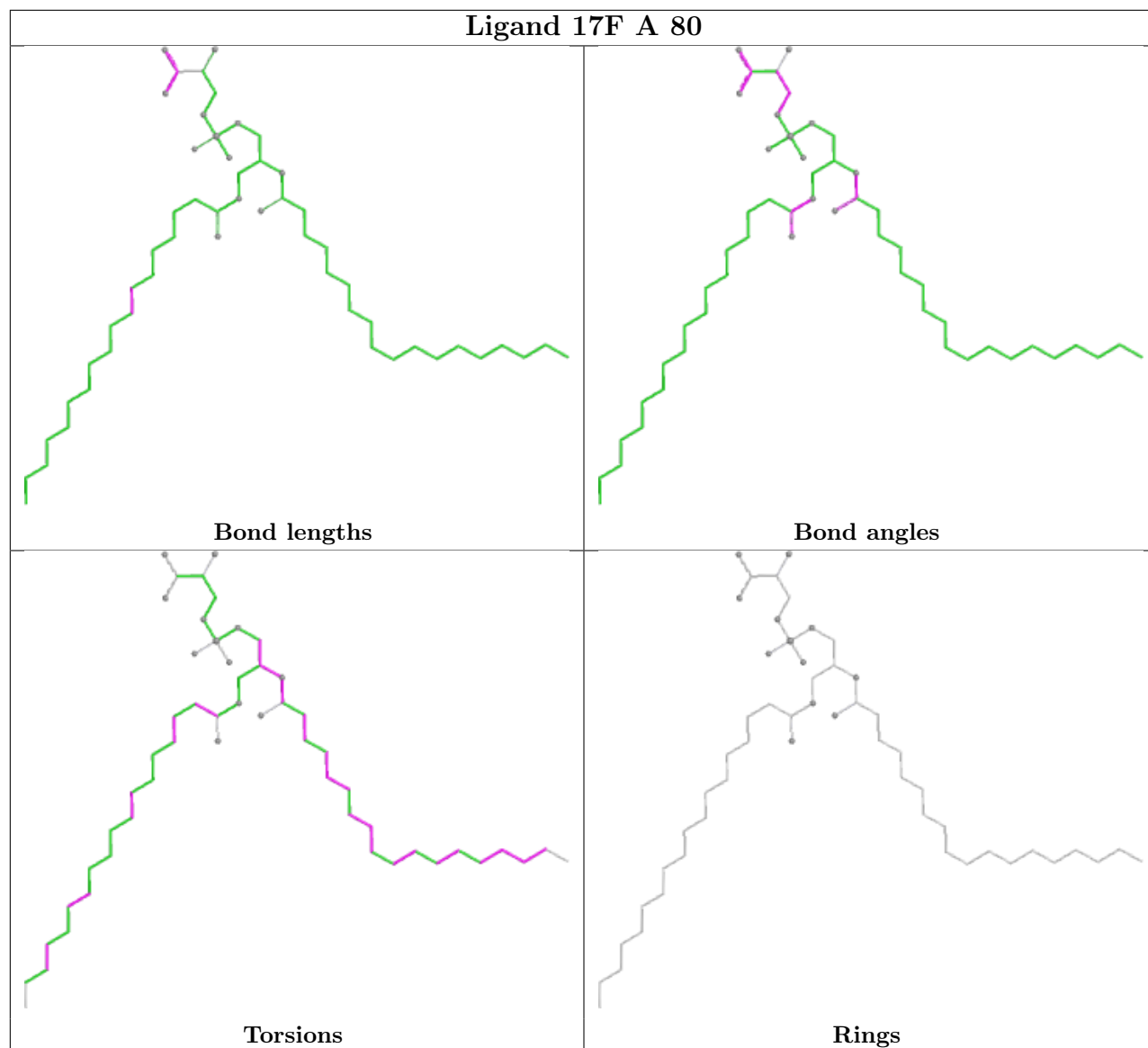


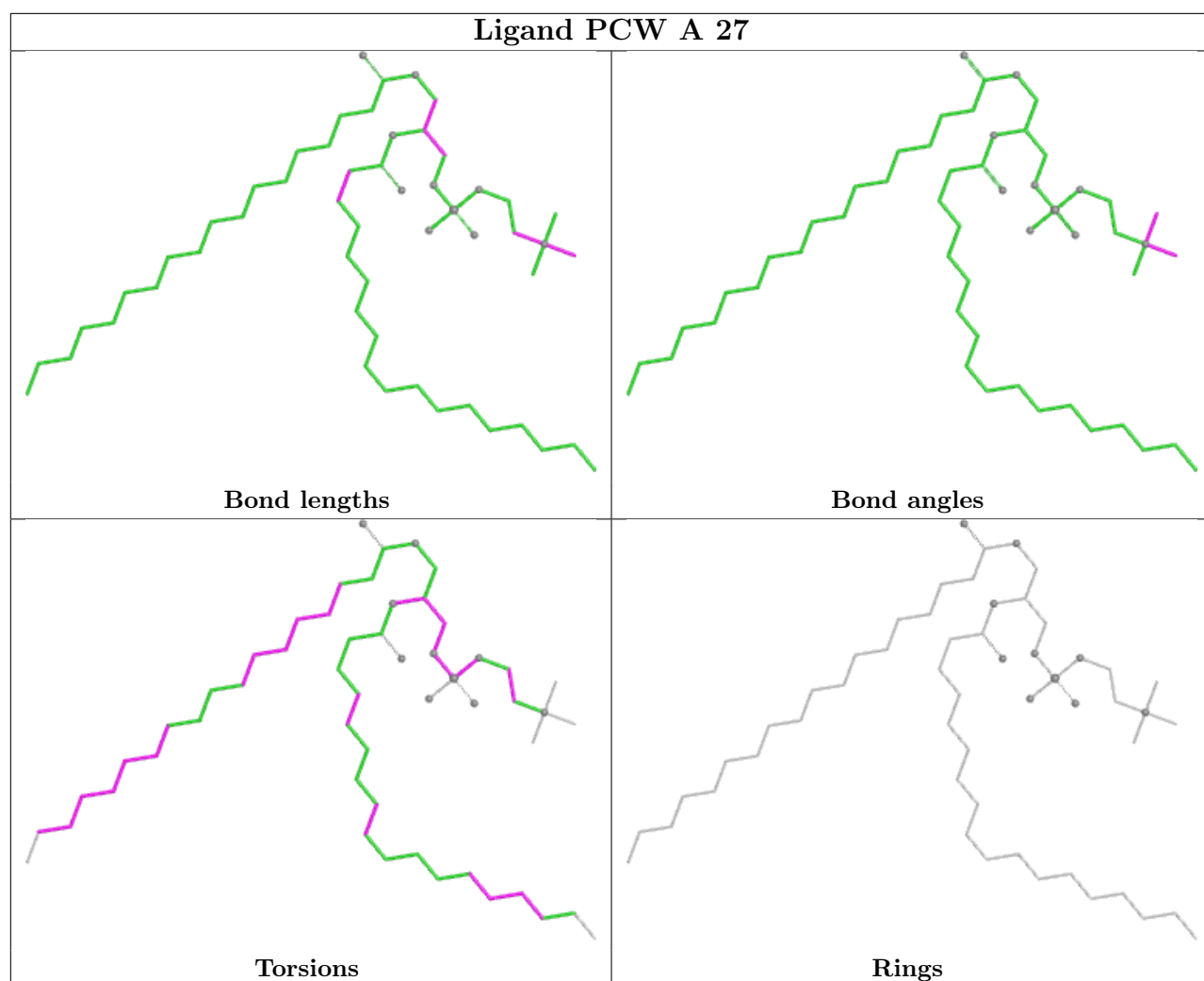


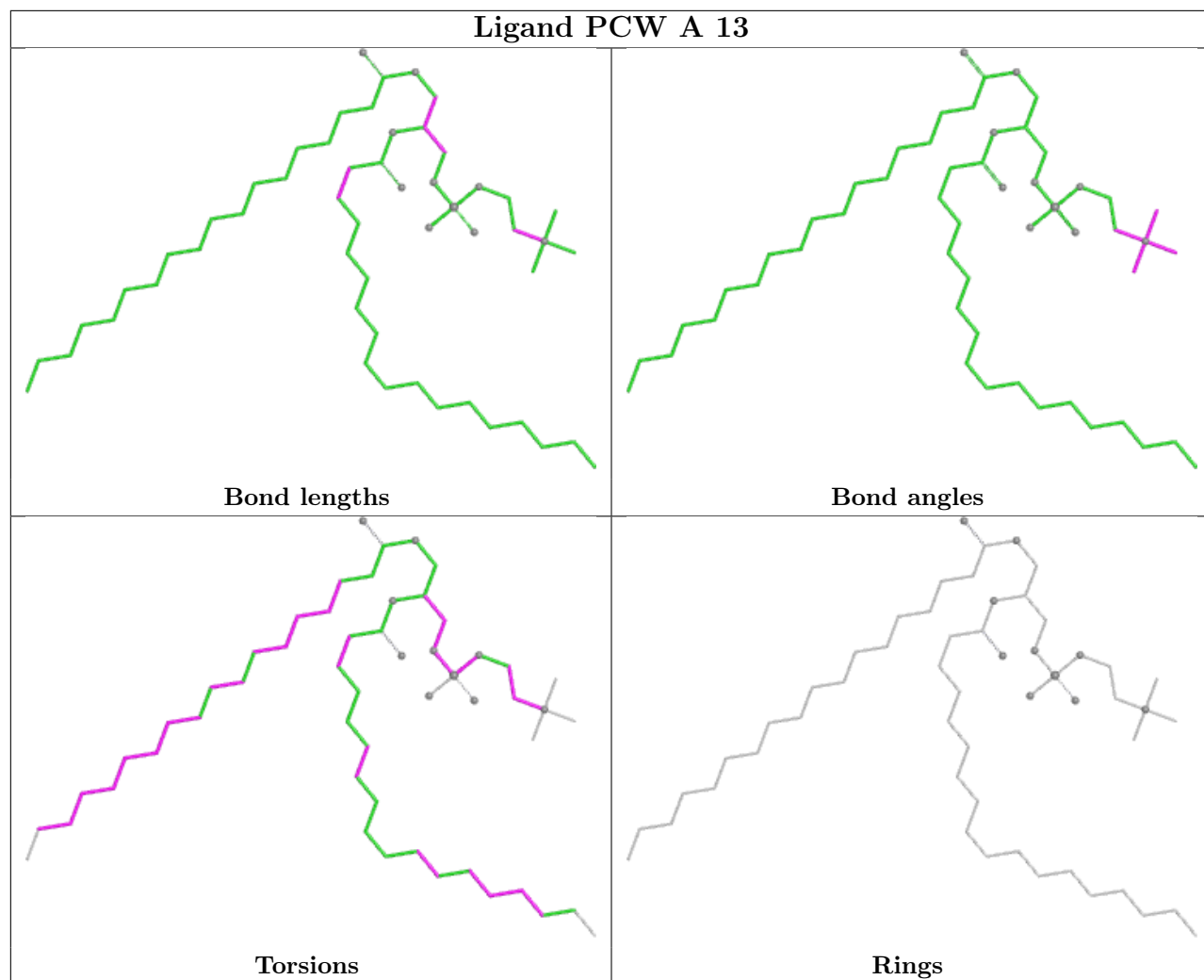


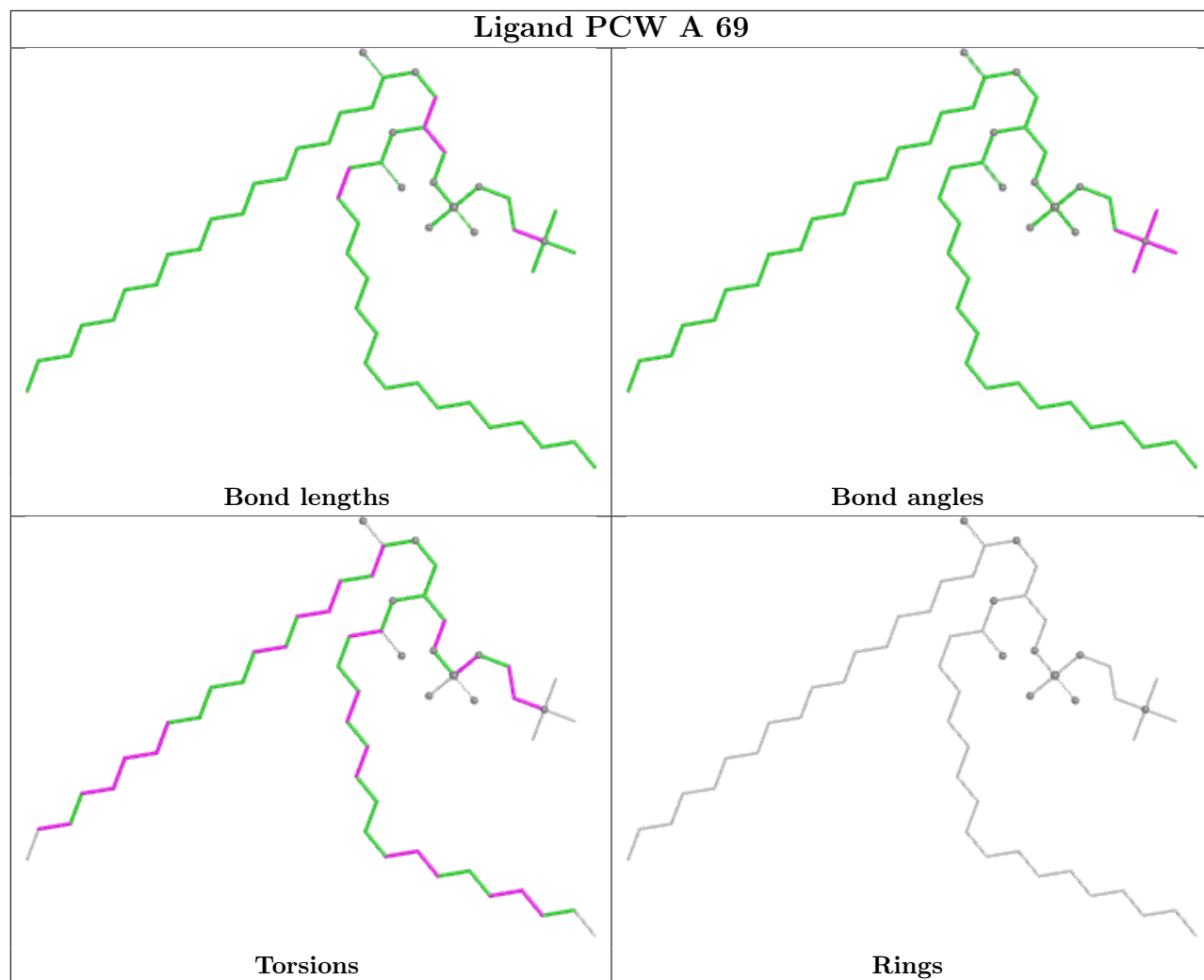


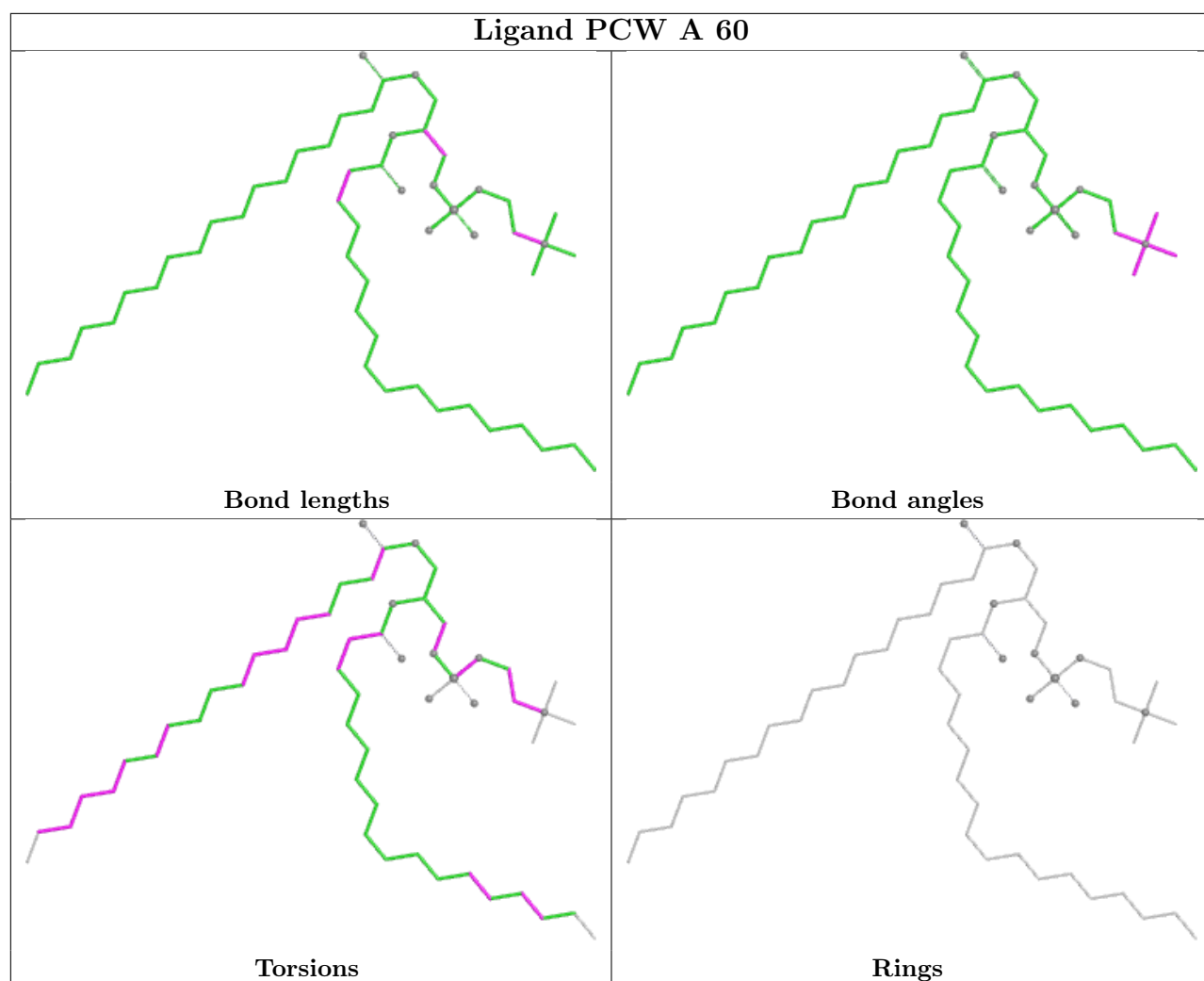
Ligand 17F A 80

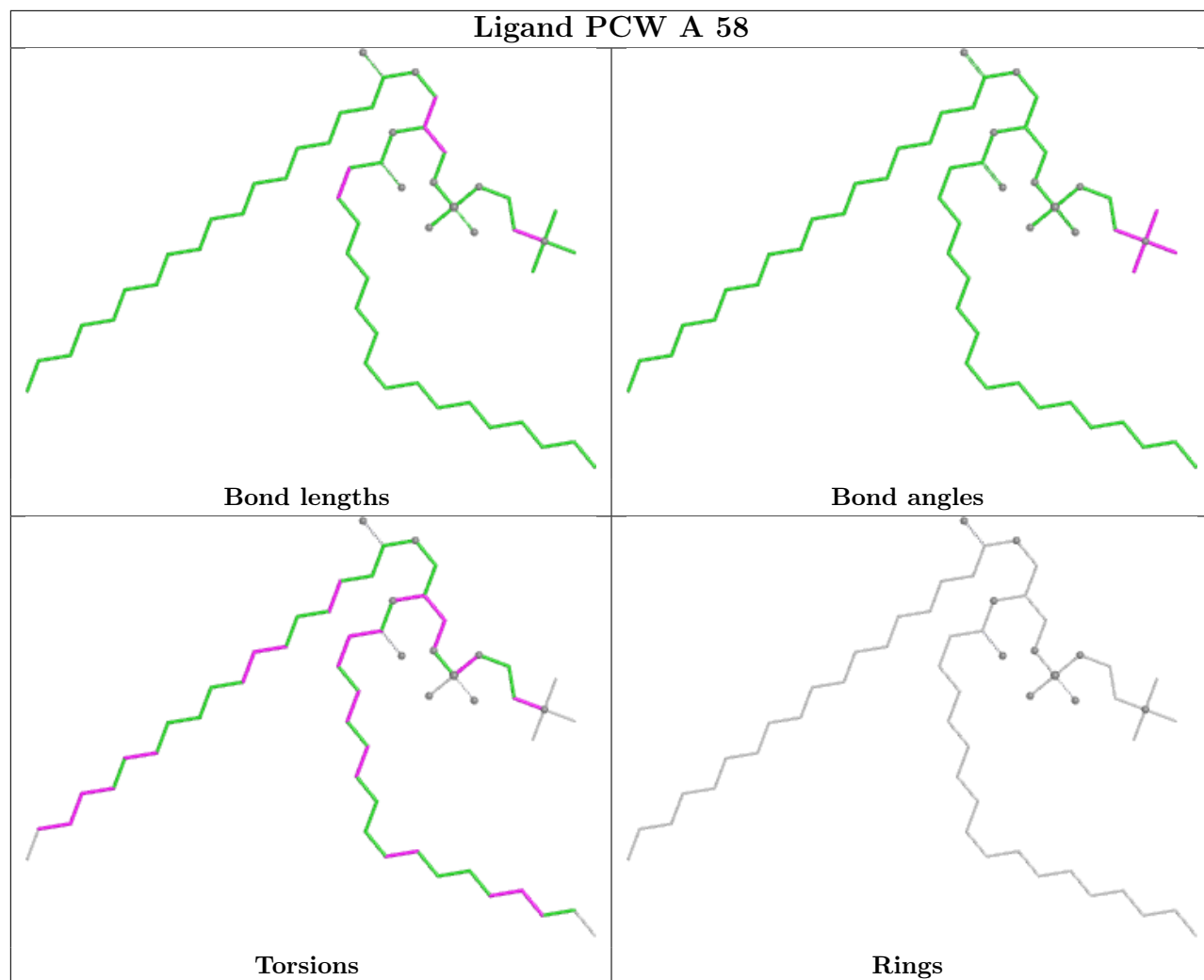


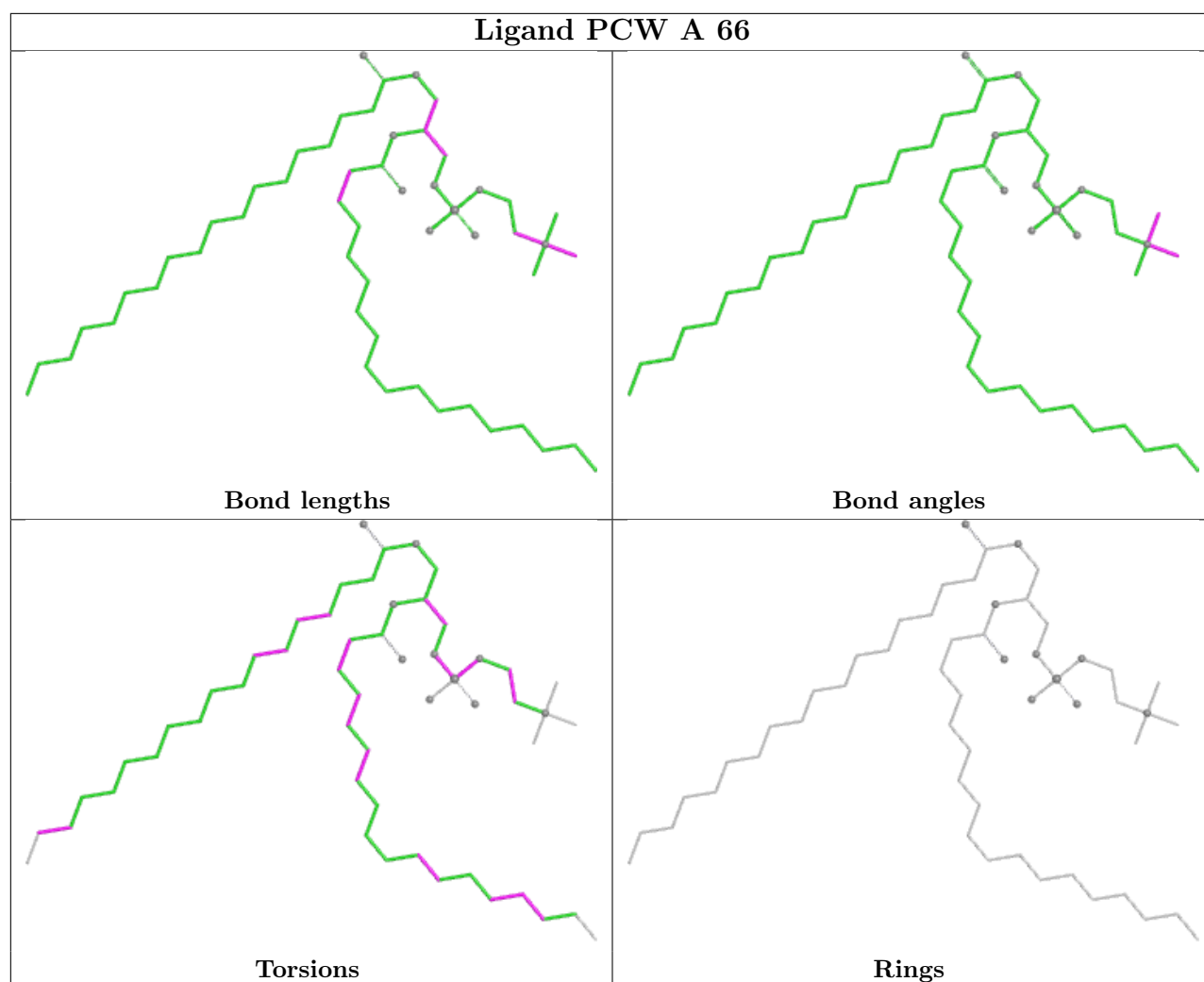


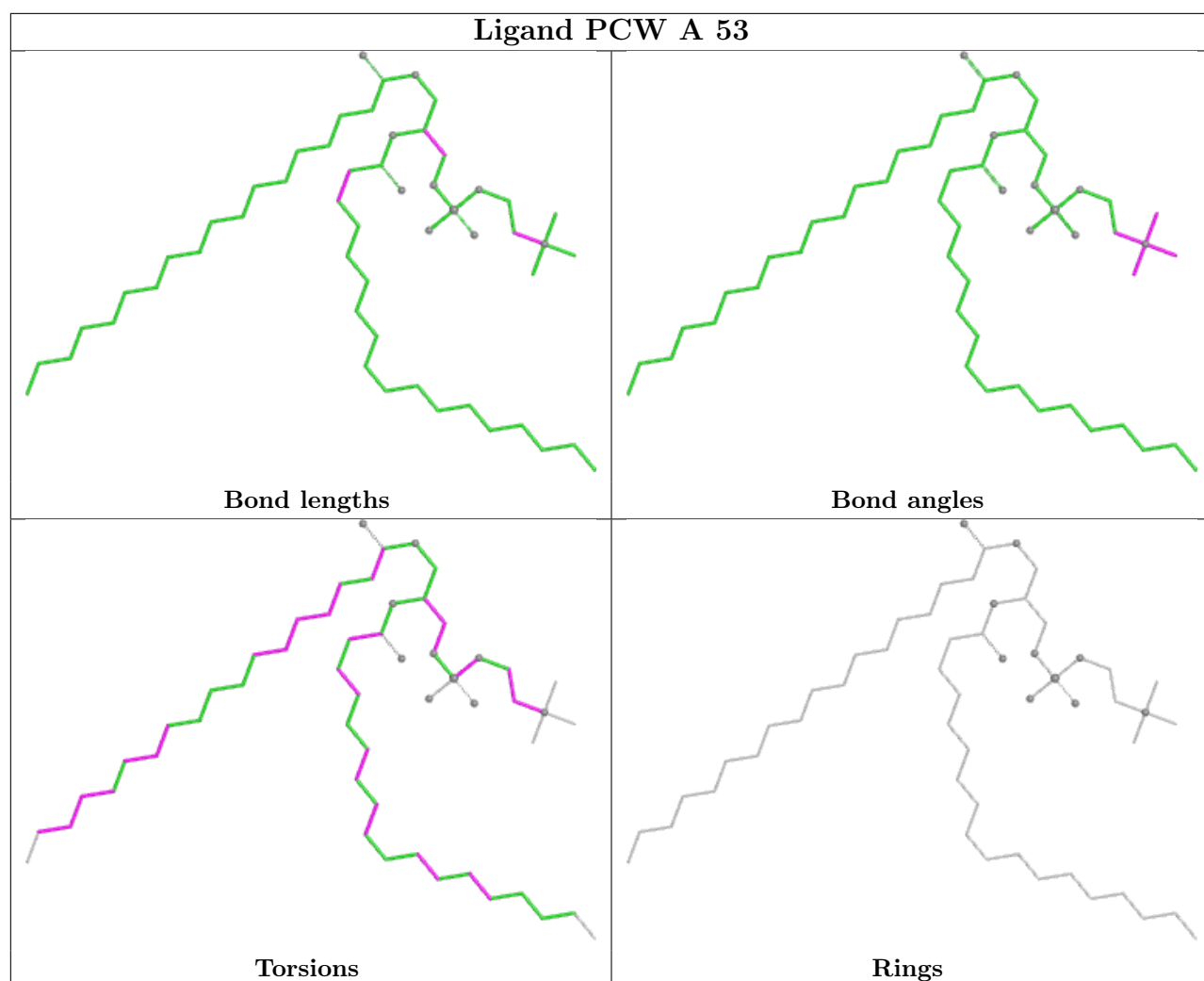


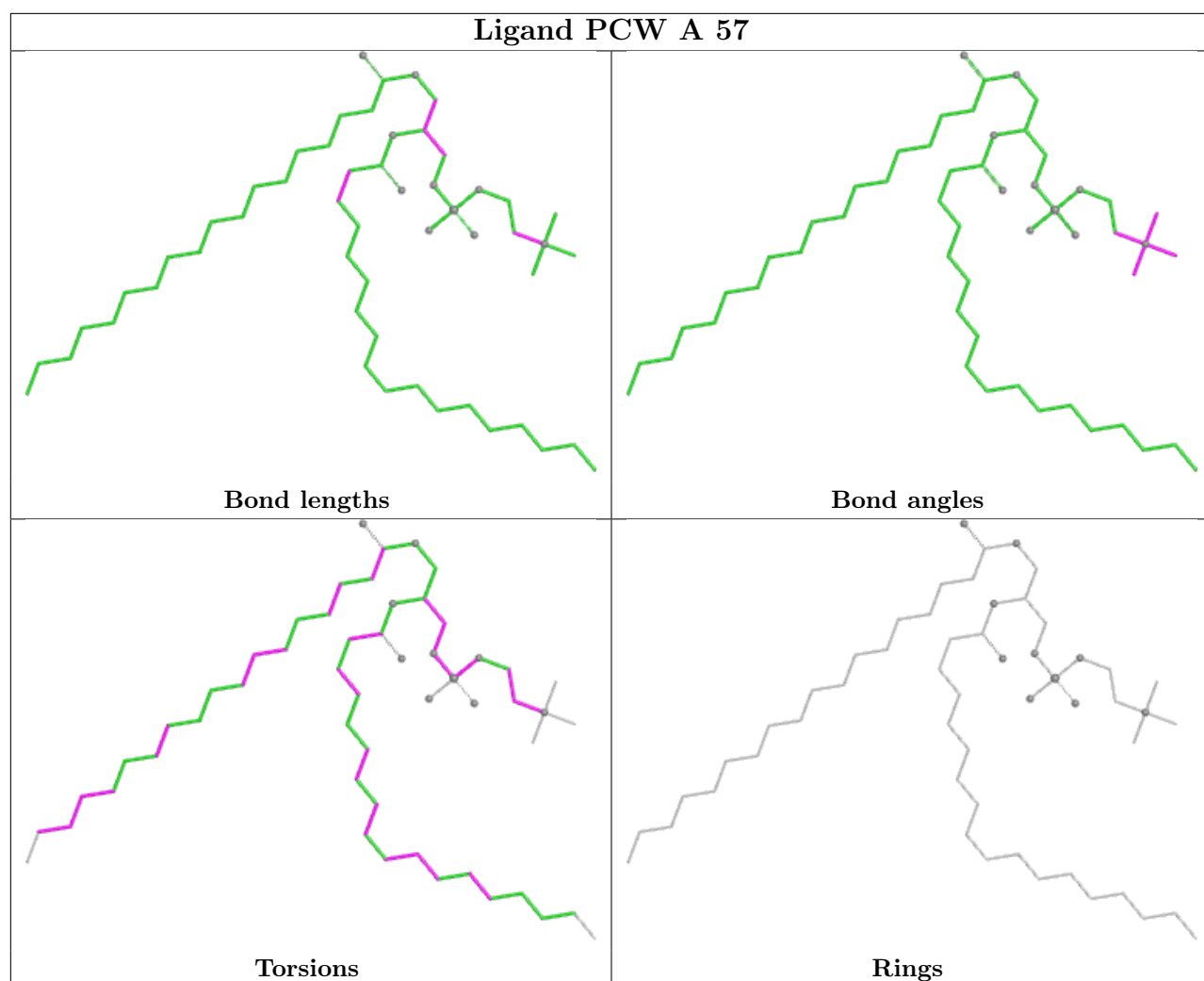


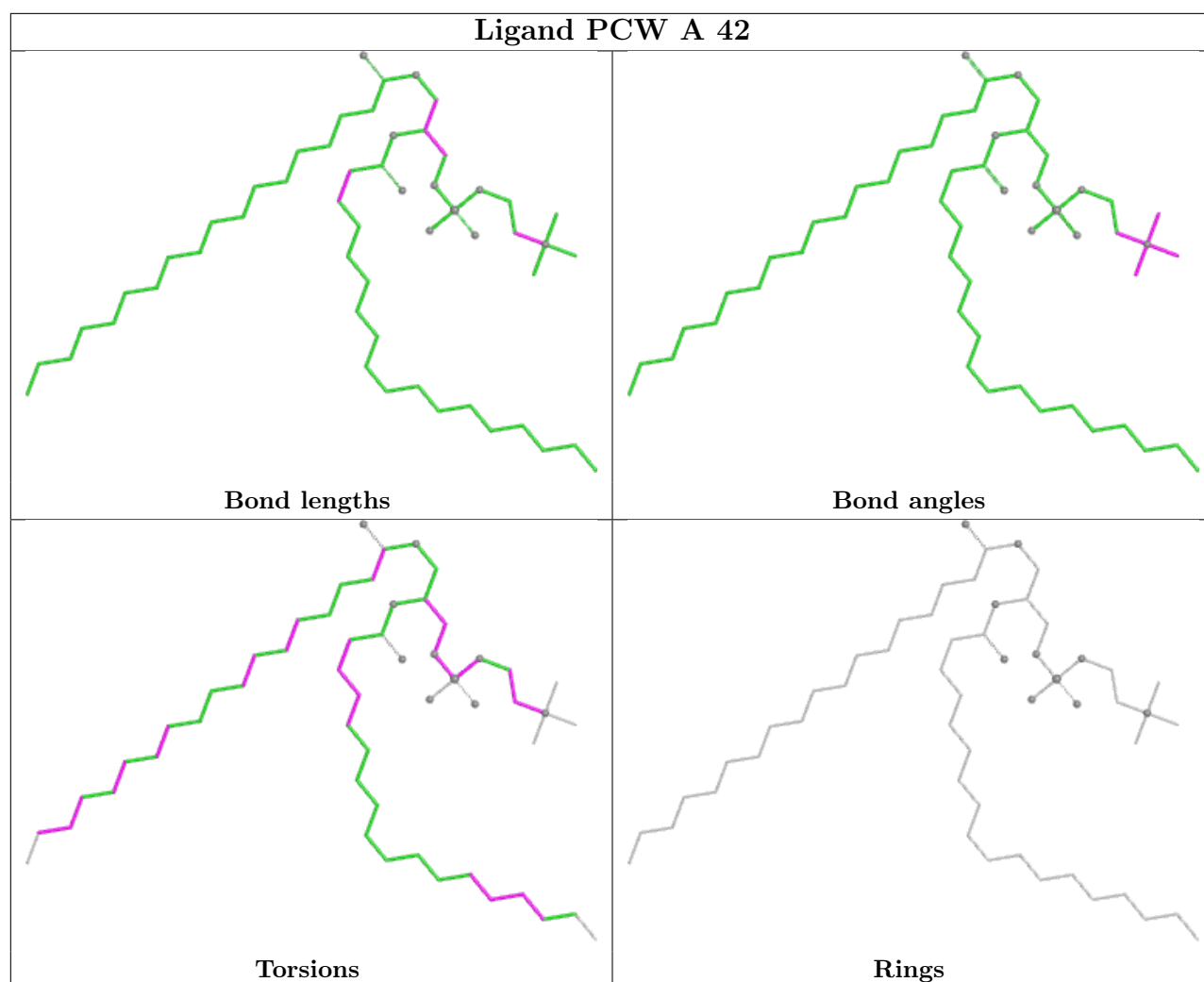


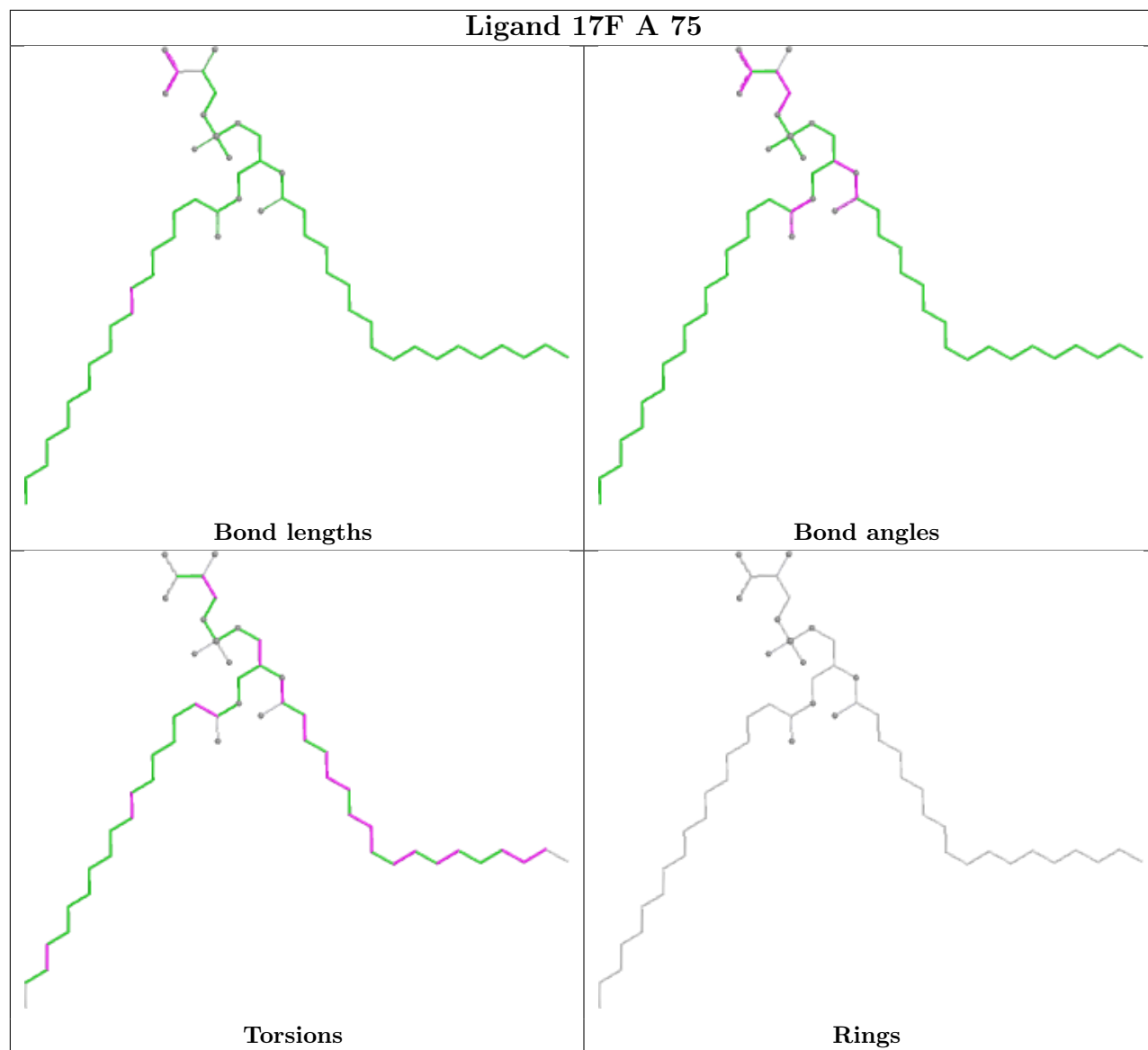


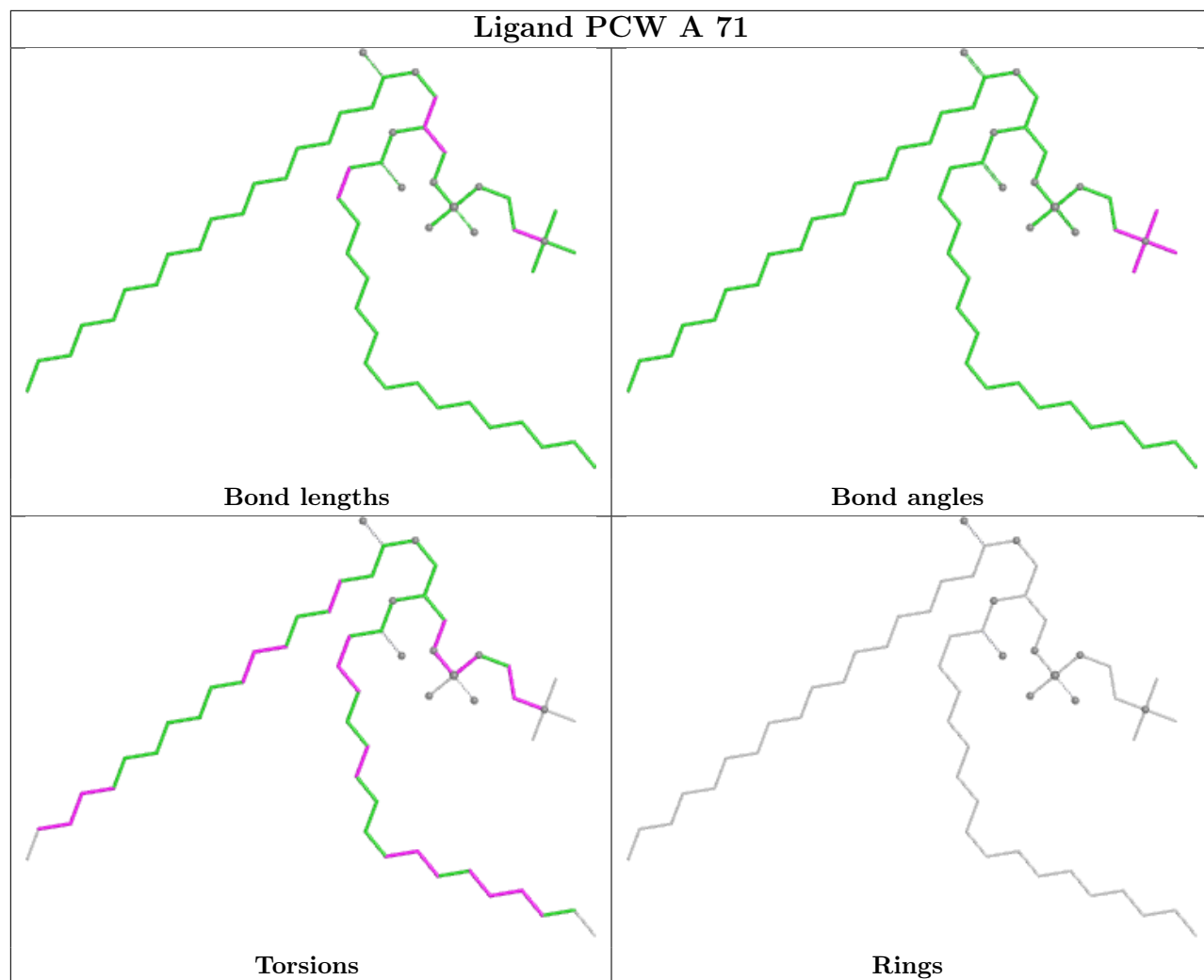


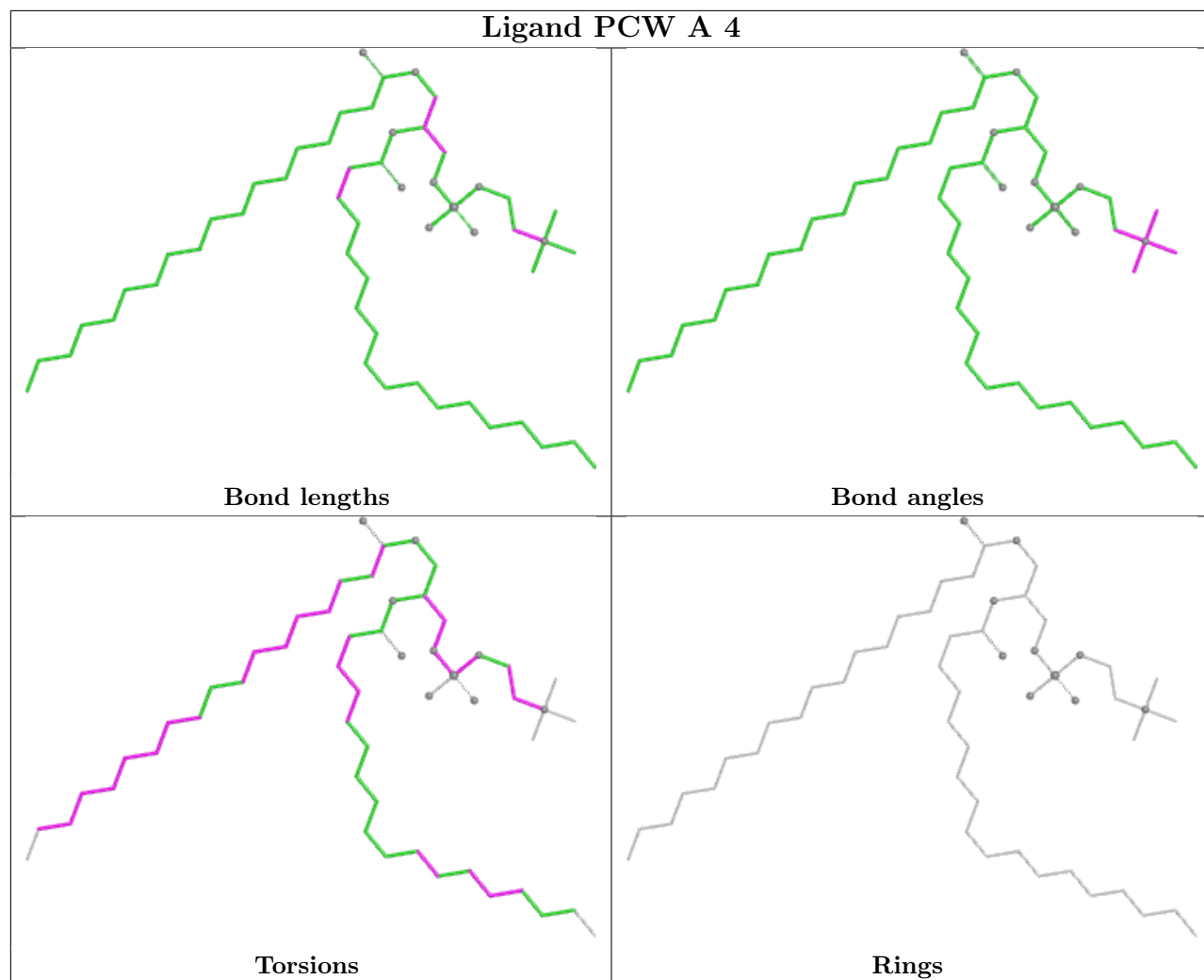


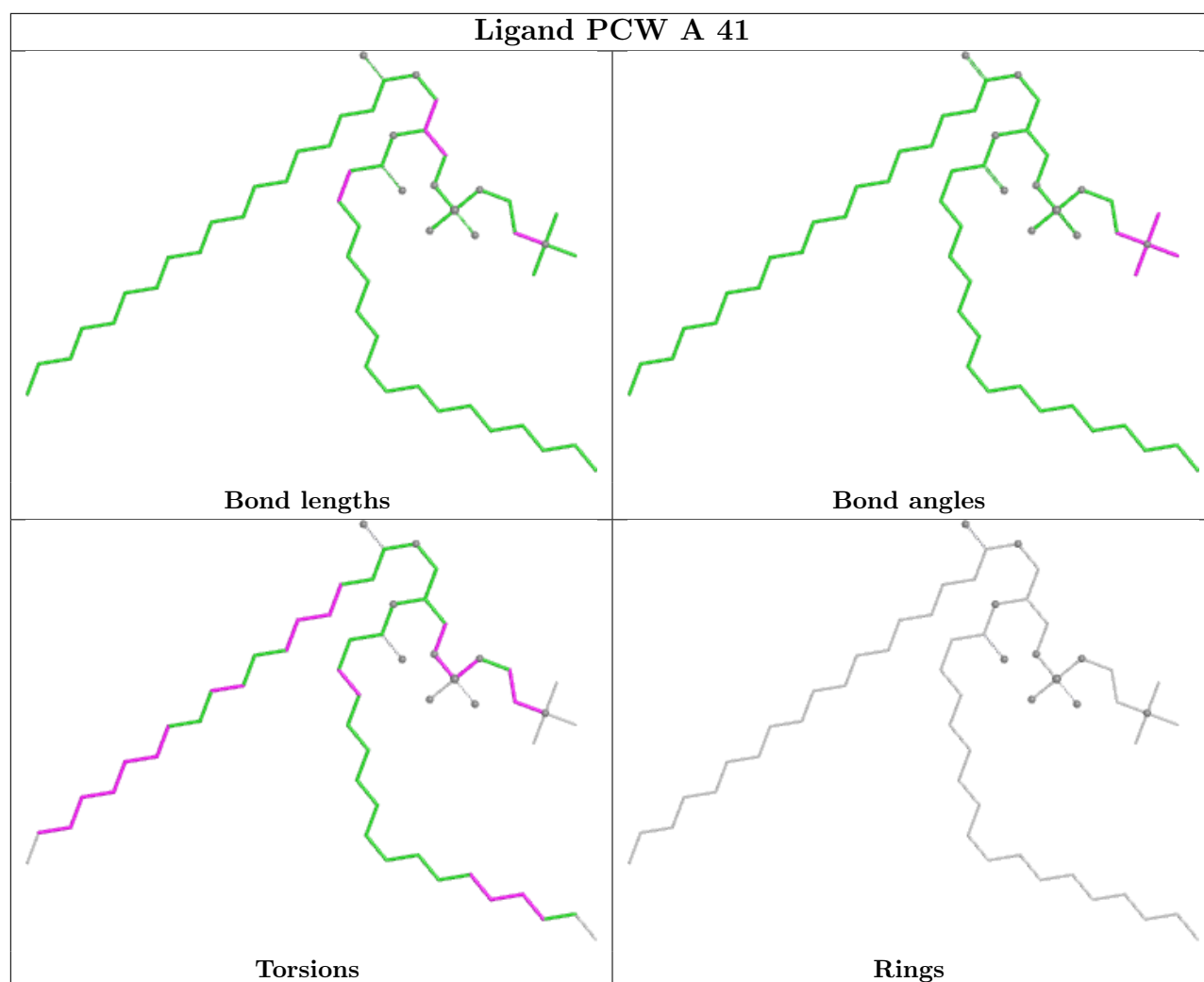












6.7 Other polymers [i](#)

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

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

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	52
Number of shifts mapped to atoms	13
Number of unparsed shifts	0
Number of shifts with mapping errors	39
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 39 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	21	ILE	HD11	0.565	?	1
1	B	21	ILE	HD12	0.565	?	1
1	B	21	ILE	HD13	0.565	?	1
1	B	24	ILE	HD11	0.379	?	1
1	B	24	ILE	HD12	0.379	?	1
1	B	24	ILE	HD13	0.379	?	1
1	B	36	ILE	HD11	0.55	?	1
1	B	36	ILE	HD12	0.55	?	1
1	B	36	ILE	HD13	0.55	?	1
1	B	46	ILE	HD11	0.381	?	1
1	B	46	ILE	HD12	0.381	?	1
1	B	46	ILE	HD13	0.381	?	1
1	B	55	ILE	HD11	0.472	?	1
1	B	55	ILE	HD12	0.472	?	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	55	ILE	HD13	0.472	?	1
1	B	84	ILE	HD11	0.705	?	1
1	B	84	ILE	HD12	0.705	?	1
1	B	84	ILE	HD13	0.705	?	1
1	B	93	ILE	HD11	0.728	?	1
1	B	93	ILE	HD12	0.728	?	1
1	B	93	ILE	HD13	0.728	?	1
1	B	100	ILE	HD11	0.245	?	1
1	B	100	ILE	HD12	0.245	?	1
1	B	100	ILE	HD13	0.245	?	1
1	B	139	ILE	HD11	0.835	?	1
1	B	139	ILE	HD12	0.835	?	1
1	B	139	ILE	HD13	0.835	?	1
1	B	142	ILE	HD11	0.619	?	1
1	B	142	ILE	HD12	0.619	?	1
1	B	142	ILE	HD13	0.619	?	1
1	D	854	ILE	HD11	0.766	?	1
1	D	854	ILE	HD12	0.766	?	1
1	D	854	ILE	HD13	0.766	?	1
1	D	867	ILE	HD11	0.708	?	1
1	D	867	ILE	HD12	0.708	?	1
1	D	867	ILE	HD13	0.708	?	1
1	D	876	ILE	HD11	0.671	?	1
1	D	876	ILE	HD12	0.671	?	1
1	D	876	ILE	HD13	0.671	?	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. 52 atoms were assigned a chemical shift out of a possible 8368. 0 out of 118 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/2970 (0%)	0/1201 (0%)	0/1192 (0%)	0/577 (0%)
Sidechain	52/4930 (1%)	39/3176 (1%)	13/1535 (1%)	0/219 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/468 (0%)	0/240 (0%)	0/228 (0%)	0/0 (—%)
Overall	52/8368 (1%)	39/4617 (1%)	13/2955 (0%)	0/796 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 52 atoms were assigned a chemical shift out of a possible 9193. 0 out of 128 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/3261 (0%)	0/1319 (0%)	0/1308 (0%)	0/634 (0%)
Sidechain	52/5422 (1%)	39/3488 (1%)	13/1693 (1%)	0/241 (0%)
Aromatic	0/510 (0%)	0/262 (0%)	0/248 (0%)	0/0 (—%)
Overall	52/9193 (1%)	39/5069 (1%)	13/3249 (0%)	0/875 (0%)

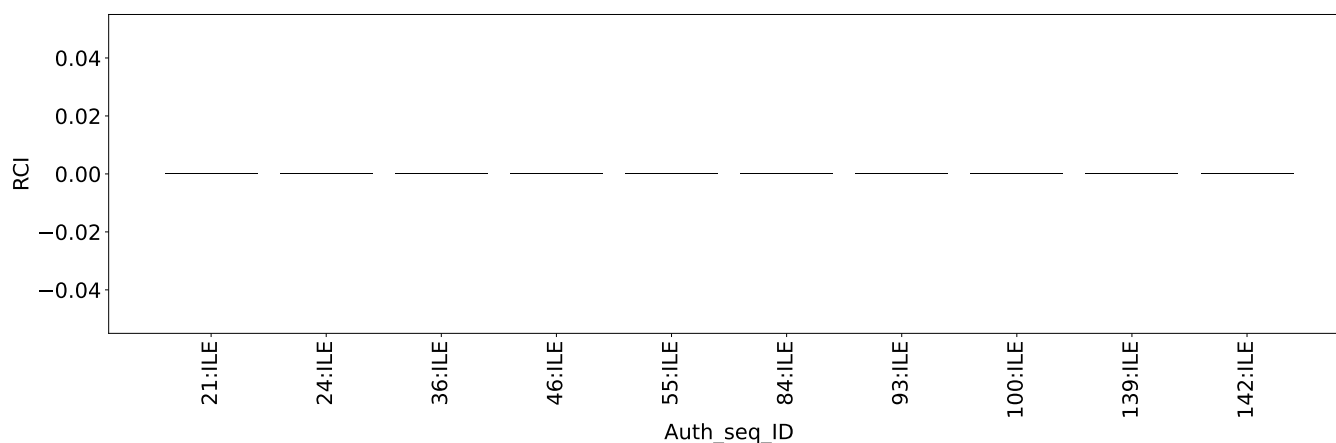
7.1.4 Statistically unusual chemical shifts [i](#)

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:



Random coil index (RCI) for chain D:

