



Full wwPDB NMR Structure Validation Report ⓘ

Mar 23, 2026 – 06:34 AM UTC

PDB ID : 6CC9 / pdb_00006cc9
BMRB ID : 30400
Title : NMR data-driven model of GTPase KRas-GMPPNP:Cmpd2 complex tethered to a nanodisc
Authors : Fang, Z.; Marshall, C.B.; Nishikawa, T.; Gossert, A.D.; Jansen, J.M.; Jahnke, W.; Ikura, M.
Deposited on : 2018-02-06

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

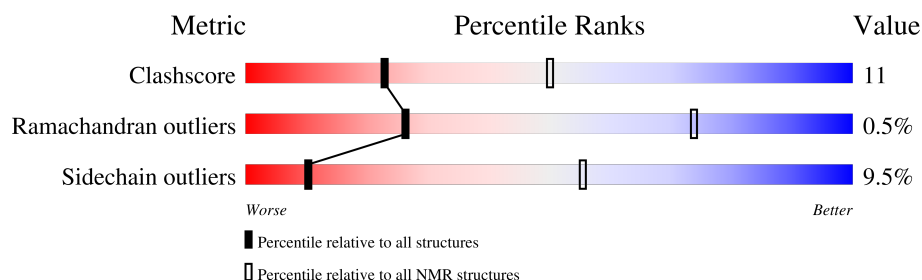
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 3%.

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% 12% ..
2	B	187	82% 9% 7% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 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	8
2	B:2-B:172 (171)	0.88	8

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

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

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

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

3 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9535 atoms, of which 429 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

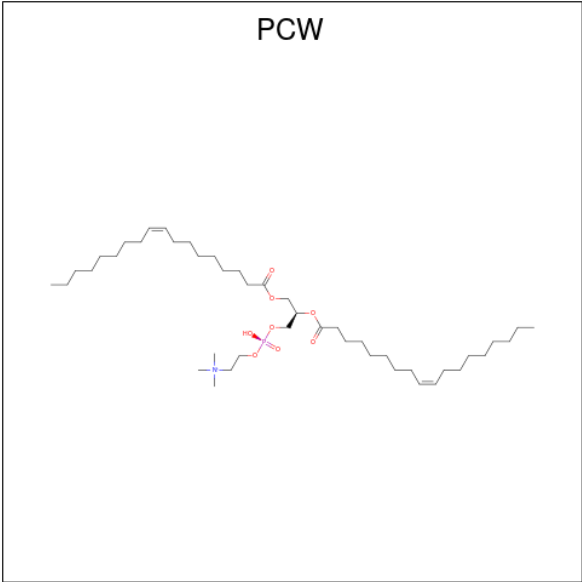
- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
2	B	185	Total	C	H	N	O	S	0
			1842	926	363	257	287	9	

There are 3 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
B	12	VAL	GLY	engineered mutation	UNP P01116

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



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

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

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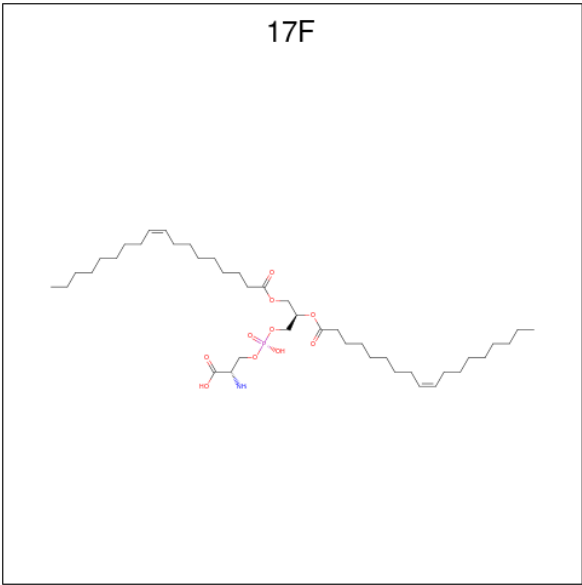
Mol	Chain	Residues	Atoms				
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44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

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

- Molecule 4 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (CCD ID: 17F) (formula: C₄₂H₇₈NO₁₀P).



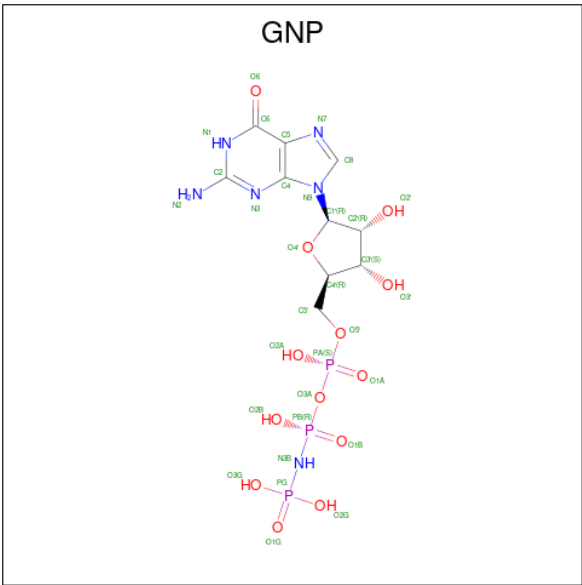
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1

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

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

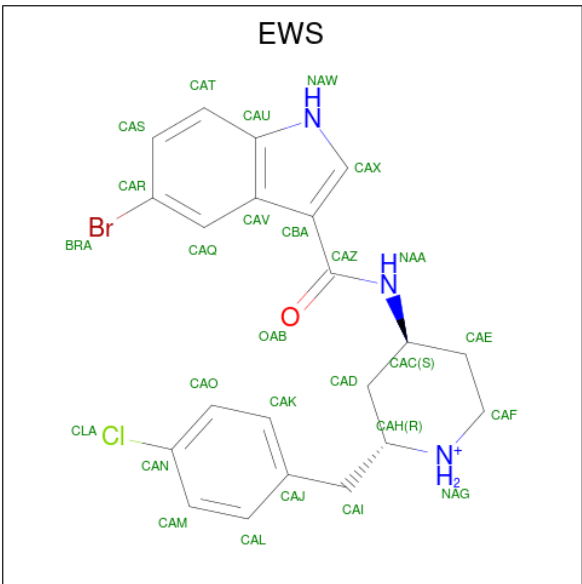


Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
5	B	1	32	10	6	13	3

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
			Total	Mg
6	B	1	1	1

- Molecule 7 is (2R,4S)-4-[(5-bromo-1H-indole-3-carbonyl)amino]-2-[(4-chlorophenyl)methyl]piperidin-1-ium (CCD ID: EWS) (formula: C₂₁H₂₂BrClN₃O).



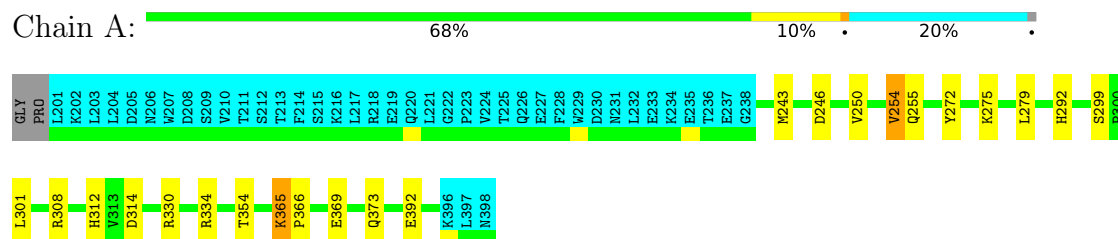
Mol	Chain	Residues	Atoms						
			Total	Br	C	Cl	H	N	O
7	B	1	49	1	21	1	22	3	1

4 Residue-property plots

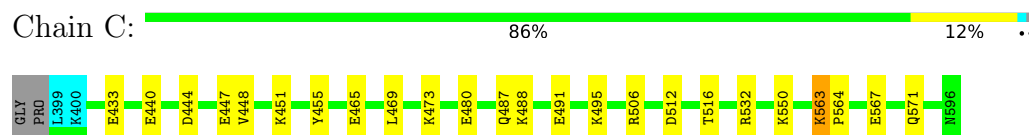
4.1 Average score per residue in the NMR ensemble

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.

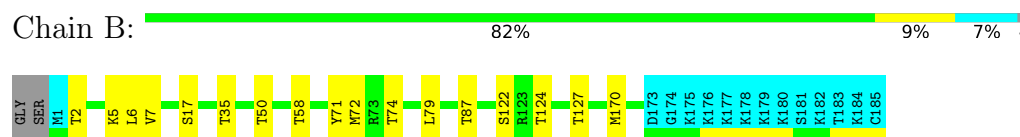
• Molecule 1: Apolipoprotein A-I



• Molecule 1: Apolipoprotein A-I



• Molecule 2: GTPase KRas



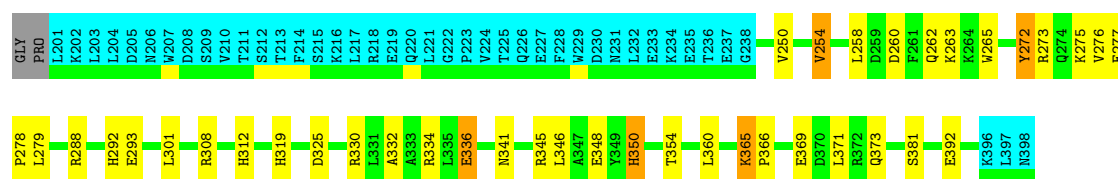
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Apolipoprotein A-I





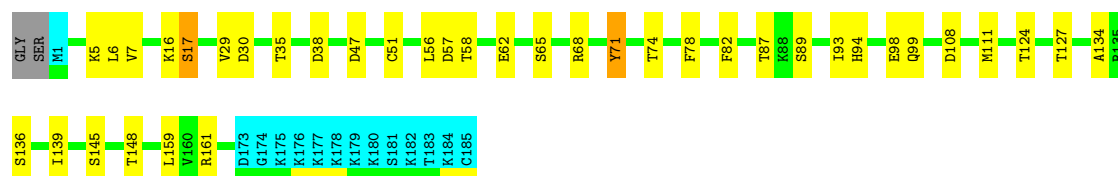
• Molecule 1: Apolipoprotein A-I

Chain C: 76% 18% ..



• Molecule 2: GTPase KRas

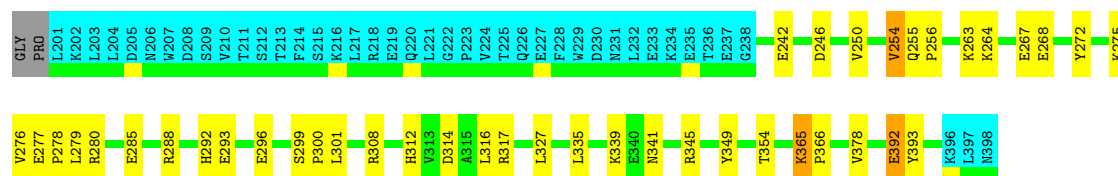
Chain B: 71% 19% 7% ..



4.2.2 Score per residue for model 2

• Molecule 1: Apolipoprotein A-I

Chain A: 58% 20% 20% ..

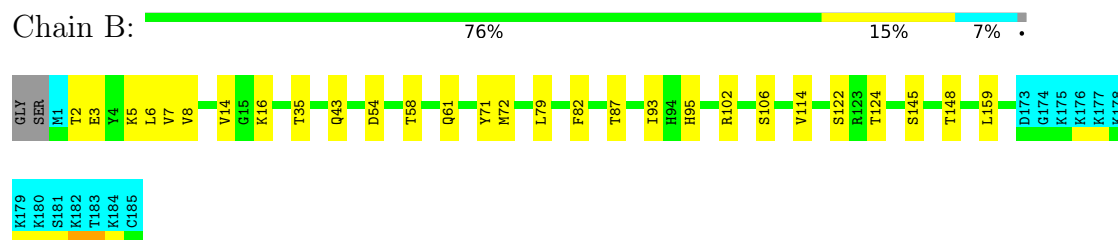


• Molecule 1: Apolipoprotein A-I

Chain C: 76% 20% ..

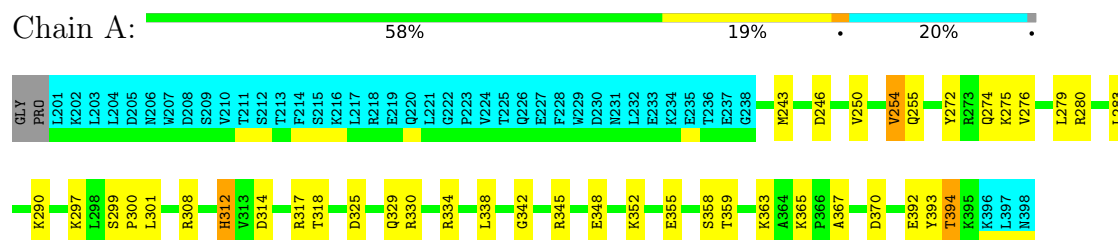


• Molecule 2: GTPase KRas

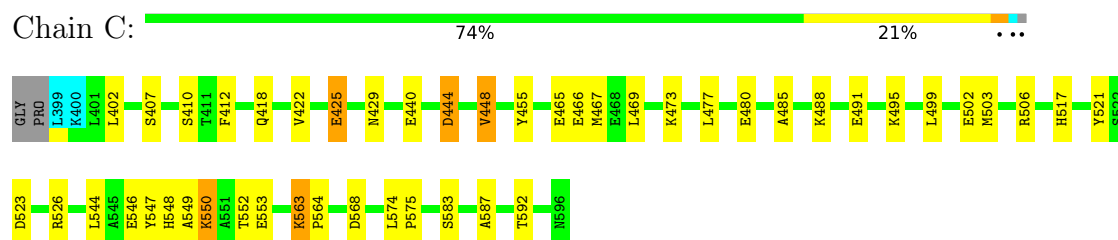


4.2.3 Score per residue for model 3

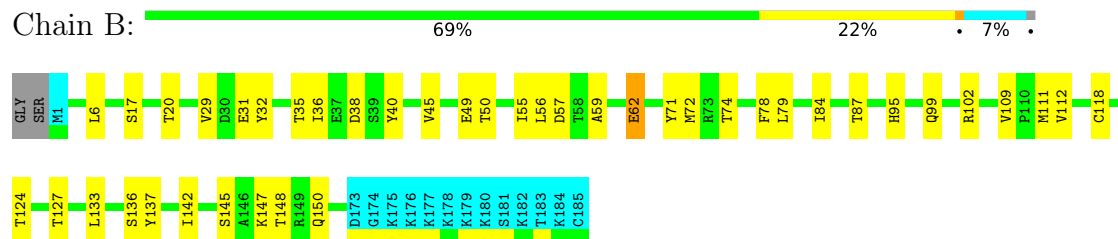
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



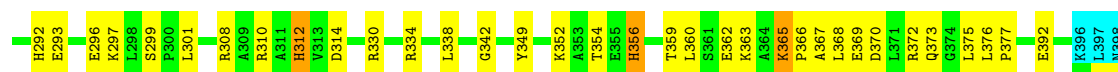
- Molecule 2: GTPase KRas



4.2.4 Score per residue for model 4

- Molecule 1: Apolipoprotein A-I





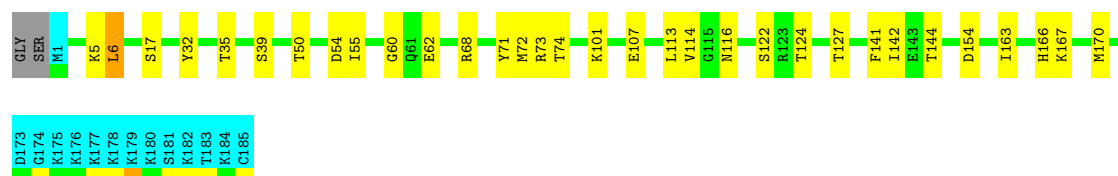
- Molecule 1: Apolipoprotein A-I

Chain C: 74% 23% ...



- Molecule 2: GTPase KRas

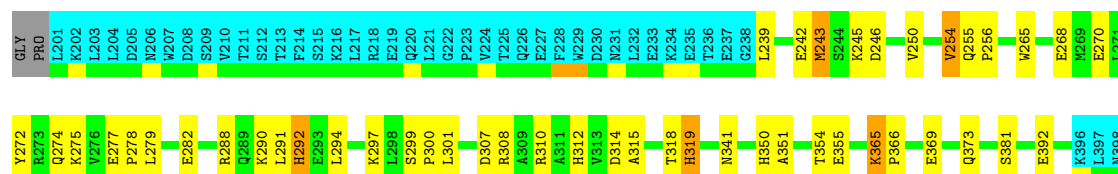
Chain B: 74% 17% 7%



4.2.5 Score per residue for model 5

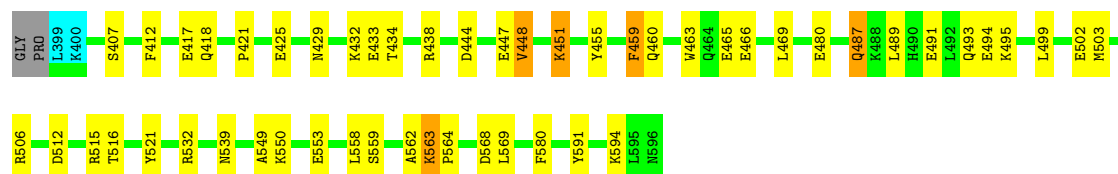
- Molecule 1: Apolipoprotein A-I

Chain A: 55% 21% 20%



- Molecule 1: Apolipoprotein A-I

Chain C: 72% 24% ...



- Molecule 2: GTPase KRas

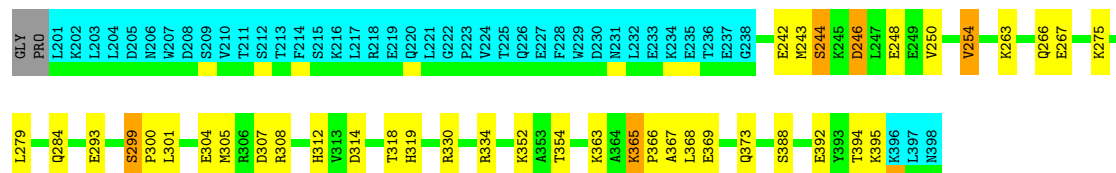
Chain B: 80% 12% 7%



4.2.6 Score per residue for model 6

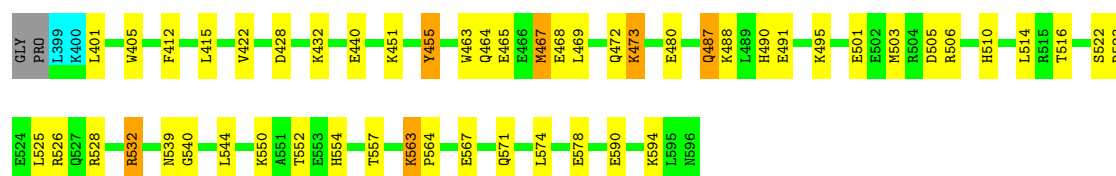
- Molecule 1: Apolipoprotein A-I

Chain A: 58% 18% 20%



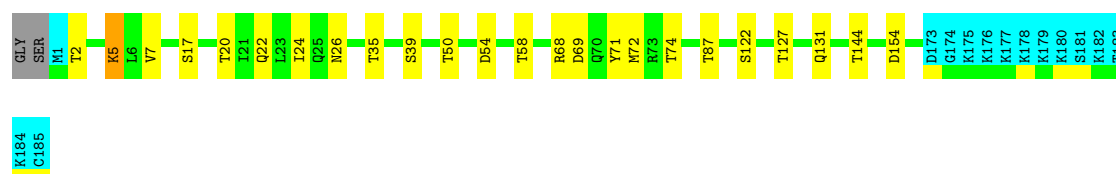
- Molecule 1: Apolipoprotein A-I

Chain C: 72% 23%



- Molecule 2: GTPase KRas

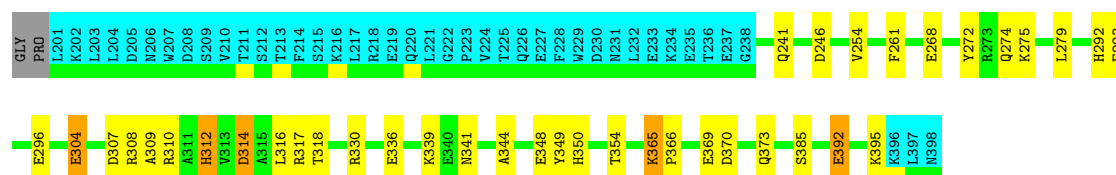
Chain B: 79% 12% 7%



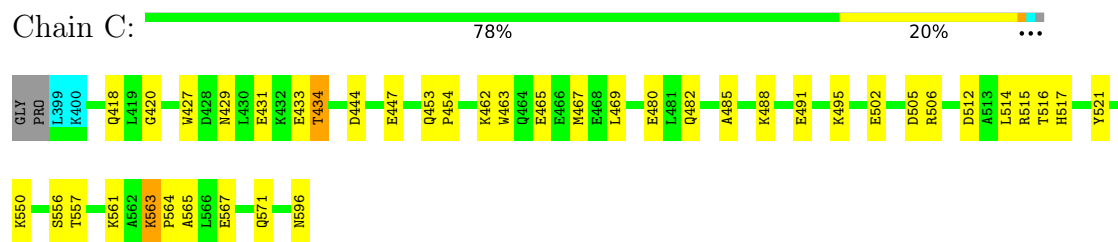
4.2.7 Score per residue for model 7

- Molecule 1: Apolipoprotein A-I

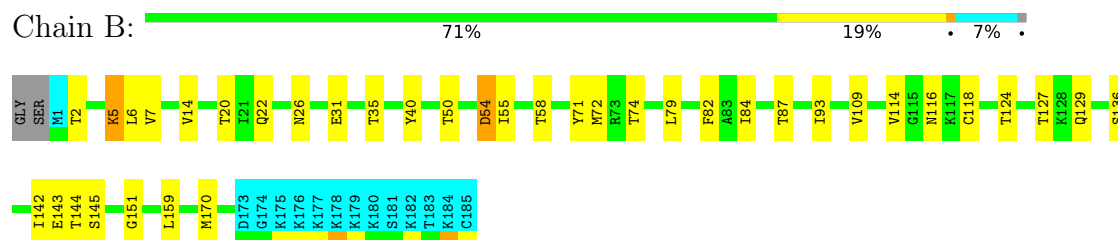
Chain A: 59% 17% 20%



- Molecule 1: Apolipoprotein A-I

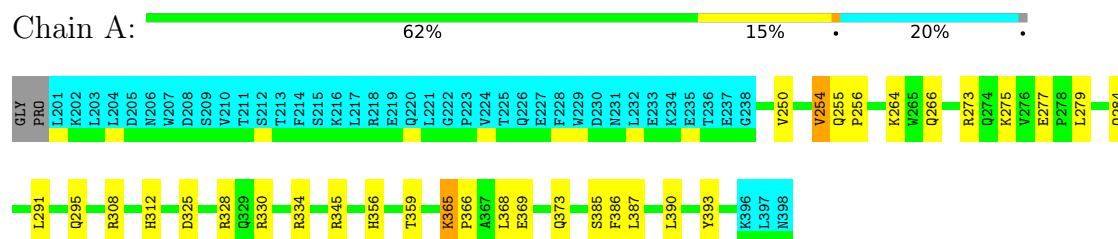


- Molecule 2: GTPase KRas

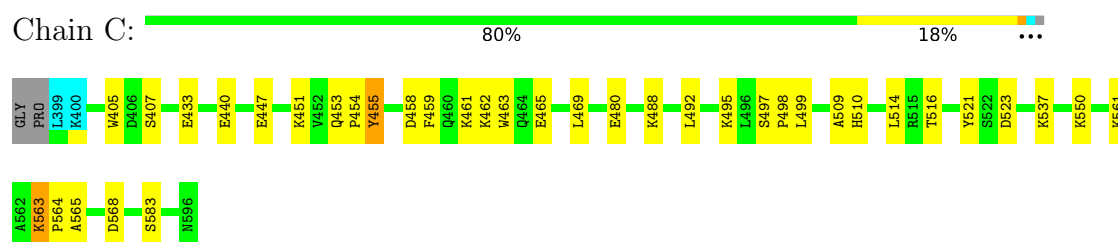


4.2.8 Score per residue for model 8 (medoid)

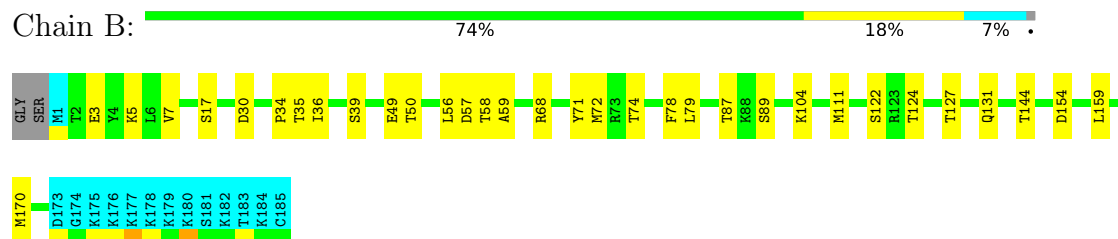
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

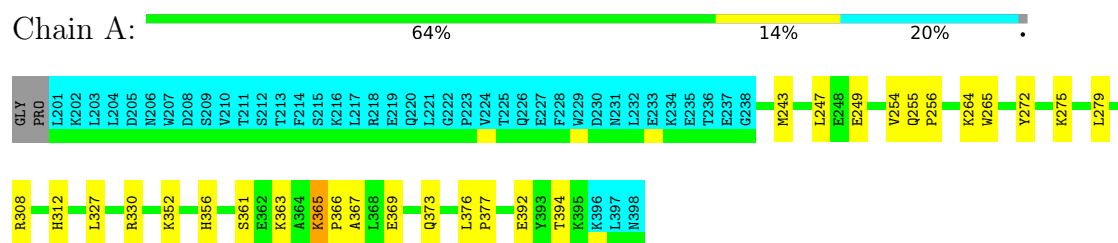


- Molecule 2: GTPase KRas

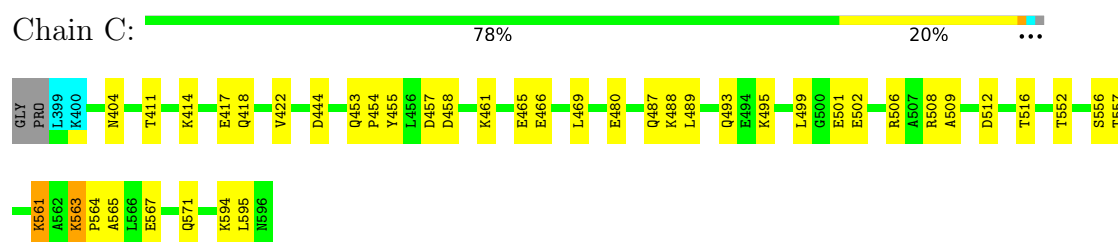


4.2.9 Score per residue for model 9

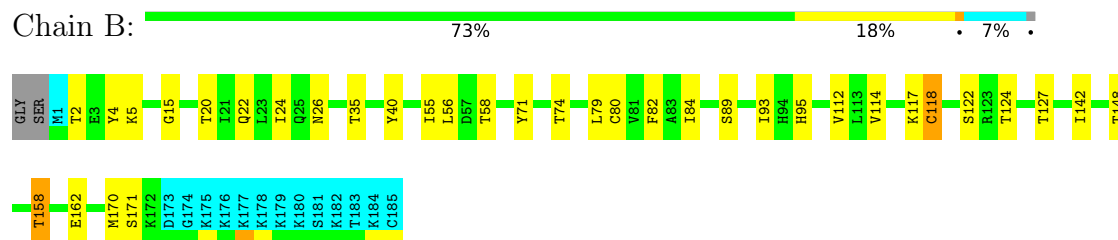
• Molecule 1: Apolipoprotein A-I



• Molecule 1: Apolipoprotein A-I

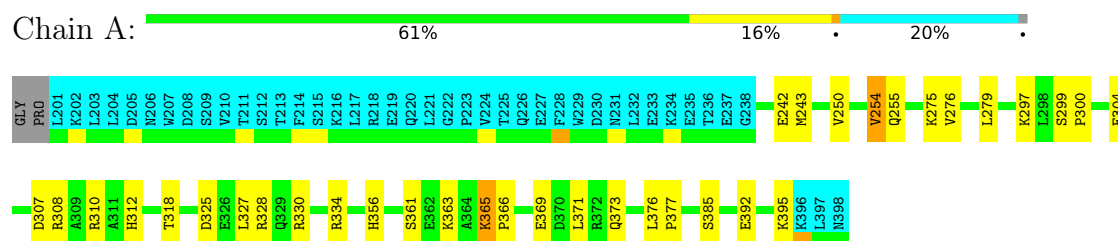


• Molecule 2: GTPase KRas

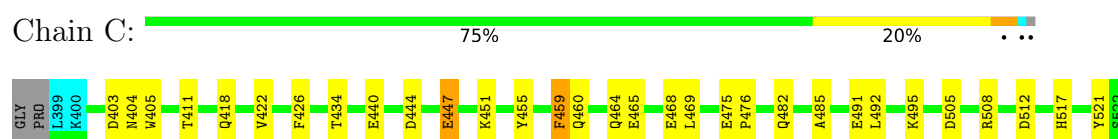


4.2.10 Score per residue for model 10

• Molecule 1: Apolipoprotein A-I

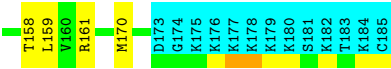
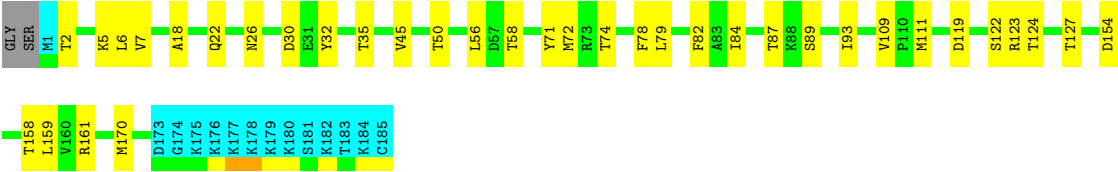


• Molecule 1: Apolipoprotein A-I





● Molecule 2: GTPase KRas



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: *10 structures for lowest energy*.

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

Software name	Classification	Version
CNS	refinement	
HADDOCK	structure calculation	

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	268
Number of shifts mapped to atoms	193
Number of unparsed shifts	0
Number of shifts with mapping errors	75
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

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: 17F, EWS, MG, PCW, GNP

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±0/1390 (0.0± 0.0%)	0.67±0.03	0±0/1875 (0.0± 0.0%)
All	All	0.38	0/43290 (0.0%)	0.75	2/58230 (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	5	LYS	CD-CE-NZ	13.26	154.32	111.90	6	2

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	28±5
1	C	1607	22	1603	35±8
2	B	1368	322	1356	17±5
3	A	540	0	840	32±9
3	B	1512	0	2351	78±17
3	C	1404	0	2182	63±16

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
4	A	54	0	76	5±2
4	B	432	0	608	37±5
4	C	378	0	532	26±7
5	B	32	0	13	1±1
7	B	27	22	0	9±4
All	All	86390	3840	108600	2184

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:72:MET:HA	7:B:239:EWS:BRA	1.57	1.53	3	5
1:A:308:ARG:CD	1:C:469:LEU:HD11	1.48	1.34	10	1
1:A:393:TYR:CE1	3:A:406:PCW:H271	1.45	1.46	8	1
1:A:393:TYR:CD1	3:A:406:PCW:C27	1.43	2.01	8	2
1:A:393:TYR:CD1	3:A:406:PCW:H271	1.37	1.51	8	1
1:A:393:TYR:HD1	3:A:406:PCW:C27	1.33	1.31	8	1
1:C:465:GLU:O	1:C:469:LEU:HG	1.28	1.19	9	9
2:B:72:MET:HB3	7:B:239:EWS:BRA	1.26	1.83	10	1
1:C:465:GLU:O	1:C:469:LEU:CG	1.26	1.82	4	6
1:A:308:ARG:CG	1:C:469:LEU:HD11	1.21	1.63	10	3
3:B:221:PCW:C5	3:C:601:PCW:H61	1.20	1.64	4	1
2:B:71:TYR:O	7:B:239:EWS:BRA	1.20	2.13	7	7
3:A:403:PCW:C38	3:B:218:PCW:H471	1.18	1.67	1	1
1:A:308:ARG:CD	1:C:469:LEU:CD1	1.18	2.21	10	1
3:B:221:PCW:O4P	3:C:601:PCW:C6	1.16	1.93	4	1
2:B:72:MET:CA	7:B:239:EWS:BRA	1.16	2.48	3	3
1:A:308:ARG:HG3	1:C:469:LEU:CD1	1.14	1.72	6	4
2:B:7:VAL:HG13	7:B:239:EWS:CAS	1.14	1.70	1	3
3:C:601:PCW:H441	4:C:627:17F:H54	1.14	1.18	8	1
1:A:308:ARG:HD3	1:C:469:LEU:CD1	1.11	1.75	10	2
1:A:393:TYR:HD1	3:A:406:PCW:H272	1.11	0.99	8	1
3:C:601:PCW:H483	3:C:605:PCW:C48	1.11	1.75	10	1
3:C:620:PCW:C16	4:C:633:17F:H29	1.10	1.76	4	1
1:A:368:LEU:HD11	4:B:230:17F:H54	1.10	1.18	8	1
3:B:221:PCW:H161	3:C:601:PCW:C38	1.10	1.72	10	1
3:B:221:PCW:H161	3:C:601:PCW:H372	1.09	1.25	8	1
2:B:72:MET:CB	7:B:239:EWS:BRA	1.08	2.55	10	1
3:B:221:PCW:C5	3:C:601:PCW:C6	1.08	2.32	4	1
1:C:488:LYS:HD2	3:C:620:PCW:H281	1.07	1.25	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ARG:CG	1:C:469:LEU:CD1	1.05	2.34	10	2
3:B:207:PCW:H222	3:C:601:PCW:H452	1.05	1.27	8	1
3:B:207:PCW:C22	3:C:601:PCW:H452	1.05	1.79	8	1
2:B:7:VAL:HB	7:B:239:EWS:CAT	1.05	1.81	10	3
3:C:620:PCW:C14	4:C:633:17F:H59	1.05	1.81	4	1
1:C:567:GLU:O	1:C:571:GLN:HG3	1.05	1.48	9	7
1:A:308:ARG:CD	1:C:469:LEU:HD21	1.04	1.82	7	2
3:C:601:PCW:C48	3:C:605:PCW:H481	1.04	1.82	10	1
3:A:403:PCW:H20	3:C:606:PCW:H282	1.04	1.30	1	1
3:B:221:PCW:H51	3:C:601:PCW:H61	1.03	1.30	4	1
1:A:308:ARG:HG3	1:C:469:LEU:HD11	1.02	1.26	2	3
1:A:349:TYR:CE2	3:A:401:PCW:H262	1.02	1.89	7	1
3:B:221:PCW:H181	3:C:601:PCW:H411	1.02	1.23	10	1
3:A:403:PCW:H222	3:C:606:PCW:H282	1.01	1.28	1	1
3:A:403:PCW:H382	3:B:218:PCW:H471	1.01	1.18	1	1
3:C:601:PCW:C48	3:C:605:PCW:C48	1.01	2.37	10	1
1:A:308:ARG:HG3	1:C:469:LEU:HD21	1.00	1.27	1	6
1:A:308:ARG:HD2	1:C:469:LEU:HD21	1.00	1.33	10	2
3:B:217:PCW:H432	3:B:223:PCW:H451	0.99	1.32	5	1
3:B:223:PCW:H471	4:C:632:17F:H76	0.99	1.34	5	1
3:B:223:PCW:H281	1:C:521:TYR:CE2	0.98	1.93	5	1
1:C:488:LYS:NZ	3:C:620:PCW:H261	0.98	1.72	4	1
3:B:221:PCW:H141	3:C:601:PCW:H351	0.98	1.31	4	1
3:B:221:PCW:H411	3:C:601:PCW:H39	0.97	1.35	10	1
1:A:369:GLU:O	1:A:373:GLN:HG3	0.97	1.58	1	8
3:C:620:PCW:H162	4:C:633:17F:C1X	0.96	1.90	4	1
1:A:308:ARG:HD3	1:C:469:LEU:HD11	0.95	0.97	10	2
3:B:217:PCW:H451	3:B:223:PCW:H462	0.95	1.32	5	1
3:B:221:PCW:C12	3:C:601:PCW:H362	0.95	1.77	10	1
3:C:620:PCW:H131	4:C:633:17F:H56	0.94	1.38	4	1
1:C:488:LYS:HD3	3:C:620:PCW:H283	0.94	1.34	9	1
3:A:410:PCW:H332	4:C:630:17F:H29	0.94	1.35	1	2
3:B:221:PCW:H52	3:C:601:PCW:C6	0.93	1.90	4	1
3:B:201:PCW:H361	3:B:220:PCW:H352	0.93	1.39	10	1
3:B:221:PCW:H161	3:C:601:PCW:C39	0.93	1.93	10	1
3:B:216:PCW:H62	3:C:601:PCW:C7	0.93	1.92	4	1
1:A:297:LYS:HE2	1:C:477:LEU:HG	0.92	1.39	4	1
3:B:216:PCW:H62	3:C:601:PCW:H73	0.92	1.41	4	1
2:B:7:VAL:HA	7:B:239:EWS:NAW	0.92	1.78	5	1
3:C:620:PCW:H162	4:C:633:17F:H29	0.92	0.94	4	2
3:A:403:PCW:H222	3:C:606:PCW:C28	0.92	1.94	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:210:PCW:H322	3:B:214:PCW:H132	0.92	1.42	4	1
1:C:465:GLU:O	1:C:469:LEU:CB	0.92	2.16	4	2
3:C:601:PCW:H483	3:C:605:PCW:H481	0.91	1.32	10	1
3:B:221:PCW:H241	3:C:601:PCW:C19	0.90	1.94	10	2
3:B:205:PCW:H41	3:B:222:PCW:H71	0.90	1.41	10	1
1:C:488:LYS:NZ	3:C:620:PCW:C26	0.90	2.34	4	1
3:B:221:PCW:O4P	3:C:601:PCW:H63	0.90	1.65	4	1
1:A:393:TYR:CE1	3:A:406:PCW:C27	0.90	2.40	8	1
3:C:618:PCW:H352	3:C:626:PCW:H162	0.89	1.43	5	2
3:B:211:PCW:H332	4:B:226:17F:H19	0.89	1.44	10	1
3:B:211:PCW:H362	4:B:226:17F:H8	0.89	1.44	10	2
3:B:217:PCW:H472	3:B:223:PCW:H483	0.88	1.43	5	1
3:B:221:PCW:H211	3:C:601:PCW:H411	0.88	1.44	4	1
3:B:201:PCW:H31	3:B:203:PCW:H342	0.88	1.43	7	1
3:C:620:PCW:H141	4:C:633:17F:H59	0.88	1.45	4	1
1:C:488:LYS:HD2	3:C:620:PCW:H272	0.88	1.43	4	1
1:A:393:TYR:HE1	3:A:406:PCW:H271	0.88	1.22	8	1
3:B:221:PCW:C18	3:C:601:PCW:H411	0.87	2.00	10	1
1:A:393:TYR:CD1	3:A:406:PCW:H272	0.87	1.83	8	1
3:B:223:PCW:C47	4:C:632:17F:H76	0.86	1.99	5	1
1:C:488:LYS:HZ1	3:C:620:PCW:H261	0.86	1.22	4	1
2:B:72:MET:CG	7:B:239:EWS:BRA	0.86	2.79	10	2
3:B:221:PCW:C16	3:C:601:PCW:C39	0.86	2.53	10	1
1:A:308:ARG:HD2	1:C:469:LEU:CD2	0.86	2.00	10	1
3:B:221:PCW:H161	3:C:601:PCW:H381	0.86	1.48	10	1
3:A:410:PCW:H372	4:C:630:17F:H36	0.85	1.46	2	2
3:C:618:PCW:H362	3:C:626:PCW:H152	0.85	1.48	9	2
1:A:393:TYR:CD1	3:A:406:PCW:H283	0.85	2.06	2	1
2:B:7:VAL:HG13	7:B:239:EWS:CAT	0.84	2.02	1	2
3:B:221:PCW:H272	3:C:601:PCW:H221	0.84	1.48	2	2
3:B:221:PCW:C4	3:C:601:PCW:C6	0.84	2.55	4	1
3:B:223:PCW:H481	4:C:632:17F:H78	0.84	1.49	5	1
3:B:210:PCW:H71	4:B:226:17F:HN1A	0.84	1.32	3	1
1:C:465:GLU:O	1:C:469:LEU:CD1	0.84	2.24	4	2
4:A:407:17F:H9A	3:B:205:PCW:H332	0.84	1.47	9	1
3:A:406:PCW:H121	4:A:407:17F:H57	0.83	1.51	1	4
3:B:221:PCW:H241	3:C:601:PCW:H19	0.83	1.50	10	1
4:C:630:17F:H1	4:C:630:17F:H4	0.83	1.48	1	3
3:B:207:PCW:C22	3:C:601:PCW:C45	0.83	2.56	8	1
4:B:230:17F:H1	4:B:230:17F:H4	0.83	1.46	9	1
1:C:488:LYS:CG	3:C:620:PCW:H281	0.82	2.03	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:221:PCW:C11	3:C:601:PCW:H362	0.82	2.03	10	1
2:B:5:LYS:HD3	7:B:239:EWS:CAX	0.82	2.05	8	3
4:C:628:17F:H65	4:C:632:17F:H11	0.82	1.48	1	4
3:A:406:PCW:H342	4:B:227:17F:H11	0.81	1.50	6	2
3:B:207:PCW:H221	3:C:601:PCW:C45	0.81	2.05	8	1
1:C:563:LYS:HB2	1:C:564:PRO:HD3	0.81	1.52	2	9
3:B:221:PCW:O4P	3:C:601:PCW:H62	0.81	1.71	4	1
1:A:279:LEU:HD22	1:C:495:LYS:HG2	0.80	1.53	10	7
3:A:410:PCW:H121	4:C:630:17F:H30	0.80	1.54	9	7
1:C:488:LYS:HD3	3:C:620:PCW:C28	0.80	2.05	9	1
3:A:403:PCW:H382	3:B:218:PCW:C47	0.80	2.05	1	1
4:C:630:17F:H2	4:C:630:17F:H4A	0.80	1.52	9	5
3:B:214:PCW:H281	4:C:627:17F:H78	0.80	1.52	6	1
3:B:223:PCW:H481	4:C:632:17F:C42	0.80	2.06	5	1
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.79	1.55	4	8
4:B:226:17F:H47	4:C:628:17F:H55	0.79	1.54	5	1
3:B:206:PCW:H332	3:B:211:PCW:H342	0.79	1.52	6	1
3:C:618:PCW:H372	3:C:626:PCW:H152	0.79	1.55	3	2
3:B:221:PCW:C16	3:C:601:PCW:C40	0.79	2.61	10	1
3:B:221:PCW:H73	4:B:229:17F:H1	0.79	1.55	4	1
3:A:402:PCW:H41	4:A:407:17F:H1	0.79	1.55	10	1
3:C:607:PCW:H182	3:C:615:PCW:H351	0.78	1.56	7	2
1:C:488:LYS:HZ1	3:C:620:PCW:C26	0.78	1.90	4	1
3:C:607:PCW:H462	4:C:633:17F:H43	0.78	1.56	4	3
1:A:308:ARG:HD3	1:C:469:LEU:HD21	0.78	1.54	7	1
3:B:208:PCW:H73	3:B:218:PCW:H42	0.78	1.56	5	1
2:B:7:VAL:CB	7:B:239:EWS:CAT	0.78	2.60	10	1
1:C:488:LYS:HD2	3:C:620:PCW:C28	0.78	2.08	8	1
3:B:211:PCW:H121	4:B:226:17F:H18A	0.78	1.55	7	3
1:C:466:GLU:OE1	1:C:469:LEU:HD12	0.77	1.78	1	1
3:B:211:PCW:H152	4:B:226:17F:H4	0.77	1.53	5	1
3:B:211:PCW:H382	4:B:226:17F:H8	0.77	1.54	7	4
2:B:5:LYS:HD3	7:B:239:EWS:CBA	0.77	2.10	8	3
3:A:408:PCW:H351	3:A:410:PCW:H341	0.77	1.55	2	1
3:C:607:PCW:H381	3:C:615:PCW:H412	0.77	1.56	5	1
3:B:204:PCW:H122	3:B:212:PCW:H371	0.77	1.56	5	1
3:B:201:PCW:H371	4:B:228:17F:H37	0.77	1.56	10	1
1:A:349:TYR:CE2	3:A:401:PCW:C26	0.76	2.67	7	1
3:B:221:PCW:H162	3:C:601:PCW:C40	0.76	2.10	10	1
3:C:606:PCW:H361	3:C:612:PCW:H151	0.76	1.56	1	2
4:B:226:17F:H11	4:B:232:17F:H59	0.76	1.56	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:206:PCW:H121	3:B:220:PCW:H82	0.76	1.55	7	1
1:C:567:GLU:O	1:C:571:GLN:CG	0.76	2.34	9	3
3:C:611:PCW:H352	3:C:623:PCW:H382	0.75	1.58	4	1
3:B:221:PCW:H421	4:B:229:17F:H66	0.75	1.56	1	1
3:C:618:PCW:H381	3:C:626:PCW:H171	0.75	1.56	5	3
3:C:618:PCW:H361	3:C:626:PCW:H212	0.75	1.58	6	3
3:B:202:PCW:H341	3:B:202:PCW:H122	0.75	1.58	4	2
3:B:217:PCW:H73	4:B:226:17F:HN1A	0.75	1.41	4	2
3:B:201:PCW:H351	3:B:220:PCW:H341	0.75	1.58	5	1
3:B:218:PCW:H231	3:C:626:PCW:H282	0.75	1.56	5	1
3:A:403:PCW:C39	3:B:218:PCW:H471	0.75	2.11	1	1
3:C:621:PCW:H431	4:C:632:17F:H58	0.75	1.57	2	3
3:B:210:PCW:H71	4:B:226:17F:N1	0.75	1.97	3	1
3:B:209:PCW:H252	3:C:601:PCW:H471	0.75	1.59	4	1
3:B:220:PCW:H341	4:B:228:17F:H30	0.74	1.56	3	1
3:B:203:PCW:H421	4:B:228:17F:H11	0.74	1.59	4	1
3:C:624:PCW:H372	3:C:625:PCW:H152	0.74	1.56	4	1
3:C:606:PCW:H141	3:C:612:PCW:H121	0.74	1.58	3	1
1:A:308:ARG:CD	1:C:469:LEU:CG	0.74	2.66	10	1
3:B:213:PCW:H141	4:B:228:17F:H18	0.74	1.58	6	1
1:A:393:TYR:HD1	3:A:406:PCW:H283	0.74	1.43	2	1
3:C:601:PCW:C44	4:C:627:17F:H54	0.74	2.09	8	1
3:B:221:PCW:H261	3:C:601:PCW:H20	0.74	1.60	9	1
3:A:403:PCW:C20	3:C:606:PCW:H282	0.73	2.11	1	1
3:B:206:PCW:H20	3:B:220:PCW:H181	0.73	1.59	1	1
3:C:618:PCW:H352	3:C:626:PCW:H152	0.73	1.58	4	2
3:B:221:PCW:H52	3:C:601:PCW:H62	0.73	1.58	4	1
3:B:223:PCW:H281	1:C:521:TYR:HE2	0.73	1.40	5	1
3:B:221:PCW:H281	3:C:601:PCW:H242	0.73	1.59	6	1
4:B:227:17F:H64	3:C:619:PCW:H481	0.73	1.61	1	1
1:A:393:TYR:HD1	3:A:406:PCW:C28	0.73	1.96	2	1
2:B:79:LEU:HG	2:B:159:LEU:HD22	0.73	1.61	7	4
2:B:5:LYS:CE	7:B:239:EWS:OAB	0.73	2.36	8	3
3:B:222:PCW:H52	4:B:227:17F:HN1A	0.73	1.44	7	1
3:B:221:PCW:H361	4:B:229:17F:H34	0.73	1.61	8	1
1:A:356:HIS:CD2	3:A:401:PCW:C27	0.73	2.72	9	1
3:B:217:PCW:C45	3:B:223:PCW:H462	0.73	2.13	5	1
3:B:223:PCW:C48	4:C:632:17F:C42	0.73	2.67	5	1
2:B:72:MET:C	7:B:239:EWS:BRA	0.73	2.87	4	2
2:B:5:LYS:HB3	7:B:239:EWS:CAX	0.73	2.14	4	3
3:C:624:PCW:H372	3:C:625:PCW:H162	0.73	1.59	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:204:PCW:H271	3:B:218:PCW:H181	0.72	1.61	6	1
4:A:407:17F:H35	4:B:227:17F:H34	0.72	1.60	2	1
3:A:403:PCW:C22	3:C:606:PCW:H262	0.72	2.13	1	1
3:B:213:PCW:H131	3:B:213:PCW:H332	0.72	1.61	5	1
3:B:211:PCW:O1P	3:B:215:PCW:H82	0.72	1.84	4	1
3:A:406:PCW:H121	4:A:407:17F:H33	0.72	1.62	10	2
3:B:221:PCW:C28	3:C:601:PCW:H242	0.72	2.15	6	1
3:B:223:PCW:H281	1:C:521:TYR:CD2	0.72	2.19	5	1
3:B:217:PCW:H40	3:B:223:PCW:H451	0.71	1.59	5	1
2:B:5:LYS:NZ	7:B:239:EWS:OAB	0.71	2.21	7	3
3:A:403:PCW:H20	3:C:606:PCW:C28	0.71	2.13	1	1
3:B:223:PCW:C28	1:C:521:TYR:CE2	0.71	2.71	5	1
3:A:409:PCW:H181	3:C:613:PCW:H341	0.71	1.61	2	1
2:B:56:LEU:HD22	7:B:239:EWS:CAQ	0.71	2.14	8	2
3:B:207:PCW:H81	4:B:228:17F:HN1	0.71	1.45	8	1
3:B:221:PCW:C16	3:C:601:PCW:H372	0.71	2.10	8	1
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.71	1.63	10	2
4:C:630:17F:H1	4:C:630:17F:C4	0.71	2.15	1	3
3:B:211:PCW:H331	4:B:226:17F:H19	0.71	1.62	2	1
1:C:465:GLU:O	1:C:469:LEU:HB2	0.71	1.86	4	1
1:C:488:LYS:HD3	3:C:620:PCW:H281	0.71	1.61	7	1
2:B:5:LYS:HE2	7:B:239:EWS:OAB	0.71	1.85	9	2
3:B:207:PCW:H481	3:C:604:PCW:H261	0.71	1.62	9	1
3:B:215:PCW:H52	3:B:217:PCW:H321	0.71	1.62	6	2
1:A:260:ASP:HA	1:A:263:LYS:HE2	0.71	1.60	1	1
3:A:408:PCW:H172	3:A:408:PCW:H382	0.70	1.62	1	1
3:C:620:PCW:C14	4:C:633:17F:C32	0.70	2.66	4	1
3:B:223:PCW:C28	1:C:521:TYR:HE2	0.70	1.98	5	1
3:B:217:PCW:H39	4:B:226:17F:H62	0.70	1.63	1	1
1:A:316:LEU:HG	1:C:462:LYS:HE3	0.70	1.63	7	2
3:B:204:PCW:H322	3:B:212:PCW:H332	0.70	1.62	5	1
2:B:5:LYS:CD	7:B:239:EWS:CAX	0.70	2.69	8	3
1:C:485:ALA:CB	3:C:620:PCW:H272	0.70	2.17	1	1
3:C:606:PCW:H351	3:C:612:PCW:H382	0.70	1.62	2	8
1:A:356:HIS:CD2	3:A:401:PCW:H272	0.70	2.20	9	1
3:B:233:PCW:H351	3:B:233:PCW:H122	0.70	1.62	9	4
3:B:211:PCW:H321	4:B:226:17F:H5	0.70	1.64	4	2
1:A:275:LYS:O	1:A:279:LEU:HG	0.70	1.87	1	9
3:A:403:PCW:H351	3:B:212:PCW:H462	0.70	1.63	1	1
1:C:473:LYS:HG2	4:C:629:17F:H76	0.70	1.64	6	1
2:B:7:VAL:HG22	7:B:239:EWS:CAS	0.70	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:H31	3:C:610:PCW:H352	0.69	1.63	1	2
1:A:341:ASN:HD21	1:C:433:GLU:HA	0.69	1.48	5	4
3:B:219:PCW:H441	3:B:225:PCW:H441	0.69	1.64	1	1
3:B:216:PCW:H42	4:B:229:17F:H1	0.69	1.64	2	1
3:C:609:PCW:H371	3:C:624:PCW:H361	0.69	1.64	10	1
4:B:227:17F:H10	4:B:227:17F:H58	0.69	1.64	6	2
1:A:393:TYR:CD1	3:A:406:PCW:C28	0.69	2.76	2	3
3:C:624:PCW:H39	3:C:625:PCW:H421	0.69	1.62	2	1
3:C:613:PCW:H281	3:C:623:PCW:H242	0.69	1.63	3	1
3:A:403:PCW:C22	3:C:606:PCW:H282	0.69	2.14	1	1
3:C:615:PCW:H211	4:C:629:17F:H41	0.69	1.64	5	1
3:B:211:PCW:H332	4:B:226:17F:C19	0.69	2.18	10	1
1:C:453:GLN:HB2	1:C:454:PRO:HD3	0.69	1.61	7	5
3:A:409:PCW:H242	3:A:410:PCW:H231	0.69	1.62	10	1
1:A:308:ARG:HD2	1:C:469:LEU:CG	0.69	2.17	10	1
3:B:210:PCW:H142	3:B:214:PCW:H151	0.68	1.64	5	4
3:B:221:PCW:C12	3:C:601:PCW:C36	0.68	2.55	10	1
4:B:226:17F:H42	4:B:232:17F:H66	0.68	1.64	10	1
4:C:632:17F:H8A	4:C:632:17F:H32	0.68	1.63	9	2
1:C:485:ALA:HB1	3:C:620:PCW:H272	0.68	1.64	1	2
3:A:406:PCW:H341	4:B:227:17F:H9	0.68	1.65	10	1
3:A:403:PCW:H52	4:B:231:17F:N1	0.68	2.03	7	1
2:B:56:LEU:HD23	7:B:239:EWS:BRA	0.68	2.43	8	2
3:B:204:PCW:H421	3:B:222:PCW:H182	0.68	1.65	10	1
2:B:56:LEU:CD2	7:B:239:EWS:BRA	0.68	2.97	8	2
3:B:211:PCW:H322	4:B:226:17F:H19	0.68	1.64	1	1
3:B:212:PCW:H152	4:B:231:17F:H6A	0.68	1.66	4	1
3:B:217:PCW:H151	4:B:226:17F:H34	0.68	1.66	7	1
1:A:308:ARG:CD	1:C:469:LEU:CD2	0.68	2.69	7	2
3:A:406:PCW:H152	4:A:407:17F:H33	0.68	1.66	3	1
3:C:607:PCW:H411	3:C:615:PCW:H432	0.68	1.66	3	2
3:B:210:PCW:H211	3:C:607:PCW:H461	0.68	1.66	4	1
3:A:406:PCW:H341	4:A:407:17F:H32	0.68	1.65	6	1
2:B:158:THR:HA	2:B:161:ARG:HD2	0.68	1.66	10	1
3:C:618:PCW:H122	3:C:626:PCW:H182	0.67	1.64	4	1
3:C:607:PCW:H242	3:C:615:PCW:H431	0.67	1.66	10	4
3:B:207:PCW:H83	4:B:228:17F:N1	0.67	2.03	3	1
1:C:418:GLN:O	1:C:422:VAL:HB	0.67	1.88	9	3
1:C:488:LYS:CD	3:C:620:PCW:H272	0.67	2.18	4	1
3:A:403:PCW:C22	3:C:606:PCW:C26	0.67	2.73	1	1
3:A:405:PCW:H431	3:C:609:PCW:H231	0.67	1.66	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:217:PCW:H40	3:B:223:PCW:C45	0.67	2.19	5	1
3:A:410:PCW:H322	4:C:630:17F:H37	0.67	1.66	8	2
3:A:401:PCW:H321	3:B:203:PCW:H152	0.67	1.66	8	1
3:C:606:PCW:H372	3:C:612:PCW:H182	0.67	1.67	10	3
4:B:232:17F:H49	3:C:624:PCW:H261	0.67	1.65	5	1
3:C:623:PCW:H371	3:C:623:PCW:H122	0.67	1.64	6	1
2:B:38:ASP:HB3	2:B:57:ASP:HB3	0.67	1.65	1	2
3:C:601:PCW:H422	4:C:627:17F:H54	0.67	1.65	3	1
4:B:236:17F:H57	3:C:622:PCW:H141	0.67	1.66	6	1
2:B:7:VAL:CG1	7:B:239:EWS:CAS	0.67	2.73	10	2
1:A:352:LYS:HG2	1:C:422:VAL:HG13	0.67	1.66	9	1
3:A:408:PCW:H371	3:A:410:PCW:H362	0.67	1.65	2	2
1:A:308:ARG:CB	1:C:469:LEU:HD11	0.67	2.20	10	3
3:C:618:PCW:H381	3:C:626:PCW:H161	0.67	1.66	8	2
3:C:617:PCW:H372	3:C:618:PCW:H121	0.67	1.67	3	1
3:B:217:PCW:H451	3:B:223:PCW:C46	0.67	2.18	5	1
3:B:202:PCW:H351	3:B:214:PCW:H321	0.66	1.65	6	1
3:B:201:PCW:H221	4:B:227:17F:H65	0.66	1.68	1	1
3:A:401:PCW:H61	3:B:213:PCW:H11	0.66	1.67	8	1
3:B:213:PCW:H251	3:B:213:PCW:H462	0.66	1.67	8	1
1:A:349:TYR:OH	3:A:401:PCW:C22	0.66	2.44	4	1
3:A:410:PCW:H331	4:C:630:17F:H29	0.66	1.65	4	1
3:C:618:PCW:H351	3:C:626:PCW:H182	0.66	1.67	10	2
3:B:215:PCW:H81	3:B:219:PCW:H73	0.66	1.65	4	1
3:A:410:PCW:H382	4:C:630:17F:H36	0.66	1.67	9	4
1:A:308:ARG:HD3	1:C:469:LEU:CD2	0.66	2.21	7	1
3:A:406:PCW:H351	4:A:407:17F:H56	0.66	1.68	1	1
3:B:201:PCW:H271	3:C:611:PCW:H472	0.66	1.68	2	1
3:C:601:PCW:C48	3:C:605:PCW:H483	0.66	2.19	10	1
3:A:403:PCW:H222	3:C:606:PCW:H262	0.66	1.67	1	1
3:C:624:PCW:H351	3:C:625:PCW:H152	0.66	1.67	1	4
3:B:216:PCW:H73	4:B:229:17F:H4A	0.66	1.68	8	1
3:C:607:PCW:H482	4:C:633:17F:H39	0.66	1.64	8	1
3:B:214:PCW:H181	4:B:229:17F:H35	0.66	1.68	2	1
1:A:349:TYR:OH	3:A:401:PCW:H221	0.66	1.89	4	1
2:B:5:LYS:HG3	7:B:239:EWS:OAB	0.66	1.90	1	1
3:C:606:PCW:H381	3:C:612:PCW:H152	0.66	1.66	2	1
3:B:221:PCW:H82	4:B:229:17F:O1	0.66	1.91	8	1
3:B:207:PCW:H131	3:B:216:PCW:H411	0.66	1.67	4	1
1:C:485:ALA:CB	3:C:620:PCW:H271	0.66	2.21	7	1
4:B:228:17F:H68	3:C:624:PCW:H481	0.66	1.66	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:617:PCW:H372	3:C:618:PCW:H142	0.65	1.68	4	2
3:C:620:PCW:H142	4:C:633:17F:H59	0.65	1.68	4	1
3:A:408:PCW:H321	3:C:610:PCW:H39	0.65	1.68	10	1
3:B:207:PCW:H131	3:B:216:PCW:H382	0.65	1.69	6	2
3:B:208:PCW:H151	3:B:222:PCW:H351	0.65	1.67	4	1
3:B:209:PCW:H252	3:C:601:PCW:C47	0.65	2.21	4	1
3:B:201:PCW:H11	4:B:230:17F:HN1	0.65	1.50	5	2
2:B:56:LEU:HD22	7:B:239:EWS:CAR	0.65	2.20	8	1
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.65	1.67	7	5
1:C:547:TYR:HA	1:C:550:LYS:HB2	0.65	1.69	3	1
2:B:7:VAL:HA	7:B:239:EWS:CAT	0.65	2.22	1	1
3:B:203:PCW:H12	3:B:213:PCW:H332	0.65	1.68	4	1
1:A:349:TYR:CZ	3:A:401:PCW:H221	0.65	2.27	4	1
3:B:211:PCW:H172	4:B:226:17F:H6	0.65	1.68	7	1
3:B:201:PCW:H12	4:B:230:17F:O1	0.65	1.92	5	2
3:B:221:PCW:H441	3:C:605:PCW:H471	0.65	1.68	3	1
3:B:223:PCW:C48	4:C:632:17F:H76	0.65	2.22	5	1
1:A:308:ARG:CG	1:C:469:LEU:HD21	0.64	2.15	3	2
3:A:406:PCW:H122	4:A:407:17F:H20	0.64	1.66	3	1
3:B:207:PCW:H483	3:C:601:PCW:H211	0.64	1.69	4	1
3:C:607:PCW:H472	4:C:633:17F:H42	0.64	1.69	10	1
3:B:207:PCW:H222	3:C:601:PCW:H361	0.64	1.69	1	1
3:B:201:PCW:H212	4:B:230:17F:H20A	0.64	1.69	8	1
3:A:410:PCW:H361	4:C:630:17F:H12A	0.64	1.67	3	2
1:C:488:LYS:HG2	3:C:620:PCW:H281	0.64	1.68	3	1
3:B:213:PCW:H381	3:B:213:PCW:H182	0.64	1.69	6	1
3:C:603:PCW:H332	3:C:607:PCW:H132	0.64	1.68	8	1
3:A:405:PCW:H181	4:B:228:17F:H58	0.64	1.67	4	1
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.64	1.69	8	2
1:A:308:ARG:HG3	1:C:469:LEU:CD2	0.64	2.16	3	6
3:A:403:PCW:H222	3:C:606:PCW:C26	0.64	2.22	1	1
3:A:409:PCW:H351	3:B:235:PCW:H412	0.64	1.69	9	1
3:C:607:PCW:H182	3:C:615:PCW:H352	0.64	1.69	9	1
3:B:221:PCW:C16	3:C:601:PCW:C38	0.64	2.64	10	1
3:A:409:PCW:H82	4:C:630:17F:HN1A	0.64	1.53	2	1
3:B:209:PCW:H372	4:B:228:17F:H34	0.64	1.70	3	1
3:B:221:PCW:C4	3:C:601:PCW:H61	0.64	2.21	4	1
3:B:216:PCW:H20	3:C:604:PCW:H482	0.64	1.67	2	1
3:B:210:PCW:H352	3:B:214:PCW:H141	0.64	1.67	10	1
1:C:465:GLU:O	1:C:469:LEU:HD12	0.63	1.92	4	2
1:A:349:TYR:CZ	3:A:401:PCW:H282	0.63	2.28	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:595:LEU:HD11	4:C:630:17F:H55	0.63	1.69	1	2
3:A:406:PCW:H331	4:A:407:17F:H56	0.63	1.70	3	1
3:C:618:PCW:H371	3:C:626:PCW:H412	0.63	1.69	7	1
3:A:403:PCW:C37	3:B:218:PCW:H471	0.63	2.23	1	1
3:A:402:PCW:H332	3:B:205:PCW:H32	0.63	1.69	7	2
3:A:410:PCW:H351	4:C:630:17F:H12A	0.63	1.71	6	2
3:C:620:PCW:H131	4:C:633:17F:C31	0.63	2.19	4	1
3:B:207:PCW:H221	3:C:601:PCW:H451	0.63	1.70	8	1
3:B:235:PCW:H32	3:C:602:PCW:H11	0.63	1.70	9	1
3:C:618:PCW:H352	3:C:626:PCW:H172	0.63	1.68	2	1
3:B:208:PCW:H20	3:B:222:PCW:H461	0.63	1.68	3	1
3:C:611:PCW:H151	3:C:623:PCW:H452	0.63	1.69	3	2
3:B:223:PCW:C27	1:C:521:TYR:HE2	0.63	2.06	5	1
3:A:406:PCW:H483	4:B:227:17F:H41	0.63	1.71	1	1
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.63	1.69	5	4
3:B:221:PCW:H262	1:C:459:PHE:CZ	0.63	2.28	5	1
3:B:223:PCW:C47	4:C:632:17F:C42	0.63	2.76	5	1
3:A:405:PCW:H352	3:B:216:PCW:H421	0.63	1.71	4	1
3:C:620:PCW:C16	4:C:633:17F:C1X	0.63	2.67	4	1
3:A:409:PCW:H181	3:C:613:PCW:H122	0.63	1.71	6	2
3:A:410:PCW:H322	4:C:630:17F:H29	0.63	1.71	10	1
3:B:234:PCW:H151	3:C:622:PCW:H162	0.62	1.70	10	1
3:B:211:PCW:H381	4:B:226:17F:H20A	0.62	1.71	1	1
3:B:212:PCW:H331	4:B:231:17F:H11	0.62	1.71	9	1
3:B:207:PCW:H441	3:B:216:PCW:H272	0.62	1.71	7	1
3:B:223:PCW:H19	3:B:225:PCW:H251	0.62	1.70	7	1
4:B:236:17F:H10	4:C:628:17F:H38	0.62	1.69	5	3
2:B:5:LYS:CG	7:B:239:EWS:OAB	0.62	2.48	1	1
3:A:406:PCW:H241	3:A:408:PCW:H272	0.62	1.72	4	1
3:A:406:PCW:H51	4:B:227:17F:O2	0.62	1.94	5	1
3:C:618:PCW:H362	3:C:626:PCW:H412	0.62	1.71	6	1
3:B:235:PCW:H342	3:C:623:PCW:H121	0.62	1.72	7	1
4:A:407:17F:H50	3:C:623:PCW:H252	0.62	1.71	5	1
3:C:609:PCW:H352	3:C:624:PCW:H361	0.62	1.70	5	1
3:B:204:PCW:H131	4:B:231:17F:H19	0.62	1.70	8	1
3:B:221:PCW:H141	3:C:601:PCW:C36	0.62	2.25	8	1
3:B:210:PCW:H181	3:B:214:PCW:H181	0.62	1.69	4	1
3:B:204:PCW:H32	3:B:208:PCW:H12	0.62	1.70	5	1
4:B:228:17F:H36	4:B:232:17F:H37	0.62	1.72	8	1
3:B:206:PCW:H40	4:B:226:17F:H73	0.62	1.71	1	1
3:C:604:PCW:H51	4:C:627:17F:N1	0.62	2.10	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:209:PCW:H151	3:B:216:PCW:H151	0.61	1.72	4	1
4:B:236:17F:H32	3:C:622:PCW:H172	0.61	1.72	2	5
3:B:203:PCW:H31	3:B:213:PCW:H351	0.61	1.72	10	1
2:B:7:VAL:HA	7:B:239:EWS:CAU	0.61	2.25	1	2
1:C:574:LEU:HB2	1:C:575:PRO:HD3	0.61	1.72	3	1
1:A:301:LEU:HD22	1:C:473:LYS:HE2	0.61	1.72	6	1
2:B:7:VAL:HB	7:B:239:EWS:CAS	0.61	2.25	8	2
3:B:202:PCW:H352	3:B:215:PCW:H152	0.61	1.73	10	1
3:C:605:PCW:H161	4:C:629:17F:H18	0.61	1.70	6	1
3:A:406:PCW:H352	4:A:407:17F:H56	0.61	1.73	8	2
3:C:620:PCW:H142	4:C:633:17F:C32	0.61	2.25	4	1
3:A:409:PCW:H472	3:C:613:PCW:H182	0.61	1.72	6	1
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.61	1.72	4	2
3:B:224:PCW:H12	3:B:224:PCW:H52	0.61	1.71	5	1
2:B:72:MET:HG2	7:B:239:EWS:BRA	0.61	2.51	10	2
3:A:410:PCW:C33	4:C:630:17F:H29	0.61	2.20	1	2
2:B:56:LEU:HD22	7:B:239:EWS:CAD	0.61	2.25	1	1
3:B:203:PCW:H12	3:B:213:PCW:H322	0.61	1.73	1	1
1:A:356:HIS:HD2	3:A:401:PCW:H272	0.61	1.53	9	1
4:B:227:17F:H10A	4:B:227:17F:H58	0.61	1.71	7	1
3:A:404:PCW:C7	7:B:239:EWS:OAB	0.61	2.49	10	1
3:C:601:PCW:H482	3:C:605:PCW:H481	0.61	1.67	10	1
3:C:607:PCW:H332	3:C:615:PCW:H361	0.60	1.73	2	1
3:B:206:PCW:H321	3:B:211:PCW:H342	0.60	1.71	1	1
3:A:405:PCW:H381	3:B:207:PCW:H372	0.60	1.73	7	1
3:B:224:PCW:H61	4:B:229:17F:O4	0.60	1.96	1	1
3:C:603:PCW:H431	3:C:607:PCW:H11	0.60	1.73	1	1
3:A:405:PCW:H332	3:B:216:PCW:H40	0.60	1.73	3	2
3:C:607:PCW:H462	4:C:633:17F:H42	0.60	1.72	5	1
3:B:233:PCW:H381	3:B:233:PCW:H141	0.60	1.72	10	2
1:A:393:TYR:CD1	3:A:406:PCW:H281	0.60	2.31	3	1
3:B:221:PCW:C16	3:C:601:PCW:C41	0.60	2.79	10	1
3:B:217:PCW:H61	4:B:226:17F:N1	0.60	2.12	2	1
3:A:404:PCW:H182	3:B:225:PCW:H381	0.60	1.71	4	1
3:B:221:PCW:C41	3:C:601:PCW:H39	0.60	2.22	10	1
3:C:604:PCW:H352	3:C:605:PCW:H352	0.60	1.74	10	1
3:C:605:PCW:H162	4:C:629:17F:H18	0.60	1.70	10	1
3:B:204:PCW:H142	3:B:212:PCW:H381	0.60	1.72	1	1
3:C:609:PCW:H412	3:C:624:PCW:H211	0.60	1.73	4	3
3:C:601:PCW:C40	4:C:627:17F:H54	0.60	2.26	4	1
3:B:203:PCW:H72	4:B:230:17F:H6A	0.60	1.72	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:210:PCW:H51	4:B:229:17F:H6A	0.60	1.74	9	1
3:A:409:PCW:H63	4:C:630:17F:HN1A	0.60	1.57	2	1
3:C:606:PCW:H362	3:C:612:PCW:H351	0.60	1.72	10	5
3:B:223:PCW:H471	4:C:631:17F:H67	0.60	1.72	2	1
2:B:40:TYR:HE1	2:B:57:ASP:HB2	0.60	1.57	3	1
1:C:488:LYS:HZ2	3:C:620:PCW:C26	0.60	2.10	4	1
3:B:211:PCW:H331	4:B:226:17F:H5	0.60	1.73	6	3
3:A:410:PCW:H382	4:C:630:17F:H12A	0.60	1.73	1	1
1:C:561:LYS:HA	1:C:565:ALA:HB3	0.60	1.73	9	1
3:B:221:PCW:H132	3:C:601:PCW:H351	0.60	1.66	10	1
3:A:403:PCW:C39	3:B:218:PCW:C47	0.59	2.80	1	1
3:C:615:PCW:H181	4:C:627:17F:H76	0.59	1.73	1	1
3:B:210:PCW:H252	3:C:607:PCW:H471	0.59	1.73	10	1
3:C:618:PCW:H331	3:C:626:PCW:H19	0.59	1.74	4	1
3:B:203:PCW:H161	4:B:230:17F:H34	0.59	1.74	4	1
3:C:607:PCW:H221	3:C:615:PCW:H411	0.59	1.73	5	3
4:C:630:17F:H2	4:C:630:17F:C4	0.59	2.27	9	2
3:B:203:PCW:H482	4:B:228:17F:H57	0.59	1.74	6	1
1:A:264:LYS:HE3	1:C:509:ALA:HB1	0.59	1.74	9	2
1:C:503:MET:HA	1:C:506:ARG:HD2	0.59	1.74	6	5
3:B:218:PCW:H31	3:B:219:PCW:H121	0.59	1.73	4	1
4:B:227:17F:H69	3:C:613:PCW:H232	0.59	1.73	7	1
1:A:250:VAL:O	1:A:254:VAL:HB	0.59	1.97	4	8
1:A:369:GLU:O	1:A:373:GLN:CG	0.59	2.43	1	2
3:C:615:PCW:H171	4:C:627:17F:H77	0.59	1.74	2	1
1:C:488:LYS:HD3	3:C:620:PCW:H272	0.59	1.73	6	1
3:C:613:PCW:H151	3:C:613:PCW:H382	0.59	1.73	9	1
3:B:234:PCW:H461	3:B:234:PCW:H252	0.59	1.73	7	1
3:A:406:PCW:H321	4:A:407:17F:H32	0.59	1.75	1	1
2:B:78:PHE:HB2	2:B:111:MET:HG2	0.59	1.73	10	3
1:C:488:LYS:HD3	3:C:620:PCW:C27	0.59	2.28	6	1
3:C:621:PCW:H412	4:C:632:17F:H34	0.59	1.75	10	1
4:B:226:17F:H65	3:C:622:PCW:H482	0.59	1.75	3	1
4:B:226:17F:H72	4:B:236:17F:H54	0.59	1.75	4	1
3:C:617:PCW:H331	3:C:618:PCW:H141	0.59	1.75	10	1
1:A:288:ARG:O	1:A:292:HIS:HB2	0.58	1.98	5	3
3:C:606:PCW:H141	3:C:612:PCW:H152	0.58	1.74	1	1
3:A:405:PCW:H212	3:C:609:PCW:H241	0.58	1.73	6	2
3:C:605:PCW:H212	4:C:629:17F:H47	0.58	1.75	7	1
3:B:201:PCW:H262	4:B:230:17F:H65	0.58	1.75	9	1
3:B:206:PCW:H171	4:B:232:17F:H62	0.58	1.75	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:330:ARG:O	1:A:334:ARG:HG2	0.58	1.98	4	5
3:A:401:PCW:H462	3:C:623:PCW:H481	0.58	1.73	2	1
2:B:114:VAL:HG12	2:B:142:ILE:HB	0.58	1.75	4	3
3:A:406:PCW:H121	4:A:407:17F:H20	0.58	1.75	5	1
3:B:206:PCW:H51	3:B:211:PCW:H332	0.58	1.75	1	1
3:C:615:PCW:H422	4:C:632:17F:H47	0.58	1.76	5	2
3:A:401:PCW:H482	3:C:614:PCW:H222	0.58	1.75	3	1
3:C:604:PCW:H82	4:C:627:17F:HN1A	0.58	1.57	2	1
3:A:405:PCW:H421	4:B:228:17F:H70	0.58	1.73	10	1
3:B:220:PCW:H11	3:B:222:PCW:H322	0.58	1.74	10	1
3:B:221:PCW:O11	3:C:601:PCW:H362	0.58	1.97	10	1
3:A:401:PCW:H331	3:A:405:PCW:H211	0.58	1.73	2	1
3:B:202:PCW:H351	3:B:214:PCW:H331	0.58	1.75	4	1
1:C:488:LYS:CE	3:C:620:PCW:H261	0.58	2.28	4	1
2:B:36:ILE:HA	2:B:59:ALA:HB2	0.58	1.76	8	2
3:B:204:PCW:H382	3:B:205:PCW:H142	0.58	1.76	3	1
3:B:221:PCW:H262	1:C:459:PHE:HZ	0.58	1.56	5	1
1:A:242:GLU:HB3	1:C:532:ARG:HH21	0.58	1.58	5	2
3:B:221:PCW:H272	3:C:601:PCW:C22	0.58	2.29	6	2
2:B:40:TYR:HB2	2:B:55:ILE:HB	0.58	1.75	7	2
3:B:208:PCW:H361	3:B:222:PCW:H121	0.58	1.74	10	1
3:A:401:PCW:H361	3:B:213:PCW:H212	0.58	1.75	1	1
3:A:410:PCW:H332	4:C:630:17F:C1X	0.58	2.25	5	2
3:B:206:PCW:H141	3:B:222:PCW:H362	0.58	1.76	6	1
3:B:203:PCW:H41	4:B:230:17F:H2	0.58	1.75	8	1
2:B:7:VAL:CG1	7:B:239:EWS:CAT	0.58	2.81	10	2
3:C:606:PCW:H341	3:C:612:PCW:H121	0.58	1.74	6	2
3:A:405:PCW:H152	4:B:228:17F:H59	0.58	1.74	1	2
3:A:403:PCW:H381	3:B:218:PCW:H452	0.58	1.74	2	1
3:A:404:PCW:H152	3:B:225:PCW:H251	0.58	1.76	10	1
3:B:207:PCW:H483	3:C:601:PCW:C21	0.57	2.29	4	1
3:C:615:PCW:H171	4:C:633:17F:H10	0.57	1.76	9	1
3:B:221:PCW:H51	4:B:229:17F:HN1	0.57	1.58	4	1
3:C:615:PCW:H221	4:C:629:17F:H38	0.57	1.75	9	2
3:A:406:PCW:C34	4:B:227:17F:H11	0.57	2.28	8	1
3:B:233:PCW:H382	3:B:233:PCW:H422	0.57	1.76	10	1
3:B:207:PCW:H212	3:C:601:PCW:H412	0.57	1.76	2	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.57	1.74	2	3
3:C:609:PCW:H82	3:C:625:PCW:H2	0.57	1.76	5	1
3:A:403:PCW:H52	4:B:231:17F:HN1	0.57	1.58	7	1
3:B:201:PCW:H152	3:B:201:PCW:H211	0.57	1.76	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:212:PCW:H322	4:B:231:17F:H11	0.57	1.75	1	1
3:B:210:PCW:H81	4:B:226:17F:O1	0.57	1.99	4	1
4:B:226:17F:H73	4:B:236:17F:H50	0.57	1.74	6	1
4:C:628:17F:H64	4:C:632:17F:H11	0.57	1.75	6	1
3:B:222:PCW:H52	4:B:227:17F:N1	0.57	2.12	7	1
4:B:236:17F:H56	3:C:622:PCW:H141	0.57	1.77	7	2
3:C:620:PCW:C13	4:C:633:17F:H56	0.57	2.24	4	1
3:C:623:PCW:H40	3:C:624:PCW:H211	0.57	1.76	8	1
3:A:405:PCW:H39	3:B:216:PCW:H451	0.57	1.76	3	1
1:A:368:LEU:CD1	4:B:230:17F:H54	0.57	2.12	8	1
3:B:201:PCW:H32	4:B:230:17F:H1A	0.57	1.75	5	1
3:B:201:PCW:H361	4:B:227:17F:H31	0.57	1.77	5	1
3:B:220:PCW:H42	4:B:232:17F:H19A	0.57	1.75	6	1
3:C:604:PCW:H31	3:C:625:PCW:H332	0.57	1.76	8	1
3:B:220:PCW:H12	3:B:222:PCW:H322	0.57	1.77	1	1
3:A:405:PCW:H162	3:C:609:PCW:H252	0.57	1.75	3	2
1:C:491:GLU:HG2	1:C:495:LYS:HE3	0.57	1.75	3	1
3:C:607:PCW:H262	3:C:615:PCW:H452	0.57	1.75	4	1
3:B:210:PCW:H382	3:B:214:PCW:H152	0.57	1.76	5	1
3:A:410:PCW:C31	4:C:630:17F:H11	0.57	2.29	7	1
2:B:170:MET:SD	3:B:211:PCW:H42	0.57	2.40	7	1
1:A:334:ARG:HD2	1:C:440:GLU:OE1	0.57	1.99	3	6
1:C:491:GLU:HB3	1:C:495:LYS:HE2	0.57	1.76	7	5
3:B:213:PCW:H221	3:B:213:PCW:H441	0.57	1.77	5	1
4:B:229:17F:H54	3:C:607:PCW:H241	0.57	1.76	6	1
1:A:368:LEU:HD11	4:B:230:17F:C30	0.57	2.12	8	1
4:B:229:17F:H75	4:C:629:17F:H54	0.57	1.75	2	1
4:C:627:17F:H10A	4:C:629:17F:H31	0.57	1.76	3	1
3:B:213:PCW:H31	3:B:213:PCW:O1P	0.57	2.00	4	1
3:B:204:PCW:H12	3:B:212:PCW:O2P	0.57	2.00	7	1
3:B:234:PCW:H39	3:C:602:PCW:H283	0.57	1.77	7	1
3:B:207:PCW:H352	3:B:216:PCW:H421	0.57	1.77	10	1
1:A:352:LYS:NZ	1:C:425:GLU:HB2	0.56	2.15	3	1
3:B:202:PCW:H182	3:B:215:PCW:H242	0.56	1.77	6	1
1:A:308:ARG:HD3	1:C:469:LEU:CG	0.56	2.30	7	1
3:B:208:PCW:H62	3:B:219:PCW:H41	0.56	1.76	9	1
3:B:209:PCW:H472	4:B:228:17F:H68	0.56	1.75	10	1
3:B:206:PCW:H461	4:B:226:17F:H78	0.56	1.74	4	1
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.56	1.77	5	2
3:A:405:PCW:H182	3:C:609:PCW:H252	0.56	1.77	8	1
3:A:408:PCW:H73	3:A:410:PCW:O1P	0.56	2.00	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:214:PCW:H262	4:C:633:17F:H48	0.56	1.77	1	1
3:C:619:PCW:H381	3:C:619:PCW:H151	0.56	1.76	1	2
1:A:393:TYR:CE1	3:A:406:PCW:H283	0.56	2.34	2	1
3:A:409:PCW:H461	3:C:613:PCW:H172	0.56	1.76	2	1
3:B:221:PCW:H342	4:B:229:17F:H19	0.56	1.77	2	1
3:B:201:PCW:H11	4:B:230:17F:N1	0.56	2.15	5	1
3:B:217:PCW:H432	3:B:223:PCW:C45	0.56	2.20	5	1
3:B:209:PCW:H442	4:B:232:17F:H43	0.56	1.75	9	1
3:C:601:PCW:H483	3:C:605:PCW:C47	0.56	2.29	10	1
1:C:451:LYS:O	1:C:455:TYR:HB2	0.56	1.99	8	6
3:A:404:PCW:H352	3:B:225:PCW:H132	0.56	1.77	2	1
3:B:207:PCW:C7	4:B:228:17F:HN1	0.56	2.13	4	1
3:C:603:PCW:H40	4:C:628:17F:H6	0.56	1.77	2	1
3:B:203:PCW:H151	3:B:213:PCW:H372	0.56	1.76	3	1
3:B:201:PCW:C37	4:B:228:17F:H37	0.56	2.29	10	1
2:B:94:HIS:O	2:B:98:GLU:HG2	0.56	2.00	1	1
4:B:228:17F:H62	3:C:624:PCW:H481	0.56	1.76	2	1
4:C:630:17F:H4A	4:C:630:17F:O4	0.56	2.00	2	1
3:C:621:PCW:H211	4:C:631:17F:H31	0.56	1.78	3	1
1:C:488:LYS:NZ	3:C:620:PCW:C25	0.56	2.68	4	1
3:B:216:PCW:H71	4:B:229:17F:H19	0.56	1.78	9	1
3:C:623:PCW:H122	3:C:623:PCW:H381	0.56	1.76	9	1
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.56	1.77	2	1
3:B:209:PCW:H471	3:C:609:PCW:H482	0.56	1.77	5	1
3:C:614:PCW:H222	3:C:614:PCW:H472	0.56	1.78	6	1
3:A:409:PCW:H51	4:C:630:17F:HN1A	0.56	1.59	10	1
3:B:208:PCW:H451	3:B:234:PCW:H241	0.56	1.76	10	1
3:B:216:PCW:O1P	3:B:221:PCW:H73	0.56	2.01	2	1
4:B:236:17F:H30	3:C:622:PCW:H271	0.56	1.77	2	1
3:B:201:PCW:H73	4:B:227:17F:O5	0.56	2.01	3	1
2:B:5:LYS:HD2	7:B:239:EWS:CAX	0.56	2.30	7	1
3:C:615:PCW:H40	4:C:632:17F:H55	0.56	1.77	8	1
3:B:221:PCW:H411	3:C:601:PCW:C39	0.56	2.23	10	1
3:B:212:PCW:H81	4:B:231:17F:O2	0.56	2.01	1	1
3:B:203:PCW:H40	4:B:228:17F:H11	0.56	1.75	2	1
3:B:204:PCW:H52	3:B:205:PCW:H81	0.56	1.78	3	1
3:C:611:PCW:H161	3:C:619:PCW:H19	0.56	1.77	4	1
3:B:204:PCW:H142	3:B:212:PCW:H39	0.56	1.76	5	1
3:C:605:PCW:H19	4:C:627:17F:H59	0.56	1.78	7	1
3:C:621:PCW:H442	4:C:632:17F:H37	0.56	1.78	7	1
3:A:404:PCW:H222	4:C:631:17F:H50	0.56	1.78	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:227:17F:H44	3:C:613:PCW:H241	0.56	1.78	1	1
2:B:72:MET:HG3	7:B:239:EWS:BRA	0.56	2.56	3	1
3:B:209:PCW:H442	4:B:228:17F:H61	0.56	1.78	4	1
3:C:618:PCW:H382	3:C:626:PCW:H171	0.56	1.79	10	2
3:B:210:PCW:H321	4:B:229:17F:H10A	0.56	1.76	10	1
3:C:609:PCW:H372	3:C:624:PCW:H181	0.56	1.77	10	1
3:C:620:PCW:H322	4:C:633:17F:H77	0.55	1.77	1	1
1:C:508:ARG:O	1:C:512:ASP:HB2	0.55	2.01	9	3
3:B:210:PCW:H211	3:B:214:PCW:H40	0.55	1.77	3	1
3:B:201:PCW:H212	4:B:230:17F:H58	0.55	1.78	6	1
3:B:209:PCW:H131	3:B:216:PCW:H152	0.55	1.78	10	1
3:B:203:PCW:H151	3:B:213:PCW:H39	0.55	1.78	1	1
2:B:79:LEU:HD23	2:B:112:VAL:HB	0.55	1.78	9	2
3:B:216:PCW:H52	4:B:229:17F:HN1	0.55	1.60	3	1
4:B:230:17F:H1	4:B:230:17F:C4	0.55	2.24	9	1
2:B:56:LEU:CD2	7:B:239:EWS:CAR	0.55	2.84	8	1
3:B:208:PCW:H381	3:B:222:PCW:H141	0.55	1.78	10	1
3:B:221:PCW:C27	3:C:601:PCW:H221	0.55	2.26	2	2
1:C:444:ASP:O	1:C:448:VAL:HB	0.55	2.02	3	2
3:B:201:PCW:H422	3:B:220:PCW:H441	0.55	1.76	8	1
4:B:230:17F:H74	3:C:611:PCW:H222	0.55	1.79	2	1
3:B:218:PCW:H73	4:B:231:17F:HN1A	0.55	1.59	6	1
3:C:601:PCW:H482	3:C:605:PCW:C48	0.55	2.25	10	1
1:A:345:ARG:HA	1:C:429:ASN:HD21	0.55	1.61	3	2
3:B:212:PCW:H362	4:B:231:17F:H10A	0.55	1.78	5	2
3:B:210:PCW:H61	4:B:229:17F:H2	0.55	1.77	2	1
1:A:393:TYR:CE1	3:A:411:PCW:H272	0.55	2.35	3	1
3:B:204:PCW:H412	3:B:205:PCW:H151	0.55	1.79	6	1
4:B:228:17F:H53	3:C:624:PCW:H271	0.55	1.78	9	1
1:C:478:ARG:O	1:C:482:GLN:HB2	0.55	2.02	4	2
3:A:405:PCW:H283	3:C:609:PCW:H261	0.55	1.79	4	1
3:C:606:PCW:H351	3:C:612:PCW:H381	0.55	1.78	7	1
3:C:604:PCW:H51	4:C:627:17F:HN1A	0.55	1.61	1	2
3:B:218:PCW:H41	4:B:231:17F:O1	0.55	2.01	3	1
1:A:352:LYS:NZ	1:C:425:GLU:HB3	0.55	2.17	4	1
3:A:406:PCW:H331	4:A:407:17F:H32	0.55	1.79	5	2
3:C:605:PCW:H82	3:C:607:PCW:H142	0.55	1.78	1	2
3:A:404:PCW:H282	3:C:618:PCW:H412	0.55	1.78	3	1
3:C:603:PCW:H39	4:C:628:17F:H6	0.55	1.78	4	1
3:B:206:PCW:H31	3:B:206:PCW:H51	0.55	1.78	6	1
3:B:213:PCW:H121	4:B:228:17F:H6	0.55	1.79	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:611:PCW:H412	3:C:611:PCW:H19	0.55	1.78	6	1
3:B:221:PCW:H141	3:C:601:PCW:H332	0.55	1.79	2	1
3:A:405:PCW:H132	3:A:405:PCW:H331	0.54	1.78	1	1
2:B:6:LEU:HD22	2:B:159:LEU:HD23	0.54	1.79	1	2
3:B:214:PCW:H441	3:B:217:PCW:H251	0.54	1.78	4	1
3:C:605:PCW:H172	4:C:629:17F:H18	0.54	1.78	5	1
3:B:203:PCW:O31	4:B:230:17F:H6	0.54	2.02	6	2
3:C:609:PCW:H382	3:C:624:PCW:H422	0.54	1.78	10	1
3:B:204:PCW:O2P	3:B:222:PCW:H71	0.54	2.01	1	1
3:C:618:PCW:H431	3:C:618:PCW:H162	0.54	1.78	2	1
3:B:217:PCW:H281	4:C:632:17F:H70	0.54	1.79	7	2
3:B:217:PCW:H272	4:C:632:17F:H38	0.54	1.79	4	1
3:B:216:PCW:H411	3:B:224:PCW:H222	0.54	1.80	5	1
2:B:62:GLU:HG2	2:B:68:ARG:HD3	0.54	1.77	1	1
3:B:201:PCW:H122	4:B:227:17F:H18A	0.54	1.78	3	1
1:C:502:GLU:HG2	1:C:506:ARG:HE	0.54	1.63	3	2
1:C:458:ASP:HA	1:C:461:LYS:HE3	0.54	1.78	4	1
1:C:488:LYS:HZ1	3:C:620:PCW:C25	0.54	2.15	4	1
3:B:204:PCW:H352	3:B:222:PCW:H161	0.54	1.79	5	1
4:B:231:17F:H33	4:B:231:17F:H8	0.54	1.80	5	2
1:A:349:TYR:HE2	3:A:401:PCW:C26	0.54	2.10	7	1
3:C:607:PCW:H261	3:C:615:PCW:H432	0.54	1.78	8	1
3:A:408:PCW:H171	3:A:411:PCW:H152	0.54	1.80	1	1
3:C:614:PCW:H171	3:C:614:PCW:H381	0.54	1.80	9	2
3:C:621:PCW:H411	4:C:632:17F:H34	0.54	1.80	4	2
3:B:201:PCW:H32	4:B:227:17F:N1	0.54	2.17	8	1
1:A:332:ALA:O	1:A:336:GLU:HB2	0.54	2.03	1	1
3:C:613:PCW:H132	3:C:619:PCW:H382	0.54	1.78	2	2
3:B:211:PCW:H121	4:B:226:17F:H18	0.54	1.80	6	1
3:B:223:PCW:H481	4:C:631:17F:H61	0.54	1.78	9	1
4:C:632:17F:H61	4:C:633:17F:H71	0.54	1.77	9	1
3:A:408:PCW:H2	3:A:410:PCW:H332	0.54	1.78	10	1
3:B:210:PCW:H162	3:B:214:PCW:H361	0.54	1.78	10	1
3:B:210:PCW:H422	4:B:229:17F:H72	0.54	1.80	1	1
3:B:224:PCW:H83	4:B:226:17F:H4A	0.54	1.79	2	1
3:B:211:PCW:H332	4:B:226:17F:O10	0.54	2.02	5	1
3:A:406:PCW:H362	4:A:407:17F:H56	0.54	1.79	6	1
3:B:214:PCW:H241	4:C:633:17F:H52	0.54	1.79	1	1
3:C:610:PCW:H20	3:C:616:PCW:H483	0.54	1.78	1	1
1:C:492:LEU:HD11	3:C:620:PCW:H482	0.54	1.79	10	1
1:A:393:TYR:HB3	3:A:406:PCW:H281	0.54	1.79	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:341:ASN:ND2	1:C:433:GLU:HA	0.54	2.17	5	1
3:C:605:PCW:H2	3:C:605:PCW:O2P	0.54	2.02	5	1
1:A:325:ASP:HA	1:A:328:ARG:HD2	0.54	1.79	8	2
3:B:203:PCW:H281	3:C:611:PCW:H242	0.54	1.80	8	1
3:A:403:PCW:C38	3:B:218:PCW:C47	0.54	2.63	1	1
1:A:308:ARG:CB	1:C:469:LEU:CD1	0.54	2.84	10	1
3:B:203:PCW:H362	3:B:213:PCW:H381	0.54	1.79	3	3
1:C:465:GLU:C	1:C:469:LEU:HG	0.54	2.23	4	1
4:C:627:17F:H71	4:C:629:17F:H53	0.54	1.80	4	1
4:C:627:17F:H66	4:C:629:17F:H55	0.54	1.80	8	1
2:B:8:VAL:HG22	2:B:79:LEU:HD12	0.53	1.81	2	1
1:C:465:GLU:HB3	1:C:469:LEU:HD11	0.53	1.80	4	2
3:C:606:PCW:H172	3:C:616:PCW:H411	0.53	1.80	4	1
3:B:214:PCW:H282	3:C:615:PCW:H432	0.53	1.80	6	1
1:C:544:LEU:O	1:C:548:HIS:HB2	0.53	2.03	3	1
3:C:607:PCW:H372	3:C:615:PCW:H412	0.53	1.79	3	2
1:A:244:SER:O	1:A:248:GLU:HB2	0.53	2.03	6	1
3:B:219:PCW:H472	3:B:223:PCW:H431	0.53	1.80	7	1
3:B:201:PCW:H361	3:B:220:PCW:C35	0.53	2.25	10	1
3:B:220:PCW:H352	3:B:220:PCW:H152	0.53	1.79	9	2
3:B:209:PCW:H131	3:B:216:PCW:H142	0.53	1.78	3	1
1:C:546:GLU:O	1:C:550:LYS:HD2	0.53	2.03	10	2
1:C:514:LEU:HA	1:C:517:HIS:HB2	0.53	1.80	7	1
3:B:221:PCW:H141	3:C:601:PCW:C37	0.53	2.32	8	1
3:B:201:PCW:H351	3:B:220:PCW:H342	0.53	1.81	2	1
1:C:528:ARG:HB3	1:C:532:ARG:NH2	0.53	2.16	10	2
3:C:611:PCW:H332	3:C:623:PCW:H411	0.53	1.79	6	1
3:B:213:PCW:H72	4:B:230:17F:O1	0.53	2.04	8	2
3:C:607:PCW:H372	3:C:615:PCW:H411	0.53	1.79	9	1
3:C:603:PCW:H411	4:C:628:17F:H9A	0.53	1.80	1	1
1:C:473:LYS:O	1:C:477:LEU:HB2	0.53	2.03	4	2
3:B:215:PCW:H83	3:B:217:PCW:P	0.53	2.44	4	1
3:C:611:PCW:H422	3:C:624:PCW:H271	0.53	1.79	3	1
3:B:223:PCW:H281	1:C:521:TYR:OH	0.53	2.03	10	1
4:B:226:17F:H71	3:C:622:PCW:H483	0.53	1.80	4	1
3:B:213:PCW:H82	3:B:213:PCW:H322	0.53	1.80	7	1
3:B:201:PCW:H32	4:B:227:17F:HN1A	0.53	1.64	8	1
3:A:404:PCW:H12	3:B:218:PCW:H352	0.53	1.80	2	1
1:C:495:LYS:O	1:C:499:LEU:HB2	0.53	2.04	2	5
3:A:409:PCW:H412	3:C:619:PCW:H412	0.53	1.79	4	1
3:B:211:PCW:H121	4:B:226:17F:C18	0.53	2.34	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ARG:HG3	1:C:469:LEU:HD13	0.53	1.76	10	1
3:B:210:PCW:H362	3:B:214:PCW:H161	0.53	1.79	5	1
1:C:469:LEU:O	1:C:473:LYS:HB2	0.53	2.03	6	1
3:B:215:PCW:H83	3:B:217:PCW:H11	0.53	1.80	7	1
3:B:207:PCW:H71	4:B:228:17F:H1	0.53	1.81	10	1
3:C:608:PCW:H31	4:C:631:17F:H4A	0.52	1.81	1	3
3:A:405:PCW:H142	3:C:609:PCW:H271	0.52	1.82	6	1
3:B:201:PCW:H381	4:B:227:17F:H56	0.52	1.79	6	1
4:B:236:17F:H40	4:B:236:17F:H72	0.52	1.80	7	1
3:B:216:PCW:H462	3:C:604:PCW:H481	0.52	1.79	2	1
3:C:611:PCW:H283	3:C:614:PCW:H441	0.52	1.81	3	1
1:A:352:LYS:HZ2	1:C:425:GLU:HB3	0.52	1.63	4	1
3:B:206:PCW:H231	3:B:220:PCW:H422	0.52	1.81	4	1
3:B:235:PCW:H341	3:C:623:PCW:H331	0.52	1.82	4	1
4:B:236:17F:H70	3:C:603:PCW:H282	0.52	1.81	6	1
4:B:232:17F:H70	3:B:233:PCW:H281	0.52	1.81	7	1
2:B:170:MET:SD	3:B:208:PCW:H61	0.52	2.45	10	1
1:C:467:MET:HE2	1:C:467:MET:HA	0.52	1.81	3	1
3:B:206:PCW:H19	4:B:226:17F:H37	0.52	1.82	4	1
3:B:222:PCW:H40	3:B:234:PCW:H252	0.52	1.81	4	1
3:B:221:PCW:H461	3:C:605:PCW:H242	0.52	1.80	5	1
1:A:388:SER:HB3	1:C:594:LYS:HE2	0.52	1.81	6	1
3:B:201:PCW:H351	3:B:220:PCW:C34	0.52	2.33	5	1
3:B:221:PCW:H51	4:B:229:17F:H1	0.52	1.81	7	1
3:B:210:PCW:H151	3:B:217:PCW:H141	0.52	1.80	8	1
3:A:406:PCW:H361	4:B:227:17F:H11	0.52	1.81	9	2
3:C:603:PCW:O1P	3:C:605:PCW:H72	0.52	2.03	5	1
4:C:628:17F:H5	4:C:632:17F:H1A	0.52	1.82	10	2
3:B:233:PCW:H141	3:B:233:PCW:H371	0.52	1.80	1	1
1:A:310:ARG:O	1:A:314:ASP:HB2	0.52	2.05	7	2
3:C:618:PCW:O3	3:C:626:PCW:H161	0.52	2.04	5	1
3:A:406:PCW:H452	3:A:409:PCW:H282	0.52	1.81	6	1
3:C:614:PCW:H412	3:C:614:PCW:H172	0.52	1.81	8	1
3:B:207:PCW:H211	3:B:209:PCW:H272	0.52	1.81	5	1
3:A:405:PCW:H162	3:C:609:PCW:H271	0.52	1.79	6	1
3:B:221:PCW:C15	3:C:601:PCW:H351	0.52	2.35	8	1
3:B:221:PCW:H161	3:C:601:PCW:C40	0.52	2.28	10	1
4:B:232:17F:H54	3:C:624:PCW:H241	0.52	1.81	3	1
3:C:609:PCW:H382	3:C:624:PCW:H381	0.52	1.81	3	1
3:A:405:PCW:H331	3:B:209:PCW:H351	0.52	1.81	6	1
3:A:410:PCW:C12	4:C:630:17F:H30	0.52	2.35	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:409:PCW:H211	3:C:613:PCW:H161	0.52	1.81	7	1
3:C:603:PCW:H431	3:C:607:PCW:H321	0.52	1.81	7	1
3:A:406:PCW:H452	3:C:613:PCW:H221	0.52	1.82	8	1
2:B:30:ASP:HA	5:B:237:GNP:H3'	0.52	1.81	10	2
3:B:211:PCW:H151	4:B:229:17F:H12	0.52	1.80	10	1
4:B:227:17F:H44	3:C:613:PCW:C24	0.52	2.35	1	1
3:C:607:PCW:H261	3:C:615:PCW:H431	0.52	1.82	2	1
3:C:621:PCW:H481	3:C:622:PCW:H481	0.52	1.82	8	2
1:C:488:LYS:HZ2	3:C:620:PCW:C27	0.52	2.18	4	1
3:B:219:PCW:O31	3:B:225:PCW:H41	0.52	2.05	5	1
2:B:7:VAL:HG11	7:B:239:EWS:CAS	0.52	2.35	10	1
3:C:606:PCW:H431	3:C:612:PCW:H162	0.52	1.82	1	1
3:B:206:PCW:H32	3:B:208:PCW:O1P	0.52	2.05	10	2
3:A:401:PCW:H472	3:C:611:PCW:H242	0.52	1.81	5	1
3:B:201:PCW:H212	4:B:230:17F:H59	0.52	1.82	9	1
1:C:595:LEU:CD1	4:C:630:17F:H55	0.51	2.35	1	2
3:B:216:PCW:H42	4:B:229:17F:C1	0.51	2.34	2	1
3:B:207:PCW:H162	3:B:209:PCW:H181	0.51	1.81	6	1
3:B:201:PCW:C1	4:B:230:17F:HN1	0.51	2.17	7	1
2:B:16:LYS:HB2	5:B:237:GNP:O2B	0.51	2.05	2	1
3:A:403:PCW:H71	4:B:231:17F:N1	0.51	2.19	6	1
3:B:212:PCW:H171	4:B:231:17F:H34	0.51	1.82	9	1
3:A:406:PCW:H342	4:B:227:17F:C9	0.51	2.35	1	1
3:A:410:PCW:H121	4:C:630:17F:C1X	0.51	2.35	1	1
3:B:201:PCW:H40	3:C:623:PCW:H242	0.51	1.81	1	1
3:B:206:PCW:H442	4:B:226:17F:H70	0.51	1.80	2	1
3:B:224:PCW:H142	4:B:232:17F:H9	0.51	1.81	6	1
3:C:605:PCW:H221	4:C:629:17F:H52	0.51	1.83	6	1
1:A:349:TYR:CD2	3:A:401:PCW:H262	0.51	2.35	7	1
3:C:603:PCW:H61	3:C:625:PCW:H251	0.51	1.82	8	1
3:B:221:PCW:H41	4:B:229:17F:O1	0.51	2.06	1	2
3:B:222:PCW:H483	3:C:622:PCW:H181	0.51	1.82	1	1
1:C:417:GLU:O	1:C:421:PRO:HD2	0.51	2.05	2	2
3:A:401:PCW:O1P	3:A:405:PCW:H11	0.51	2.06	3	1
3:B:211:PCW:H131	3:B:217:PCW:H82	0.51	1.83	8	2
3:A:406:PCW:H472	4:B:227:17F:H41	0.51	1.83	5	1
3:A:404:PCW:H462	3:B:225:PCW:H232	0.51	1.81	9	1
3:A:406:PCW:H132	4:A:407:17F:H20A	0.51	1.83	1	2
3:B:206:PCW:H332	3:B:211:PCW:H321	0.51	1.82	1	1
3:C:620:PCW:H322	4:C:633:17F:C42	0.51	2.36	1	1
3:B:204:PCW:H422	3:B:205:PCW:H172	0.51	1.81	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:465:GLU:C	1:C:469:LEU:HD12	0.51	2.30	4	1
3:B:224:PCW:H281	3:B:233:PCW:H283	0.51	1.81	6	1
3:A:404:PCW:H172	3:B:225:PCW:H381	0.51	1.83	7	1
4:B:232:17F:H4	4:B:232:17F:HN1	0.51	1.65	9	1
1:C:489:LEU:O	1:C:493:GLN:HB2	0.51	2.06	9	1
3:C:618:PCW:H431	3:C:626:PCW:H19	0.51	1.81	10	1
3:A:403:PCW:H362	3:B:218:PCW:H451	0.51	1.82	1	1
3:A:410:PCW:O2P	3:A:411:PCW:H52	0.51	2.06	1	3
3:B:202:PCW:H442	3:B:215:PCW:H283	0.51	1.82	1	1
4:C:628:17F:H9	4:C:628:17F:H18A	0.51	1.82	9	1
2:B:71:TYR:CD2	7:B:239:EWS:CAO	0.51	2.94	10	1
3:B:211:PCW:H122	4:B:226:17F:C19	0.51	2.36	10	1
3:B:211:PCW:H82	3:B:219:PCW:C32	0.51	2.35	4	1
3:C:621:PCW:H461	4:C:632:17F:H35	0.51	1.83	5	1
3:A:408:PCW:H422	3:B:205:PCW:H452	0.51	1.82	6	1
3:B:212:PCW:H121	4:B:231:17F:H6A	0.51	1.83	10	1
1:C:447:GLU:O	1:C:451:LYS:HB2	0.51	2.06	5	2
3:C:615:PCW:C18	4:C:633:17F:H12	0.51	2.36	2	1
3:A:405:PCW:H361	3:A:405:PCW:H141	0.51	1.83	3	1
3:C:618:PCW:H342	3:C:626:PCW:H371	0.51	1.82	4	1
3:B:201:PCW:H42	4:B:230:17F:H2	0.51	1.83	7	1
3:B:220:PCW:H251	4:B:232:17F:H76	0.51	1.82	9	1
3:A:410:PCW:H352	4:C:630:17F:H29	0.51	1.82	2	1
2:B:43:GLN:OE1	3:B:202:PCW:H62	0.51	2.06	2	1
3:B:219:PCW:H471	3:B:223:PCW:H432	0.51	1.83	4	1
4:B:236:17F:H34	4:B:236:17F:H10A	0.51	1.82	5	1
4:B:228:17F:H8	4:B:232:17F:H9A	0.51	1.82	9	2
3:A:404:PCW:H231	3:B:225:PCW:H422	0.51	1.82	10	1
1:C:492:LEU:CD1	3:C:620:PCW:H482	0.51	2.36	10	1
3:B:220:PCW:H83	3:B:222:PCW:H321	0.51	1.82	7	1
3:A:409:PCW:H471	3:C:613:PCW:H182	0.50	1.83	1	1
3:B:202:PCW:H212	3:B:215:PCW:H232	0.50	1.83	4	1
3:B:213:PCW:H141	4:B:228:17F:H9	0.50	1.82	9	1
3:C:603:PCW:H242	4:C:632:17F:H53	0.50	1.82	9	1
3:C:601:PCW:C39	4:C:627:17F:H54	0.50	2.36	4	1
1:A:239:LEU:O	1:A:243:MET:HB2	0.50	2.06	5	1
3:A:404:PCW:H32	3:B:218:PCW:H372	0.50	1.83	5	1
3:A:405:PCW:H232	3:C:609:PCW:H261	0.50	1.81	8	1
1:A:275:LYS:O	1:A:279:LEU:HB2	0.50	2.07	9	1
4:B:236:17F:H57	3:C:622:PCW:H161	0.50	1.83	9	1
3:B:220:PCW:H212	3:B:235:PCW:H262	0.50	1.82	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:409:PCW:H372	3:B:235:PCW:H371	0.50	1.84	5	1
1:C:421:PRO:O	1:C:425:GLU:HG2	0.50	2.06	5	1
3:B:203:PCW:H132	3:B:213:PCW:H351	0.50	1.84	9	1
3:A:403:PCW:H342	3:B:212:PCW:H272	0.50	1.83	1	1
3:B:203:PCW:H431	4:B:228:17F:H12A	0.50	1.83	3	1
3:B:212:PCW:H261	3:B:212:PCW:H462	0.50	1.83	6	1
3:B:233:PCW:H242	3:C:609:PCW:H441	0.50	1.83	6	1
3:B:214:PCW:H283	4:C:633:17F:H52	0.50	1.82	7	1
4:C:632:17F:H61	4:C:633:17F:H69	0.50	1.83	8	1
1:C:414:LYS:HA	1:C:417:GLU:HG3	0.50	1.82	9	1
3:C:603:PCW:H332	3:C:607:PCW:H121	0.50	1.81	9	1
2:B:72:MET:SD	7:B:239:EWS:BRA	0.50	3.24	10	1
3:A:406:PCW:H342	4:B:227:17F:H9	0.50	1.84	1	1
1:C:491:GLU:O	1:C:495:LYS:HG3	0.50	2.06	5	5
1:A:279:LEU:HB3	1:C:495:LYS:HE3	0.50	1.83	2	1
3:B:207:PCW:H441	3:B:209:PCW:H241	0.50	1.82	4	1
3:A:403:PCW:H412	3:B:218:PCW:H462	0.50	1.84	5	1
3:B:204:PCW:H32	3:B:208:PCW:C1	0.50	2.36	5	1
3:A:404:PCW:H81	3:B:225:PCW:O2P	0.50	2.06	7	1
3:B:209:PCW:H31	3:B:224:PCW:H132	0.50	1.83	7	2
1:C:492:LEU:HD13	3:C:620:PCW:H441	0.50	1.84	8	1
3:B:202:PCW:H181	3:B:215:PCW:H242	0.50	1.83	9	1
3:C:607:PCW:H283	4:C:632:17F:H52	0.50	1.84	1	1
3:C:621:PCW:H483	4:C:632:17F:H35	0.50	1.84	1	1
3:B:209:PCW:H83	4:B:228:17F:N1	0.50	2.21	2	1
3:B:210:PCW:H152	3:B:214:PCW:H352	0.50	1.84	6	1
1:C:525:LEU:HD23	1:C:528:ARG:HD2	0.50	1.83	6	1
3:B:208:PCW:H441	3:B:234:PCW:H262	0.50	1.84	7	1
1:A:276:VAL:O	1:A:280:ARG:HB2	0.50	2.07	2	2
4:A:407:17F:H10A	3:B:205:PCW:H361	0.50	1.83	2	1
3:C:606:PCW:H431	3:C:612:PCW:H172	0.50	1.82	3	1
3:B:222:PCW:H332	3:B:222:PCW:H131	0.50	1.82	5	1
3:C:615:PCW:H182	4:C:629:17F:H42	0.50	1.83	5	1
3:C:601:PCW:H483	3:C:601:PCW:H212	0.50	1.83	7	1
3:C:605:PCW:H162	4:C:627:17F:H34	0.50	1.82	8	1
3:A:410:PCW:O3	4:C:630:17F:H30	0.50	2.05	7	2
3:C:615:PCW:H221	4:C:629:17F:H42	0.50	1.83	1	1
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.50	1.84	3	3
3:B:222:PCW:H131	3:B:222:PCW:H351	0.50	1.83	5	1
3:B:209:PCW:O11	3:B:216:PCW:H131	0.50	2.07	6	1
3:A:403:PCW:H342	3:B:212:PCW:C27	0.50	2.37	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:630:17F:C4	4:C:630:17F:H1	0.50	2.37	2	1
3:B:204:PCW:H52	3:B:205:PCW:H61	0.50	1.82	3	1
3:B:211:PCW:H352	4:B:226:17F:O10	0.50	2.06	3	1
3:B:214:PCW:H281	4:C:627:17F:H75	0.50	1.84	3	1
3:B:203:PCW:H481	4:B:228:17F:H20	0.50	1.84	6	2
3:B:205:PCW:H221	3:B:205:PCW:H461	0.50	1.84	6	1
1:A:312:HIS:HE1	1:C:465:GLU:HB2	0.49	1.66	9	4
1:A:279:LEU:HD22	1:C:495:LYS:HE2	0.49	1.83	3	1
3:A:409:PCW:C6	4:C:630:17F:HN1A	0.49	2.20	3	1
3:C:606:PCW:H361	3:C:612:PCW:H152	0.49	1.84	7	3
3:B:219:PCW:H351	3:B:225:PCW:H351	0.49	1.84	7	1
3:B:234:PCW:H141	3:C:602:PCW:H461	0.49	1.82	7	1
1:C:485:ALA:HB1	3:C:620:PCW:H271	0.49	1.82	7	1
3:A:408:PCW:H322	3:C:610:PCW:H371	0.49	1.84	8	1
3:A:409:PCW:H262	3:C:613:PCW:H181	0.49	1.83	8	1
3:C:607:PCW:H352	3:C:615:PCW:H381	0.49	1.83	8	1
1:A:363:LYS:HD3	1:C:411:THR:HG23	0.49	1.84	9	2
3:B:209:PCW:H19	3:B:216:PCW:H211	0.49	1.82	1	1
4:B:227:17F:H10	4:B:227:17F:H33	0.49	1.84	8	2
3:B:201:PCW:H82	3:B:222:PCW:O2P	0.49	2.07	4	1
1:C:465:GLU:C	1:C:469:LEU:CD1	0.49	2.85	4	1
3:B:225:PCW:H282	3:C:626:PCW:H481	0.49	1.82	1	1
3:C:607:PCW:H471	4:C:633:17F:H39	0.49	1.84	9	2
1:A:365:LYS:O	1:A:369:GLU:HB2	0.49	2.06	8	1
3:B:221:PCW:C13	3:C:601:PCW:C35	0.49	2.67	10	1
3:A:410:PCW:H352	4:C:630:17F:C1X	0.49	2.37	2	1
3:B:201:PCW:H42	4:B:232:17F:N1	0.49	2.22	2	1
1:A:338:LEU:O	1:A:342:GLY:HA3	0.49	2.08	3	2
3:A:406:PCW:H121	4:A:407:17F:H20A	0.49	1.84	4	1
4:A:407:17F:H37	3:B:222:PCW:C3	0.49	2.36	5	1
4:B:236:17F:H47	4:B:236:17F:H76	0.49	1.85	5	1
1:A:308:ARG:HD2	1:C:465:GLU:OE1	0.49	2.08	6	1
3:B:212:PCW:H151	4:B:231:17F:H10	0.49	1.83	6	1
3:B:211:PCW:H231	4:B:229:17F:H44	0.49	1.83	8	1
3:A:402:PCW:H122	4:B:231:17F:H76	0.49	1.82	9	1
1:A:301:LEU:HB3	1:C:473:LYS:HE2	0.49	1.84	1	1
1:A:314:ASP:HA	1:A:317:ARG:HD2	0.49	1.82	2	3
3:A:409:PCW:H82	4:C:630:17F:N1	0.49	2.23	2	1
3:C:607:PCW:H482	4:C:633:17F:H42	0.49	1.83	2	1
3:B:221:PCW:P	3:C:601:PCW:H63	0.49	2.48	4	1
3:C:606:PCW:H381	3:C:612:PCW:H162	0.49	1.85	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:7:VAL:HG13	7:B:239:EWS:CAU	0.49	2.38	5	1
3:B:204:PCW:H121	3:B:208:PCW:H352	0.49	1.82	5	1
3:A:402:PCW:C32	3:B:205:PCW:H32	0.49	2.37	6	1
2:B:5:LYS:HG2	2:B:54:ASP:HB3	0.49	1.83	6	1
3:B:214:PCW:H261	3:C:615:PCW:H472	0.49	1.83	7	1
2:B:15:GLY:HA2	5:B:237:GNP:O2B	0.49	2.07	9	1
3:A:405:PCW:H461	3:C:609:PCW:H20	0.49	1.83	10	1
3:B:223:PCW:C28	1:C:521:TYR:OH	0.49	2.61	10	1
3:A:406:PCW:H322	4:B:227:17F:H6A	0.49	1.83	1	1
4:B:236:17F:H11A	3:C:622:PCW:H272	0.49	1.85	3	1
1:C:574:LEU:O	1:C:578:GLU:HG3	0.49	2.07	6	1
3:C:607:PCW:H272	3:C:615:PCW:H451	0.49	1.85	10	1
2:B:6:LEU:O	7:B:239:EWS:NAW	0.49	2.46	1	1
3:B:210:PCW:H142	3:B:214:PCW:H162	0.49	1.84	1	1
2:B:116:ASN:HA	2:B:144:THR:O	0.49	2.08	7	2
3:B:211:PCW:H151	4:B:226:17F:H20	0.49	1.83	4	1
1:C:489:LEU:O	1:C:493:GLN:HG3	0.49	2.08	5	1
2:B:5:LYS:CG	7:B:239:EWS:CAX	0.49	2.91	8	1
4:B:226:17F:H39	4:C:628:17F:H55	0.49	1.83	8	1
3:B:202:PCW:H231	3:B:215:PCW:H242	0.49	1.85	2	1
3:B:207:PCW:H242	3:B:216:PCW:H182	0.49	1.84	2	1
1:C:488:LYS:HG2	3:C:620:PCW:C28	0.49	2.36	3	1
1:C:466:GLU:OE1	1:C:469:LEU:CD1	0.49	2.58	1	1
3:C:601:PCW:H461	3:C:601:PCW:H171	0.49	1.84	2	1
3:B:215:PCW:H461	4:C:632:17F:H75	0.49	1.85	3	1
3:C:615:PCW:C19	4:C:633:17F:H12	0.49	2.38	4	2
3:A:402:PCW:H11	3:B:212:PCW:H31	0.49	1.84	6	1
3:B:221:PCW:H212	4:C:627:17F:H54	0.49	1.84	10	1
4:C:627:17F:H68	4:C:629:17F:H53	0.49	1.84	10	1
3:B:202:PCW:H71	3:B:217:PCW:H31	0.49	1.85	1	1
3:B:221:PCW:H242	3:C:601:PCW:H172	0.49	1.85	2	1
1:C:517:HIS:O	1:C:521:TYR:HB2	0.49	2.07	7	3
3:B:210:PCW:H121	3:B:214:PCW:H341	0.49	1.85	10	1
3:B:214:PCW:H232	4:B:229:17F:H50	0.49	1.83	10	1
3:B:207:PCW:H83	4:B:228:17F:HN1A	0.48	1.64	3	1
3:A:406:PCW:C16	4:A:407:17F:H33	0.48	2.38	6	1
3:C:612:PCW:H242	3:C:612:PCW:H422	0.48	1.84	6	1
1:A:336:GLU:HA	1:A:339:LYS:HE3	0.48	1.85	7	1
2:B:143:GLU:O	2:B:151:GLY:HA3	0.48	2.08	7	1
3:C:615:PCW:H212	4:C:629:17F:H42	0.48	1.84	8	1
4:A:407:17F:H50	3:C:613:PCW:H283	0.48	1.84	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:236:17F:H77	3:C:603:PCW:H272	0.48	1.85	1	1
1:A:268:GLU:O	1:A:272:TYR:HB2	0.48	2.08	2	3
4:B:231:17F:H12A	4:B:231:17F:H61	0.48	1.85	3	1
3:C:605:PCW:H261	4:C:629:17F:H66	0.48	1.85	4	1
4:B:228:17F:O8	4:B:232:17F:H6A	0.48	2.08	6	1
3:B:204:PCW:H141	3:B:208:PCW:H371	0.48	1.85	7	1
3:C:604:PCW:H31	3:C:625:PCW:H341	0.48	1.86	7	1
3:B:214:PCW:H231	4:B:229:17F:H39	0.48	1.84	1	1
3:C:610:PCW:H62	3:C:617:PCW:H61	0.48	1.85	1	1
2:B:147:LYS:HG3	5:B:237:GNP:HN1	0.48	1.69	3	1
3:A:405:PCW:H2	4:B:228:17F:H19	0.48	1.84	6	1
4:A:407:17F:H44	3:B:220:PCW:H421	0.48	1.85	6	1
3:C:626:PCW:H41	3:C:626:PCW:O31	0.48	2.08	6	1
1:C:479:ALA:O	1:C:483:GLU:HG2	0.48	2.08	2	1
3:A:409:PCW:H142	3:A:410:PCW:H172	0.48	1.84	3	1
1:A:359:THR:HA	1:A:362:GLU:OE1	0.48	2.09	4	1
3:C:615:PCW:H231	4:C:629:17F:H45	0.48	1.85	5	1
3:A:408:PCW:H11	3:C:610:PCW:H321	0.48	1.85	7	1
1:A:291:LEU:O	1:A:295:GLN:HG3	0.48	2.08	8	1
3:B:215:PCW:H121	3:B:217:PCW:H122	0.48	1.84	9	1
3:C:615:PCW:H20	4:C:633:17F:H40	0.48	1.85	10	1
3:B:224:PCW:H71	4:B:229:17F:O5	0.48	2.08	2	1
1:C:563:LYS:HB2	1:C:564:PRO:CD	0.48	2.39	10	5
4:C:627:17F:H10A	4:C:629:17F:H19	0.48	1.86	2	1
3:B:204:PCW:H142	3:B:208:PCW:H362	0.48	1.84	4	1
3:C:607:PCW:O11	3:C:615:PCW:H51	0.48	2.08	7	1
3:A:405:PCW:H142	3:C:609:PCW:H272	0.48	1.85	10	1
2:B:17:SER:HB2	2:B:29:VAL:HG21	0.48	1.84	1	1
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.48	2.39	2	4
3:B:204:PCW:O2P	3:B:204:PCW:H73	0.48	2.08	2	1
1:A:297:LYS:O	1:A:301:LEU:HB2	0.48	2.08	3	2
3:B:208:PCW:H272	3:B:219:PCW:H272	0.48	1.85	4	1
3:A:406:PCW:H331	4:B:227:17F:C8	0.48	2.39	6	1
3:B:208:PCW:H39	3:B:234:PCW:H272	0.48	1.84	8	1
3:C:604:PCW:H152	3:C:625:PCW:H462	0.48	1.84	9	1
3:A:401:PCW:H41	3:B:213:PCW:O11	0.48	2.09	1	1
3:B:210:PCW:H71	4:B:229:17F:O4	0.48	2.08	2	1
3:B:203:PCW:H422	4:B:228:17F:H40	0.48	1.86	3	1
3:B:214:PCW:H221	3:C:615:PCW:H483	0.48	1.85	4	1
2:B:22:GLN:O	2:B:26:ASN:HA	0.48	2.08	9	4
4:B:236:17F:H73	4:C:628:17F:H72	0.48	1.86	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:212:PCW:H152	4:B:231:17F:H59	0.48	1.84	5	1
3:A:402:PCW:H152	3:A:402:PCW:H351	0.48	1.84	9	1
3:B:203:PCW:O2	3:B:213:PCW:H322	0.48	2.08	9	1
3:A:405:PCW:H151	4:B:228:17F:H33	0.48	1.86	10	1
2:B:71:TYR:CD1	7:B:239:EWS:BRA	0.48	3.22	1	1
3:A:401:PCW:H261	3:C:614:PCW:H281	0.48	1.86	4	1
3:A:406:PCW:H382	4:B:227:17F:H8A	0.48	1.84	4	1
3:B:214:PCW:H81	4:B:229:17F:O1	0.48	2.09	4	1
3:A:405:PCW:H152	3:C:609:PCW:H262	0.48	1.84	5	1
1:C:559:SER:HB2	1:C:563:LYS:HE2	0.48	1.85	5	1
3:B:206:PCW:H162	3:B:208:PCW:H161	0.48	1.86	9	1
3:B:210:PCW:H122	3:B:214:PCW:H162	0.48	1.86	9	1
3:B:215:PCW:H40	4:C:632:17F:H76	0.48	1.84	9	1
3:B:235:PCW:H251	3:C:622:PCW:H251	0.48	1.86	9	1
3:C:614:PCW:H412	3:C:619:PCW:H20	0.48	1.86	9	1
2:B:5:LYS:HB3	7:B:239:EWS:NAW	0.48	2.23	6	2
3:B:207:PCW:H63	4:B:228:17F:HN1	0.48	1.68	6	1
3:A:403:PCW:H51	4:B:231:17F:H4	0.48	1.86	7	1
3:B:221:PCW:H82	4:B:229:17F:C3	0.48	2.39	7	1
3:B:213:PCW:H83	4:B:230:17F:O1	0.48	2.08	8	1
1:A:308:ARG:CG	1:C:469:LEU:CD2	0.48	2.91	10	1
3:B:217:PCW:H483	3:B:219:PCW:H481	0.48	1.85	10	1
3:C:621:PCW:H162	4:C:632:17F:H6	0.47	1.85	1	1
3:B:220:PCW:H121	3:B:220:PCW:H372	0.47	1.85	2	2
3:C:615:PCW:H212	4:C:629:17F:H41	0.47	1.85	2	1
3:C:603:PCW:H332	3:C:607:PCW:H122	0.47	1.86	3	1
3:A:410:PCW:H331	4:C:630:17F:C1X	0.47	2.39	4	1
3:B:201:PCW:H432	4:B:228:17F:H45	0.47	1.84	5	1
2:B:5:LYS:HD3	2:B:54:ASP:HB3	0.47	1.85	7	1
2:B:3:GLU:HG3	3:B:223:PCW:H81	0.47	1.85	8	1
3:B:205:PCW:H483	3:C:610:PCW:H432	0.47	1.86	8	1
1:A:273:ARG:HA	1:A:276:VAL:HG12	0.47	1.85	1	1
1:C:430:LEU:HA	1:C:433:GLU:HB2	0.47	1.86	1	1
3:C:608:PCW:H31	4:C:631:17F:C4	0.47	2.39	1	2
1:A:363:LYS:O	1:A:367:ALA:HB3	0.47	2.10	4	4
3:C:621:PCW:H442	4:C:632:17F:H12	0.47	1.84	4	1
3:B:203:PCW:H52	3:B:203:PCW:H2	0.47	1.85	10	1
1:C:488:LYS:CB	3:C:620:PCW:H281	0.47	2.38	3	1
3:C:605:PCW:H152	4:C:627:17F:H34	0.47	1.86	6	1
1:A:242:GLU:HB3	1:C:532:ARG:NH2	0.47	2.24	10	1
3:C:607:PCW:H132	3:C:615:PCW:H342	0.47	1.86	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:402:PCW:O1P	3:B:212:PCW:H51	0.47	2.09	6	1
3:B:220:PCW:H142	4:B:232:17F:H60	0.47	1.86	8	1
3:A:404:PCW:H72	7:B:239:EWS:OAB	0.47	2.08	10	1
3:A:406:PCW:H51	4:B:230:17F:N1	0.47	2.24	1	1
3:B:210:PCW:H282	3:B:214:PCW:H40	0.47	1.86	2	1
3:B:211:PCW:H62	3:B:211:PCW:H12	0.47	1.85	2	1
3:C:615:PCW:H182	4:C:633:17F:H12	0.47	1.87	2	1
3:B:209:PCW:H382	3:B:224:PCW:H221	0.47	1.86	3	1
3:B:204:PCW:H342	3:B:212:PCW:H12	0.47	1.87	4	1
1:C:429:ASN:HA	1:C:432:LYS:HD2	0.47	1.85	4	2
4:B:236:17F:H43	4:B:236:17F:H75	0.47	1.85	5	1
3:B:216:PCW:O1P	3:C:601:PCW:H71	0.47	2.09	7	1
3:C:623:PCW:H39	3:C:623:PCW:H141	0.47	1.86	8	1
3:B:202:PCW:H332	3:B:215:PCW:H141	0.47	1.86	1	1
3:B:216:PCW:H32	4:B:229:17F:H2	0.47	1.87	1	1
4:B:236:17F:H73	4:C:628:17F:H68	0.47	1.86	1	2
4:B:230:17F:H78	3:C:619:PCW:H451	0.47	1.85	2	1
2:B:5:LYS:HD3	7:B:239:EWS:OAB	0.47	2.08	6	1
3:B:221:PCW:H121	3:C:601:PCW:H351	0.47	1.85	6	1
3:B:221:PCW:H452	3:C:605:PCW:H471	0.47	1.87	6	1
3:B:201:PCW:H361	4:B:227:17F:H20	0.47	1.86	7	1
3:A:402:PCW:H482	3:C:610:PCW:H261	0.47	1.87	8	1
3:A:406:PCW:H121	4:A:407:17F:C31	0.47	2.34	8	1
3:C:607:PCW:H332	3:C:615:PCW:H341	0.47	1.86	8	1
3:B:210:PCW:O2P	3:B:214:PCW:H41	0.47	2.09	10	1
3:C:604:PCW:H12	3:C:625:PCW:H332	0.47	1.86	1	1
3:C:607:PCW:H352	3:C:615:PCW:H382	0.47	1.85	1	1
3:A:408:PCW:H151	3:A:411:PCW:H152	0.47	1.84	2	1
3:B:208:PCW:H82	3:B:219:PCW:O1P	0.47	2.10	2	1
3:C:621:PCW:H132	4:C:632:17F:H4A	0.47	1.87	2	2
3:B:211:PCW:C12	4:B:226:17F:H18A	0.47	2.39	3	1
3:C:607:PCW:H152	3:C:615:PCW:H321	0.47	1.85	7	2
3:B:209:PCW:H451	3:B:224:PCW:H242	0.47	1.86	4	1
3:B:205:PCW:H152	3:B:205:PCW:H351	0.47	1.85	6	1
3:B:216:PCW:H231	3:C:604:PCW:H462	0.47	1.86	6	1
4:B:232:17F:H4A	4:B:232:17F:O10	0.47	2.09	6	1
3:C:626:PCW:H422	4:C:631:17F:H48	0.47	1.86	6	1
3:B:209:PCW:H131	3:B:216:PCW:H122	0.47	1.87	7	1
3:C:603:PCW:H252	4:C:628:17F:H39	0.47	1.85	8	1
3:A:408:PCW:H11	3:C:610:PCW:H352	0.47	1.87	9	1
3:B:224:PCW:H82	4:B:226:17F:O1	0.47	2.09	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:615:PCW:H151	4:C:633:17F:H8	0.47	1.85	9	1
3:A:409:PCW:H222	3:A:410:PCW:H212	0.47	1.86	10	1
3:B:203:PCW:H251	4:B:230:17F:H64	0.47	1.87	10	1
3:B:205:PCW:H461	3:C:610:PCW:H272	0.47	1.87	10	1
3:C:607:PCW:H152	3:C:615:PCW:H352	0.47	1.87	1	1
3:B:203:PCW:H482	3:B:213:PCW:H19	0.47	1.86	3	1
3:B:220:PCW:H131	4:B:232:17F:H31	0.47	1.87	3	1
4:B:236:17F:H68	3:C:603:PCW:H271	0.47	1.86	3	1
1:C:549:ALA:O	1:C:553:GLU:HG3	0.47	2.09	3	2
3:B:208:PCW:H41	3:B:219:PCW:H32	0.47	1.86	4	1
3:B:233:PCW:H62	3:B:233:PCW:H331	0.47	1.87	6	2
3:A:411:PCW:H452	3:C:616:PCW:H251	0.47	1.87	1	1
3:C:613:PCW:H31	3:C:613:PCW:O31	0.47	2.08	1	8
1:C:586:SER:O	1:C:590:GLU:HG3	0.47	2.10	10	2
3:B:204:PCW:H231	3:B:218:PCW:H212	0.47	1.87	3	1
1:A:375:LEU:HD11	4:B:230:17F:H54	0.47	1.87	4	1
3:B:203:PCW:H322	3:B:213:PCW:H352	0.47	1.86	9	1
3:B:201:PCW:O2P	3:B:213:PCW:H72	0.47	2.10	2	1
3:A:405:PCW:H161	4:B:228:17F:H34	0.47	1.87	4	1
3:B:204:PCW:H162	3:B:208:PCW:H382	0.47	1.86	4	1
3:A:410:PCW:H462	3:A:411:PCW:H241	0.47	1.86	6	1
4:B:227:17F:H58	4:B:227:17F:C10	0.47	2.39	9	2
3:A:406:PCW:H341	4:B:227:17F:H9A	0.47	1.87	7	1
3:B:211:PCW:O11	3:B:217:PCW:H12	0.47	2.10	7	1
3:B:234:PCW:H62	3:C:617:PCW:O1P	0.47	2.10	7	1
3:A:402:PCW:H372	4:B:231:17F:H74	0.47	1.87	8	1
3:B:207:PCW:H232	3:B:216:PCW:H162	0.47	1.86	9	1
3:B:209:PCW:H161	3:B:224:PCW:H211	0.47	1.86	10	1
3:B:214:PCW:H212	4:B:229:17F:H36	0.46	1.86	1	1
3:C:621:PCW:H432	4:C:632:17F:H69	0.46	1.87	2	1
3:B:206:PCW:O2P	3:B:211:PCW:H82	0.46	2.10	3	1
1:A:376:LEU:HB2	1:A:377:PRO:CD	0.46	2.40	9	3
3:B:223:PCW:H471	4:C:632:17F:C42	0.46	2.25	5	1
3:C:603:PCW:H421	3:C:607:PCW:H11	0.46	1.86	5	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.46	1.86	7	1
3:B:221:PCW:O31	3:B:221:PCW:H12	0.46	2.10	7	1
4:B:226:17F:H40	4:B:236:17F:H42	0.46	1.87	10	1
3:C:605:PCW:H221	4:C:627:17F:H37	0.46	1.85	10	1
1:C:440:GLU:O	1:C:444:ASP:HB2	0.46	2.10	1	1
3:B:211:PCW:O3	4:B:226:17F:H4	0.46	2.11	3	1
1:A:356:HIS:HD2	3:A:401:PCW:C27	0.46	2.16	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:212:PCW:H241	3:B:218:PCW:H451	0.46	1.87	4	1
3:A:405:PCW:O2P	3:B:207:PCW:H72	0.46	2.10	7	1
3:C:607:PCW:H341	3:C:615:PCW:H362	0.46	1.87	9	1
3:C:612:PCW:H161	3:C:617:PCW:H19	0.46	1.88	9	1
3:B:213:PCW:H441	3:B:213:PCW:H251	0.46	1.88	1	1
3:A:401:PCW:H482	3:C:614:PCW:H221	0.46	1.86	2	1
3:C:626:PCW:H40	4:C:631:17F:H44	0.46	1.87	6	2
1:A:372:ARG:O	1:A:376:LEU:HG	0.46	2.10	4	1
3:A:401:PCW:H481	3:C:614:PCW:H20	0.46	1.86	4	1
3:A:406:PCW:H381	4:B:227:17F:H11	0.46	1.87	4	1
3:B:207:PCW:H231	3:C:601:PCW:H322	0.46	1.87	4	1
1:A:351:ALA:O	1:A:355:GLU:HG2	0.46	2.10	5	1
3:B:208:PCW:H62	4:B:231:17F:O1	0.46	2.10	5	1
3:B:218:PCW:H41	3:B:219:PCW:O11	0.46	2.10	7	1
3:B:201:PCW:H32	4:B:230:17F:O1	0.46	2.10	10	1
4:B:226:17F:H35	4:B:236:17F:H50	0.46	1.86	10	1
3:C:603:PCW:H411	4:C:628:17F:C7	0.46	2.40	10	1
3:B:206:PCW:H482	3:B:218:PCW:H221	0.46	1.88	1	1
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.46	1.86	4	2
3:B:203:PCW:O2	3:B:213:PCW:H321	0.46	2.11	5	1
3:B:233:PCW:H481	3:C:603:PCW:H2	0.46	1.87	5	1
3:C:617:PCW:H411	3:C:618:PCW:H182	0.46	1.88	7	1
3:C:608:PCW:H73	4:C:631:17F:O1	0.46	2.10	8	1
3:B:202:PCW:H332	3:B:215:PCW:H152	0.46	1.88	9	1
4:C:628:17F:H1A	4:C:628:17F:H4	0.46	1.86	1	1
4:C:630:17F:C4	4:C:630:17F:C1	0.46	2.92	1	3
2:B:45:VAL:HG22	2:B:50:THR:HG23	0.46	1.88	10	2
3:A:409:PCW:H483	3:C:619:PCW:H40	0.46	1.86	4	1
3:A:403:PCW:H442	3:A:404:PCW:H141	0.46	1.87	5	1
2:B:171:SER:HA	3:B:209:PCW:H61	0.46	1.86	5	1
3:B:209:PCW:H381	4:B:228:17F:H20A	0.46	1.87	7	1
1:C:561:LYS:O	1:C:565:ALA:HB3	0.46	2.10	8	2
3:B:201:PCW:H371	4:B:228:17F:H41	0.46	1.87	9	1
1:A:392:GLU:HA	1:A:395:LYS:HG2	0.46	1.87	10	1
3:B:212:PCW:H382	4:B:231:17F:H10A	0.46	1.88	4	1
2:B:5:LYS:CD	7:B:239:EWS:OAB	0.46	2.63	6	1
3:B:210:PCW:H352	3:B:214:PCW:H142	0.46	1.86	7	1
3:C:611:PCW:H411	3:C:611:PCW:H19	0.46	1.86	8	1
3:B:212:PCW:H352	4:B:231:17F:H29	0.46	1.87	9	1
3:B:221:PCW:H422	4:B:229:17F:H63	0.46	1.86	9	1
3:C:606:PCW:H142	3:C:612:PCW:H171	0.46	1.87	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:409:PCW:H351	3:B:235:PCW:H382	0.46	1.87	5	1
3:B:214:PCW:H281	4:C:627:17F:H73	0.46	1.88	7	1
3:B:219:PCW:H452	3:B:219:PCW:H232	0.46	1.87	8	1
3:B:209:PCW:H131	3:B:224:PCW:H182	0.46	1.87	9	1
1:A:272:TYR:HD2	1:C:506:ARG:HH22	0.46	1.53	1	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.46	2.38	6	5
3:A:408:PCW:H252	3:A:411:PCW:H251	0.46	1.87	1	1
3:A:410:PCW:H382	4:C:630:17F:C12	0.46	2.40	1	1
2:B:145:SER:HB3	2:B:148:THR:HG22	0.46	1.88	1	1
1:C:563:LYS:CB	1:C:564:PRO:HD3	0.46	2.36	2	3
3:A:410:PCW:H51	3:A:410:PCW:H11	0.46	1.87	5	1
3:B:213:PCW:H141	4:B:228:17F:O9	0.46	2.11	5	1
3:B:206:PCW:O2P	3:B:211:PCW:H12	0.46	2.11	7	1
3:C:605:PCW:H451	4:C:627:17F:H51	0.46	1.88	8	1
3:A:408:PCW:H351	3:A:410:PCW:C34	0.46	2.34	2	1
1:A:315:ALA:O	1:A:319:HIS:HB2	0.46	2.11	5	1
3:A:409:PCW:H461	3:C:613:PCW:H171	0.46	1.88	5	1
3:B:201:PCW:H52	3:B:222:PCW:H42	0.46	1.86	6	1
3:C:607:PCW:H222	3:C:615:PCW:H411	0.46	1.87	6	1
3:C:609:PCW:H412	3:C:624:PCW:H222	0.46	1.88	8	1
3:B:205:PCW:H52	3:B:212:PCW:O2P	0.46	2.11	9	1
3:B:219:PCW:H411	3:B:223:PCW:H372	0.46	1.86	9	1
3:B:225:PCW:H19	3:B:225:PCW:H381	0.46	1.87	9	1
3:C:621:PCW:H252	3:C:622:PCW:H431	0.46	1.87	9	1
3:B:210:PCW:H132	3:B:217:PCW:H151	0.45	1.87	1	1
4:B:236:17F:H33	3:C:622:PCW:H19	0.45	1.87	10	2
1:C:455:TYR:OH	3:C:601:PCW:H231	0.45	2.10	9	2
3:C:622:PCW:H282	4:C:628:17F:H52	0.45	1.87	3	2
3:B:222:PCW:H481	3:C:622:PCW:H181	0.45	1.86	4	1
3:C:603:PCW:H412	3:C:607:PCW:H31	0.45	1.88	6	1
1:A:355:GLU:OE1	1:A:355:GLU:HA	0.45	2.11	3	1
3:C:615:PCW:H19	4:C:633:17F:H12	0.45	1.88	4	1
3:B:204:PCW:H2	3:B:208:PCW:H322	0.45	1.87	5	1
3:B:208:PCW:H451	4:B:231:17F:H48	0.45	1.88	5	1
1:C:466:GLU:HA	1:C:469:LEU:HD12	0.45	1.87	5	1
3:C:618:PCW:O3	3:C:626:PCW:H162	0.45	2.11	6	1
3:B:220:PCW:H442	3:B:222:PCW:H221	0.45	1.88	8	1
3:B:221:PCW:H172	3:C:601:PCW:H381	0.45	1.88	8	1
3:A:404:PCW:H20	3:B:225:PCW:H252	0.45	1.88	9	1
3:A:406:PCW:H472	3:A:409:PCW:H262	0.45	1.86	9	1
1:A:346:LEU:O	1:A:350:HIS:HB2	0.45	2.11	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:603:PCW:H231	4:C:632:17F:H54	0.45	1.87	1	1
3:C:604:PCW:H131	3:C:625:PCW:H372	0.45	1.88	3	1
3:B:217:PCW:H232	4:B:226:17F:H64	0.45	1.88	5	1
3:B:210:PCW:H181	3:B:214:PCW:H19	0.45	1.88	6	1
3:A:411:PCW:H431	3:C:616:PCW:H261	0.45	1.88	9	1
3:C:611:PCW:H31	3:C:619:PCW:O3	0.45	2.11	9	1
3:B:201:PCW:H371	4:B:228:17F:C21	0.45	2.37	10	1
3:B:207:PCW:C21	3:C:601:PCW:H412	0.45	2.40	2	1
3:B:221:PCW:H131	3:B:221:PCW:H341	0.45	1.88	3	1
3:C:607:PCW:H181	3:C:615:PCW:H352	0.45	1.89	4	1
1:A:352:LYS:HG2	1:C:422:VAL:HG22	0.45	1.88	6	1
3:B:204:PCW:P	3:B:212:PCW:O2P	0.45	2.74	6	1
3:B:212:PCW:H121	4:B:231:17F:H9A	0.45	1.88	7	1
3:B:216:PCW:H71	4:B:229:17F:H19A	0.45	1.88	8	1
3:C:603:PCW:H441	3:C:607:PCW:H11	0.45	1.88	8	1
3:A:402:PCW:O2P	3:B:205:PCW:H32	0.45	2.11	9	1
3:B:203:PCW:H122	4:B:230:17F:O8	0.45	2.11	10	1
3:B:210:PCW:H232	3:B:214:PCW:H461	0.45	1.87	10	1
4:B:230:17F:H9	4:B:230:17F:H19	0.45	1.88	10	1
3:A:403:PCW:C39	3:B:218:PCW:C48	0.45	2.95	1	1
3:A:403:PCW:H221	3:C:606:PCW:C26	0.45	2.40	1	1
3:B:203:PCW:H41	4:B:230:17F:O2	0.45	2.11	3	1
3:C:607:PCW:H232	3:C:615:PCW:H411	0.45	1.88	3	1
2:B:163:ILE:HG22	2:B:167:LYS:HE2	0.45	1.87	4	1
4:B:227:17F:H33	4:B:227:17F:O8	0.45	2.12	5	1
3:B:213:PCW:N	4:B:232:17F:N1	0.45	2.65	7	1
3:A:409:PCW:H62	4:C:630:17F:H1A	0.45	1.87	9	1
3:B:202:PCW:H162	3:B:215:PCW:H182	0.45	1.88	9	1
3:B:234:PCW:H172	3:B:234:PCW:H421	0.45	1.87	9	1
3:B:210:PCW:H51	4:B:226:17F:H2	0.45	1.88	10	1
3:C:615:PCW:H212	4:C:629:17F:H45	0.45	1.88	10	1
1:C:464:GLN:O	1:C:468:GLU:HG3	0.45	2.12	6	1
3:A:410:PCW:H472	3:A:411:PCW:H283	0.45	1.87	7	1
3:A:409:PCW:H261	3:C:613:PCW:H181	0.45	1.88	10	1
3:B:221:PCW:H61	4:B:229:17F:O2	0.45	2.11	10	1
3:B:221:PCW:C17	3:C:601:PCW:H411	0.45	2.41	10	1
3:C:603:PCW:C40	4:C:628:17F:H6	0.45	2.42	2	1
1:C:455:TYR:CE1	3:C:601:PCW:H252	0.45	2.47	3	1
1:A:363:LYS:HG2	1:C:411:THR:HG22	0.45	1.87	4	1
3:B:211:PCW:H372	4:B:226:17F:H19A	0.45	1.89	5	1
3:B:233:PCW:H51	4:B:236:17F:O2	0.45	2.12	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:223:PCW:H461	3:C:622:PCW:H452	0.45	1.87	7	1
3:B:234:PCW:H442	3:B:234:PCW:H212	0.45	1.89	7	1
3:B:221:PCW:H141	3:C:601:PCW:H372	0.45	1.88	8	1
1:A:352:LYS:HZ2	1:C:425:GLU:CB	0.45	2.24	4	1
3:B:212:PCW:H172	4:B:231:17F:H34	0.45	1.89	5	1
4:B:226:17F:H20A	4:B:229:17F:H10	0.45	1.88	6	1
1:C:487:GLN:O	1:C:491:GLU:HG3	0.45	2.12	6	1
3:B:209:PCW:H342	4:B:228:17F:O8	0.45	2.12	1	1
1:C:461:LYS:O	1:C:465:GLU:HG3	0.45	2.11	1	2
3:A:408:PCW:H251	3:A:411:PCW:H232	0.45	1.87	2	1
3:B:214:PCW:H271	3:C:615:PCW:H432	0.45	1.89	2	1
3:C:611:PCW:H182	3:C:619:PCW:H181	0.45	1.89	2	3
3:A:405:PCW:H242	3:C:609:PCW:H261	0.45	1.88	3	1
3:B:220:PCW:H451	3:B:235:PCW:H232	0.45	1.88	5	1
4:B:236:17F:H72	3:C:603:PCW:H262	0.45	1.89	5	1
3:A:406:PCW:H331	4:B:227:17F:H8A	0.45	1.88	6	1
3:B:235:PCW:H11	3:C:602:PCW:H11	0.45	1.88	6	1
3:B:208:PCW:H261	3:B:219:PCW:H283	0.45	1.88	7	1
3:B:217:PCW:H342	3:B:217:PCW:H152	0.45	1.87	7	1
1:A:327:LEU:HD23	1:A:330:ARG:HD3	0.45	1.88	9	1
4:B:236:17F:H44	4:C:628:17F:H78	0.45	1.88	10	1
3:B:234:PCW:H251	3:C:617:PCW:H481	0.45	1.89	1	1
3:B:213:PCW:H121	4:B:228:17F:O9	0.45	2.12	9	2
1:C:431:GLU:HA	1:C:434:THR:OG1	0.45	2.12	7	1
3:B:201:PCW:H362	3:B:220:PCW:H382	0.45	1.89	8	1
3:B:204:PCW:H422	3:B:205:PCW:H351	0.45	1.88	8	1
4:C:628:17F:H6A	4:C:632:17F:HN1	0.45	1.72	8	1
3:A:405:PCW:H40	3:C:609:PCW:H20	0.44	1.89	2	1
3:C:615:PCW:H421	4:C:632:17F:H52	0.44	1.89	3	1
3:A:410:PCW:H352	4:C:630:17F:H37	0.44	1.89	7	1
3:B:203:PCW:H483	4:B:228:17F:H57	0.44	1.87	7	1
3:B:203:PCW:H411	3:B:213:PCW:H162	0.44	1.89	7	1
3:C:611:PCW:H382	3:C:611:PCW:H171	0.44	1.89	7	1
4:C:628:17F:H65	4:C:632:17F:H29	0.44	1.89	7	1
4:B:227:17F:H65	3:C:623:PCW:H281	0.44	1.90	9	1
3:C:607:PCW:H322	3:C:615:PCW:H341	0.44	1.88	10	1
3:C:613:PCW:H171	3:C:613:PCW:H431	0.44	1.88	10	1
3:B:206:PCW:H451	3:B:208:PCW:H282	0.44	1.90	1	1
2:B:5:LYS:HA	2:B:54:ASP:O	0.44	2.12	2	1
3:B:204:PCW:H42	3:B:218:PCW:O4P	0.44	2.12	1	1
3:B:208:PCW:O1P	3:B:211:PCW:H83	0.44	2.13	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H231	4:A:407:17F:H75	0.44	1.88	2	1
3:C:611:PCW:H141	3:C:619:PCW:H172	0.44	1.88	2	1
3:B:212:PCW:H332	4:B:231:17F:H8A	0.44	1.88	4	1
4:B:227:17F:H58	4:B:227:17F:H9A	0.44	1.88	5	1
3:B:223:PCW:H462	3:C:622:PCW:H452	0.44	1.88	9	1
4:B:230:17F:H2	4:B:230:17F:O2	0.44	2.12	9	1
3:C:622:PCW:H73	3:C:622:PCW:H331	0.44	1.88	9	1
4:A:407:17F:H54	3:B:204:PCW:H481	0.44	1.89	1	1
3:B:201:PCW:H382	3:B:220:PCW:H361	0.44	1.89	2	1
2:B:113:LEU:O	2:B:141:PHE:HA	0.44	2.12	4	1
3:A:403:PCW:H432	3:B:218:PCW:H472	0.44	1.89	10	1
4:B:236:17F:H10	4:C:628:17F:H41	0.44	1.90	10	1
1:C:530:ALA:O	1:C:534:GLU:HG2	0.44	2.12	2	1
3:B:220:PCW:H251	4:B:232:17F:H75	0.44	1.90	3	1
3:A:404:PCW:H261	4:C:631:17F:H49	0.44	1.88	4	1
3:B:219:PCW:O2P	3:B:225:PCW:H62	0.44	2.13	4	1
4:B:229:17F:H4	4:B:229:17F:H2	0.44	1.89	4	1
3:C:607:PCW:H121	3:C:615:PCW:O31	0.44	2.12	4	1
1:A:307:ASP:HA	1:A:310:ARG:CD	0.44	2.41	5	1
1:A:242:GLU:OE1	1:C:528:ARG:HA	0.44	2.12	6	1
3:A:401:PCW:H40	3:B:203:PCW:H271	0.44	1.88	6	1
3:B:211:PCW:H242	3:B:216:PCW:H161	0.44	1.90	6	1
3:B:224:PCW:H52	4:B:226:17F:P1	0.44	2.52	8	1
3:B:204:PCW:H372	3:B:222:PCW:H141	0.44	1.89	9	1
3:B:210:PCW:H52	4:B:229:17F:HN1	0.44	1.72	9	1
1:C:455:TYR:O	1:C:459:PHE:HB2	0.44	2.12	10	1
3:C:611:PCW:H172	3:C:623:PCW:H451	0.44	1.89	2	1
3:B:221:PCW:H182	3:C:601:PCW:H412	0.44	1.90	3	1
3:C:618:PCW:H122	3:C:626:PCW:H181	0.44	1.89	3	2
3:B:210:PCW:C14	3:B:214:PCW:H151	0.44	2.40	5	1
3:B:221:PCW:H411	3:C:601:PCW:H372	0.44	1.89	7	1
3:C:605:PCW:H221	4:C:629:17F:H51	0.44	1.89	8	1
4:A:407:17F:H20A	4:A:407:17F:H8	0.44	1.88	10	1
1:A:277:GLU:HB3	1:A:278:PRO:CD	0.44	2.43	1	1
4:A:407:17F:H30	4:B:227:17F:H19	0.44	1.89	2	1
3:B:208:PCW:H332	3:B:222:PCW:H362	0.44	1.90	4	1
3:A:404:PCW:H40	3:B:225:PCW:H261	0.44	1.89	5	1
1:A:243:MET:HA	1:A:246:ASP:HB2	0.44	1.90	6	1
1:A:299:SER:HB2	1:A:300:PRO:CD	0.44	2.42	10	2
3:B:210:PCW:H73	4:B:226:17F:H2	0.44	1.89	6	1
1:C:428:ASP:O	1:C:432:LYS:HG3	0.44	2.12	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:405:PCW:O2P	3:B:207:PCW:H83	0.44	2.13	7	1
3:A:409:PCW:H211	3:C:613:PCW:H142	0.44	1.87	8	1
3:B:216:PCW:H32	4:B:229:17F:HN1	0.44	1.71	8	1
3:A:410:PCW:C32	4:C:630:17F:H29	0.44	2.43	10	1
3:C:607:PCW:H142	3:C:615:PCW:H321	0.44	1.90	10	1
3:B:218:PCW:H152	3:B:219:PCW:H121	0.44	1.90	1	1
3:B:219:PCW:H482	4:C:631:17F:H63	0.44	1.89	1	1
3:B:204:PCW:H322	3:B:222:PCW:H121	0.44	1.89	2	1
1:C:458:ASP:O	1:C:462:LYS:HG3	0.44	2.13	2	1
3:B:205:PCW:H19	3:B:205:PCW:H412	0.44	1.89	3	1
4:A:407:17F:H41	4:B:227:17F:H31	0.44	1.87	7	1
3:B:207:PCW:H162	3:B:209:PCW:H211	0.44	1.90	7	1
1:A:345:ARG:HD3	1:C:433:GLU:OE2	0.44	2.13	8	1
3:B:201:PCW:H181	4:B:230:17F:H18	0.44	1.89	8	1
3:B:207:PCW:H422	3:B:209:PCW:H231	0.44	1.90	10	1
3:B:233:PCW:H82	4:B:236:17F:O1	0.44	2.13	10	1
3:C:618:PCW:C35	3:C:626:PCW:H212	0.44	2.43	10	1
1:C:485:ALA:HA	1:C:488:LYS:HG2	0.44	1.90	4	1
2:B:62:GLU:OE1	2:B:68:ARG:HD3	0.44	2.13	5	1
3:C:609:PCW:H132	3:C:625:PCW:H40	0.44	1.89	5	1
3:A:409:PCW:H211	3:C:613:PCW:H171	0.44	1.89	6	1
3:A:401:PCW:O1P	3:A:405:PCW:H12	0.44	2.12	7	1
3:A:410:PCW:H322	4:C:630:17F:C21	0.44	2.41	8	1
3:B:216:PCW:H11	4:B:229:17F:N1	0.44	2.28	8	1
3:C:621:PCW:H422	4:C:632:17F:H34	0.44	1.88	9	1
3:B:221:PCW:C17	3:C:601:PCW:C41	0.44	2.96	10	1
3:C:618:PCW:H412	3:C:626:PCW:C17	0.44	2.43	10	1
3:B:220:PCW:H331	3:B:220:PCW:H132	0.43	1.90	1	1
1:C:512:ASP:O	1:C:515:ARG:HB2	0.43	2.13	1	1
3:A:406:PCW:H462	4:A:407:17F:H74	0.43	1.90	5	1
3:B:221:PCW:H362	4:B:229:17F:H58	0.43	1.90	5	1
3:C:626:PCW:H271	4:C:631:17F:H41	0.43	1.89	5	1
1:A:392:GLU:HA	1:A:395:LYS:HD2	0.43	1.89	7	1
1:C:567:GLU:HG2	1:C:571:GLN:NE2	0.43	2.27	9	1
3:B:212:PCW:H351	4:B:231:17F:H8A	0.43	1.88	1	1
1:A:278:PRO:O	1:A:282:GLU:HG3	0.43	2.12	5	2
3:C:615:PCW:H222	4:C:633:17F:H41	0.43	1.90	8	2
3:A:405:PCW:H152	4:B:228:17F:H34	0.43	1.88	6	1
1:C:491:GLU:HB3	1:C:495:LYS:CE	0.43	2.44	7	2
3:C:605:PCW:H171	4:C:627:17F:H34	0.43	1.90	9	1
3:B:221:PCW:H241	3:C:601:PCW:C20	0.43	2.40	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:608:PCW:H82	4:C:631:17F:O1	0.43	2.12	10	1
3:C:609:PCW:O1P	3:C:614:PCW:H32	0.43	2.13	10	1
3:A:403:PCW:H222	3:C:606:PCW:C27	0.43	2.41	1	1
1:C:485:ALA:HA	3:C:620:PCW:H271	0.43	1.90	3	1
3:C:603:PCW:H251	3:C:607:PCW:H281	0.43	1.88	3	1
3:C:606:PCW:H171	3:C:616:PCW:H39	0.43	1.88	3	1
3:C:621:PCW:H441	4:C:632:17F:H37	0.43	1.89	3	1
3:B:210:PCW:H122	3:B:214:PCW:H121	0.43	1.88	4	1
4:B:226:17F:H51	4:C:628:17F:H54	0.43	1.90	4	1
3:C:620:PCW:C13	4:C:633:17F:H59	0.43	2.39	4	1
2:B:32:TYR:HD1	5:B:237:GNP:HNB3	0.43	1.56	5	1
3:B:212:PCW:H252	3:B:218:PCW:H412	0.43	1.91	5	1
3:B:203:PCW:H40	4:B:228:17F:H12A	0.43	1.90	7	1
1:C:458:ASP:HA	1:C:461:LYS:HD2	0.43	1.90	9	1
3:C:607:PCW:H151	3:C:615:PCW:C35	0.43	2.43	10	1
3:B:207:PCW:H42	3:B:216:PCW:H351	0.43	1.90	2	1
2:B:40:TYR:CE1	2:B:57:ASP:HB2	0.43	2.44	3	1
1:A:376:LEU:HB2	1:A:377:PRO:HD3	0.43	1.91	9	2
1:A:291:LEU:HD23	1:A:294:LEU:HD12	0.43	1.88	5	1
3:B:219:PCW:O2P	3:B:225:PCW:H82	0.43	2.13	6	1
3:B:233:PCW:H83	3:C:602:PCW:H32	0.43	1.90	6	1
1:A:330:ARG:HD3	1:C:444:ASP:OD2	0.43	2.14	7	1
3:B:203:PCW:H19	4:B:230:17F:H10	0.43	1.89	7	1
3:B:208:PCW:H352	3:B:222:PCW:H352	0.43	1.89	10	1
3:C:618:PCW:H122	3:C:626:PCW:H171	0.43	1.91	2	1
3:B:203:PCW:H441	3:B:213:PCW:H262	0.43	1.90	3	1
3:B:221:PCW:H222	3:C:601:PCW:H483	0.43	1.90	3	1
3:B:235:PCW:O4P	3:B:235:PCW:H2	0.43	2.13	4	1
3:B:215:PCW:H73	3:B:217:PCW:O1P	0.43	2.13	5	1
3:B:216:PCW:H241	3:C:605:PCW:H461	0.43	1.90	8	1
1:A:356:HIS:HA	1:C:418:GLN:OE1	0.43	2.13	10	1
3:A:408:PCW:O31	3:A:410:PCW:H332	0.43	2.13	10	1
2:B:84:ILE:HD12	2:B:123:ARG:HG3	0.43	1.90	10	1
3:B:204:PCW:O3P	3:B:222:PCW:H61	0.43	2.13	1	1
1:A:263:LYS:O	1:A:267:GLU:HG3	0.43	2.14	6	2
2:B:14:VAL:HG23	2:B:16:LYS:HG2	0.43	1.91	2	1
3:B:201:PCW:H132	4:B:230:17F:H18	0.43	1.91	3	1
3:B:214:PCW:H42	3:B:217:PCW:H61	0.43	1.90	4	1
3:B:212:PCW:H332	4:B:231:17F:H11	0.43	1.89	6	1
3:B:223:PCW:H451	3:C:622:PCW:H431	0.43	1.90	6	1
3:B:221:PCW:H141	3:C:601:PCW:H362	0.43	1.91	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:618:PCW:O1P	3:C:626:PCW:H2	0.43	2.12	9	1
3:B:209:PCW:O31	3:B:216:PCW:H31	0.43	2.13	10	1
4:B:228:17F:H47	3:C:611:PCW:H462	0.43	1.89	1	1
3:C:605:PCW:H171	4:C:629:17F:H18	0.43	1.91	1	1
3:B:204:PCW:H231	3:B:212:PCW:H461	0.43	1.91	2	1
2:B:109:VAL:HB	2:B:111:MET:HE2	0.43	1.90	3	2
1:A:365:LYS:HB2	1:A:366:PRO:CD	0.43	2.43	9	2
3:A:410:PCW:H381	4:C:630:17F:H36	0.43	1.90	4	2
3:B:222:PCW:H71	3:B:222:PCW:O31	0.43	2.13	6	1
3:B:206:PCW:H431	3:B:217:PCW:H382	0.43	1.89	8	1
2:B:68:ARG:O	2:B:72:MET:HB2	0.43	2.13	4	3
3:A:406:PCW:H321	4:B:227:17F:O7	0.43	2.14	5	1
1:C:510:HIS:O	1:C:514:LEU:HG	0.43	2.14	8	2
3:B:222:PCW:H272	3:B:235:PCW:H221	0.43	1.89	4	1
3:B:210:PCW:C7	4:B:226:17F:HN1A	0.43	2.26	5	1
3:B:235:PCW:H32	3:C:602:PCW:H31	0.43	1.91	5	1
3:A:402:PCW:H471	4:B:231:17F:H46	0.43	1.90	8	1
3:C:611:PCW:H221	3:C:619:PCW:H242	0.43	1.91	8	1
3:A:406:PCW:H282	3:A:411:PCW:H481	0.43	1.90	10	1
3:B:217:PCW:H131	4:B:226:17F:H63	0.43	1.90	10	1
1:A:258:LEU:O	1:A:262:GLN:HB2	0.43	2.14	1	1
3:B:215:PCW:H72	3:B:219:PCW:H63	0.43	1.91	1	1
1:A:335:LEU:O	1:A:339:LYS:HG3	0.43	2.13	2	1
3:B:211:PCW:H382	4:B:226:17F:H10	0.43	1.91	4	1
4:B:236:17F:H8A	4:C:628:17F:H41	0.43	1.91	4	1
3:B:204:PCW:H181	3:B:218:PCW:H132	0.43	1.90	5	1
3:B:206:PCW:H351	3:B:211:PCW:H331	0.43	1.90	5	1
3:B:214:PCW:H40	3:B:215:PCW:H39	0.43	1.91	5	1
1:A:304:GLU:O	1:A:308:ARG:HG2	0.43	2.14	6	1
1:A:344:ALA:O	1:A:348:GLU:HG2	0.43	2.14	7	1
3:B:201:PCW:H42	4:B:230:17F:C2	0.43	2.44	7	1
4:C:633:17F:H58	4:C:633:17F:H30	0.43	1.90	7	1
1:A:386:PHE:O	1:A:390:LEU:HG	0.43	2.14	8	1
4:B:228:17F:H39	4:B:232:17F:H38	0.43	1.91	8	1
3:B:205:PCW:C4	3:B:222:PCW:H71	0.43	2.30	10	1
1:A:270:GLU:O	1:A:274:GLN:HB2	0.42	2.14	5	1
4:B:231:17F:H50	3:C:610:PCW:H483	0.42	1.91	5	1
2:B:20:THR:O	2:B:24:ILE:HG12	0.42	2.14	6	2
3:B:208:PCW:H19	3:B:222:PCW:H442	0.42	1.90	6	1
1:A:279:LEU:HB3	1:C:495:LYS:HD3	0.42	1.90	7	1
3:B:224:PCW:H52	4:B:226:17F:O1	0.42	2.14	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:607:PCW:H151	3:C:615:PCW:H351	0.42	1.90	10	1
3:A:401:PCW:H441	3:C:614:PCW:H272	0.42	1.90	1	1
3:C:604:PCW:H371	3:C:605:PCW:H331	0.42	1.91	1	1
3:B:209:PCW:H332	3:B:224:PCW:H19	0.42	1.90	3	1
3:B:235:PCW:C34	3:C:623:PCW:H331	0.42	2.44	4	1
3:C:625:PCW:O11	3:C:625:PCW:H52	0.42	2.15	7	1
3:B:207:PCW:H71	4:B:228:17F:C1	0.42	2.44	10	1
3:C:605:PCW:H242	4:C:629:17F:H52	0.42	1.92	10	1
3:B:211:PCW:H131	3:B:217:PCW:H2	0.42	1.90	1	1
3:C:604:PCW:H52	3:C:604:PCW:C1	0.42	2.44	2	1
3:A:404:PCW:H11	3:B:218:PCW:H372	0.42	1.89	3	1
2:B:6:LEU:O	2:B:55:ILE:HA	0.42	2.14	3	2
2:B:59:ALA:HB3	2:B:62:GLU:HG2	0.42	1.91	3	1
3:B:209:PCW:H342	4:B:228:17F:H18A	0.42	1.90	3	1
3:C:607:PCW:C15	3:C:615:PCW:H321	0.42	2.45	3	2
3:A:402:PCW:H321	3:B:205:PCW:H32	0.42	1.91	6	1
3:A:406:PCW:C31	4:A:407:17F:H31	0.42	2.44	8	1
3:C:610:PCW:H272	3:C:610:PCW:H482	0.42	1.92	8	1
4:B:236:17F:H75	3:C:603:PCW:H271	0.42	1.92	9	1
3:B:204:PCW:H412	3:B:205:PCW:H382	0.42	1.91	10	1
3:B:209:PCW:H151	3:B:216:PCW:H142	0.42	1.90	2	1
2:B:145:SER:HB2	2:B:150:GLN:HB2	0.42	1.92	3	1
3:B:224:PCW:H11	4:B:232:17F:H6	0.42	1.91	4	1
1:A:304:GLU:O	1:A:308:ARG:HG3	0.42	2.14	7	1
3:C:609:PCW:H382	3:C:624:PCW:H431	0.42	1.89	7	1
4:B:232:17F:H49	3:C:609:PCW:H451	0.42	1.91	9	1
1:A:330:ARG:HD3	1:C:444:ASP:CG	0.42	2.39	10	1
3:A:410:PCW:H442	3:A:410:PCW:H272	0.42	1.92	10	1
3:B:210:PCW:H71	4:B:226:17F:O1	0.42	2.14	1	1
3:B:219:PCW:H461	3:B:223:PCW:H482	0.42	1.89	1	1
3:B:233:PCW:H41	4:B:236:17F:O2	0.42	2.15	8	2
4:C:628:17F:H4A	4:C:632:17F:HN1	0.42	1.75	3	1
3:A:406:PCW:H321	4:A:407:17F:H8	0.42	1.91	4	1
2:B:62:GLU:HB3	2:B:68:ARG:NH1	0.42	2.30	4	1
3:B:233:PCW:H172	3:C:624:PCW:C15	0.42	2.44	4	1
2:B:170:MET:HB3	3:B:211:PCW:H52	0.42	1.92	9	1
3:B:217:PCW:H222	4:B:226:17F:H65	0.42	1.91	9	1
3:C:618:PCW:H372	3:C:626:PCW:H412	0.42	1.91	9	1
3:A:405:PCW:H432	3:C:609:PCW:H231	0.42	1.92	10	1
3:A:406:PCW:H211	4:A:407:17F:H70	0.42	1.90	2	1
3:C:610:PCW:H482	3:C:610:PCW:H252	0.42	1.89	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:356:HIS:O	1:A:360:LEU:HB2	0.42	2.14	4	1
3:B:215:PCW:H11	3:B:223:PCW:O1P	0.42	2.15	4	1
3:B:212:PCW:H412	4:B:231:17F:H57	0.42	1.90	5	1
3:C:615:PCW:H222	4:C:633:17F:H35	0.42	1.91	6	1
3:B:207:PCW:H71	4:B:228:17F:HN1	0.42	1.74	7	1
4:A:407:17F:H37	4:B:227:17F:H19	0.42	1.91	10	1
3:B:211:PCW:H11	3:B:217:PCW:O1P	0.42	2.14	10	1
4:A:407:17F:H30	4:B:227:17F:O10	0.42	2.15	1	1
2:B:78:PHE:O	2:B:111:MET:HA	0.42	2.15	3	1
2:B:133:LEU:HG	2:B:137:TYR:HE2	0.42	1.73	3	1
3:B:214:PCW:H241	3:C:615:PCW:H471	0.42	1.92	3	1
3:B:221:PCW:C7	4:B:229:17F:H1	0.42	2.36	4	1
3:B:201:PCW:H40	3:C:623:PCW:H272	0.42	1.90	5	1
3:A:409:PCW:H2	3:A:409:PCW:O1P	0.42	2.14	7	2
3:B:219:PCW:H231	3:B:219:PCW:H461	0.42	1.92	7	1
3:A:406:PCW:H331	4:A:407:17F:H31	0.42	1.91	8	1
1:C:458:ASP:HA	1:C:461:LYS:NZ	0.42	2.30	8	1
3:C:625:PCW:O11	3:C:625:PCW:H83	0.42	2.15	8	1
3:C:608:PCW:C1	4:C:631:17F:H4A	0.42	2.44	2	1
1:A:325:ASP:O	1:A:329:GLN:HG3	0.42	2.15	3	1
3:B:210:PCW:H73	4:B:226:17F:P1	0.42	2.55	10	1
3:C:615:PCW:H242	4:C:629:17F:H45	0.42	1.92	1	1
1:C:451:LYS:C	1:C:454:PRO:HD2	0.42	2.40	4	1
1:C:589:GLU:O	1:C:593:LYS:HG3	0.42	2.14	4	1
3:C:605:PCW:H481	4:C:627:17F:H53	0.42	1.91	4	1
3:B:210:PCW:H41	4:B:226:17F:O5	0.42	2.15	5	1
3:B:214:PCW:H381	3:B:217:PCW:H162	0.42	1.90	6	1
3:A:401:PCW:H362	3:B:213:PCW:H432	0.42	1.92	8	1
3:B:207:PCW:H232	3:C:601:PCW:H421	0.42	1.90	8	1
3:C:607:PCW:H283	3:C:615:PCW:H422	0.42	1.92	3	1
4:B:226:17F:H45	4:B:232:17F:H62	0.42	1.91	4	1
3:C:605:PCW:H212	4:C:627:17F:H37	0.42	1.92	6	1
3:B:210:PCW:H82	4:B:229:17F:H6A	0.42	1.91	7	1
3:A:410:PCW:H132	4:C:630:17F:H11A	0.42	1.92	8	1
3:B:216:PCW:H221	3:C:604:PCW:H462	0.42	1.91	8	1
1:C:427:TRP:O	1:C:431:GLU:HG2	0.41	2.15	1	1
3:B:218:PCW:H71	4:B:231:17F:H2	0.41	1.90	2	1
3:B:209:PCW:H73	3:B:216:PCW:H12	0.41	1.92	3	1
3:B:221:PCW:H371	4:B:229:17F:H31	0.41	1.91	3	1
3:B:211:PCW:H82	3:B:219:PCW:H321	0.41	1.91	4	1
3:A:408:PCW:H39	3:A:410:PCW:H432	0.41	1.92	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:602:PCW:H63	3:C:602:PCW:O11	0.41	2.15	6	1
1:C:574:LEU:HB2	1:C:575:PRO:CD	0.41	2.45	1	1
3:B:211:PCW:H121	4:B:226:17F:O9	0.41	2.14	3	1
3:A:409:PCW:H63	4:C:630:17F:N1	0.41	2.30	4	1
1:C:488:LYS:NZ	3:C:620:PCW:C27	0.41	2.83	4	1
3:B:209:PCW:H61	3:B:216:PCW:O2P	0.41	2.14	6	1
3:B:205:PCW:H62	3:B:212:PCW:O2P	0.41	2.14	7	1
3:B:210:PCW:H20	4:C:633:17F:H51	0.41	1.91	9	1
3:C:603:PCW:H371	3:C:607:PCW:C3	0.41	2.46	9	1
3:C:612:PCW:H241	3:C:612:PCW:H452	0.41	1.91	9	1
3:B:215:PCW:H83	3:B:217:PCW:O2P	0.41	2.14	1	1
1:A:243:MET:HA	1:A:246:ASP:HB3	0.41	1.92	3	1
3:B:212:PCW:H461	3:B:218:PCW:H442	0.41	1.91	4	1
3:B:203:PCW:O31	3:B:203:PCW:H41	0.41	2.16	6	1
3:A:411:PCW:H172	3:A:411:PCW:H211	0.41	1.92	10	1
4:B:236:17F:H6A	3:C:603:PCW:H142	0.41	1.92	10	1
3:B:203:PCW:H132	3:B:213:PCW:H372	0.41	1.91	1	1
1:A:345:ARG:O	1:A:349:TYR:HB2	0.41	2.15	2	1
3:B:204:PCW:O1P	3:B:222:PCW:H81	0.41	2.14	3	1
4:A:407:17F:H37	3:B:222:PCW:H32	0.41	1.91	5	1
3:B:220:PCW:O2P	3:B:222:PCW:H322	0.41	2.15	5	1
3:A:405:PCW:H331	3:B:209:PCW:H361	0.41	1.91	7	1
3:B:207:PCW:H71	4:B:228:17F:O3	0.41	2.15	7	1
4:A:407:17F:H54	3:C:613:PCW:H281	0.41	1.92	9	1
3:B:212:PCW:H432	4:B:231:17F:H60	0.41	1.93	1	1
3:B:216:PCW:H52	3:B:216:PCW:O31	0.41	2.14	1	1
1:C:458:ASP:HA	1:C:461:LYS:HE2	0.41	1.91	1	1
1:A:264:LYS:O	1:A:268:GLU:HG3	0.41	2.15	2	1
1:C:576:VAL:O	1:C:580:PHE:HB2	0.41	2.15	2	1
3:A:401:PCW:H381	3:B:213:PCW:H483	0.41	1.92	3	1
3:B:210:PCW:H332	3:B:214:PCW:H142	0.41	1.91	3	1
3:B:208:PCW:H432	3:B:234:PCW:H221	0.41	1.92	5	1
3:B:209:PCW:H151	3:B:216:PCW:H171	0.41	1.92	5	1
1:C:502:GLU:O	1:C:506:ARG:HG3	0.41	2.15	9	3
3:C:615:PCW:H442	4:C:632:17F:H47	0.41	1.93	5	1
4:B:232:17F:H44	3:C:609:PCW:H482	0.41	1.93	6	1
3:C:604:PCW:H131	3:C:625:PCW:H381	0.41	1.93	6	1
3:A:409:PCW:H121	3:C:613:PCW:H2	0.41	1.92	9	1
1:A:330:ARG:HH12	1:C:448:VAL:HG23	0.41	1.76	1	1
1:A:285:GLU:HA	1:A:288:ARG:HD2	0.41	1.92	2	1
2:B:71:TYR:HD1	7:B:239:EWS:BRA	0.41	2.53	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:201:PCW:H212	4:B:230:17F:H33	0.41	1.92	2	1
3:B:218:PCW:H172	3:B:225:PCW:H372	0.41	1.91	2	1
3:C:611:PCW:O31	3:C:623:PCW:H361	0.41	2.15	2	1
1:A:239:LEU:HA	1:A:242:GLU:HB2	0.41	1.91	4	1
1:A:290:LYS:HE3	1:C:487:GLN:OE1	0.41	2.16	5	1
3:B:220:PCW:H71	4:B:232:17F:O1	0.41	2.16	8	1
3:A:410:PCW:C38	4:C:630:17F:H36	0.41	2.44	9	1
3:A:404:PCW:H352	3:B:225:PCW:H162	0.41	1.91	10	1
3:B:213:PCW:H161	3:B:213:PCW:H342	0.41	1.91	10	1
3:B:208:PCW:H341	3:B:222:PCW:H362	0.41	1.90	1	1
3:B:235:PCW:H481	3:C:610:PCW:H452	0.41	1.91	1	1
3:C:626:PCW:O31	3:C:626:PCW:H42	0.41	2.15	1	1
3:B:208:PCW:H242	3:B:218:PCW:H281	0.41	1.93	3	1
2:B:101:LYS:HE3	2:B:107:GLU:HA	0.41	1.93	4	1
3:B:201:PCW:H172	4:B:227:17F:O8	0.41	2.15	4	1
3:B:233:PCW:H451	3:B:233:PCW:H321	0.41	1.93	5	1
4:B:226:17F:H70	4:B:236:17F:H55	0.41	1.92	6	1
3:B:221:PCW:H132	3:C:601:PCW:H12	0.41	1.92	7	1
3:B:205:PCW:O2P	3:B:212:PCW:H73	0.41	2.16	10	1
1:A:341:ASN:O	1:A:345:ARG:HG3	0.41	2.16	2	1
3:A:411:PCW:H162	4:C:630:17F:H38	0.41	1.92	2	1
3:B:206:PCW:H32	3:B:220:PCW:H63	0.41	1.91	4	1
3:A:405:PCW:H322	3:B:207:PCW:H322	0.41	1.92	5	1
3:B:201:PCW:H132	4:B:227:17F:O8	0.41	2.16	6	1
1:C:540:GLY:O	1:C:544:LEU:HG	0.41	2.16	6	1
3:A:406:PCW:H131	4:A:407:17F:H20A	0.41	1.92	7	1
3:B:224:PCW:H151	4:B:232:17F:H9	0.41	1.92	7	1
3:B:203:PCW:H321	3:B:213:PCW:H81	0.41	1.92	9	1
1:A:330:ARG:NH2	1:C:447:GLU:HB3	0.41	2.31	10	1
3:B:221:PCW:H452	4:C:627:17F:H50	0.41	1.93	1	1
1:C:490:HIS:HA	1:C:493:GLN:OE1	0.41	2.15	1	1
1:C:578:GLU:O	1:C:582:VAL:HG23	0.41	2.16	1	1
1:A:375:LEU:HD11	4:B:230:17F:C30	0.41	2.46	4	1
3:B:204:PCW:H151	3:B:212:PCW:H39	0.41	1.92	4	1
4:B:226:17F:C40	4:B:236:17F:H54	0.41	2.45	4	1
1:A:277:GLU:HB2	1:A:278:PRO:CD	0.41	2.45	5	1
4:A:407:17F:C2X	3:B:201:PCW:H381	0.41	2.45	5	1
3:A:406:PCW:H341	4:A:407:17F:C1Y	0.41	2.43	6	1
3:B:219:PCW:H381	3:B:223:PCW:H372	0.41	1.92	6	1
3:B:220:PCW:H2	3:B:220:PCW:H41	0.41	1.91	6	1
3:C:611:PCW:H152	3:C:623:PCW:H431	0.41	1.92	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:621:PCW:H482	4:C:632:17F:H35	0.41	1.92	6	1
3:A:404:PCW:O1P	3:B:218:PCW:H71	0.41	2.15	7	1
3:B:205:PCW:H371	3:B:205:PCW:H19	0.41	1.93	7	1
3:C:607:PCW:H282	3:C:615:PCW:H451	0.41	1.93	7	1
3:B:206:PCW:H40	3:B:217:PCW:H351	0.41	1.92	10	1
4:A:407:17F:H51	3:C:623:PCW:H251	0.41	1.93	2	1
3:B:207:PCW:H82	3:B:209:PCW:O2P	0.41	2.16	3	1
3:B:204:PCW:N	3:B:204:PCW:O2P	0.41	2.54	4	1
3:C:617:PCW:H181	3:C:617:PCW:H152	0.41	1.65	4	1
2:B:35:THR:HG21	2:B:57:ASP:CG	0.41	2.41	8	1
3:B:201:PCW:H372	4:B:227:17F:H32	0.41	1.93	8	1
3:B:206:PCW:H431	3:B:217:PCW:H411	0.41	1.91	8	1
3:B:216:PCW:H32	4:B:229:17F:N1	0.41	2.31	8	1
1:A:264:LYS:CE	1:C:509:ALA:HB1	0.41	2.44	9	1
3:B:224:PCW:H421	4:B:226:17F:H49	0.41	1.93	9	1
3:C:607:PCW:H251	3:C:615:PCW:H441	0.41	1.93	9	1
3:B:209:PCW:O1P	3:B:216:PCW:H12	0.40	2.16	1	1
3:B:207:PCW:H172	3:B:209:PCW:H241	0.40	1.92	2	1
3:C:615:PCW:H222	4:C:633:17F:H40	0.40	1.92	3	1
3:B:207:PCW:H11	4:B:228:17F:O1	0.40	2.16	4	1
3:B:207:PCW:H19	3:C:601:PCW:H122	0.40	1.92	4	1
3:B:209:PCW:H39	4:B:228:17F:H18A	0.40	1.92	4	1
3:B:220:PCW:C4	4:B:232:17F:H19A	0.40	2.46	6	1
3:B:213:PCW:C6	4:B:232:17F:HN1A	0.40	2.28	7	1
3:B:218:PCW:H283	3:B:234:PCW:H462	0.40	1.93	9	1
3:B:210:PCW:O1P	3:B:217:PCW:H41	0.40	2.16	10	1
3:A:409:PCW:H232	3:C:613:PCW:H172	0.40	1.93	3	1
1:C:488:LYS:HB3	3:C:620:PCW:H281	0.40	1.93	3	1
3:C:603:PCW:H481	4:C:633:17F:H60	0.40	1.93	3	1
1:A:349:TYR:OH	3:A:401:PCW:H222	0.40	2.15	4	1
1:C:559:SER:HA	1:C:562:ALA:HB3	0.40	1.94	4	2
3:A:401:PCW:H483	3:C:623:PCW:H482	0.40	1.93	5	1
3:B:201:PCW:C1	4:B:230:17F:H1A	0.40	2.45	5	1
3:A:401:PCW:H51	3:B:203:PCW:H12	0.40	1.92	6	1
3:B:210:PCW:H83	4:B:229:17F:H2	0.40	1.93	7	1
3:B:217:PCW:H152	3:B:217:PCW:C34	0.40	2.46	7	1
1:A:243:MET:O	1:A:247:LEU:HB2	0.40	2.16	9	1
4:A:407:17F:H52	3:B:201:PCW:H411	0.40	1.93	9	1
3:A:408:PCW:C32	3:C:610:PCW:H39	0.40	2.43	10	1
3:B:206:PCW:H162	4:B:226:17F:H37	0.40	1.91	10	1
1:C:475:GLU:HB2	1:C:476:PRO:CD	0.40	2.46	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:202:PCW:C7	3:B:217:PCW:H31	0.40	2.46	1	1
3:A:404:PCW:H72	3:B:225:PCW:O2P	0.40	2.15	2	1
3:B:210:PCW:H171	3:B:214:PCW:H352	0.40	1.92	2	1
3:B:221:PCW:H51	4:B:229:17F:N1	0.40	2.30	4	1
3:A:403:PCW:H462	3:A:404:PCW:H372	0.40	1.92	5	1
3:B:233:PCW:H381	3:B:233:PCW:C42	0.40	2.47	5	1
4:B:236:17F:H72	3:C:603:PCW:H282	0.40	1.92	5	1
1:C:412:PHE:O	1:C:415:LEU:HB2	0.40	2.16	6	1
3:A:404:PCW:H322	3:A:404:PCW:H41	0.40	1.92	7	1
3:B:201:PCW:H41	4:B:230:17F:O1	0.40	2.16	7	1
3:C:613:PCW:H72	3:C:619:PCW:H12	0.40	1.93	7	1
3:B:220:PCW:O1P	3:B:220:PCW:H2	0.40	2.17	8	1
3:A:409:PCW:H62	4:C:630:17F:N1	0.40	2.32	9	1
3:A:410:PCW:H462	3:A:411:PCW:H231	0.40	1.93	9	1
2:B:158:THR:O	2:B:162:GLU:HG2	0.40	2.16	9	1
4:B:236:17F:C31	3:C:622:PCW:H141	0.40	2.47	9	1
3:B:211:PCW:C36	4:B:226:17F:H8	0.40	2.32	10	1
1:A:260:ASP:HA	1:A:263:LYS:CE	0.40	2.38	1	1
1:C:508:ARG:O	1:C:512:ASP:HB3	0.40	2.16	1	1
3:A:406:PCW:H351	4:A:407:17F:H32	0.40	1.92	5	1
3:B:211:PCW:H251	3:B:211:PCW:H461	0.40	1.93	6	1
3:C:611:PCW:H19	3:C:611:PCW:H381	0.40	1.93	6	1
3:B:233:PCW:H381	3:B:233:PCW:H422	0.40	1.92	9	1
3:A:411:PCW:H41	3:A:411:PCW:O11	0.40	2.16	1	1
2:B:134:ALA:HB1	2:B:139:ILE:O	0.40	2.16	1	1
1:A:352:LYS:O	1:A:356:HIS:HB2	0.40	2.17	4	1
3:B:206:PCW:H431	3:B:206:PCW:H372	0.40	1.94	4	1
4:B:226:17F:H74	3:C:621:PCW:H483	0.40	1.93	5	1
1:C:434:THR:HB	1:C:438:ARG:CZ	0.40	2.47	5	1
3:B:208:PCW:H361	3:B:234:PCW:H282	0.40	1.92	6	1
3:B:217:PCW:H421	3:B:223:PCW:H382	0.40	1.92	6	1
1:C:463:TRP:O	1:C:467:MET:HB2	0.40	2.17	6	1
1:A:268:GLU:OE1	1:C:506:ARG:HD3	0.40	2.17	7	1
3:A:410:PCW:H381	4:C:630:17F:H12A	0.40	1.94	7	1
4:B:228:17F:C2X	4:B:232:17F:H37	0.40	2.43	8	1
3:C:611:PCW:H372	3:C:624:PCW:H283	0.40	1.93	8	1
2:B:18:ALA:HB2	5:B:237:GNP:O2A	0.40	2.15	10	1
3:C:603:PCW:H371	3:C:603:PCW:H412	0.40	1.94	10	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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	171/187 (91%)	160±4 (94±2%)	10±4 (6±3%)	0±0 (0±0%)	37	78
All	All	5230/5870 (89%)	5036 (96%)	169 (3%)	25 (0%)	26	74

All 8 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	60	GLY	1
2	B	119	ASP	1
2	B	14	VAL	1
1	C	420	GLY	1
2	B	34	PRO	1
2	B	117	LYS	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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	152/166 (92%)	137±1 (90±1%)	15±1 (10±1%)	9	54
All	All	4590/5160 (89%)	4155 (91%)	435 (9%)	10	55

All 177 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
2	B	35	THR	9
2	B	74	THR	9
2	B	124	THR	9
2	B	127	THR	9
1	A	392	GLU	8
2	B	58	THR	8
2	B	87	THR	8
1	C	516	THR	8
1	A	312	HIS	8
1	C	550	LYS	8
1	C	480	GLU	7
2	B	122	SER	7
1	A	354	THR	6
2	B	2	THR	6
1	A	293	GLU	5
2	B	17	SER	5
1	A	318	THR	5
2	B	89	SER	4
1	C	405	TRP	4
1	C	447	GLU	4
1	C	448	VAL	4
1	C	455	TYR	4
1	A	246	ASP	4
1	C	407	SER	4
1	C	568	ASP	4
2	B	39	SER	4
2	B	50	THR	4
2	B	154	ASP	4
1	C	463	TRP	4
1	C	487	GLN	4
1	C	505	ASP	4
1	A	265	TRP	3
1	A	272	TYR	3
1	A	319	HIS	3
1	A	350	HIS	3
2	B	136	SER	3
1	C	403	ASP	3
1	C	444	ASP	3
1	C	451	LYS	3
1	C	466	GLU	3
1	C	467	MET	3

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Mol	Chain	Res	Type	Models (Total)
1	A	292	HIS	3
1	A	296	GLU	3
2	B	95	HIS	3
2	B	148	THR	3
1	C	482	GLN	3
1	C	594	LYS	3
1	A	274	GLN	3
1	A	370	ASP	3
1	A	394	THR	3
2	B	20	THR	3
2	B	32	TYR	3
1	C	412	PHE	3
1	C	552	THR	3
2	B	6	LEU	3
1	A	314	ASP	3
1	C	459	PHE	3
1	A	385	SER	3
1	A	348	GLU	2
1	A	371	LEU	2
1	A	381	SER	2
2	B	16	LYS	2
2	B	99	GLN	2
2	B	108	ASP	2
1	C	592	THR	2
1	A	327	LEU	2
2	B	102	ARG	2
2	B	145	SER	2
1	C	512	ASP	2
1	C	548	HIS	2
1	A	255	GLN	2
1	A	359	THR	2
2	B	31	GLU	2
2	B	49	GLU	2
1	C	410	SER	2
1	C	583	SER	2
1	A	249	GLU	2
1	A	299	SER	2
1	A	356	HIS	2
1	A	368	LEU	2
2	B	54	ASP	2
1	C	490	HIS	2
1	C	546	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	C	561	LYS	2
1	C	580	PHE	2
1	A	243	MET	2
2	B	158	THR	2
2	B	170	MET	2
1	C	418	GLN	2
1	C	460	GLN	2
1	A	266	GLN	2
1	A	284	GLN	2
2	B	131	GLN	2
2	B	144	THR	2
1	C	501	GLU	2
1	C	532	ARG	2
1	C	557	THR	2
1	A	304	GLU	2
1	C	434	THR	2
1	C	556	SER	2
1	C	523	ASP	2
1	A	361	SER	2
1	C	404	ASN	2
1	A	325	ASP	1
1	A	336	GLU	1
1	A	360	LEU	1
2	B	30	ASP	1
2	B	47	ASP	1
2	B	51	CYS	1
2	B	65	SER	1
2	B	71	TYR	1
2	B	161	ARG	1
1	C	433	GLU	1
1	A	378	VAL	1
2	B	3	GLU	1
2	B	61	GLN	1
2	B	106	SER	1
2	B	114	VAL	1
1	C	559	SER	1
1	C	576	VAL	1
1	C	584	PHE	1
1	A	283	LEU	1
1	A	290	LYS	1
1	A	358	SER	1
2	B	29	VAL	1

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Mol	Chain	Res	Type	Models (Total)
2	B	62	GLU	1
2	B	142	ILE	1
1	C	402	LEU	1
1	C	425	GLU	1
1	A	270	GLU	1
2	B	73	ARG	1
2	B	166	HIS	1
1	C	409	THR	1
1	C	477	LEU	1
1	A	245	LYS	1
2	B	96	TYR	1
1	C	494	GLU	1
1	C	558	LEU	1
1	A	244	SER	1
1	A	305	MET	1
1	A	307	ASP	1
2	B	69	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
1	A	241	GLN	1
1	A	261	PHE	1
2	B	109	VAL	1
2	B	129	GLN	1
1	C	427	TRP	1
1	C	429	ASN	1
1	C	596	ASN	1
1	A	273	ARG	1
1	A	277	GLU	1
1	A	387	LEU	1
2	B	104	LYS	1
1	C	462	LYS	1
1	C	521	TYR	1
1	C	537	LYS	1
2	B	4	TYR	1
2	B	80	CYS	1
2	B	118	CYS	1
2	B	171	SER	1
1	C	457	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	276	VAL	1
1	A	297	LYS	1
2	B	56	LEU	1
2	B	119	ASP	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

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

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	B	218	-	53,53,53	1.06±0.01	4±0 (7±0%)
3	PCW	B	225	-	53,53,53	1.05±0.01	4±1 (7±1%)
3	PCW	B	233	-	53,53,53	1.06±0.01	4±0 (7±0%)
3	PCW	B	209	-	53,53,53	1.05±0.01	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	C	609	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	603	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	408	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	B	204	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	402	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	C	601	-	53,53,53	1.04±0.01	5±0 (8±0%)
4	17F	B	229	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	C	605	-	53,53,53	1.06±0.01	5±0 (8±0%)
3	PCW	A	410	-	53,53,53	1.07±0.01	4±0 (7±0%)
4	17F	C	627	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	B	205	-	53,53,53	1.04±0.01	4±1 (8±1%)
3	PCW	B	216	-	53,53,53	1.05±0.01	4±0 (6±0%)
4	17F	C	629	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	B	214	-	53,53,53	1.05±0.02	4±0 (7±0%)
3	PCW	B	210	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	C	618	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	B	235	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	611	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	17F	B	232	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	B	202	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	A	407	-	52,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	C	614	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	B	212	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	17F	B	236	-	52,53,53	0.92±0.01	1±0 (1±0%)
4	17F	B	231	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	B	224	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	B	234	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	C	615	-	53,53,53	1.05±0.01	4±0 (6±0%)
7	EWS	B	239	-	30,30,30	2.27±0.00	10±0 (33±0%)
3	PCW	B	208	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	B	223	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	C	633	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	C	623	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	607	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	610	-	53,53,53	1.04±0.01	4±0 (6±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	C	625	-	53,53,53	1.04±0.01	4±1 (7±1%)
5	GNP	B	237	-	34,34,34	1.42±0.02	5±0 (14±0%)
3	PCW	B	219	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	C	608	-	53,53,53	1.05±0.01	5±0 (8±0%)
4	17F	B	226	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	C	604	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	C	606	-	53,53,53	1.04±0.01	4±0 (8±0%)
3	PCW	B	222	-	53,53,53	1.06±0.01	4±0 (7±0%)
3	PCW	A	403	-	53,53,53	1.05±0.01	5±0 (8±0%)
3	PCW	B	217	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	C	602	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	411	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	17F	C	632	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	C	616	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	B	201	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	C	628	-	52,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	B	220	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	626	-	53,53,53	1.04±0.01	5±0 (8±0%)
3	PCW	B	215	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	17F	B	227	-	52,53,53	0.93±0.01	1±0 (1±0%)
3	PCW	B	203	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	C	631	-	52,53,53	0.92±0.01	1±0 (1±0%)
4	17F	B	228	-	52,53,53	0.92±0.01	0±0 (0±0%)
3	PCW	B	213	-	53,53,53	1.05±0.01	3±0 (6±0%)
3	PCW	C	617	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	404	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	B	206	-	53,53,53	1.05±0.01	4±0 (8±0%)
3	PCW	C	613	-	53,53,53	1.08±0.01	6±0 (10±0%)
3	PCW	C	621	-	53,53,53	1.05±0.01	4±0 (8±0%)
3	PCW	B	207	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	C	630	-	52,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	A	401	-	53,53,53	1.04±0.02	4±0 (7±0%)
3	PCW	A	405	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	C	624	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	B	221	-	53,53,53	1.07±0.01	5±0 (9±0%)

Mol	Type	Chain	Res	Link	Counts	Bond lengths	
						RMSZ	#Z>2
3	PCW	B	211	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	A	406	-	53,53,53	1.06±0.01	5±0 (9±0%)
3	PCW	C	622	-	53,53,53	1.06±0.01	4±0 (7±0%)
4	17F	B	230	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	C	612	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	C	619	-	53,53,53	1.04±0.01	3±0 (6±0%)
3	PCW	A	409	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	C	620	-	53,53,53	1.04±0.01	5±0 (8±0%)

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

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	B	218	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	225	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	233	-	59,61,61	2.31±0.01	5±0 (8±0%)
3	PCW	B	209	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	C	609	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	603	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	408	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	204	-	59,61,61	2.77±0.01	9±0 (15±0%)
3	PCW	A	402	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	601	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	B	229	-	54,60,60	1.07±0.04	5±0 (9±0%)
3	PCW	C	605	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	410	-	59,61,61	2.33±0.01	5±0 (8±0%)
4	17F	C	627	-	54,60,60	1.06±0.01	5±0 (9±0%)
3	PCW	B	205	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	B	216	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	C	629	-	54,60,60	1.04±0.02	5±0 (9±0%)
3	PCW	B	214	-	59,61,61	2.32±0.00	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	B	210	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	618	-	59,61,61	2.33±0.01	5±0 (8±0%)
3	PCW	B	235	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	611	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	B	232	-	54,60,60	1.05±0.03	5±0 (9±0%)
3	PCW	B	202	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	407	-	54,60,60	1.77±0.03	10±1 (17±1%)
3	PCW	C	614	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	212	-	59,61,61	0.84±0.00	1±0 (1±0%)
4	17F	B	236	-	54,60,60	1.05±0.03	5±0 (9±0%)
4	17F	B	231	-	54,60,60	1.06±0.03	5±0 (9±0%)
3	PCW	B	224	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	234	-	59,61,61	2.77±0.01	9±0 (15±0%)
3	PCW	C	615	-	59,61,61	2.32±0.01	5±0 (8±0%)
7	EWS	B	239	-	37,42,42	1.39±0.01	2±0 (5±0%)
3	PCW	B	208	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	B	223	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	C	633	-	54,60,60	1.04±0.02	4±0 (7±0%)
3	PCW	C	623	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	607	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	610	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	625	-	59,61,61	2.32±0.01	5±0 (8±0%)
5	GNP	B	237	-	47,54,54	0.96±0.01	2±0 (4±0%)
3	PCW	B	219	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	C	608	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	B	226	-	54,60,60	1.07±0.02	5±0 (9±0%)
3	PCW	C	604	-	59,61,61	2.33±0.00	5±0 (8±0%)
3	PCW	C	606	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	222	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	403	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	B	217	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	602	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	411	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	C	632	-	54,60,60	1.05±0.03	5±0 (9±0%)
3	PCW	C	616	-	59,61,61	2.32±0.00	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	B	201	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	C	628	-	54,60,60	1.12±0.03	6±0 (10±0%)
3	PCW	B	220	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	626	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	215	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	B	227	-	54,60,60	1.05±0.02	5±0 (8±0%)
3	PCW	B	203	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	C	631	-	54,60,60	1.05±0.03	5±0 (9±0%)
4	17F	B	228	-	54,60,60	1.08±0.03	5±1 (9±1%)
3	PCW	B	213	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	617	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	404	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	B	206	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	C	613	-	59,61,61	0.83±0.01	1±0 (1±0%)
3	PCW	C	621	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	207	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	C	630	-	54,60,60	1.80±0.03	10±0 (17±0%)
3	PCW	A	401	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	405	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	624	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	B	221	-	59,61,61	0.83±0.01	1±0 (1±0%)
3	PCW	B	211	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	406	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	C	622	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	B	230	-	54,60,60	1.10±0.05	5±0 (9±0%)
3	PCW	C	612	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	619	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	409	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	620	-	59,61,61	0.85±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
3	PCW	B	218	-	-	0±0,57,57,57	-
3	PCW	C	618	-	-	0±0,57,57,57	-
3	PCW	C	611	-	-	0±0,57,57,57	-
3	PCW	C	614	-	-	0±0,57,57,57	-
3	PCW	B	223	-	-	0±0,57,57,57	-
3	PCW	C	610	-	-	0±0,57,57,57	-
3	PCW	C	606	-	-	0±0,57,57,57	-
3	PCW	B	233	-	-	0±0,57,57,57	-
3	PCW	B	209	-	-	0±0,57,57,57	-
4	17F	B	236	-	-	0±0,59,59,59	-
4	17F	C	631	-	-	0±0,59,59,59	-
4	17F	C	627	-	-	0±0,59,59,59	-
4	17F	C	629	-	-	0±0,59,59,59	-
3	PCW	A	404	-	-	0±0,57,57,57	-
3	PCW	C	623	-	-	0±0,57,57,57	-
4	17F	C	630	-	-	0±0,59,59,59	-
3	PCW	B	208	-	-	0±0,57,57,57	-
4	17F	B	226	-	-	0±0,59,59,59	-
3	PCW	B	205	-	-	0±0,57,57,57	-
7	EWS	B	239	-	-	0±0,12,22,22	1±0,4,4,4
3	PCW	C	613	-	-	0±0,57,57,57	-
3	PCW	C	619	-	-	0±0,57,57,57	-
3	PCW	B	203	-	-	0±0,57,57,57	-
4	17F	B	230	-	-	0±0,59,59,59	-
3	PCW	B	204	-	-	0±0,57,57,57	-
3	PCW	B	213	-	-	0±0,57,57,57	-
3	PCW	C	626	-	-	0±0,57,57,57	-
3	PCW	A	409	-	-	0±0,57,57,57	-
3	PCW	B	206	-	-	0±0,57,57,57	-
3	PCW	C	602	-	-	0±0,57,57,57	-
3	PCW	C	608	-	-	0±0,57,57,57	-
3	PCW	C	622	-	-	0±0,57,57,57	-
3	PCW	A	408	-	-	0±0,57,57,57	-
3	PCW	C	617	-	-	0±0,57,57,57	-
3	PCW	B	221	-	-	0±0,57,57,57	-
3	PCW	C	612	-	-	0±0,57,57,57	-
3	PCW	B	212	-	-	0±0,57,57,57	-
3	PCW	C	625	-	-	0±0,57,57,57	-
3	PCW	C	601	-	-	0±0,57,57,57	-
4	17F	B	227	-	-	0±0,59,59,59	-
3	PCW	B	235	-	-	0±0,57,57,57	-
4	17F	C	632	-	-	0±0,59,59,59	-
4	17F	A	407	-	-	0±0,59,59,59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	406	-	-	0±0,57,57,57	-
3	PCW	C	620	-	-	0±0,57,57,57	-
5	GNP	B	237	-	-	0±0,18,38,38	0±0,3,3,3
3	PCW	B	211	-	-	0±0,57,57,57	-
3	PCW	C	621	-	-	0±0,57,57,57	-
3	PCW	C	605	-	-	0±0,57,57,57	-
4	17F	B	228	-	-	0±0,59,59,59	-
3	PCW	C	603	-	-	0±0,57,57,57	-
3	PCW	B	207	-	-	0±0,57,57,57	-
3	PCW	B	219	-	-	0±0,57,57,57	-
3	PCW	B	225	-	-	0±0,57,57,57	-
3	PCW	C	609	-	-	0±0,57,57,57	-
3	PCW	B	224	-	-	0±0,57,57,57	-
3	PCW	A	410	-	-	0±0,57,57,57	-
3	PCW	B	215	-	-	0±0,57,57,57	-
3	PCW	B	222	-	-	0±0,57,57,57	-
3	PCW	B	220	-	-	0±0,57,57,57	-
3	PCW	C	616	-	-	0±0,57,57,57	-
4	17F	C	628	-	-	0±0,59,59,59	-
3	PCW	B	202	-	-	0±0,57,57,57	-
3	PCW	A	405	-	-	0±0,57,57,57	-
3	PCW	C	604	-	-	0±0,57,57,57	-
3	PCW	C	615	-	-	0±0,57,57,57	-
4	17F	B	231	-	-	0±0,59,59,59	-
3	PCW	B	201	-	-	0±0,57,57,57	-
3	PCW	B	214	-	-	0±0,57,57,57	-
3	PCW	B	210	-	-	0±0,57,57,57	-
3	PCW	C	624	-	-	0±0,57,57,57	-
3	PCW	B	216	-	-	0±0,57,57,57	-
3	PCW	B	217	-	-	0±0,57,57,57	-
4	17F	B	229	-	-	0±0,59,59,59	-
3	PCW	A	411	-	-	0±0,57,57,57	-
3	PCW	A	401	-	-	0±0,57,57,57	-
4	17F	B	232	-	-	0±0,59,59,59	-
3	PCW	B	234	-	-	0±0,57,57,57	-
4	17F	C	633	-	-	0±0,59,59,59	-
3	PCW	C	607	-	-	0±0,57,57,57	-
3	PCW	A	403	-	-	0±0,57,57,57	-
3	PCW	A	402	-	-	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
7	B	239	EWS	CAV-CBA	6.58	1.34	1.45	8	10
7	B	239	EWS	CAI-CAJ	5.02	1.39	1.51	8	10
5	B	237	GNP	PG-O1G	4.61	1.53	1.46	4	10
7	B	239	EWS	CAV-CAU	3.94	1.36	1.41	2	10
5	B	237	GNP	PG-O3G	3.36	1.47	1.56	4	10
5	B	237	GNP	PB-O2B	3.29	1.48	1.56	1	10
7	B	239	EWS	CAX-CBA	3.15	1.33	1.38	2	10
3	A	411	PCW	C5-N	2.94	1.42	1.51	1	10
3	C	615	PCW	C5-N	2.93	1.42	1.51	3	10
3	B	218	PCW	C5-N	2.89	1.42	1.51	5	10
3	C	604	PCW	C5-N	2.87	1.42	1.51	1	10
3	C	618	PCW	C5-N	2.87	1.42	1.51	4	10
3	B	222	PCW	C5-N	2.86	1.42	1.51	7	10
3	A	410	PCW	C5-N	2.86	1.42	1.51	8	10
3	A	405	PCW	C5-N	2.85	1.42	1.51	10	10
3	C	616	PCW	C5-N	2.85	1.42	1.51	6	10
3	A	404	PCW	C5-N	2.85	1.42	1.51	3	10
3	B	216	PCW	C5-N	2.84	1.42	1.51	2	10
3	C	609	PCW	C5-N	2.83	1.42	1.51	1	10
3	A	402	PCW	C5-N	2.83	1.42	1.51	4	10
3	A	409	PCW	C5-N	2.83	1.42	1.51	1	10
3	C	624	PCW	C5-N	2.81	1.42	1.51	2	10
3	B	212	PCW	C1-C2	2.81	1.59	1.50	7	10
3	B	201	PCW	C5-N	2.80	1.42	1.51	6	10
3	B	225	PCW	C5-N	2.80	1.42	1.51	3	10
3	B	220	PCW	C5-N	2.79	1.43	1.51	6	10
3	B	203	PCW	C5-N	2.79	1.43	1.51	9	10
3	B	233	PCW	C5-N	2.78	1.43	1.51	6	10
5	B	237	GNP	PB-O3A	2.78	1.55	1.59	5	10
3	B	202	PCW	C5-N	2.78	1.43	1.51	4	10
3	B	214	PCW	C5-N	2.78	1.43	1.51	7	10
3	B	219	PCW	C5-N	2.78	1.43	1.51	1	10
3	C	623	PCW	C5-N	2.78	1.43	1.51	7	10
3	C	619	PCW	C5-N	2.78	1.43	1.51	9	10
3	B	223	PCW	C5-N	2.77	1.43	1.51	6	10
3	C	603	PCW	C5-N	2.77	1.43	1.51	5	10
3	B	213	PCW	C5-N	2.76	1.43	1.51	1	10
3	B	217	PCW	C5-N	2.76	1.43	1.51	8	10
3	B	211	PCW	C5-N	2.76	1.43	1.51	6	10
3	B	235	PCW	C5-N	2.76	1.43	1.51	7	10
3	C	602	PCW	C5-N	2.76	1.43	1.51	5	10
3	C	625	PCW	C5-N	2.76	1.43	1.51	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	617	PCW	C5-N	2.76	1.43	1.51	2	10
3	B	204	PCW	C5-N	2.76	1.43	1.51	6	10
3	C	622	PCW	C5-N	2.76	1.43	1.51	6	10
3	B	207	PCW	C5-N	2.74	1.43	1.51	1	10
3	B	208	PCW	C1-C2	2.74	1.59	1.50	2	10
5	B	237	GNP	PG-O2G	2.73	1.49	1.56	3	10
3	C	622	PCW	C1-C2	2.72	1.59	1.50	9	10
3	B	210	PCW	C5-N	2.72	1.43	1.51	7	10
3	C	610	PCW	C5-N	2.72	1.43	1.51	2	10
3	C	612	PCW	C5-N	2.71	1.43	1.51	9	10
3	A	401	PCW	C5-N	2.71	1.43	1.51	10	10
3	C	613	PCW	C1-C2	2.71	1.59	1.50	5	10
3	A	406	PCW	C1-C2	2.70	1.59	1.50	1	10
3	C	602	PCW	C1-C2	2.70	1.59	1.50	9	10
3	B	221	PCW	C1-C2	2.70	1.59	1.50	6	10
3	C	607	PCW	C5-N	2.70	1.43	1.51	3	10
3	A	409	PCW	C1-C2	2.70	1.59	1.50	10	10
3	B	233	PCW	C1-C2	2.69	1.59	1.50	5	10
3	B	209	PCW	C1-C2	2.68	1.59	1.50	9	10
3	B	213	PCW	C1-C2	2.67	1.59	1.50	9	10
3	B	218	PCW	C1-C2	2.66	1.59	1.50	4	10
3	A	405	PCW	C1-C2	2.66	1.59	1.50	10	10
7	B	239	EWS	CBA-CAZ	2.66	1.34	1.51	9	10
3	C	625	PCW	C1-C2	2.65	1.59	1.50	6	10
3	B	202	PCW	C1-C2	2.64	1.59	1.50	4	10
7	B	239	EWS	CAT-CAU	2.64	1.35	1.39	10	10
3	C	607	PCW	C1-C2	2.64	1.59	1.50	10	10
3	B	214	PCW	C1-C2	2.64	1.59	1.50	3	10
3	B	203	PCW	C1-C2	2.64	1.59	1.50	8	10
3	B	224	PCW	C1-C2	2.64	1.59	1.50	8	10
3	C	611	PCW	C5-N	2.64	1.43	1.51	9	10
3	B	211	PCW	C1-C2	2.63	1.59	1.50	8	10
3	C	610	PCW	C1-C2	2.63	1.59	1.50	10	10
3	C	614	PCW	C5-N	2.63	1.43	1.51	5	10
3	A	408	PCW	C5-N	2.62	1.43	1.51	3	10
3	C	626	PCW	C1-C2	2.62	1.59	1.50	10	10
3	A	410	PCW	C1-C2	2.62	1.59	1.50	8	10
3	B	207	PCW	C1-C2	2.61	1.59	1.50	5	10
3	C	615	PCW	C1-C2	2.61	1.59	1.50	5	10
3	A	411	PCW	C1-C2	2.61	1.59	1.50	2	10
3	B	234	PCW	C5-N	2.60	1.43	1.51	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	408	PCW	C1-C2	2.60	1.58	1.50	5	10
3	C	609	PCW	C1-C2	2.60	1.58	1.50	3	10
3	A	402	PCW	C1-C2	2.60	1.58	1.50	7	10
3	B	210	PCW	C1-C2	2.60	1.58	1.50	10	10
3	B	217	PCW	C1-C2	2.60	1.58	1.50	10	10
3	B	204	PCW	C1-C2	2.59	1.58	1.50	4	10
3	C	621	PCW	C5-N	2.59	1.43	1.51	10	10
3	B	223	PCW	C1-C2	2.58	1.58	1.50	7	10
3	C	603	PCW	C1-C2	2.58	1.58	1.50	2	10
3	C	606	PCW	C1-C2	2.58	1.58	1.50	9	10
3	B	216	PCW	C1-C2	2.58	1.58	1.50	3	10
3	C	604	PCW	C1-C2	2.58	1.58	1.50	1	10
3	B	205	PCW	C5-N	2.57	1.43	1.51	6	10
3	C	624	PCW	C1-C2	2.57	1.58	1.50	3	10
3	A	401	PCW	C1-C2	2.57	1.58	1.50	5	10
3	C	601	PCW	C1-C2	2.57	1.58	1.50	1	10
3	C	614	PCW	C1-C2	2.57	1.58	1.50	7	10
3	B	225	PCW	C1-C2	2.57	1.58	1.50	6	10
3	C	621	PCW	C1-C2	2.57	1.58	1.50	5	10
3	C	618	PCW	C1-C2	2.56	1.58	1.50	3	10
3	C	611	PCW	C1-C2	2.56	1.58	1.50	6	10
3	B	222	PCW	C1-C2	2.55	1.58	1.50	5	10
7	B	239	EWS	CAU-NAW	2.55	1.33	1.37	1	10
3	B	206	PCW	C1-C2	2.55	1.58	1.50	4	10
3	C	617	PCW	C1-C2	2.54	1.58	1.50	7	10
3	A	403	PCW	C5-N	2.54	1.43	1.51	9	10
3	B	220	PCW	C1-C2	2.54	1.58	1.50	2	10
3	A	404	PCW	C1-C2	2.54	1.58	1.50	3	10
3	B	205	PCW	C1-C2	2.54	1.58	1.50	1	10
3	B	215	PCW	C1-C2	2.54	1.58	1.50	8	10
3	A	410	PCW	C33-C32	2.53	1.61	1.52	3	10
3	B	219	PCW	C1-C2	2.53	1.58	1.50	7	10
3	C	620	PCW	C5-N	2.53	1.43	1.51	1	10
3	B	235	PCW	C1-C2	2.53	1.58	1.50	6	10
3	C	626	PCW	C5-N	2.53	1.43	1.51	2	10
3	C	616	PCW	C1-C2	2.53	1.58	1.50	1	10
3	C	605	PCW	C5-N	2.52	1.43	1.51	7	10
3	C	620	PCW	C1-C2	2.52	1.58	1.50	7	10
3	A	403	PCW	C1-C2	2.52	1.58	1.50	8	10
3	B	234	PCW	C1-C2	2.52	1.58	1.50	4	10
3	A	406	PCW	C5-N	2.52	1.43	1.51	5	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	208	PCW	C5-N	2.52	1.43	1.51	9	10
3	C	608	PCW	C1-C2	2.52	1.58	1.50	3	10
3	C	605	PCW	C1-C2	2.51	1.58	1.50	6	10
3	A	404	PCW	C33-C32	2.51	1.61	1.52	9	10
7	B	239	EWS	CAX-NAW	2.51	1.33	1.37	8	10
3	B	221	PCW	C5-N	2.50	1.43	1.51	3	10
3	B	224	PCW	C5-N	2.50	1.43	1.51	4	10
3	C	612	PCW	C1-C2	2.50	1.58	1.50	6	10
3	C	619	PCW	C33-C32	2.50	1.61	1.52	5	10
3	C	615	PCW	C33-C32	2.50	1.61	1.52	4	10
3	B	216	PCW	C33-C32	2.49	1.61	1.52	2	10
3	B	209	PCW	C5-N	2.49	1.43	1.51	3	10
3	C	608	PCW	C5-N	2.49	1.43	1.51	9	10
3	C	622	PCW	C33-C32	2.49	1.61	1.52	10	10
3	B	207	PCW	C33-C32	2.49	1.61	1.52	9	10
3	B	210	PCW	C33-C32	2.48	1.61	1.52	6	10
3	C	619	PCW	C1-C2	2.48	1.58	1.50	6	10
3	B	212	PCW	C5-N	2.47	1.43	1.51	6	10
3	B	218	PCW	C33-C32	2.48	1.61	1.52	4	10
3	A	403	PCW	C33-C32	2.47	1.61	1.52	5	10
3	C	601	PCW	C5-N	2.47	1.43	1.51	2	10
3	C	623	PCW	C1-C2	2.47	1.58	1.50	1	10
3	C	606	PCW	C5-N	2.47	1.43	1.51	10	10
3	B	201	PCW	C1-C2	2.47	1.58	1.50	1	10
3	C	605	PCW	C33-C32	2.47	1.61	1.52	7	10
3	B	202	PCW	C33-C32	2.46	1.61	1.52	6	10
3	C	613	PCW	C5-N	2.46	1.44	1.51	10	10
3	C	626	PCW	C33-C32	2.45	1.61	1.52	6	10
3	A	406	PCW	C33-C32	2.45	1.61	1.52	7	10
3	A	401	PCW	C33-C32	2.44	1.61	1.52	3	10
3	B	206	PCW	C5-N	2.44	1.44	1.51	5	10
3	C	606	PCW	C33-C32	2.44	1.61	1.52	6	10
3	B	204	PCW	C33-C32	2.43	1.61	1.52	10	10
3	B	219	PCW	C33-C32	2.43	1.61	1.52	1	10
3	B	225	PCW	C33-C32	2.43	1.61	1.52	4	10
3	B	221	PCW	C33-C32	2.43	1.61	1.52	1	10
3	B	201	PCW	C33-C32	2.43	1.61	1.52	4	10
3	C	603	PCW	C33-C32	2.43	1.61	1.52	7	10
3	C	623	PCW	C33-C32	2.43	1.61	1.52	7	10
3	C	624	PCW	C33-C32	2.43	1.61	1.52	8	10
3	A	408	PCW	C33-C32	2.43	1.61	1.52	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	205	PCW	C33-C32	2.43	1.61	1.52	10	10
3	C	611	PCW	C33-C32	2.43	1.61	1.52	5	10
3	A	402	PCW	C33-C32	2.42	1.61	1.52	7	10
3	A	409	PCW	C33-C32	2.42	1.61	1.52	3	10
3	C	625	PCW	C33-C32	2.42	1.61	1.52	6	10
3	C	612	PCW	C33-C32	2.42	1.61	1.52	8	10
3	B	234	PCW	C33-C32	2.42	1.61	1.52	5	10
3	C	604	PCW	C33-C32	2.42	1.61	1.52	8	10
3	C	607	PCW	C33-C32	2.42	1.61	1.52	4	10
3	B	233	PCW	C33-C32	2.42	1.61	1.52	3	10
3	C	601	PCW	C33-C32	2.41	1.61	1.52	9	10
3	C	617	PCW	C33-C32	2.41	1.61	1.52	9	10
3	B	217	PCW	C33-C32	2.41	1.61	1.52	9	10
3	C	614	PCW	C33-C32	2.41	1.61	1.52	8	10
3	C	618	PCW	C33-C32	2.41	1.61	1.52	1	10
3	C	621	PCW	C33-C32	2.41	1.61	1.52	5	10
3	B	208	PCW	C33-C32	2.41	1.61	1.52	5	10
3	B	214	PCW	C33-C32	2.41	1.61	1.52	4	10
3	C	609	PCW	C33-C32	2.41	1.61	1.52	1	10
3	B	209	PCW	C33-C32	2.40	1.61	1.52	9	10
3	B	222	PCW	C33-C32	2.40	1.61	1.52	2	10
3	B	206	PCW	C33-C32	2.40	1.61	1.52	9	10
3	C	602	PCW	C33-C32	2.40	1.61	1.52	8	10
3	B	211	PCW	C33-C32	2.39	1.60	1.52	6	10
3	C	613	PCW	C33-C32	2.39	1.60	1.52	10	10
3	C	610	PCW	C33-C32	2.39	1.60	1.52	7	10
3	C	616	PCW	C33-C32	2.39	1.60	1.52	6	10
3	B	215	PCW	C5-N	2.38	1.44	1.51	5	10
3	B	215	PCW	C33-C32	2.38	1.60	1.52	2	10
3	C	608	PCW	C33-C32	2.38	1.60	1.52	7	10
3	B	213	PCW	C33-C32	2.38	1.60	1.52	6	10
3	B	203	PCW	C33-C32	2.37	1.60	1.52	2	10
3	B	220	PCW	C33-C32	2.37	1.60	1.52	2	10
3	B	206	PCW	C7-N	2.37	1.43	1.50	7	10
3	C	613	PCW	O2-C2	2.37	1.52	1.46	3	5
3	A	405	PCW	C33-C32	2.36	1.60	1.52	10	10
3	B	224	PCW	C33-C32	2.36	1.60	1.52	8	10
3	A	411	PCW	C33-C32	2.35	1.60	1.52	2	10
3	B	223	PCW	C33-C32	2.34	1.60	1.52	3	10
3	C	620	PCW	C33-C32	2.34	1.60	1.52	5	10
3	B	212	PCW	C33-C32	2.34	1.60	1.52	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	621	PCW	C7-N	2.32	1.43	1.50	9	10
3	B	235	PCW	C33-C32	2.32	1.60	1.52	4	10
3	C	613	PCW	C7-N	2.31	1.43	1.50	3	10
3	B	203	PCW	C3-C2	2.29	1.58	1.50	8	8
3	B	209	PCW	C7-N	2.29	1.43	1.50	5	10
3	C	620	PCW	C7-N	2.29	1.43	1.50	6	10
3	A	403	PCW	C7-N	2.29	1.43	1.50	9	9
3	A	406	PCW	C7-N	2.28	1.43	1.50	5	10
7	B	239	EWS	CAO-CAN	2.28	1.42	1.38	1	10
3	B	224	PCW	C7-N	2.27	1.43	1.50	7	10
3	C	608	PCW	C7-N	2.27	1.43	1.50	6	10
3	B	208	PCW	C7-N	2.27	1.43	1.50	7	10
3	A	401	PCW	C3-C2	2.26	1.57	1.50	2	9
3	A	406	PCW	C3-C2	2.26	1.57	1.50	7	9
3	B	212	PCW	C7-N	2.26	1.43	1.50	9	10
3	B	216	PCW	C3-C2	2.26	1.57	1.50	8	7
3	A	410	PCW	C3-C2	2.25	1.57	1.50	6	10
3	C	623	PCW	C3-C2	2.25	1.57	1.50	10	7
3	A	402	PCW	C3-C2	2.24	1.57	1.50	1	8
3	B	218	PCW	C3-C2	2.24	1.57	1.50	2	8
3	B	212	PCW	C3-C2	2.24	1.57	1.50	7	8
3	B	215	PCW	C7-N	2.24	1.43	1.50	1	10
3	B	221	PCW	C3-C2	2.24	1.57	1.50	8	10
3	C	605	PCW	C7-N	2.24	1.43	1.50	1	10
3	B	221	PCW	C7-N	2.23	1.43	1.50	9	9
3	C	625	PCW	C3-C2	2.23	1.57	1.50	5	8
3	C	608	PCW	C3-C2	2.23	1.57	1.50	10	6
3	C	612	PCW	C3-C2	2.23	1.57	1.50	8	10
3	C	606	PCW	C7-N	2.23	1.43	1.50	6	10
3	C	626	PCW	C7-N	2.23	1.43	1.50	8	10
3	C	602	PCW	C3-C2	2.22	1.57	1.50	2	8
3	B	219	PCW	C3-C2	2.22	1.57	1.50	10	8
3	B	205	PCW	C7-N	2.21	1.43	1.50	2	9
3	C	601	PCW	C7-N	2.21	1.43	1.50	6	9
3	C	616	PCW	C3-C2	2.21	1.57	1.50	3	9
3	C	626	PCW	C3-C2	2.20	1.57	1.50	1	6
3	B	207	PCW	C3-C2	2.19	1.57	1.50	5	9
3	C	601	PCW	C3-C2	2.19	1.57	1.50	8	8
3	C	614	PCW	C3-C2	2.19	1.57	1.50	7	5
3	B	222	PCW	C3-C2	2.19	1.57	1.50	6	10
3	B	233	PCW	C3-C2	2.18	1.57	1.50	7	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	204	PCW	C3-C2	2.18	1.57	1.50	4	6
3	B	234	PCW	C3-C2	2.17	1.57	1.50	9	8
3	C	611	PCW	C3-C2	2.17	1.57	1.50	6	8
3	B	214	PCW	C3-C2	2.17	1.57	1.50	4	8
3	B	225	PCW	C3-C2	2.17	1.57	1.50	4	8
3	A	403	PCW	C3-C2	2.17	1.57	1.50	6	7
3	B	223	PCW	C3-C2	2.17	1.57	1.50	6	10
3	B	211	PCW	C3-C2	2.17	1.57	1.50	5	7
3	C	605	PCW	C3-C2	2.16	1.57	1.50	10	7
4	B	227	17F	C1X-C2X	2.16	1.61	1.52	6	10
3	C	610	PCW	C3-C2	2.16	1.57	1.50	5	5
3	A	411	PCW	C3-C2	2.16	1.57	1.50	2	9
3	A	405	PCW	C3-C2	2.15	1.57	1.50	5	9
4	C	630	17F	C1X-C2X	2.15	1.61	1.52	9	2
3	A	404	PCW	C3-C2	2.15	1.57	1.50	5	6
3	B	208	PCW	C3-C2	2.15	1.57	1.50	3	9
3	B	201	PCW	C3-C2	2.15	1.57	1.50	6	8
3	B	202	PCW	C3-C2	2.15	1.57	1.50	4	8
3	C	603	PCW	C3-C2	2.15	1.57	1.50	1	7
3	C	613	PCW	C3-C2	2.15	1.57	1.50	5	10
3	C	622	PCW	C3-C2	2.15	1.57	1.50	4	8
3	C	624	PCW	C3-C2	2.15	1.57	1.50	6	8
4	C	632	17F	C1X-C2X	2.15	1.61	1.52	3	8
3	B	215	PCW	C3-C2	2.15	1.57	1.50	4	9
3	B	224	PCW	C3-C2	2.14	1.57	1.50	8	9
3	B	209	PCW	C3-C2	2.14	1.57	1.50	2	7
3	B	235	PCW	C3-C2	2.14	1.57	1.50	7	7
3	C	619	PCW	P-O4P	2.14	1.51	1.59	2	1
3	C	604	PCW	C3-C2	2.14	1.57	1.50	9	7
4	B	229	17F	C1X-C2X	2.14	1.61	1.52	9	7
3	B	205	PCW	C3-C2	2.13	1.57	1.50	6	6
3	C	609	PCW	C3-C2	2.13	1.57	1.50	7	6
3	C	617	PCW	C3-C2	2.13	1.57	1.50	2	5
3	C	607	PCW	C3-C2	2.13	1.57	1.50	3	6
3	C	620	PCW	C3-C2	2.13	1.57	1.50	10	7
3	B	210	PCW	C3-C2	2.13	1.57	1.50	9	5
4	B	236	17F	C1X-C2X	2.13	1.61	1.52	3	10
3	B	213	PCW	C3-C2	2.13	1.57	1.50	7	4
3	C	606	PCW	C3-C2	2.12	1.57	1.50	9	5
3	C	618	PCW	C3-C2	2.12	1.57	1.50	7	8
3	A	408	PCW	C3-C2	2.11	1.57	1.50	2	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	B	226	17F	C1X-C2X	2.12	1.61	1.52	4	8
7	B	239	EWS	CAQ-CAV	2.11	1.36	1.39	5	10
3	B	220	PCW	C3-C2	2.10	1.57	1.50	7	7
3	C	619	PCW	C3-C2	2.10	1.57	1.50	5	3
4	C	633	17F	C1X-C2X	2.10	1.61	1.52	7	9
4	B	230	17F	C1X-C2X	2.10	1.61	1.52	1	7
3	A	409	PCW	C3-C2	2.10	1.57	1.50	9	6
4	A	407	17F	C1X-C2X	2.10	1.61	1.52	10	5
4	B	231	17F	C1X-C2X	2.09	1.61	1.52	9	7
4	C	629	17F	C1X-C2X	2.09	1.61	1.52	4	7
3	C	615	PCW	C3-C2	2.09	1.57	1.50	7	6
4	B	232	17F	C1X-C2X	2.09	1.61	1.52	2	8
3	B	217	PCW	C3-C2	2.09	1.57	1.50	2	6
4	C	627	17F	C1X-C2X	2.08	1.61	1.52	3	6
3	B	206	PCW	C3-C2	2.07	1.57	1.50	9	5
3	C	621	PCW	C3-C2	2.07	1.57	1.50	6	4
4	C	631	17F	C1X-C2X	2.06	1.61	1.52	3	7
4	B	228	17F	C1X-C2X	2.05	1.60	1.52	7	5
3	C	615	PCW	P-O4P	2.04	1.51	1.59	3	1
3	B	225	PCW	P-O4P	2.04	1.51	1.59	5	1
3	C	625	PCW	P-O4P	2.02	1.51	1.59	1	1
3	B	207	PCW	P-O4P	2.02	1.51	1.59	9	1
4	C	628	17F	C1X-C2X	2.01	1.60	1.52	1	1
4	C	627	17F	C4-C5	2.01	1.57	1.50	2	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	210	PCW	C8-N-C7	12.13	77.11	108.98	10	10
3	A	409	PCW	C8-N-C7	12.06	77.30	108.98	6	10
3	C	604	PCW	C8-N-C7	12.02	77.40	108.98	7	10
3	C	612	PCW	C8-N-C7	12.02	77.41	108.98	7	10
3	A	408	PCW	C8-N-C7	12.01	77.42	108.98	1	10
3	C	618	PCW	C8-N-C7	12.01	77.44	108.98	4	10
3	B	225	PCW	C8-N-C7	11.99	77.47	108.98	5	10
3	A	411	PCW	C8-N-C7	11.99	77.49	108.98	9	10
3	A	404	PCW	C8-N-C7	11.97	77.53	108.98	6	10
3	B	235	PCW	C8-N-C7	11.97	77.54	108.98	6	10
3	C	610	PCW	C8-N-C7	11.96	77.56	108.98	10	10
3	C	607	PCW	C8-N-C7	11.96	77.57	108.98	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	410	PCW	C8-N-C7	11.95	77.57	108.98	10	10
3	B	211	PCW	C8-N-C7	11.95	77.58	108.98	5	10
3	C	603	PCW	C8-N-C7	11.95	77.59	108.98	3	10
3	C	617	PCW	C8-N-C7	11.95	77.59	108.98	3	10
3	B	222	PCW	C8-N-C7	11.95	77.60	108.98	5	10
3	A	401	PCW	C8-N-C7	11.94	77.60	108.98	1	10
3	C	625	PCW	C8-N-C7	11.94	77.60	108.98	9	10
3	B	216	PCW	C8-N-C7	11.94	77.61	108.98	6	10
3	B	223	PCW	C8-N-C7	11.94	77.61	108.98	6	10
3	B	201	PCW	C8-N-C7	11.94	77.62	108.98	6	10
3	B	234	PCW	C8-N-C7	11.93	77.64	108.98	3	10
3	C	624	PCW	C8-N-C7	11.93	77.64	108.98	7	10
3	C	614	PCW	C8-N-C7	11.93	77.64	108.98	4	10
3	B	214	PCW	C8-N-C7	11.93	77.65	108.98	10	10
3	A	405	PCW	C8-N-C7	11.93	77.65	108.98	6	10
3	C	611	PCW	C8-N-C7	11.92	77.66	108.98	10	10
3	A	402	PCW	C8-N-C7	11.92	77.68	108.98	10	10
3	B	217	PCW	C8-N-C7	11.91	77.69	108.98	6	10
3	B	207	PCW	C8-N-C7	11.91	77.69	108.98	4	10
3	C	623	PCW	C8-N-C7	11.91	77.69	108.98	1	10
3	B	220	PCW	C8-N-C7	11.91	77.70	108.98	5	10
3	B	204	PCW	C8-N-C7	11.90	77.70	108.98	9	10
3	C	615	PCW	C8-N-C7	11.90	77.71	108.98	1	10
3	B	233	PCW	C8-N-C7	11.90	77.72	108.98	7	10
3	B	219	PCW	C8-N-C7	11.90	77.73	108.98	10	10
3	C	602	PCW	C8-N-C7	11.89	77.74	108.98	8	10
3	B	202	PCW	C8-N-C7	11.89	77.74	108.98	10	10
3	C	616	PCW	C8-N-C7	11.89	77.74	108.98	2	10
3	C	619	PCW	C8-N-C7	11.89	77.75	108.98	5	10
3	B	203	PCW	C8-N-C7	11.88	77.76	108.98	1	10
3	B	213	PCW	C8-N-C7	11.87	77.79	108.98	6	10
3	C	609	PCW	C8-N-C7	11.85	77.86	108.98	5	10
3	C	622	PCW	C8-N-C7	11.84	77.88	108.98	4	10
3	B	218	PCW	C8-N-C7	11.83	77.91	108.98	10	10
3	A	409	PCW	C8-N-C6	10.17	82.27	108.98	7	10
3	B	219	PCW	C8-N-C6	10.14	82.34	108.98	2	10
3	C	617	PCW	C8-N-C6	10.13	82.35	108.98	2	10
3	C	624	PCW	C8-N-C6	10.13	82.37	108.98	2	10
3	A	411	PCW	C8-N-C6	10.12	82.40	108.98	3	10
3	B	233	PCW	C8-N-C6	10.11	82.41	108.98	3	10
3	B	214	PCW	C8-N-C6	10.11	82.43	108.98	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	220	PCW	C8-N-C6	10.11	82.43	108.98	6	10
3	B	225	PCW	C8-N-C6	10.11	82.43	108.98	10	10
3	C	609	PCW	C8-N-C6	10.11	82.43	108.98	2	10
3	B	203	PCW	C8-N-C6	10.10	82.44	108.98	2	10
3	B	213	PCW	C8-N-C6	10.10	82.45	108.98	8	10
3	A	410	PCW	C8-N-C6	10.10	82.45	108.98	6	10
3	B	218	PCW	C8-N-C6	10.10	82.46	108.98	2	10
3	B	204	PCW	C8-N-C6	10.09	82.46	108.98	5	10
3	C	614	PCW	C8-N-C6	10.09	82.46	108.98	2	10
3	B	223	PCW	C8-N-C6	10.09	82.47	108.98	5	10
3	B	202	PCW	C8-N-C6	10.08	82.49	108.98	6	10
3	B	222	PCW	C8-N-C6	10.08	82.49	108.98	10	10
3	C	623	PCW	C8-N-C6	10.08	82.49	108.98	9	10
3	B	207	PCW	C8-N-C6	10.08	82.50	108.98	10	10
3	C	619	PCW	C8-N-C6	10.08	82.50	108.98	3	10
3	B	217	PCW	C8-N-C6	10.08	82.50	108.98	7	10
3	C	622	PCW	C8-N-C6	10.08	82.51	108.98	6	10
3	A	401	PCW	C8-N-C6	10.06	82.56	108.98	8	10
3	A	405	PCW	C8-N-C6	10.06	82.56	108.98	9	10
3	C	625	PCW	C8-N-C6	10.06	82.55	108.98	5	10
3	C	612	PCW	C8-N-C6	10.05	82.56	108.98	5	10
3	A	402	PCW	C8-N-C6	10.05	82.58	108.98	5	10
3	C	615	PCW	C8-N-C6	10.05	82.58	108.98	2	10
3	C	607	PCW	C8-N-C6	10.05	82.59	108.98	3	10
3	A	408	PCW	C8-N-C6	10.04	82.59	108.98	9	10
3	B	210	PCW	C8-N-C6	10.04	82.60	108.98	4	10
3	B	216	PCW	C8-N-C6	10.04	82.61	108.98	9	10
3	B	234	PCW	C8-N-C6	10.03	82.62	108.98	5	10
3	C	603	PCW	C8-N-C6	10.03	82.64	108.98	8	10
3	A	404	PCW	C8-N-C6	10.02	82.64	108.98	2	10
3	C	616	PCW	C8-N-C6	10.02	82.64	108.98	8	10
3	C	611	PCW	C8-N-C6	10.02	82.65	108.98	3	10
3	C	618	PCW	C8-N-C6	10.02	82.65	108.98	9	10
3	B	201	PCW	C8-N-C6	10.01	82.68	108.98	3	10
3	C	602	PCW	C8-N-C6	10.01	82.68	108.98	9	10
3	B	235	PCW	C8-N-C6	9.99	82.73	108.98	2	10
3	C	604	PCW	C8-N-C6	9.98	82.76	108.98	3	10
3	B	211	PCW	C8-N-C6	9.98	82.76	108.98	7	10
3	C	610	PCW	C8-N-C6	9.95	82.85	108.98	7	10
3	B	234	PCW	O4P-P-O2P	7.60	78.83	108.94	6	10
3	B	204	PCW	O4P-P-O2P	7.58	78.88	108.94	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	407	17F	O2-P1-O6	6.39	78.61	107.57	5	10
4	C	630	17F	O2-P1-O6	6.37	78.71	107.57	7	10
4	C	630	17F	O2-P1-O3	6.19	79.52	107.57	6	10
4	A	407	17F	O2-P1-O3	6.19	79.53	107.57	4	10
3	B	204	PCW	O1P-P-O2P	5.95	84.75	112.44	9	10
3	B	234	PCW	O1P-P-O2P	5.90	85.02	112.44	5	10
3	B	204	PCW	O3P-P-O2P	5.89	85.58	108.94	6	10
3	B	234	PCW	O3P-P-O2P	5.86	85.71	108.94	6	10
7	B	239	EWS	CAV-CBA-CAX	5.80	109.35	106.15	5	10
3	B	207	PCW	C8-N-C5	5.54	87.89	109.91	6	10
3	C	616	PCW	C8-N-C5	5.50	88.06	109.91	5	10
3	A	411	PCW	C8-N-C5	5.49	88.09	109.91	7	10
3	C	622	PCW	C8-N-C5	5.48	88.13	109.91	5	10
3	C	603	PCW	C8-N-C5	5.47	88.17	109.91	7	10
3	B	217	PCW	C8-N-C5	5.46	88.21	109.91	1	10
3	C	610	PCW	C8-N-C5	5.45	88.24	109.91	9	10
3	B	222	PCW	C8-N-C5	5.45	88.25	109.91	4	10
3	C	623	PCW	C8-N-C5	5.45	88.25	109.91	8	10
3	A	408	PCW	C8-N-C5	5.44	88.28	109.91	10	10
3	B	201	PCW	C8-N-C5	5.44	88.27	109.91	10	10
3	C	615	PCW	C8-N-C5	5.44	88.29	109.91	5	10
3	C	617	PCW	C8-N-C5	5.44	88.30	109.91	9	10
3	A	405	PCW	C8-N-C5	5.43	88.33	109.91	10	10
3	C	619	PCW	C8-N-C5	5.43	88.33	109.91	8	10
3	B	223	PCW	C8-N-C5	5.43	88.34	109.91	3	10
3	B	213	PCW	C8-N-C5	5.42	88.36	109.91	10	10
3	C	625	PCW	C8-N-C5	5.42	88.37	109.91	2	10
3	B	210	PCW	C8-N-C5	5.42	88.38	109.91	1	10
3	A	402	PCW	C8-N-C5	5.41	88.39	109.91	8	10
3	C	609	PCW	C8-N-C5	5.41	88.39	109.91	6	10
3	B	218	PCW	C8-N-C5	5.41	88.40	109.91	9	10
3	C	607	PCW	C8-N-C5	5.41	88.40	109.91	6	10
3	A	404	PCW	C8-N-C5	5.41	88.41	109.91	9	10
3	C	612	PCW	C8-N-C5	5.41	88.41	109.91	4	10
3	B	216	PCW	C8-N-C5	5.40	88.43	109.91	3	10
3	B	219	PCW	C8-N-C5	5.40	88.44	109.91	4	10
3	B	225	PCW	C8-N-C5	5.39	88.47	109.91	2	10
3	A	401	PCW	C8-N-C5	5.39	88.48	109.91	2	10
3	B	234	PCW	C8-N-C5	5.39	88.48	109.91	4	10
3	C	618	PCW	C8-N-C5	5.39	88.50	109.91	8	10
3	B	202	PCW	C8-N-C5	5.38	88.51	109.91	5	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	214	PCW	C8-N-C5	5.39	88.50	109.91	2	10
3	B	220	PCW	C8-N-C5	5.38	88.52	109.91	2	10
3	B	235	PCW	C8-N-C5	5.38	88.52	109.91	1	10
3	C	602	PCW	C8-N-C5	5.38	88.52	109.91	10	10
3	A	410	PCW	C8-N-C5	5.38	88.53	109.91	10	10
3	B	204	PCW	C8-N-C5	5.38	88.53	109.91	7	10
3	C	624	PCW	C8-N-C5	5.38	88.53	109.91	4	10
3	C	611	PCW	C8-N-C5	5.38	88.54	109.91	8	10
3	C	604	PCW	C8-N-C5	5.37	88.55	109.91	6	10
3	C	614	PCW	C8-N-C5	5.37	88.57	109.91	5	10
3	B	233	PCW	C8-N-C5	5.36	88.59	109.91	1	10
3	B	211	PCW	C8-N-C5	5.35	88.63	109.91	2	10
3	B	203	PCW	C8-N-C5	5.35	88.66	109.91	8	10
3	A	409	PCW	C8-N-C5	5.32	88.75	109.91	9	10
4	C	630	17F	O3-C1-C2	5.00	112.42	108.06	5	10
4	B	230	17F	O3-C1-C2	4.89	112.32	108.06	8	10
4	A	407	17F	O2-P1-O1	4.84	89.91	112.44	1	10
4	C	630	17F	O2-P1-O1	4.81	90.06	112.44	10	10
4	B	229	17F	O3-C1-C2	4.26	111.77	108.06	9	10
4	B	231	17F	O3-C1-C2	4.23	111.75	108.06	1	10
4	B	228	17F	O3-C1-C2	4.13	111.66	108.06	4	10
4	C	631	17F	O3-C1-C2	4.11	111.64	108.06	2	10
4	B	226	17F	O3-C1-C2	4.09	111.62	108.06	7	10
7	B	239	EWS	CBA-CAX-NAW	4.06	107.47	110.22	8	10
4	B	236	17F	O3-C1-C2	3.87	111.43	108.06	4	10
4	B	227	17F	O3-C1-C2	3.85	111.41	108.06	10	10
4	B	232	17F	O3-C1-C2	3.80	111.37	108.06	5	10
4	C	628	17F	O3-C1-C2	3.75	111.33	108.06	7	10
5	B	237	GNP	O1B-PB-N3B	3.69	106.33	111.77	5	10
4	C	632	17F	O3-C1-C2	3.66	111.25	108.06	2	10
4	C	627	17F	O3-C1-C2	3.62	111.22	108.06	10	10
3	B	204	PCW	O1P-P-O4P	3.59	123.82	107.57	9	10
4	A	407	17F	O3-C1-C2	3.57	111.17	108.06	1	10
4	C	633	17F	O3-C1-C2	3.49	111.10	108.06	3	10
3	B	214	PCW	C6-N-C5	3.45	123.63	109.91	1	10
4	C	628	17F	O7-C7-O8	3.45	132.26	123.63	7	10
3	B	234	PCW	O1P-P-O4P	3.44	123.18	107.57	5	10
4	C	632	17F	O5-C3-O4	3.44	116.27	124.08	4	10
4	B	229	17F	O5-C3-O4	3.44	116.28	124.08	5	10
4	C	629	17F	O3-C1-C2	3.43	111.05	108.06	10	10
3	B	233	PCW	C6-N-C5	3.42	123.52	109.91	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	219	PCW	C6-N-C5	3.42	123.51	109.91	4	10
4	C	631	17F	O5-C3-O4	3.41	116.33	124.08	5	10
3	A	402	PCW	C6-N-C5	3.41	123.46	109.91	5	10
4	B	226	17F	O5-C3-O4	3.40	116.36	124.08	3	10
3	A	409	PCW	C6-N-C5	3.40	123.42	109.91	9	10
4	B	232	17F	O5-C3-O4	3.39	116.38	124.08	4	10
4	B	236	17F	O5-C3-O4	3.39	116.39	124.08	4	10
3	A	401	PCW	C6-N-C5	3.38	123.36	109.91	3	10
4	C	630	17F	O5-C3-O4	3.38	116.41	124.08	10	10
4	C	627	17F	O5-C3-O4	3.38	116.41	124.08	9	10
3	C	609	PCW	C6-N-C5	3.37	123.32	109.91	7	10
3	C	624	PCW	C6-N-C5	3.37	123.32	109.91	2	10
4	B	227	17F	O5-C3-O4	3.37	116.43	124.08	9	10
4	C	628	17F	O5-C3-O4	3.37	116.42	124.08	4	10
3	A	408	PCW	C6-N-C5	3.37	123.31	109.91	7	10
3	C	623	PCW	C6-N-C5	3.37	123.31	109.91	9	10
3	B	213	PCW	C6-N-C5	3.37	123.30	109.91	9	10
3	C	611	PCW	C6-N-C5	3.37	123.30	109.91	8	10
4	C	629	17F	O5-C3-O4	3.37	116.44	124.08	7	10
4	B	228	17F	O5-C3-O4	3.36	116.45	124.08	1	10
3	C	622	PCW	C6-N-C5	3.36	123.28	109.91	5	10
4	B	231	17F	O5-C3-O4	3.36	116.46	124.08	7	10
3	C	607	PCW	C6-N-C5	3.36	123.26	109.91	6	10
3	C	614	PCW	C6-N-C5	3.36	123.25	109.91	5	10
4	B	230	17F	O5-C3-O4	3.36	116.47	124.08	5	10
3	A	410	PCW	C6-N-C5	3.35	123.24	109.91	9	10
4	C	633	17F	O5-C3-O4	3.35	116.47	124.08	9	10
3	C	603	PCW	C6-N-C5	3.35	123.22	109.91	9	10
3	B	220	PCW	C6-N-C5	3.35	123.21	109.91	8	10
3	C	602	PCW	C6-N-C5	3.35	123.22	109.91	9	10
3	A	411	PCW	C6-N-C5	3.34	123.20	109.91	7	10
3	B	223	PCW	C6-N-C5	3.34	123.20	109.91	5	10
3	C	615	PCW	C6-N-C5	3.34	123.18	109.91	4	10
3	A	404	PCW	C6-N-C5	3.33	123.15	109.91	4	10
3	B	207	PCW	C6-N-C5	3.33	123.15	109.91	2	10
3	C	625	PCW	C6-N-C5	3.33	123.14	109.91	2	10
3	C	617	PCW	C6-N-C5	3.33	123.14	109.91	10	10
4	A	407	17F	O5-C3-O4	3.33	116.53	124.08	3	10
3	B	204	PCW	C6-N-C5	3.32	123.11	109.91	5	10
3	B	218	PCW	C6-N-C5	3.32	123.12	109.91	1	10
3	B	225	PCW	C6-N-C5	3.32	123.11	109.91	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	610	PCW	C6-N-C5	3.32	123.09	109.91	7	10
3	B	203	PCW	C6-N-C5	3.31	123.08	109.91	2	10
3	C	616	PCW	C6-N-C5	3.31	123.08	109.91	10	10
3	B	210	PCW	C6-N-C5	3.30	123.04	109.91	3	10
3	B	216	PCW	C6-N-C5	3.30	123.04	109.91	7	10
3	B	202	PCW	C6-N-C5	3.30	123.02	109.91	5	10
3	B	201	PCW	C6-N-C5	3.29	123.00	109.91	7	10
3	B	235	PCW	C6-N-C5	3.29	123.00	109.91	3	10
3	B	222	PCW	C6-N-C5	3.29	122.97	109.91	9	10
3	B	217	PCW	C6-N-C5	3.28	122.96	109.91	1	10
3	C	619	PCW	C6-N-C5	3.28	122.96	109.91	9	10
3	C	604	PCW	C6-N-C5	3.28	122.96	109.91	4	10
3	C	618	PCW	C6-N-C5	3.27	122.92	109.91	3	10
3	C	612	PCW	C6-N-C5	3.27	122.90	109.91	4	10
3	A	405	PCW	C6-N-C5	3.27	122.90	109.91	9	10
3	B	234	PCW	C6-N-C5	3.27	122.89	109.91	8	10
3	B	211	PCW	C6-N-C5	3.25	122.82	109.91	8	10
4	B	230	17F	O7-C7-O8	3.16	131.53	123.63	7	10
4	C	633	17F	O7-C7-O8	3.09	131.35	123.63	1	10
4	B	232	17F	O7-C7-O8	3.08	131.34	123.63	7	10
4	B	229	17F	O7-C7-O8	3.08	131.34	123.63	1	10
4	A	407	17F	O7-C7-O8	3.07	131.31	123.63	3	10
4	C	629	17F	O7-C7-O8	3.06	131.27	123.63	5	10
4	C	631	17F	O7-C7-O8	3.05	131.27	123.63	3	10
4	C	627	17F	O7-C7-O8	3.01	131.17	123.63	4	10
4	A	407	17F	O3-P1-O1	2.99	120.80	108.94	5	10
4	B	236	17F	O7-C7-O8	2.99	131.10	123.63	10	10
4	C	632	17F	O7-C7-O8	2.95	131.01	123.63	1	10
4	B	228	17F	O7-C7-O8	2.94	130.99	123.63	1	10
4	B	231	17F	O7-C7-O8	2.89	130.85	123.63	4	10
4	B	226	17F	O7-C7-O8	2.88	130.84	123.63	10	10
4	C	630	17F	O7-C7-O8	2.87	130.81	123.63	8	10
4	B	227	17F	O7-C7-O8	2.84	130.74	123.63	1	10
4	C	630	17F	O3-P1-O1	2.82	120.10	108.94	8	10
3	B	215	PCW	C8-N-C7	2.75	101.74	108.98	4	10
3	B	224	PCW	C8-N-C7	2.75	101.75	108.98	5	10
3	C	605	PCW	C8-N-C7	2.74	101.78	108.98	5	10
3	A	403	PCW	C8-N-C7	2.73	101.81	108.98	4	10
3	A	406	PCW	C8-N-C7	2.72	101.82	108.98	3	10
3	C	620	PCW	C8-N-C7	2.70	101.89	108.98	7	10
3	B	212	PCW	C8-N-C7	2.69	101.91	108.98	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	C	628	17F	C5-O9-C17	2.68	111.38	117.80	2	10
3	B	221	PCW	C8-N-C7	2.68	101.94	108.98	10	10
3	B	206	PCW	C8-N-C7	2.67	101.96	108.98	7	10
3	B	208	PCW	C8-N-C7	2.67	101.97	108.98	3	10
3	C	613	PCW	C8-N-C7	2.67	101.97	108.98	1	10
3	B	205	PCW	C8-N-C7	2.67	101.97	108.98	7	10
3	C	621	PCW	C8-N-C7	2.67	101.97	108.98	2	10
3	B	209	PCW	C8-N-C7	2.66	101.99	108.98	1	10
3	C	626	PCW	C8-N-C7	2.64	102.03	108.98	10	10
4	C	633	17F	O9-C17-O10	2.64	129.87	123.70	10	10
3	C	606	PCW	C8-N-C7	2.63	102.08	108.98	6	10
3	C	608	PCW	C8-N-C7	2.63	102.08	108.98	6	10
3	B	235	PCW	C7-N-C5	2.61	120.30	109.91	6	10
3	C	601	PCW	C8-N-C7	2.59	102.17	108.98	6	10
3	C	610	PCW	C7-N-C5	2.59	120.20	109.91	1	10
4	A	407	17F	O6-P1-O1	2.59	119.20	108.94	9	10
4	C	630	17F	O6-P1-O1	2.57	119.12	108.94	9	9
4	C	631	17F	C5-O9-C17	2.56	111.66	117.80	9	10
3	C	612	PCW	C7-N-C5	2.56	120.09	109.91	2	10
3	B	201	PCW	C7-N-C5	2.54	119.99	109.91	9	10
4	B	232	17F	C5-O9-C17	2.53	111.73	117.80	8	9
3	C	619	PCW	C7-N-C5	2.53	119.96	109.91	7	10
3	B	220	PCW	C7-N-C5	2.53	119.95	109.91	10	10
3	A	405	PCW	C7-N-C5	2.52	119.92	109.91	1	10
4	C	630	17F	C5-O9-C17	2.52	111.77	117.80	7	8
3	B	207	PCW	C7-N-C5	2.52	119.91	109.91	6	10
3	B	225	PCW	C7-N-C5	2.51	119.88	109.91	7	10
3	B	222	PCW	C7-N-C5	2.51	119.87	109.91	4	10
3	A	408	PCW	C7-N-C5	2.50	119.87	109.91	1	10
3	B	217	PCW	C7-N-C5	2.50	119.86	109.91	4	10
3	A	401	PCW	C7-N-C5	2.49	119.81	109.91	1	10
3	C	622	PCW	C7-N-C5	2.49	119.81	109.91	2	10
4	A	407	17F	O9-C17-O10	2.49	129.53	123.70	1	10
3	B	234	PCW	C7-N-C5	2.49	119.80	109.91	4	10
3	C	624	PCW	C7-N-C5	2.48	119.78	109.91	5	10
4	B	231	17F	C5-O9-C17	2.48	111.86	117.80	4	9
3	B	210	PCW	C7-N-C5	2.48	119.75	109.91	6	10
3	B	203	PCW	C7-N-C5	2.48	119.75	109.91	6	10
4	C	632	17F	O9-C17-O10	2.47	129.48	123.70	5	10
3	B	211	PCW	C7-N-C5	2.47	119.73	109.91	4	10
3	C	623	PCW	C7-N-C5	2.47	119.71	109.91	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	226	17F	C5-O9-C17	2.47	111.89	117.80	2	9
3	B	214	PCW	C7-N-C5	2.46	119.70	109.91	9	10
3	C	602	PCW	C7-N-C5	2.46	119.70	109.91	5	10
3	A	404	PCW	C7-N-C5	2.46	119.69	109.91	9	10
3	C	615	PCW	C7-N-C5	2.46	119.69	109.91	5	10
3	A	411	PCW	C7-N-C5	2.46	119.69	109.91	10	10
3	C	616	PCW	C7-N-C5	2.46	119.69	109.91	5	10
4	B	230	17F	C5-O9-C17	2.46	111.92	117.80	4	10
3	B	218	PCW	C7-N-C5	2.45	119.66	109.91	4	10
3	B	223	PCW	C7-N-C5	2.45	119.66	109.91	7	10
3	B	233	PCW	C7-N-C5	2.45	119.66	109.91	1	10
4	C	627	17F	O9-C17-O10	2.45	129.43	123.70	8	10
3	C	607	PCW	C7-N-C5	2.44	119.63	109.91	10	10
4	B	229	17F	C5-O9-C17	2.44	111.95	117.80	8	9
3	C	603	PCW	C7-N-C5	2.44	119.61	109.91	6	10
3	C	625	PCW	C7-N-C5	2.44	119.61	109.91	10	10
3	C	614	PCW	C7-N-C5	2.44	119.59	109.91	6	10
3	C	617	PCW	C7-N-C5	2.43	119.58	109.91	9	10
4	B	228	17F	C5-O9-C17	2.43	111.97	117.80	7	10
3	A	402	PCW	C7-N-C5	2.43	119.56	109.91	4	10
3	B	213	PCW	C7-N-C5	2.43	119.55	109.91	5	10
3	C	618	PCW	C7-N-C5	2.43	119.55	109.91	4	10
4	B	227	17F	C5-O9-C17	2.43	111.99	117.80	3	8
4	B	226	17F	O9-C17-O10	2.42	129.37	123.70	6	10
3	C	604	PCW	C7-N-C5	2.42	119.54	109.91	7	10
5	B	237	GNP	O1G-PG-N3B	2.42	108.20	111.77	8	9
4	B	228	17F	O9-C17-O10	2.42	129.36	123.70	4	10
3	B	202	PCW	C7-N-C5	2.42	119.52	109.91	9	10
3	A	409	PCW	C7-N-C5	2.41	119.49	109.91	8	10
4	B	231	17F	O9-C17-O10	2.41	129.33	123.70	8	10
3	B	216	PCW	C7-N-C5	2.41	119.47	109.91	4	10
3	B	204	PCW	C7-N-C5	2.40	119.45	109.91	2	10
3	C	609	PCW	C7-N-C5	2.40	119.44	109.91	5	10
3	C	611	PCW	C7-N-C5	2.40	119.43	109.91	10	10
3	A	410	PCW	C7-N-C5	2.39	119.42	109.91	4	10
3	B	219	PCW	C7-N-C5	2.39	119.41	109.91	8	10
4	B	227	17F	O9-C17-O10	2.39	129.29	123.70	10	10
4	B	236	17F	O9-C17-O10	2.39	129.29	123.70	3	10
4	C	629	17F	O9-C17-O10	2.39	129.28	123.70	9	10
4	C	630	17F	O9-C17-O10	2.38	129.28	123.70	6	10
4	B	229	17F	O9-C17-O10	2.38	129.27	123.70	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	C	627	17F	C5-O9-C17	2.36	112.15	117.80	1	9
4	C	629	17F	C5-O9-C17	2.35	112.17	117.80	3	10
4	B	232	17F	O9-C17-O10	2.35	129.19	123.70	10	10
4	C	631	17F	O9-C17-O10	2.32	129.13	123.70	7	10
4	C	632	17F	C5-O9-C17	2.32	112.25	117.80	8	10
4	B	230	17F	O9-C17-O10	2.30	129.08	123.70	5	10
4	C	628	17F	O7-C7-C8	2.30	104.83	111.83	7	9
4	A	407	17F	C5-O9-C17	2.26	112.38	117.80	7	4
4	B	236	17F	C5-O9-C17	2.25	112.41	117.80	9	10
4	C	628	17F	O9-C17-O10	2.24	128.94	123.70	1	10
4	B	228	17F	C6-C5-C4	2.15	106.77	111.78	10	1
4	B	228	17F	O7-C6-C5	2.14	114.56	108.40	6	2
3	C	616	PCW	C7-N-C6	2.12	114.55	108.98	2	1
3	C	618	PCW	C7-N-C6	2.09	114.47	108.98	4	1
3	A	404	PCW	C7-N-C6	2.07	114.40	108.98	3	1
3	B	204	PCW	C7-N-C6	2.06	114.39	108.98	10	1
3	A	405	PCW	C7-N-C6	2.05	114.37	108.98	8	2
3	B	204	PCW	O1P-P-O3P	2.05	116.87	107.57	6	3
3	A	409	PCW	C7-N-C6	2.05	114.36	108.98	6	1
3	B	222	PCW	C7-N-C6	2.05	114.36	108.98	10	2
3	A	402	PCW	C7-N-C6	2.04	114.32	108.98	10	1
3	C	617	PCW	C7-N-C6	2.03	114.32	108.98	5	2
4	A	407	17F	O7-C6-C5	2.03	114.25	108.40	3	1
3	A	401	PCW	C7-N-C6	2.03	114.30	108.98	8	1
3	B	219	PCW	C7-N-C6	2.02	114.29	108.98	5	1
3	C	604	PCW	C7-N-C6	2.02	114.27	108.98	1	1
3	C	612	PCW	C7-N-C6	2.02	114.27	108.98	10	1
3	B	207	PCW	C7-N-C6	2.01	114.27	108.98	1	1
3	B	217	PCW	C7-N-C6	2.01	114.26	108.98	7	1
3	B	225	PCW	C7-N-C6	2.00	114.23	108.98	5	1
3	C	609	PCW	C7-N-C6	2.00	114.23	108.98	10	1

There are no chirality outliers.

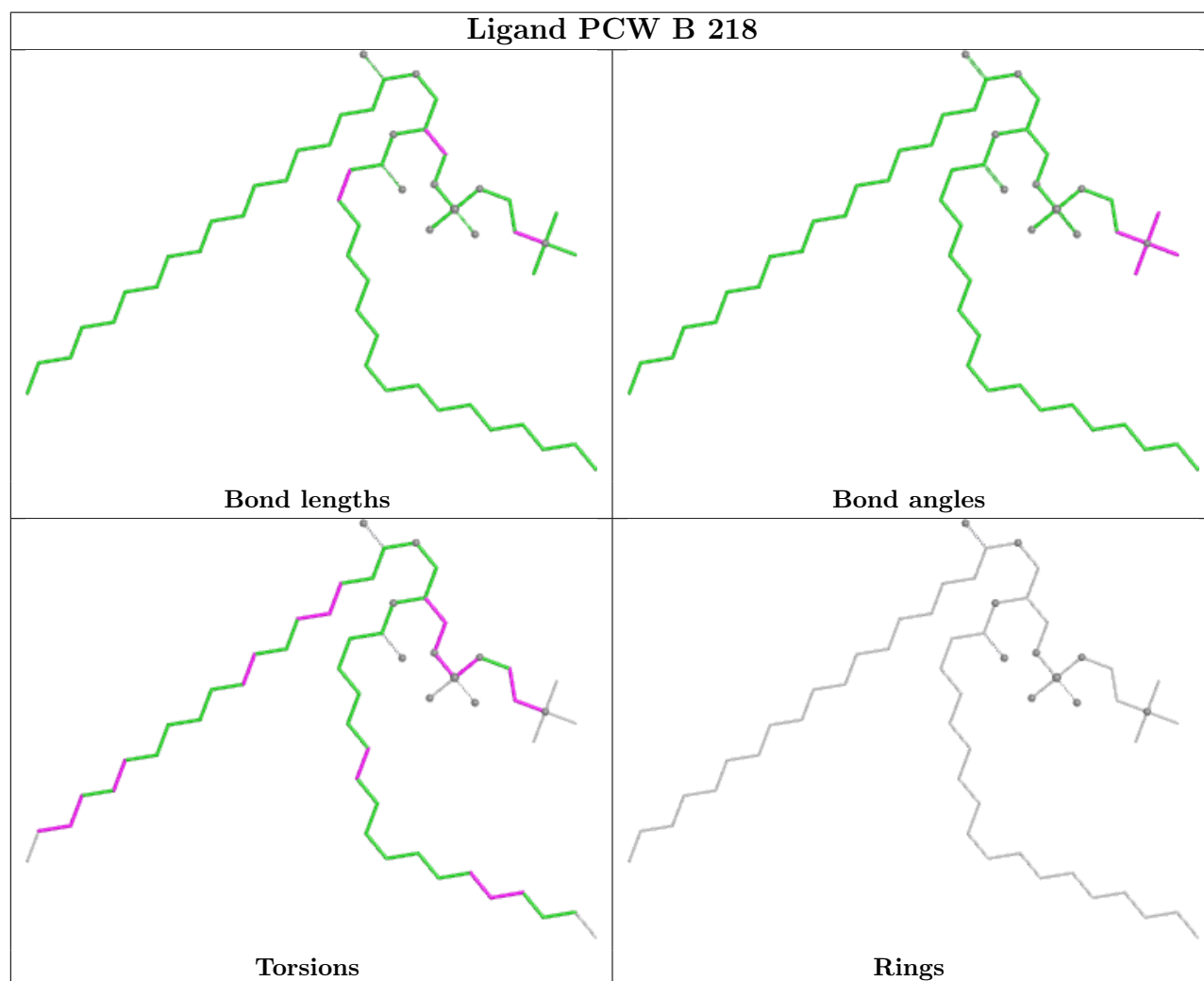
All unique torsion outliers are listed below.

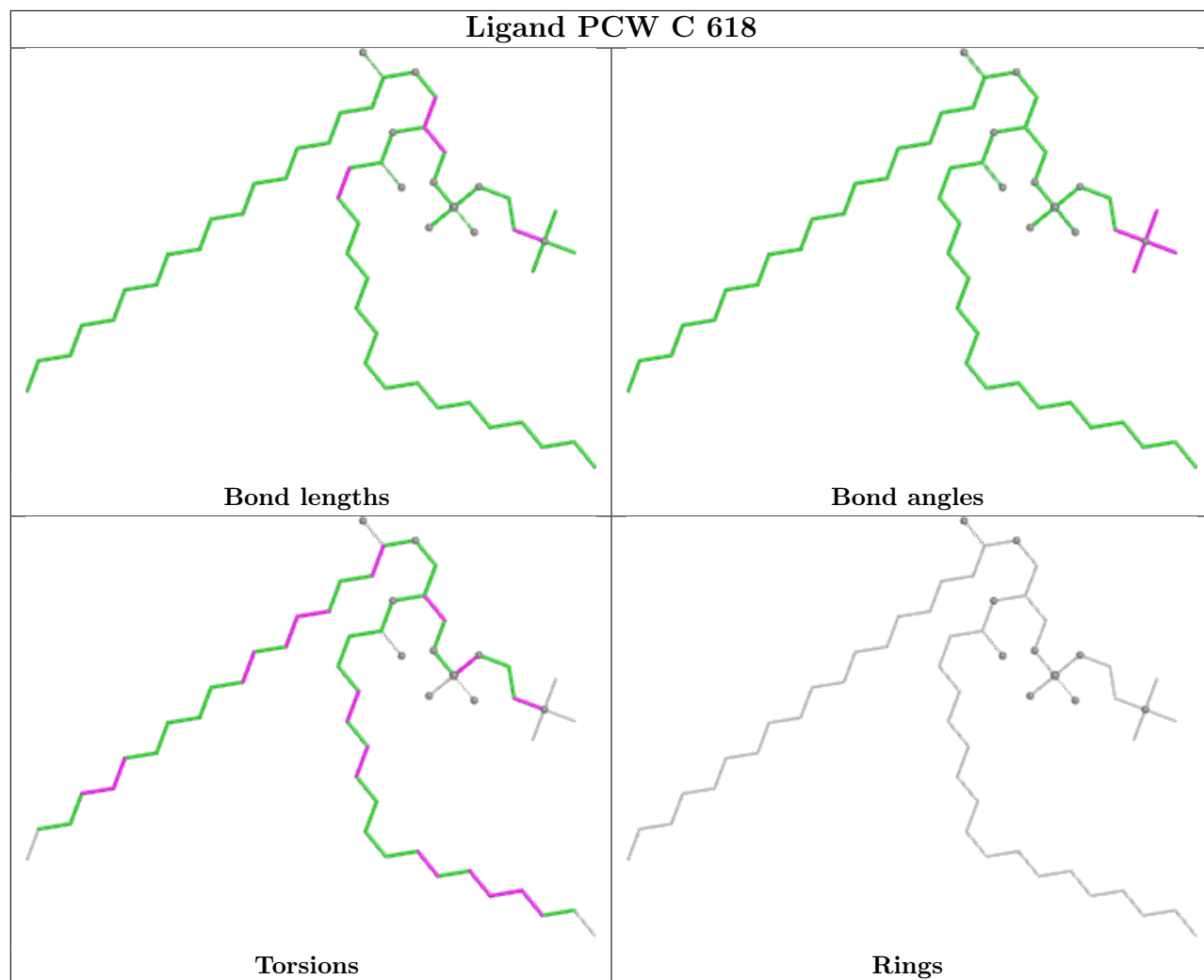
Mol	Chain	Res	Type	Atoms	Models (Total)
5	B	237	GNP	PG-N3B-PB-O1B	1

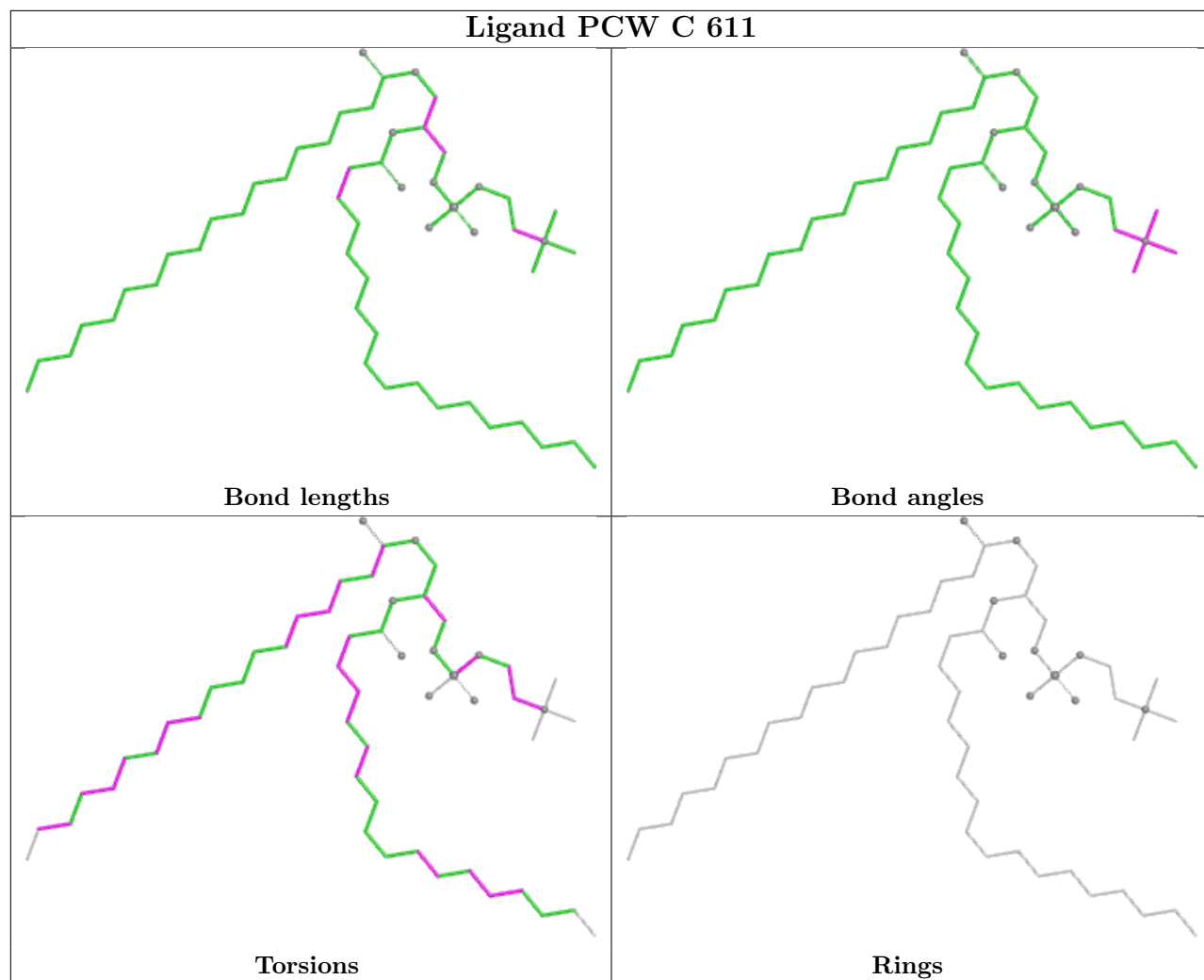
All unique ring outliers are listed below.

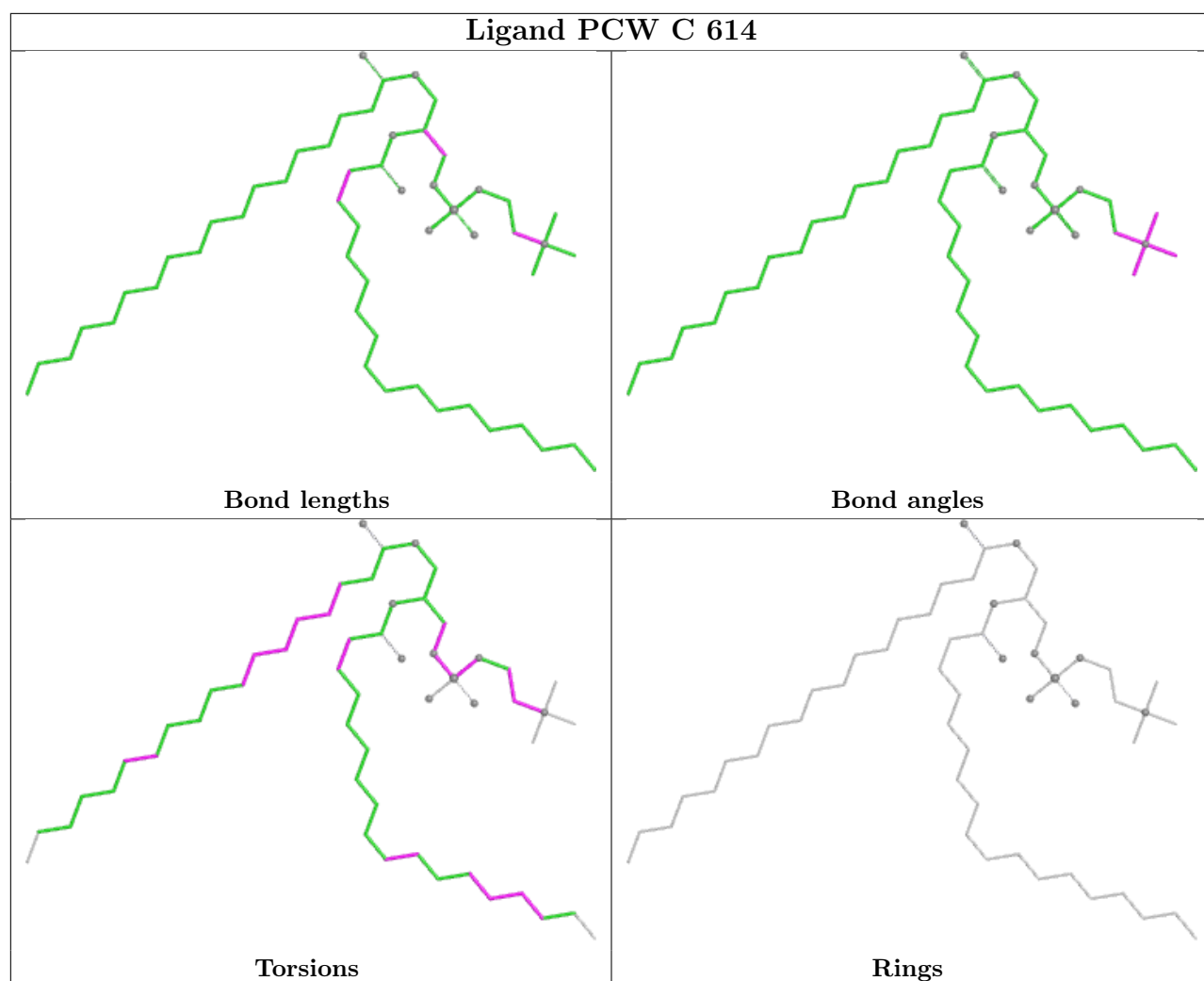
Mol	Chain	Res	Type	Atoms	Models (Total)
7	B	239	EWS	CAC-CAD-CAE-CAF-CAH-NAG	10

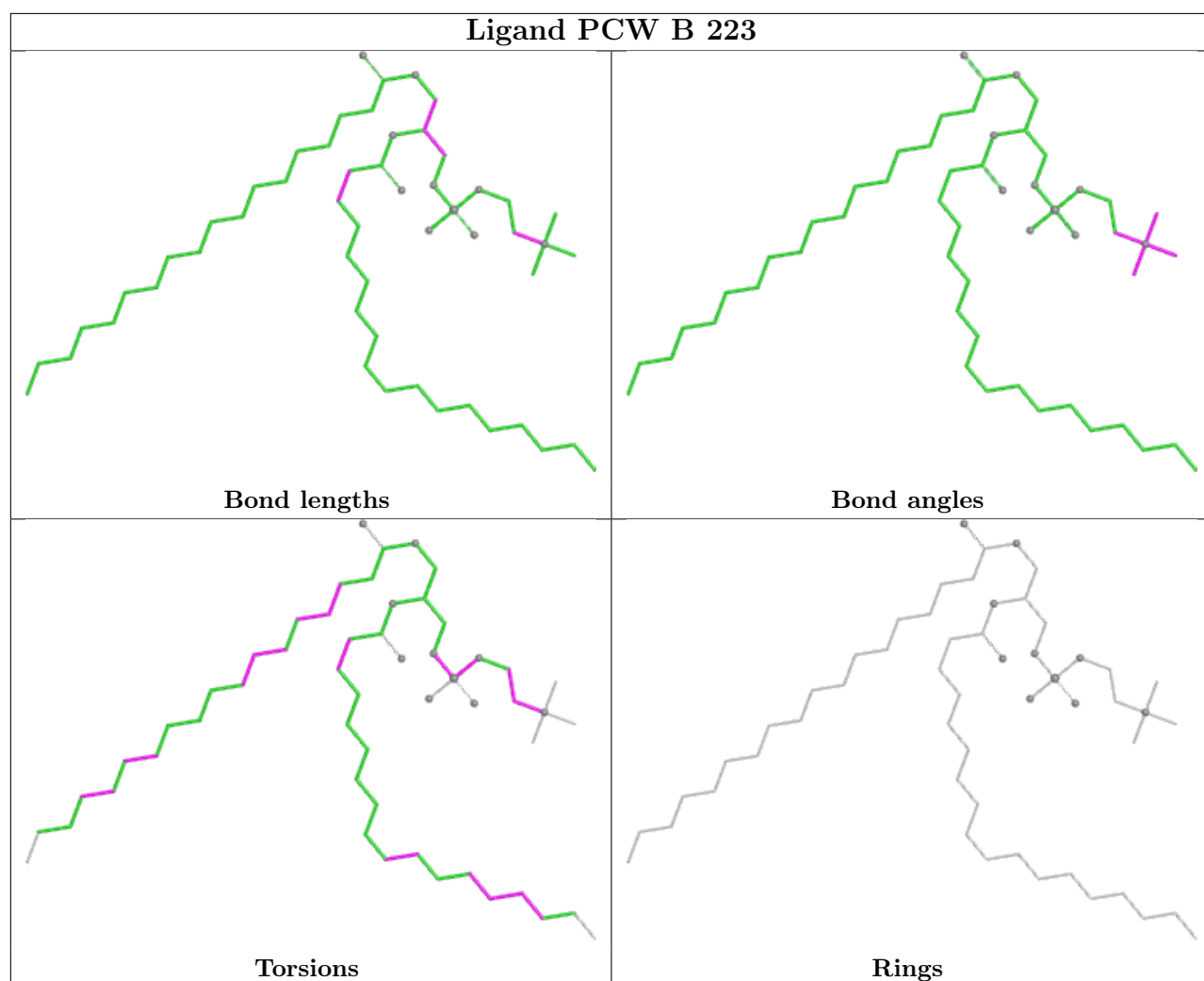
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

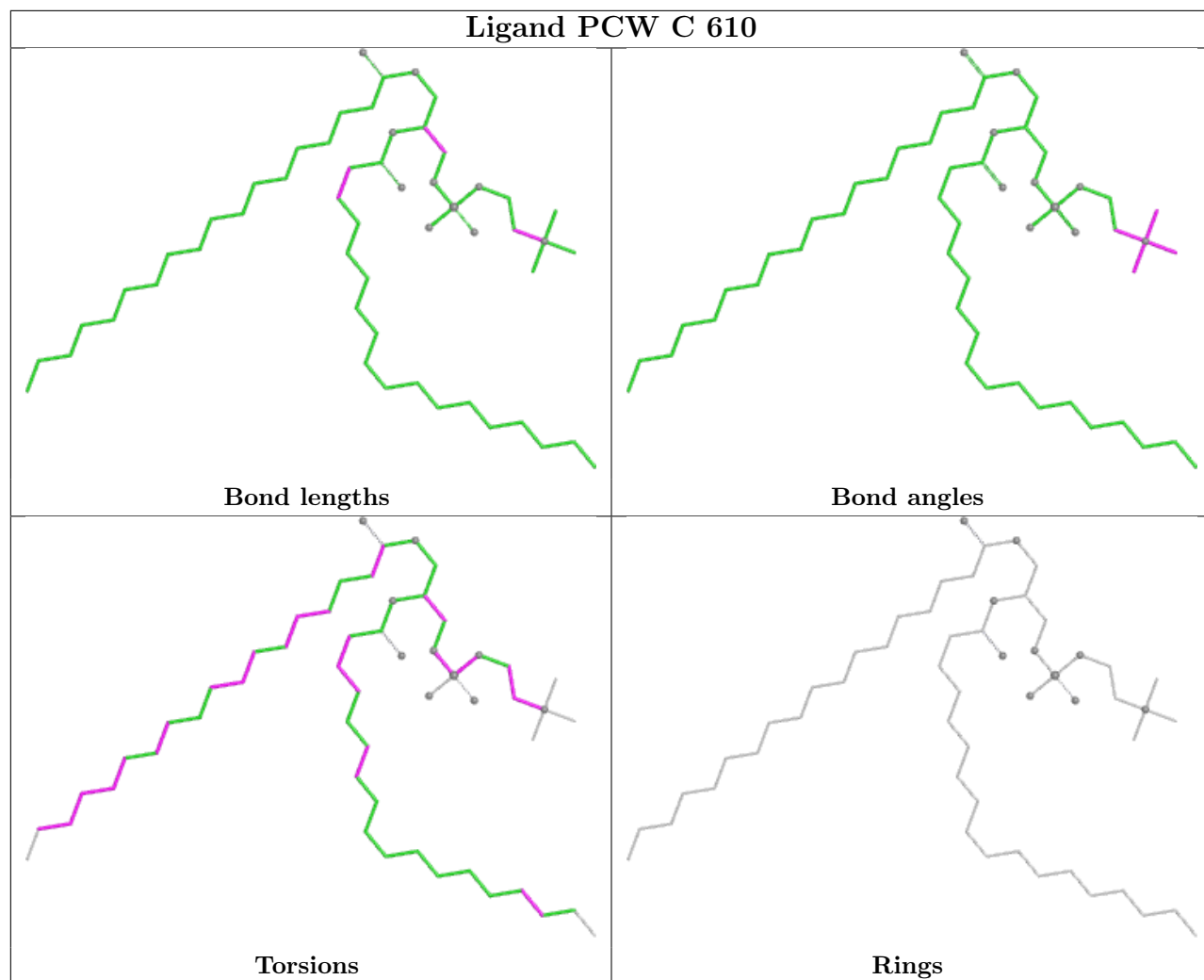


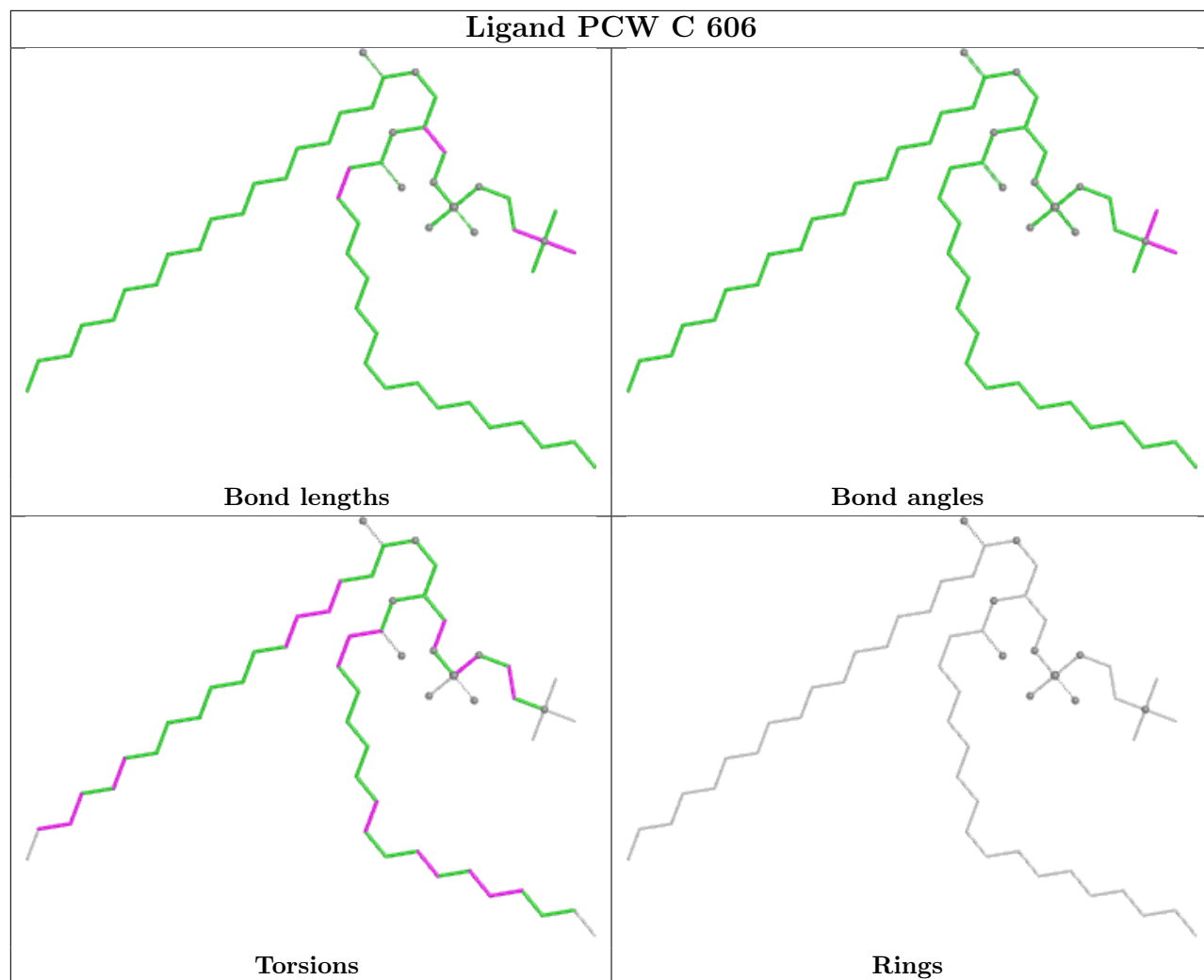


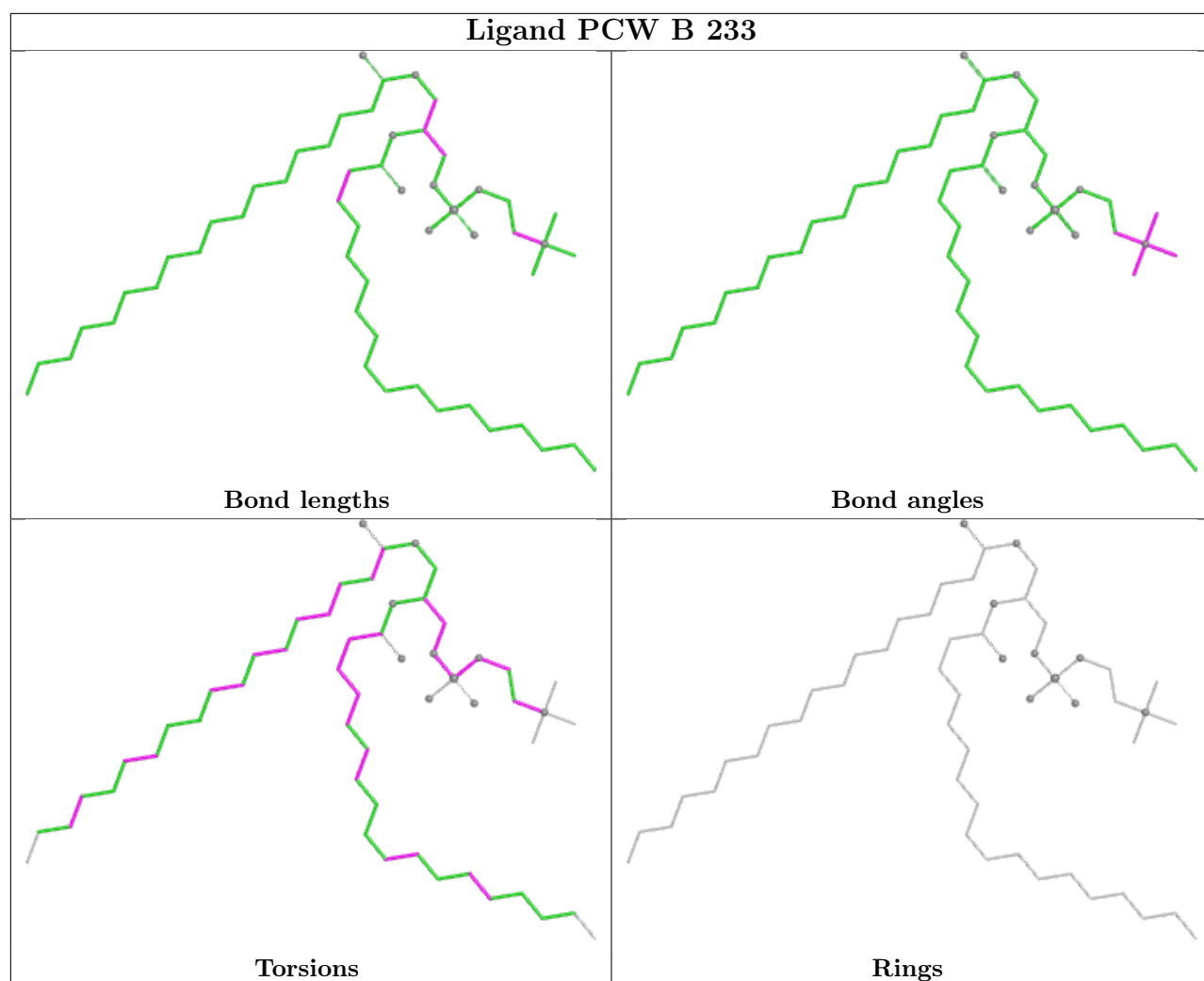


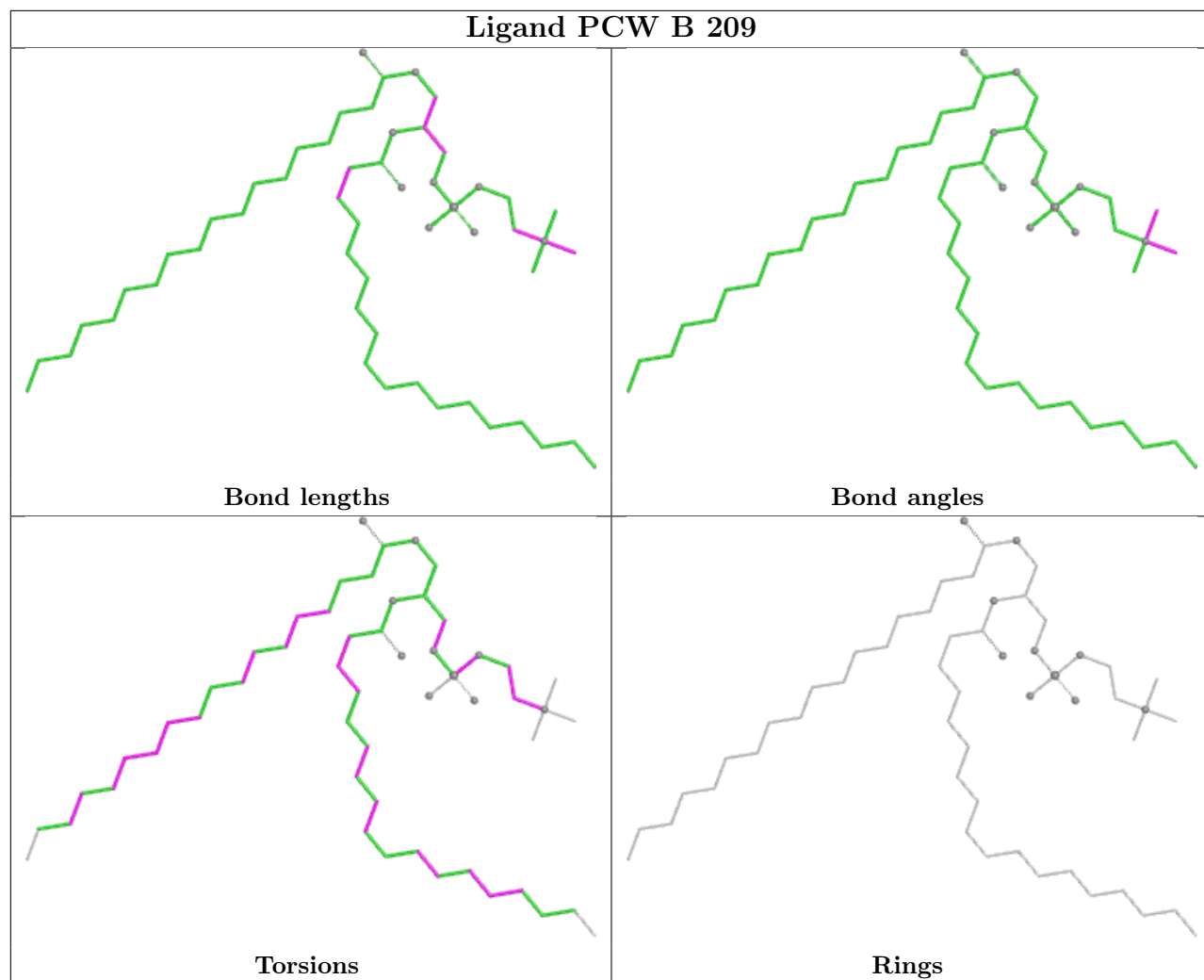


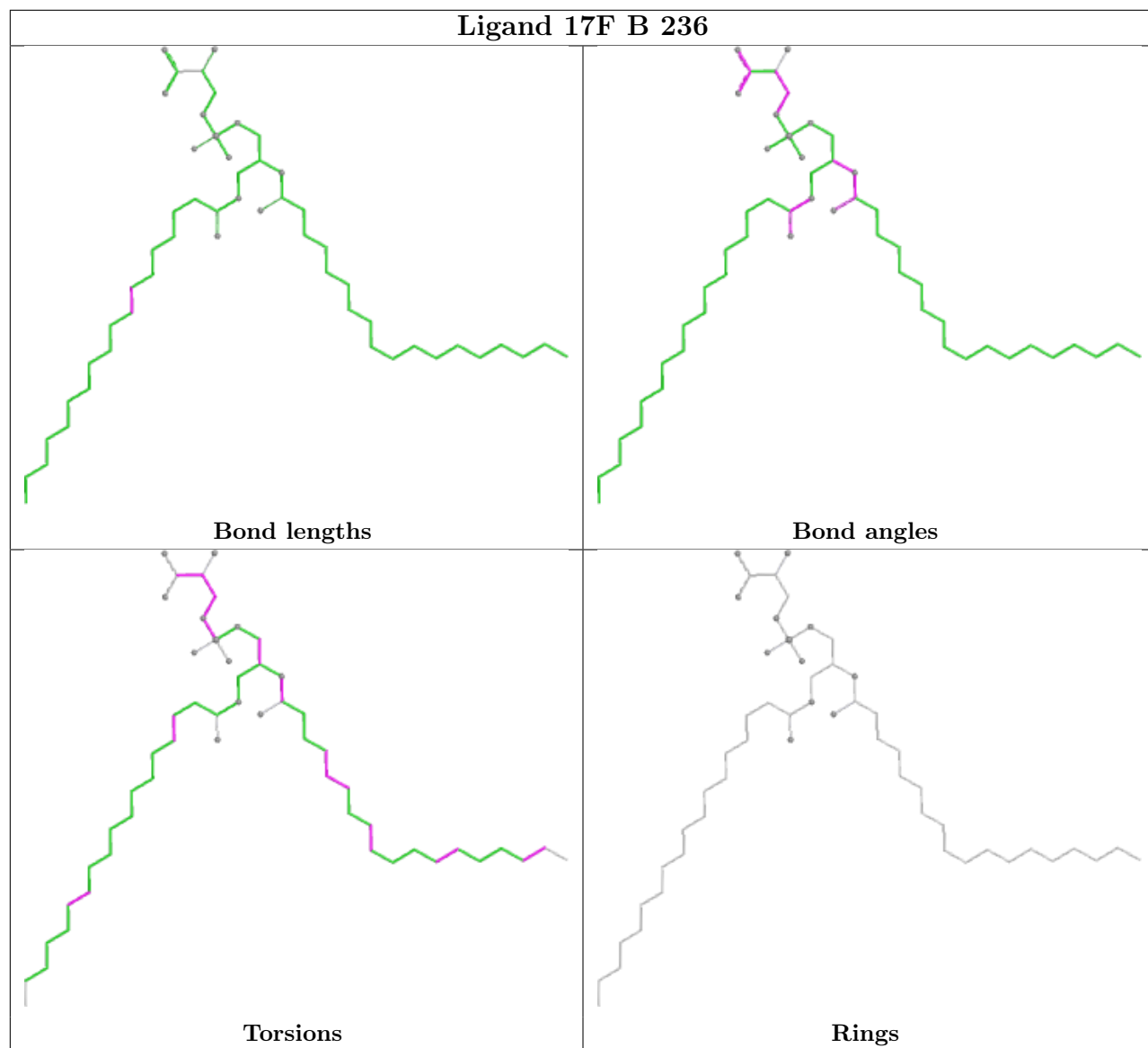


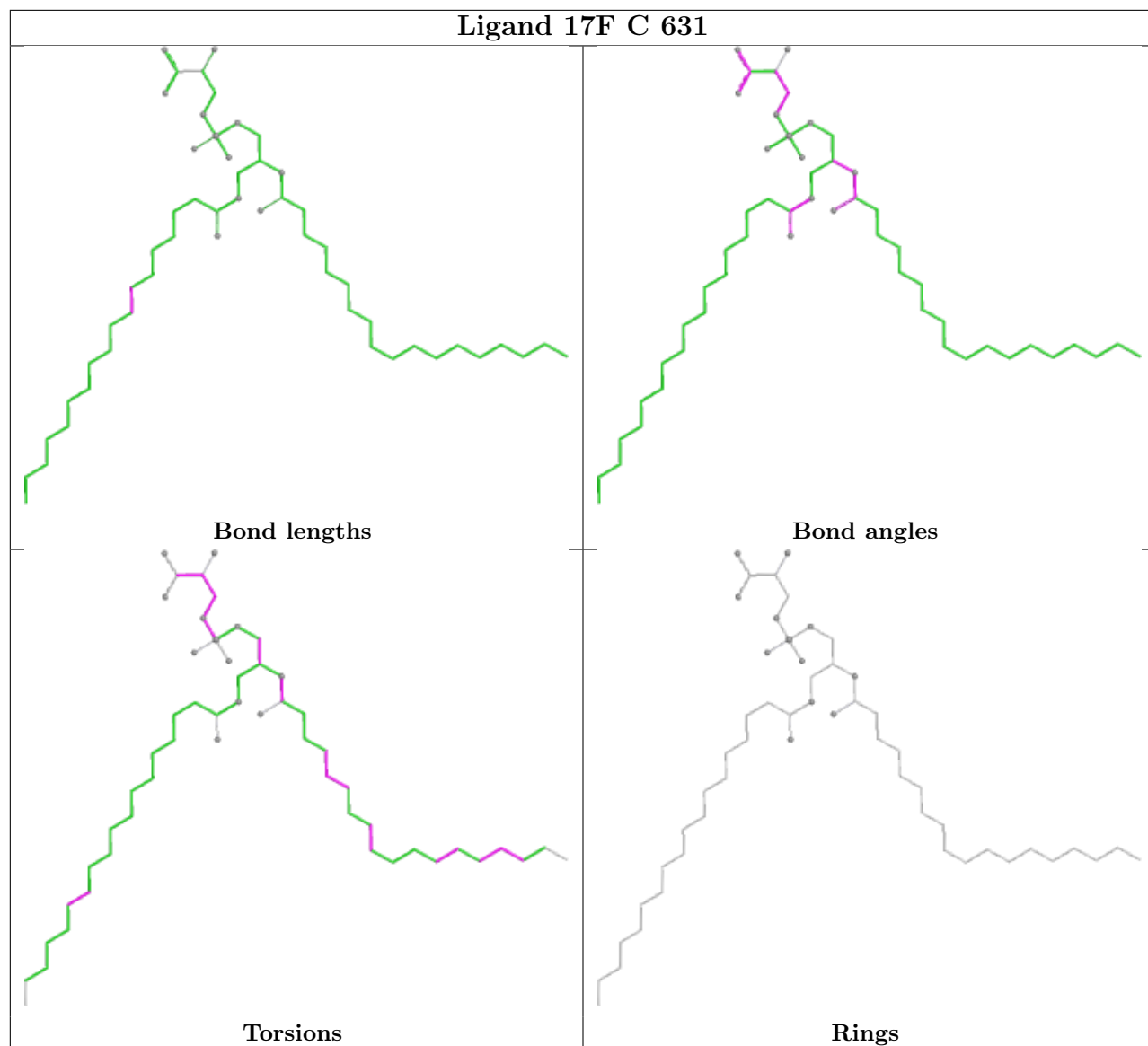


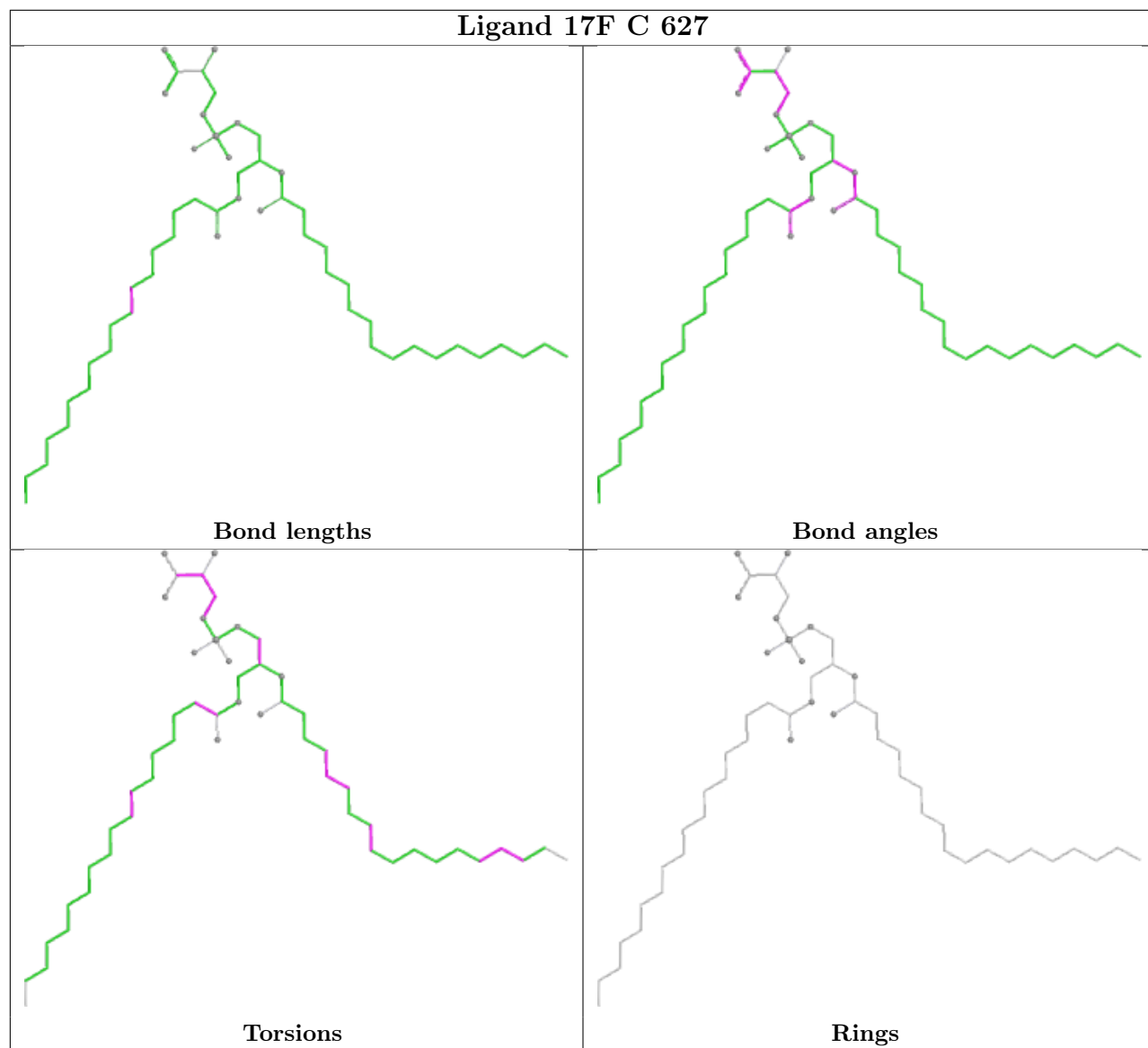


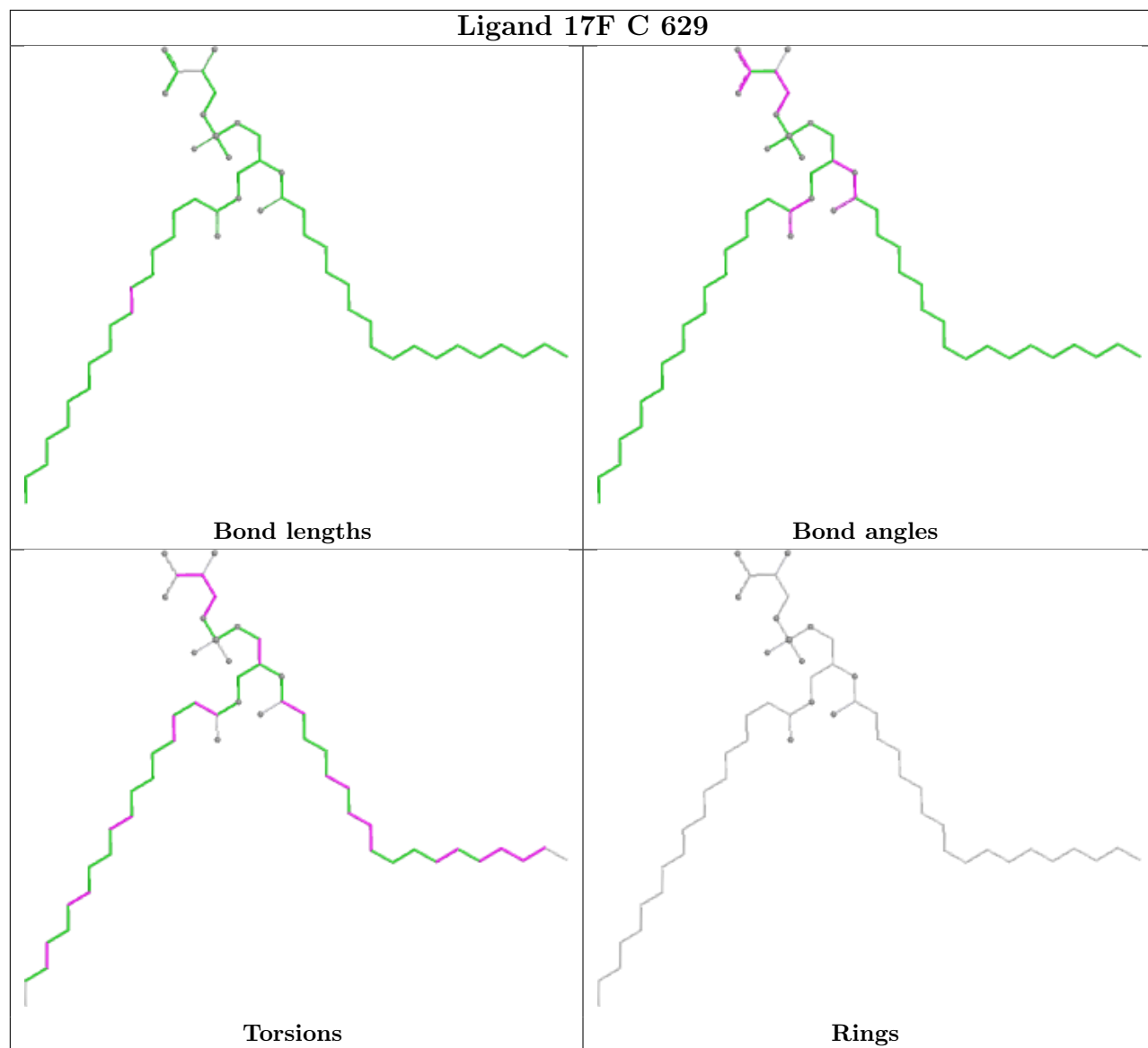


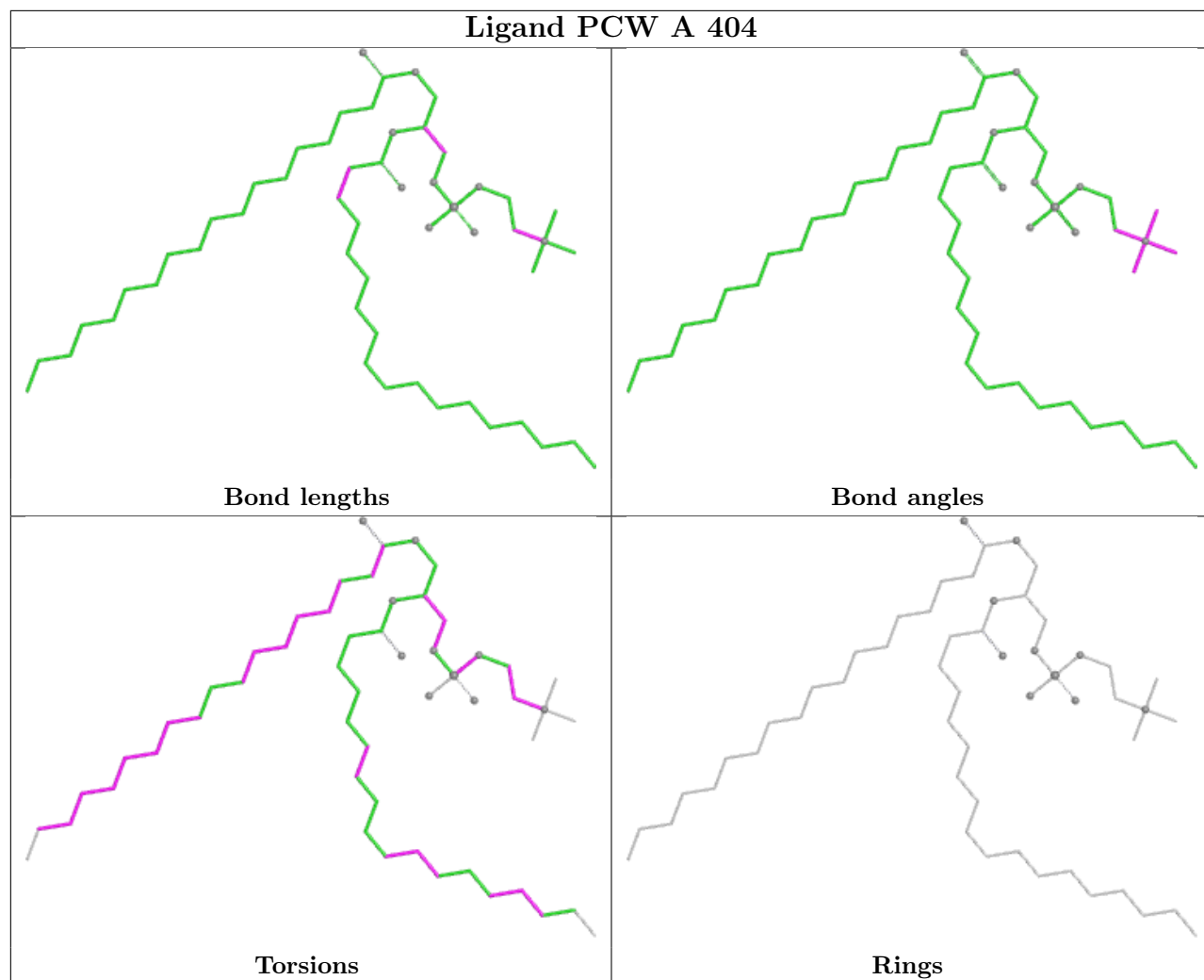


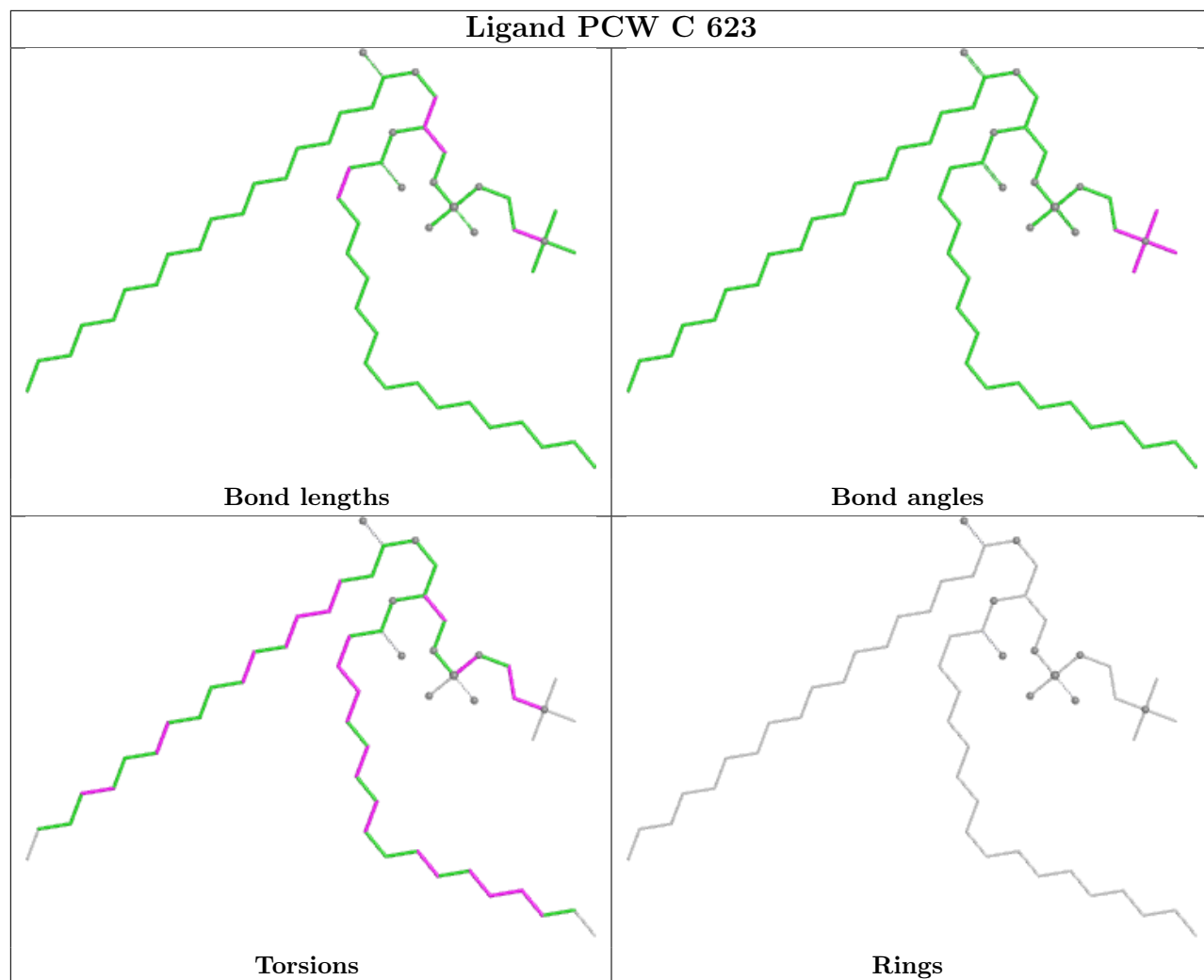




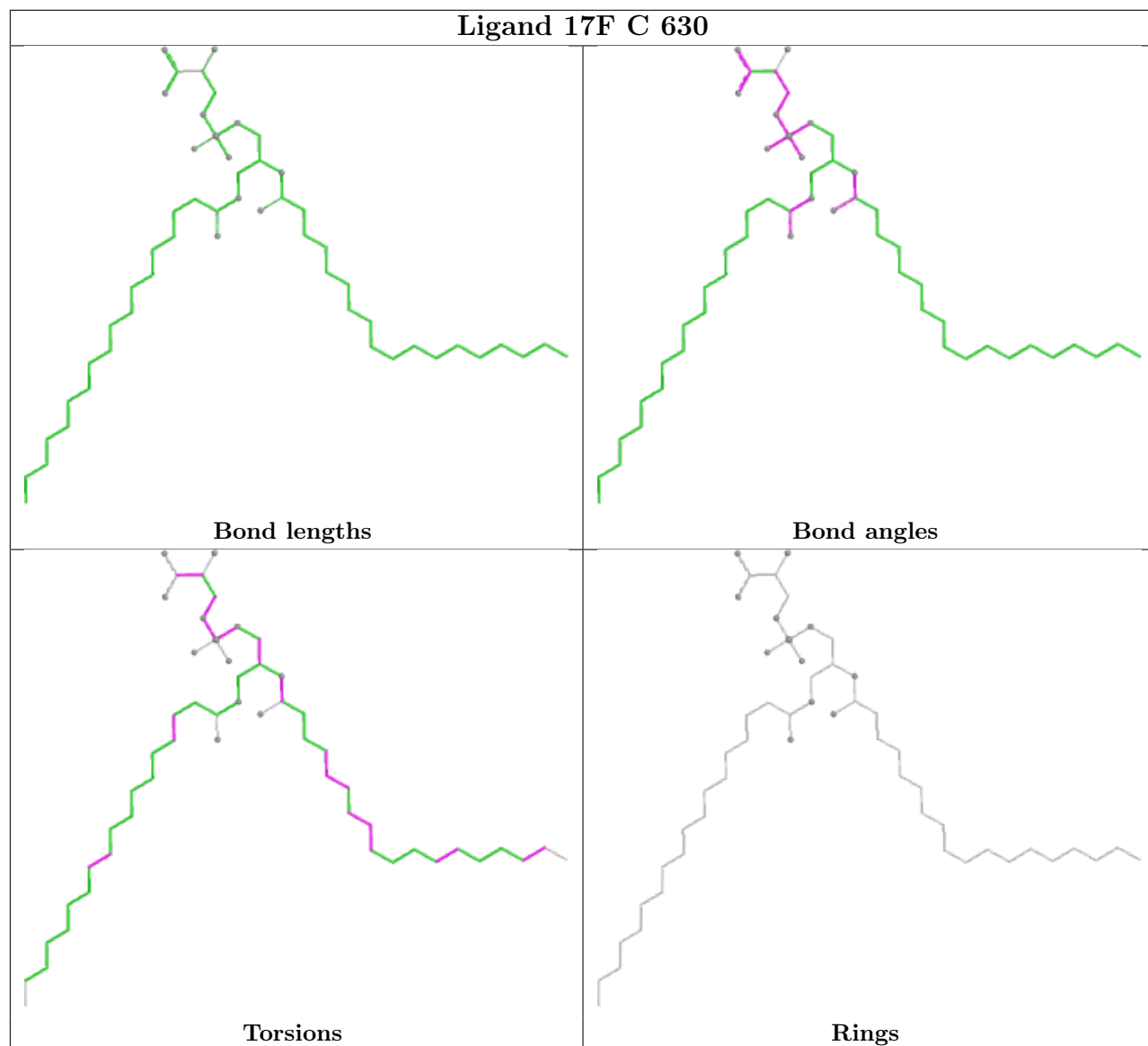


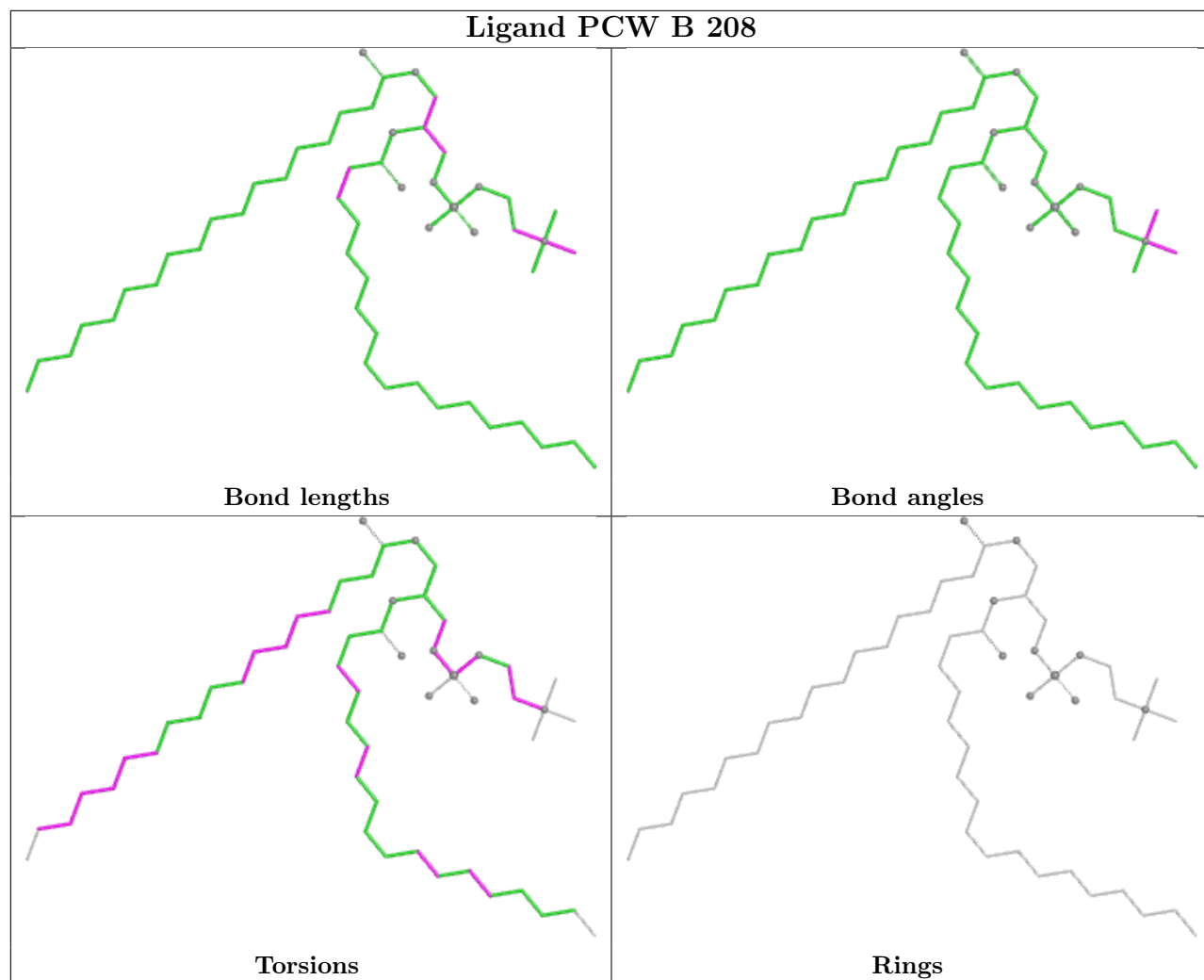


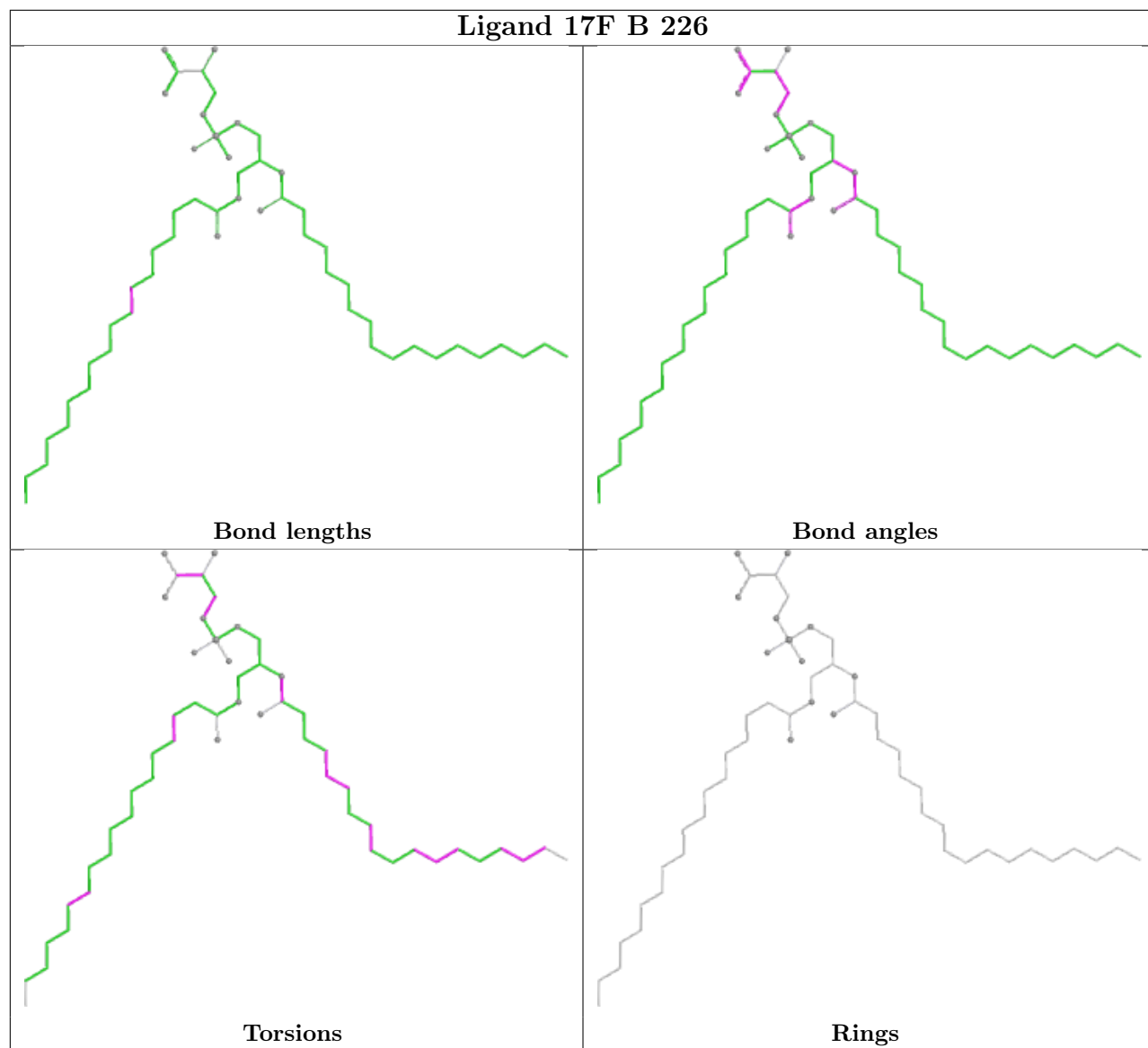


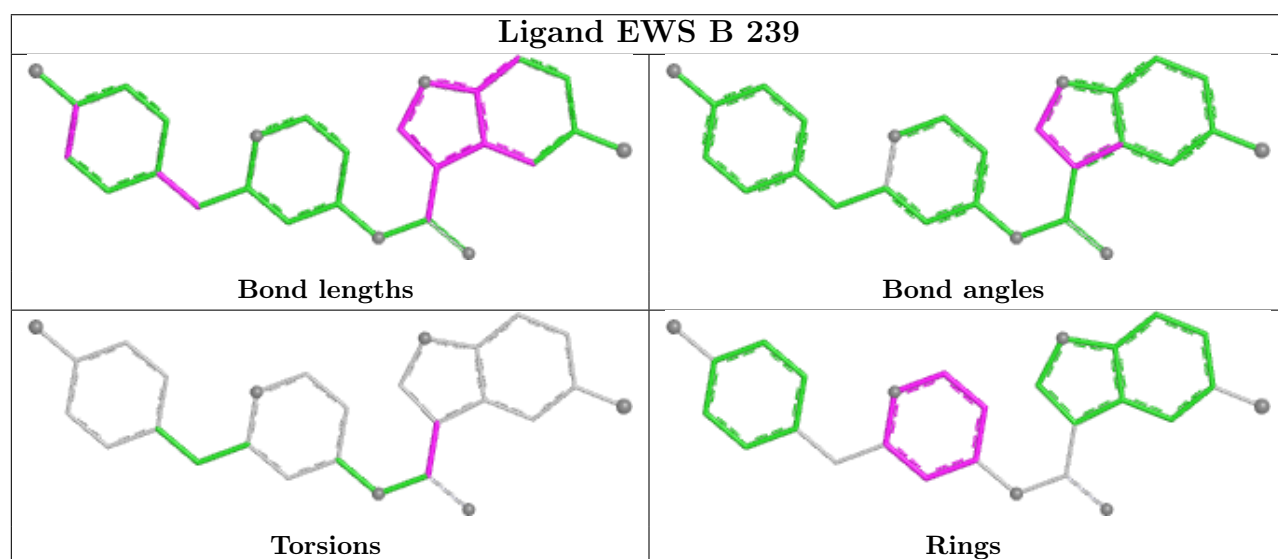
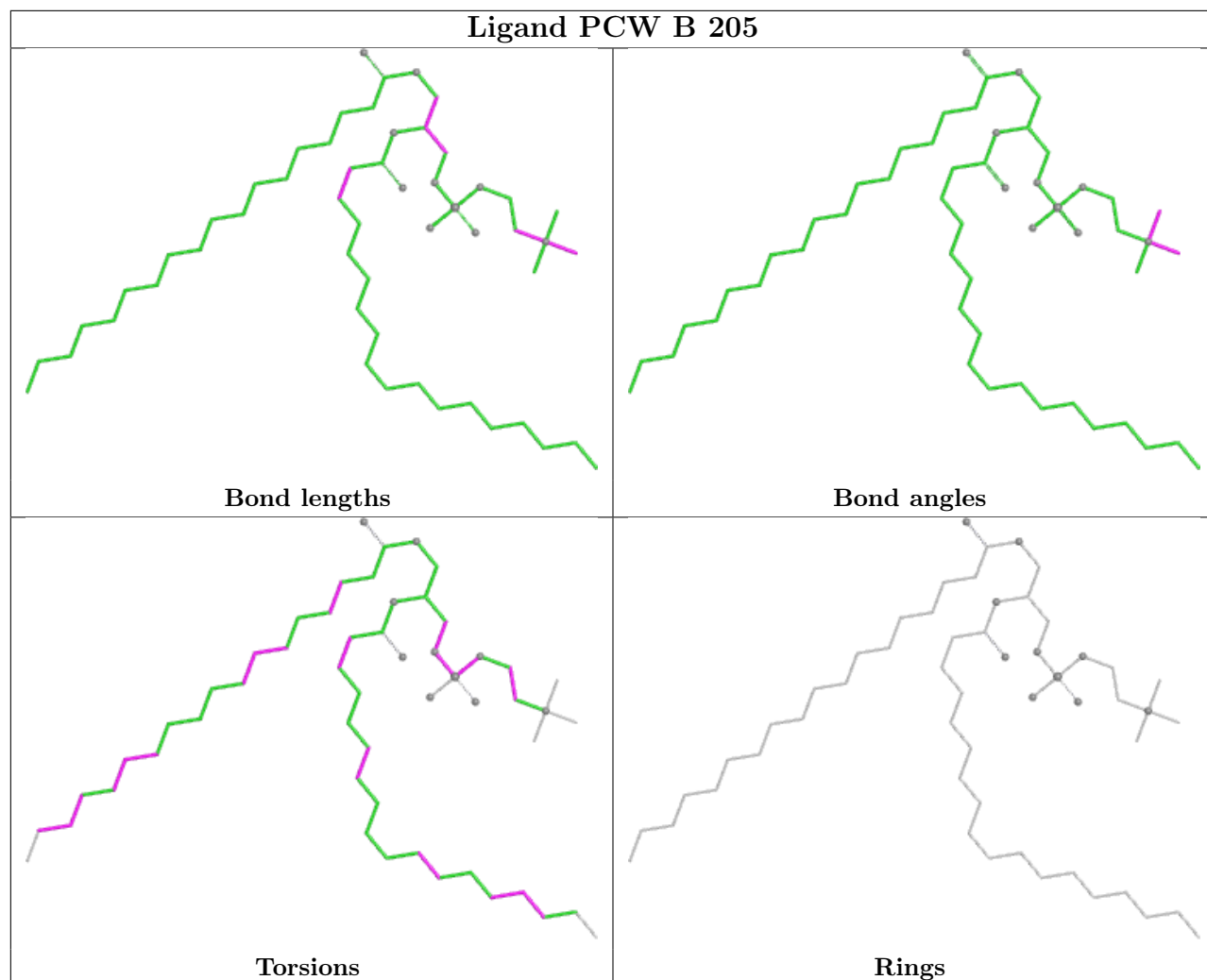


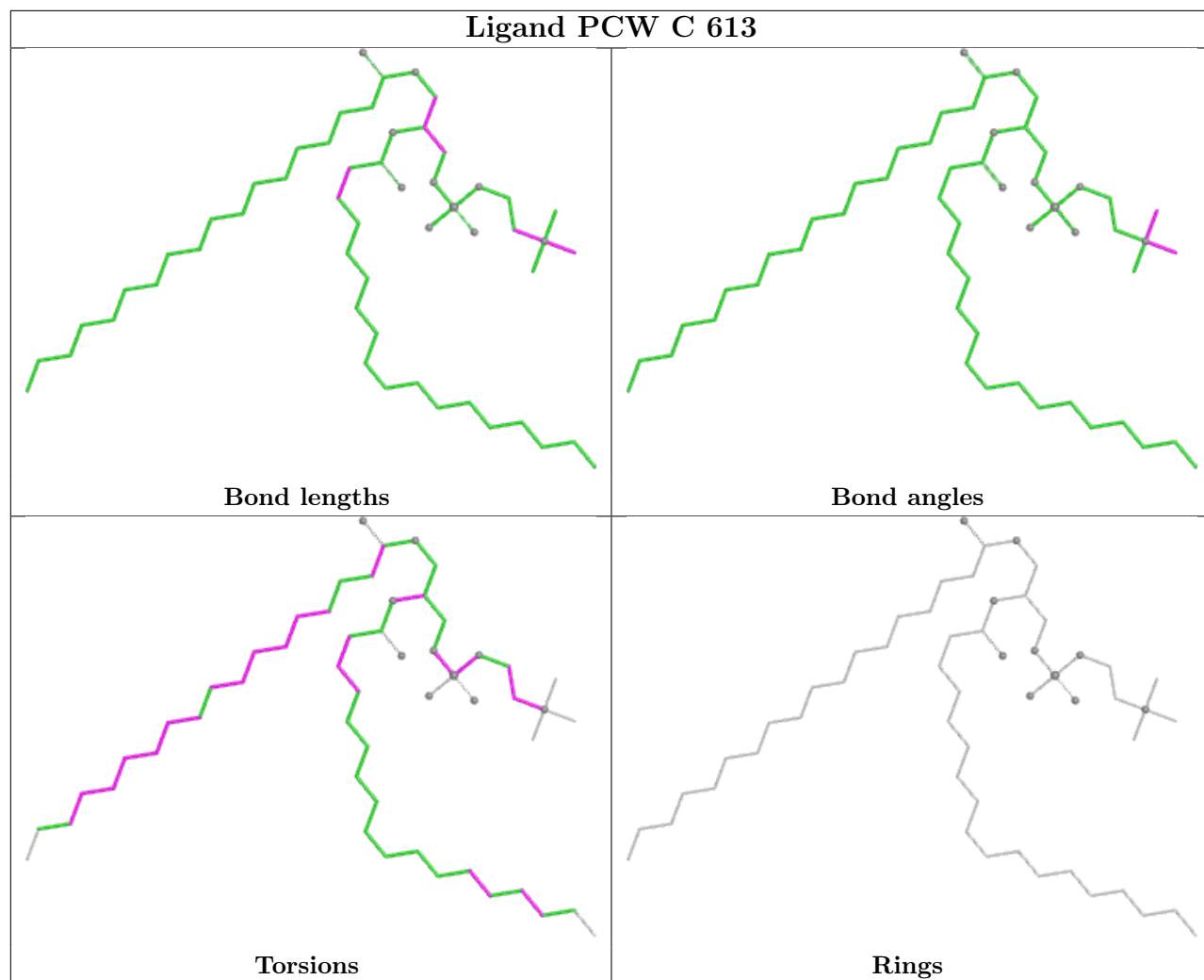
Ligand 17F C 630

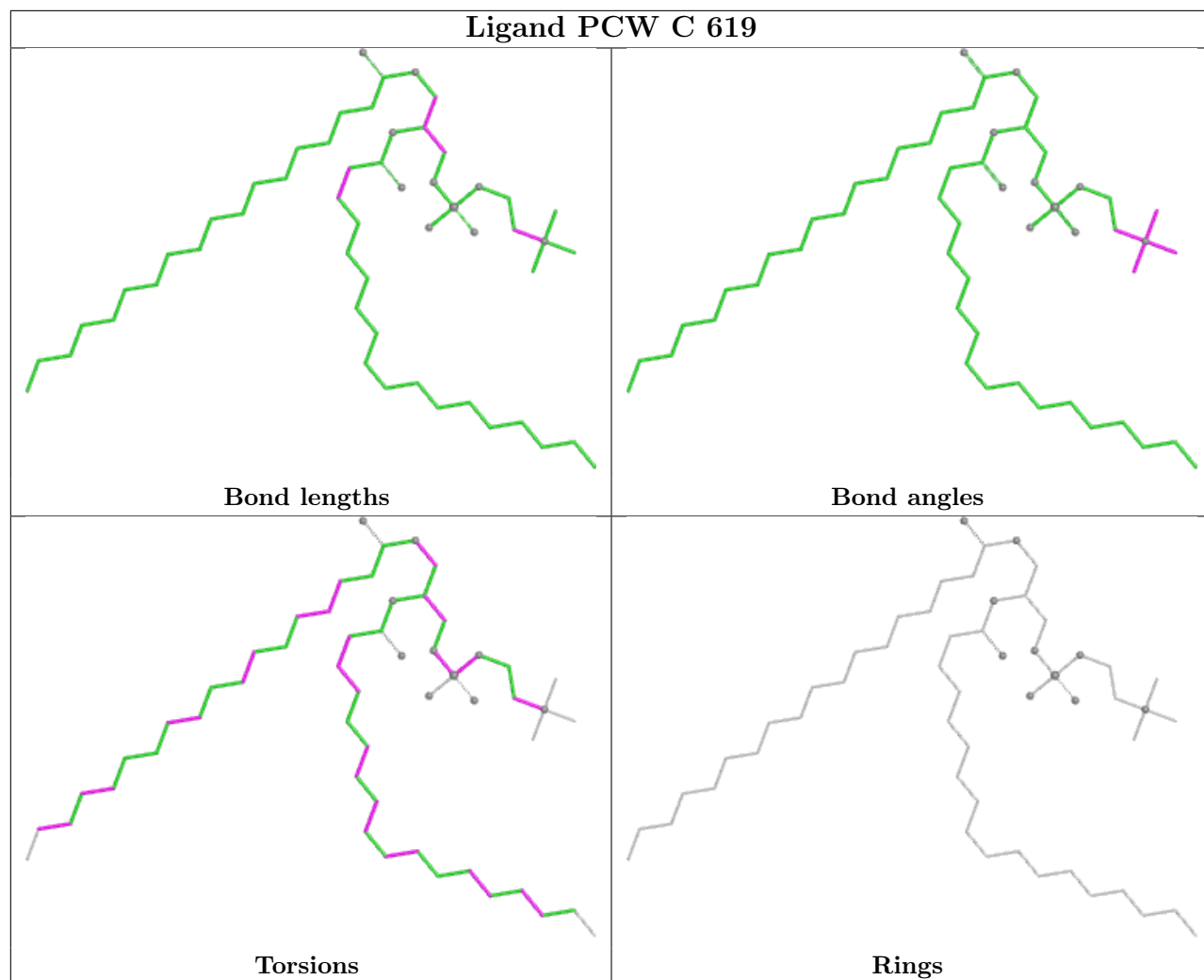


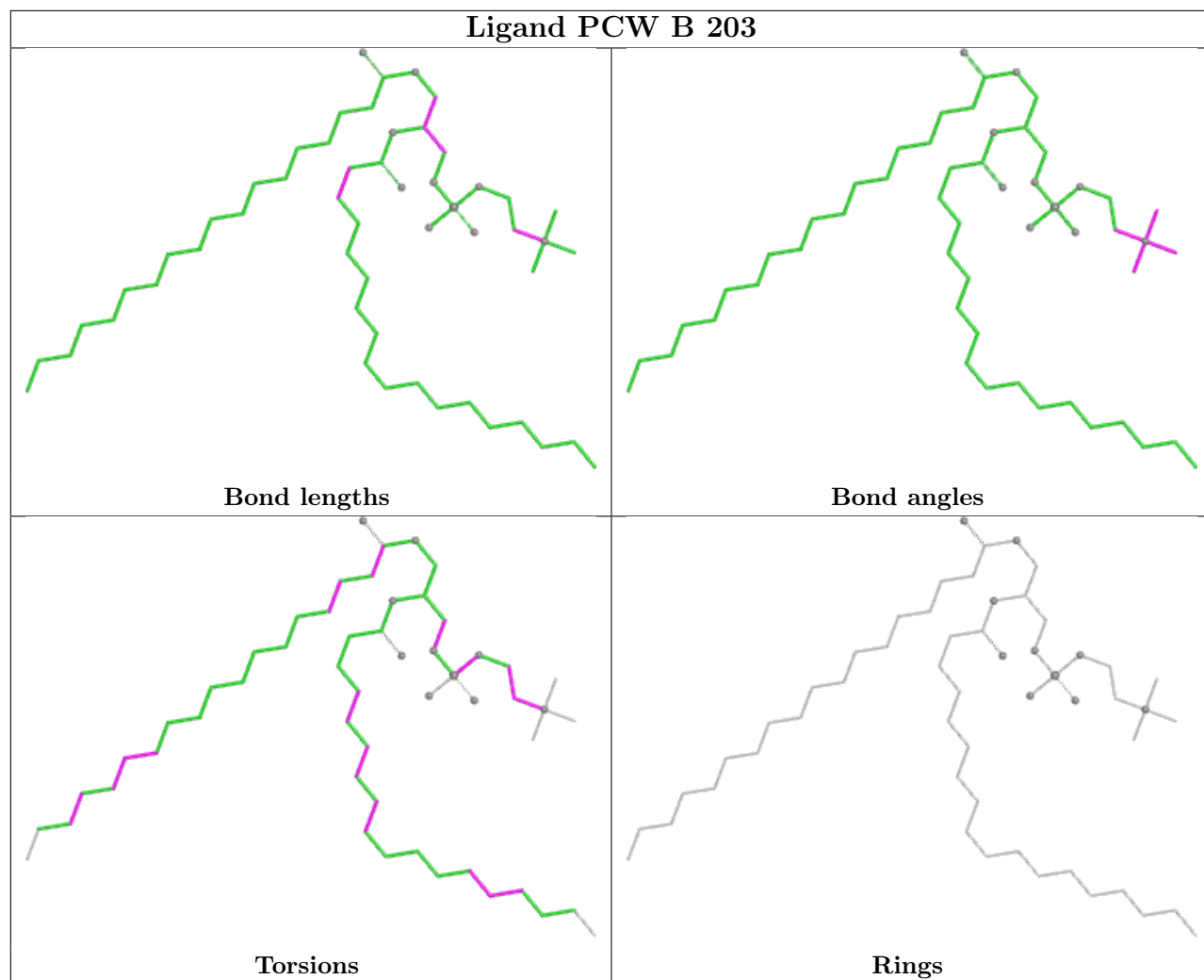


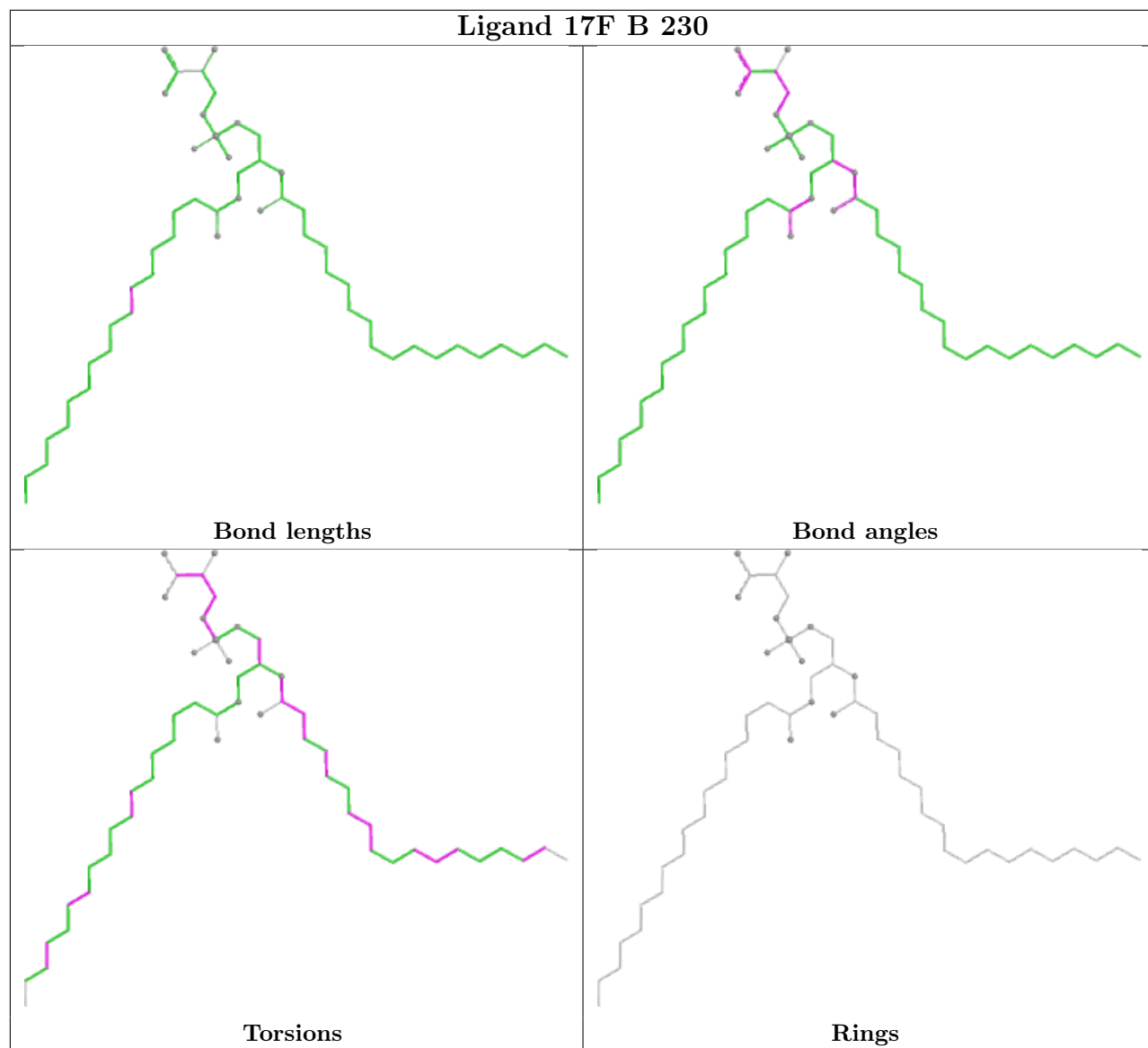


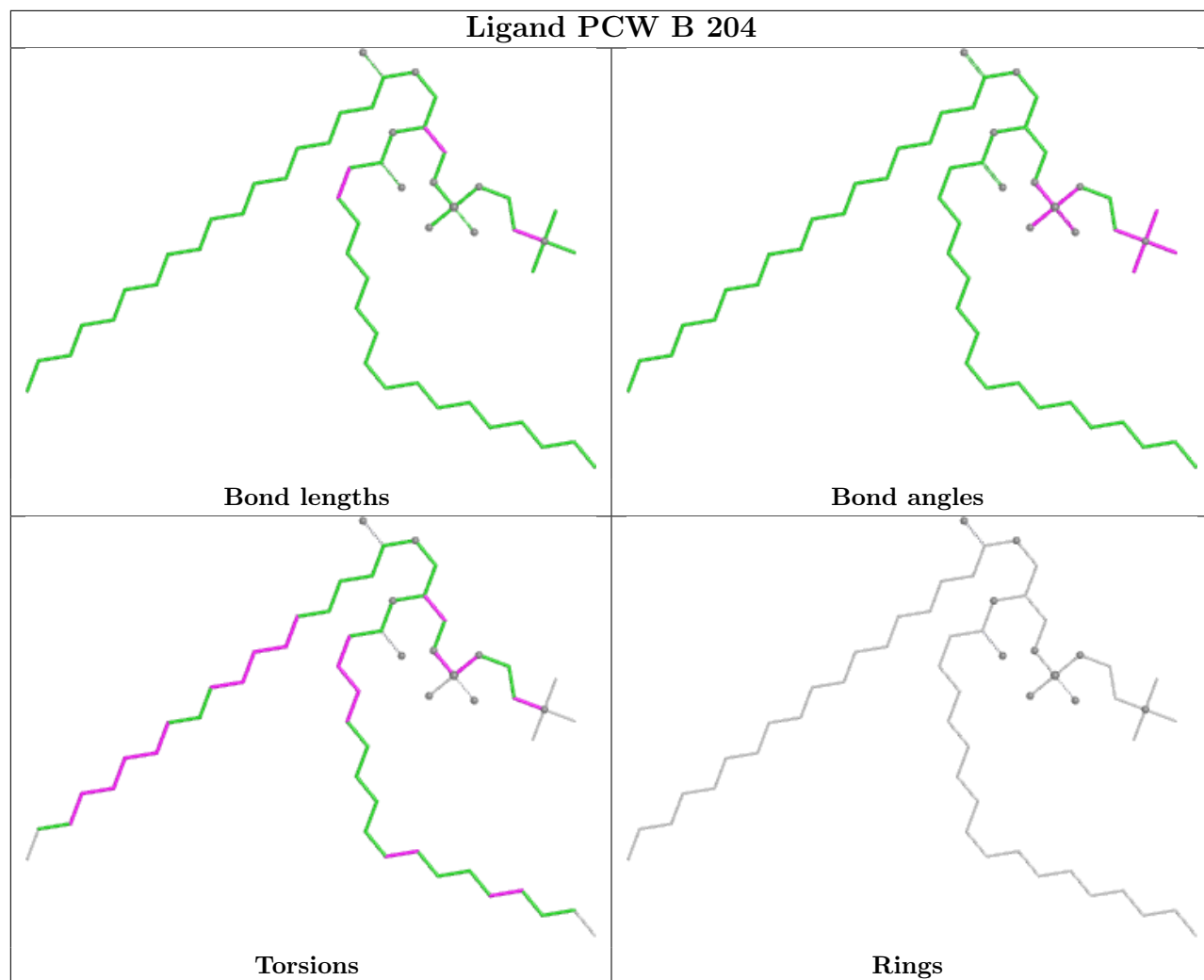


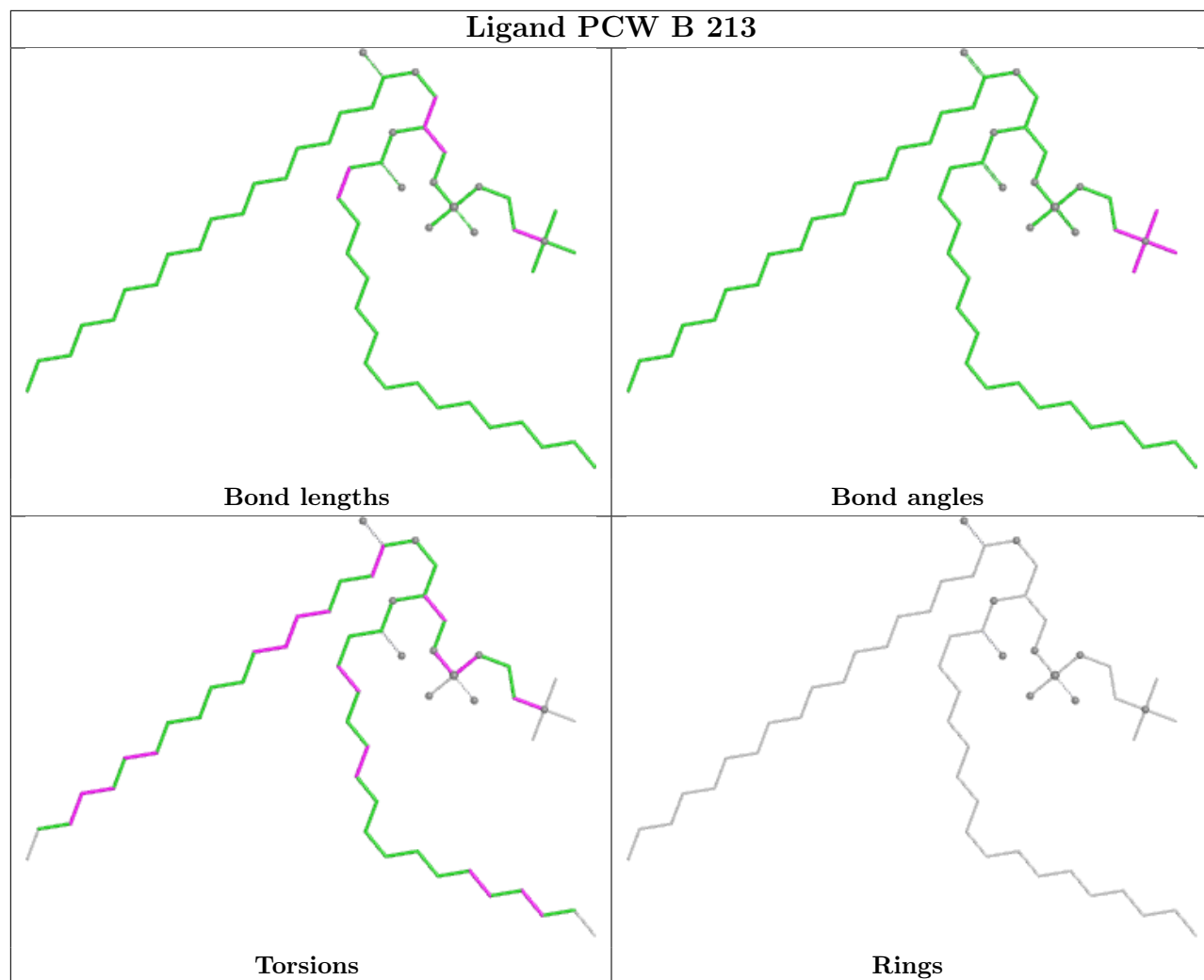


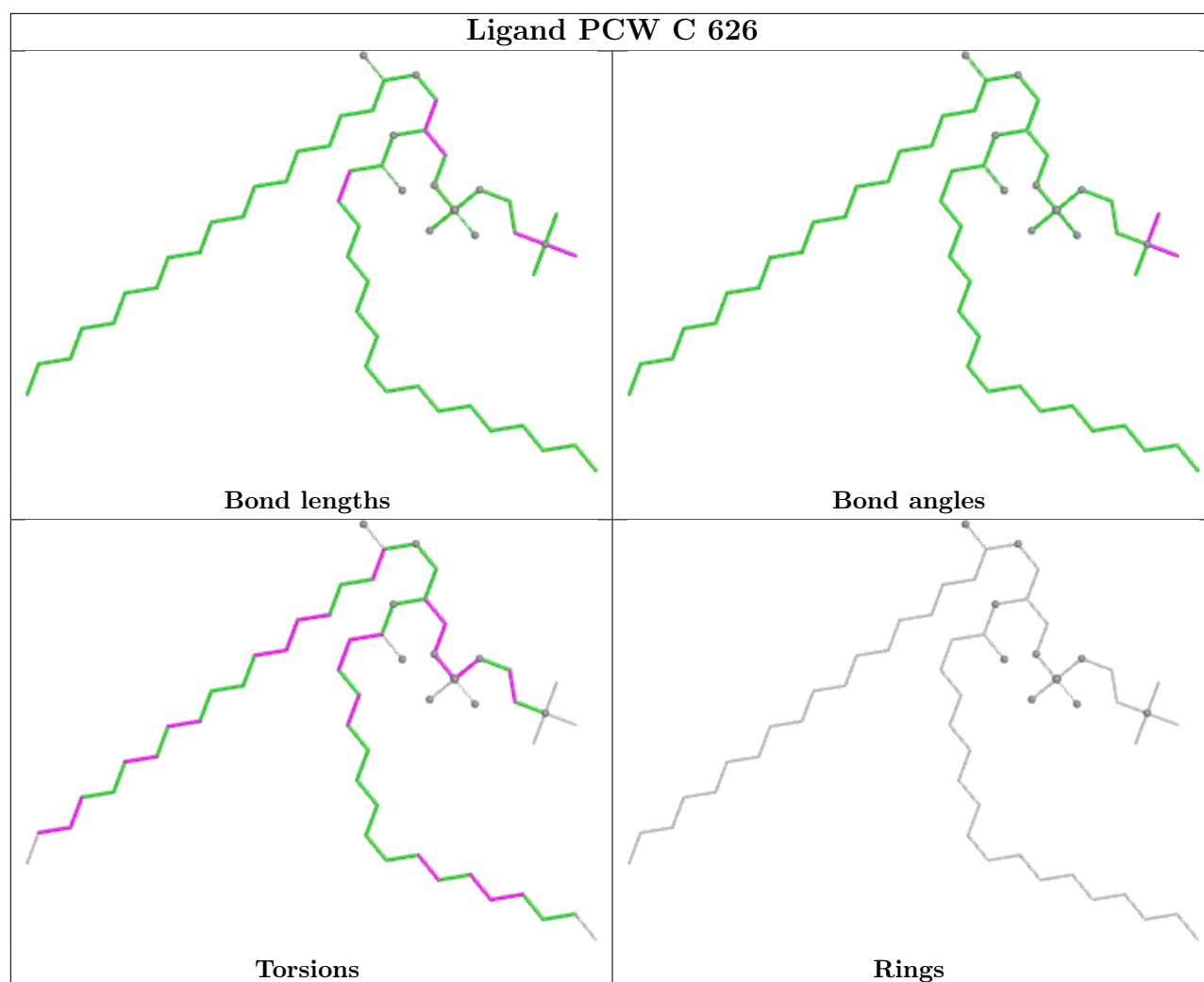


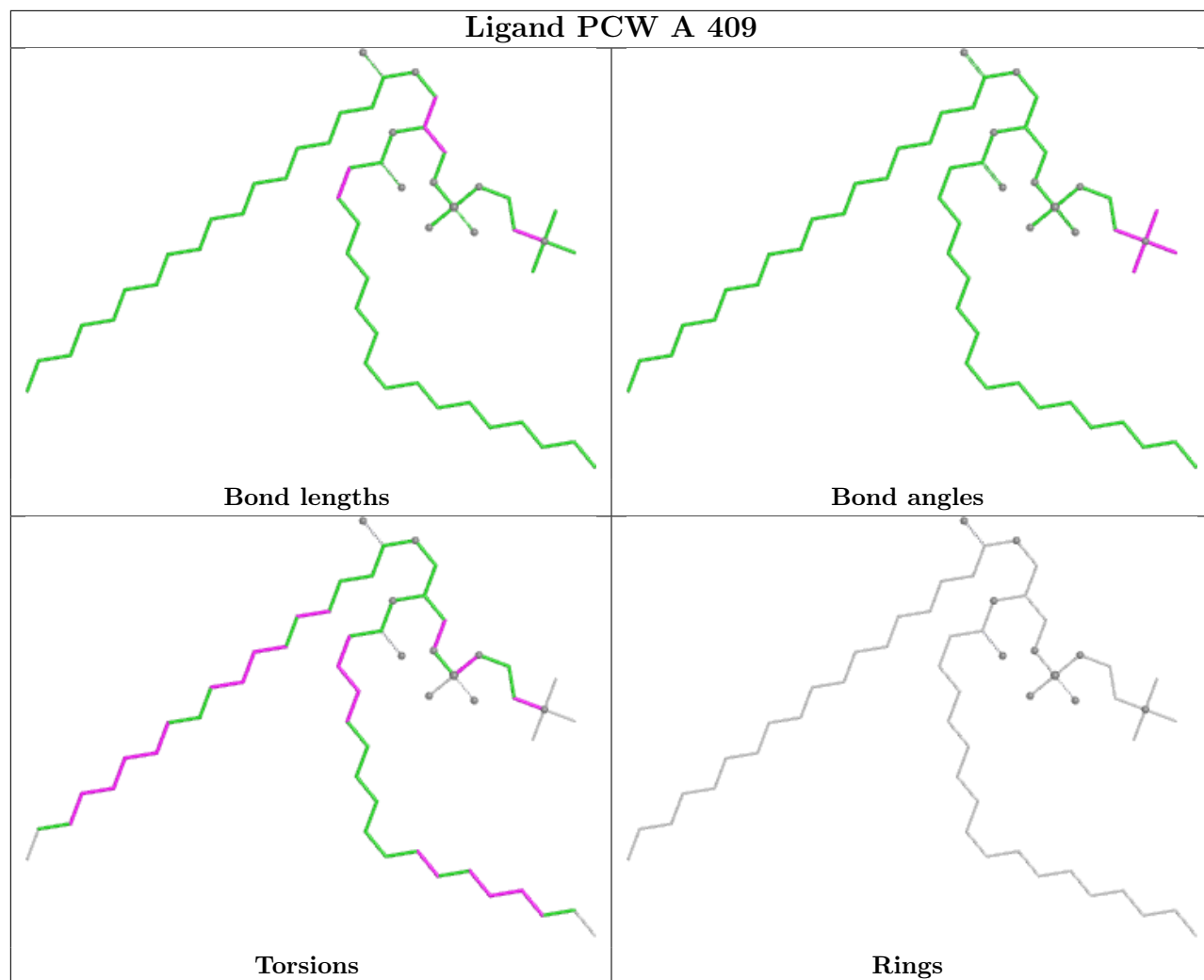


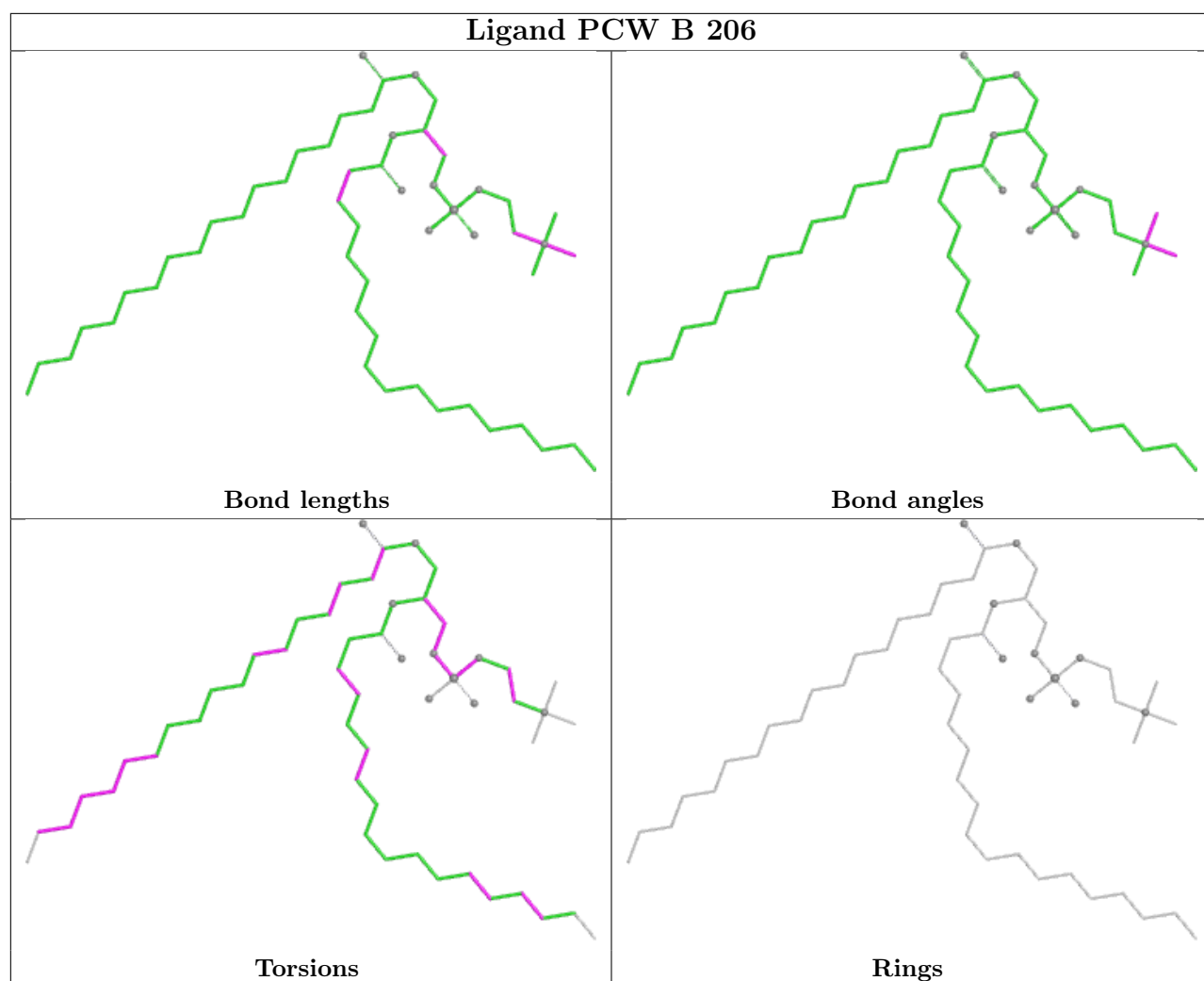


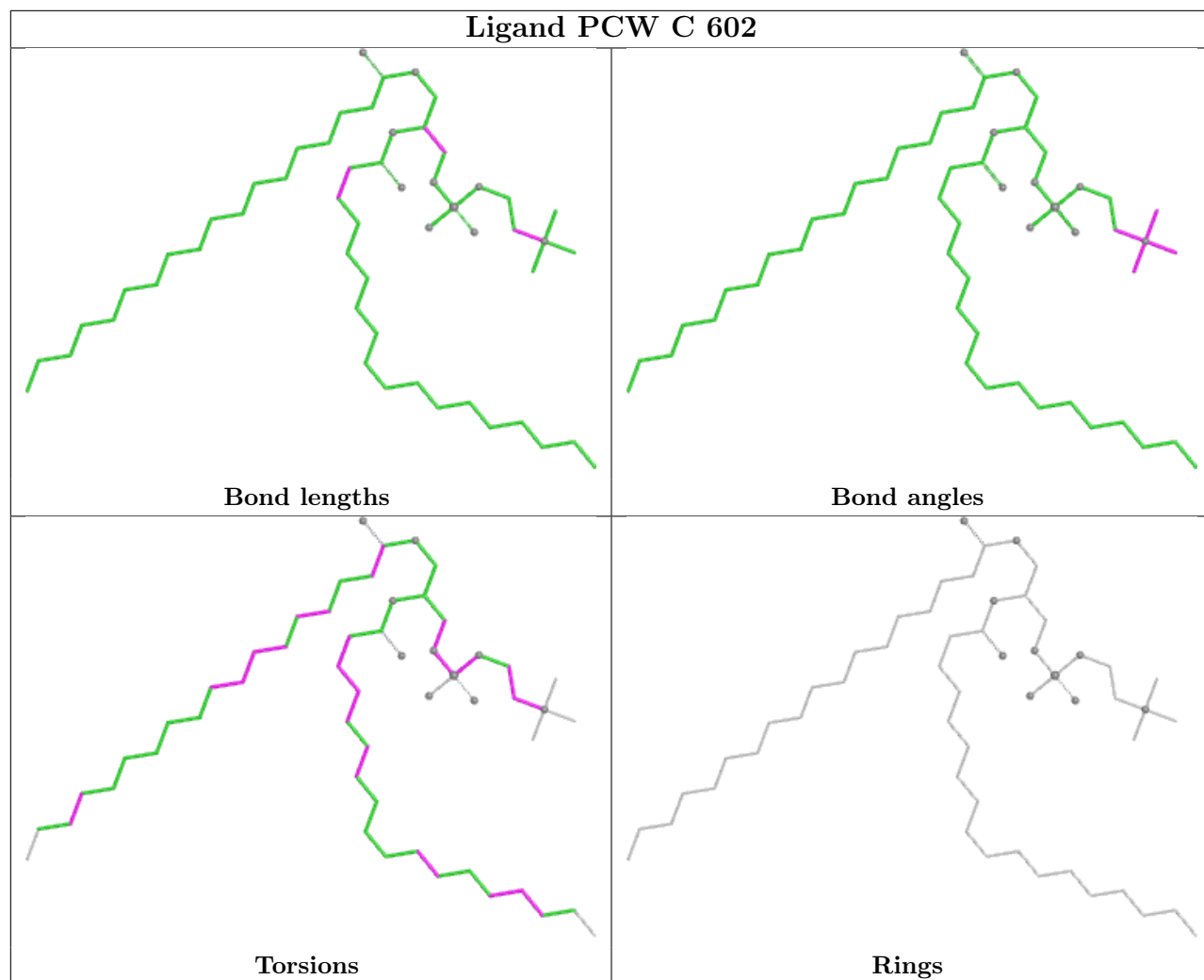


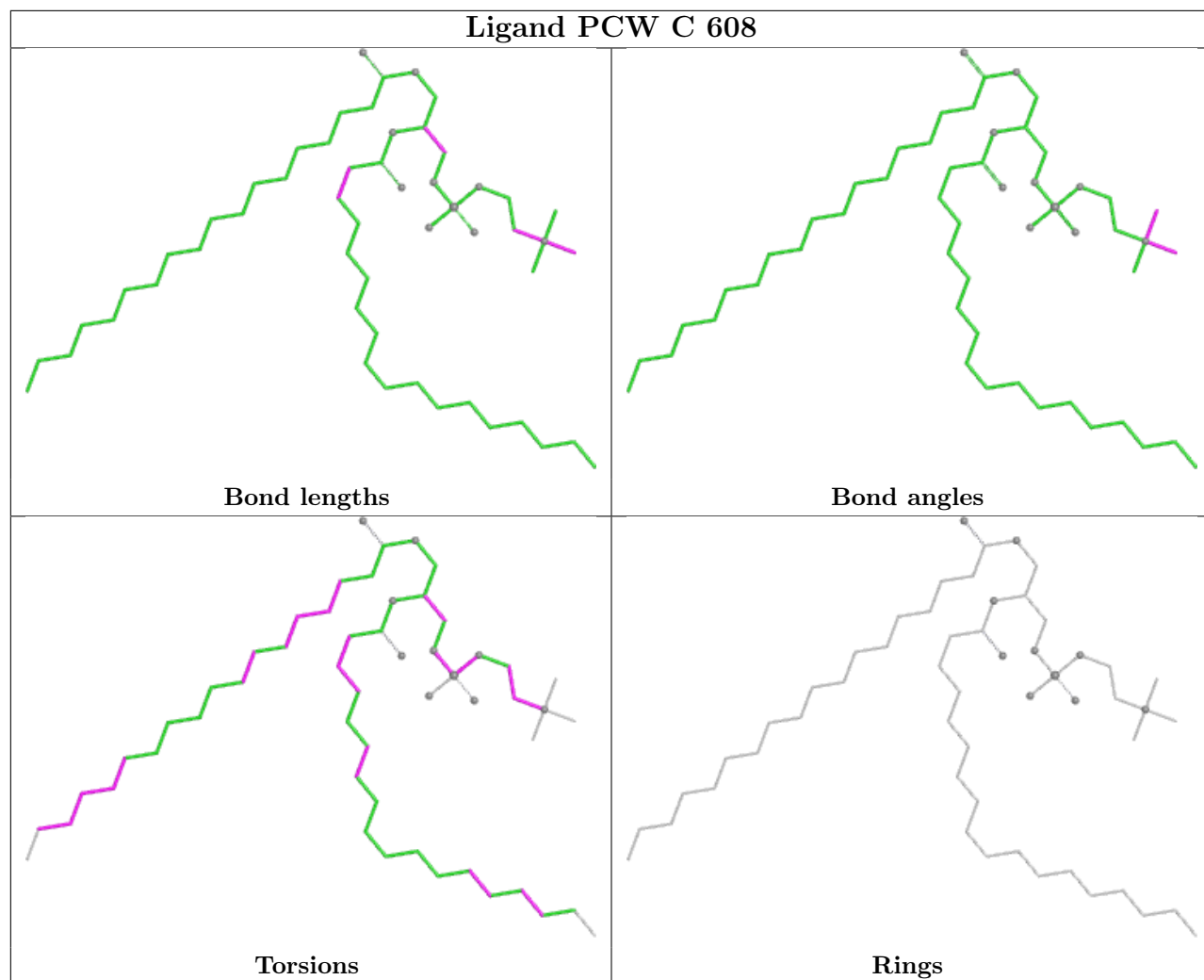


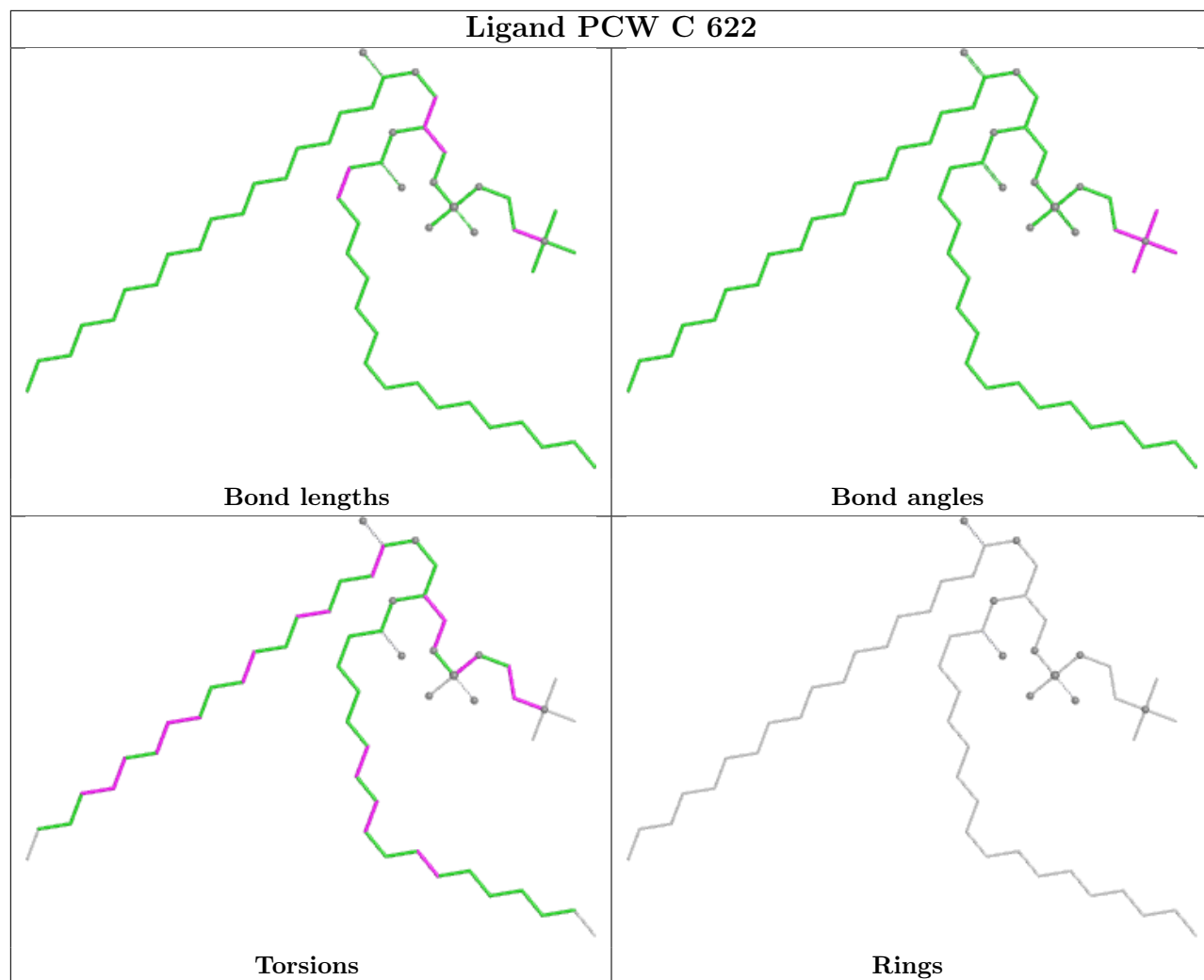


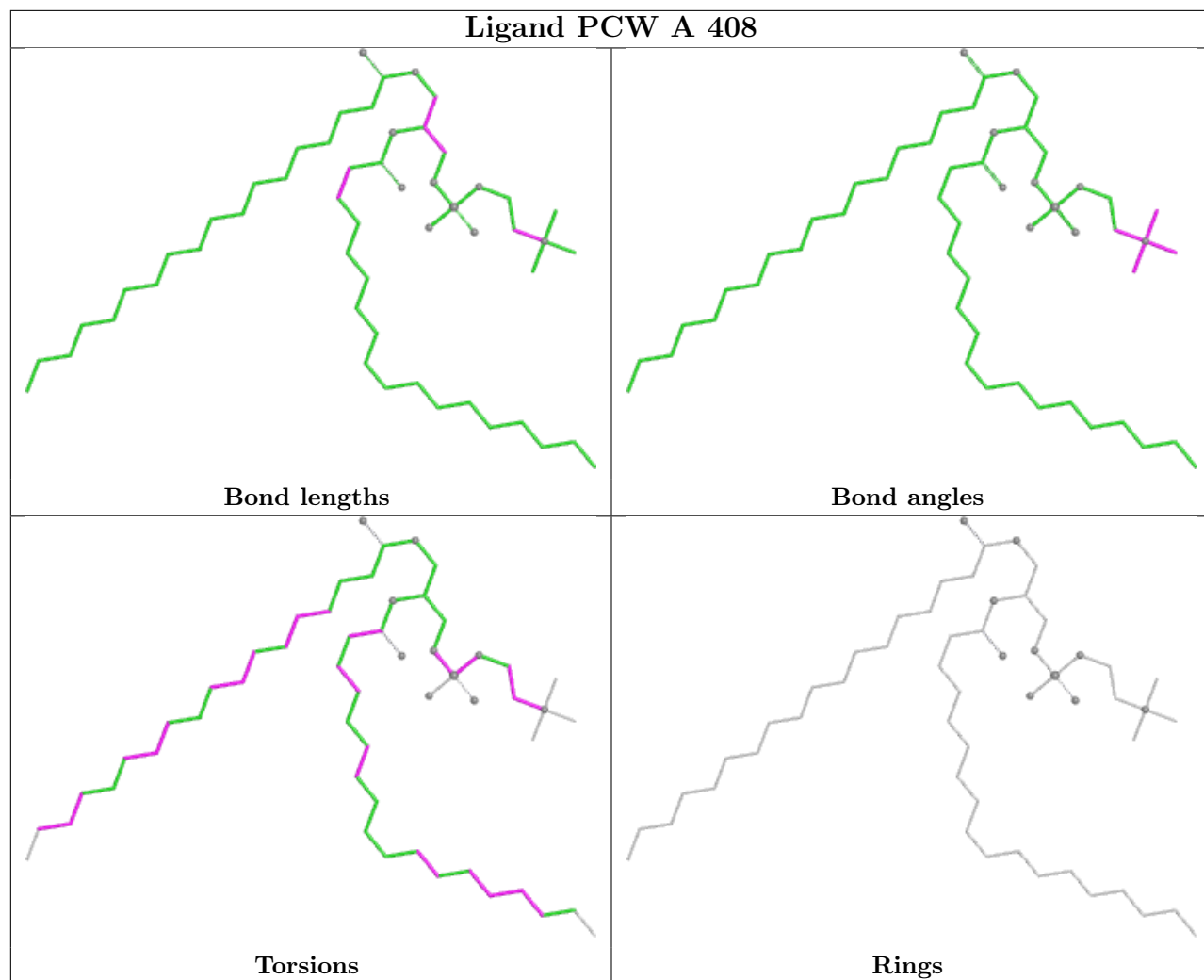


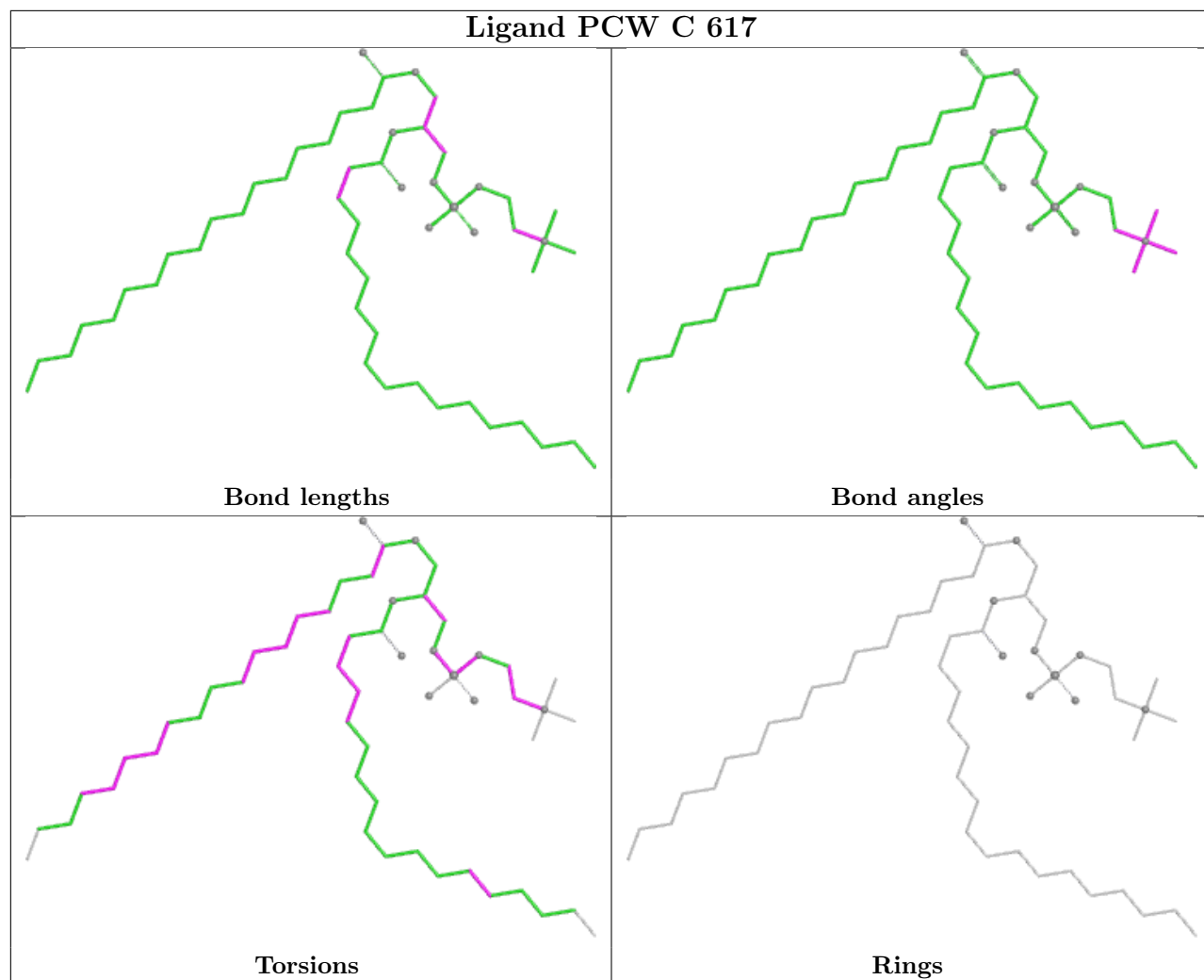


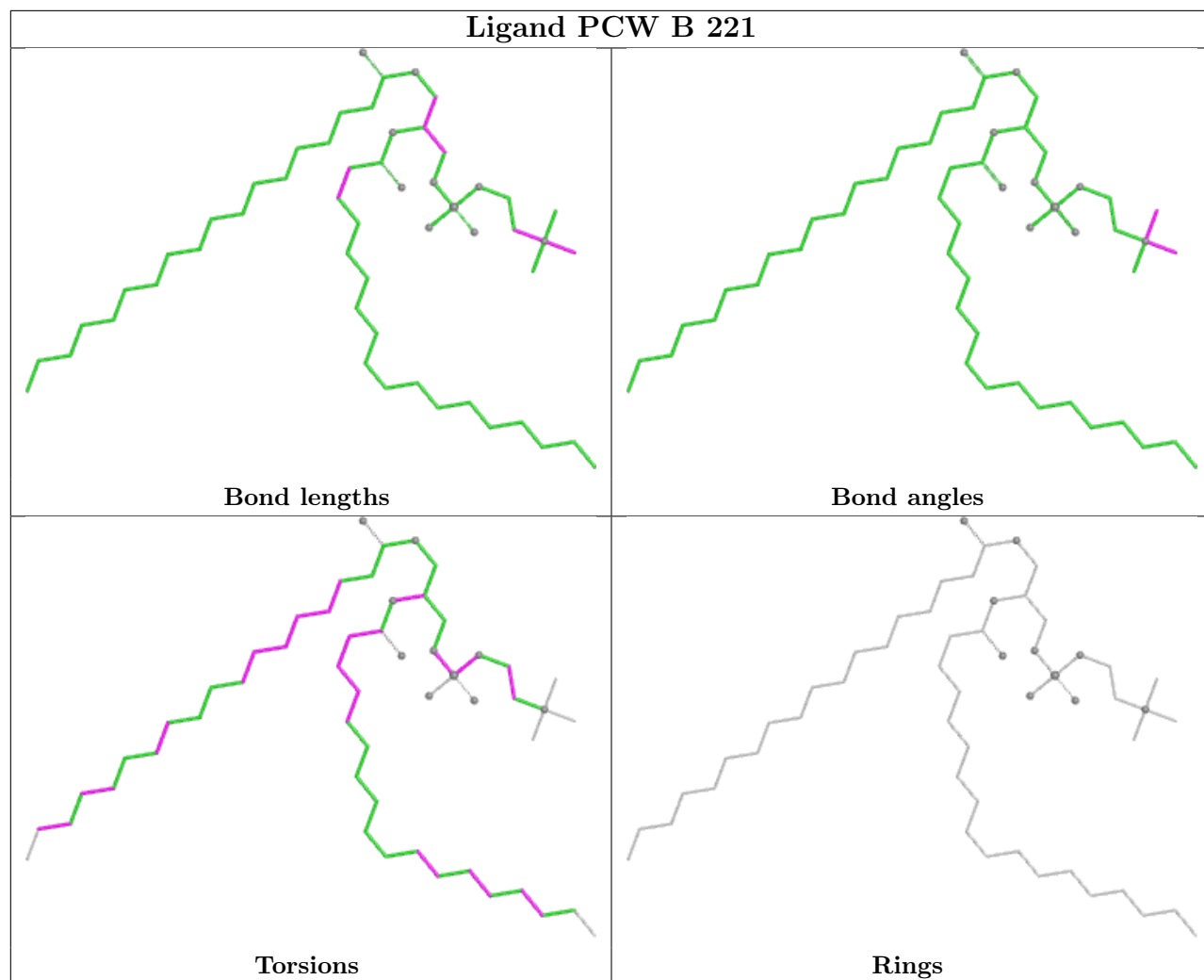


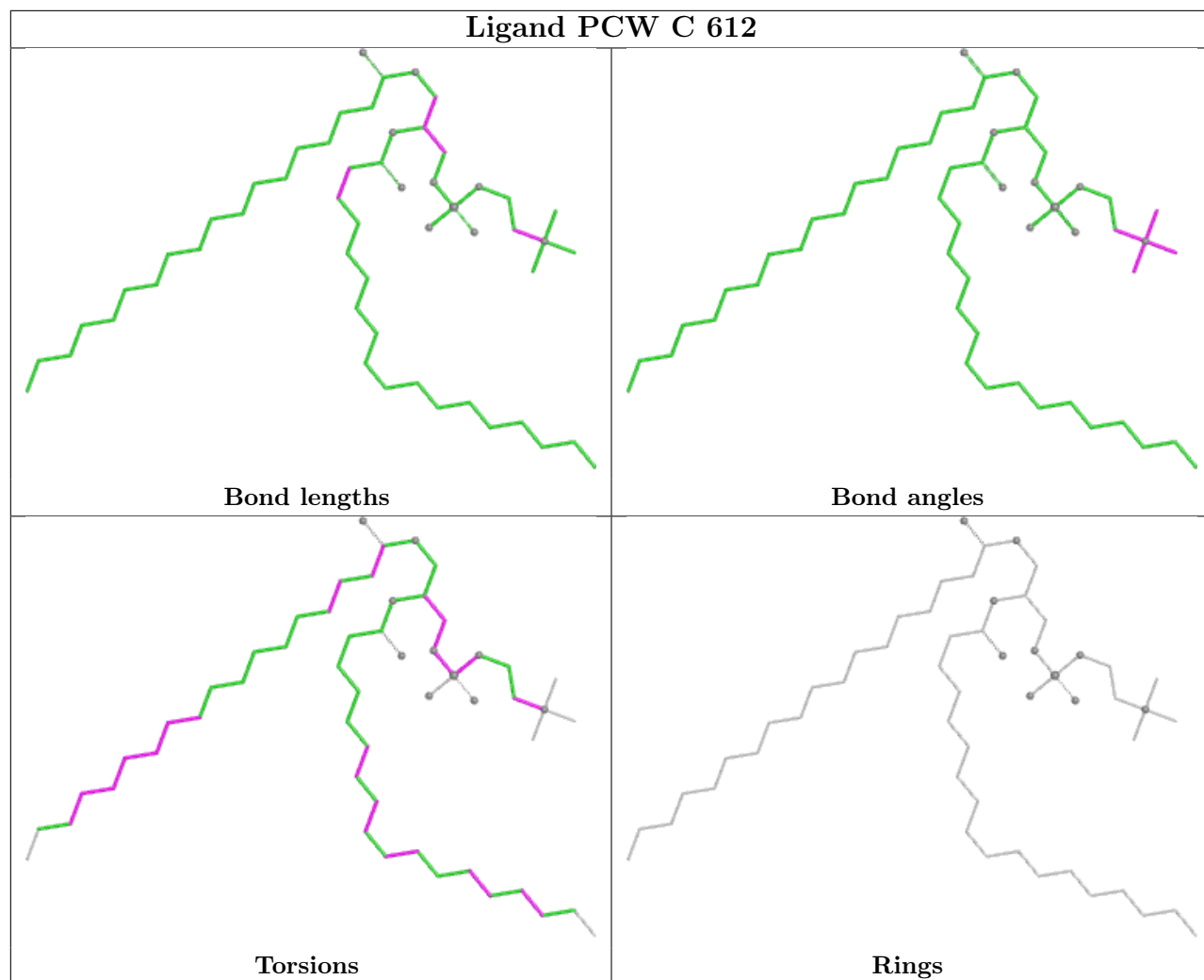


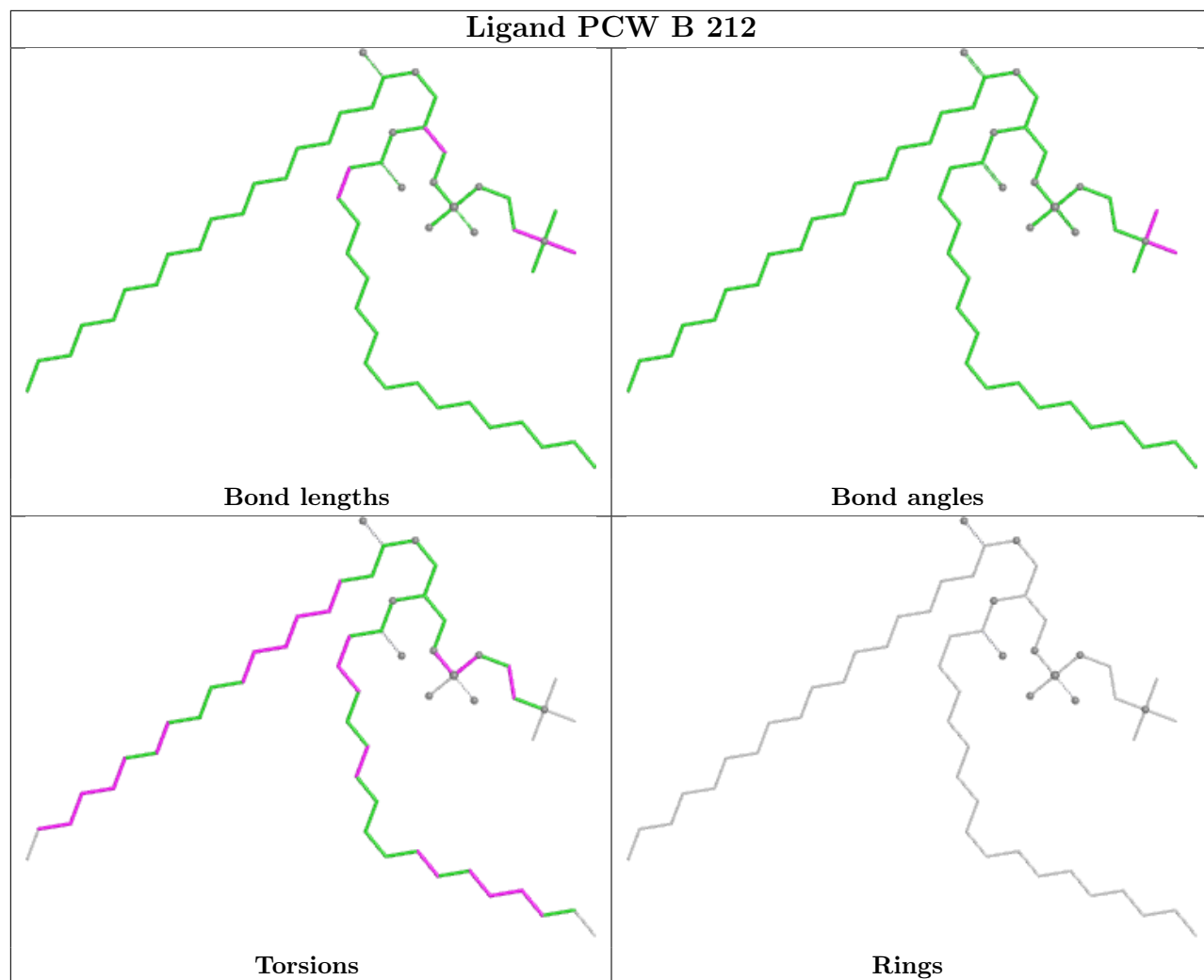


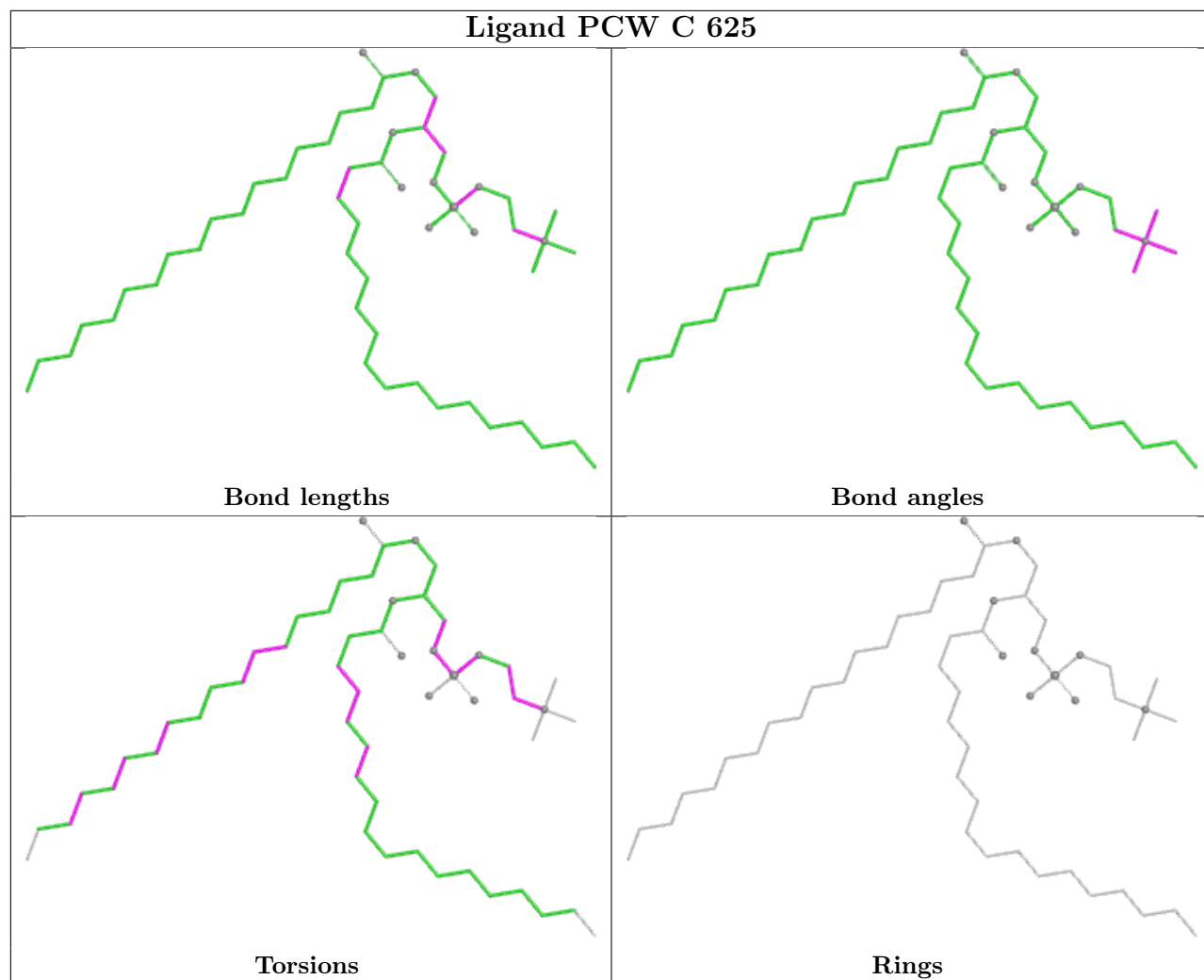


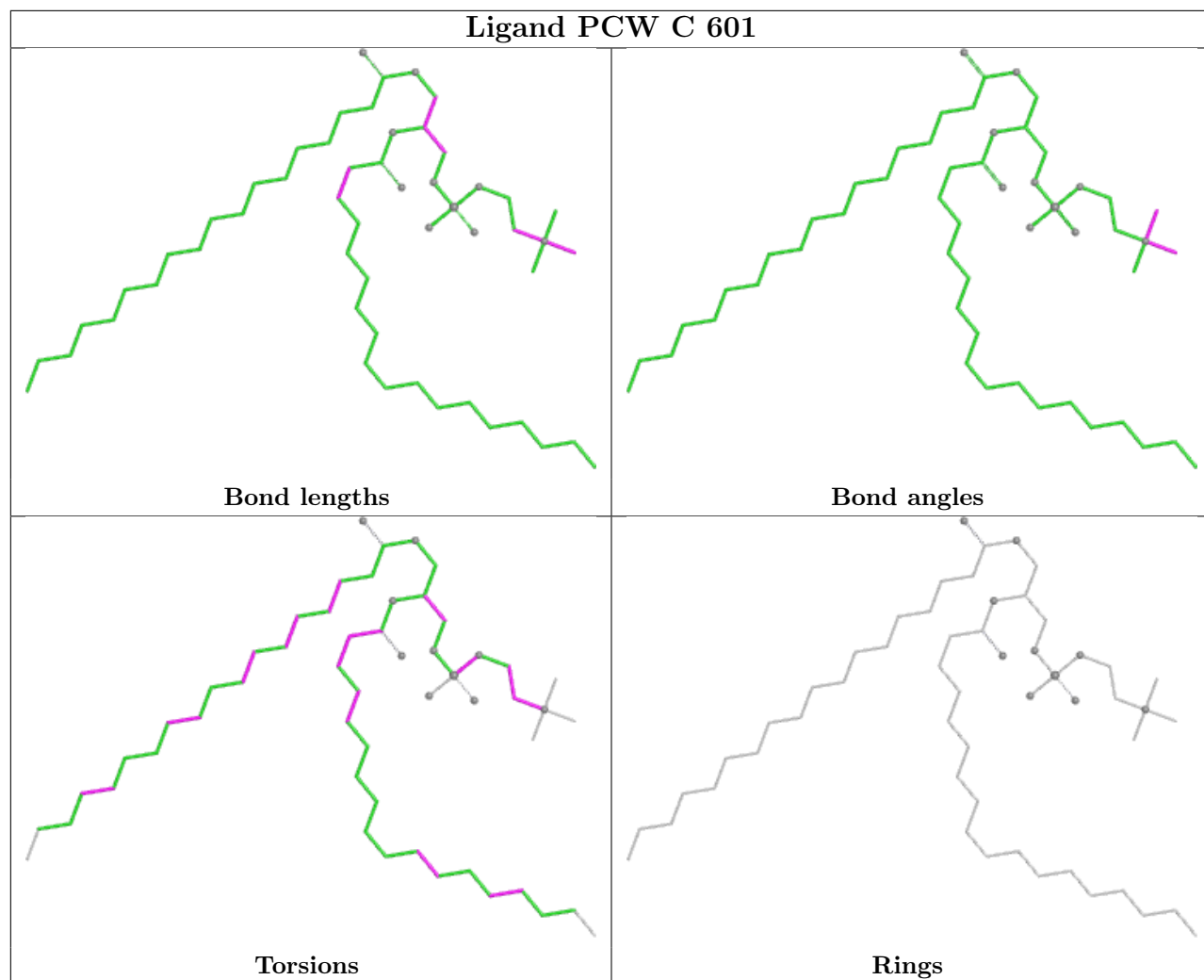


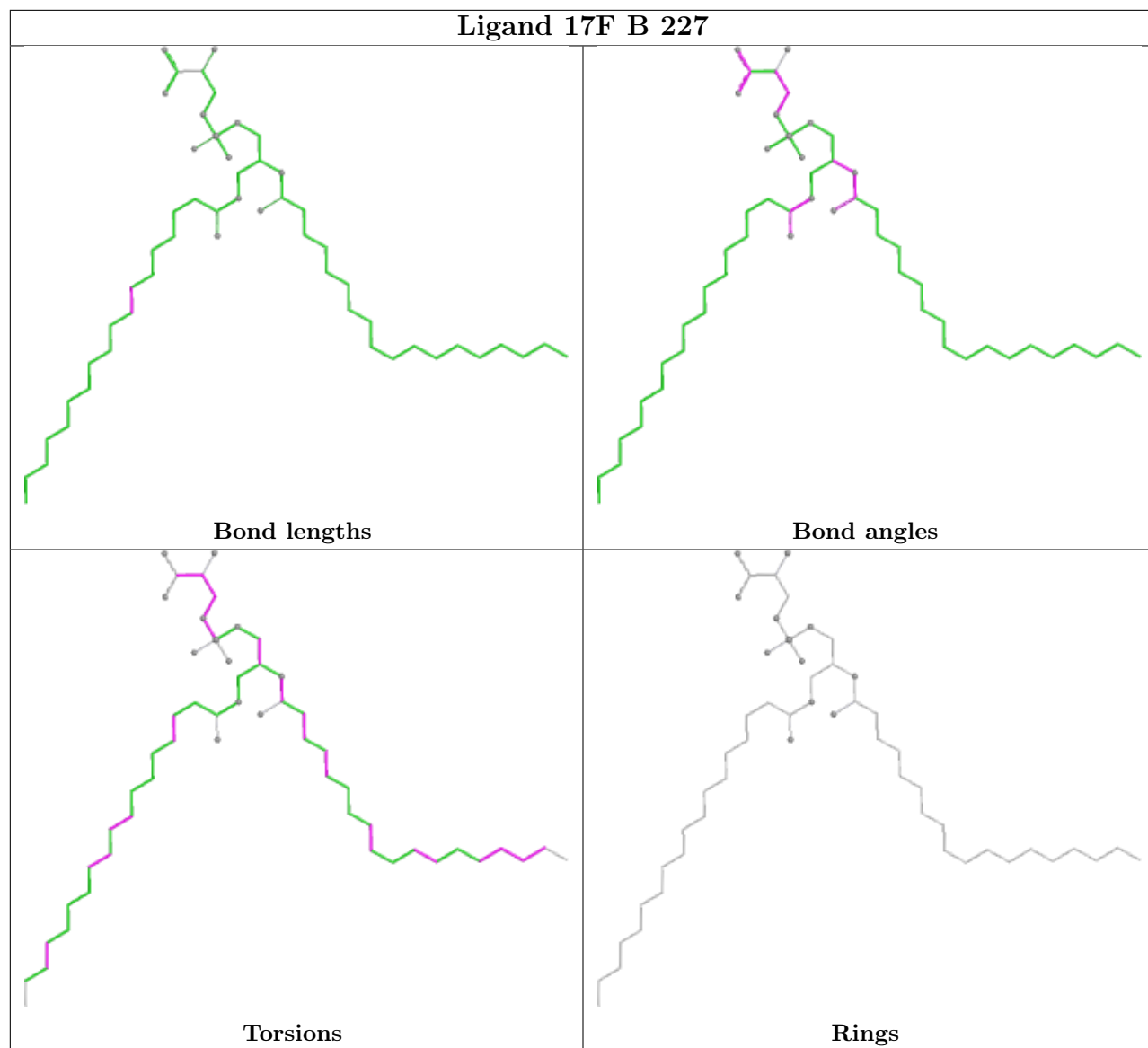


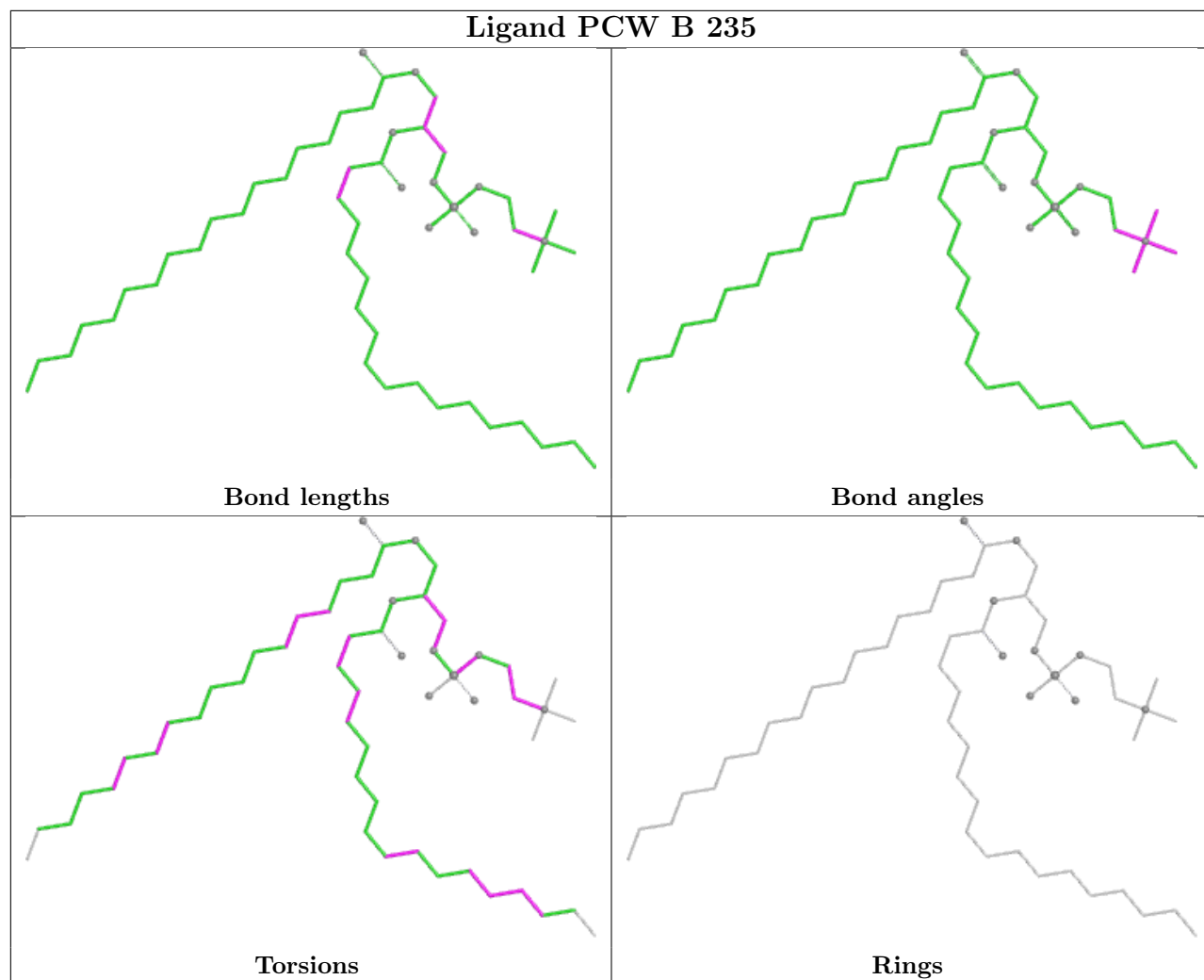


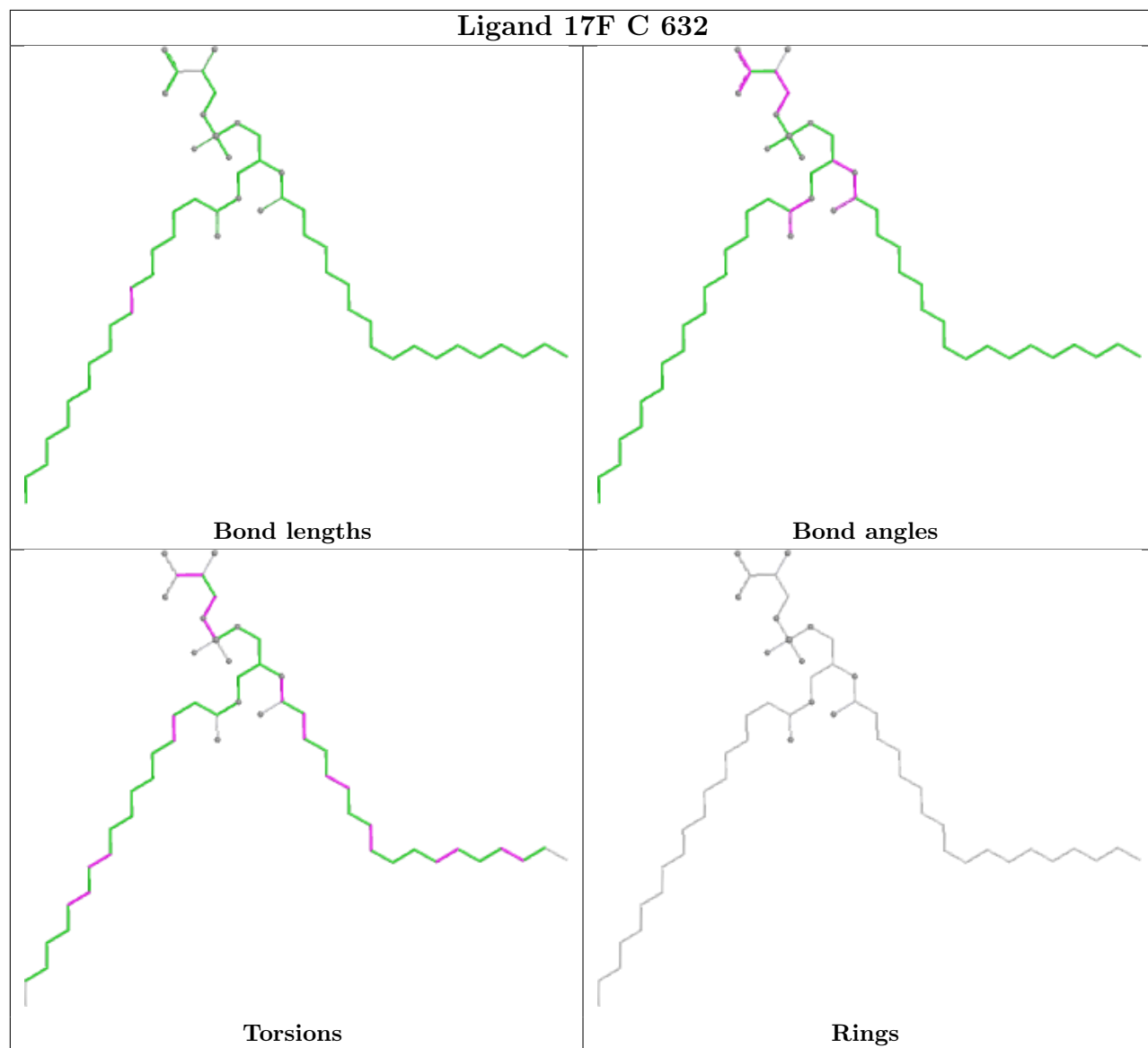


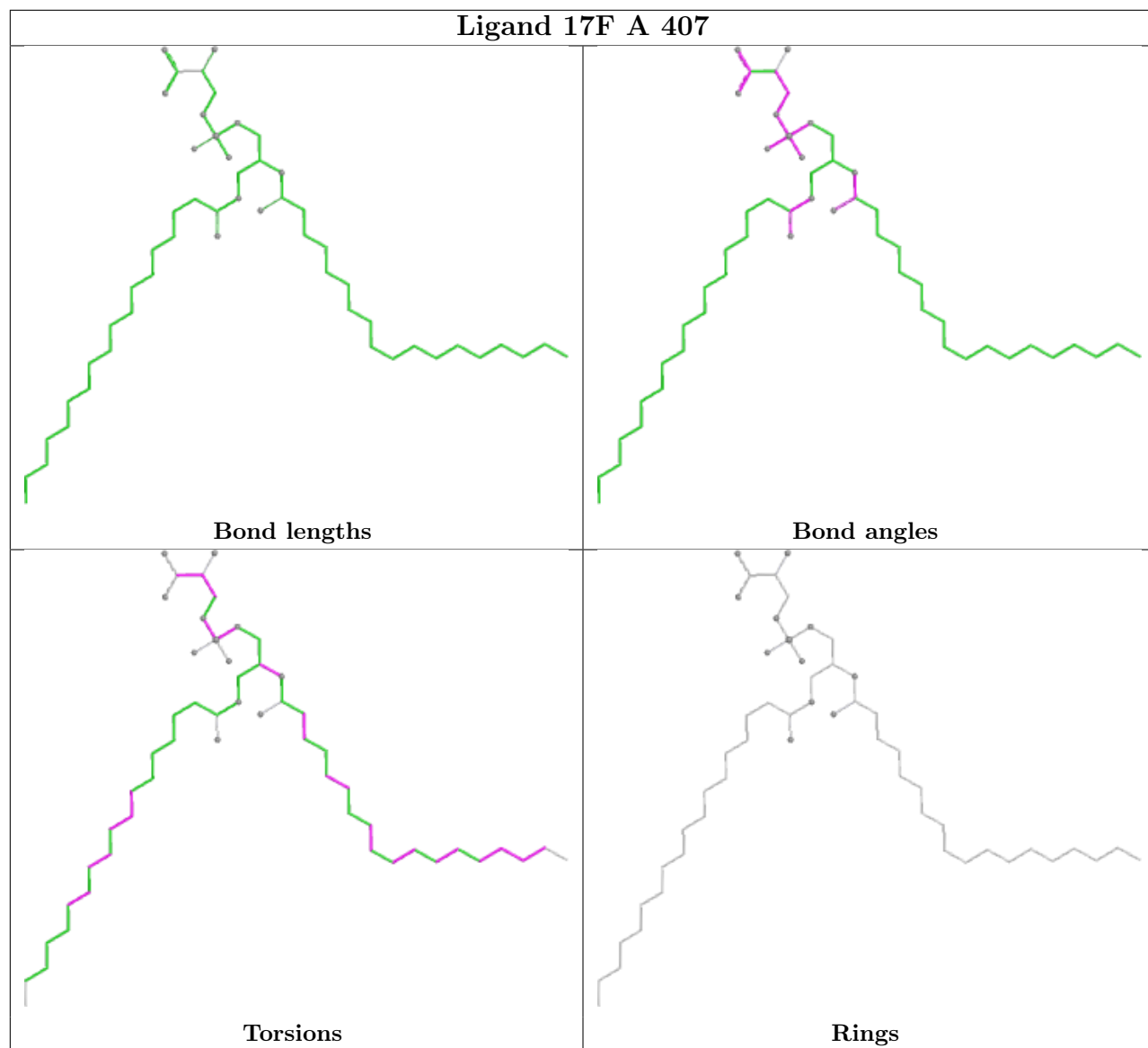


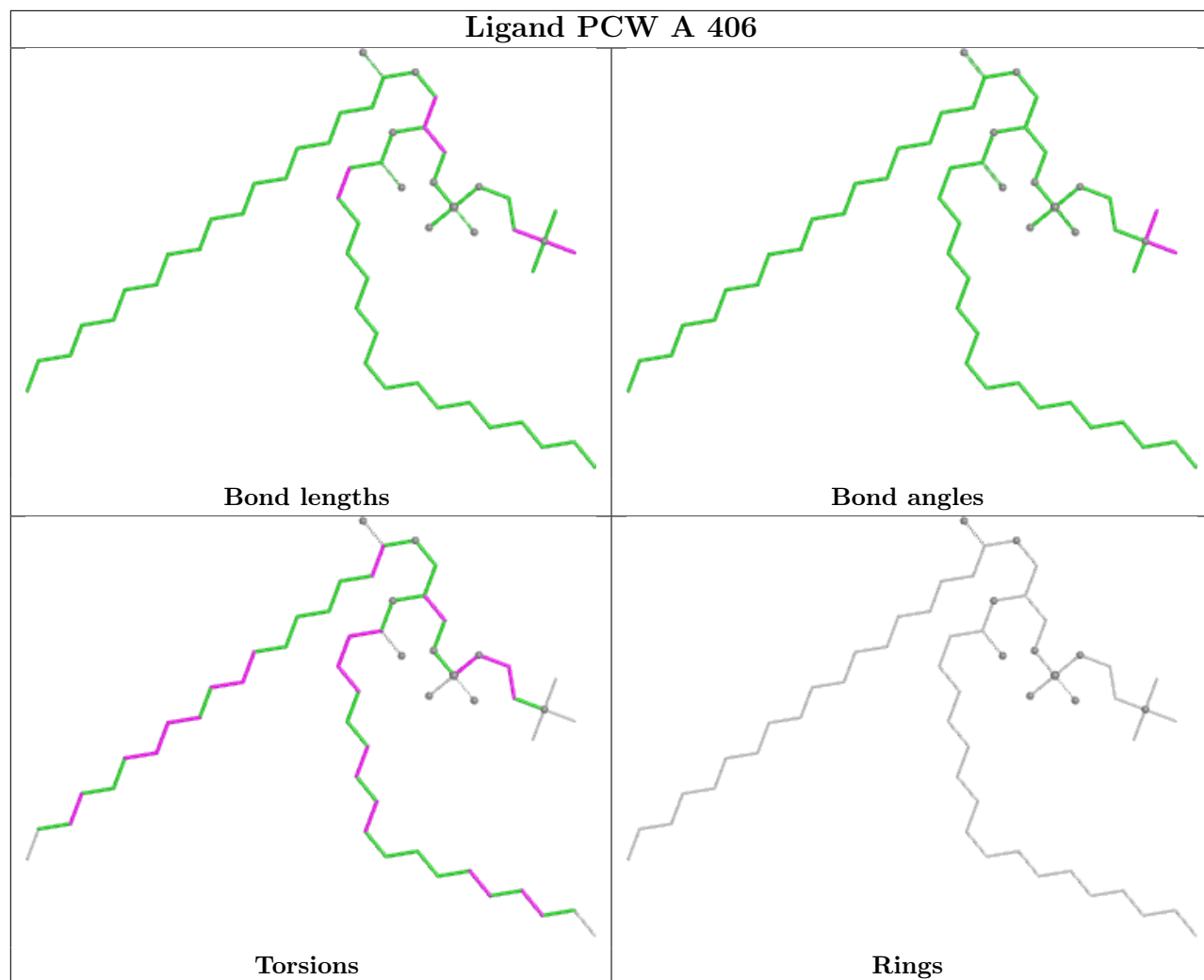


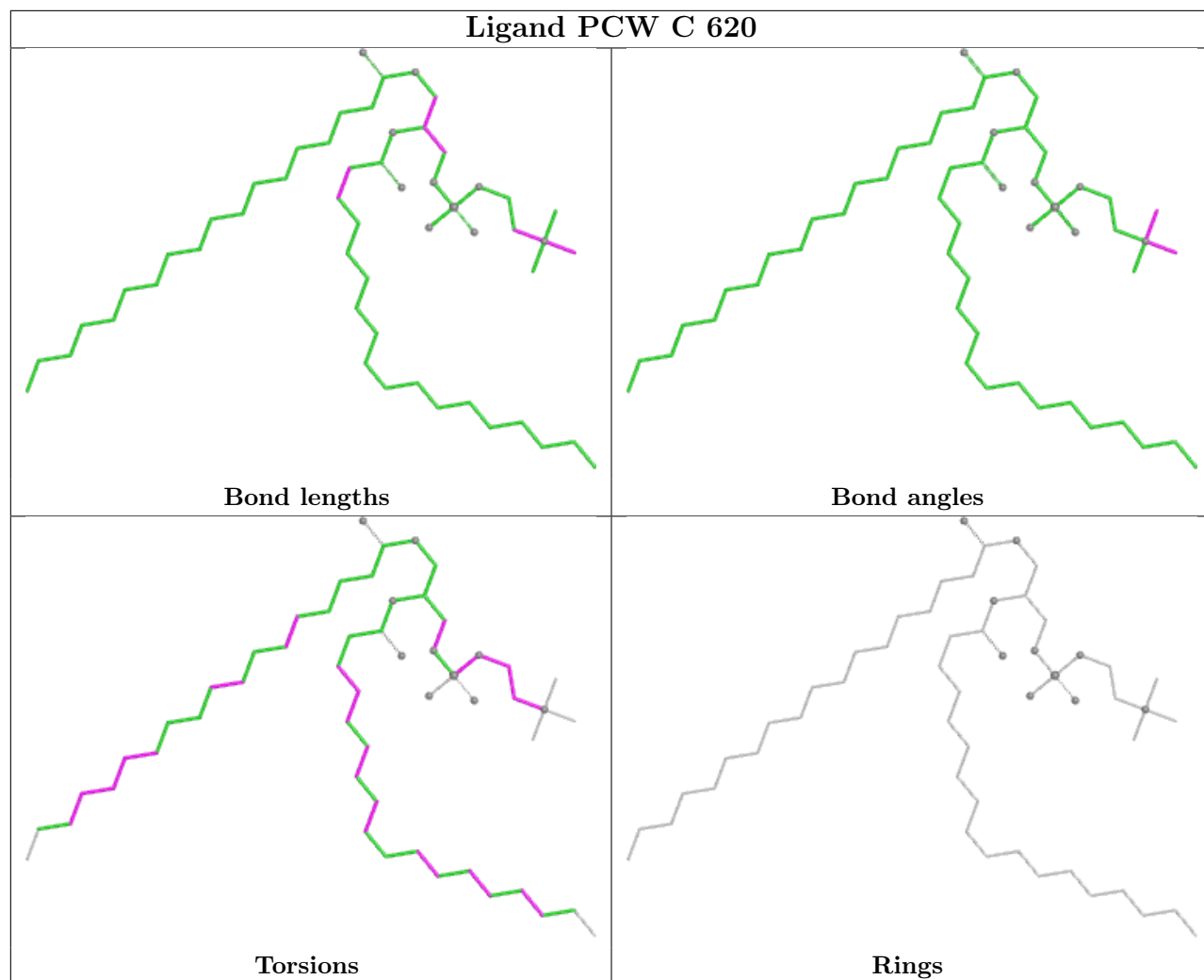


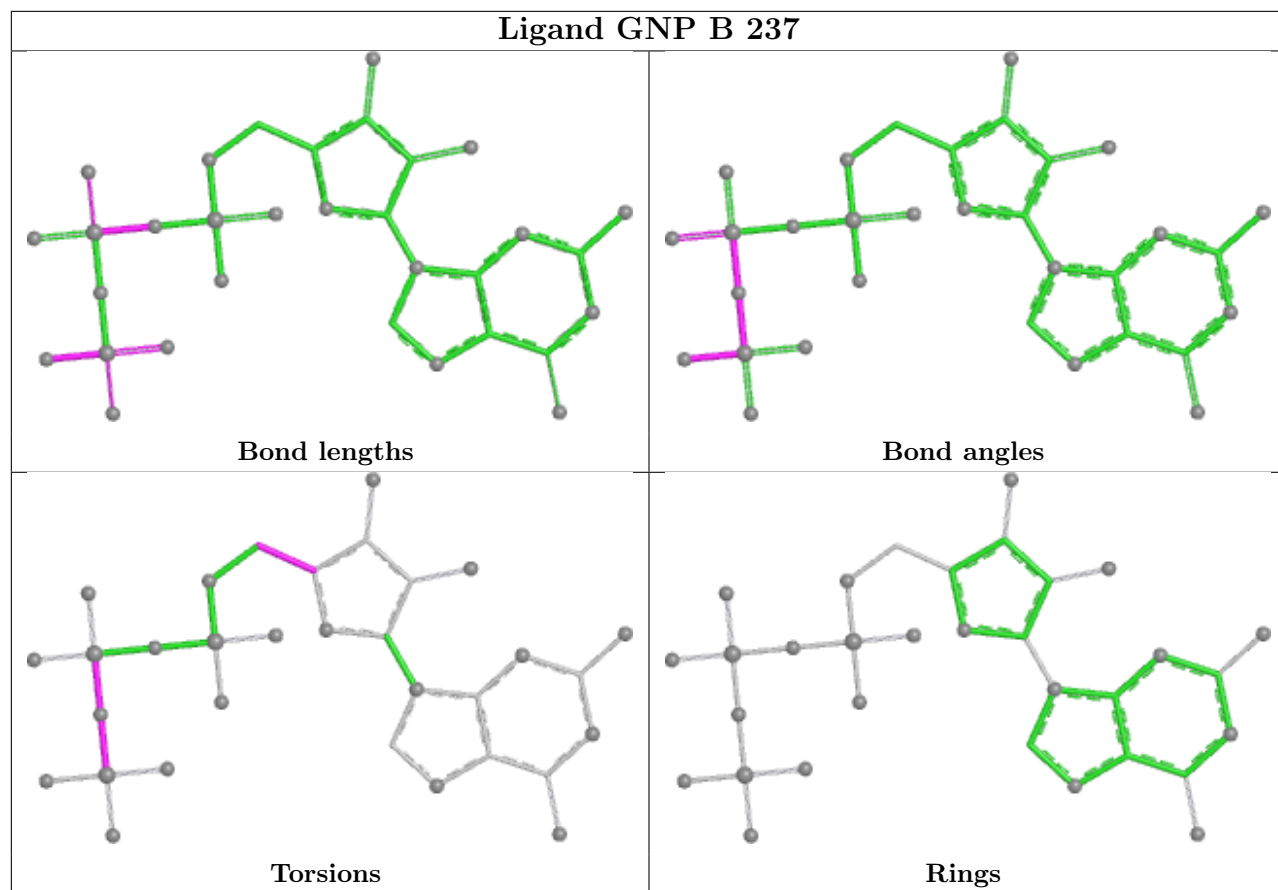


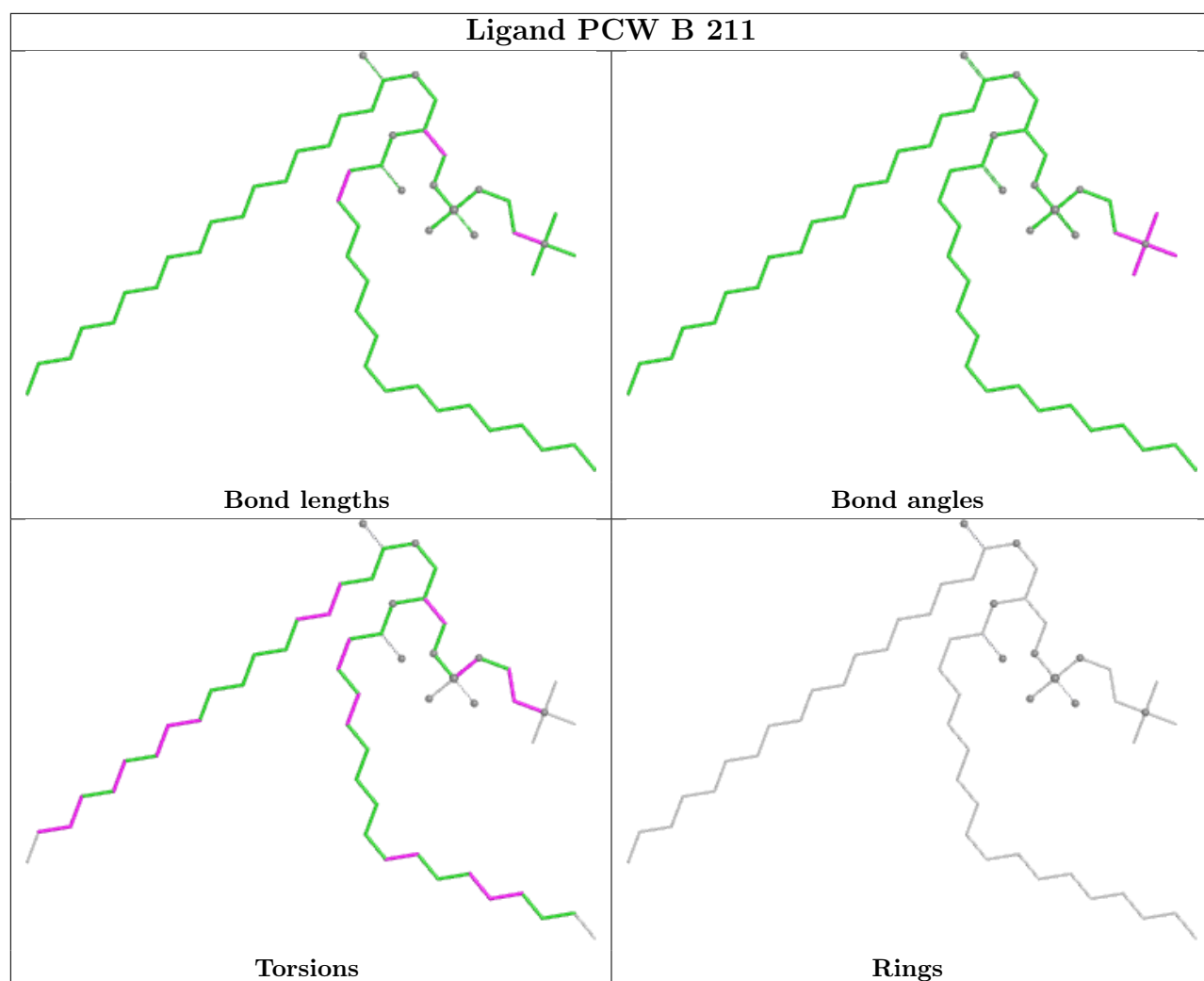


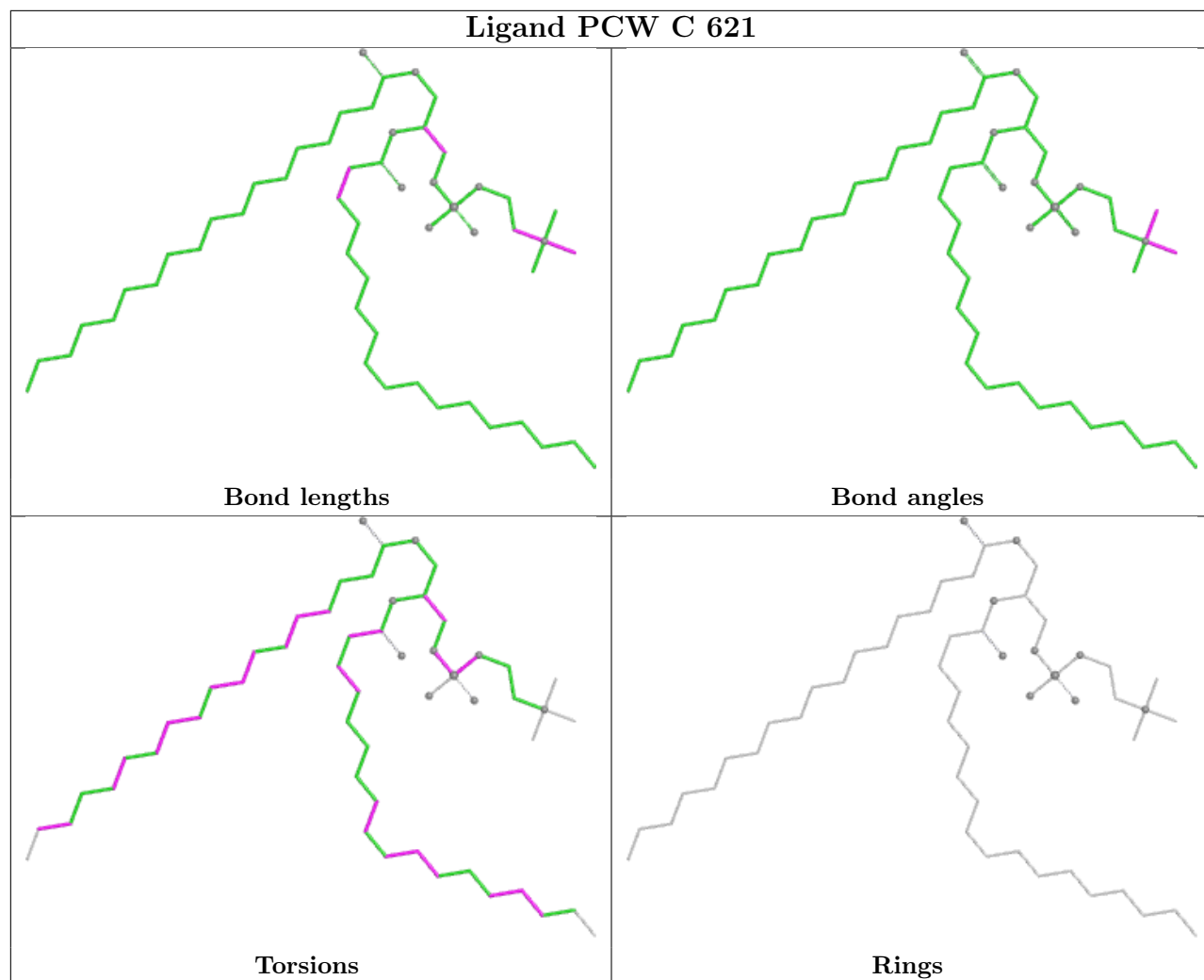


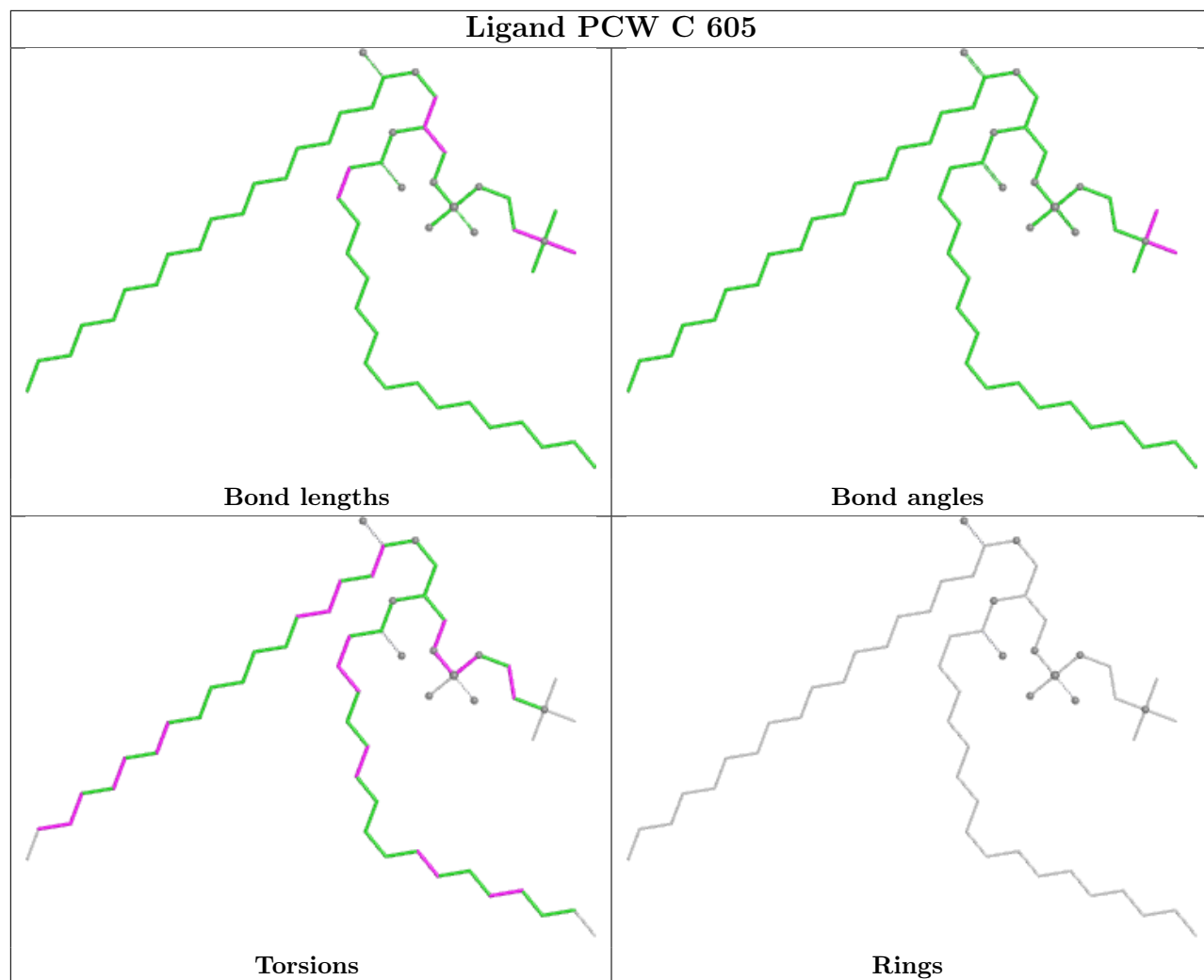


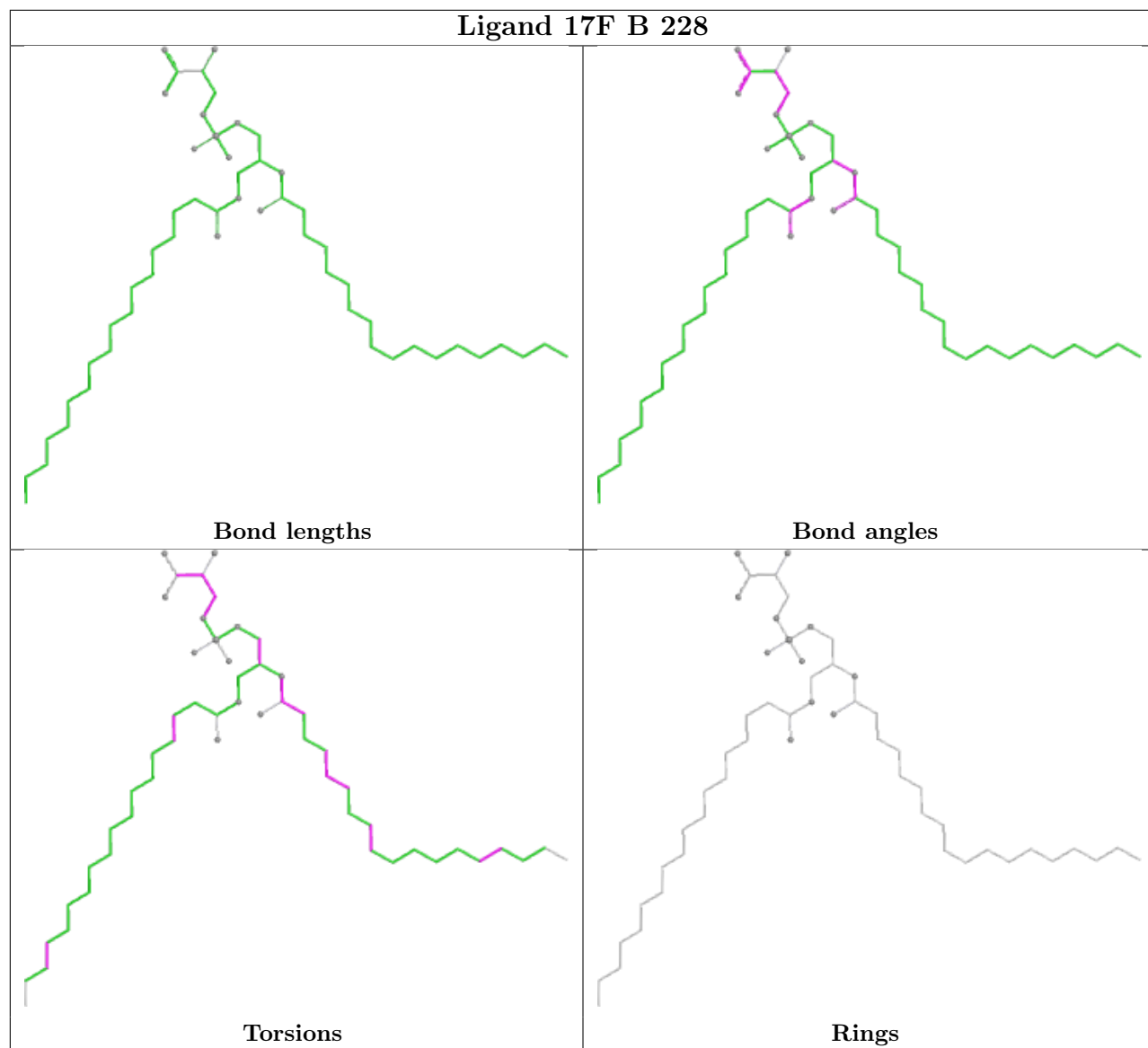


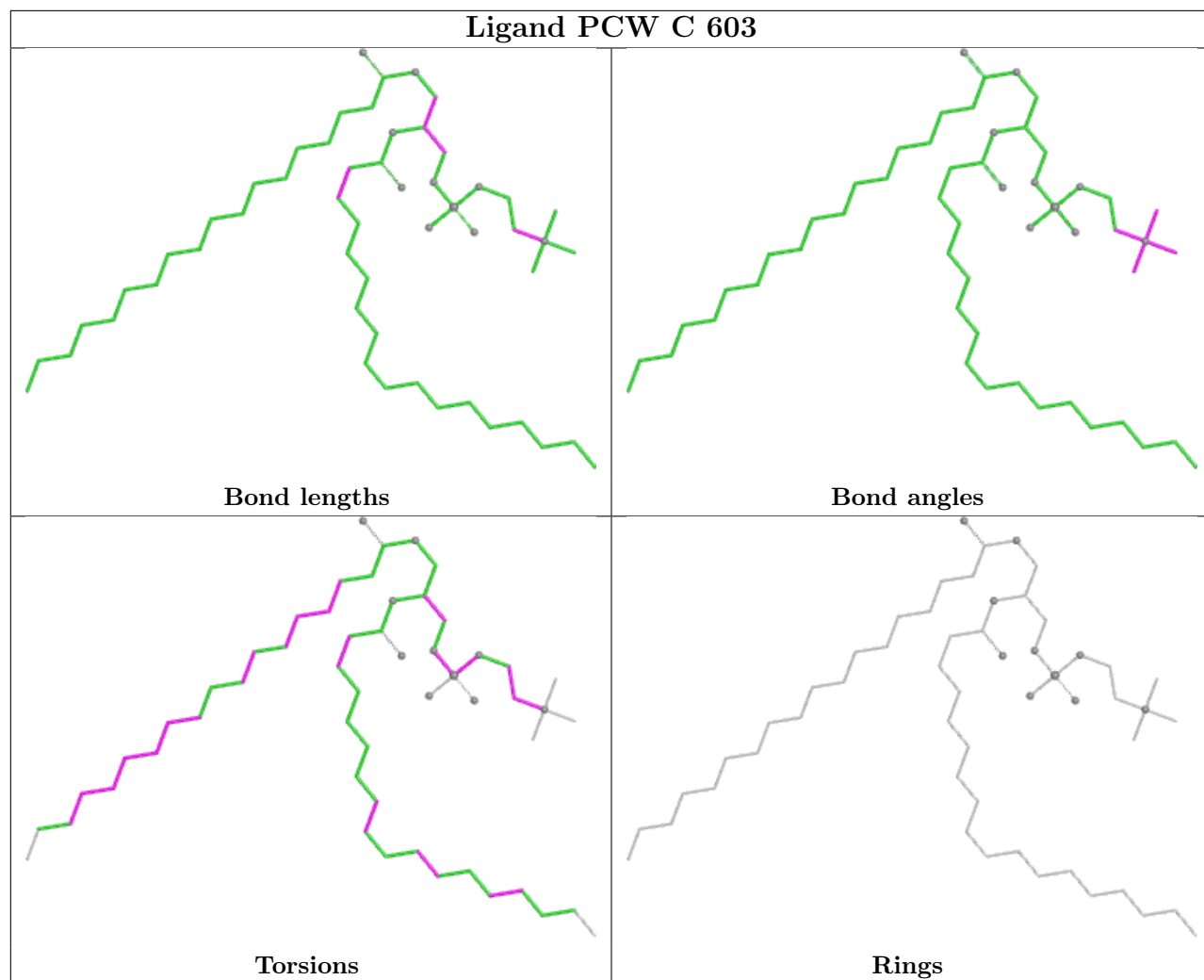


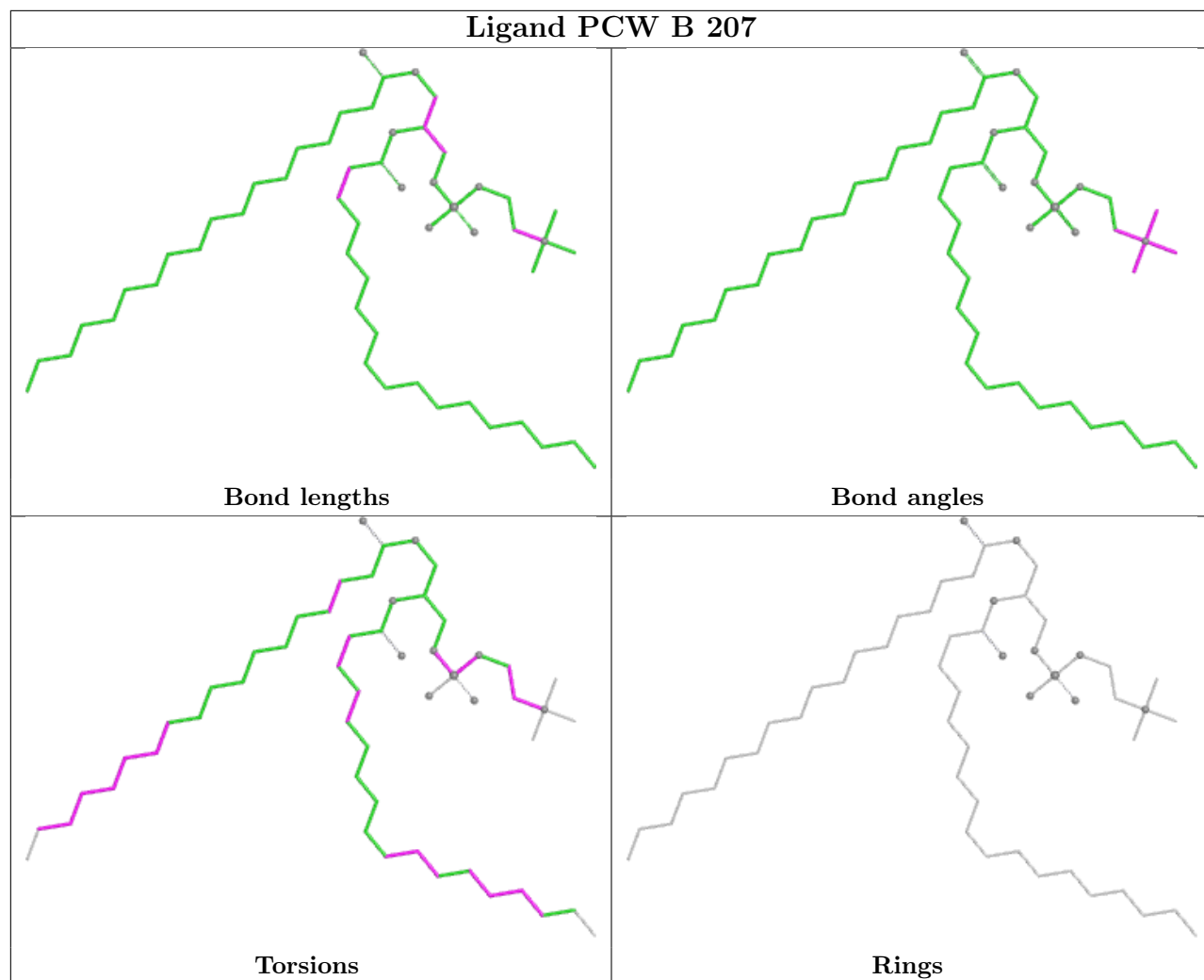


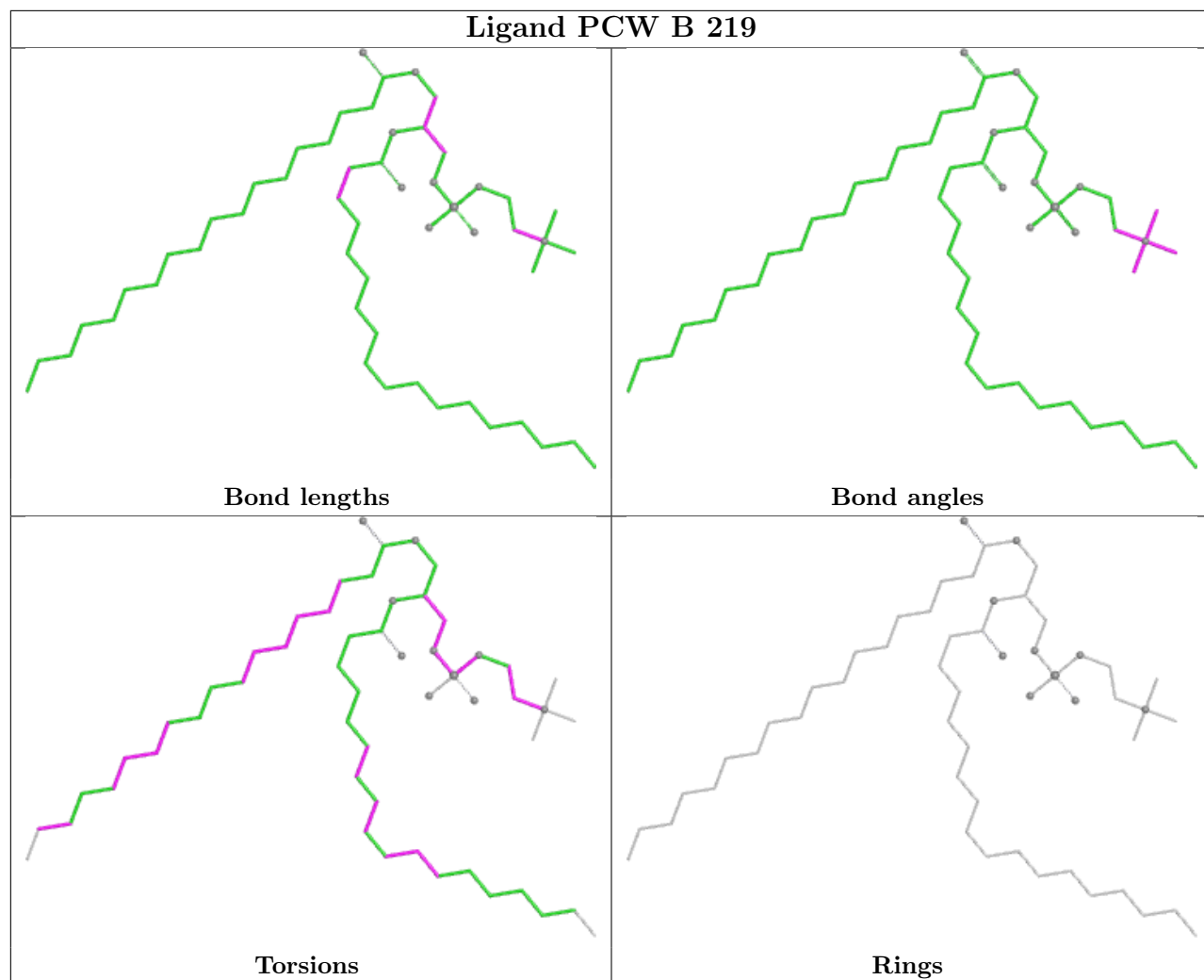


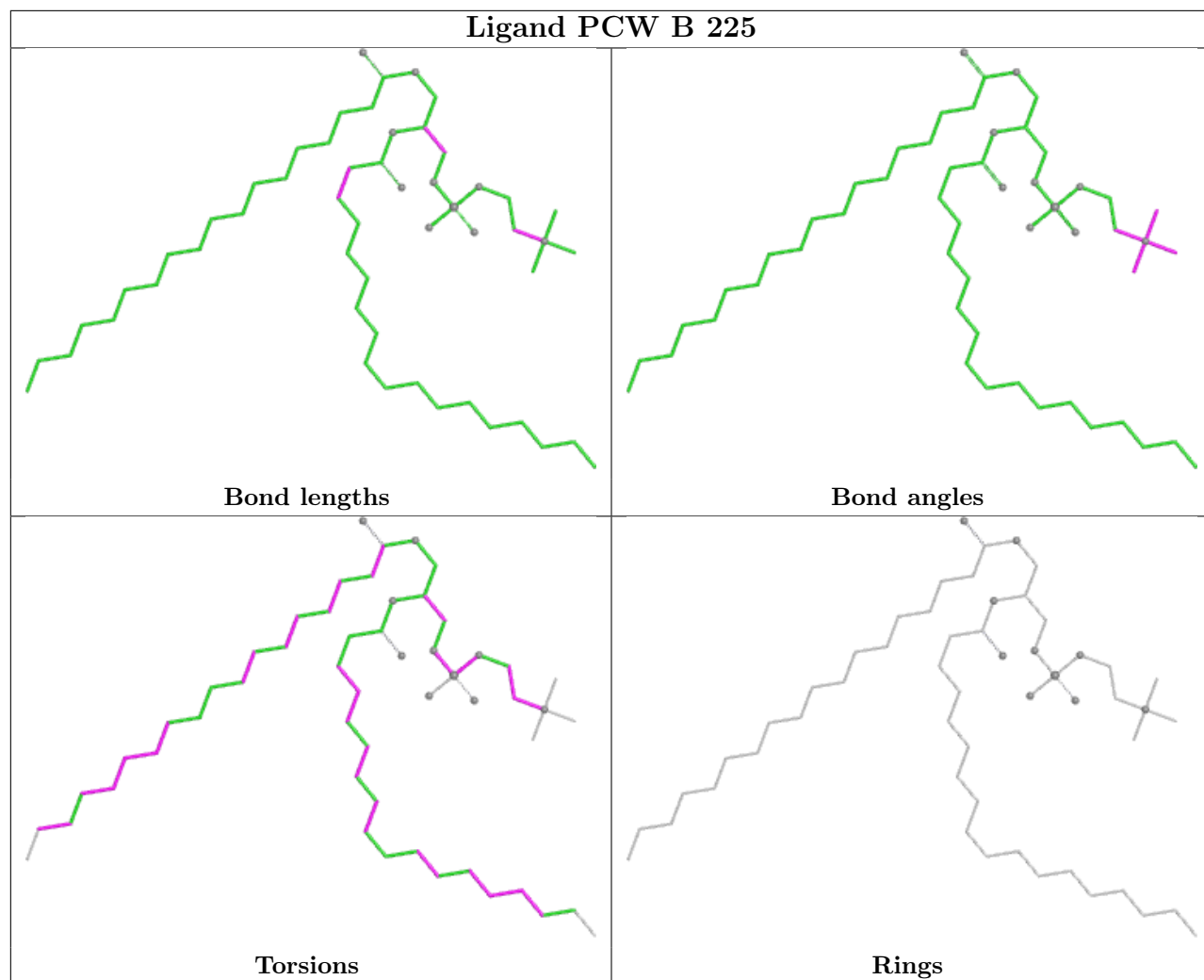


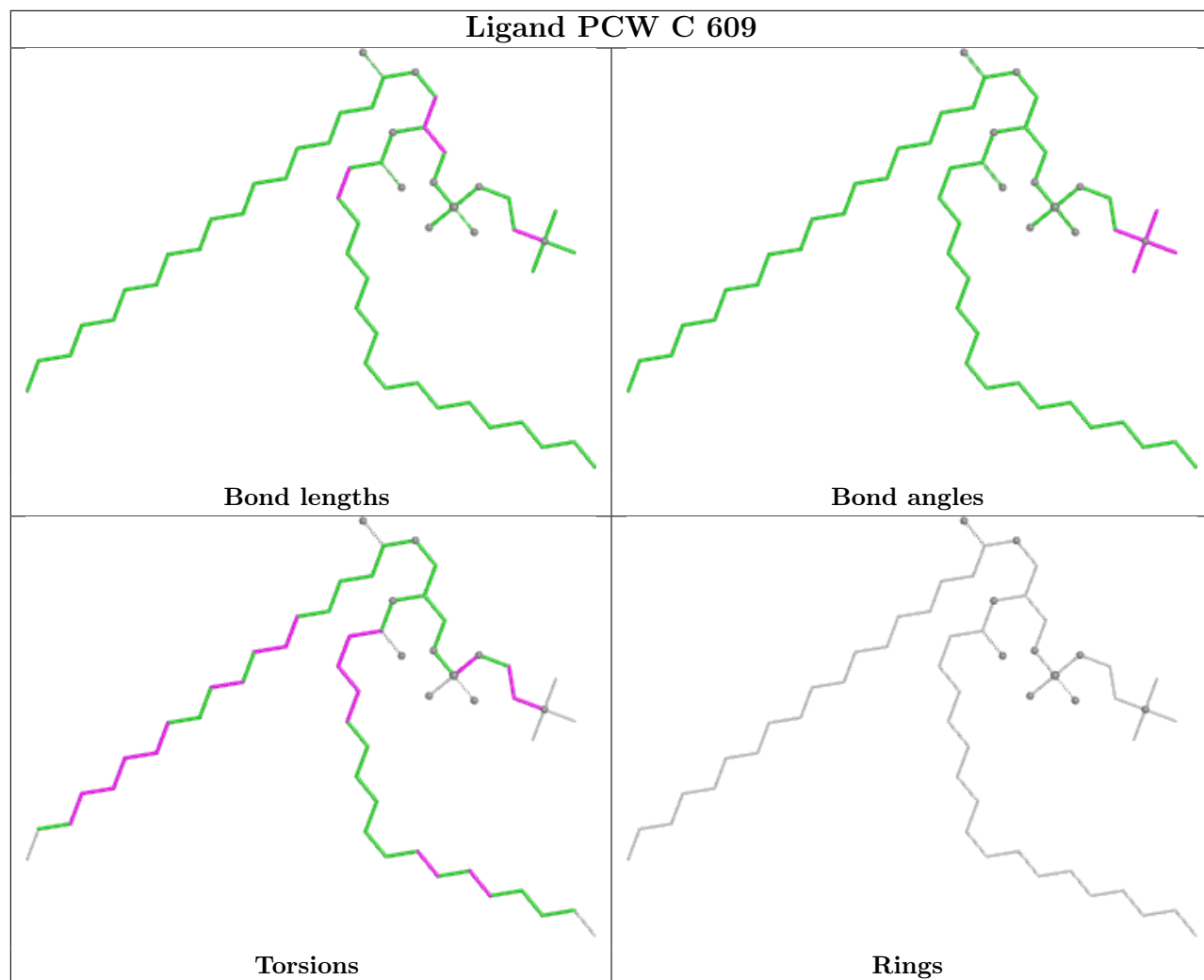


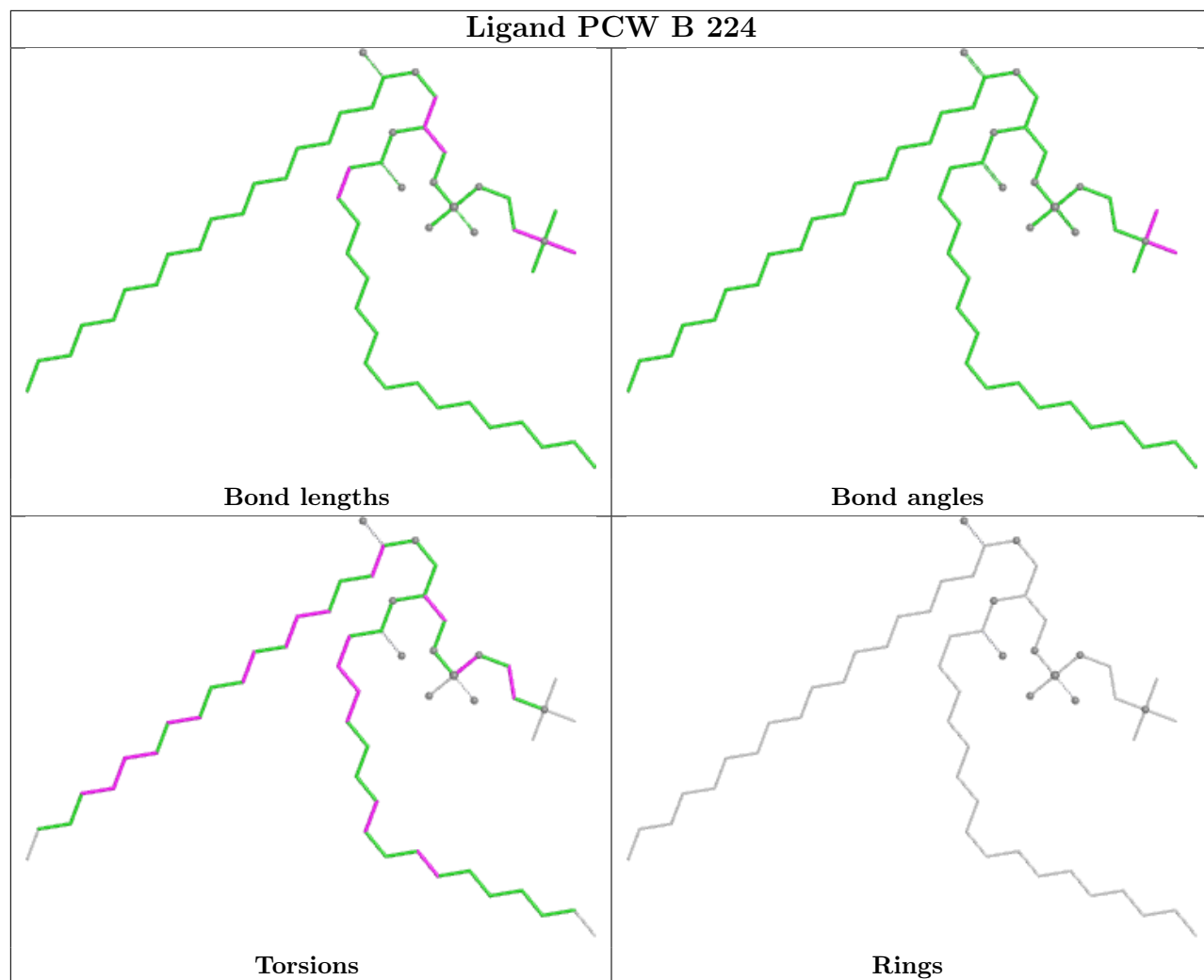


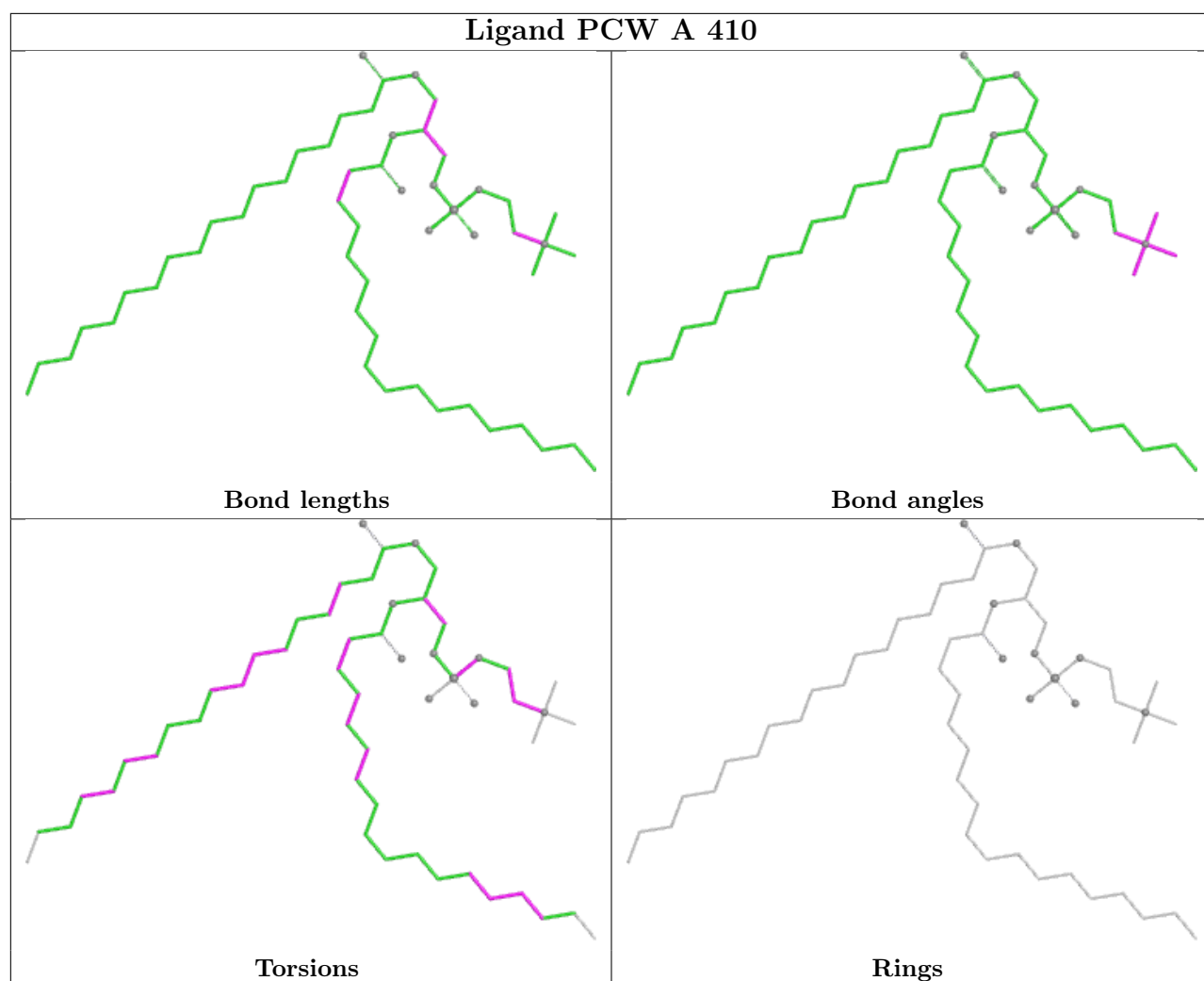


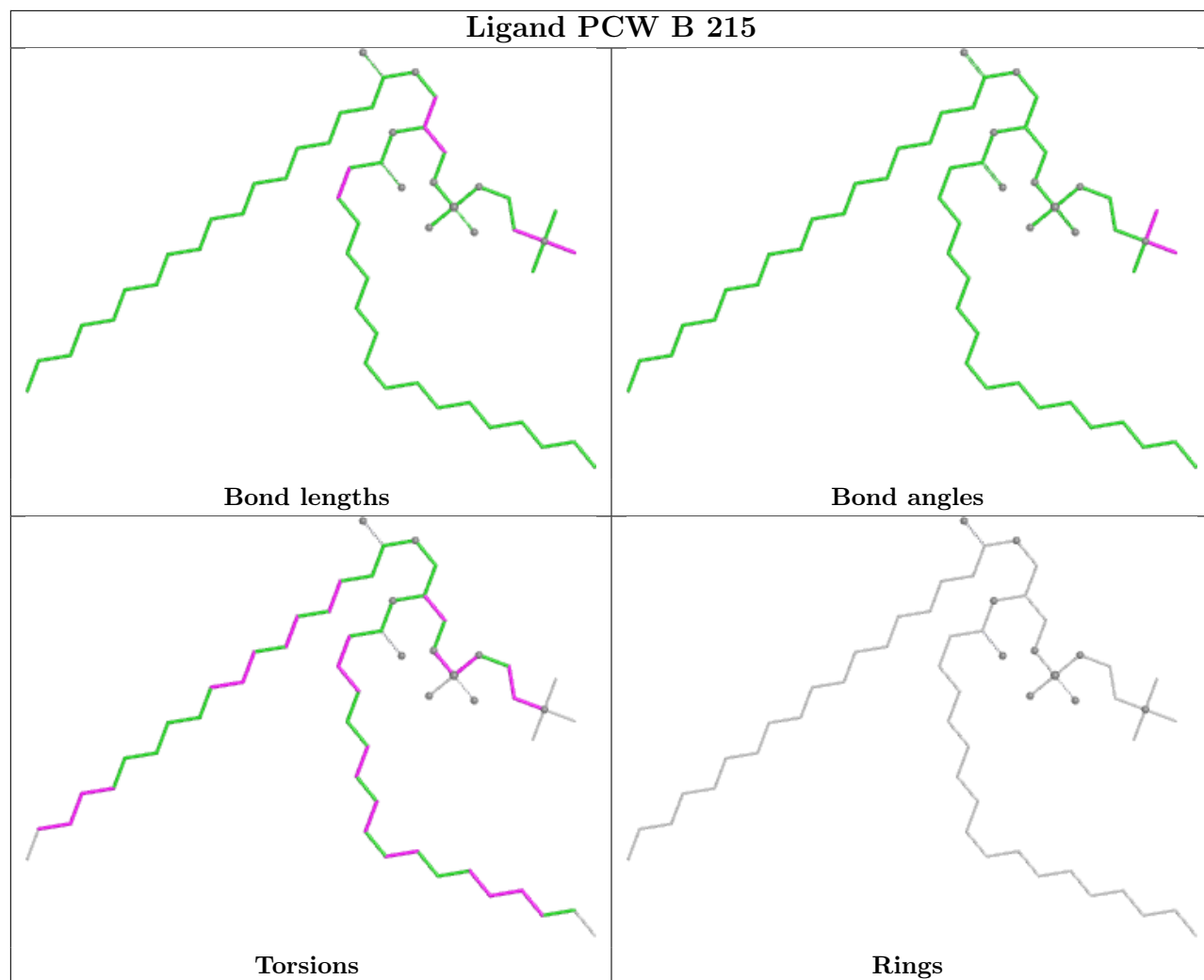


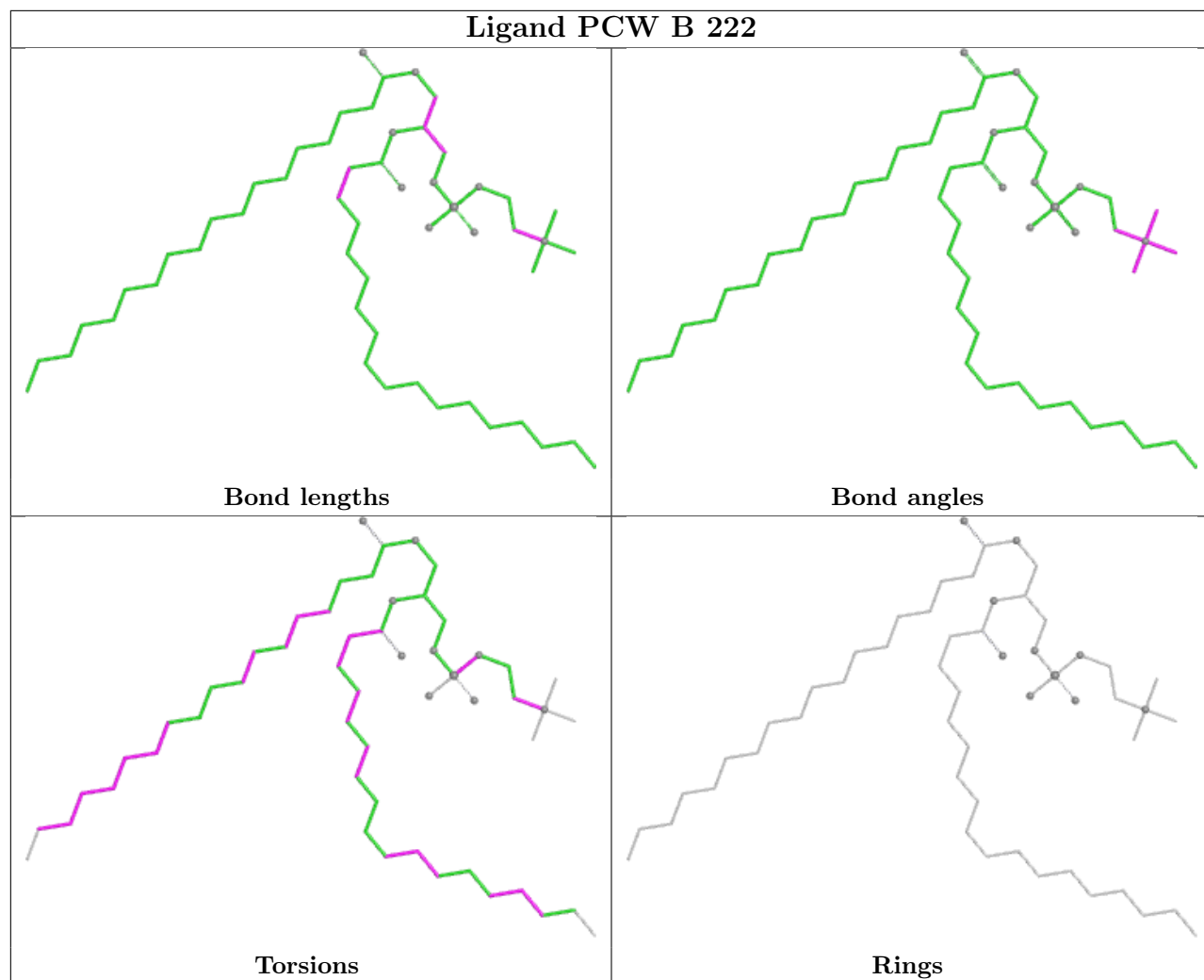


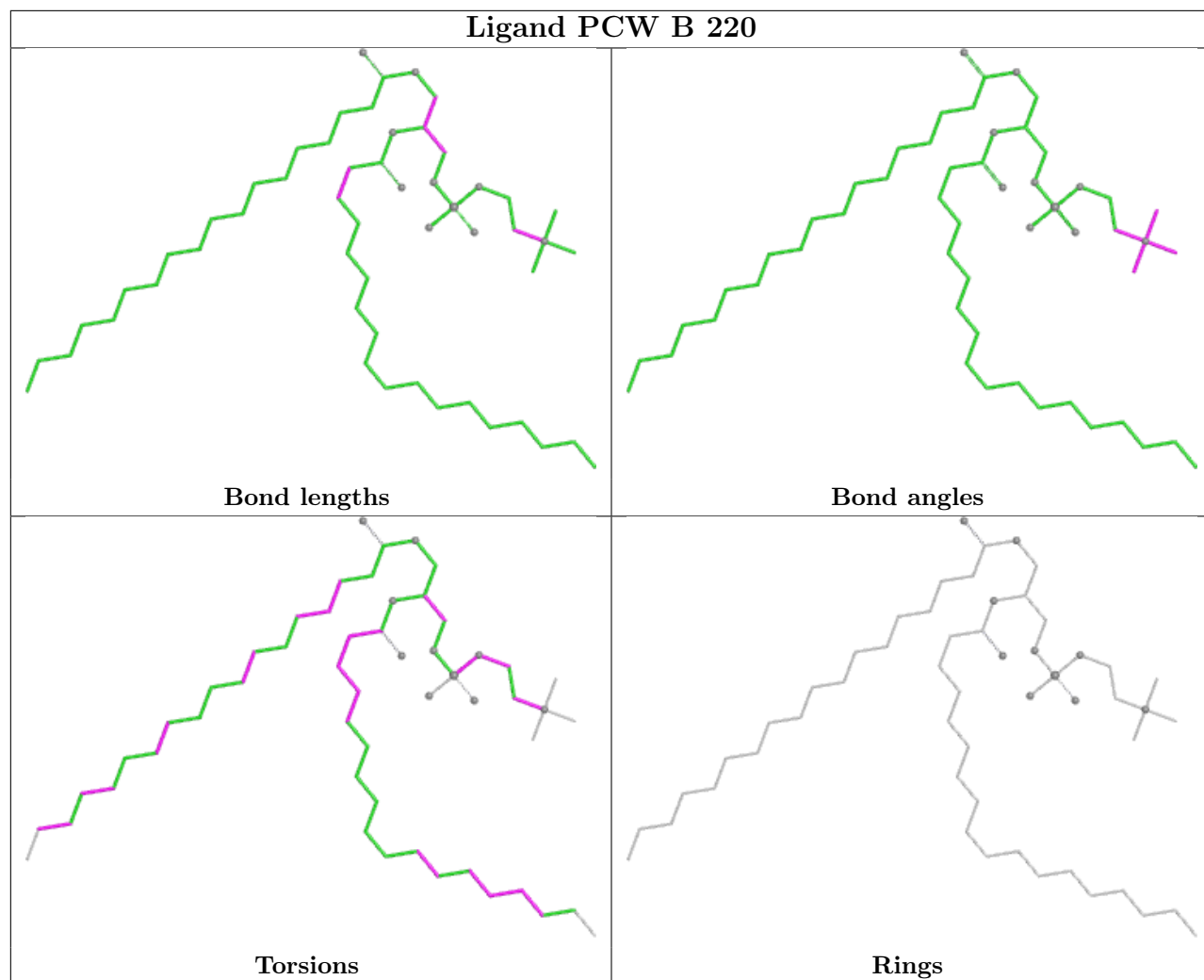


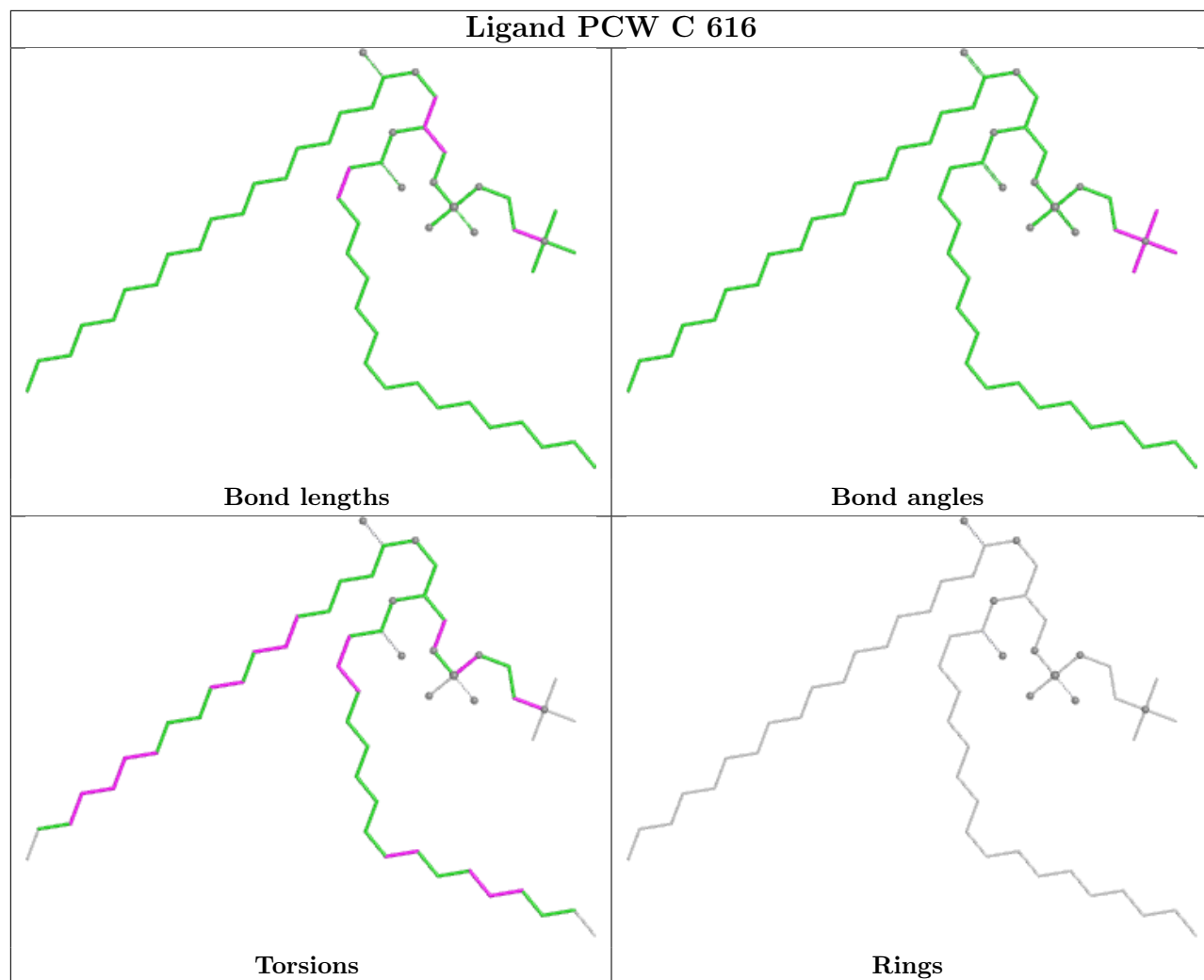


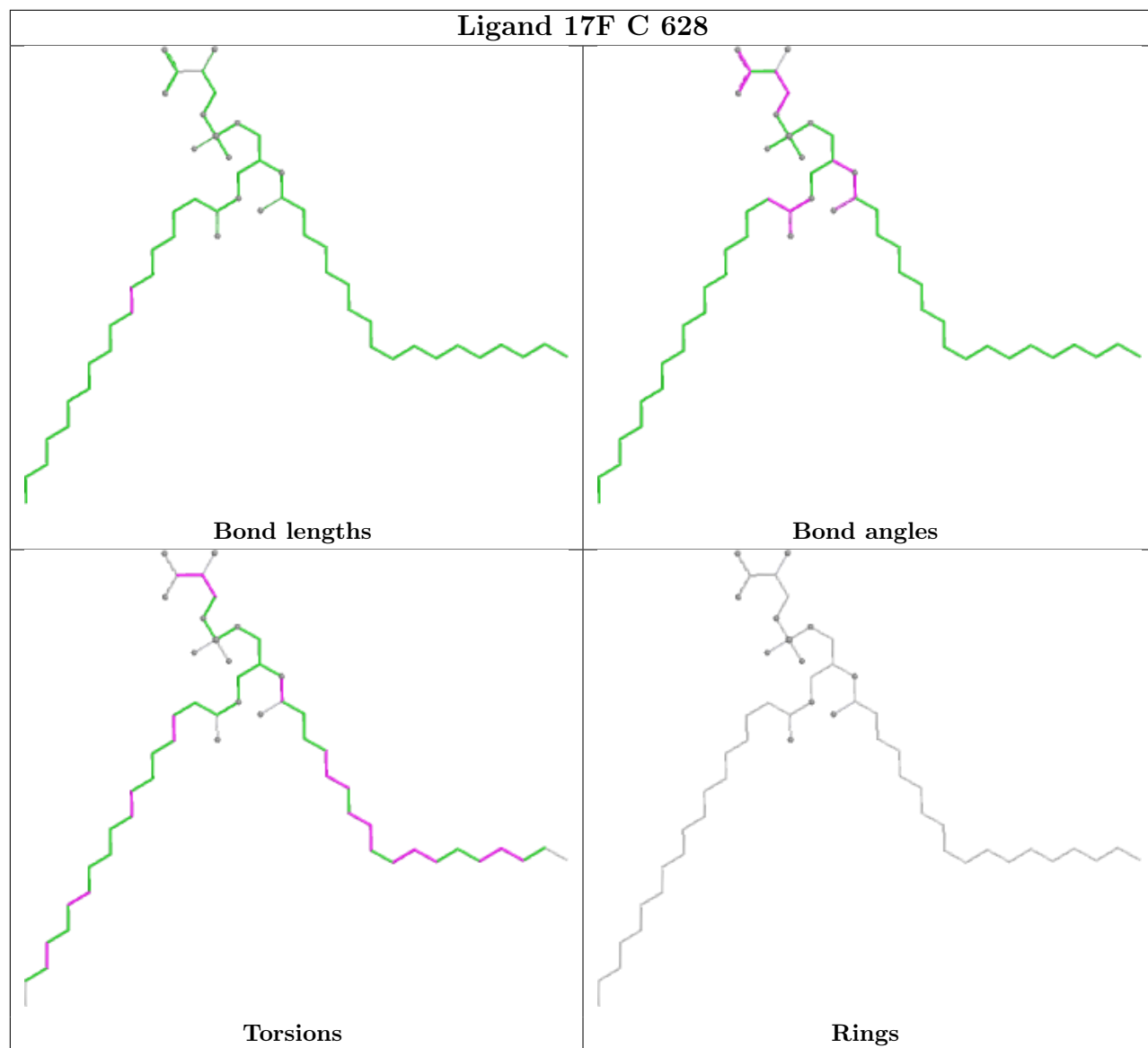


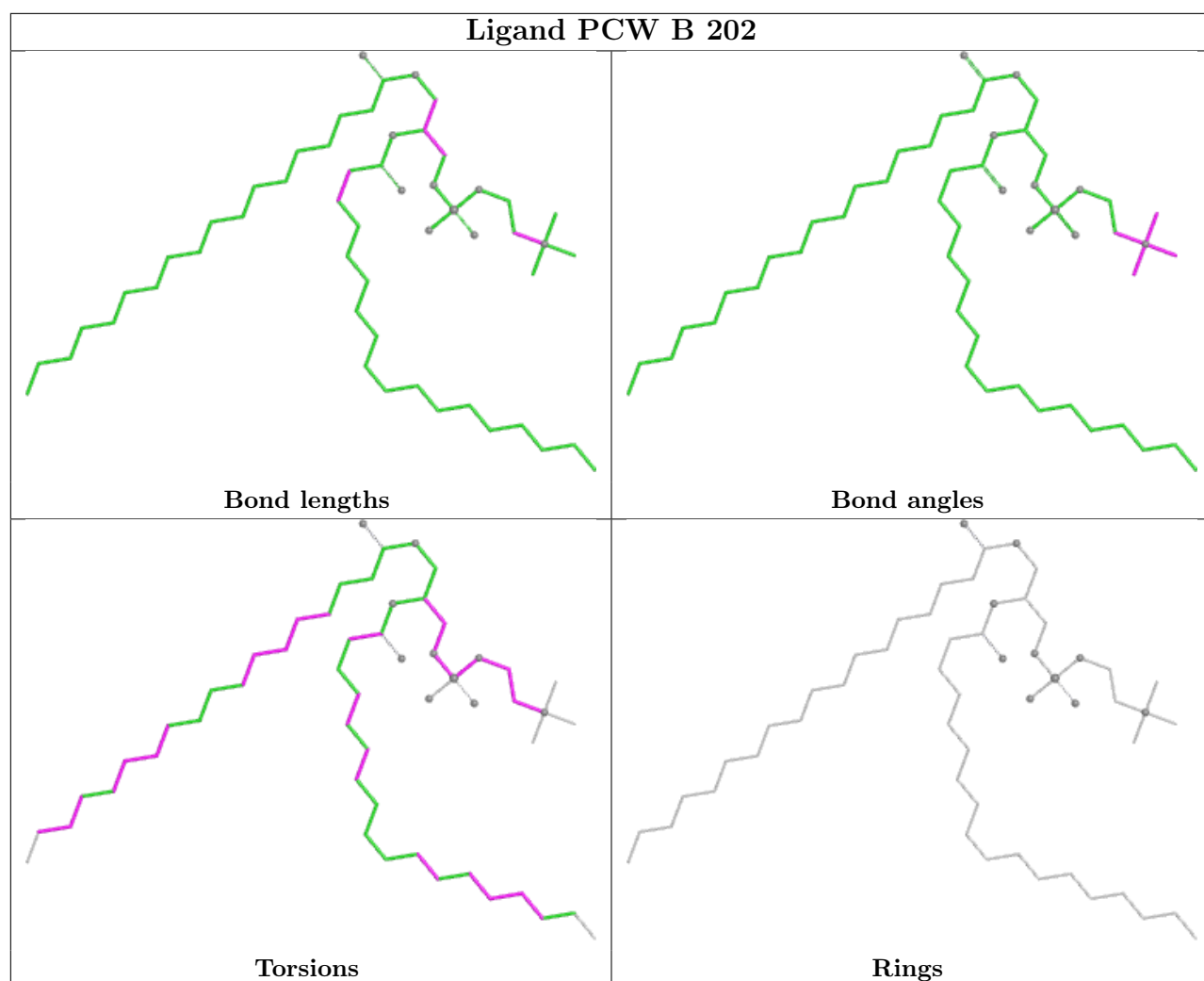


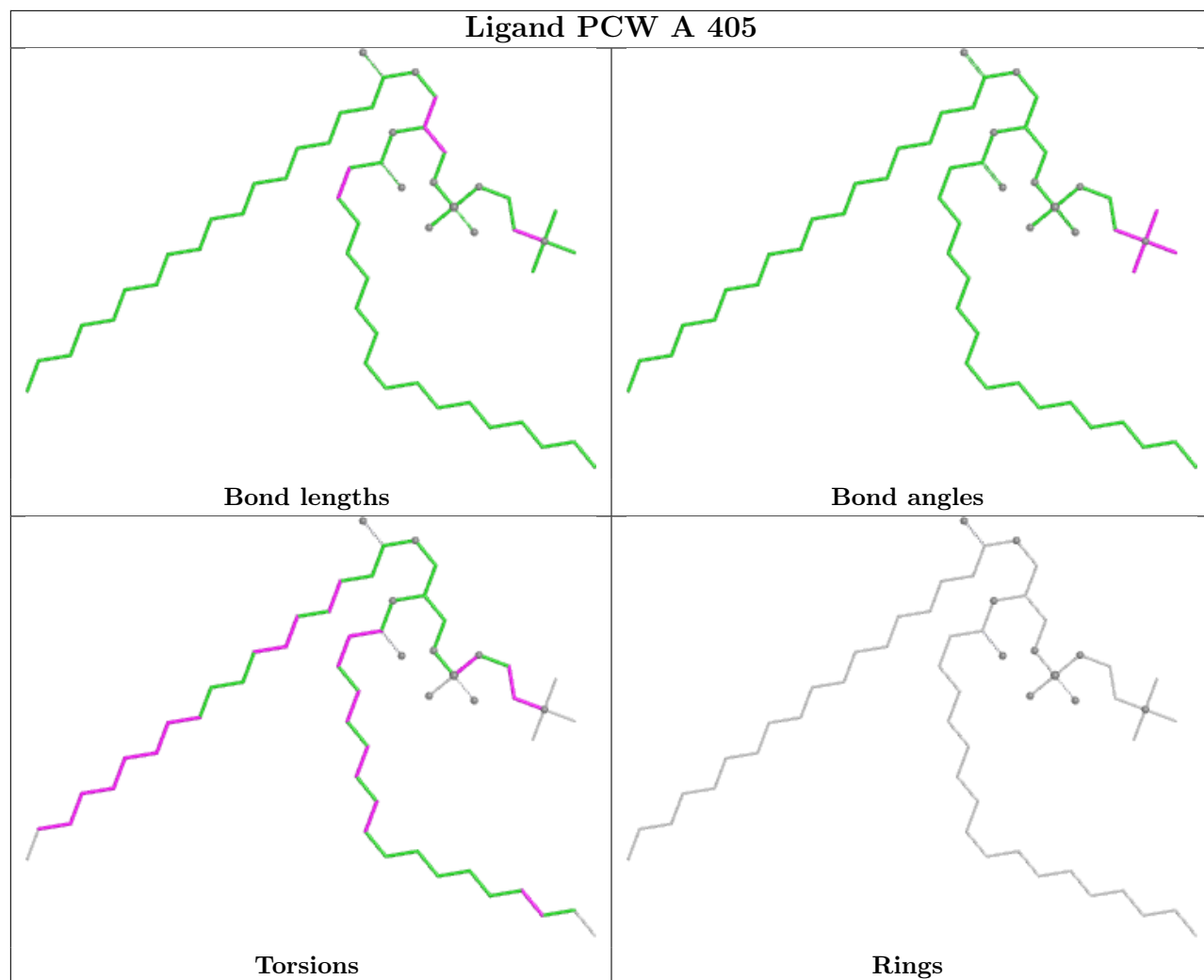


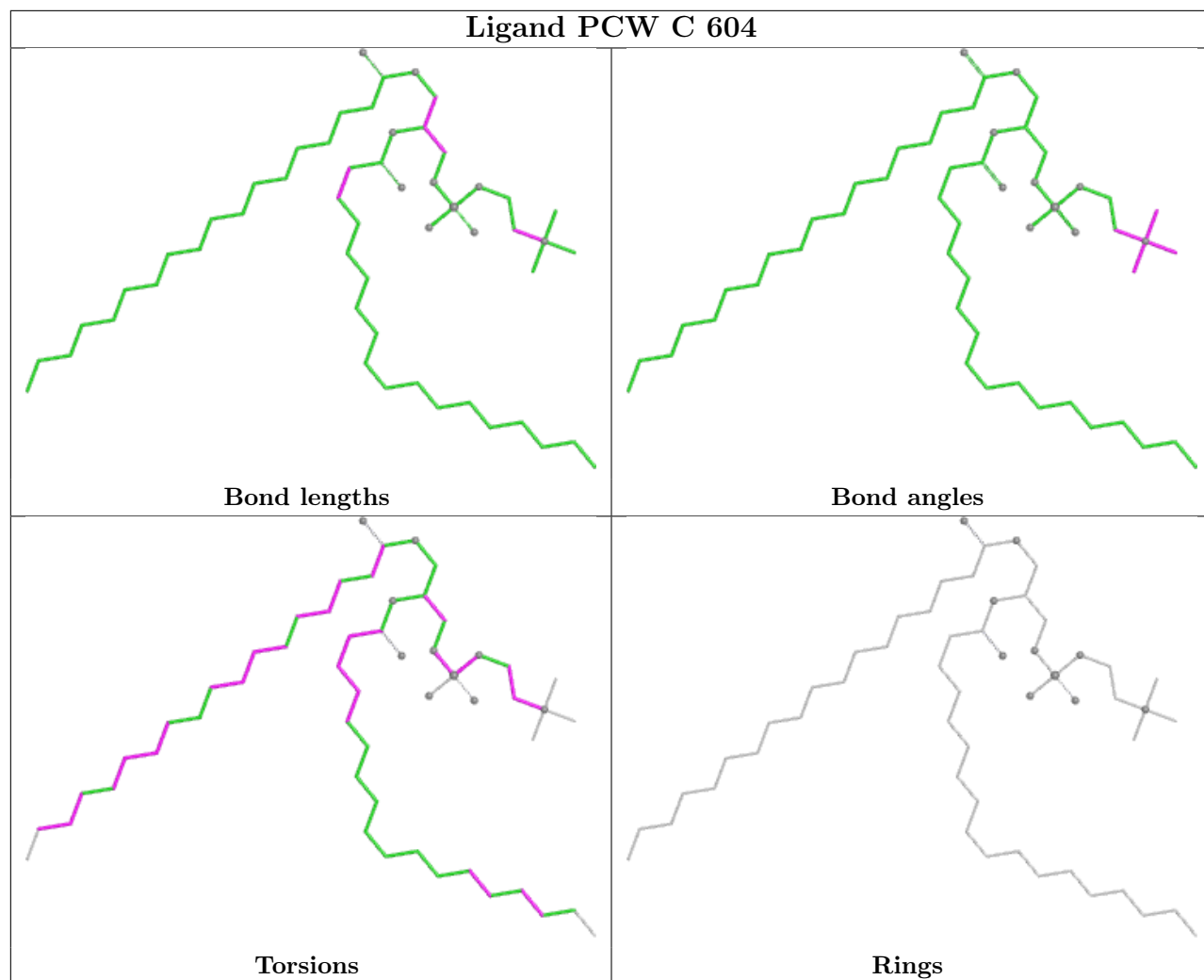


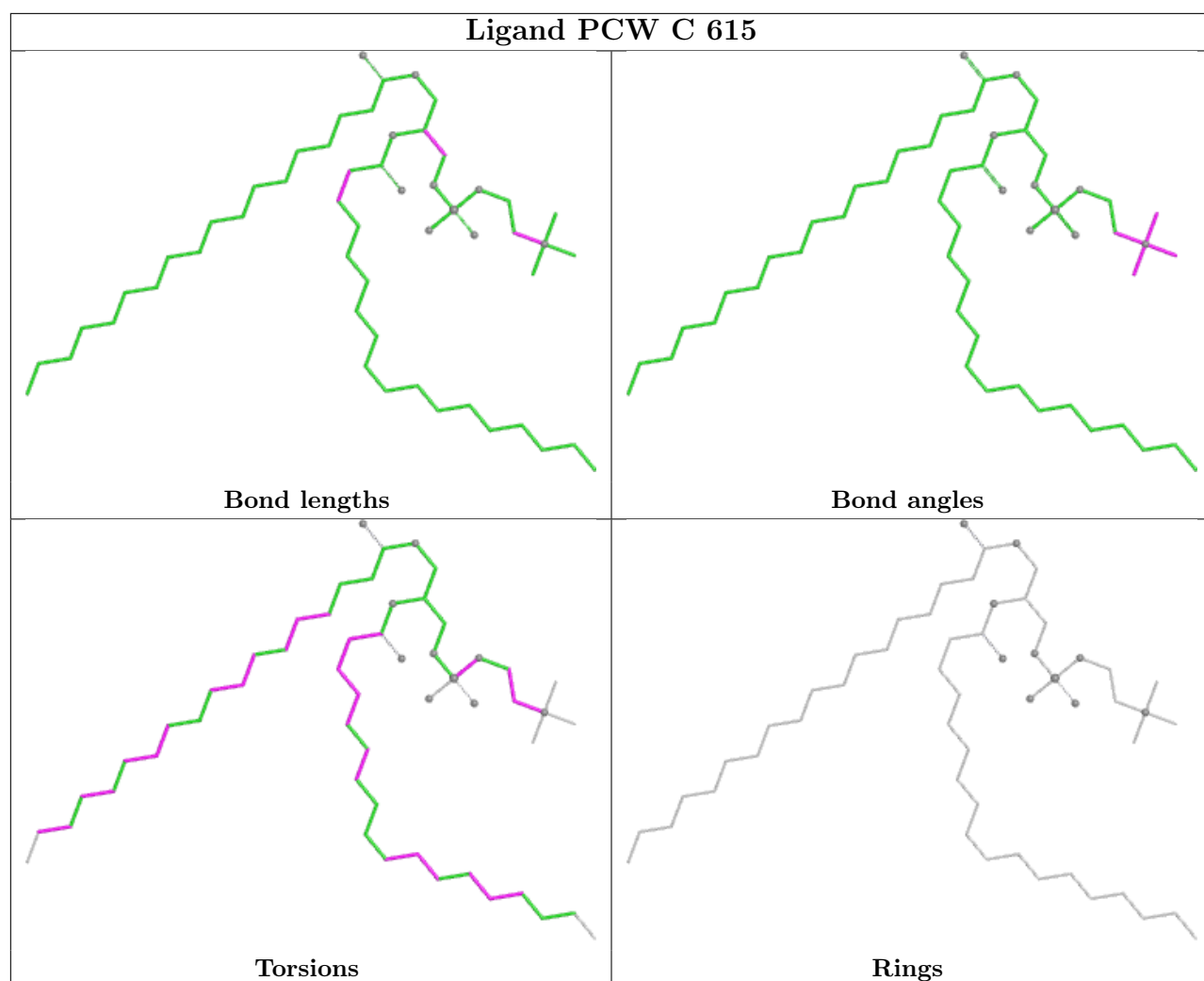


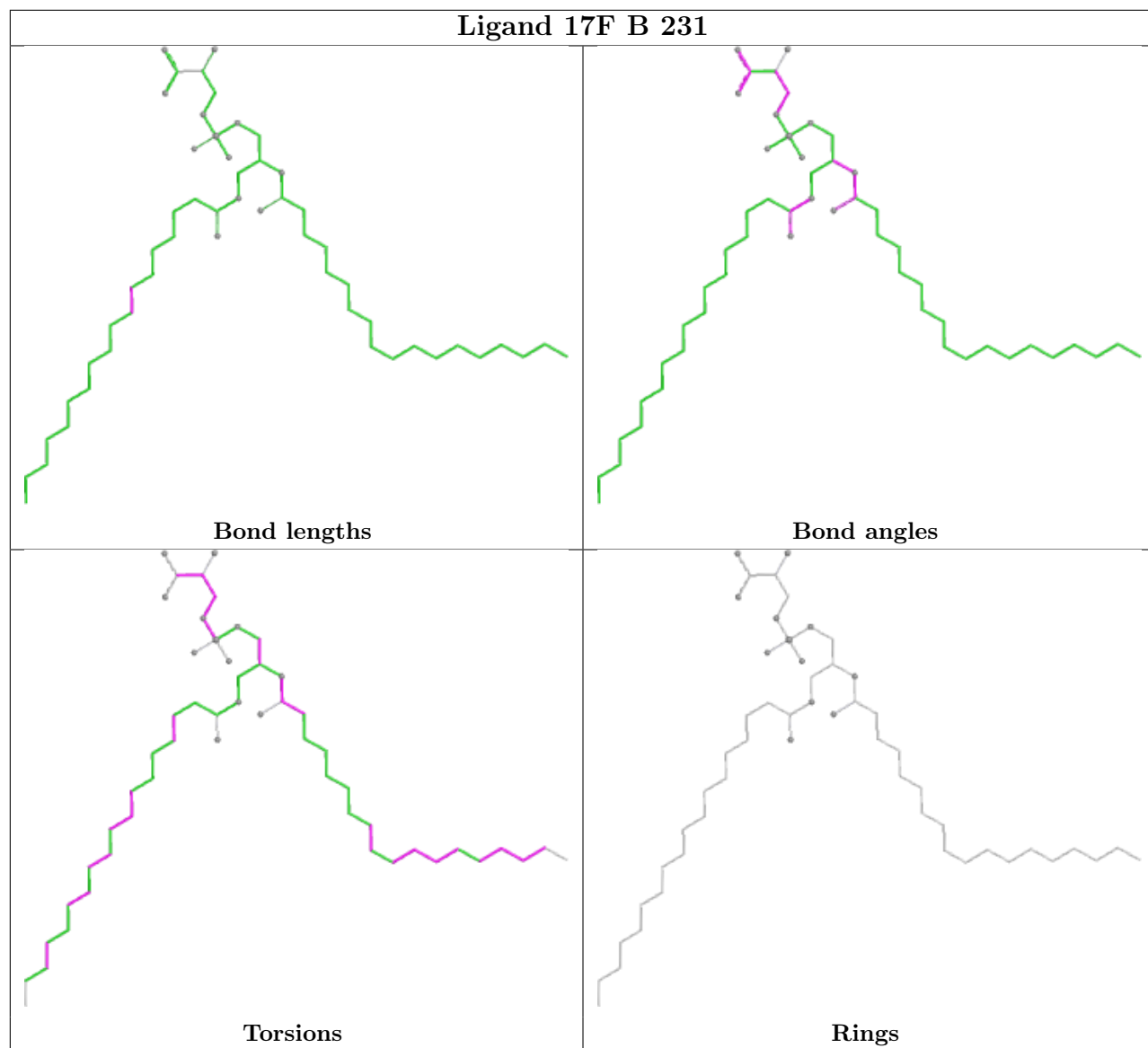


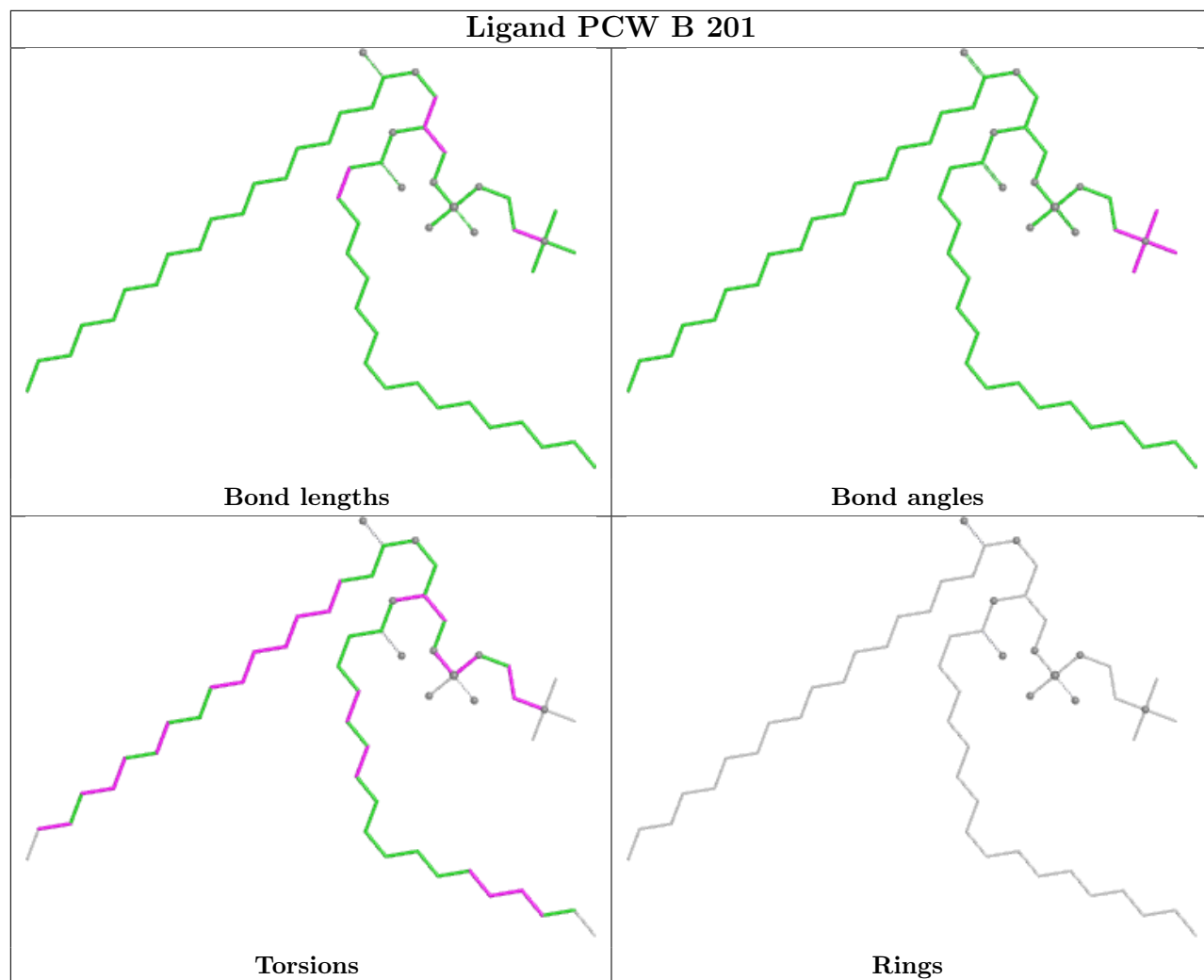


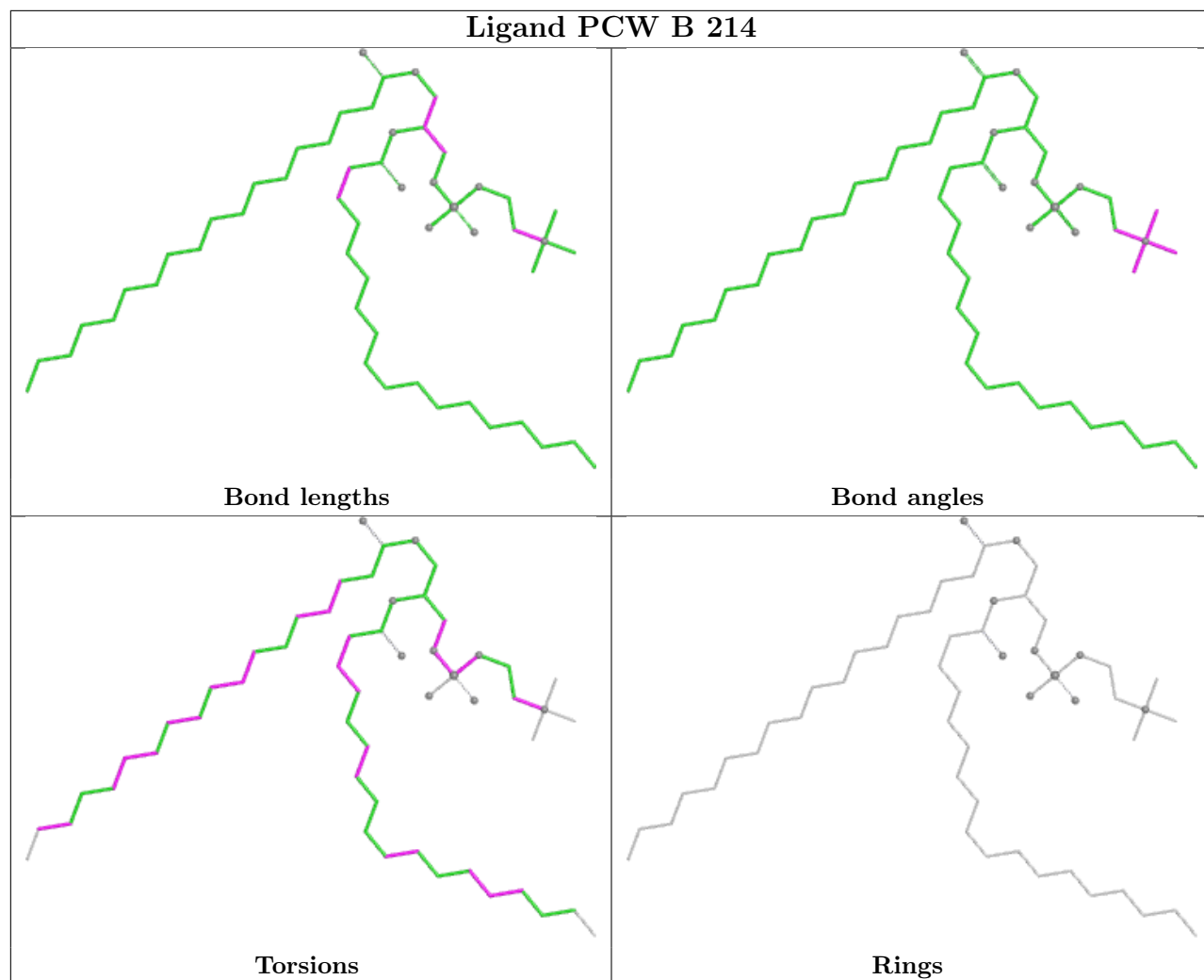


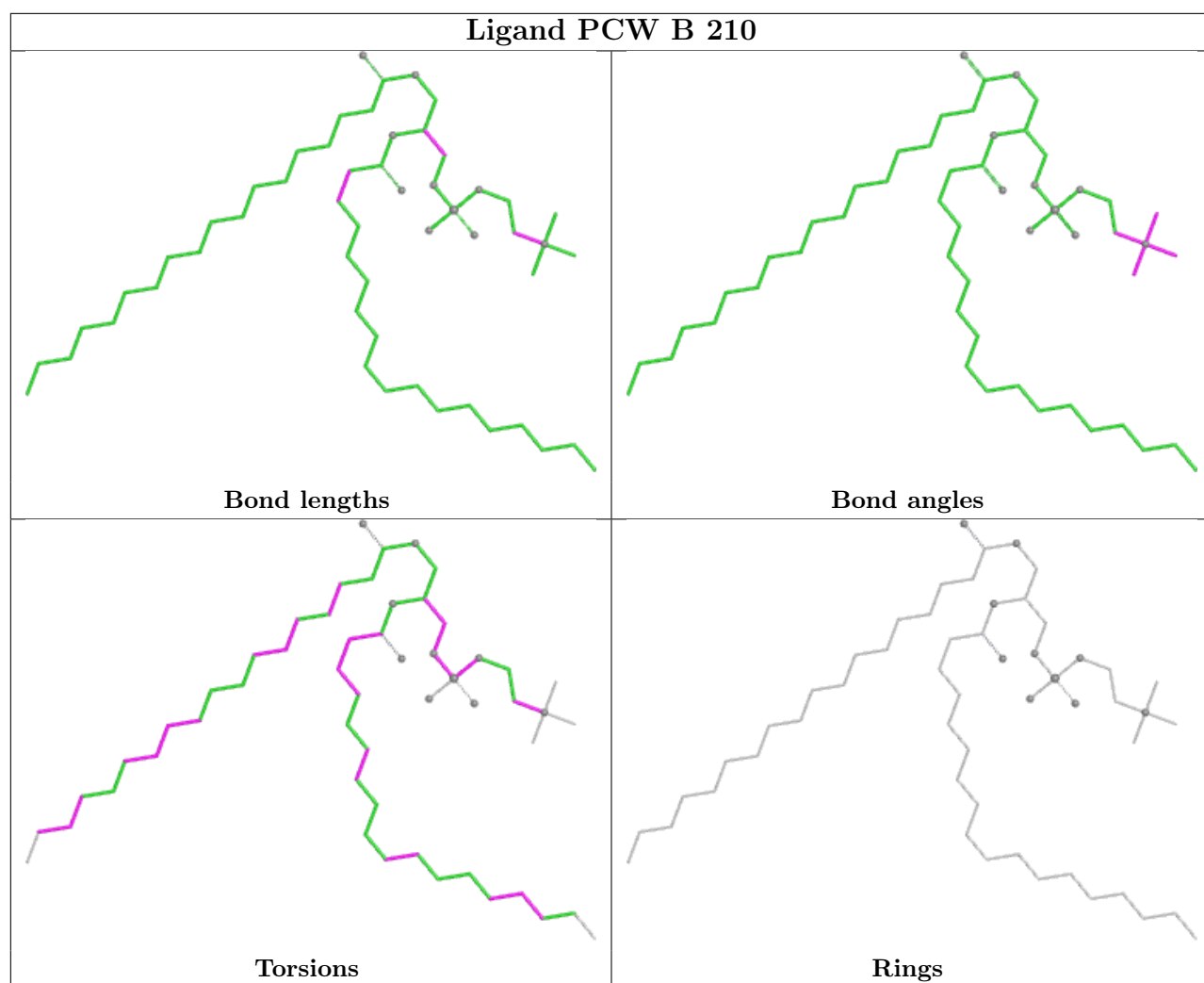


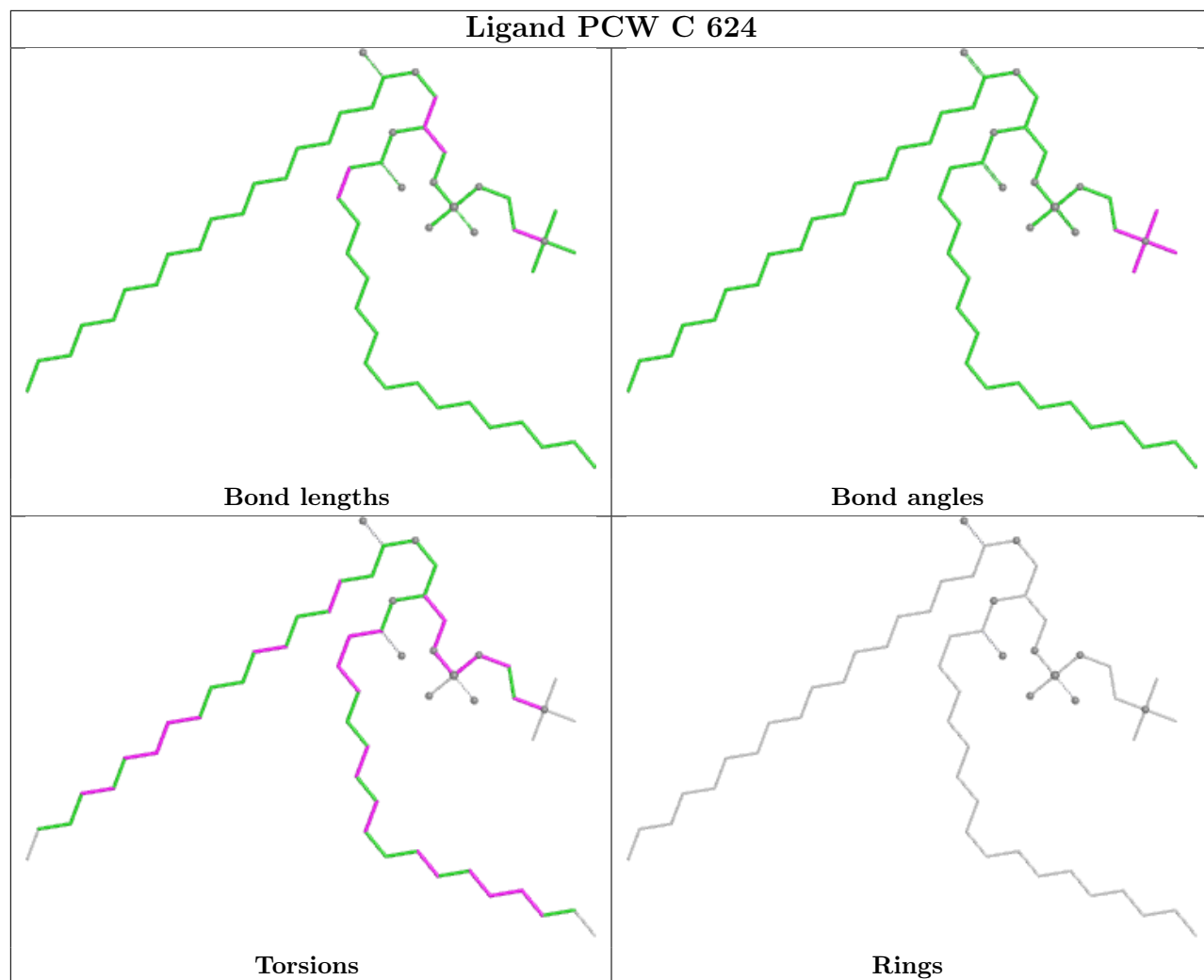


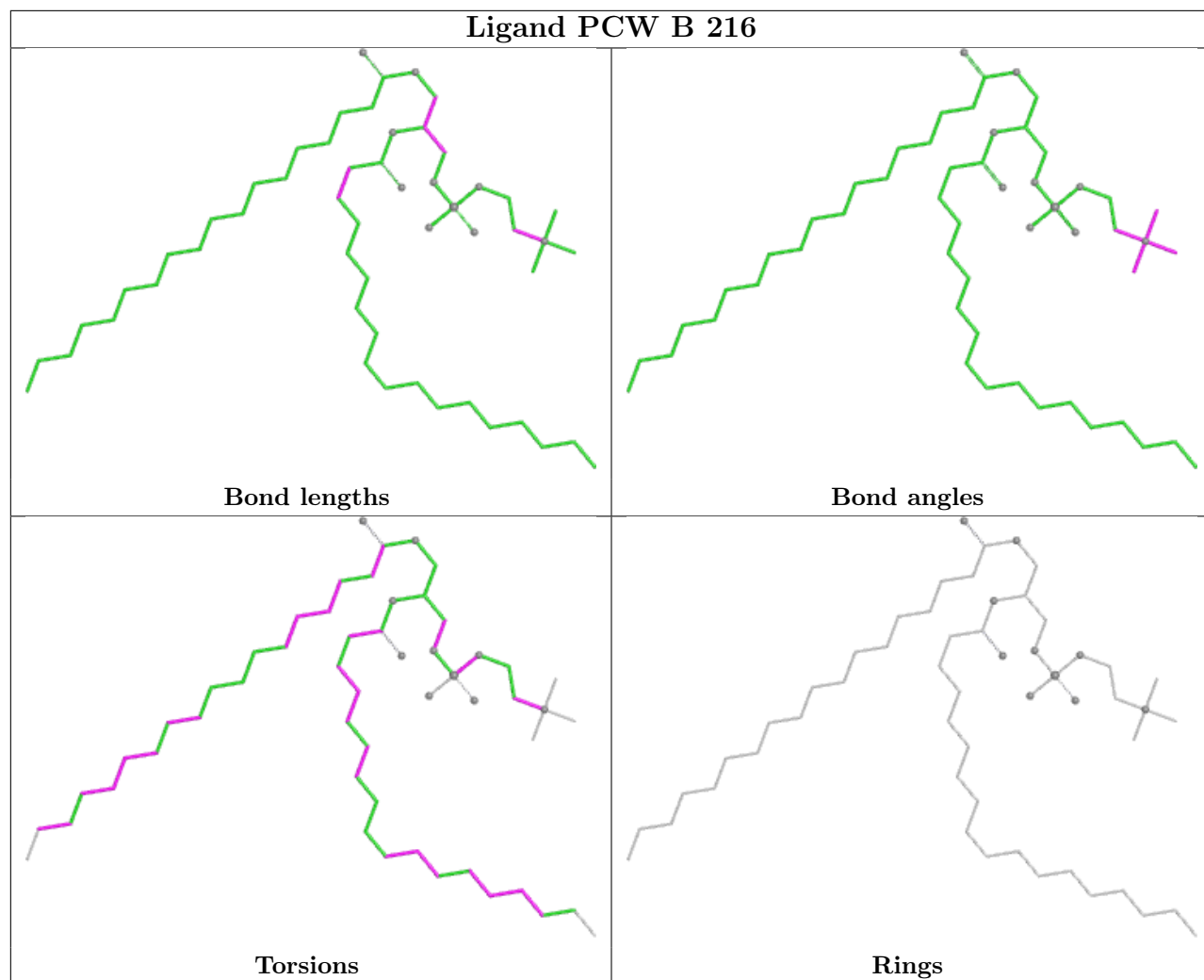


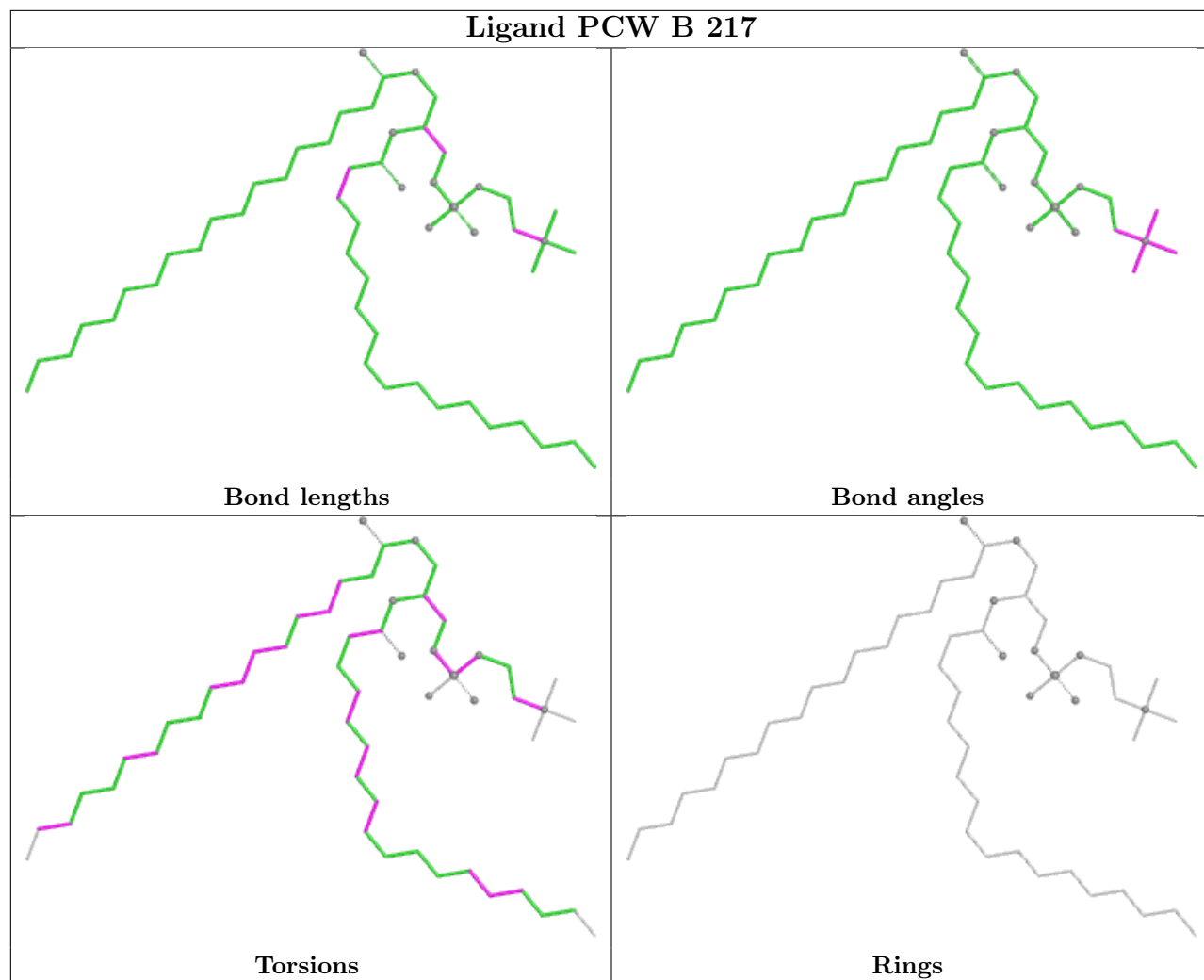


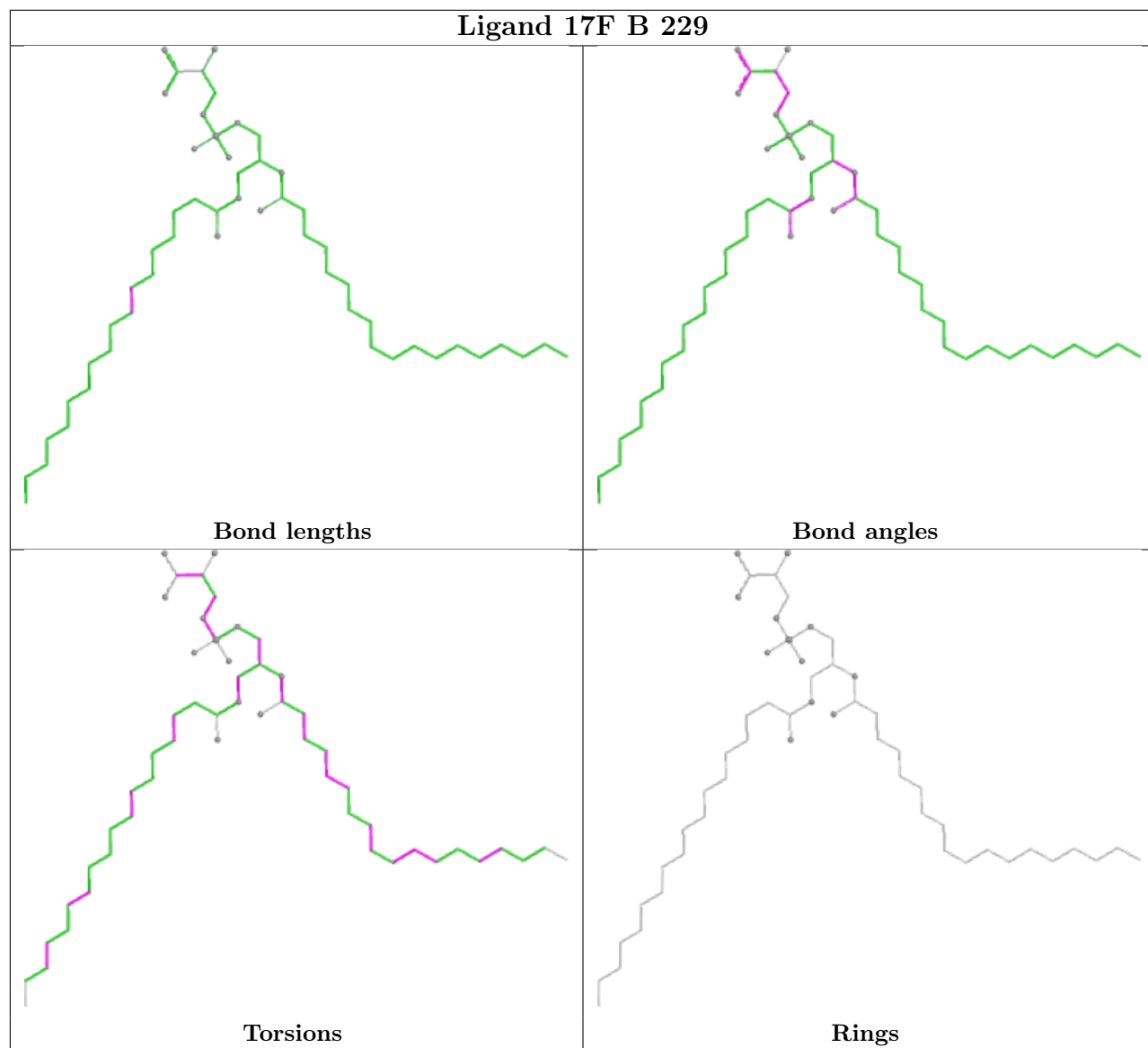


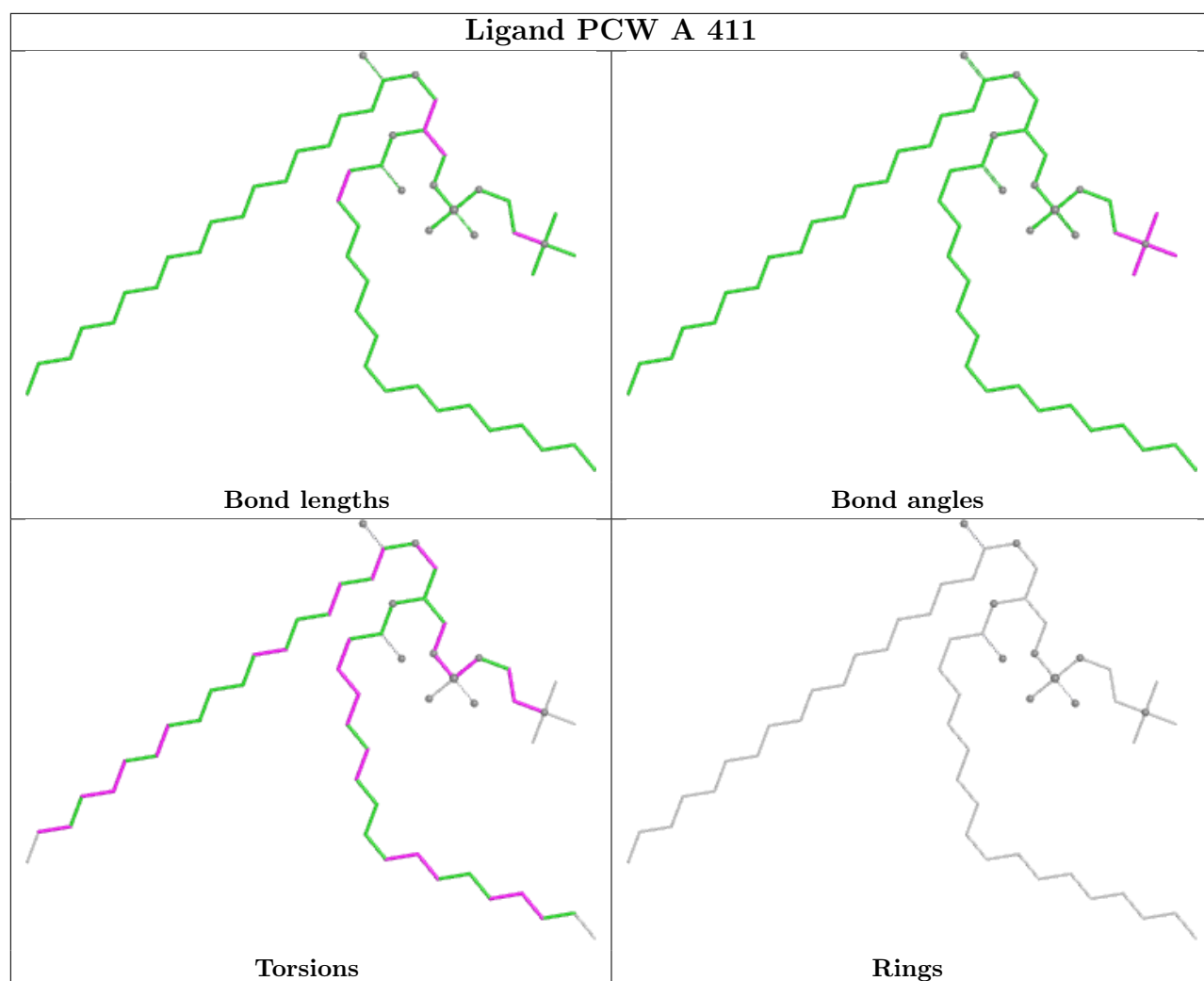


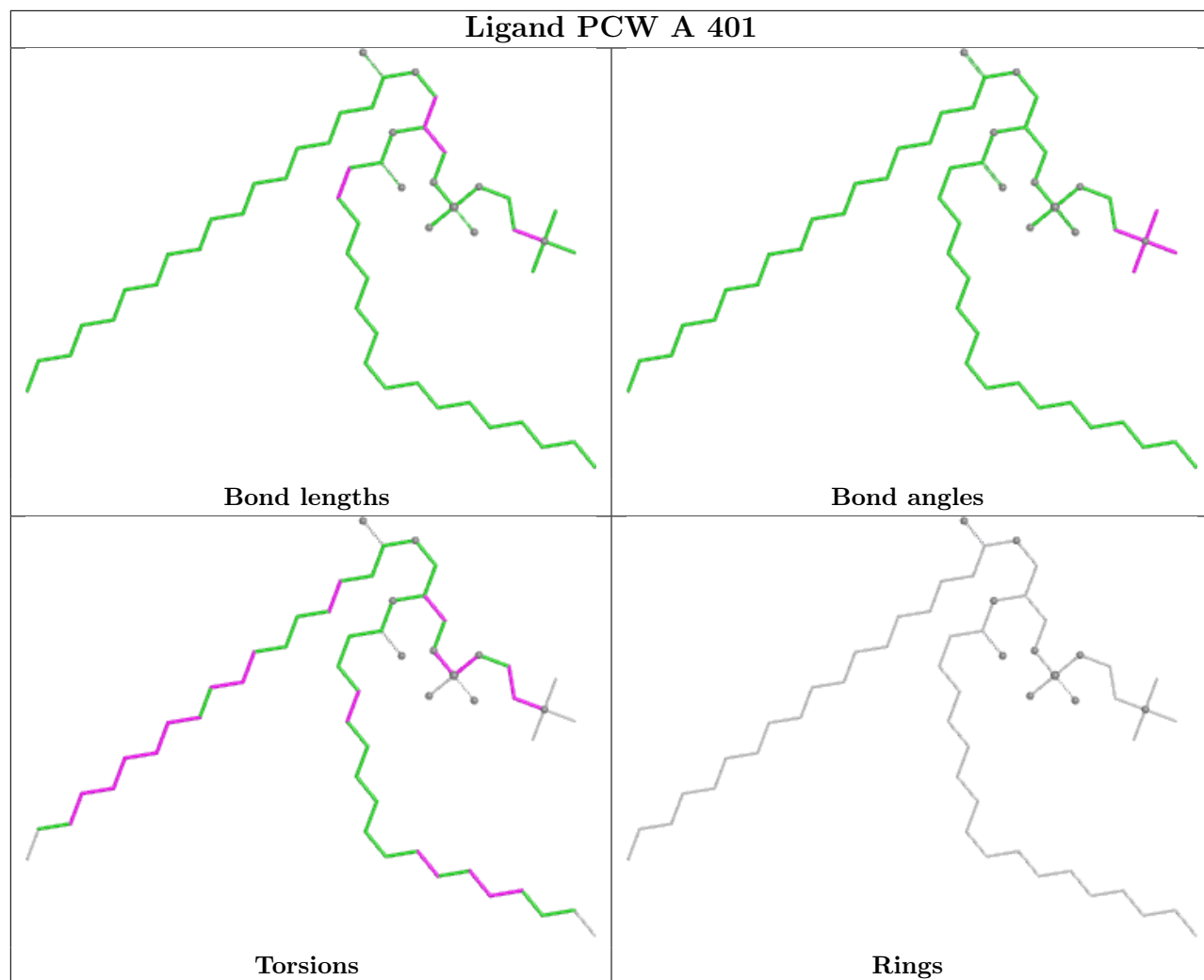


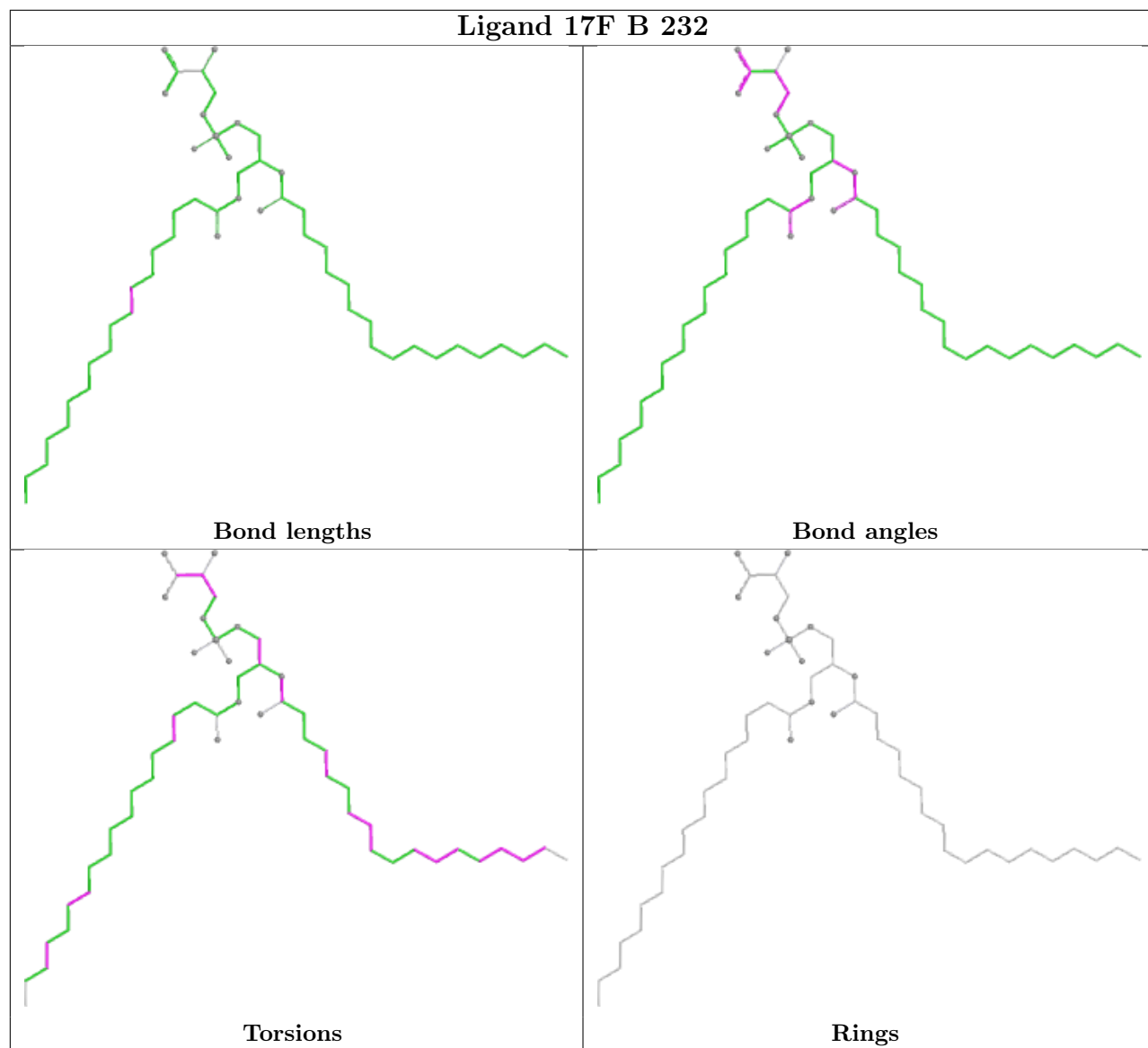


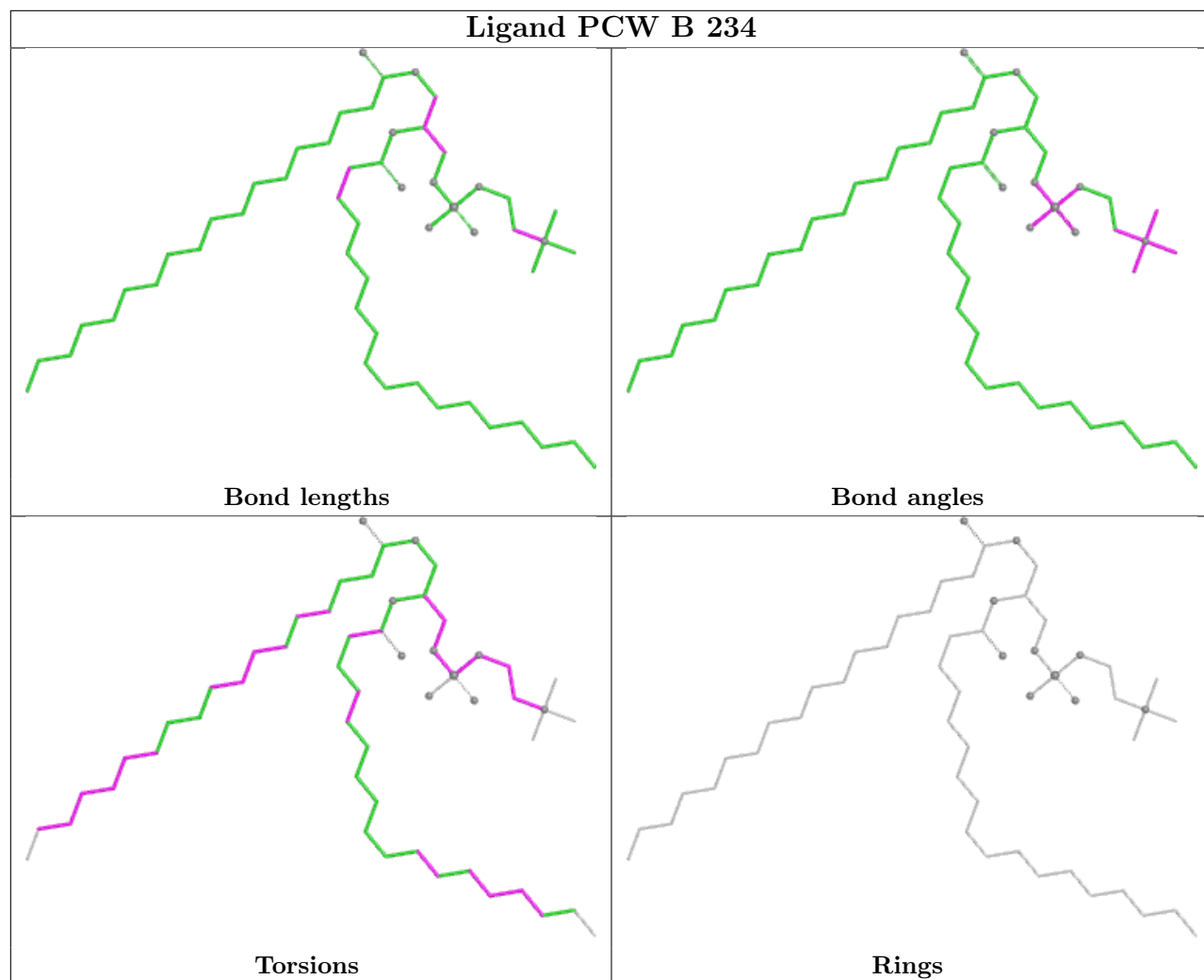


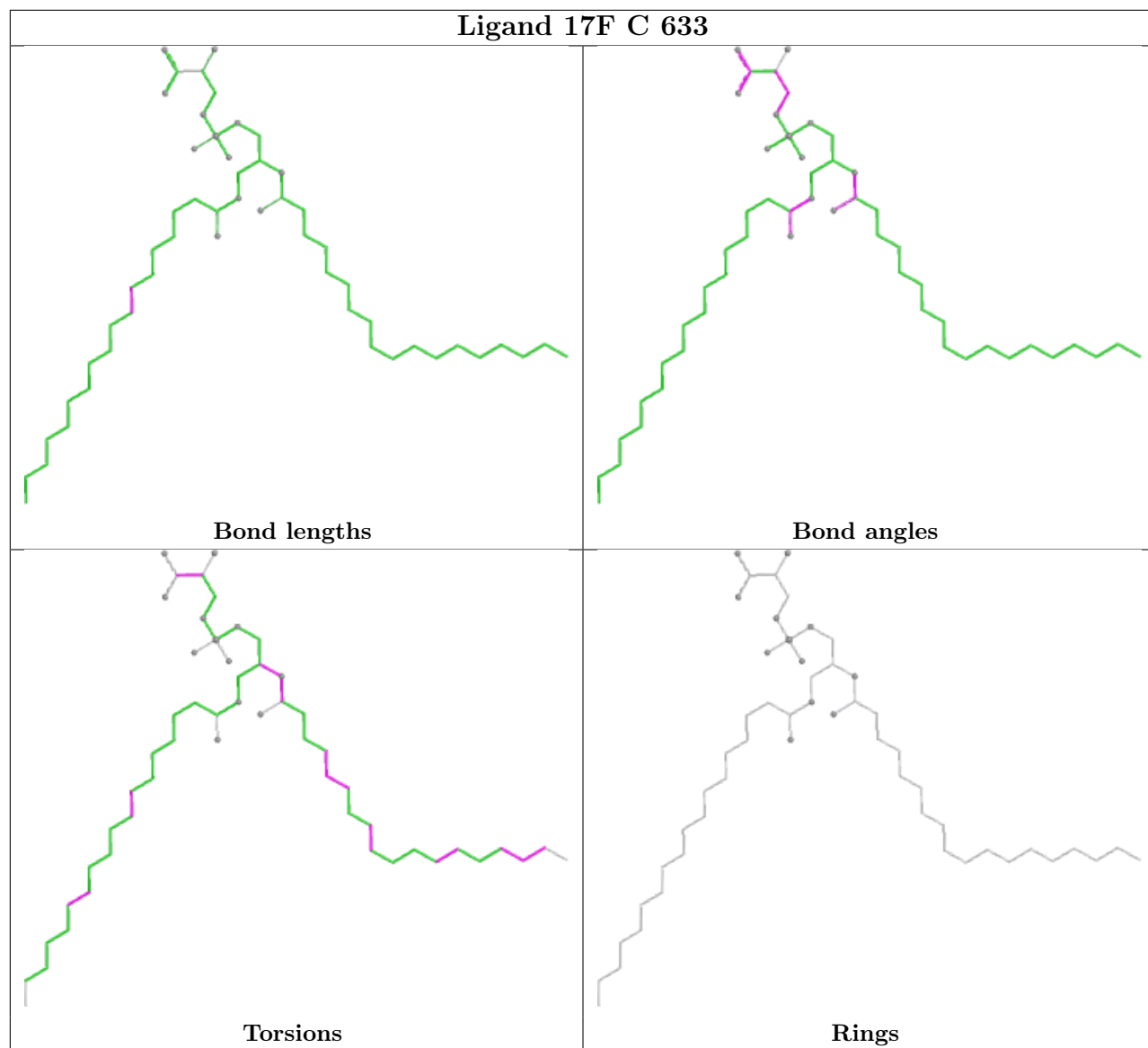


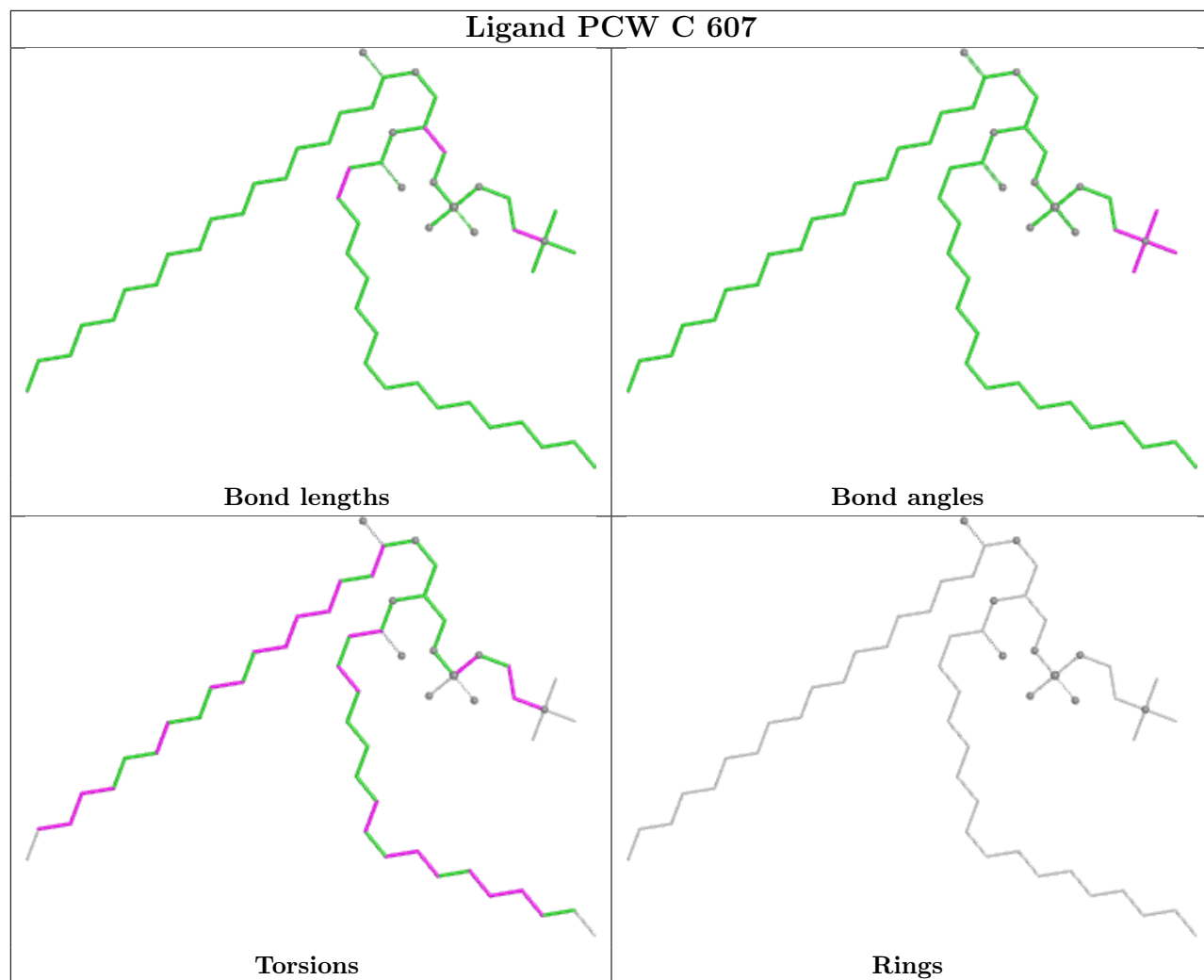


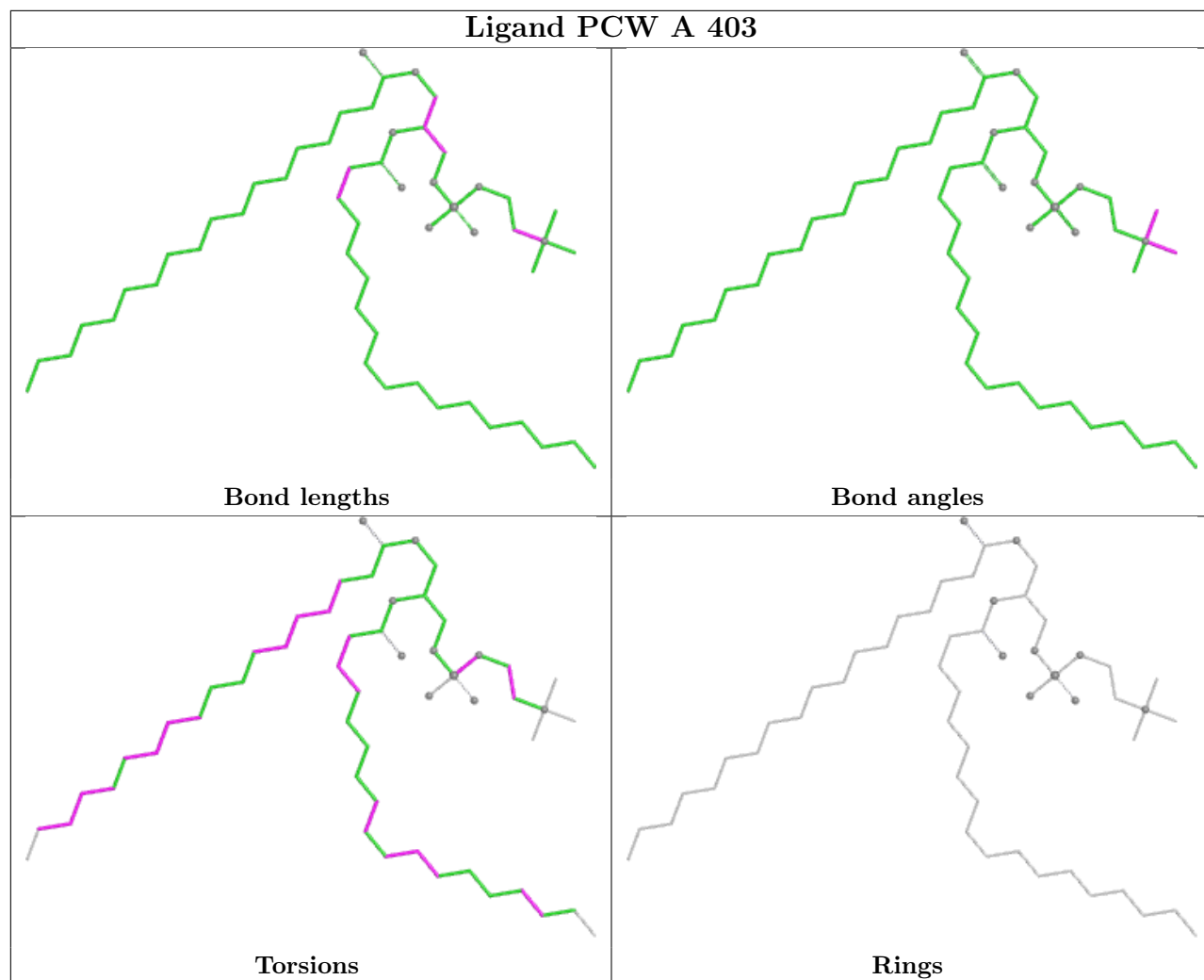


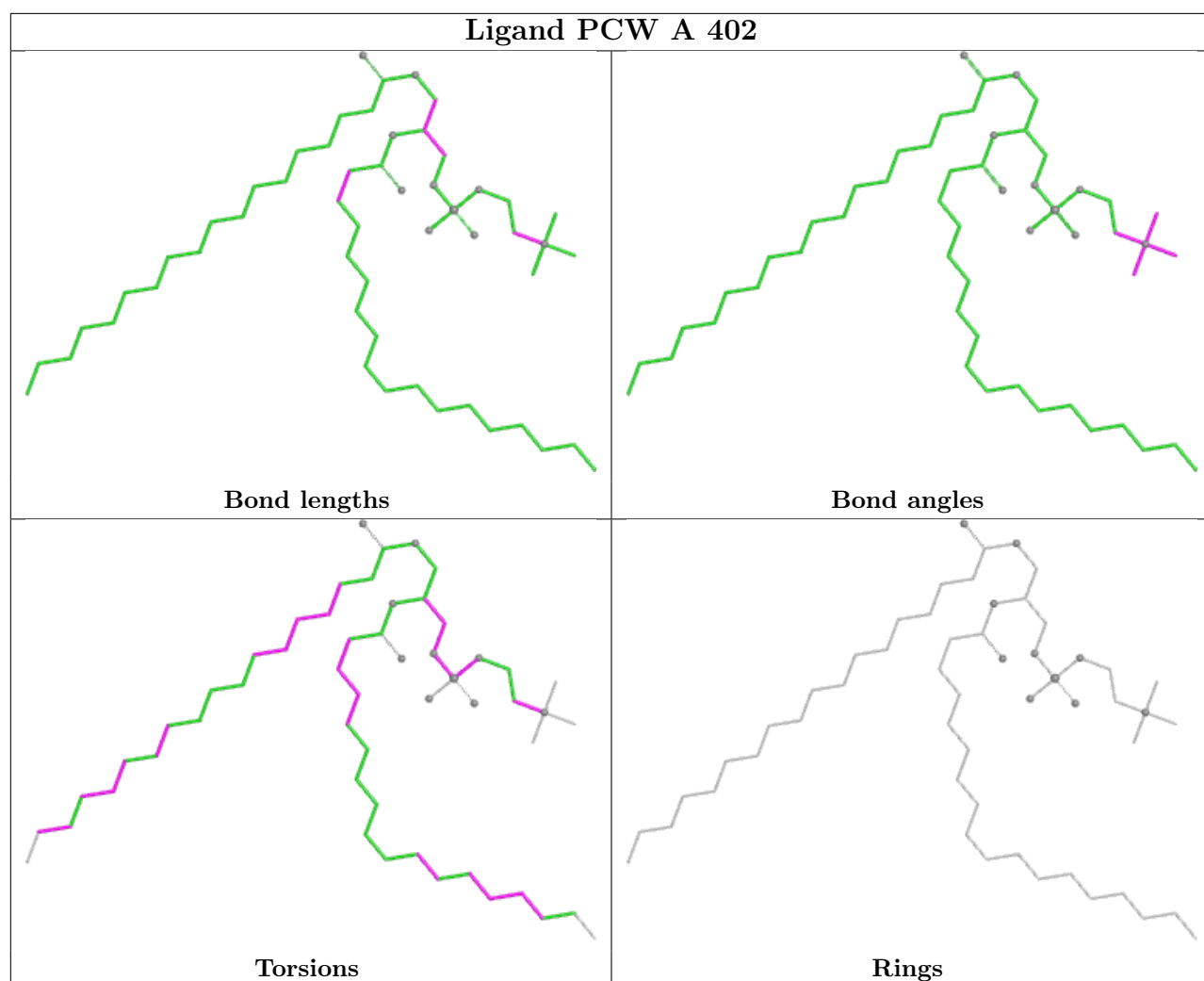












6.7 Other polymers [i](#)

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 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *resonance_list_nmrstar_50_51.txt*

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	268
Number of shifts mapped to atoms	193
Number of unparsed shifts	0
Number of shifts with mapping errors	75
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 75 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	6	LEU	HD21	0.865	?	.
1	B	6	LEU	HD22	0.865	?	.
1	B	6	LEU	HD23	0.865	?	.
1	B	14	VAL	HG11	0.892	?	.
1	B	14	VAL	HG12	0.892	?	.
1	B	14	VAL	HG13	0.892	?	.
1	B	19	LEU	HD11	0.547	?	.
1	B	19	LEU	HD12	0.547	?	.
1	B	19	LEU	HD13	0.547	?	.
1	B	21	ILE	HD11	0.513	?	1
1	B	21	ILE	HD12	0.513	?	1
1	B	21	ILE	HD13	0.513	?	1
1	B	23	LEU	HD11	-0.325	?	.
1	B	23	LEU	HD12	-0.325	?	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	23	LEU	HD13	-0.325	?	.
1	B	24	ILE	HD11	0.389	?	1
1	B	24	ILE	HD12	0.389	?	1
1	B	24	ILE	HD13	0.389	?	1
1	B	36	ILE	HD11	0.714	?	1
1	B	36	ILE	HD12	0.714	?	1
1	B	36	ILE	HD13	0.714	?	1
1	B	46	ILE	HD11	0.361	?	1
1	B	46	ILE	HD12	0.361	?	1
1	B	46	ILE	HD13	0.361	?	1
1	B	55	ILE	HD11	0.451	?	1
1	B	55	ILE	HD12	0.451	?	1
1	B	55	ILE	HD13	0.451	?	1
1	B	79	LEU	HD11	0.023	?	.
1	B	79	LEU	HD12	0.023	?	.
1	B	79	LEU	HD13	0.023	?	.
1	B	79	LEU	HD21	0.081	?	.
1	B	79	LEU	HD22	0.081	?	.
1	B	79	LEU	HD23	0.081	?	.
1	B	84	ILE	HD11	0.7	?	1
1	B	84	ILE	HD12	0.7	?	1
1	B	84	ILE	HD13	0.7	?	1
1	B	93	ILE	HD11	0.724	?	1
1	B	93	ILE	HD12	0.724	?	1
1	B	93	ILE	HD13	0.724	?	1
1	B	100	ILE	HD11	0.234	?	1
1	B	100	ILE	HD12	0.234	?	1
1	B	100	ILE	HD13	0.234	?	1
1	B	113	LEU	HD11	0.989	?	.
1	B	113	LEU	HD12	0.989	?	.
1	B	113	LEU	HD13	0.989	?	.
1	B	113	LEU	HD21	1.261	?	.
1	B	113	LEU	HD22	1.261	?	.
1	B	113	LEU	HD23	1.261	?	.
1	B	120	LEU	HD21	0.8	?	.
1	B	120	LEU	HD22	0.8	?	.
1	B	120	LEU	HD23	0.8	?	.
1	B	125	VAL	HG11	-0.21	?	.
1	B	125	VAL	HG12	-0.21	?	.
1	B	125	VAL	HG13	-0.21	?	.
1	B	133	LEU	HD11	0.344	?	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	133	LEU	HD12	0.344	?	.
1	B	133	LEU	HD13	0.344	?	.
1	B	133	LEU	HD21	0.39	?	.
1	B	133	LEU	HD22	0.39	?	.
1	B	133	LEU	HD23	0.39	?	.
1	B	139	ILE	HD11	0.809	?	1
1	B	139	ILE	HD12	0.809	?	1
1	B	139	ILE	HD13	0.809	?	1
1	B	142	ILE	HD11	0.618	?	1
1	B	142	ILE	HD12	0.618	?	1
1	B	142	ILE	HD13	0.618	?	1
1	B	159	LEU	HD11	0.613	?	.
1	B	159	LEU	HD12	0.613	?	.
1	B	159	LEU	HD13	0.613	?	.
1	B	160	VAL	HG11	-0.056	?	.
1	B	160	VAL	HG12	-0.056	?	.
1	B	160	VAL	HG13	-0.056	?	.
1	B	163	ILE	HD11	0.612	?	1
1	B	163	ILE	HD12	0.612	?	1
1	B	163	ILE	HD13	0.612	?	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	84	-0.47 ± 0.76	None needed (< 0.5 ppm)

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 3%, i.e. 254 atoms were assigned a chemical shift out of a possible 7385. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	154/2608 (6%)	77/1053 (7%)	0/1048 (0%)	77/507 (15%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	100/4339 (2%)	75/2790 (3%)	25/1354 (2%)	0/195 (0%)
Aromatic	0/438 (0%)	0/222 (0%)	0/208 (0%)	0/8 (0%)
Overall	254/7385 (3%)	152/4065 (4%)	25/2610 (1%)	77/710 (11%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 268 atoms were assigned a chemical shift out of a possible 8192. 0 out of 109 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	168/2894 (6%)	84/1169 (7%)	0/1162 (0%)	84/563 (15%)
Sidechain	100/4818 (2%)	75/3094 (2%)	25/1508 (2%)	0/216 (0%)
Aromatic	0/480 (0%)	0/244 (0%)	0/228 (0%)	0/8 (0%)
Overall	268/8192 (3%)	159/4507 (4%)	25/2898 (1%)	84/787 (11%)

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:

