



## wwPDB EM Validation Summary Report ⓘ

Oct 21, 2023 – 12:36 PM EDT

PDB ID : 8SS3  
EMDB ID : EMD-40742  
Title : Structure of LBD-TMD of AMPA receptor GluA2 in complex with auxiliary subunits TARP gamma-5 and cornichon-2 bound to competitive antagonist ZK and channel blocker spermidine (closed state)  
Authors : Gangwar, S.P.; Yen, L.Y.; Yelshanskaya, M.V.; Sobolevsky, A.I.  
Deposited on : 2023-05-08  
Resolution : 3.21 Å (reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

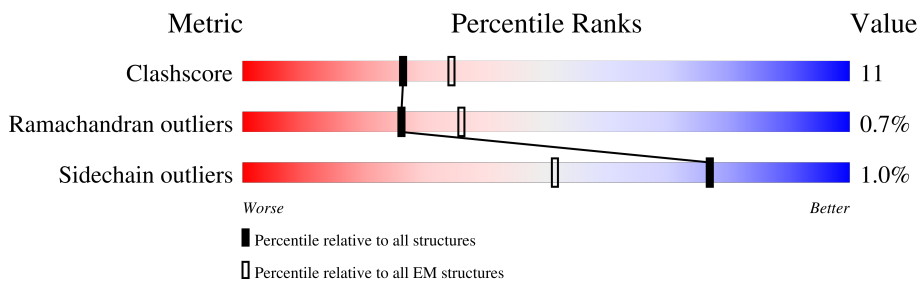
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1026	 19% 51% 7% 42%
1	B	1026	 35% 5% 61%
1	C	1026	 19% 51% 7% 42%
1	D	1026	 34% 5% 61%
2	E	160	 19% 72% 12% .. 12%
2	F	160	 18% 72% 12% .. 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLR	A	1107	X	-	-	-
5	CLR	A	1112	X	-	-	-
5	CLR	C	1106	X	-	-	-
5	CLR	C	1111	X	-	-	-
6	AJP	A	1110	X	-	X	-
6	AJP	A	1111	X	-	X	-
6	AJP	A	1116	X	-	X	-
6	AJP	C	1109	X	-	X	-
6	AJP	C	1110	X	-	X	-
6	AJP	C	1114	X	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19887 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	596	4671	3049	753	838	31	0	0
1	B	404	3156	2048	511	576	21	0	0
1	C	596	4671	3049	753	838	31	0	0
1	D	404	3156	2048	511	576	21	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	754	SER	ASN	conflict	UNP P19491
A	758	VAL	LEU	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
A	830	SER	-	linker	UNP P19491
A	831	ALA	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	754	SER	ASN	conflict	UNP P19491
B	758	VAL	LEU	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
B	830	SER	-	linker	UNP P19491
B	831	ALA	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	754	SER	ASN	conflict	UNP P19491
C	758	VAL	LEU	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
C	830	SER	-	linker	UNP P19491
C	831	ALA	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491

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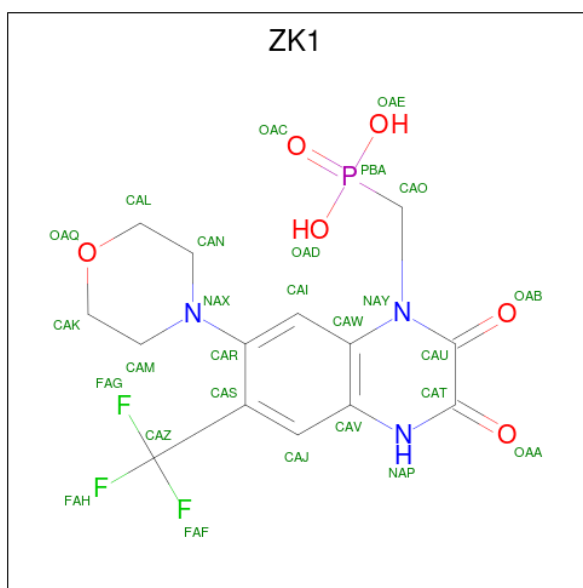
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Chain	Residue	Modelled	Actual	Comment	Reference
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	754	SER	ASN	conflict	UNP P19491
D	758	VAL	LEU	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
D	830	SER	-	linker	UNP P19491
D	831	ALA	-	linker	UNP P19491

- Molecule 2 is a protein called Protein cornichon homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	140	Total	C	N	O	S	0	0
			1166	787	175	191	13		
2	F	140	Total	C	N	O	S	0	0
			1166	787	175	191	13		

- Molecule 3 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C<sub>14</sub>H<sub>15</sub>F<sub>3</sub>N<sub>3</sub>O<sub>6</sub>P) (labeled as "Ligand of Interest" by depositor).



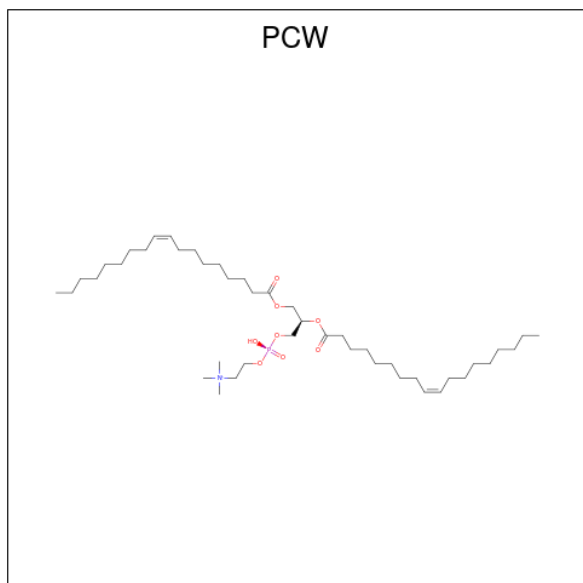
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	F	N	O		P
3	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

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Mol	Chain	Residues	Atoms					AltConf	
3	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula:  $C_{44}H_{85}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C				0
			11	11				
4	A	1	Total	C				0
			11	11				
4	A	1	Total	C				0
			11	11				
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C				0
			11	11				
4	A	1	Total	C				0
			11	11				
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C				0
			11	11				
4	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	B	1	Total	C	N	O	P	0
			32	22	1	8	1	
4	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	B	1	Total	C				0
			11	11				
4	B	1	Total	C				0
			11	11				
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	C	1	Total	C				0
			11	11				
4	C	1	Total	C				0
			11	11				
4	C	1	Total	C				0
			11	11				
4	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	C	1	Total	C				0
			11	11				

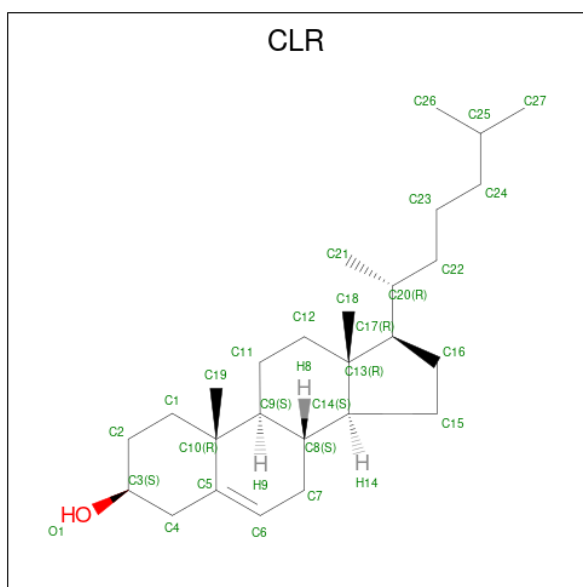
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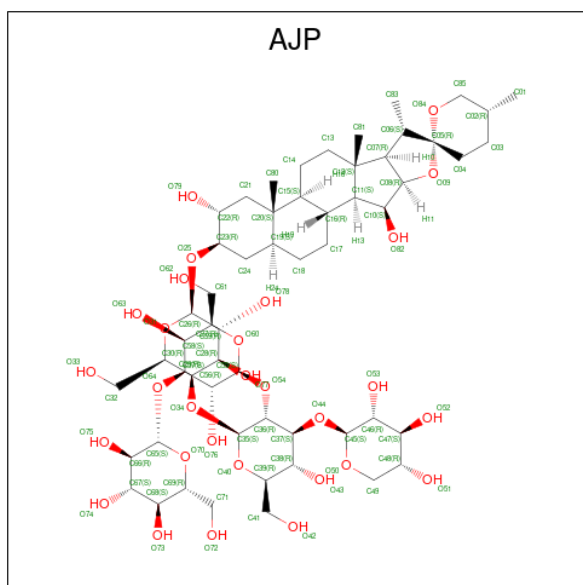
Mol	Chain	Residues	Atoms	AltConf
4	C	1	Total C 11 11	0
4	D	1	Total C 11 11	0
4	D	1	Total C N O P 41 31 1 8 1	0
4	D	1	Total C N O P 43 33 1 8 1	0
4	D	1	Total C N O P 32 22 1 8 1	0
4	D	1	Total C N O P 41 31 1 8 1	0
4	D	1	Total C N O P 39 29 1 8 1	0
4	D	1	Total C 11 11	0
4	D	1	Total C N O P 51 41 1 8 1	0
4	D	1	Total C 11 11	0
4	E	1	Total C 11 11	0
4	E	1	Total C 11 11	0
4	E	1	Total C N O P 43 33 1 8 1	0
4	E	1	Total C 11 11	0
4	E	1	Total C 11 11	0
4	F	1	Total C 11 11	0
4	F	1	Total C N O P 43 33 1 8 1	0
4	F	1	Total C 11 11	0
4	F	1	Total C 11 11	0
4	F	1	Total C 11 11	0

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



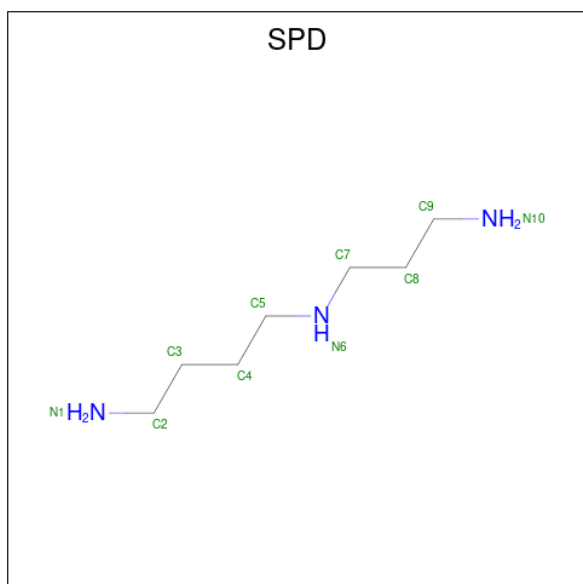
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	C	1	Total	C	O	0
			28	27	1	
5	C	1	Total	C	O	0
			28	27	1	

- Molecule 6 is Digitonin (three-letter code: AJP) (formula:  $C_{56}H_{92}O_{29}$ ).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			42	33	9	
6	A	1	Total	C	O	0
			42	33	9	
6	A	1	Total	C	O	0
			42	33	9	
6	C	1	Total	C	O	0
			41	33	8	
6	C	1	Total	C	O	0
			42	33	9	
6	C	1	Total	C	O	0
			42	33	9	

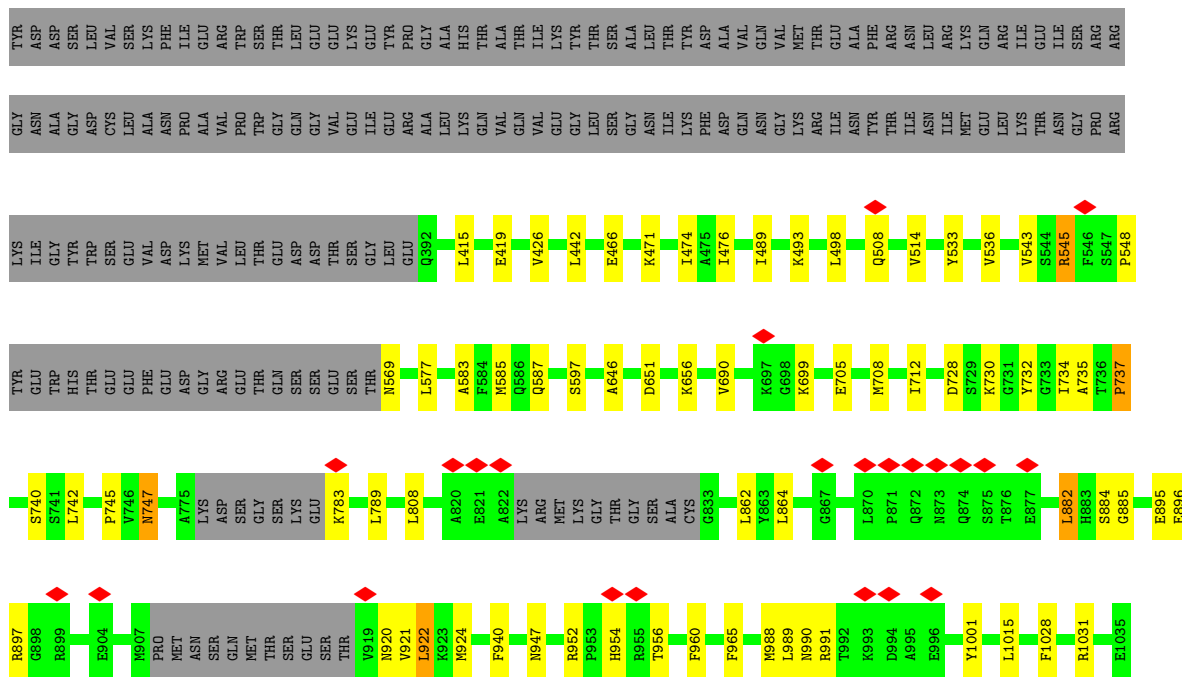
- Molecule 7 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



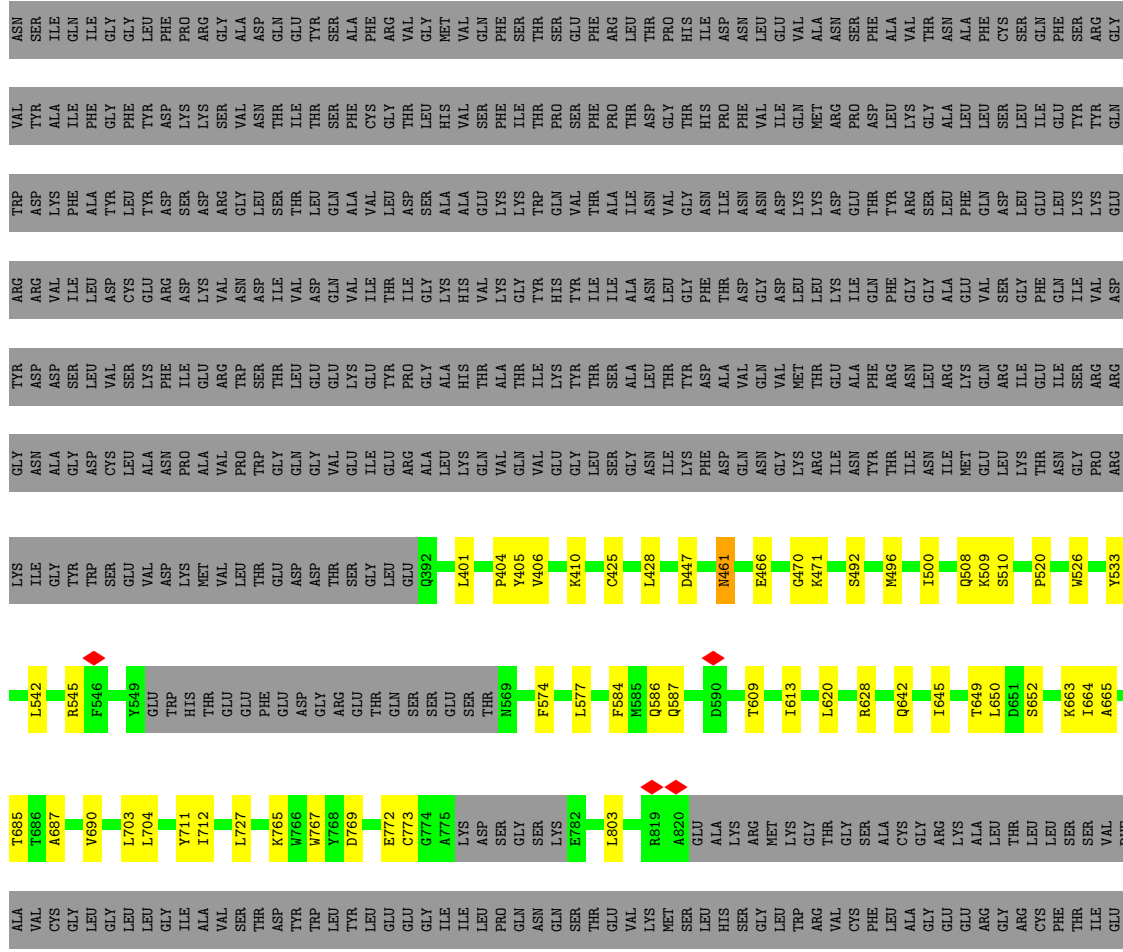
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	N	0
			10	7	3	







● Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	81723	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.924	Depositor
Minimum map value	-1.802	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.25	Depositor
Map size ( $\text{\AA}$ )	345.28, 345.28, 345.28	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, CLR, PCW, AJP, ZK1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	0/4774	0.64	3/6446 (0.0%)
1	B	0.52	0/3224	0.64	1/4350 (0.0%)
1	C	0.52	0/4774	0.64	3/6446 (0.0%)
1	D	0.52	0/3224	0.64	1/4350 (0.0%)
2	E	0.38	0/1203	0.61	0/1636
2	F	0.38	0/1203	0.61	0/1636
All	All	0.51	0/18402	0.64	8/24864 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	3
2	E	0	4
2	F	0	4
All	All	0	18

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	704	LEU	CA-CB-CG	5.93	128.94	115.30
1	D	704	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	1015	LEU	CA-CB-CG	5.19	127.24	115.30
1	C	1015	LEU	CA-CB-CG	5.19	127.23	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	882	LEU	CB-CG-CD2	-5.09	102.34	111.00

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	545	ARG	Peptide
1	A	922	LEU	Peptide
1	B	510	SER	Peptide
1	B	663	LYS	Peptide
1	B	772	GLU	Peptide

## 5.2 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 the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4671	0	4745	43	0
1	B	3156	0	3201	28	0
1	C	4671	0	4745	43	0
1	D	3156	0	3201	32	0
2	E	1166	0	1152	13	0
2	F	1166	0	1152	14	0
3	A	27	0	13	2	0
3	B	27	0	13	0	0
3	C	27	0	13	1	0
3	D	27	0	13	0	0
4	A	394	0	566	22	0
4	B	331	0	450	18	0
4	C	241	0	341	16	0
4	D	280	0	375	15	0
4	E	87	0	121	4	0
4	F	87	0	121	6	0
5	A	56	0	74	9	0
5	C	56	0	74	9	0
6	A	126	0	0	108	0
6	C	125	0	0	107	0
7	A	10	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19887	0	20389	447	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 447 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1107:CLR:C14	5:A:1107:CLR:C15	1.75	1.63
5:A:1107:CLR:C15	5:A:1107:CLR:C16	1.77	1.61
6:C:1109:AJP:C19	6:C:1109:AJP:C24	1.78	1.61
5:C:1106:CLR:C15	5:C:1106:CLR:C16	1.77	1.61
6:C:1114:AJP:C14	6:C:1114:AJP:C15	1.79	1.61

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	586/1026 (57%)	538 (92%)	46 (8%)	2 (0%)	41 74
1	B	398/1026 (39%)	369 (93%)	27 (7%)	2 (0%)	29 66
1	C	586/1026 (57%)	538 (92%)	46 (8%)	2 (0%)	41 74
1	D	398/1026 (39%)	369 (93%)	27 (7%)	2 (0%)	29 66
2	E	136/160 (85%)	120 (88%)	12 (9%)	4 (3%)	4 27
2	F	136/160 (85%)	120 (88%)	12 (9%)	4 (3%)	4 27
All	All	2240/4424 (51%)	2054 (92%)	170 (8%)	16 (1%)	26 60

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	773	CYS
1	D	773	CYS
2	E	116	MET
2	E	117	TYR
2	F	116	MET

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	504/877 (58%)	498 (99%)	6 (1%)	71	87
1	B	340/877 (39%)	338 (99%)	2 (1%)	86	93
1	C	504/877 (58%)	498 (99%)	6 (1%)	71	87
1	D	340/877 (39%)	338 (99%)	2 (1%)	86	93
2	E	126/143 (88%)	124 (98%)	2 (2%)	62	83
2	F	126/143 (88%)	124 (98%)	2 (2%)	62	83
All	All	1940/3794 (51%)	1920 (99%)	20 (1%)	77	89

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	410	LYS
2	E	124	ASN
2	F	124	ASN
2	F	122	ILE
1	B	410	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	586	GLN
2	E	124	ASN
2	F	124	ASN
2	F	75	HIS

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Mol	Chain	Res	Type
2	E	94	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

65 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PCW	A	1105	-	50,50,53	1.14	4 (8%)	56,58,61	1.06	3 (5%)
4	PCW	B	1105	-	31,31,53	1.23	2 (6%)	36,39,61	1.36	3 (8%)
4	PCW	D	1107	-	38,38,53	1.26	5 (13%)	43,46,61	1.23	4 (9%)
4	PCW	D	1109	-	50,50,53	1.18	4 (8%)	56,58,61	0.94	3 (5%)
3	ZK1	A	1101	-	28,29,29	2.73	8 (28%)	42,45,45	1.92	9 (21%)
4	PCW	A	1113	-	50,50,53	1.18	4 (8%)	56,58,61	1.00	3 (5%)
4	PCW	D	1108	-	10,10,53	0.77	0	9,9,61	0.37	0
4	PCW	D	1110	-	10,10,53	0.79	0	9,9,61	0.31	0
5	CLR	C	1111	-	31,31,31	9.03	22 (70%)	48,48,48	3.98	26 (54%)
4	PCW	F	204	-	10,10,53	0.80	0	9,9,61	0.29	0
4	PCW	C	1105	-	10,10,53	0.78	0	9,9,61	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PCW	D	1105	-	31,31,53	1.23	2 (6%)	36,39,61	1.40	4 (11%)
4	PCW	B	1111	-	50,50,53	1.12	3 (6%)	56,58,61	1.01	4 (7%)
3	ZK1	B	1102	-	28,29,29	2.77	8 (28%)	42,45,45	1.83	9 (21%)
4	PCW	C	1107	-	10,10,53	0.76	0	9,9,61	0.35	0
4	PCW	D	1101	-	10,10,53	0.72	0	9,9,61	0.42	0
4	PCW	E	204	-	10,10,53	0.78	0	9,9,61	0.38	0
4	PCW	B	1106	-	40,40,53	1.27	5 (12%)	45,48,61	1.17	3 (6%)
4	PCW	D	1103	-	40,40,53	1.22	3 (7%)	46,48,61	1.05	3 (6%)
6	AJP	C	1110	-	48,48,95	19.05	41 (85%)	71,78,149	3.10	36 (50%)
4	PCW	E	203	-	42,42,53	1.25	4 (9%)	48,50,61	1.06	3 (6%)
4	PCW	A	1106	-	10,10,53	0.78	0	9,9,61	0.35	0
4	PCW	A	1115	-	10,10,53	0.78	0	9,9,61	0.34	0
4	PCW	D	1106	-	40,40,53	1.26	5 (12%)	45,48,61	1.18	3 (6%)
4	PCW	F	205	-	10,10,53	0.78	0	9,9,61	0.35	0
4	PCW	C	1113	-	10,10,53	0.77	0	9,9,61	0.34	0
4	PCW	C	1112	-	50,50,53	1.18	4 (8%)	56,58,61	0.99	3 (5%)
4	PCW	A	1103	-	42,42,53	1.22	4 (9%)	48,50,61	0.99	3 (6%)
3	ZK1	C	1101	-	28,29,29	2.72	8 (28%)	42,45,45	1.90	9 (21%)
7	SPD	A	1119	-	9,9,9	0.32	0	8,8,8	0.51	0
4	PCW	A	1118	-	50,50,53	1.17	4 (8%)	56,58,61	0.93	3 (5%)
4	PCW	B	1110	-	50,50,53	1.14	4 (8%)	56,58,61	1.06	3 (5%)
4	PCW	F	203	-	10,10,53	0.79	0	9,9,61	0.38	0
5	CLR	C	1106	-	31,31,31	9.02	22 (70%)	48,48,48	4.23	24 (50%)
4	PCW	A	1117	-	10,10,53	0.80	0	9,9,61	0.28	0
4	PCW	C	1108	-	10,10,53	0.79	0	9,9,61	0.28	0
4	PCW	A	1102	-	50,50,53	1.15	3 (6%)	56,58,61	0.98	3 (5%)
4	PCW	E	205	-	10,10,53	0.81	0	9,9,61	0.28	0
6	AJP	C	1109	-	47,47,95	17.09	38 (80%)	70,76,149	3.04	30 (42%)
4	PCW	A	1104	-	40,40,53	1.23	4 (10%)	46,48,61	1.10	3 (6%)
3	ZK1	D	1102	-	28,29,29	2.77	7 (25%)	42,45,45	1.83	10 (23%)
6	AJP	A	1116	-	48,48,95	18.83	40 (83%)	71,78,149	3.25	34 (47%)
4	PCW	B	1104	-	42,42,53	1.18	3 (7%)	48,50,61	1.16	3 (6%)
4	PCW	A	1109	-	10,10,53	0.80	0	9,9,61	0.28	0
5	CLR	A	1112	-	31,31,31	9.03	22 (70%)	48,48,48	3.97	24 (50%)
6	AJP	A	1111	-	48,48,95	18.86	41 (85%)	71,78,149	3.11	35 (49%)
4	PCW	A	1108	-	10,10,53	0.76	0	9,9,61	0.34	0
4	PCW	B	1107	-	38,38,53	1.27	5 (13%)	43,46,61	1.19	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PCW	C	1103	-	42,42,53	1.22	4 (9%)	48,50,61	0.97	3 (6%)
6	AJP	A	1110	-	48,48,95	18.86	39 (81%)	71,78,149	3.42	38 (53%)
4	PCW	D	1104	-	42,42,53	1.17	3 (7%)	48,50,61	1.19	3 (6%)
4	PCW	C	1104	-	40,40,53	1.23	4 (10%)	46,48,61	1.10	3 (6%)
4	PCW	B	1108	-	10,10,53	0.79	0	9,9,61	0.30	0
4	PCW	B	1103	-	40,40,53	1.22	3 (7%)	46,48,61	1.04	3 (6%)
4	PCW	B	1109	-	10,10,53	0.78	0	9,9,61	0.31	0
4	PCW	F	201	-	10,10,53	0.77	0	9,9,61	0.32	0
4	PCW	C	1115	-	10,10,53	0.80	0	9,9,61	0.28	0
5	CLR	A	1107	-	31,31,31	9.01	22 (70%)	48,48,48	4.20	24 (50%)
4	PCW	E	201	-	10,10,53	0.77	0	9,9,61	0.36	0
6	AJP	C	1114	-	48,48,95	18.96	40 (83%)	71,78,149	3.26	37 (52%)
4	PCW	A	1114	-	50,50,53	1.12	3 (6%)	56,58,61	1.09	4 (7%)
4	PCW	F	202	-	42,42,53	1.25	4 (9%)	48,50,61	1.06	3 (6%)
4	PCW	E	202	-	10,10,53	0.78	0	9,9,61	0.30	0
4	PCW	C	1102	-	50,50,53	1.15	4 (8%)	56,58,61	0.98	3 (5%)
4	PCW	B	1101	-	10,10,53	0.72	0	9,9,61	0.42	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	A	1105	-	-	24/54/54/57	-
4	PCW	B	1105	-	-	15/34/34/57	-
4	PCW	D	1107	-	-	25/42/42/57	-
4	PCW	D	1109	-	-	24/54/54/57	-
3	ZK1	A	1101	-	-	6/13/23/23	0/3/3/3
4	PCW	A	1113	-	-	24/54/54/57	-
4	PCW	D	1108	-	-	4/8/8/57	-
4	PCW	D	1110	-	-	5/8/8/57	-
5	CLR	C	1111	-	2/2/10/11	5/10/68/68	0/4/4/4
4	PCW	F	204	-	-	4/8/8/57	-
4	PCW	C	1105	-	-	4/8/8/57	-
4	PCW	D	1105	-	-	14/34/34/57	-
4	PCW	B	1111	-	-	23/54/54/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZK1	B	1102	-	-	5/13/23/23	0/3/3/3
4	PCW	C	1107	-	-	6/8/8/57	-
4	PCW	D	1101	-	-	5/8/8/57	-
4	PCW	E	204	-	-	4/8/8/57	-
6	AJP	C	1110	-	9/9/18/38	4/6/117/220	1/7/7/11
4	PCW	B	1106	-	-	24/44/44/57	-
4	PCW	D	1103	-	-	26/44/44/57	-
4	PCW	E	203	-	-	24/46/46/57	-
4	PCW	A	1106	-	-	4/8/8/57	-
4	PCW	A	1115	-	-	3/8/8/57	-
4	PCW	D	1106	-	-	23/44/44/57	-
4	PCW	F	205	-	-	7/8/8/57	-
4	PCW	C	1113	-	-	3/8/8/57	-
4	PCW	C	1112	-	-	26/54/54/57	-
4	PCW	A	1103	-	-	24/46/46/57	-
3	ZK1	C	1101	-	-	8/13/23/23	0/3/3/3
7	SPD	A	1119	-	-	0/7/7/7	-
4	PCW	A	1118	-	-	22/54/54/57	-
4	PCW	B	1110	-	-	29/54/54/57	-
4	PCW	F	203	-	-	4/8/8/57	-
5	CLR	C	1106	-	2/2/10/11	7/10/68/68	0/4/4/4
4	PCW	A	1117	-	-	4/8/8/57	-
6	AJP	C	1109	-	12/12/17/38	2/6/113/220	0/7/7/11
4	PCW	A	1102	-	-	27/54/54/57	-
4	PCW	C	1108	-	-	6/8/8/57	-
4	PCW	E	205	-	-	4/8/8/57	-
4	PCW	A	1104	-	-	25/44/44/57	-
6	AJP	A	1116	-	9/9/18/38	2/6/117/220	0/7/7/11
3	ZK1	D	1102	-	-	5/13/23/23	0/3/3/3
4	PCW	B	1104	-	-	32/46/46/57	-
6	AJP	A	1111	-	9/9/18/38	4/6/117/220	1/7/7/11
5	CLR	A	1112	-	2/2/10/11	4/10/68/68	0/4/4/4
4	PCW	A	1109	-	-	6/8/8/57	-
4	PCW	A	1108	-	-	3/8/8/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	B	1107	-	-	24/42/42/57	-
4	PCW	C	1103	-	-	24/46/46/57	-
6	AJP	A	1110	-	13/13/18/38	3/6/117/220	0/7/7/11
4	PCW	D	1104	-	-	31/46/46/57	-
4	PCW	C	1104	-	-	24/44/44/57	-
4	PCW	B	1108	-	-	4/8/8/57	-
4	PCW	B	1103	-	-	26/44/44/57	-
4	PCW	B	1109	-	-	5/8/8/57	-
4	PCW	F	201	-	-	4/8/8/57	-
5	CLR	A	1107	-	2/2/10/11	7/10/68/68	0/4/4/4
4	PCW	C	1115	-	-	4/8/8/57	-
4	PCW	E	201	-	-	7/8/8/57	-
6	AJP	C	1114	-	9/9/18/38	2/6/117/220	0/7/7/11
4	PCW	A	1114	-	-	24/54/54/57	-
4	PCW	F	202	-	-	23/46/46/57	-
4	PCW	E	202	-	-	4/8/8/57	-
4	PCW	C	1102	-	-	26/54/54/57	-
4	PCW	B	1101	-	-	6/8/8/57	-

The worst 5 of 455 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1110	AJP	O78-C27	-59.85	0.02	1.43
6	A	1111	AJP	O78-C27	-58.47	0.05	1.43
6	C	1114	AJP	O78-C27	-58.06	0.06	1.43
6	A	1110	AJP	O78-C27	-57.53	0.07	1.43
6	A	1116	AJP	O78-C27	-56.79	0.09	1.43

The worst 5 of 428 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1107	CLR	C18-C13-C17	-13.44	86.65	111.71
5	C	1106	CLR	C18-C13-C17	-13.37	86.77	111.71
5	A	1112	CLR	C18-C13-C17	-12.44	88.52	111.71
5	C	1111	CLR	C18-C13-C17	-12.03	89.27	111.71
5	C	1106	CLR	C12-C13-C17	10.68	132.55	116.57

5 of 69 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1107	CLR	C9
5	A	1107	CLR	C17
5	A	1112	CLR	C9
5	A	1112	CLR	C17
5	C	1106	CLR	C9

5 of 807 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1102	ZK1	NAY-CAO-PBA-OAC
3	B	1102	ZK1	NAY-CAO-PBA-OAD
3	D	1102	ZK1	NAY-CAO-PBA-OAC
3	D	1102	ZK1	NAY-CAO-PBA-OAD
4	A	1102	PCW	O2-C2-C3-O3

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1110	AJP	C02-C03-C04-C05-C85-O84
6	A	1111	AJP	C02-C03-C04-C05-C85-O84

48 monomers are involved in 312 short contacts:

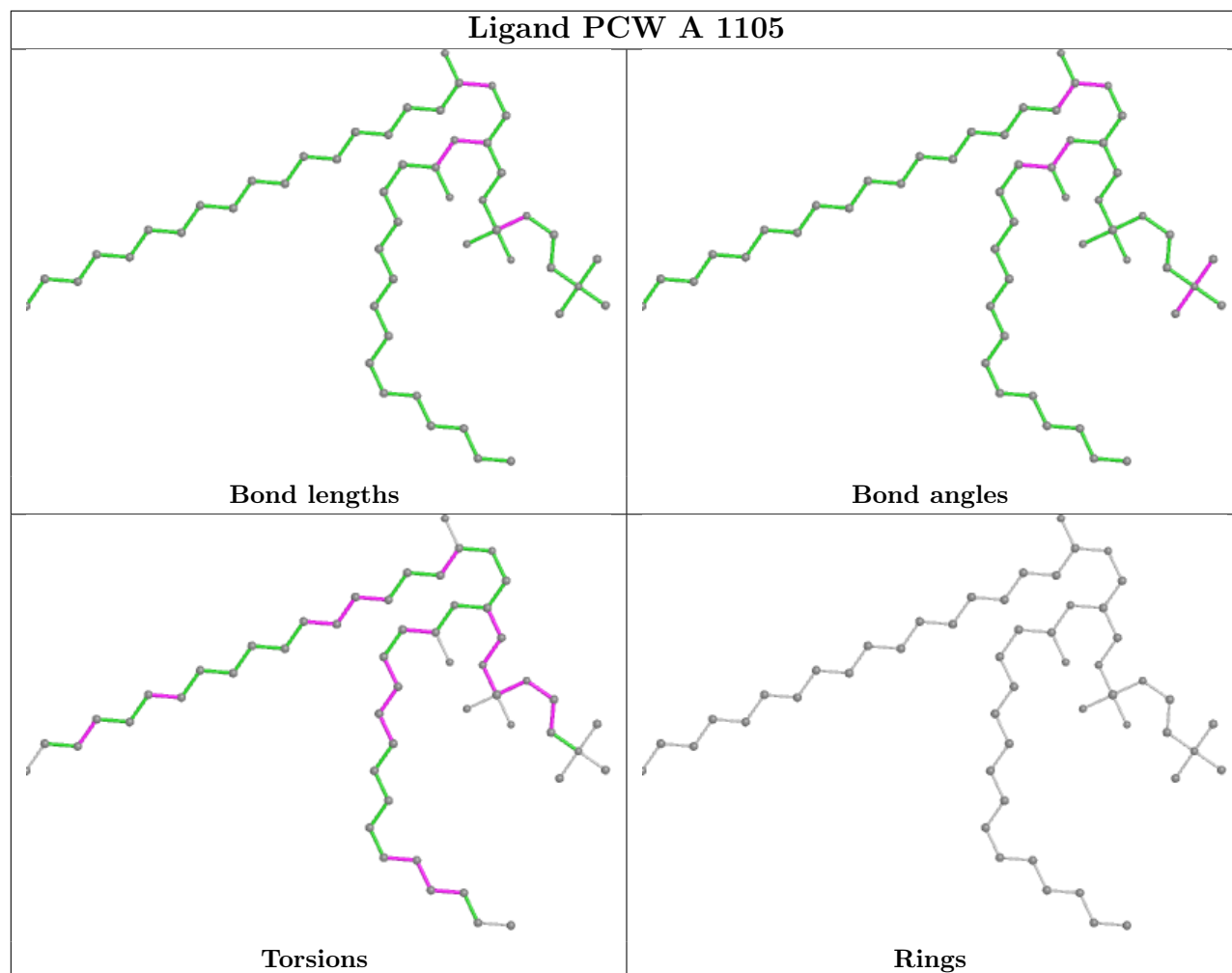
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1105	PCW	3	0
4	D	1107	PCW	3	0
4	D	1109	PCW	3	0
3	A	1101	ZK1	2	0
4	A	1113	PCW	2	0
4	D	1110	PCW	1	0
5	C	1111	CLR	2	0
4	F	204	PCW	2	0
4	B	1111	PCW	6	0
4	C	1107	PCW	1	0
4	D	1101	PCW	3	0
4	B	1106	PCW	1	0
4	D	1103	PCW	4	0
6	C	1110	AJP	34	0
4	E	203	PCW	1	0
4	D	1106	PCW	2	0
4	C	1112	PCW	1	0
4	A	1103	PCW	3	0
3	C	1101	ZK1	1	0

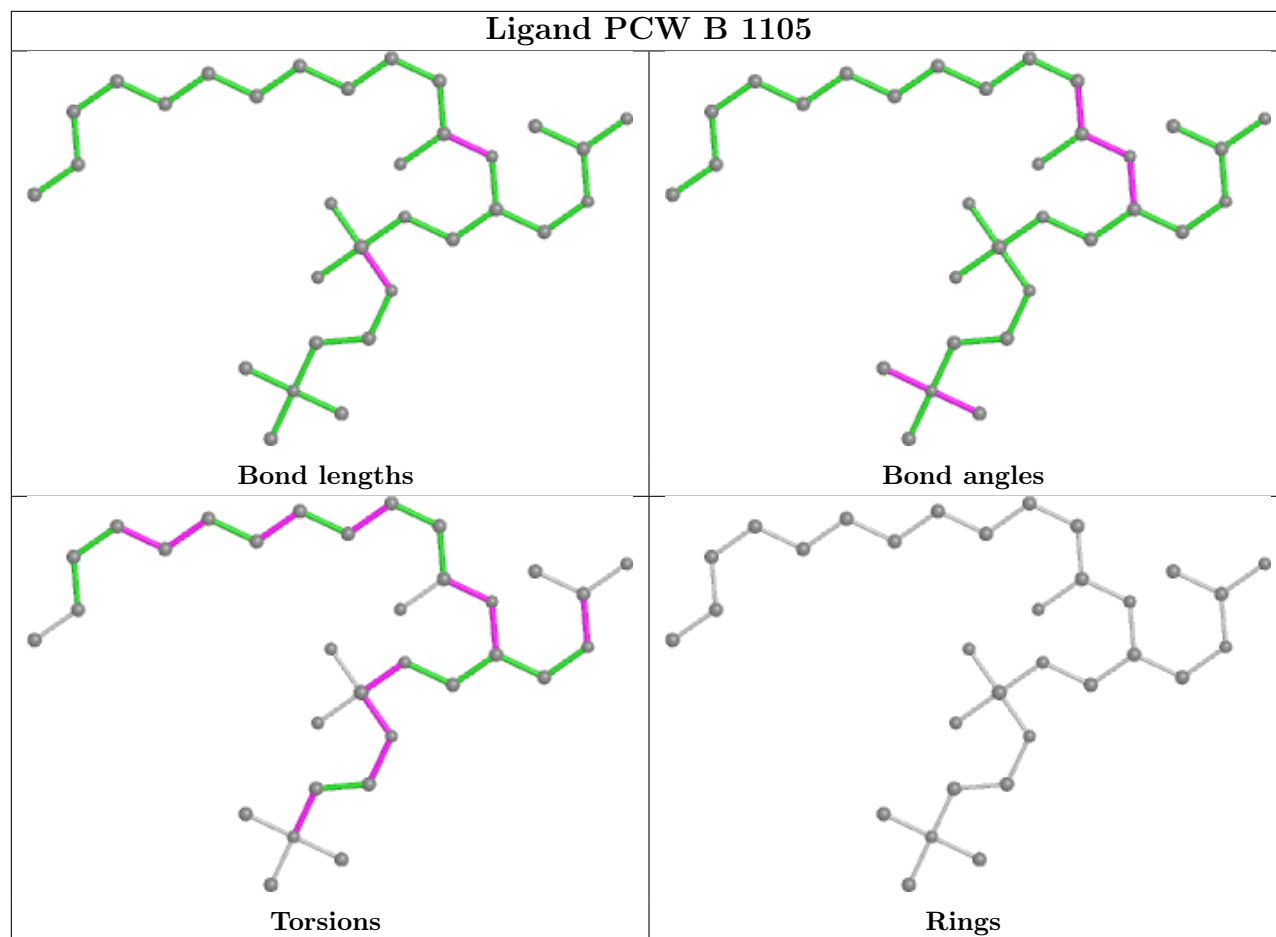
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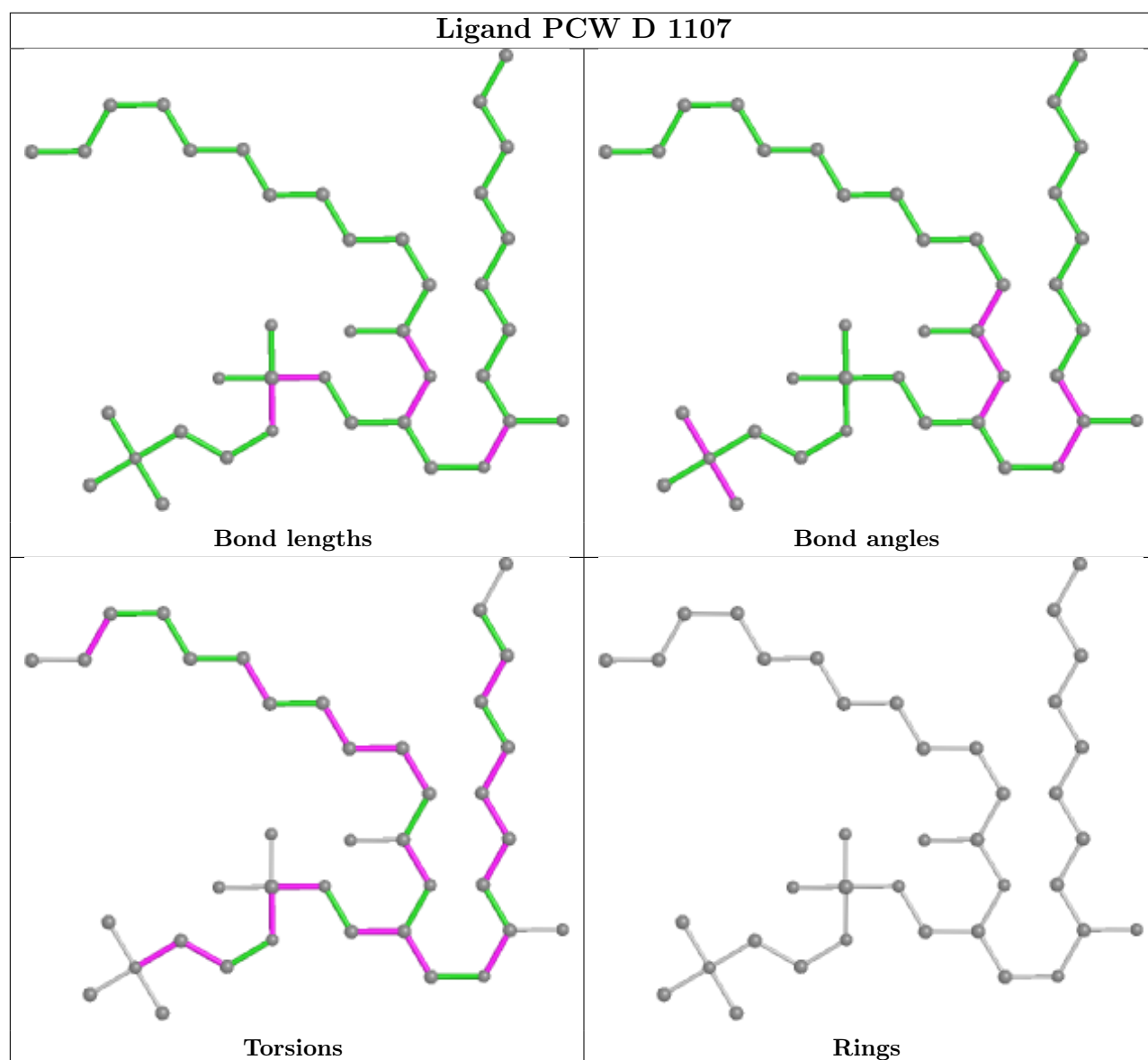
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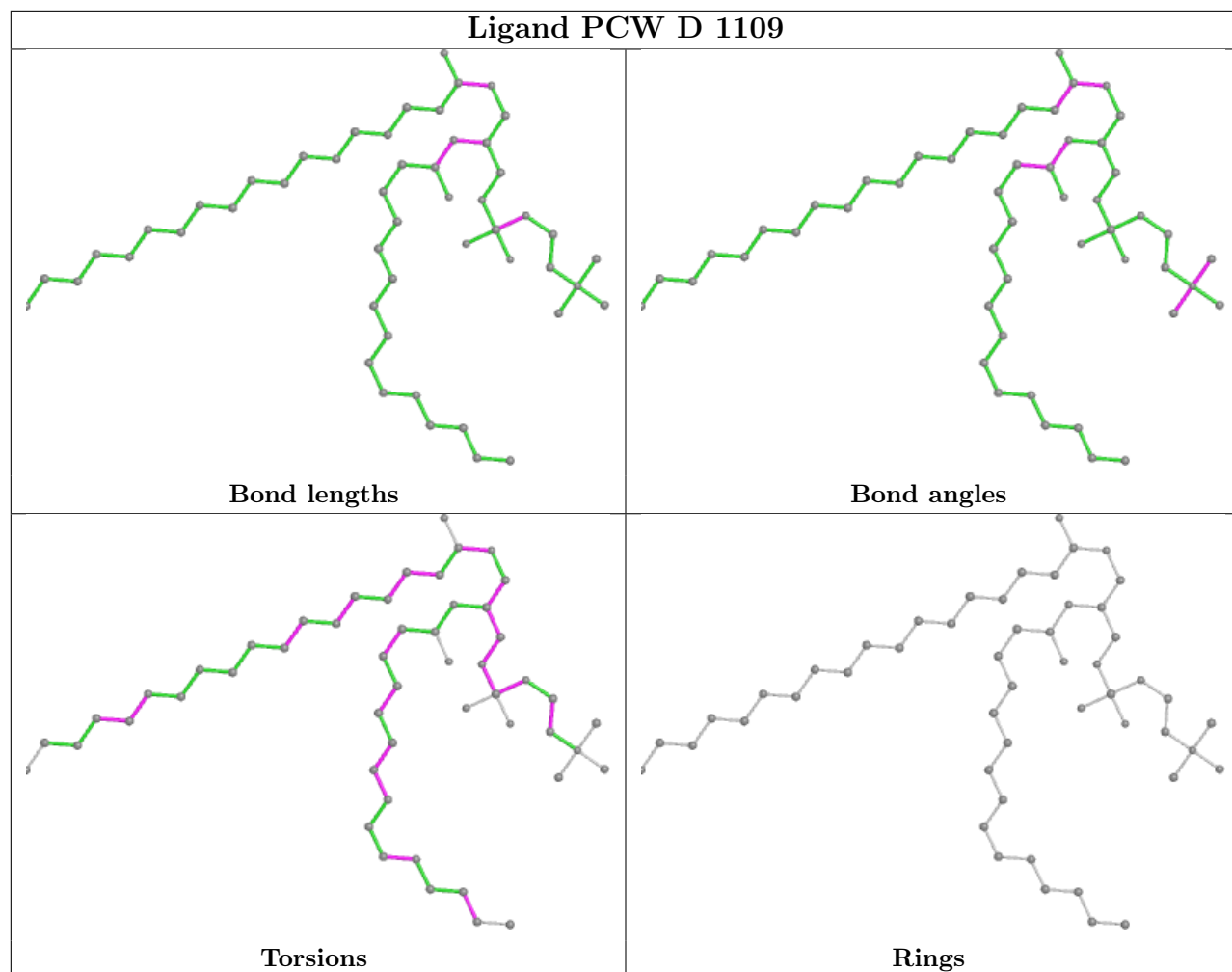
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1118	PCW	3	0
4	B	1110	PCW	5	0
5	C	1106	CLR	7	0
4	A	1102	PCW	5	0
4	E	205	PCW	1	0
6	C	1109	AJP	33	0
4	A	1104	PCW	3	0
6	A	1116	AJP	38	0
4	B	1104	PCW	1	0
5	A	1112	CLR	3	0
6	A	1111	AJP	36	0
4	A	1108	PCW	2	0
4	B	1107	PCW	2	0
4	C	1103	PCW	2	0
6	A	1110	AJP	34	0
4	D	1104	PCW	2	0
4	C	1104	PCW	5	0
4	B	1103	PCW	2	0
4	B	1109	PCW	1	0
4	F	201	PCW	1	0
4	C	1115	PCW	1	0
5	A	1107	CLR	6	0
4	E	201	PCW	1	0
6	C	1114	AJP	40	0
4	A	1114	PCW	3	0
4	F	202	PCW	3	0
4	E	202	PCW	1	0
4	C	1102	PCW	6	0
4	B	1101	PCW	2	0

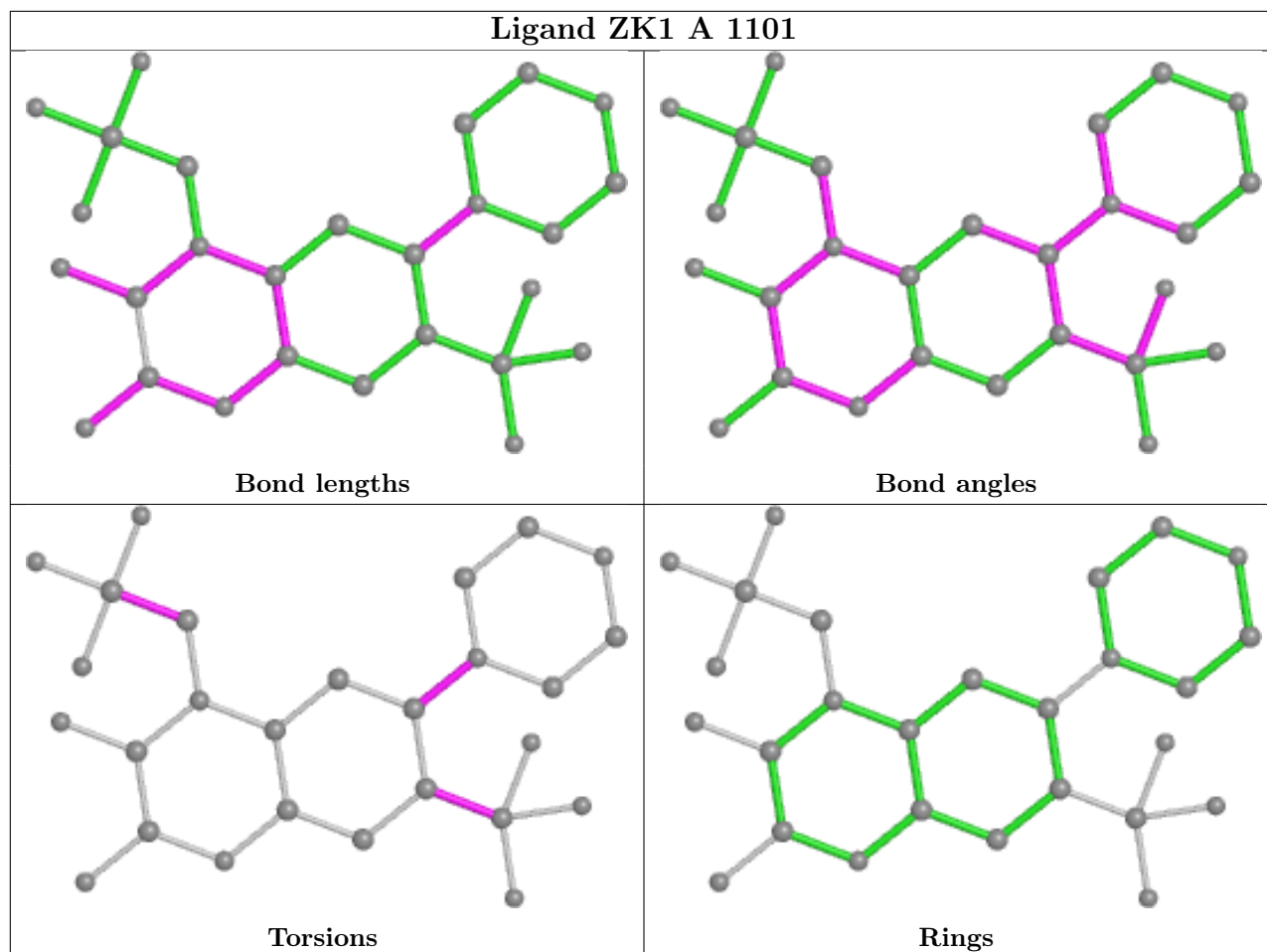
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



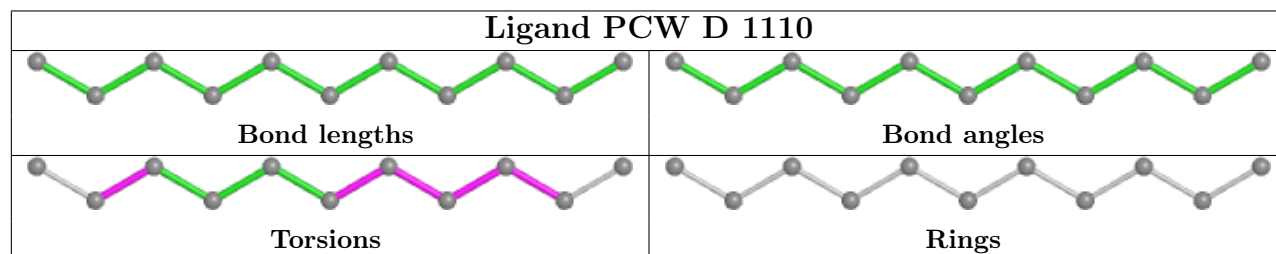
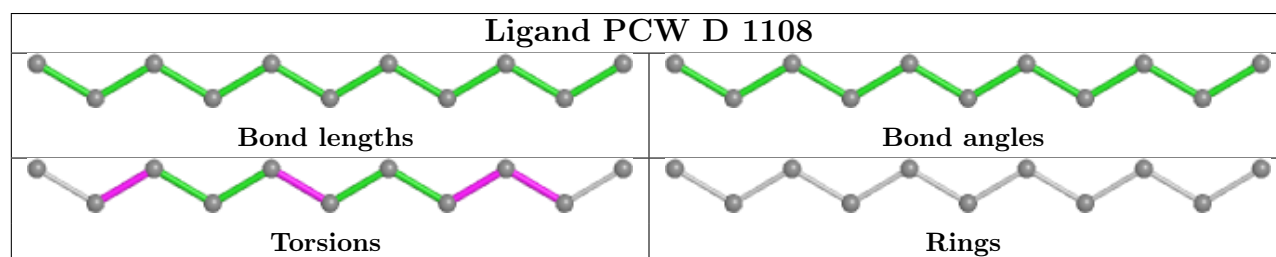
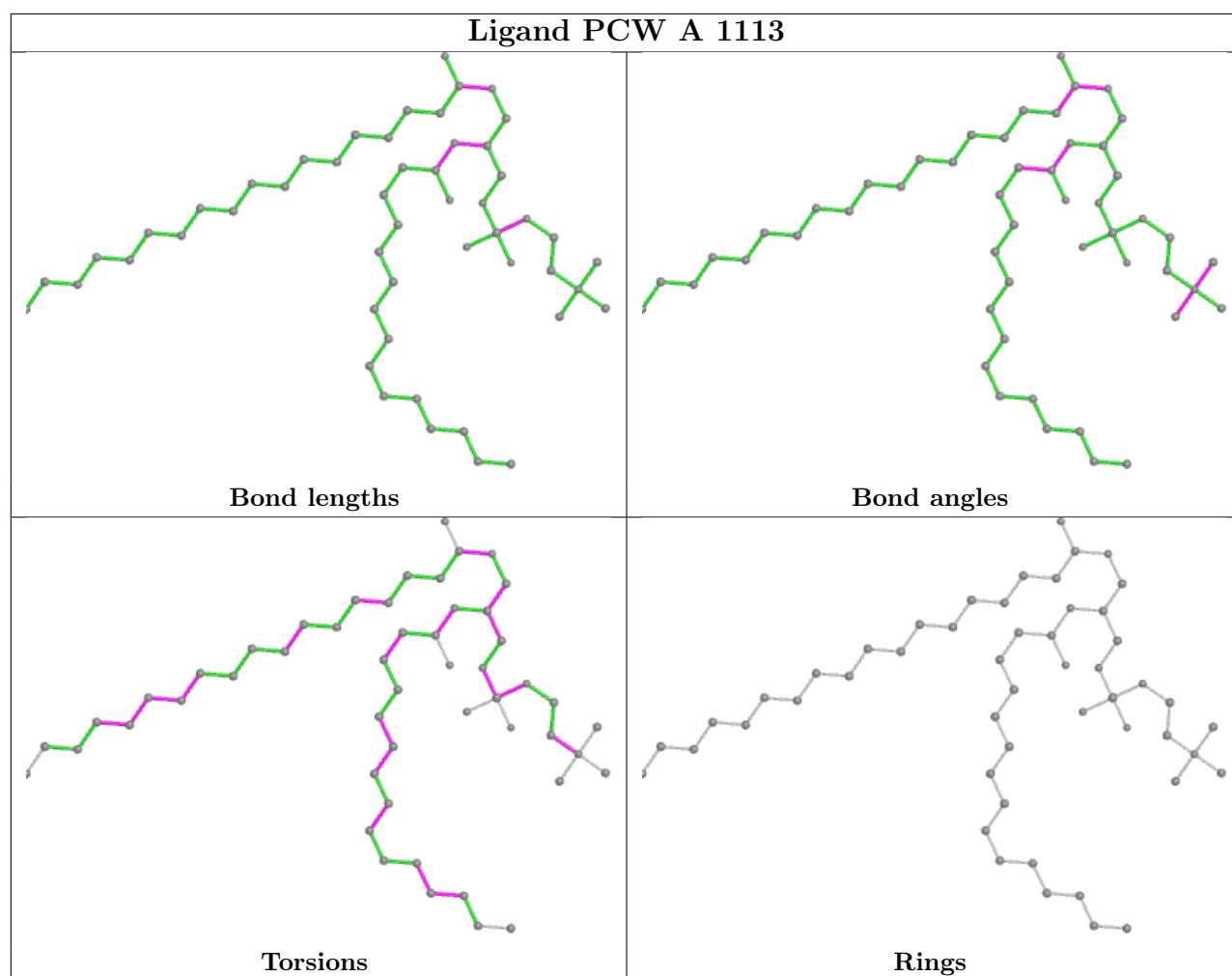


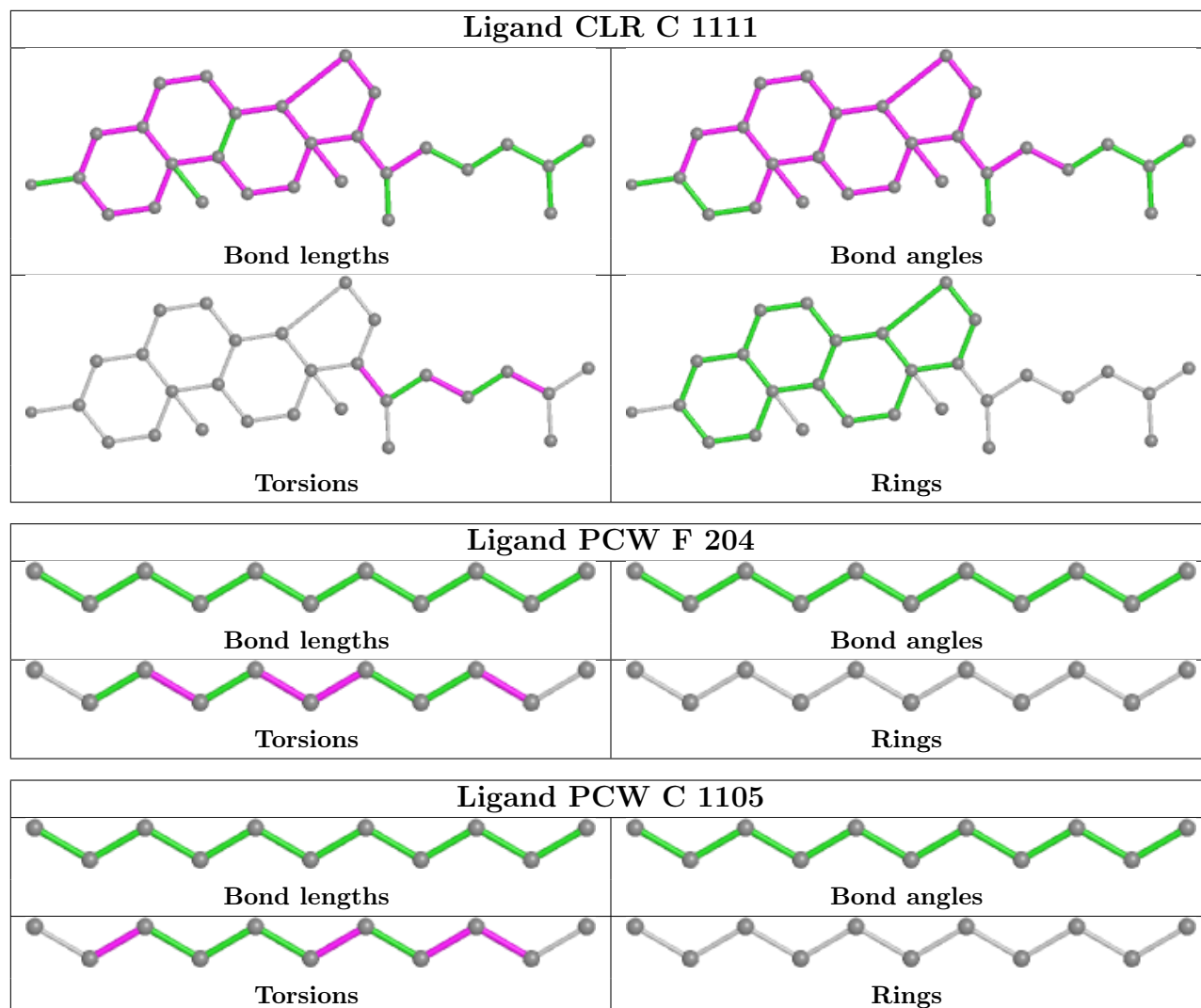


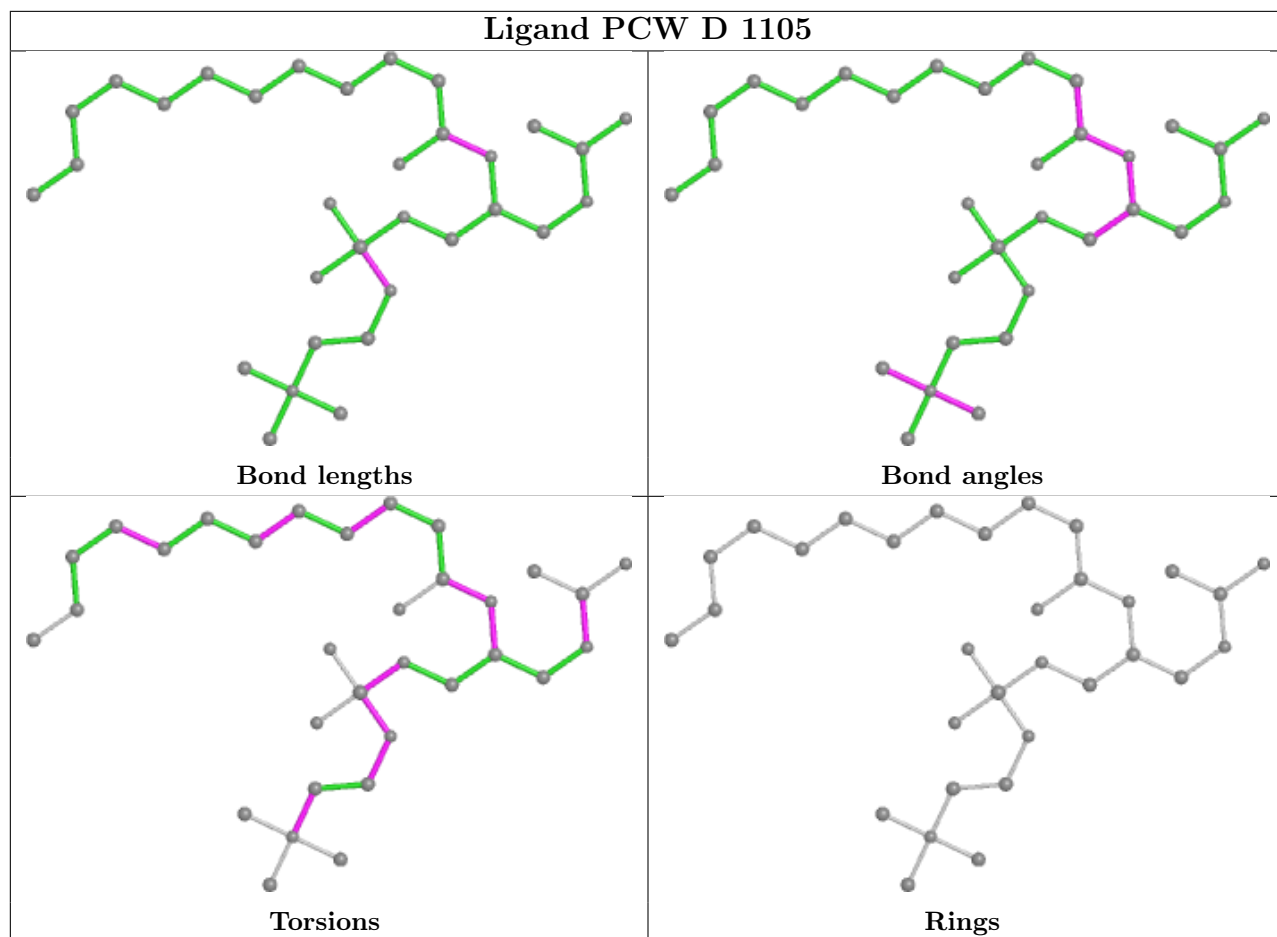


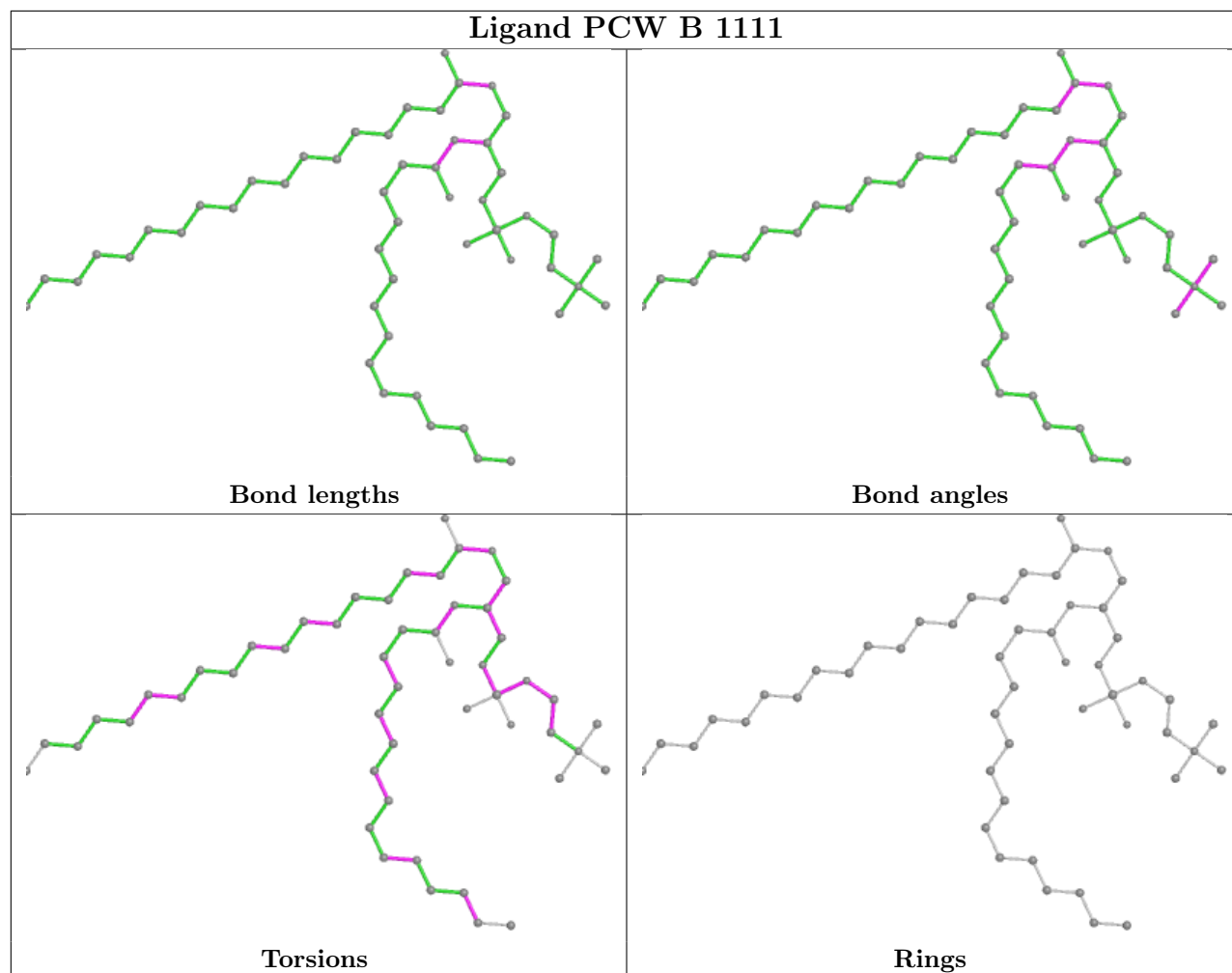


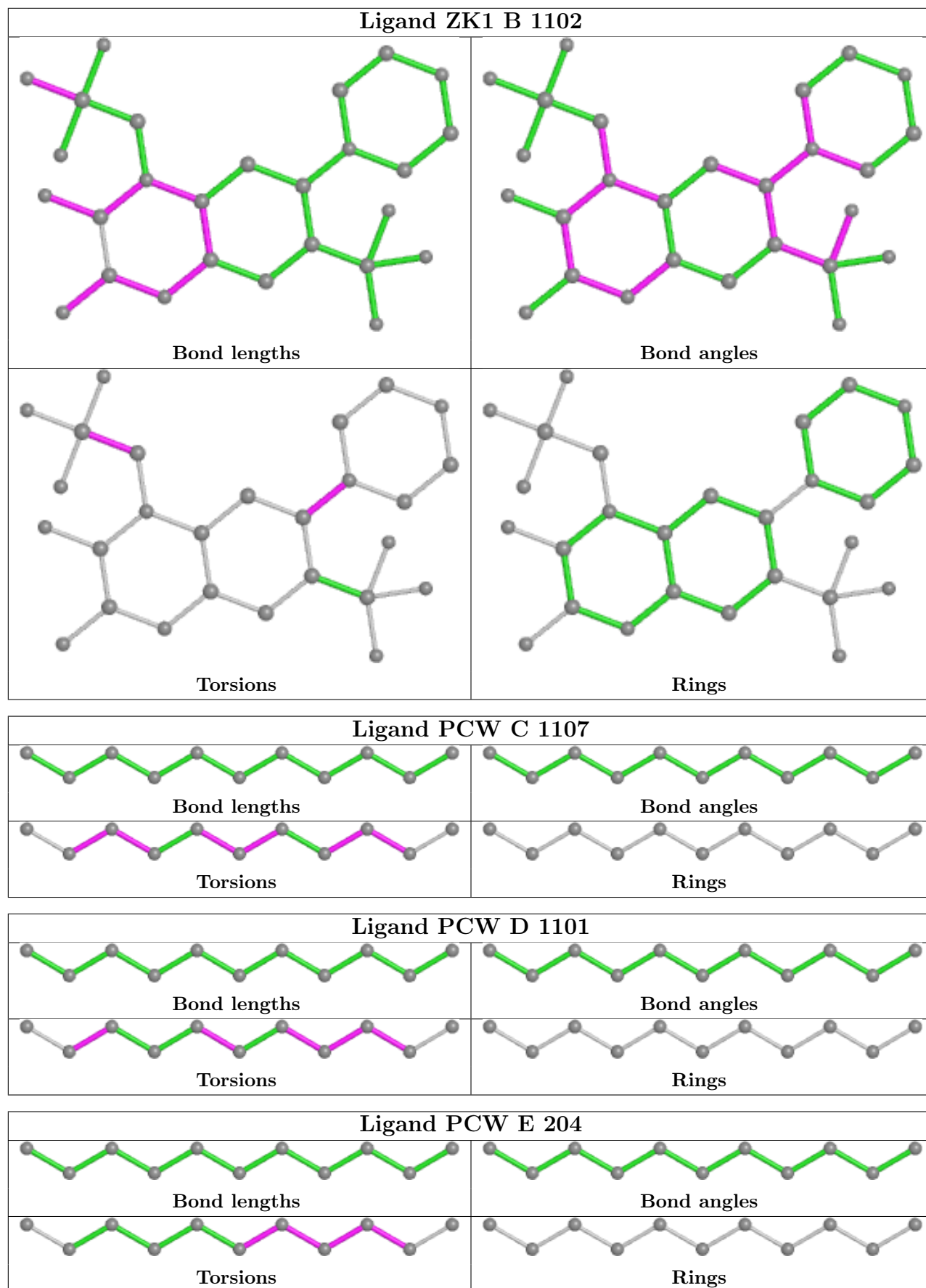


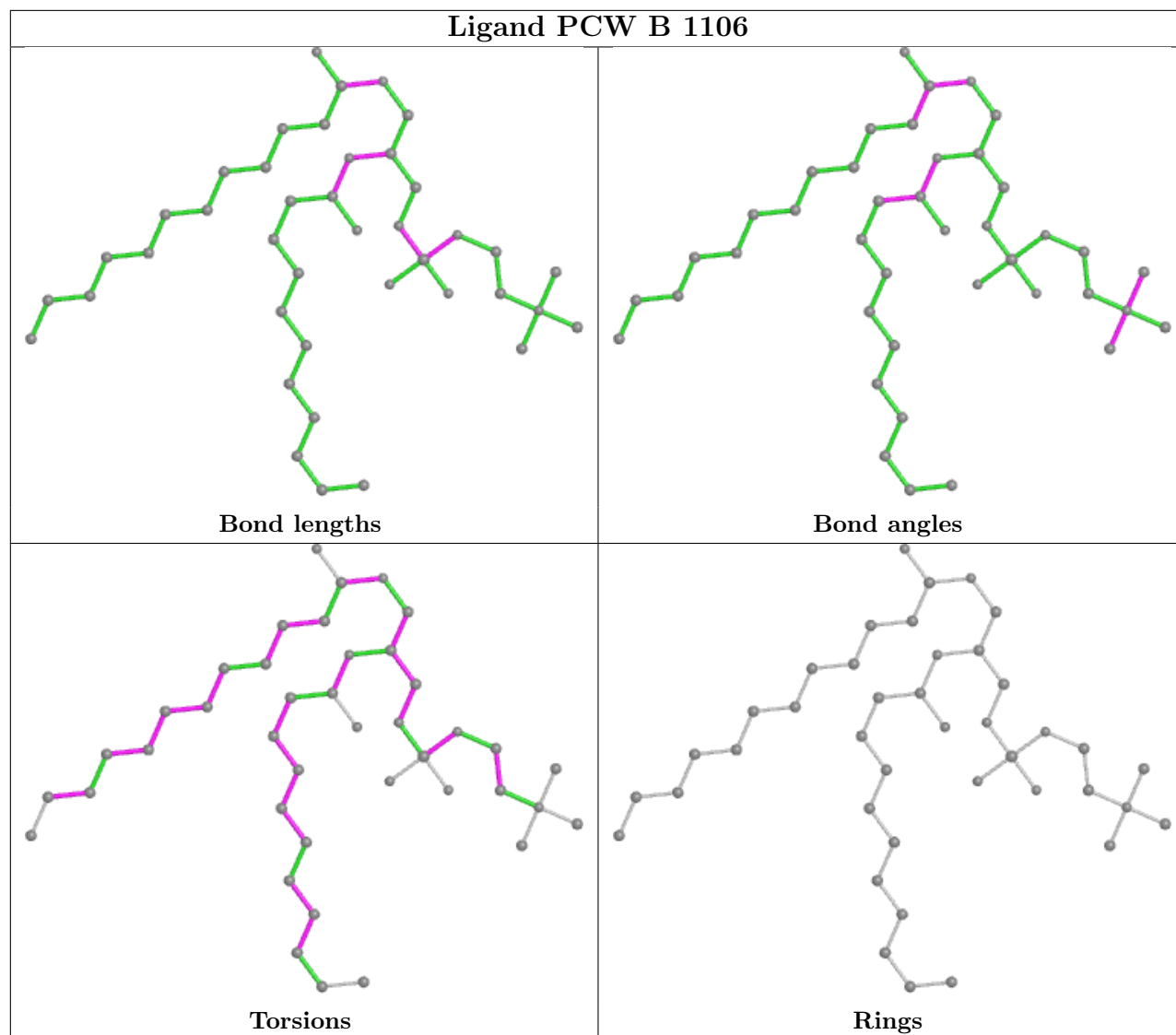


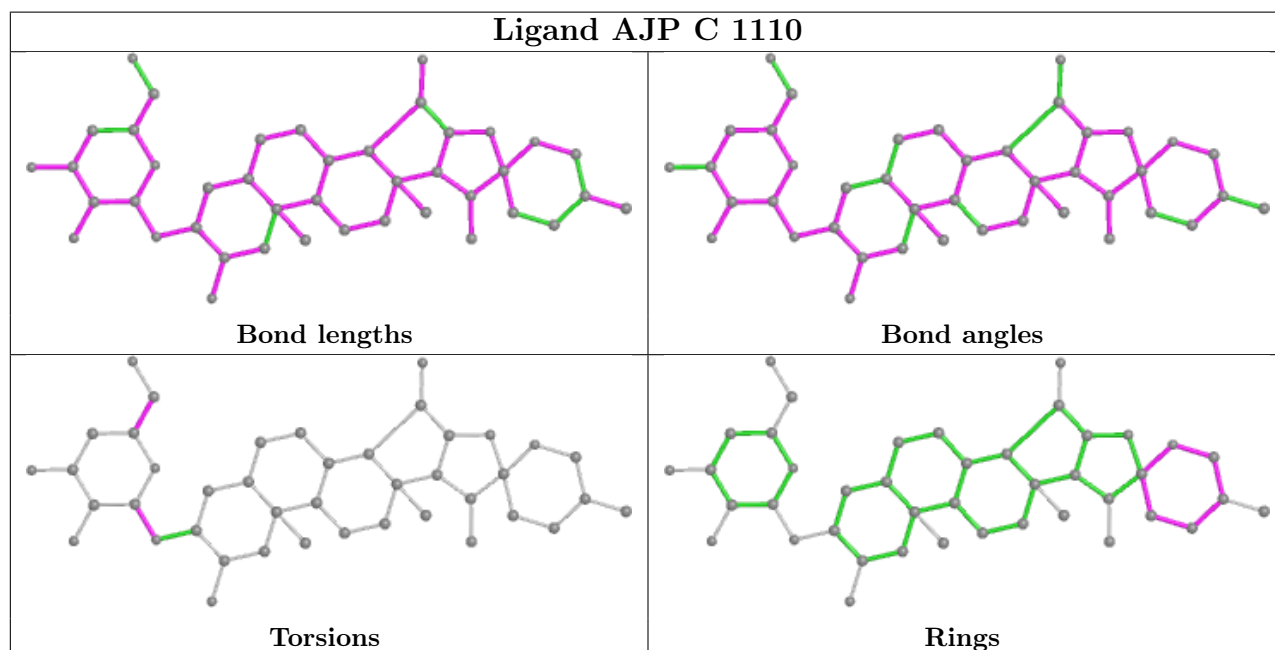
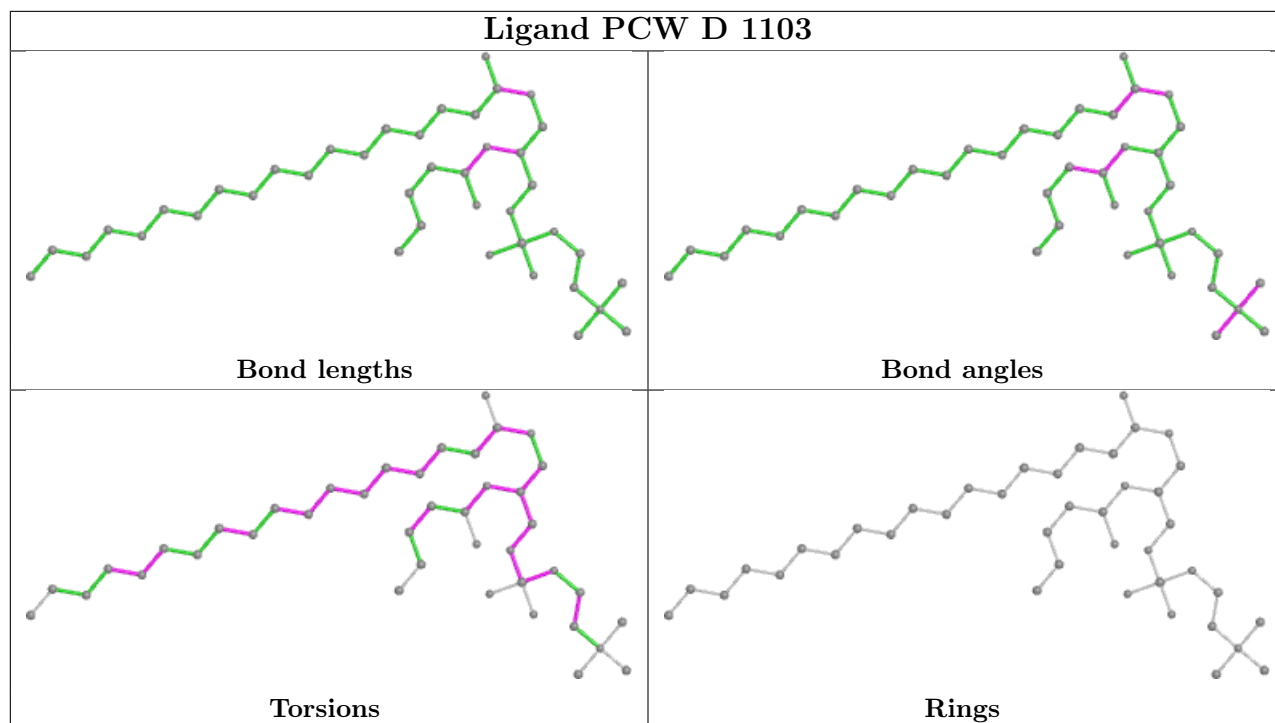


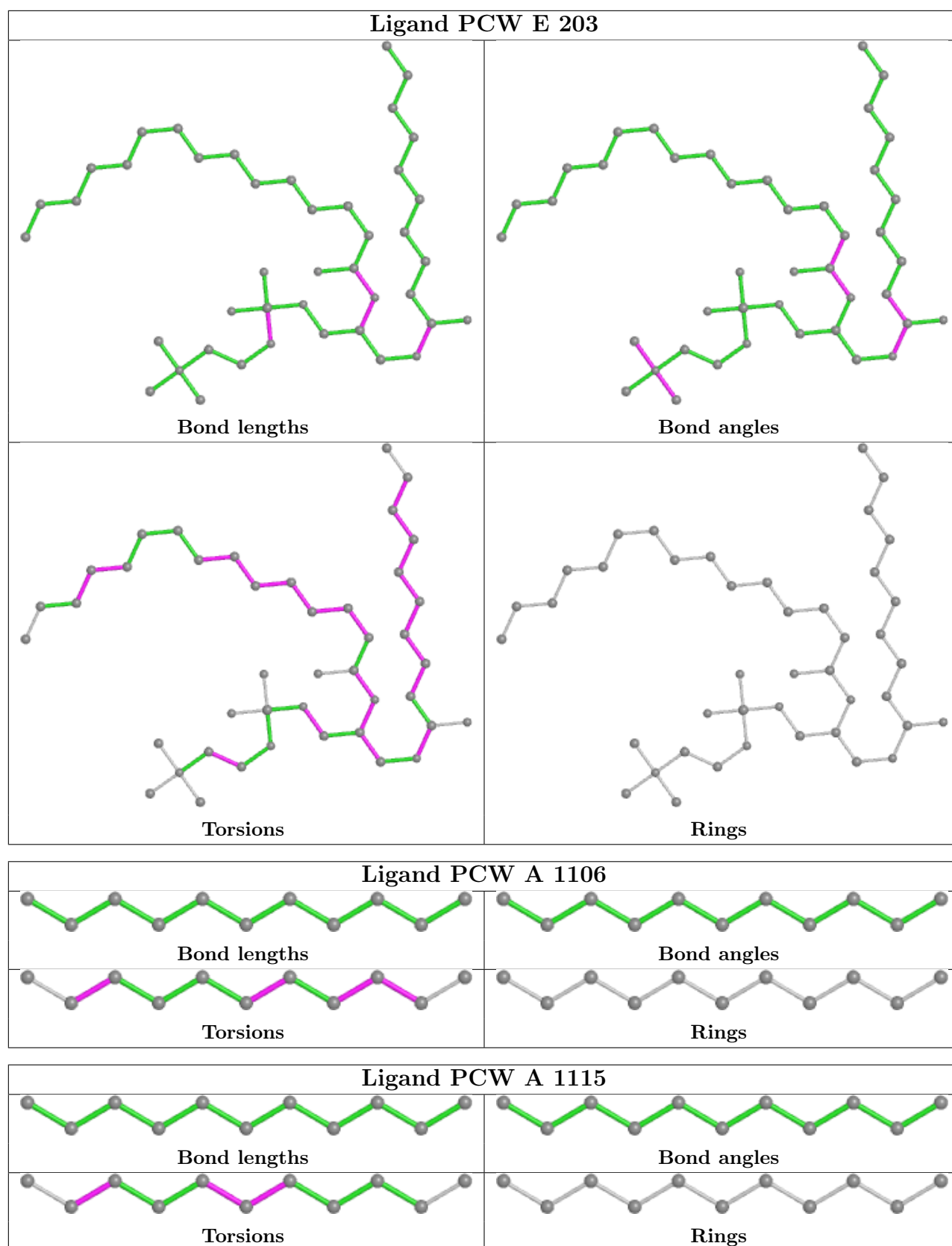




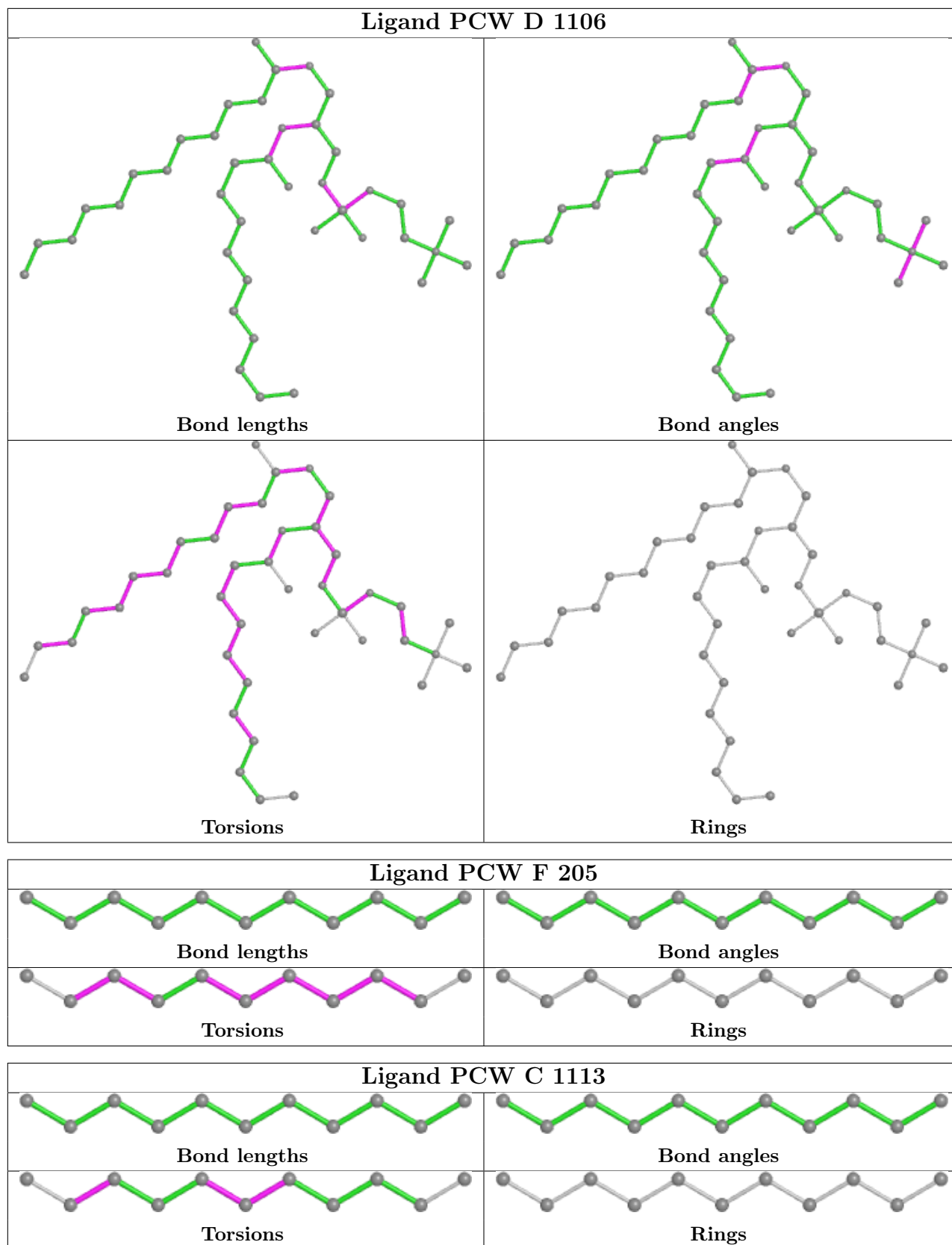


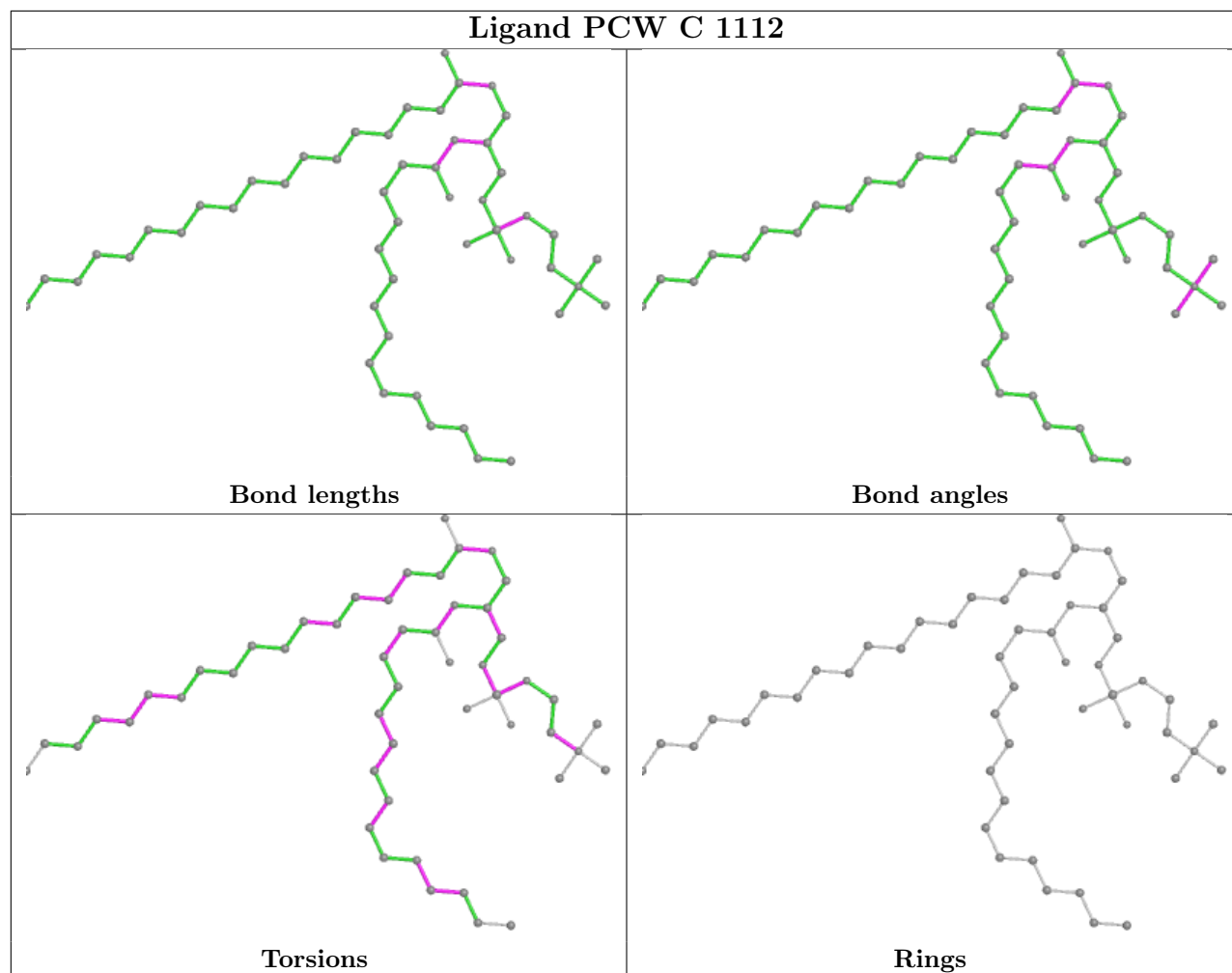


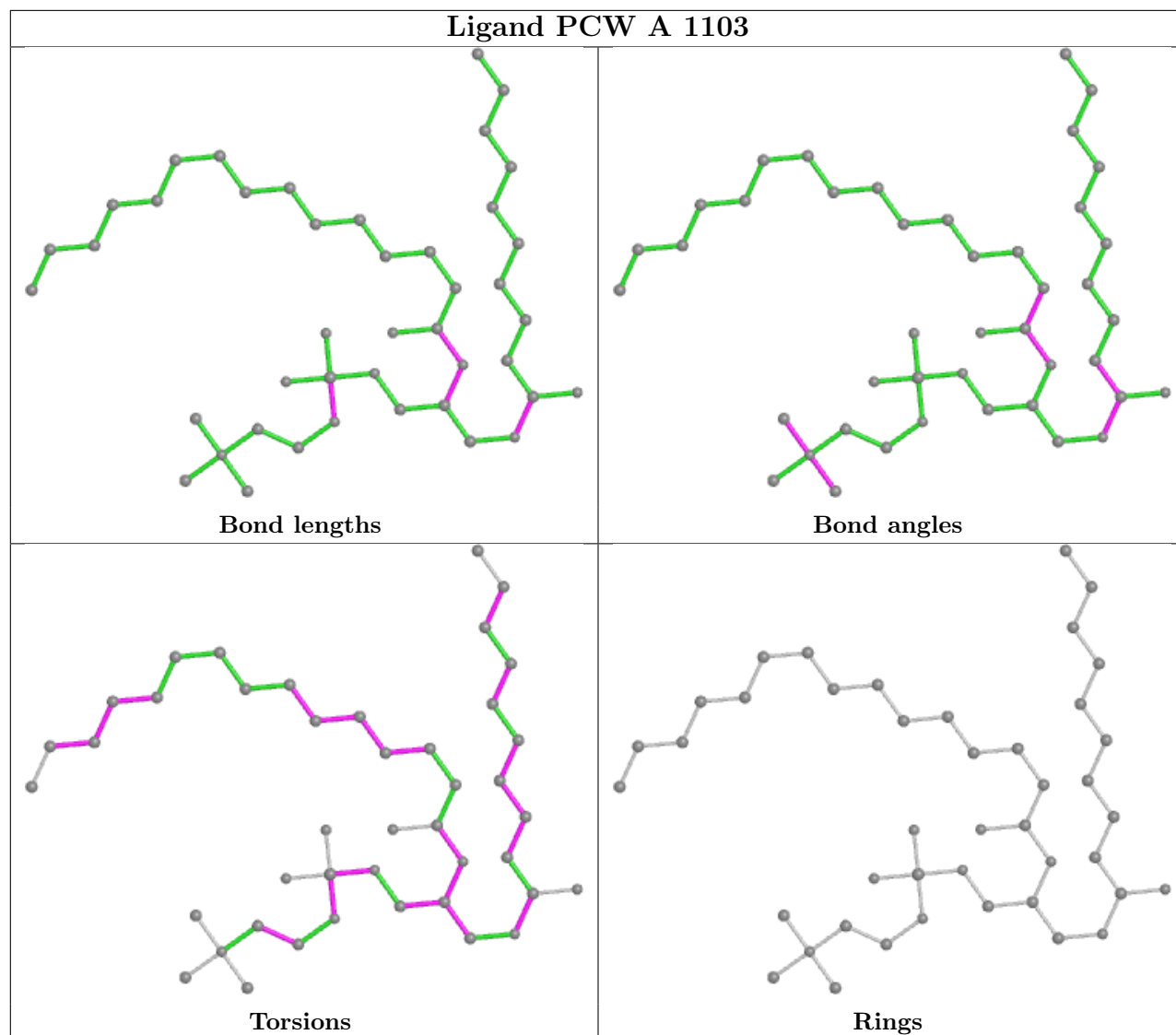


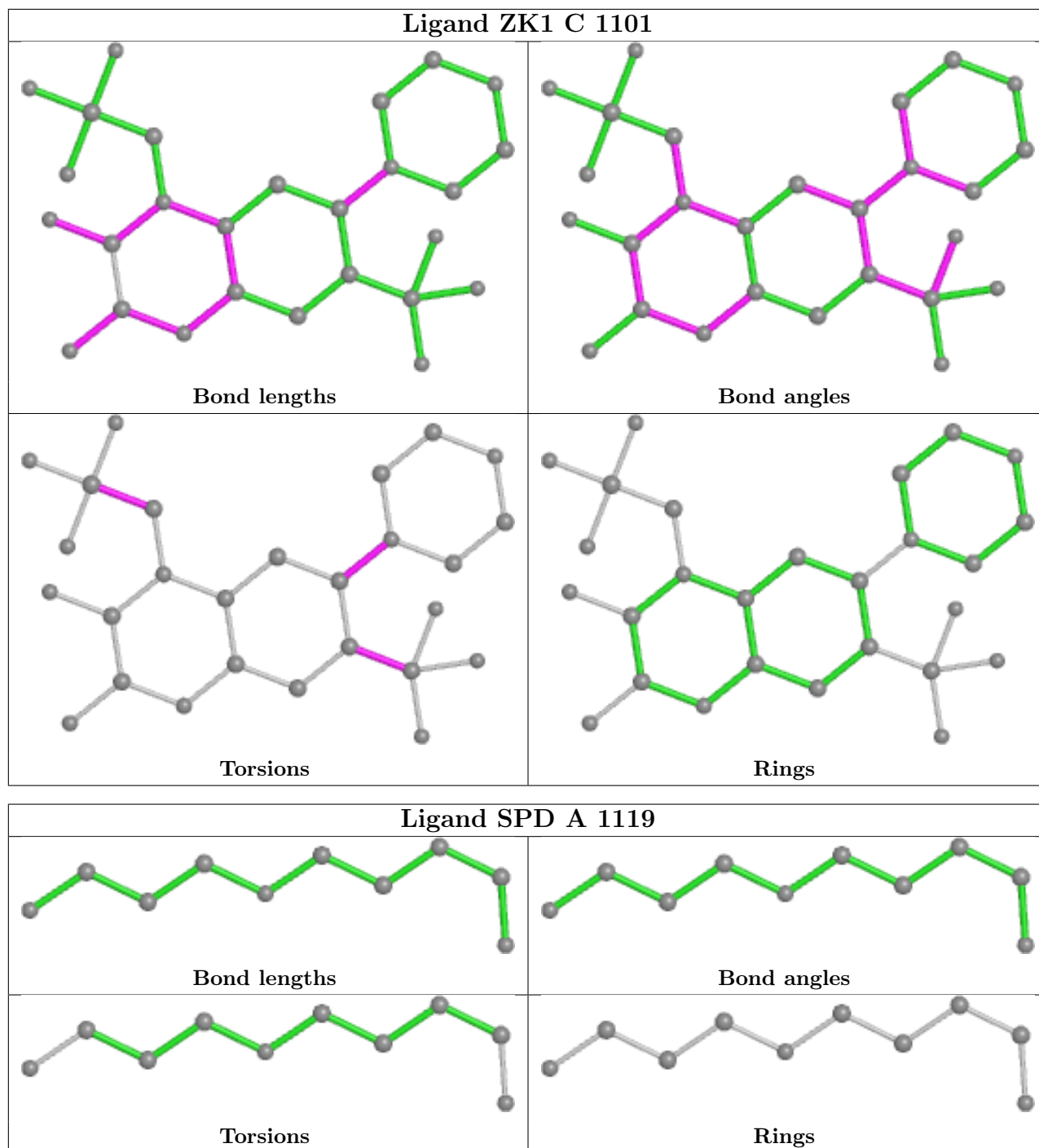


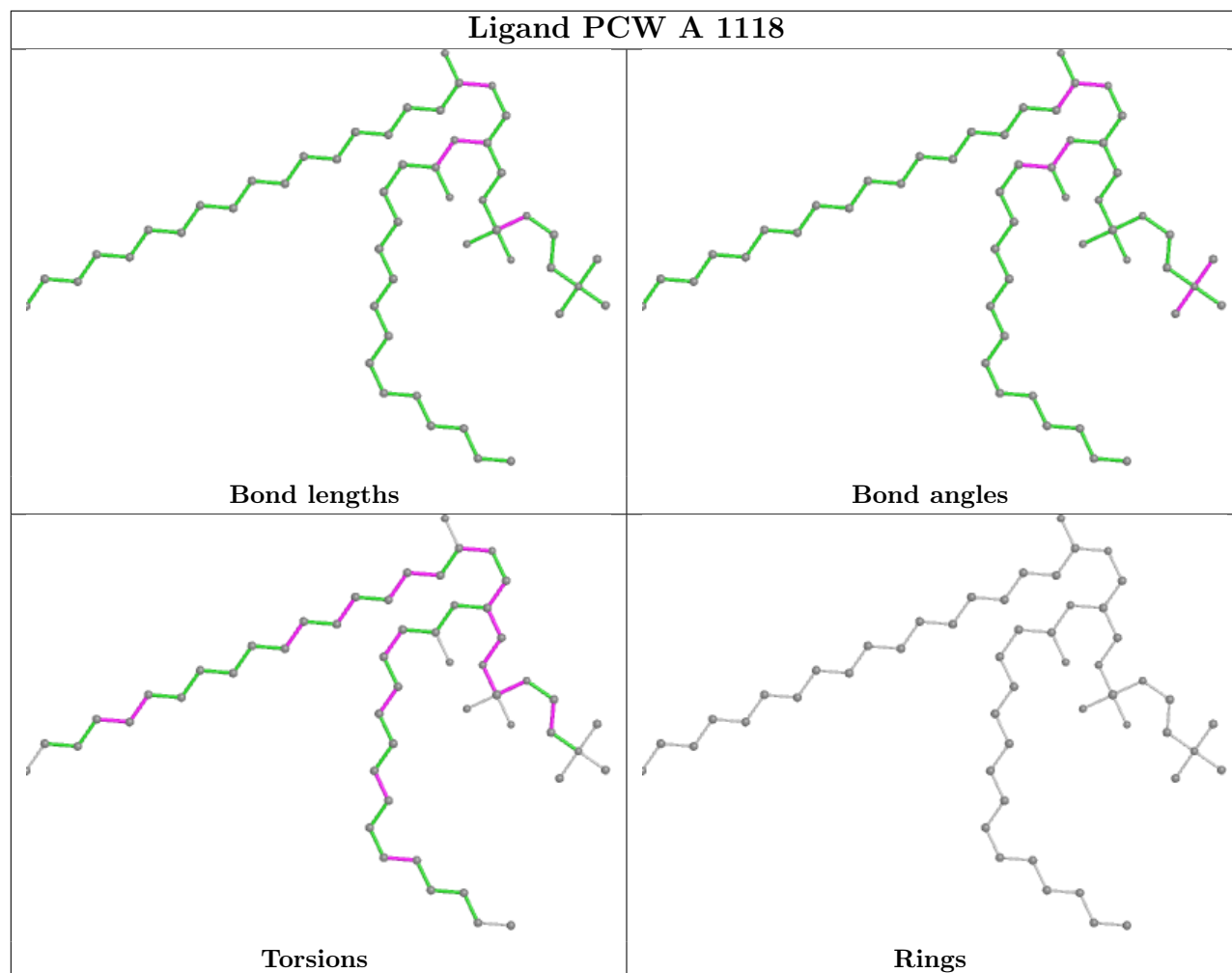


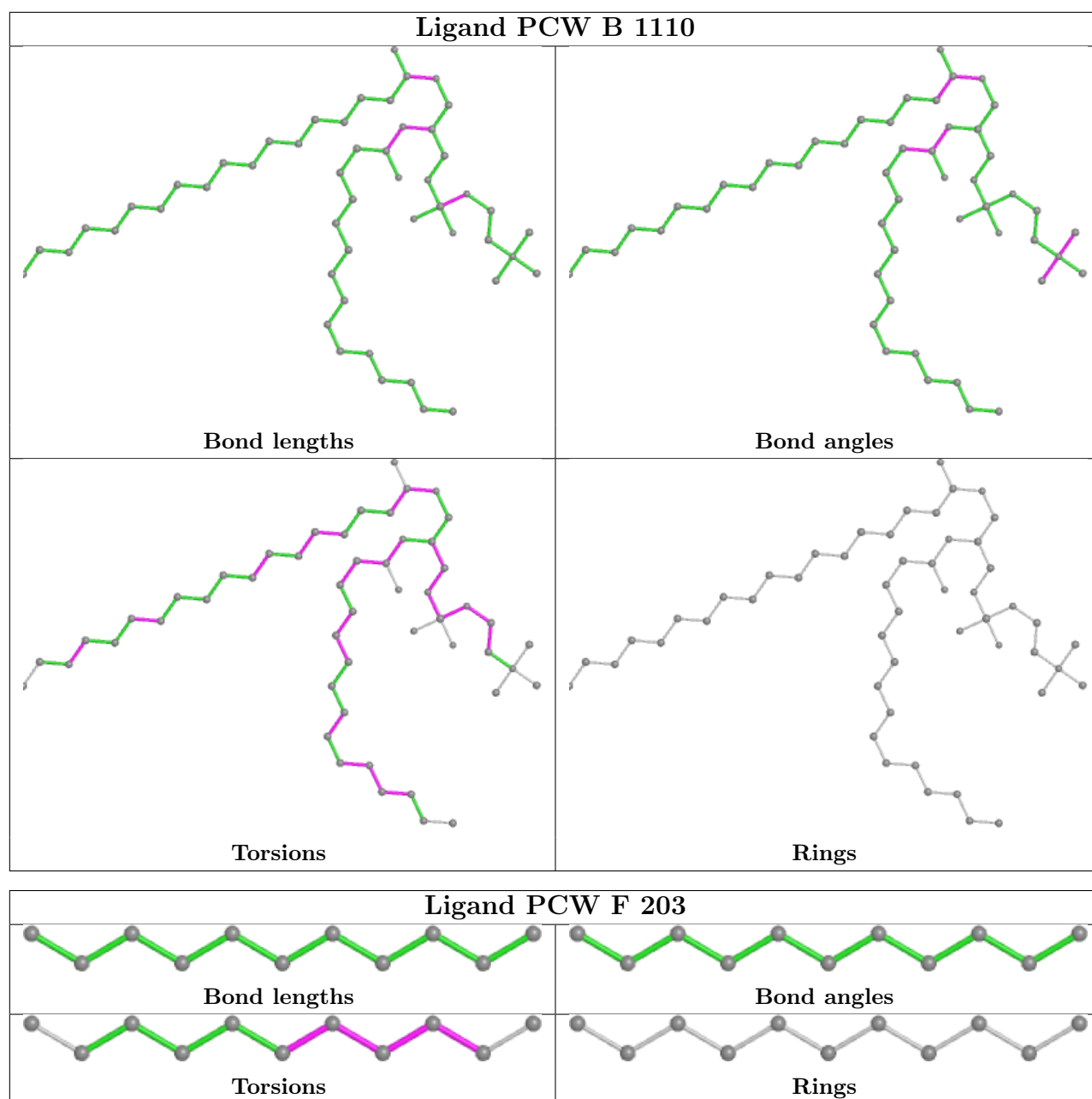


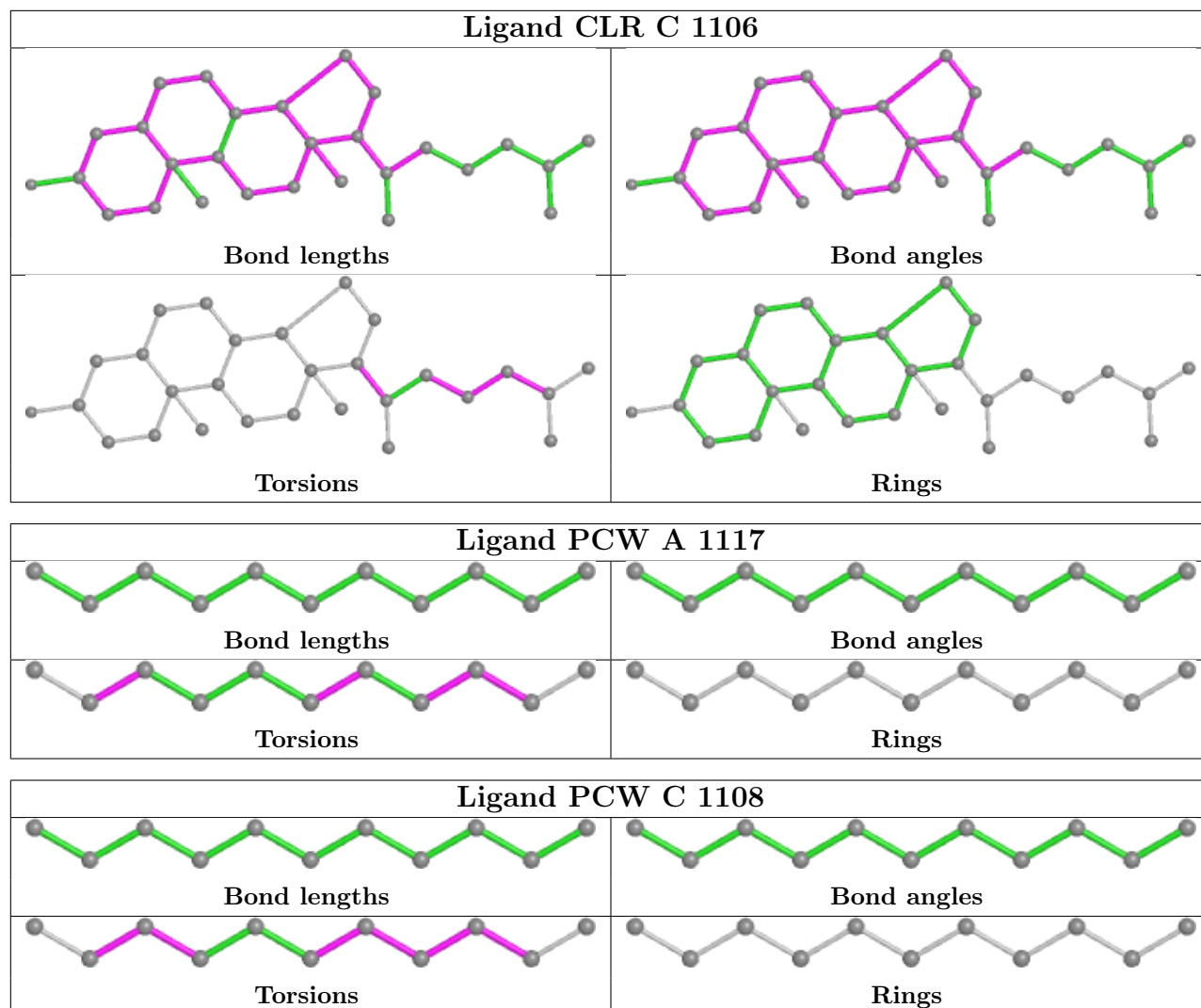


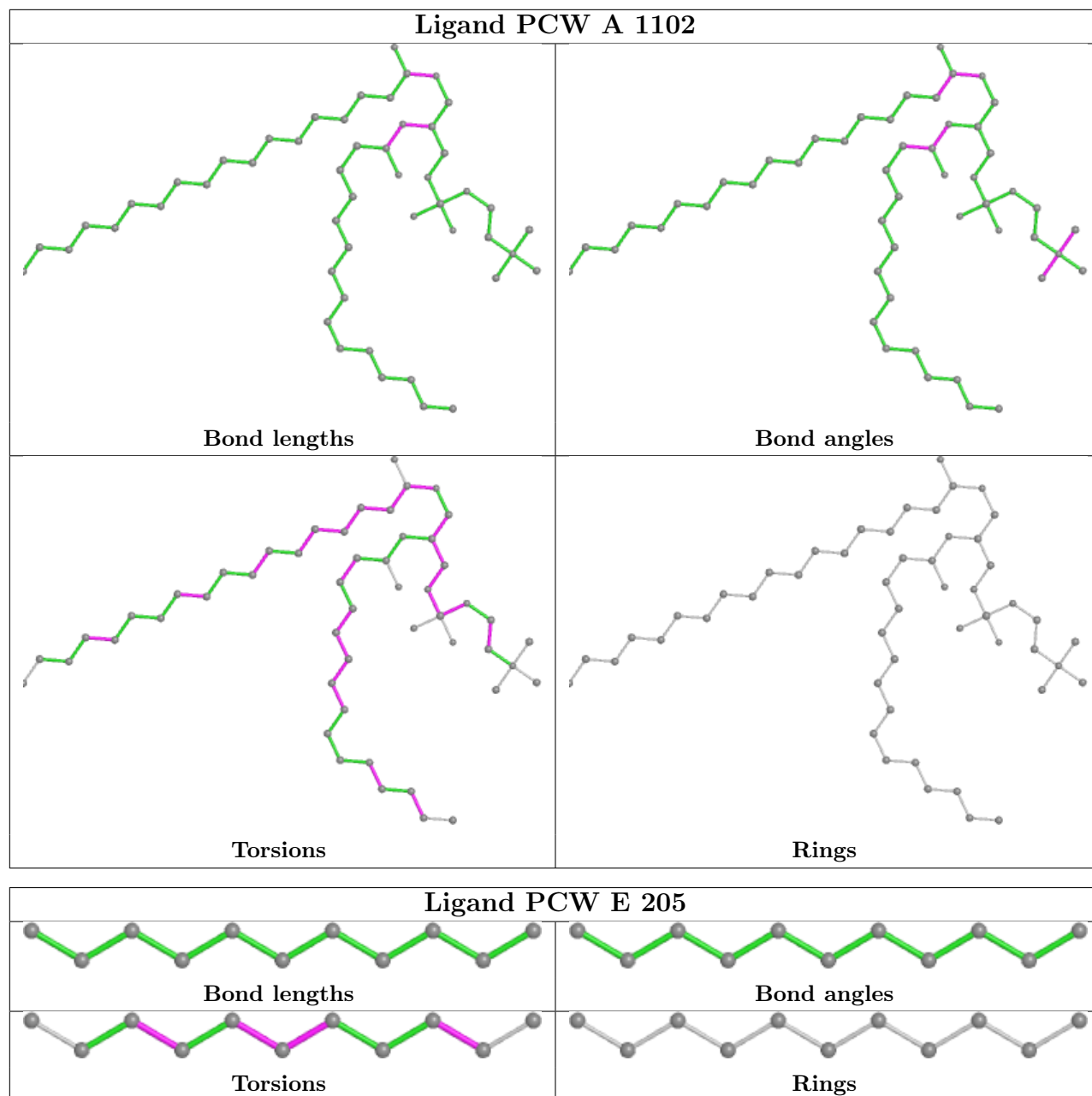




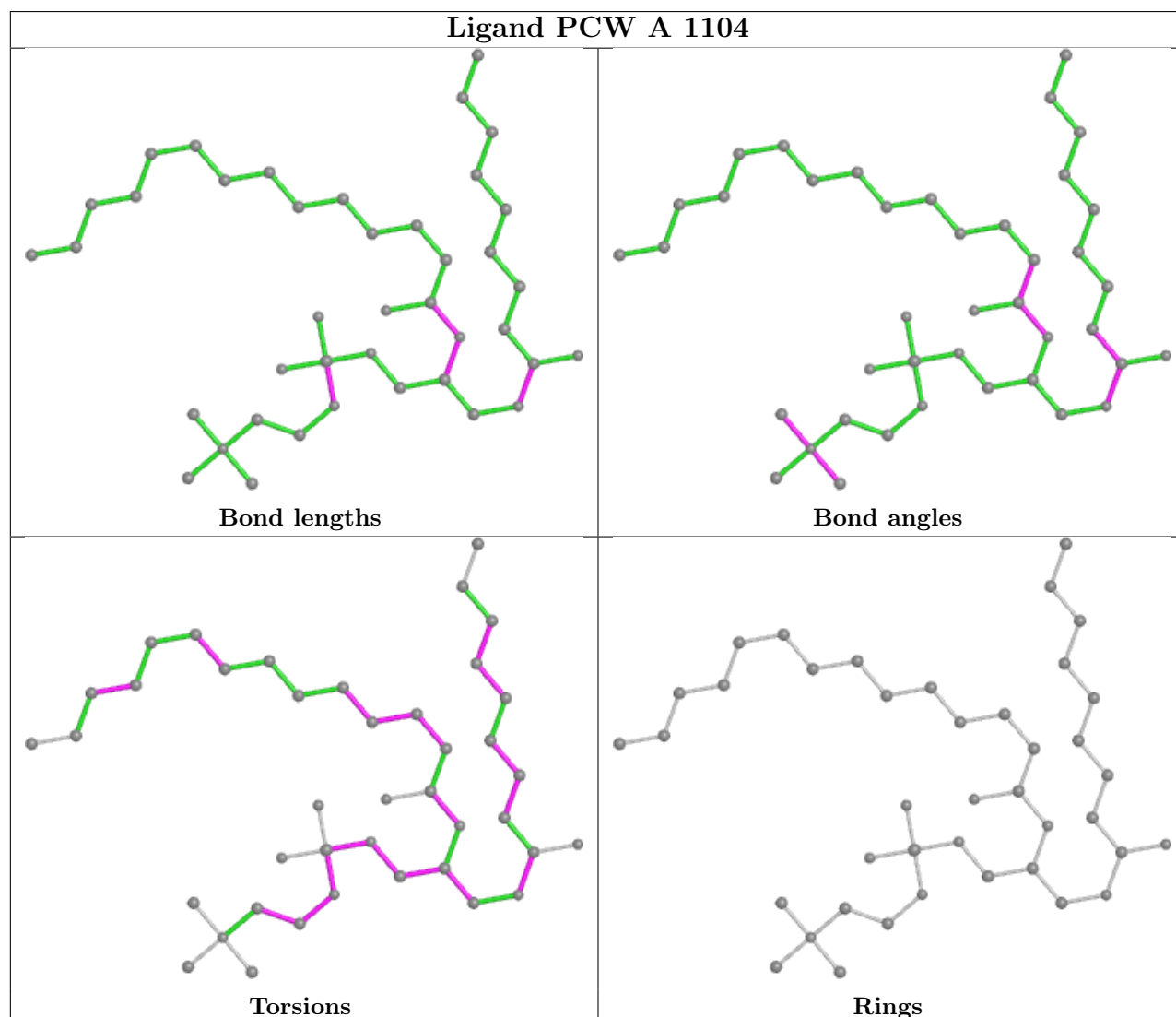
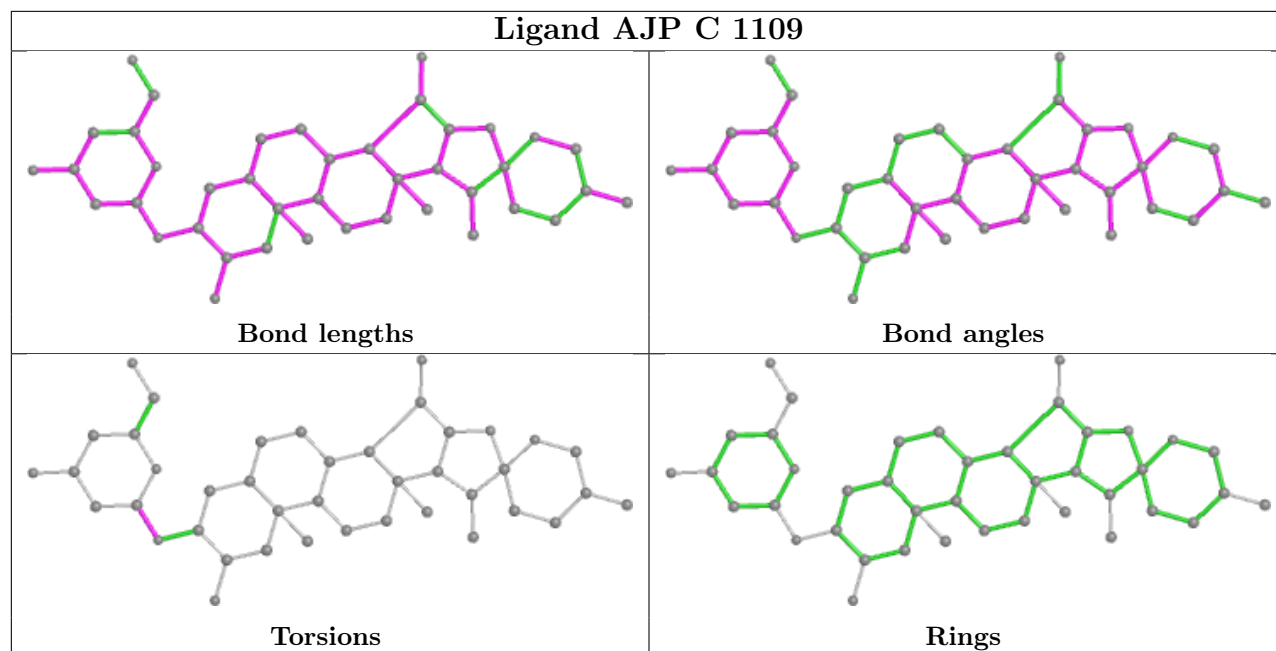


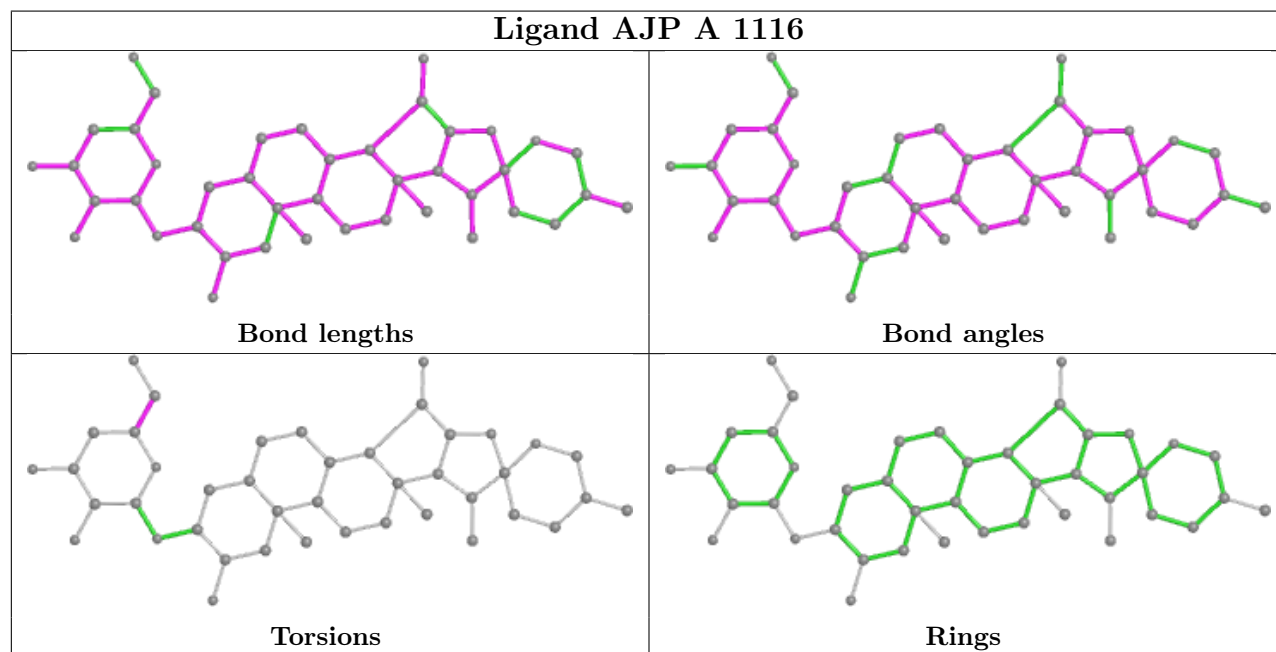
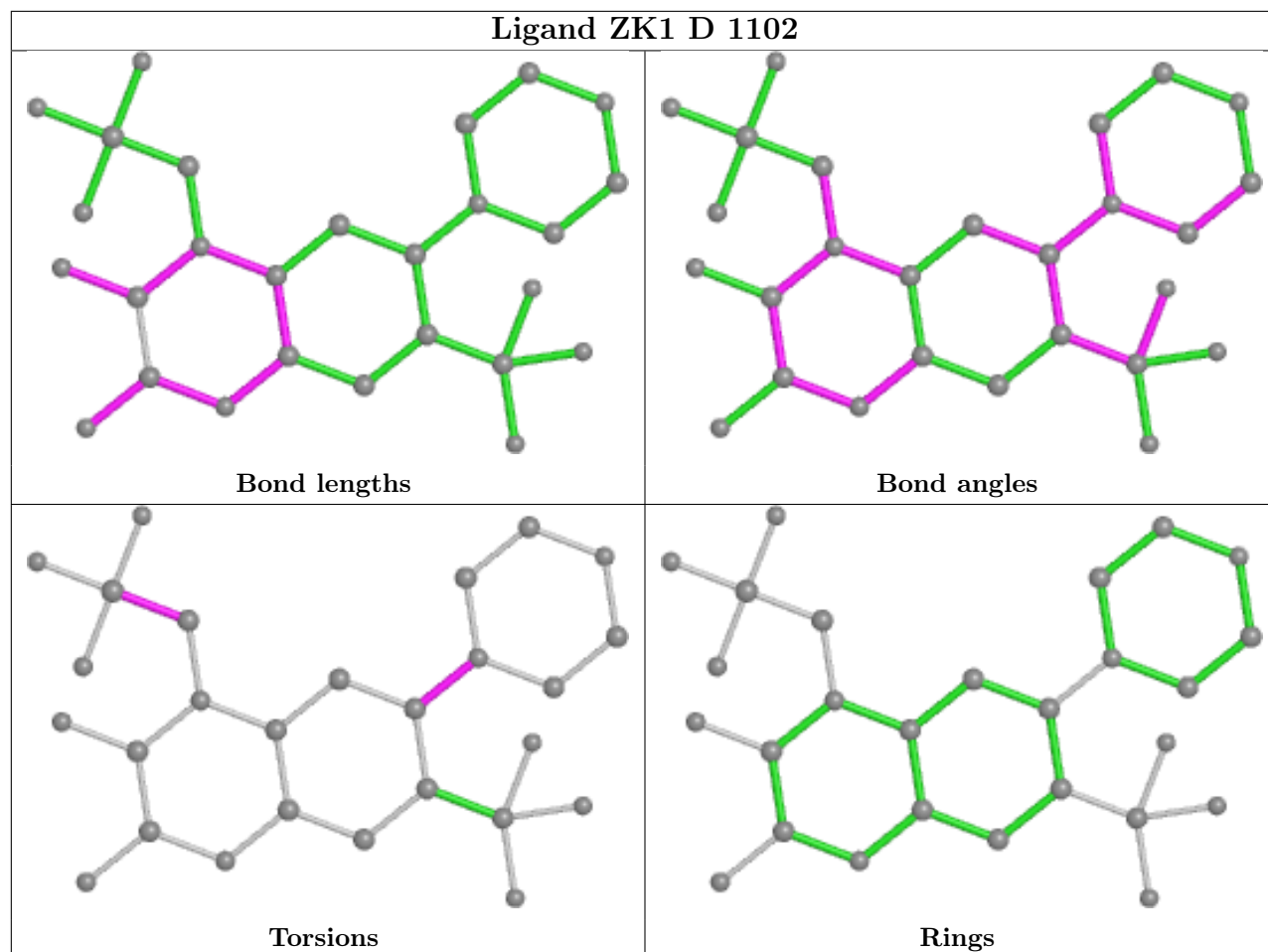


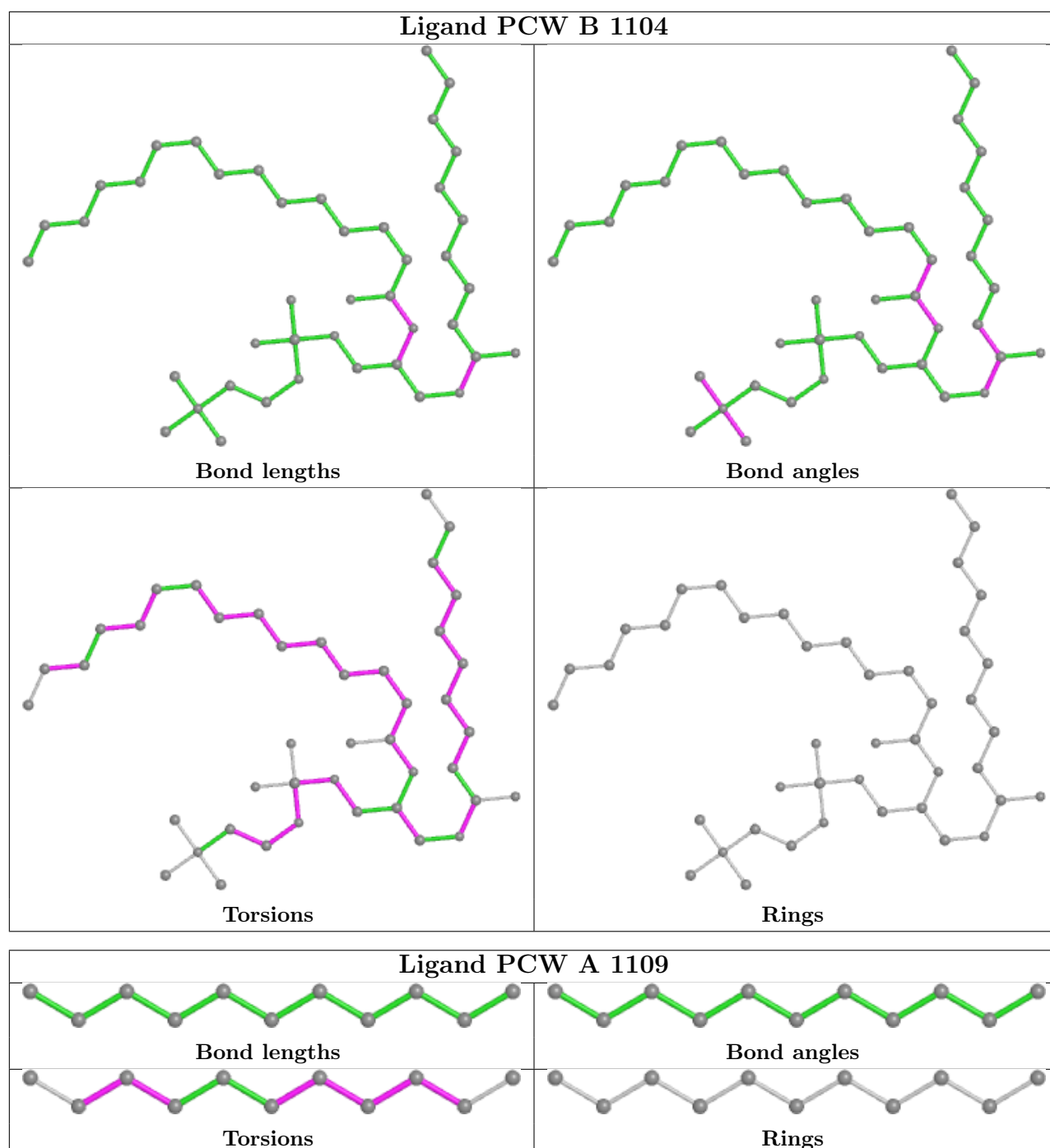


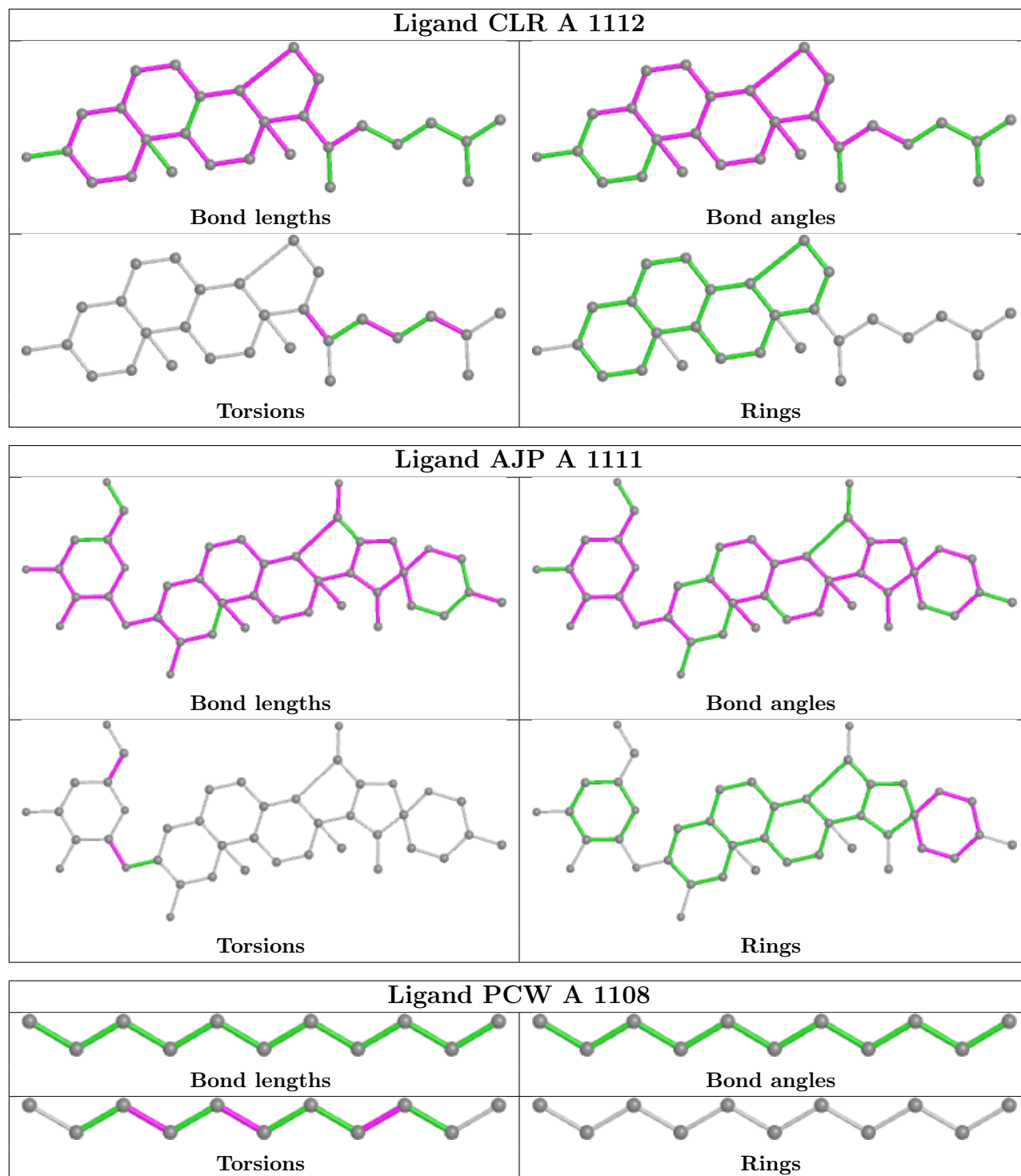


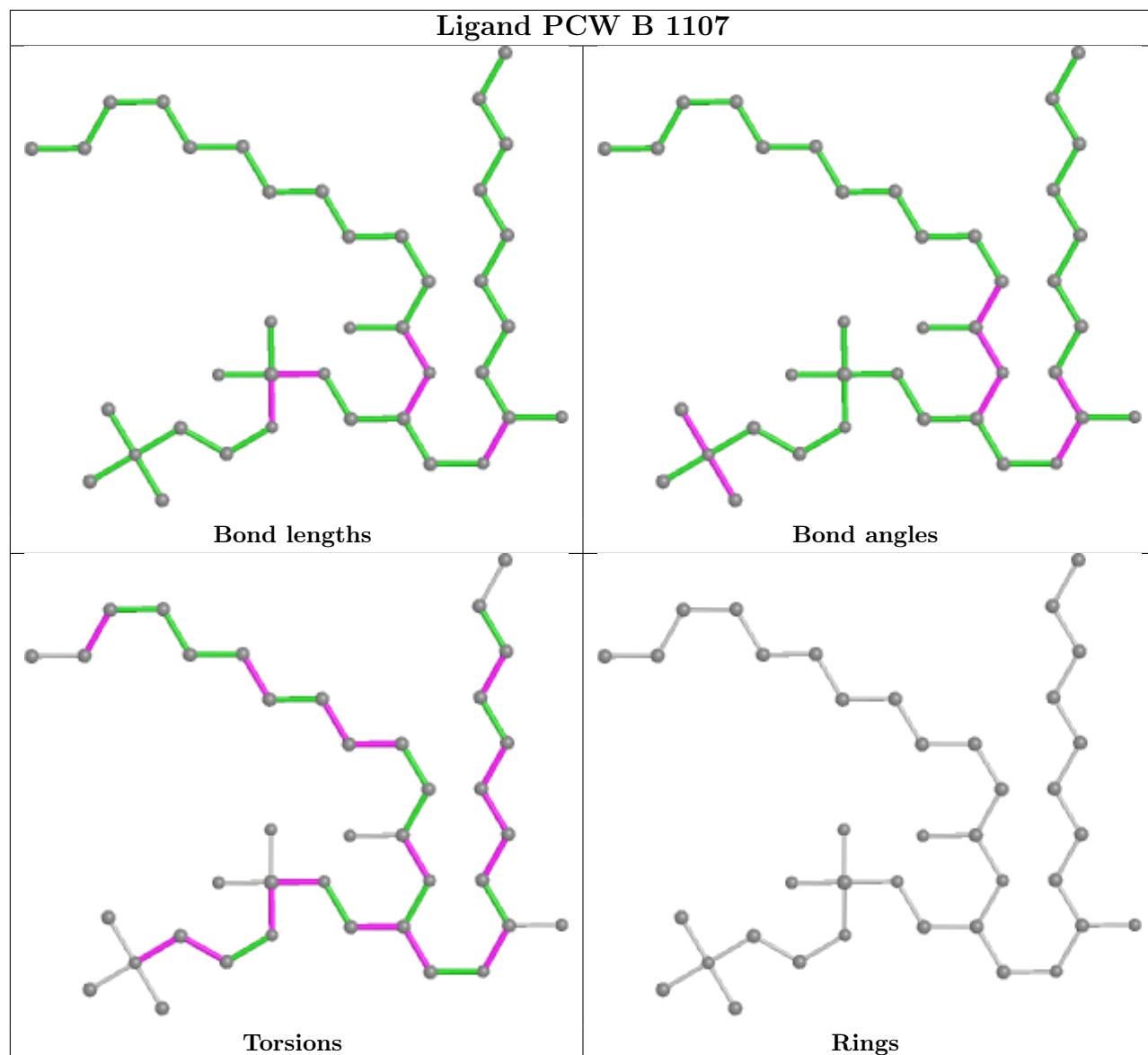


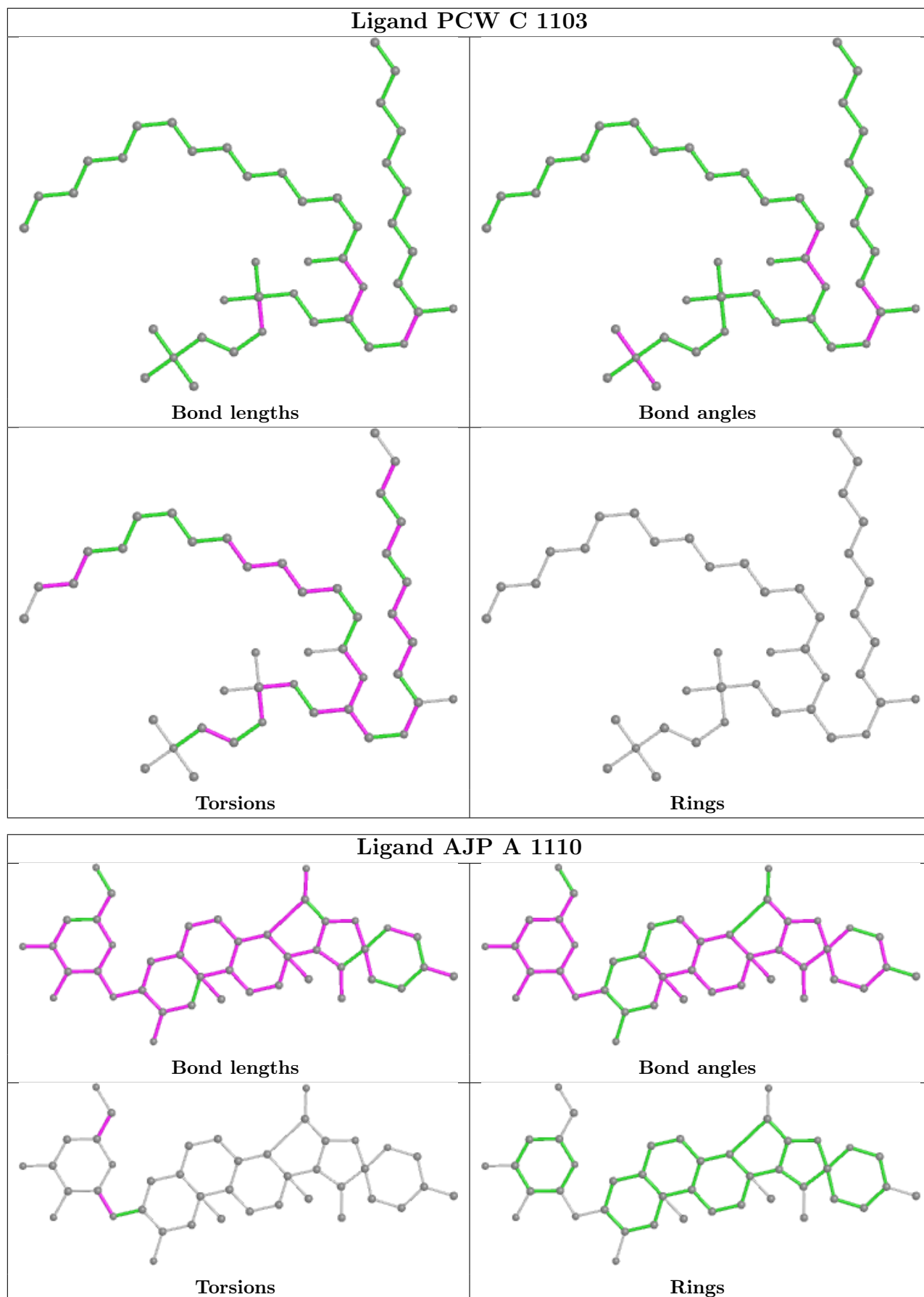


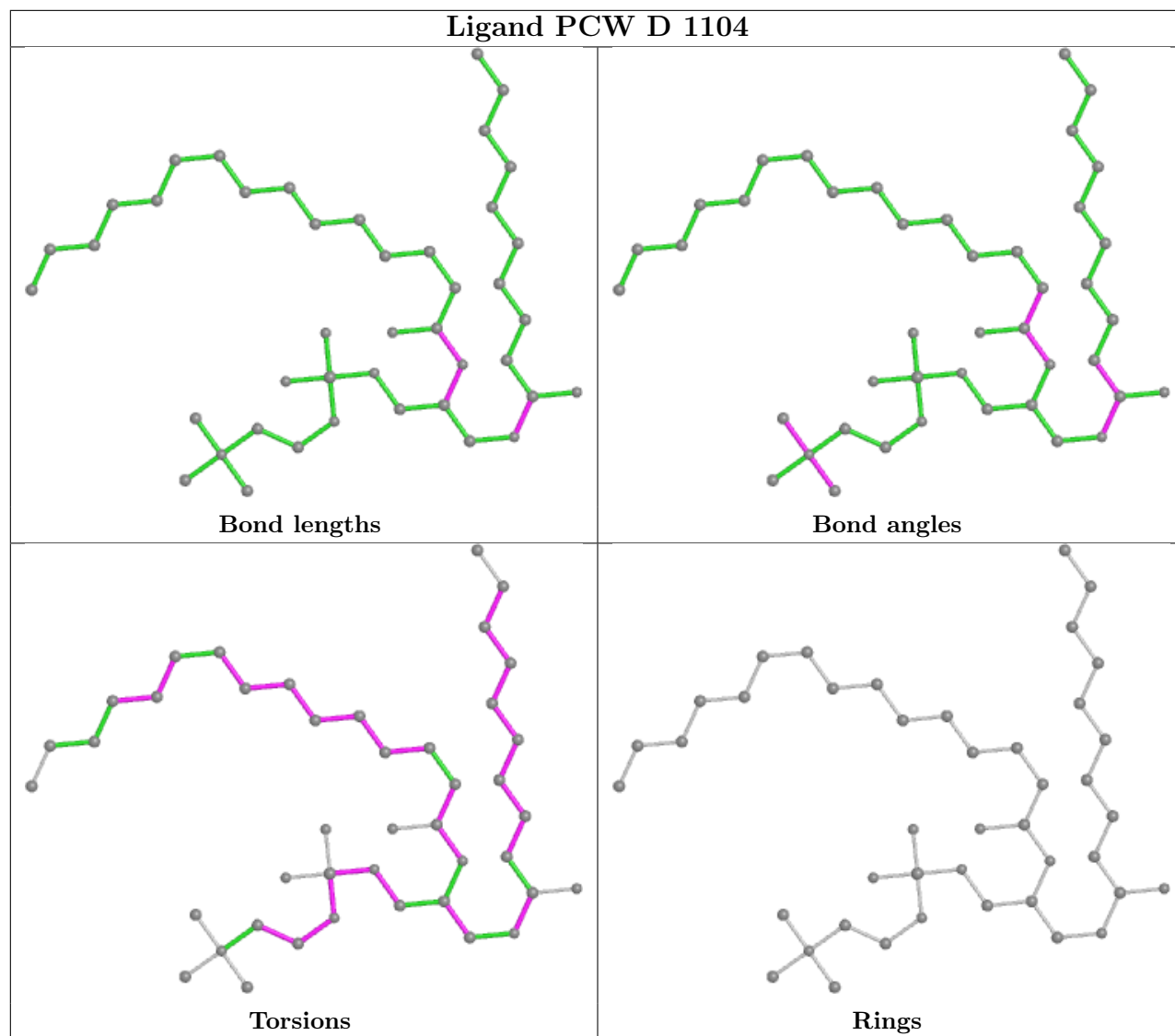


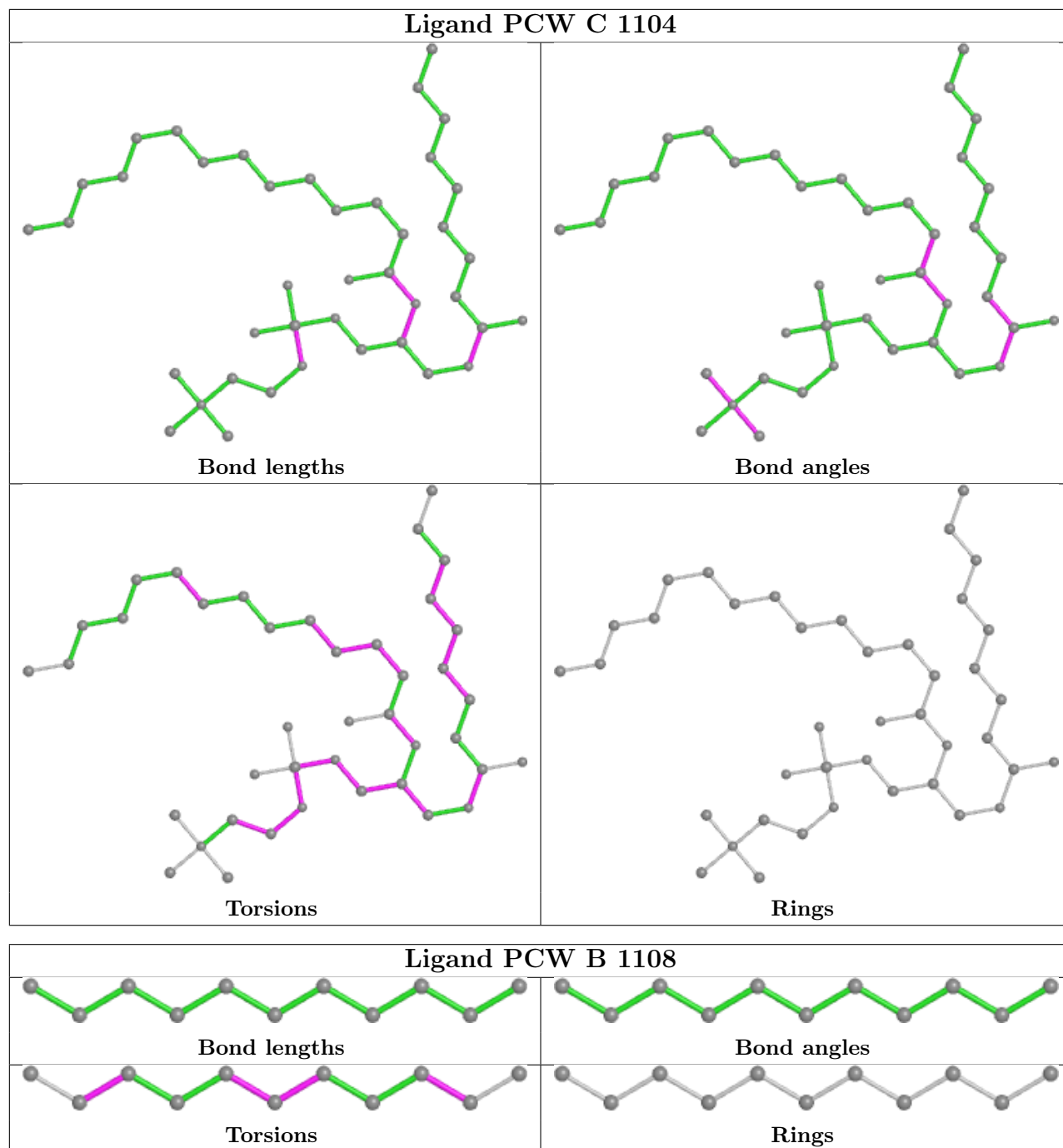




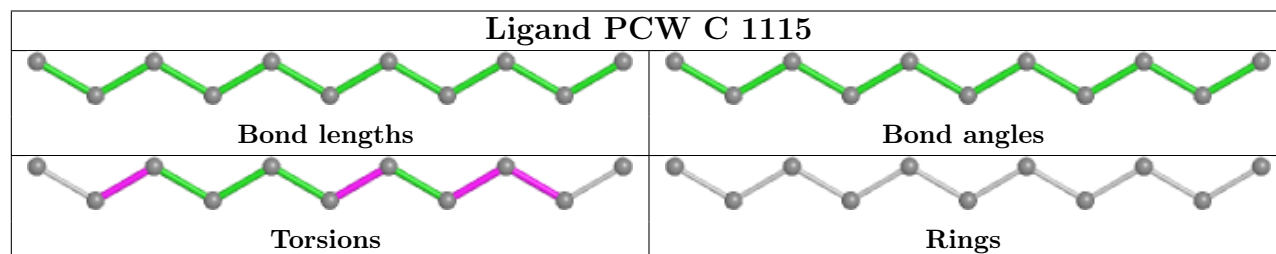
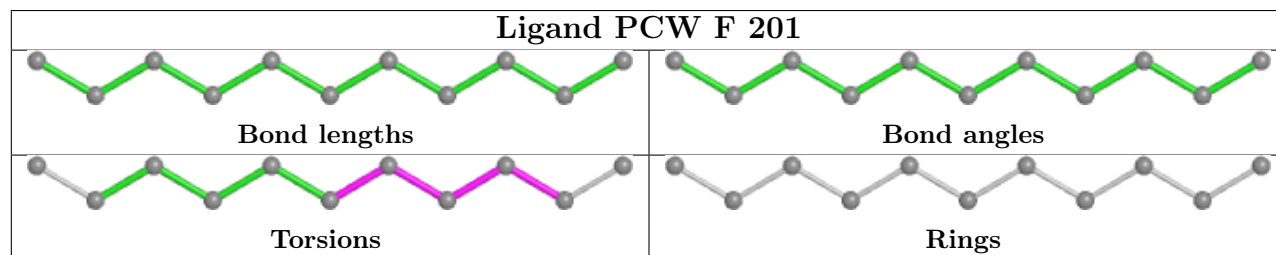
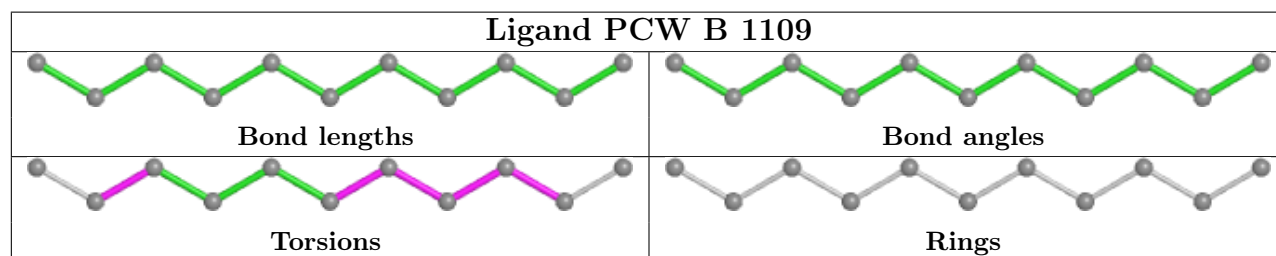
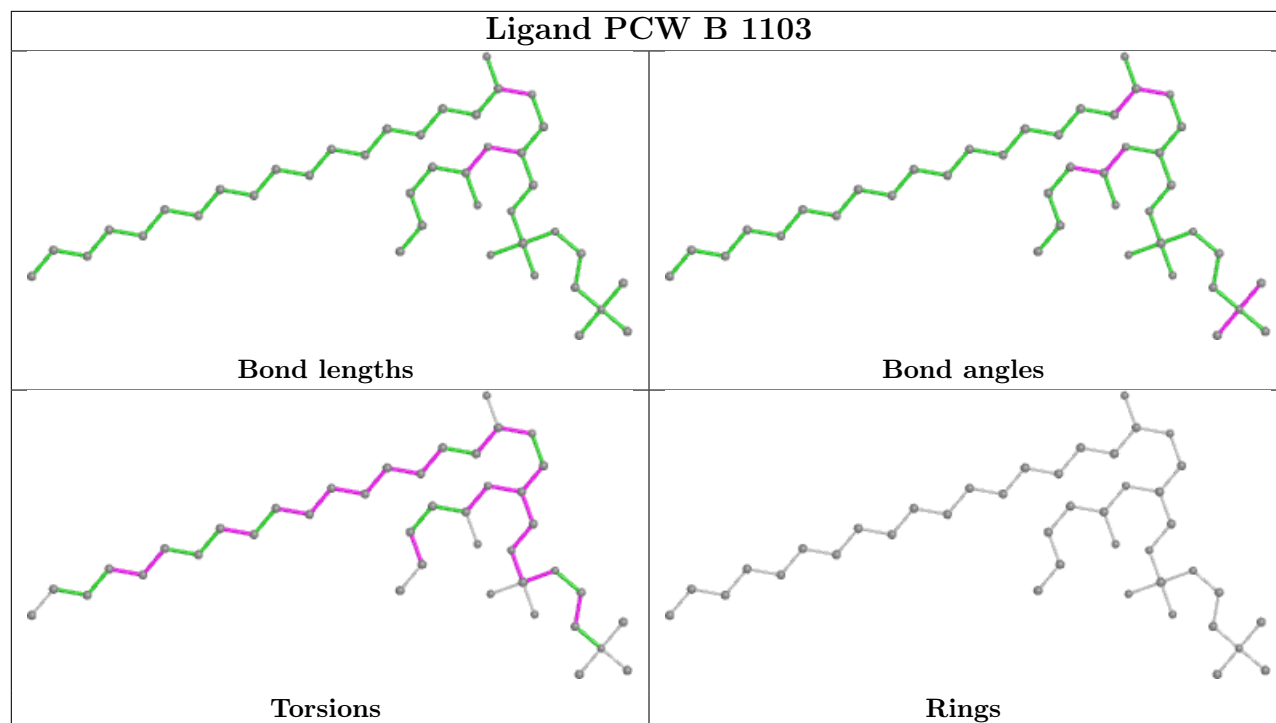


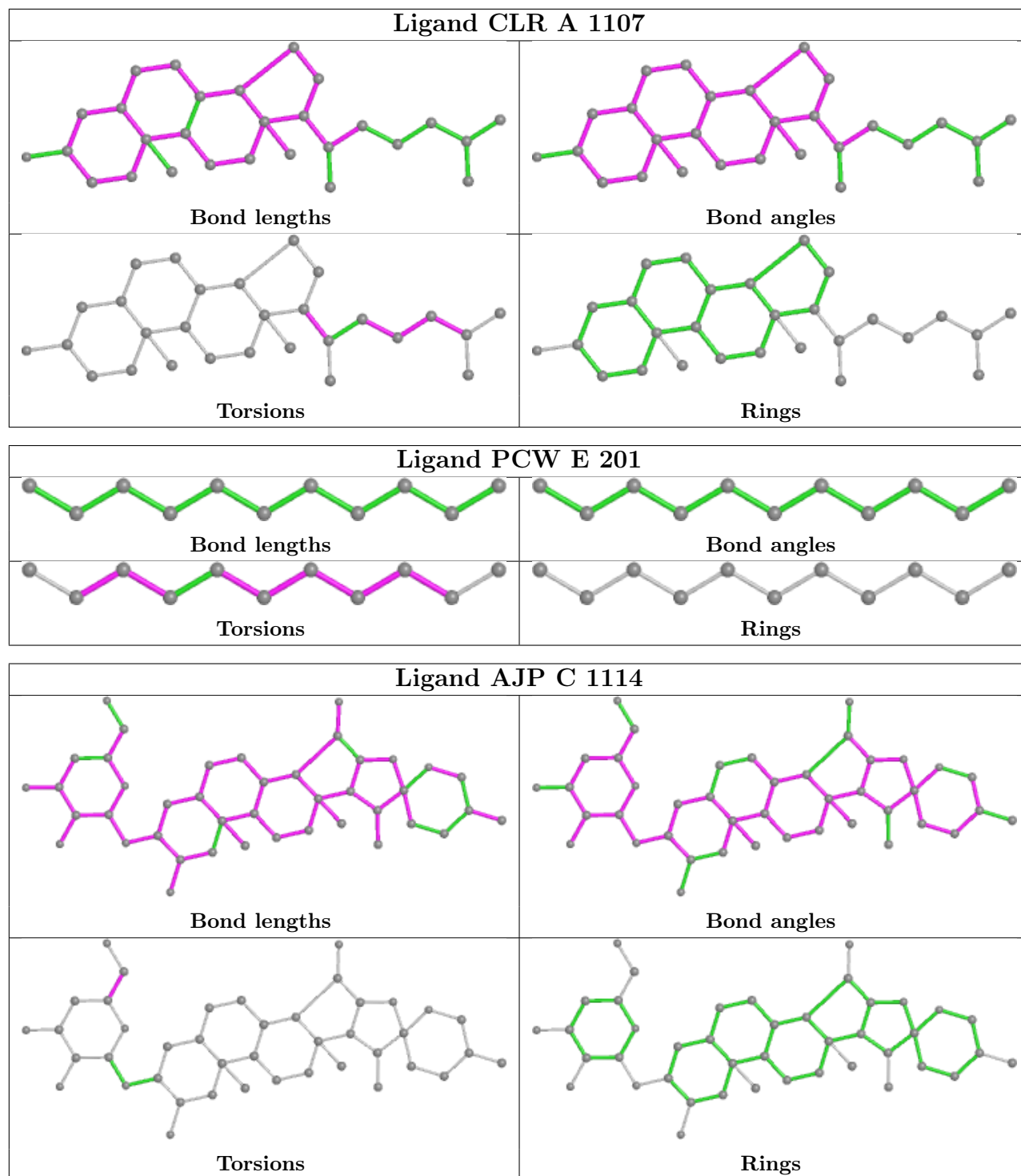


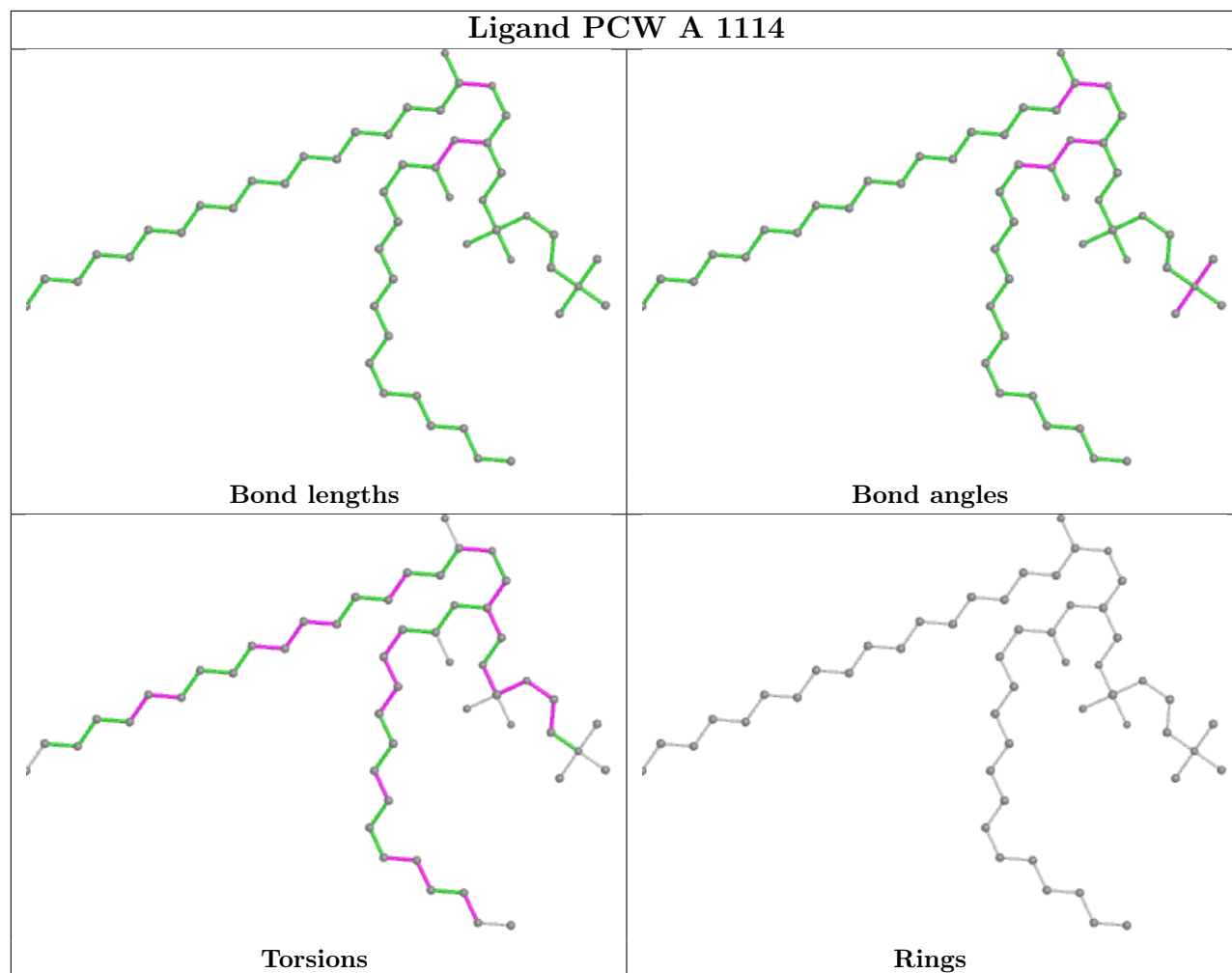


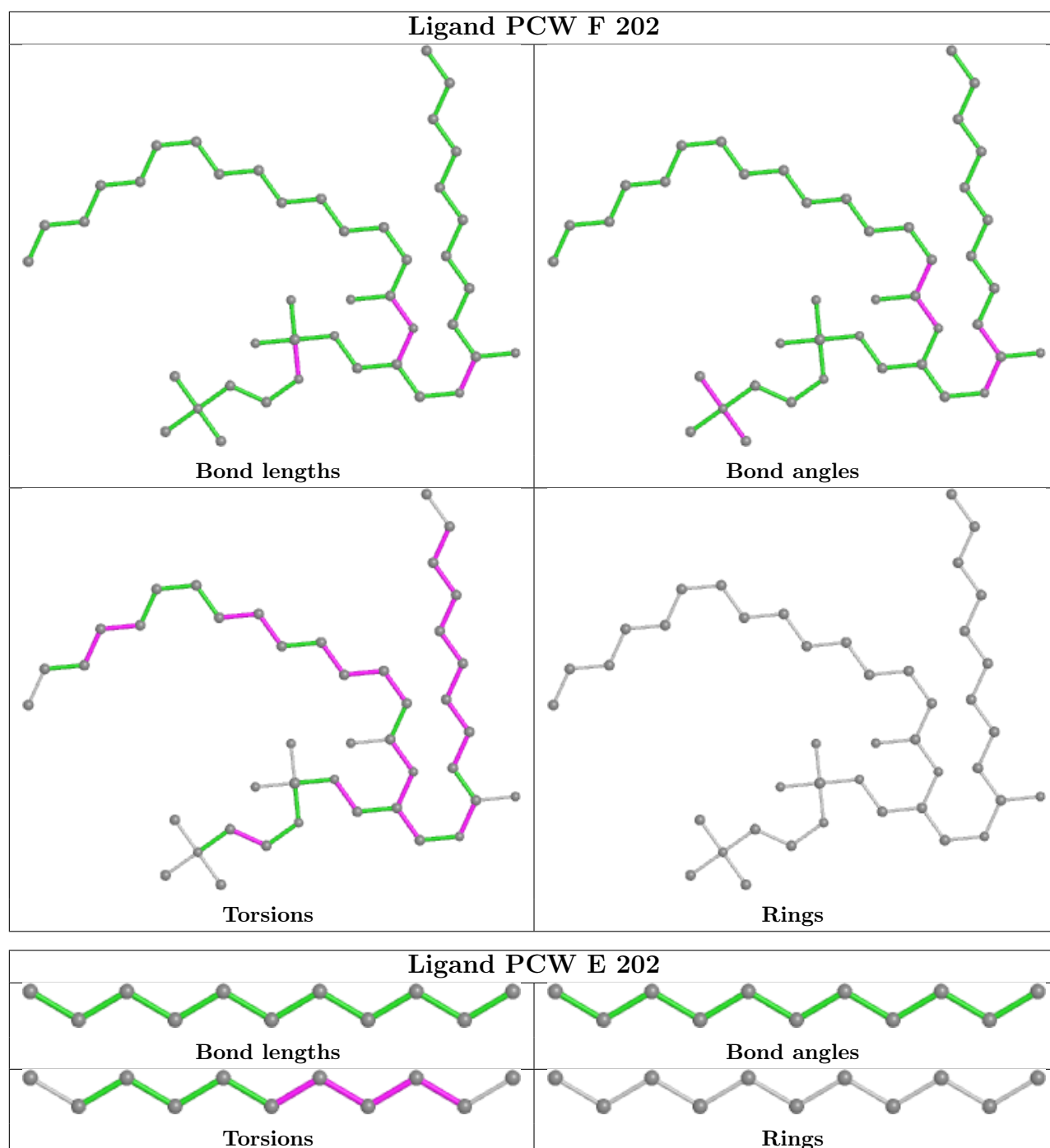


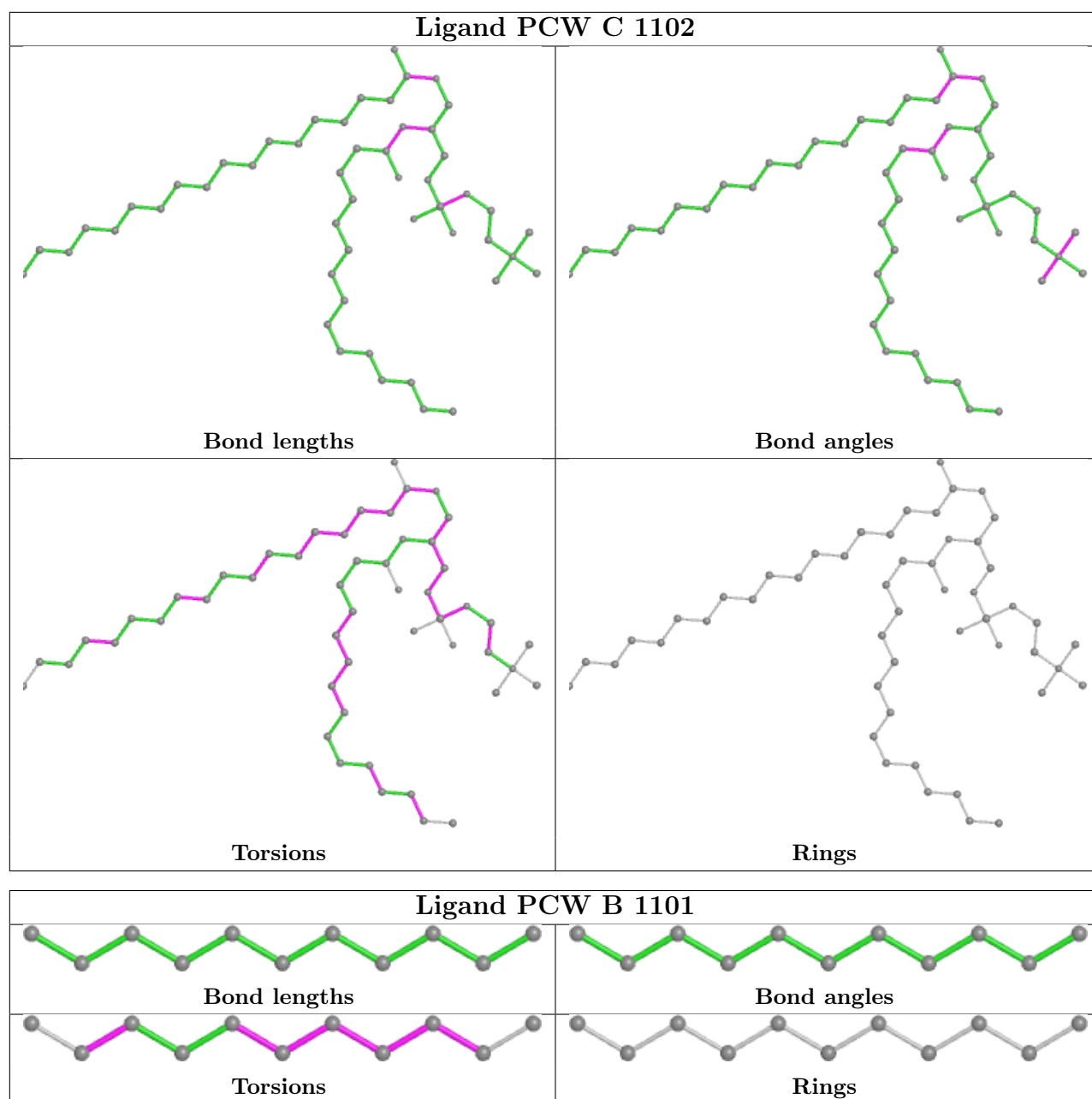












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

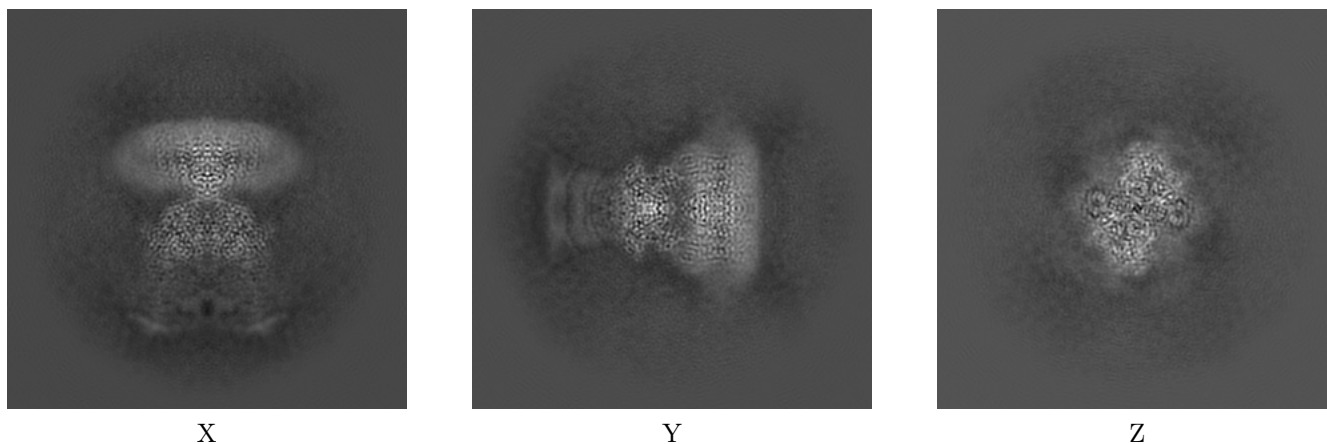
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40742. These allow visual inspection of the internal detail of the map and identification of artifacts.

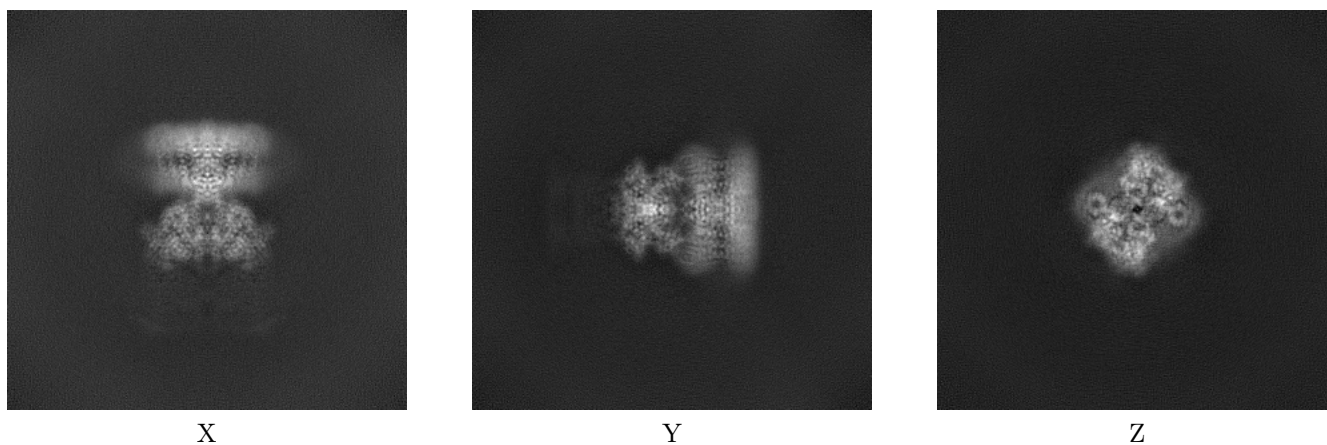
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



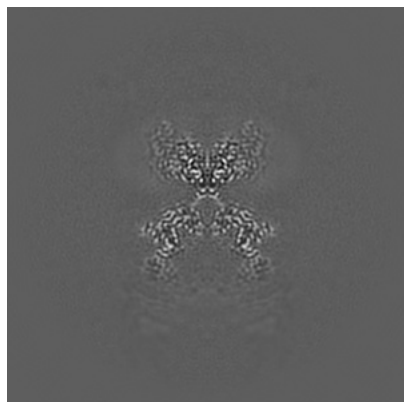
#### 6.1.2 Raw map



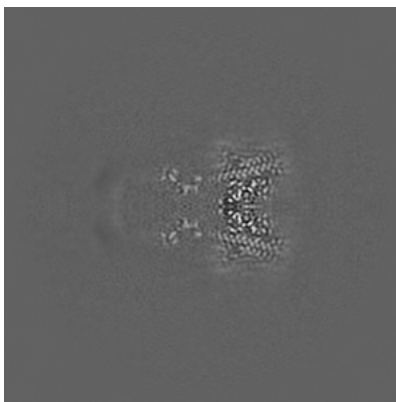
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

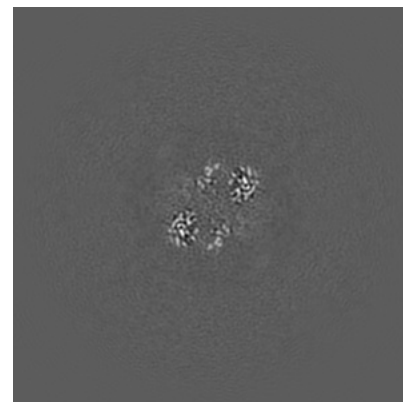
### 6.2.1 Primary map



X Index: 208

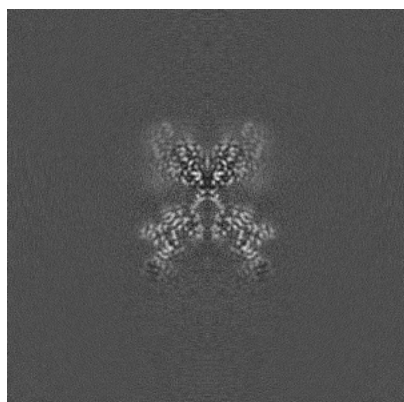


Y Index: 208

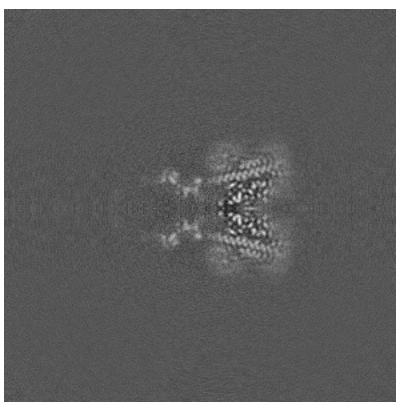


Z Index: 208

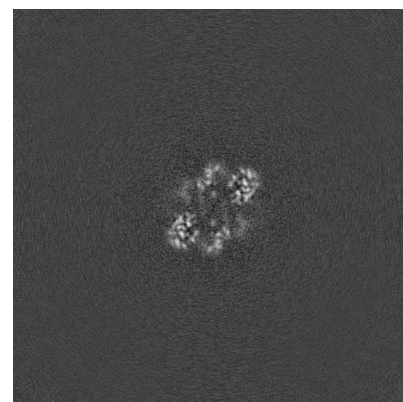
### 6.2.2 Raw map



X Index: 208



Y Index: 208



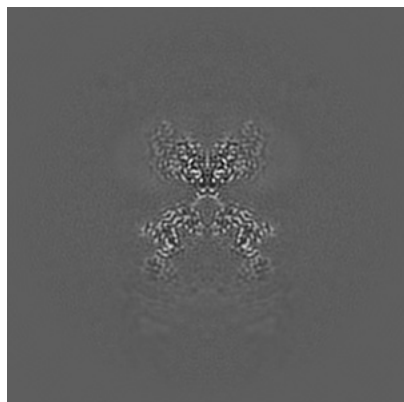
Z Index: 208

The images above show central slices of the map in three orthogonal directions.

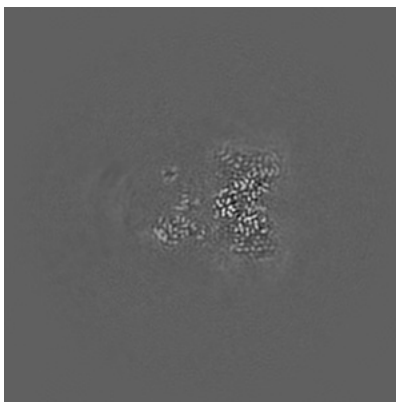


## 6.3 Largest variance slices [i](#)

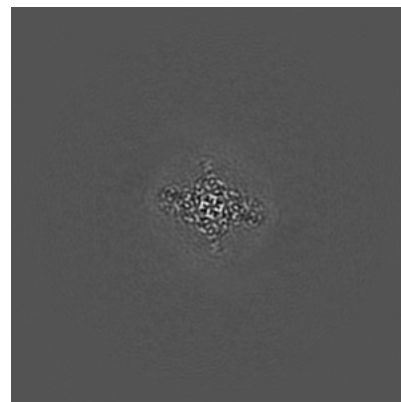
### 6.3.1 Primary map



X Index: 208

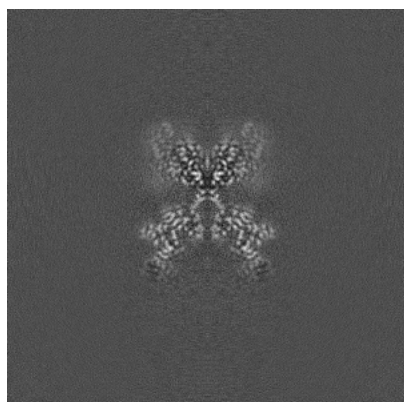


Y Index: 202

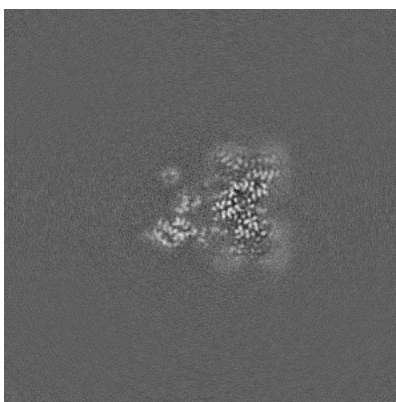


Z Index: 239

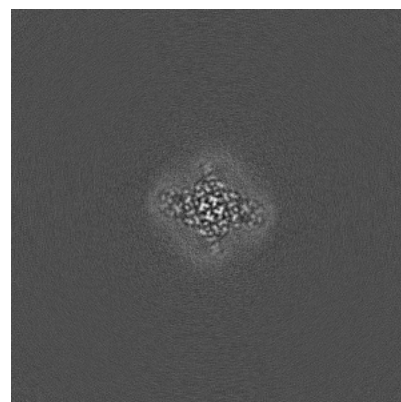
### 6.3.2 Raw map



X Index: 208



Y Index: 201



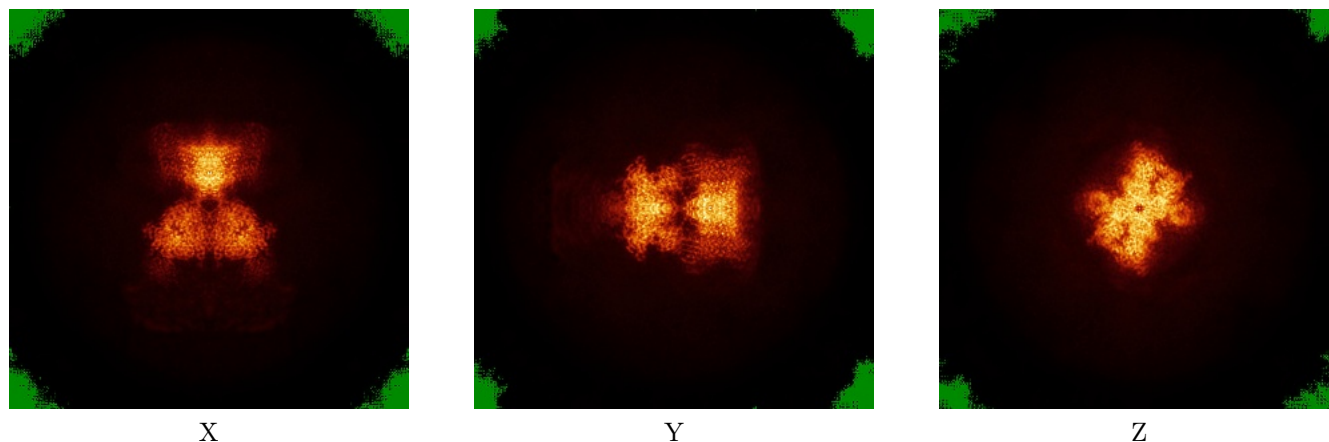
Z Index: 239

The images above show the largest variance slices of the map in three orthogonal directions.

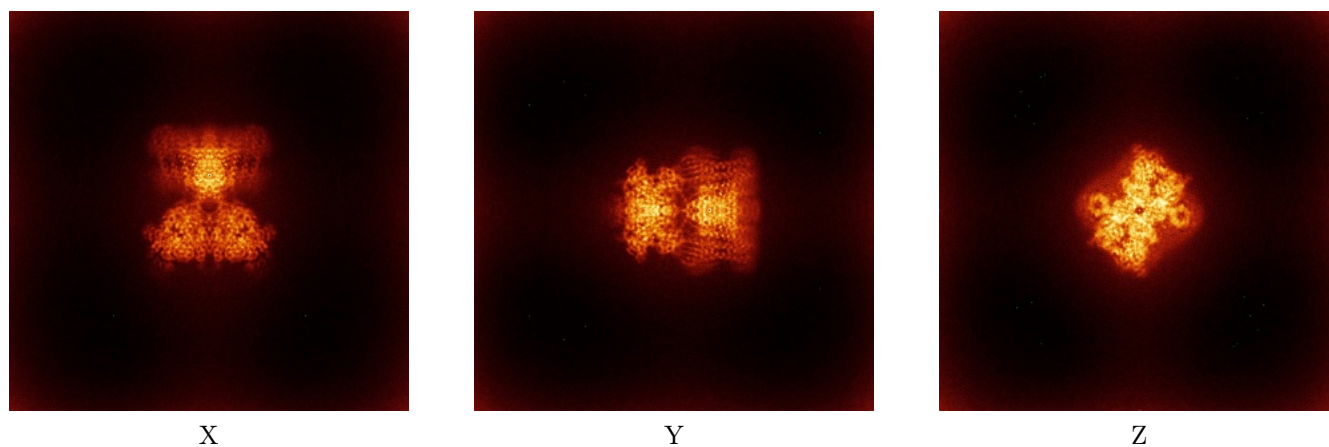


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



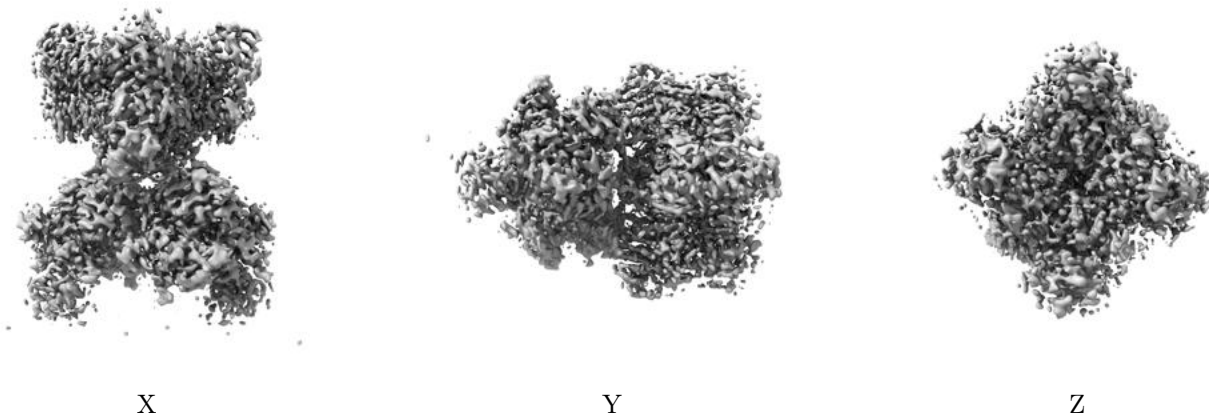
### 6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

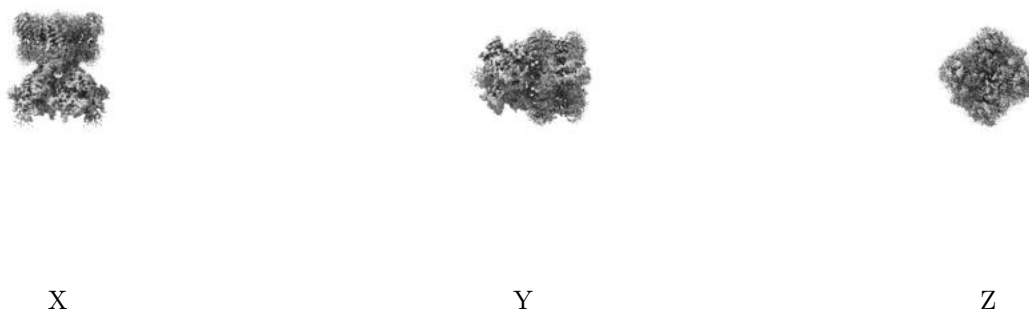
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

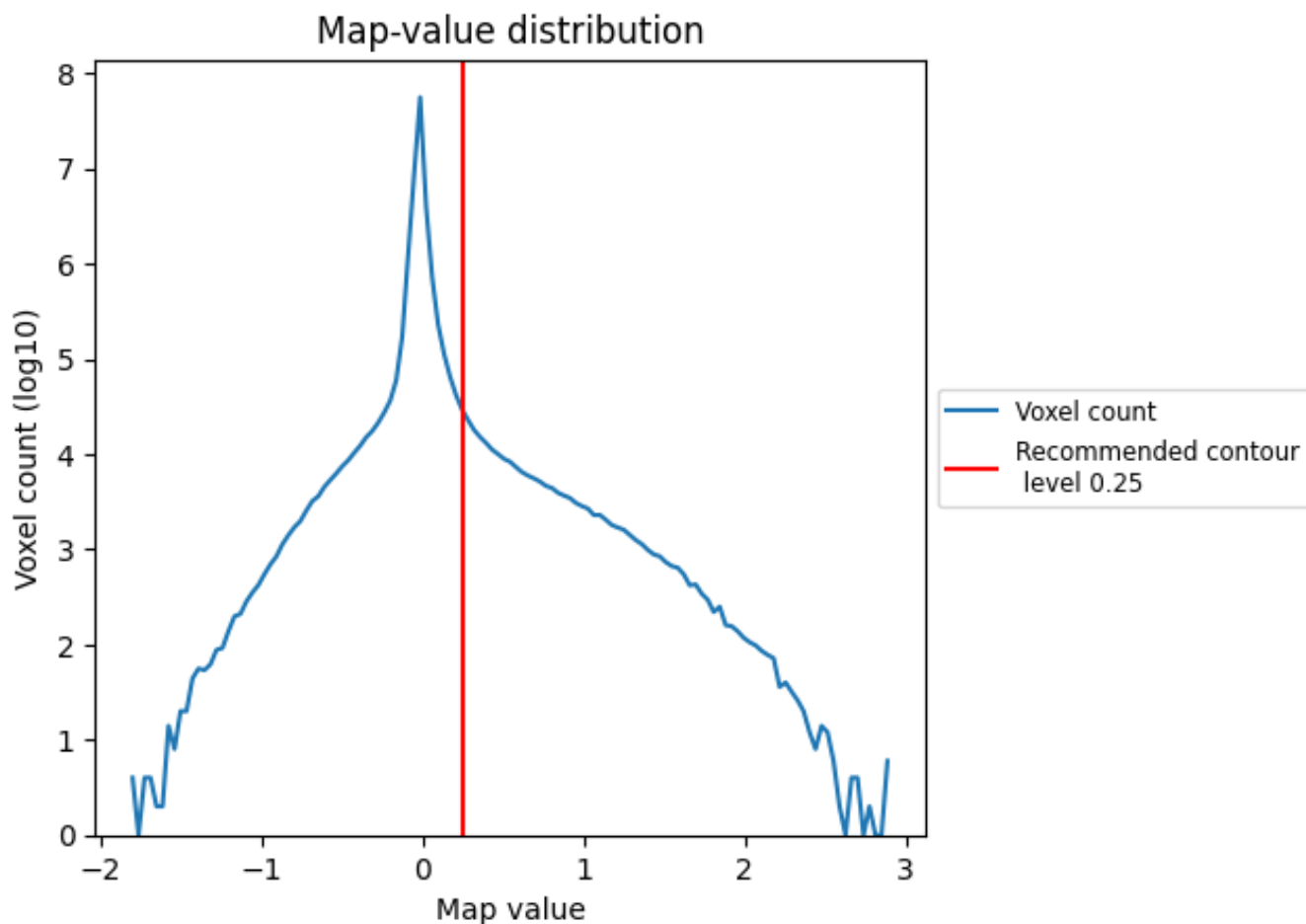
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

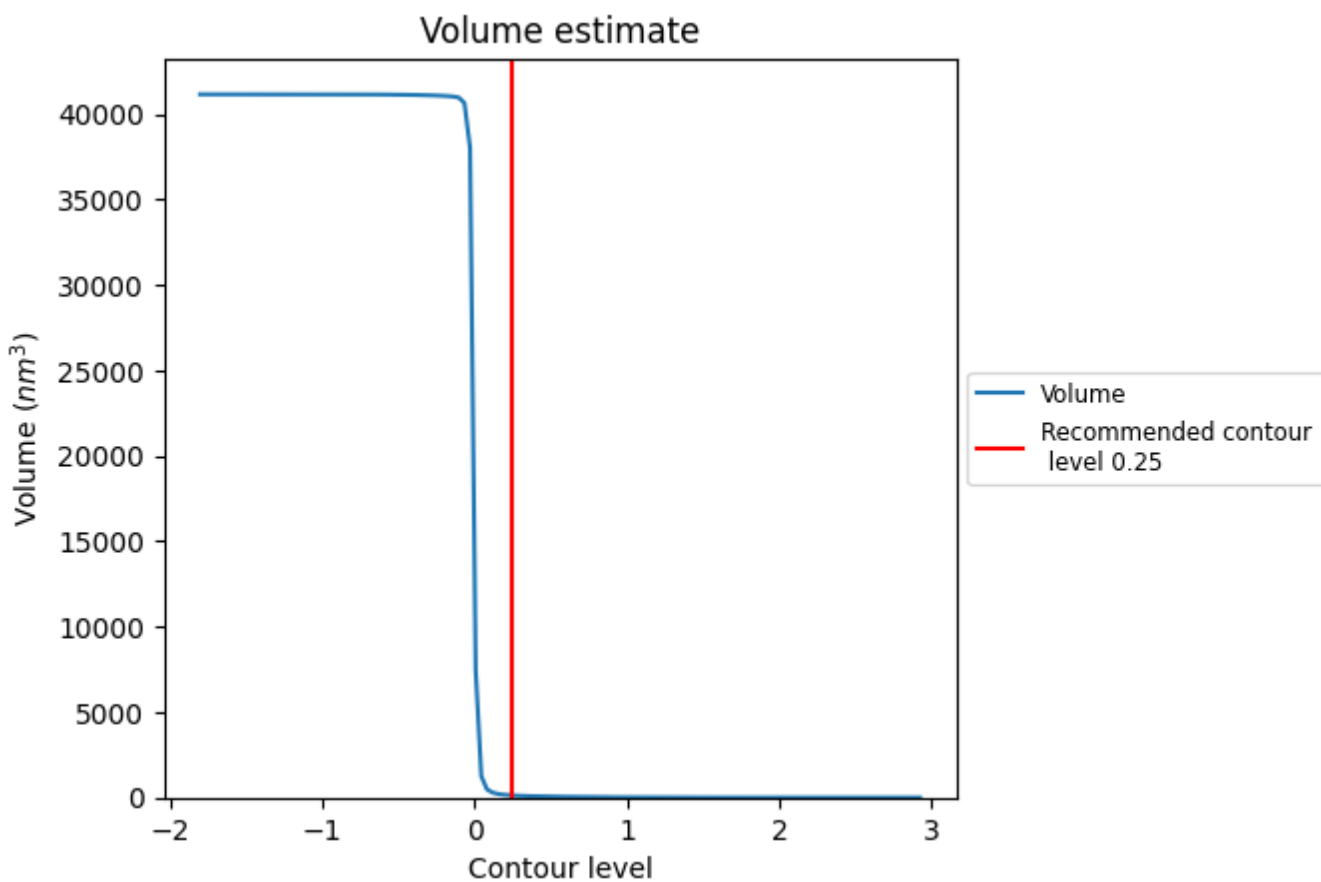
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

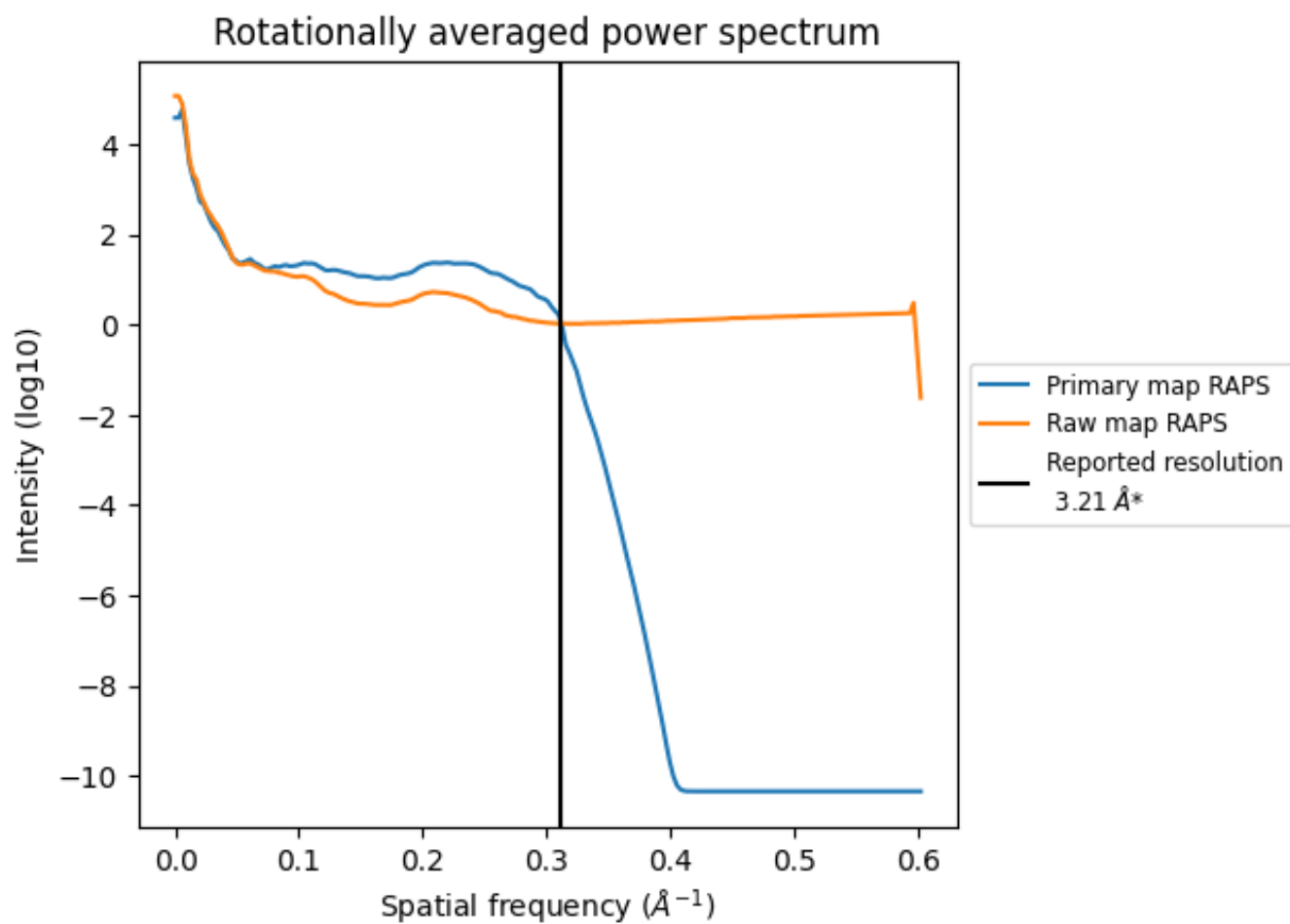
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 124 nm<sup>3</sup>; this corresponds to an approximate mass of 112 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

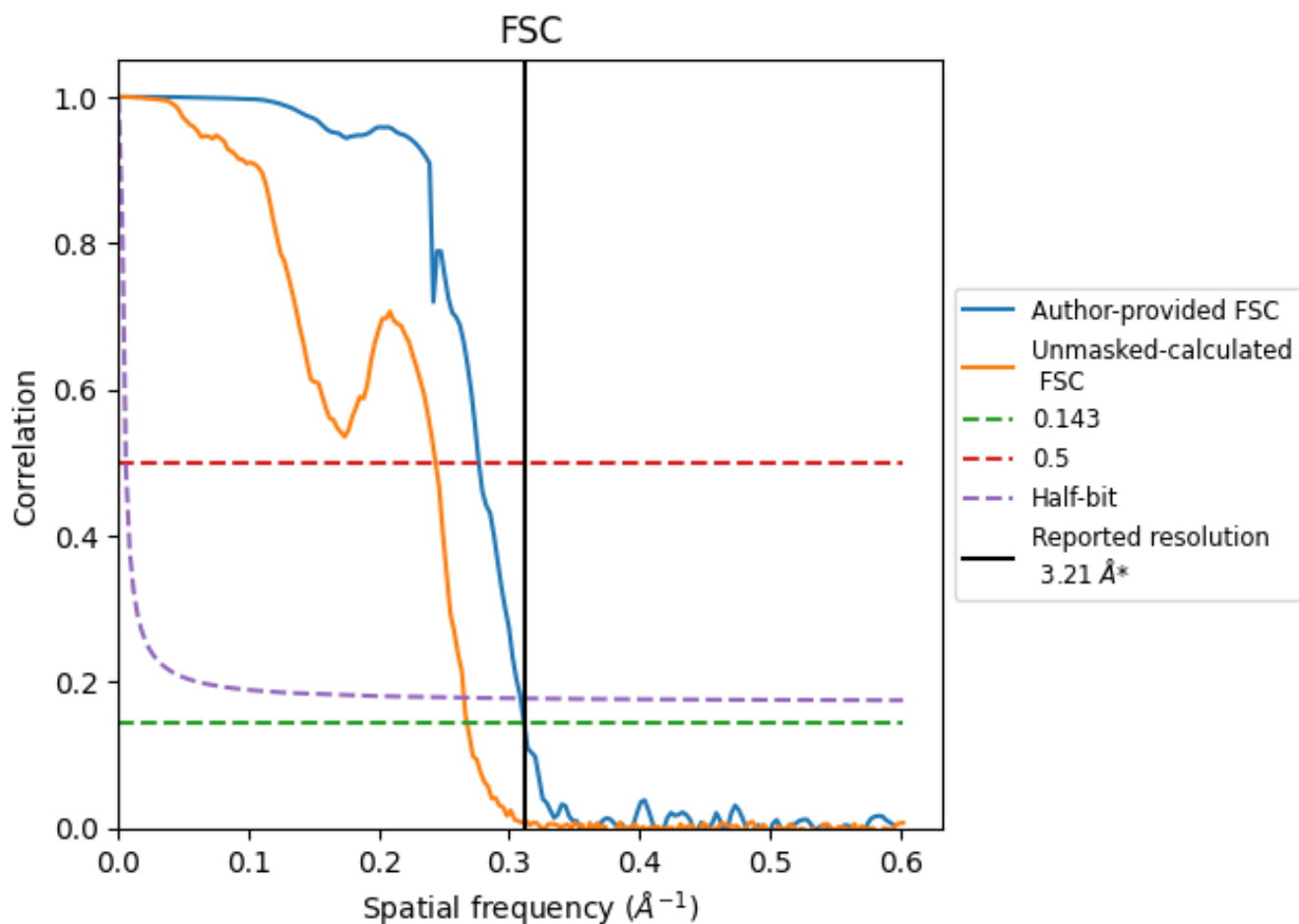


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

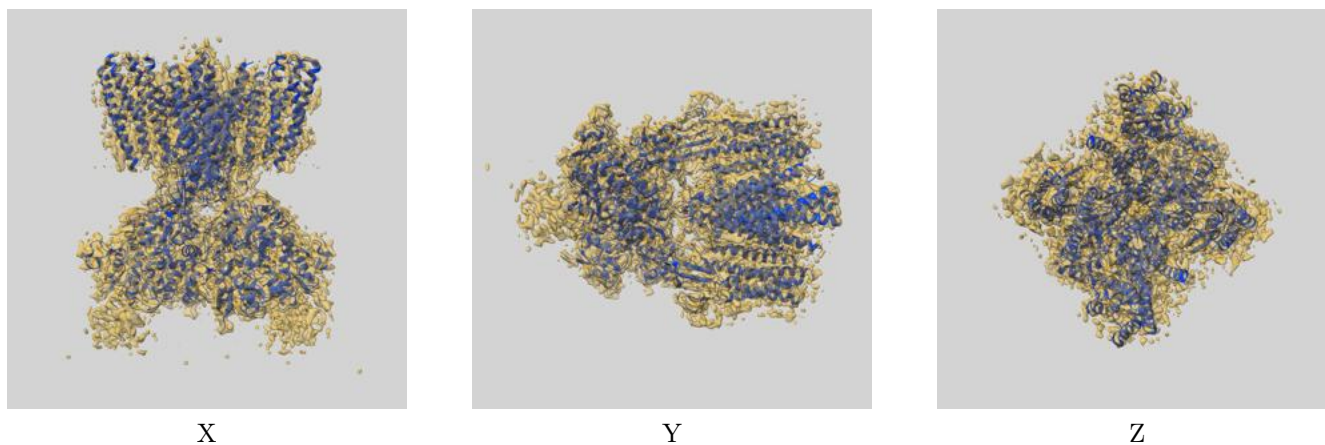
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	3.62	3.24
Unmasked-calculated*	3.74	4.11	3.77

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 3.21 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40742 and PDB model 8SS3. Per-residue inclusion information can be found in section 3 on page 12.

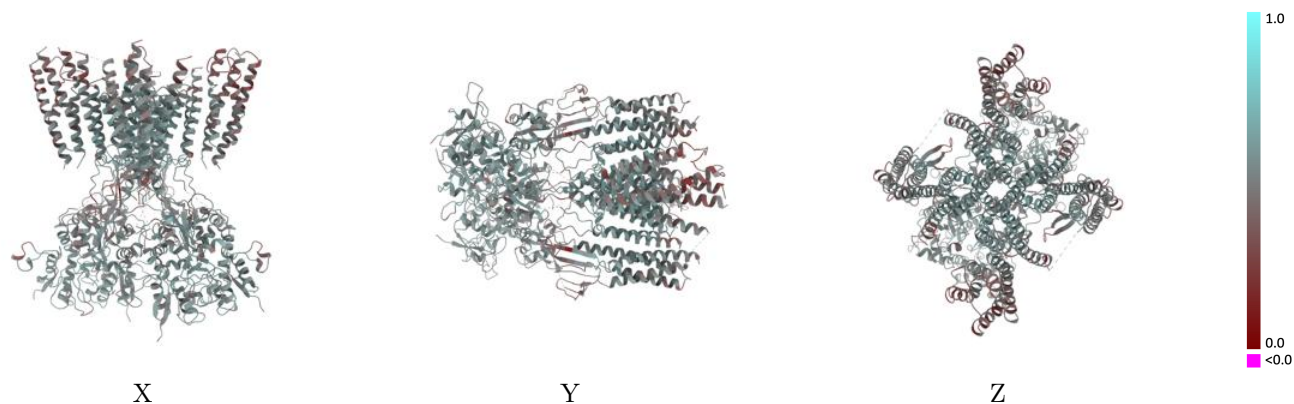
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

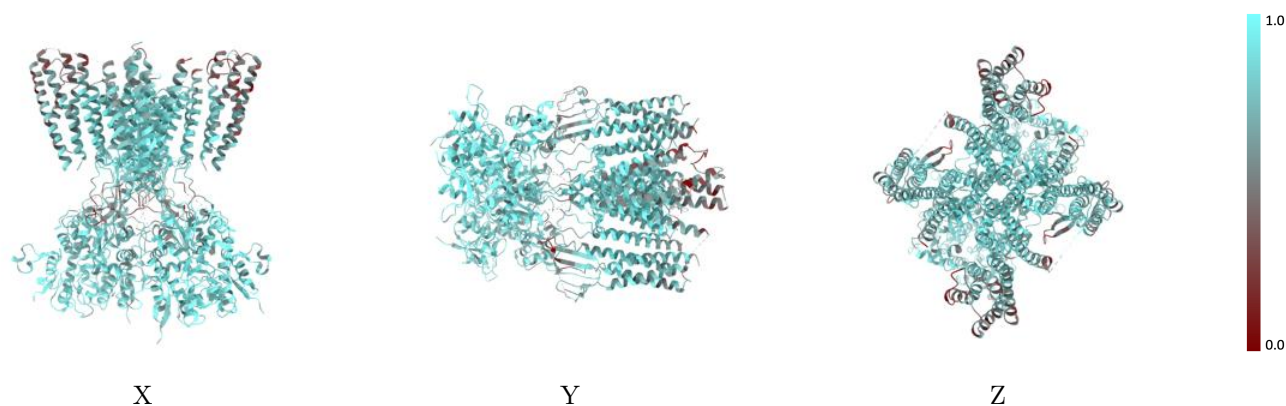


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



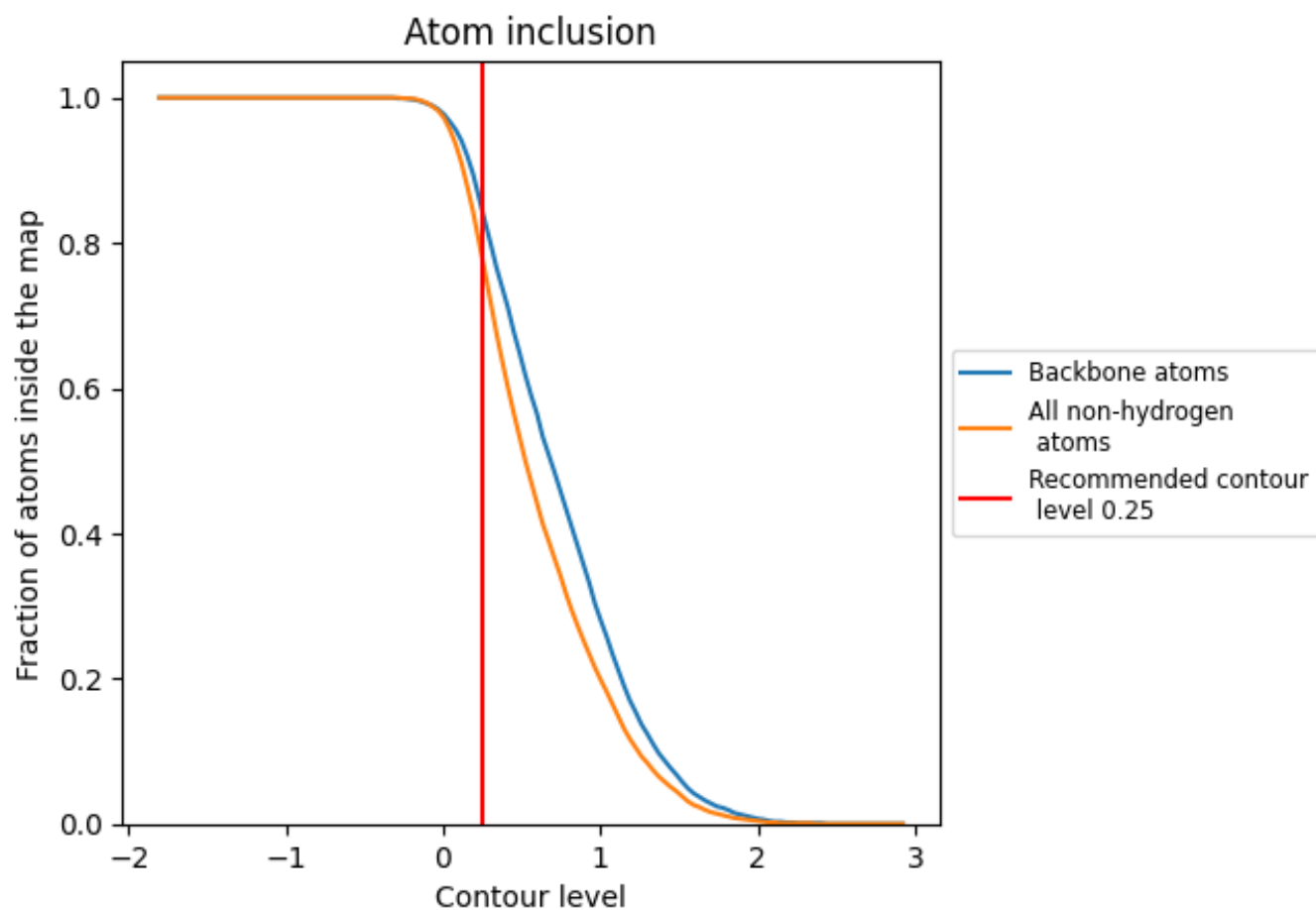
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7790	 0.5070
A	 0.7830	 0.5110
B	 0.8310	 0.5290
C	 0.7870	 0.5090
D	 0.8350	 0.5260
E	 0.6090	 0.4340
F	 0.6030	 0.4360

