



## wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 04:02 PM JST

PDB ID : 6JB1  
EMDB ID : EMD-9787  
Title : Structure of pancreatic ATP-sensitive potassium channel bound with repaglinide and ATPgammaS at 3.3A resolution  
Authors : Chen, L.; Ding, D.; Wang, M.; Wu, J.-X.; Kang, Y.  
Deposited on : 2019-01-25  
Resolution : 3.30 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:

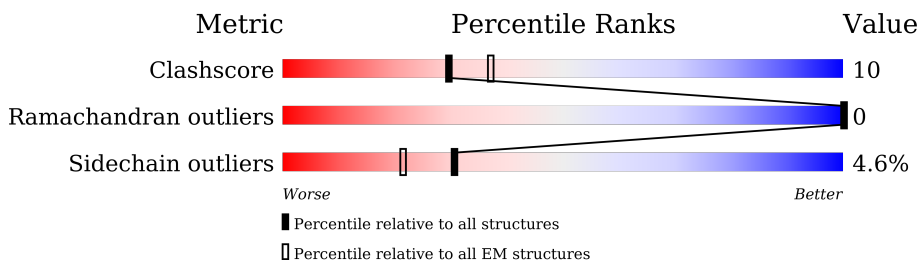
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 3.30 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	390	 55% 27% 16%
1	C	390	 55% 28% 16%
1	E	390	 54% 28% 16%
1	G	390	 54% 28% 16%
2	B	1582	 16% 69% 16% 14%
2	D	1582	 16% 69% 16% 14%
2	F	1582	 16% 70% 16% 14%
2	H	1582	 16% 70% 15% 14%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
5	AJP	B	1601	X	-	-	-
5	AJP	D	1601	X	-	-	-
5	AJP	F	1601	X	-	-	-
5	AJP	H	1601	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 52028 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.

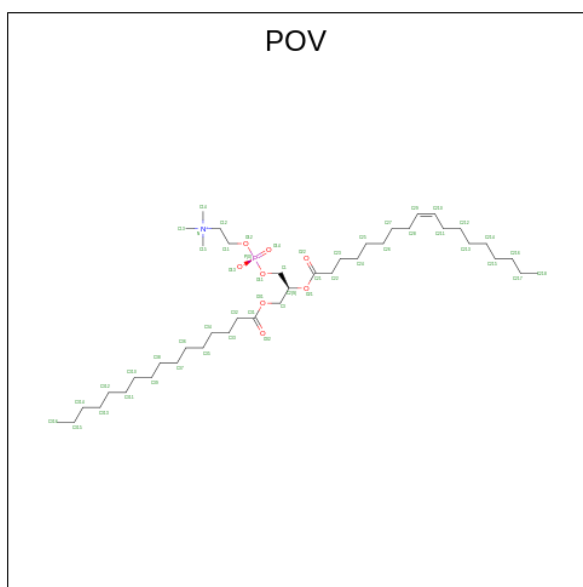
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	327	2543	1641	440	446	16	0	0
1	C	327	2543	1641	440	446	16	0	0
1	E	327	2543	1641	440	446	16	0	0
1	G	327	2543	1641	440	446	16	0	0

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8 isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1366	9890	6419	1693	1735	43	0	0
2	D	1366	9890	6419	1693	1735	43	0	0
2	F	1366	9890	6419	1693	1735	43	0	0
2	H	1366	9890	6419	1693	1735	43	0	0

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total 31	22	1	7	1	0
3	B	1	Total 272	199	7	59	7	0
3	B	1	Total 272	199	7	59	7	0
3	B	1	Total 272	199	7	59	7	0
3	B	1	Total 272	199	7	59	7	0
3	B	1	Total 272	199	7	59	7	0
3	B	1	Total 272	199	7	59	7	0
3	B	1	Total 272	199	7	59	7	0
3	B	1	Total 272	199	7	59	7	0
3	B	1	Total 272	199	7	59	7	0
3	C	1	Total 31	22	1	7	1	0
3	D	1	Total 272	199	7	59	7	0
3	D	1	Total 272	199	7	59	7	0
3	D	1	Total 272	199	7	59	7	0
3	D	1	Total 272	199	7	59	7	0

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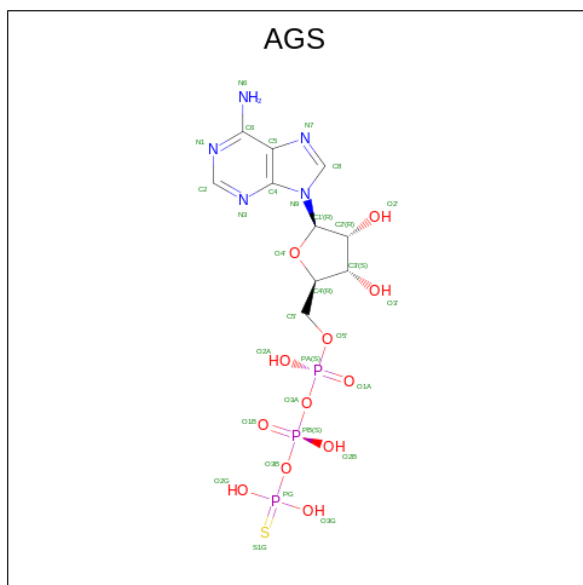
Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	E	1	Total	C	N	O	P	0
			31	22	1	7	1	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	G	1	Total	C	N	O	P	0
			31	22	1	7	1	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	

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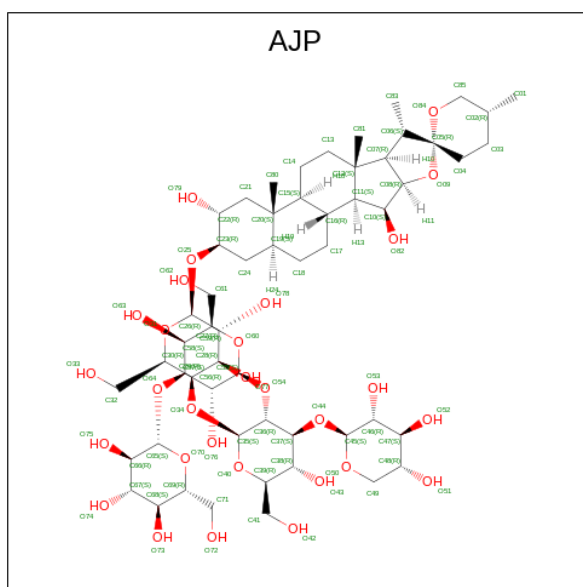
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	H	1	272	199	7	59	7	0

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula:  $C_{10}H_{16}N_5O_{12}P_3S$ ).



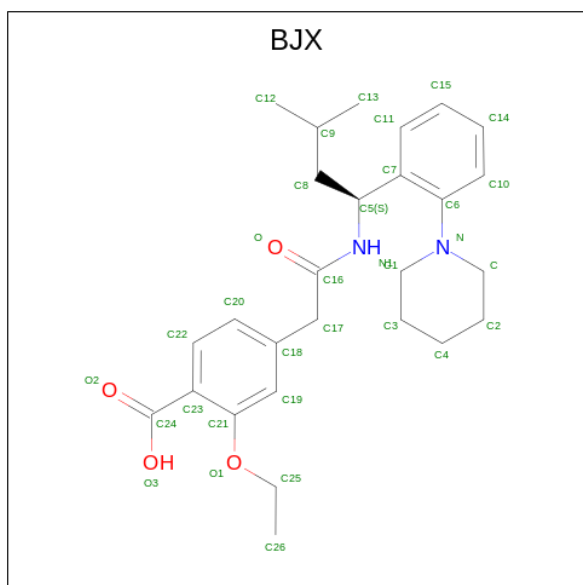
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
4	A	1	31	10	5	12	3	1	0
4	B	1	31	10	5	12	3	1	0
4	C	1	31	10	5	12	3	1	0
4	D	1	31	10	5	12	3	1	0
4	E	1	31	10	5	12	3	1	0
4	F	1	31	10	5	12	3	1	0
4	G	1	31	10	5	12	3	1	0
4	H	1	31	10	5	12	3	1	0

- Molecule 5 is Digitonin (three-letter code: AJP) (formula:  $C_{56}H_{92}O_{29}$ ).



Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	C O	0
			74	50 24	
5	D	1	Total	C O	0
			74	50 24	
5	F	1	Total	C O	0
			74	50 24	
5	H	1	Total	C O	0
			74	50 24	

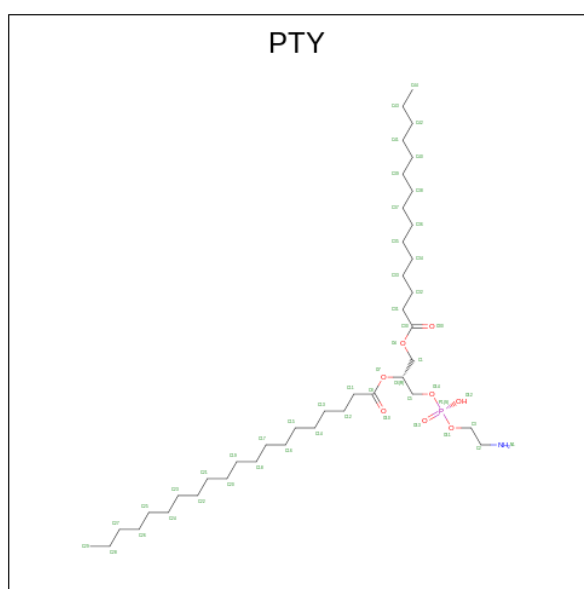
- Molecule 6 is Repaglinide (three-letter code: BJX) (formula:  $C_{27}H_{36}N_2O_4$ ).





Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	B	1	33	27	2	4	0
6	D	1	33	27	2	4	0
6	F	1	33	27	2	4	0
6	H	1	33	27	2	4	0

- Molecule 7 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	B	1	102	65	4	29	4	0
7	B	1	102	65	4	29	4	0
7	B	1	102	65	4	29	4	0
7	B	1	102	65	4	29	4	0
7	D	1	102	65	4	29	4	0
7	D	1	102	65	4	29	4	0
7	D	1	102	65	4	29	4	0

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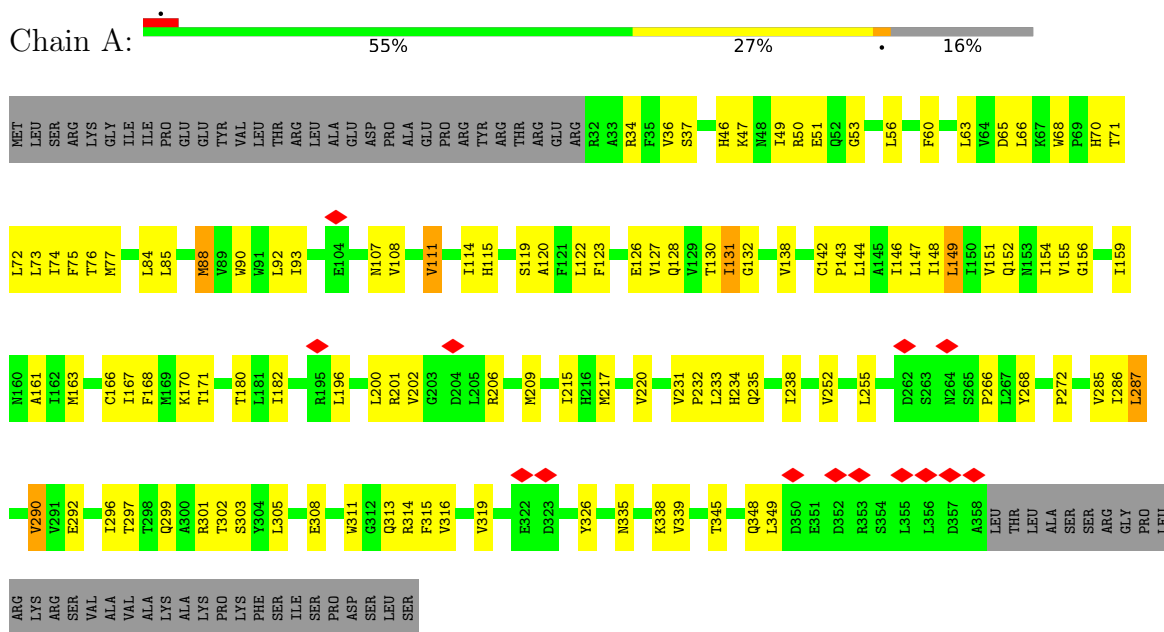
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>					<b>AltConf</b>
7	D	1	Total 102	C 65	N 4	O 29	P 4	0
7	F	1	Total 102	C 65	N 4	O 29	P 4	0
7	F	1	Total 102	C 65	N 4	O 29	P 4	0
7	F	1	Total 102	C 65	N 4	O 29	P 4	0
7	F	1	Total 102	C 65	N 4	O 29	P 4	0
7	H	1	Total 102	C 65	N 4	O 29	P 4	0
7	H	1	Total 102	C 65	N 4	O 29	P 4	0
7	H	1	Total 102	C 65	N 4	O 29	P 4	0
7	H	1	Total 102	C 65	N 4	O 29	P 4	0

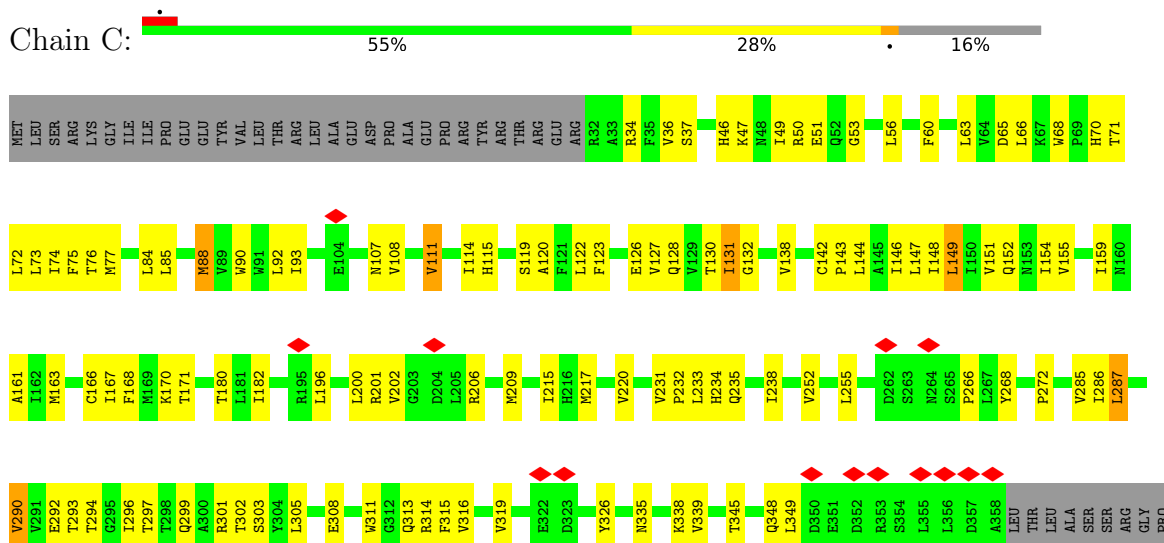
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



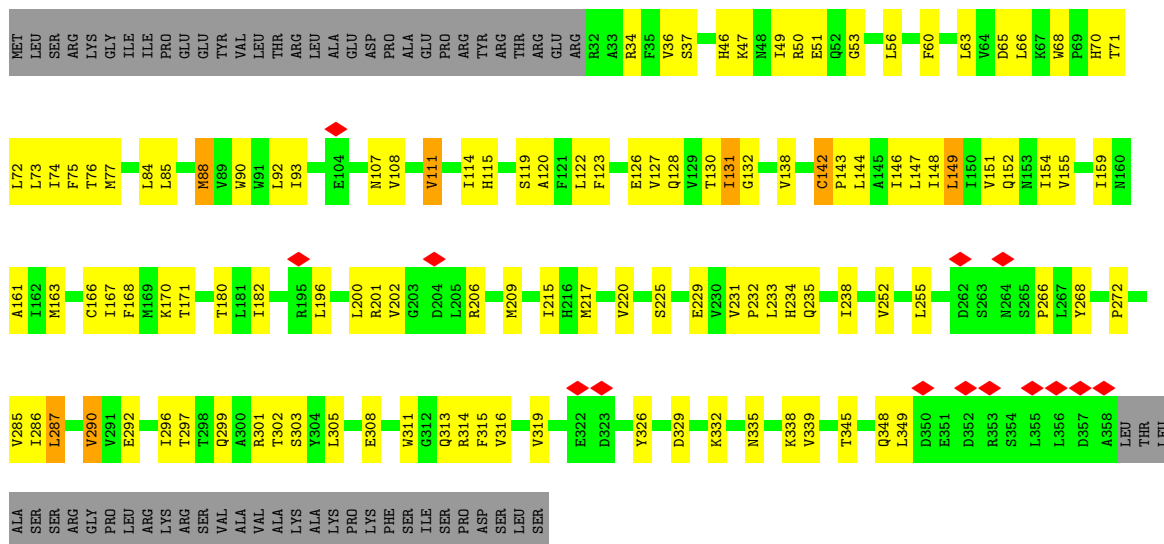
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



LEU  
ARG  
LYS  
SER  
ARG  
VAL  
SER  
VAL  
VAL  
ALA  
ALA  
ALA  
PRO  
LYS  
LYS  
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PHE  
SER  
ILE  
SER  
SER  
PRO  
ASP  
SER  
LEU  
SER

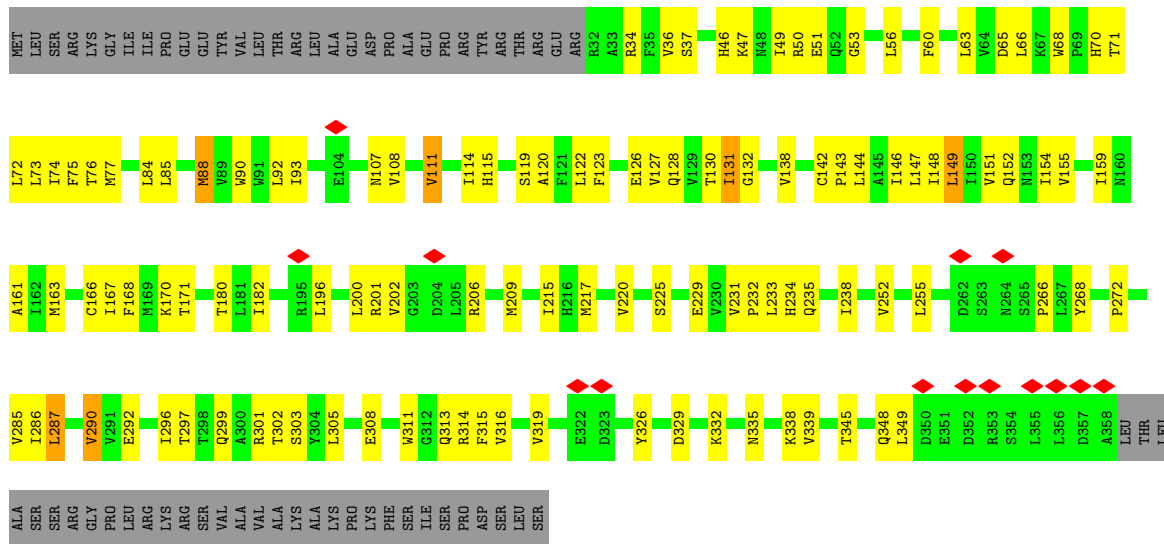
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain E:



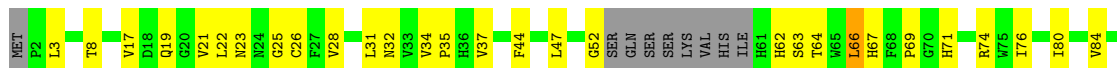
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

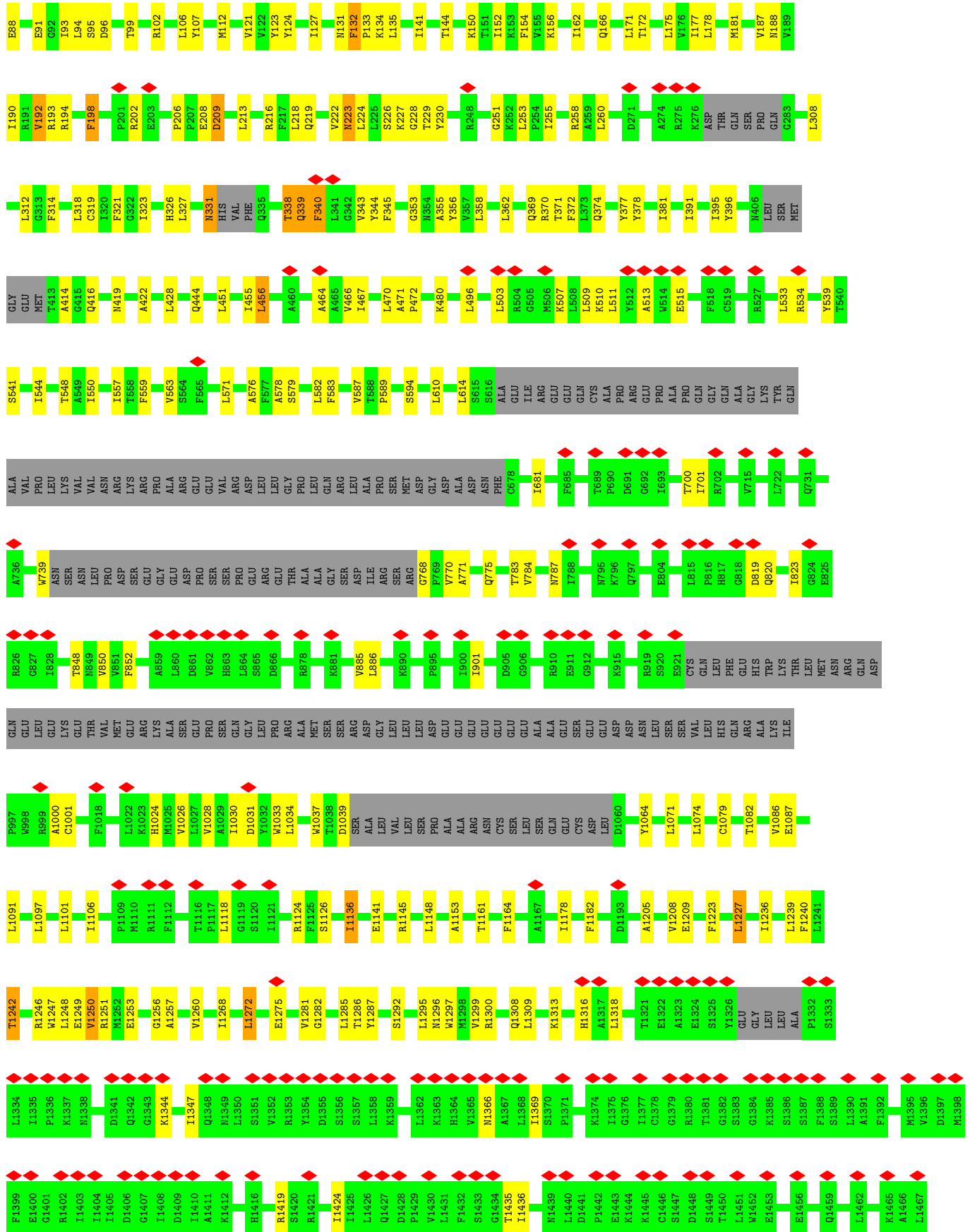
Chain G:

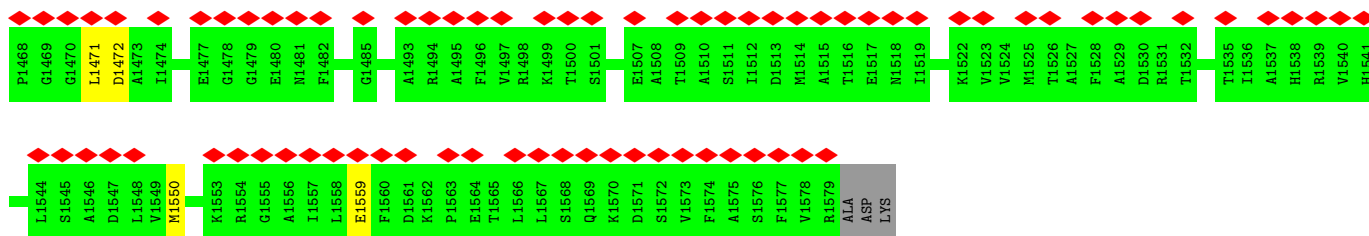


• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

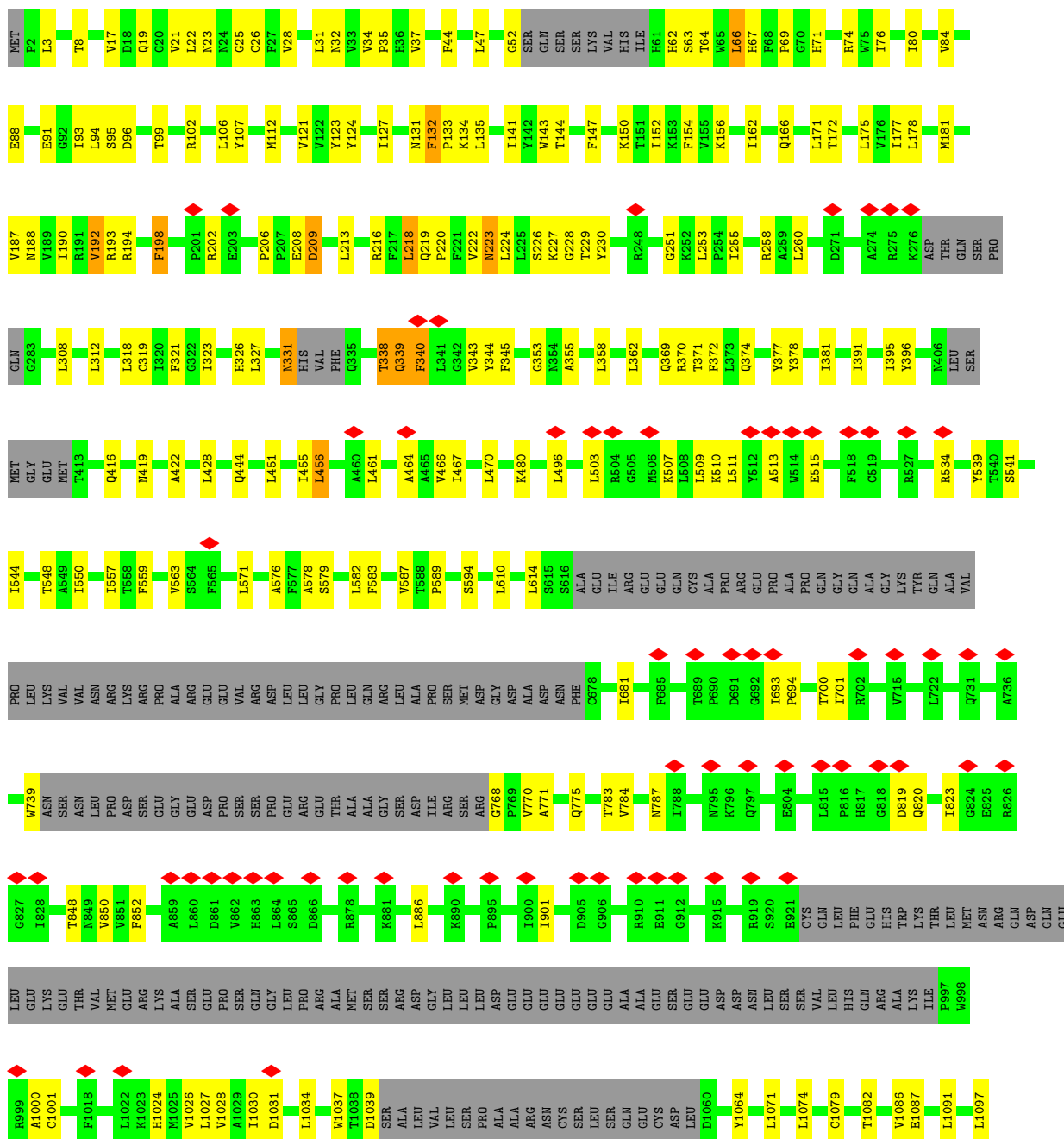
Chain B:

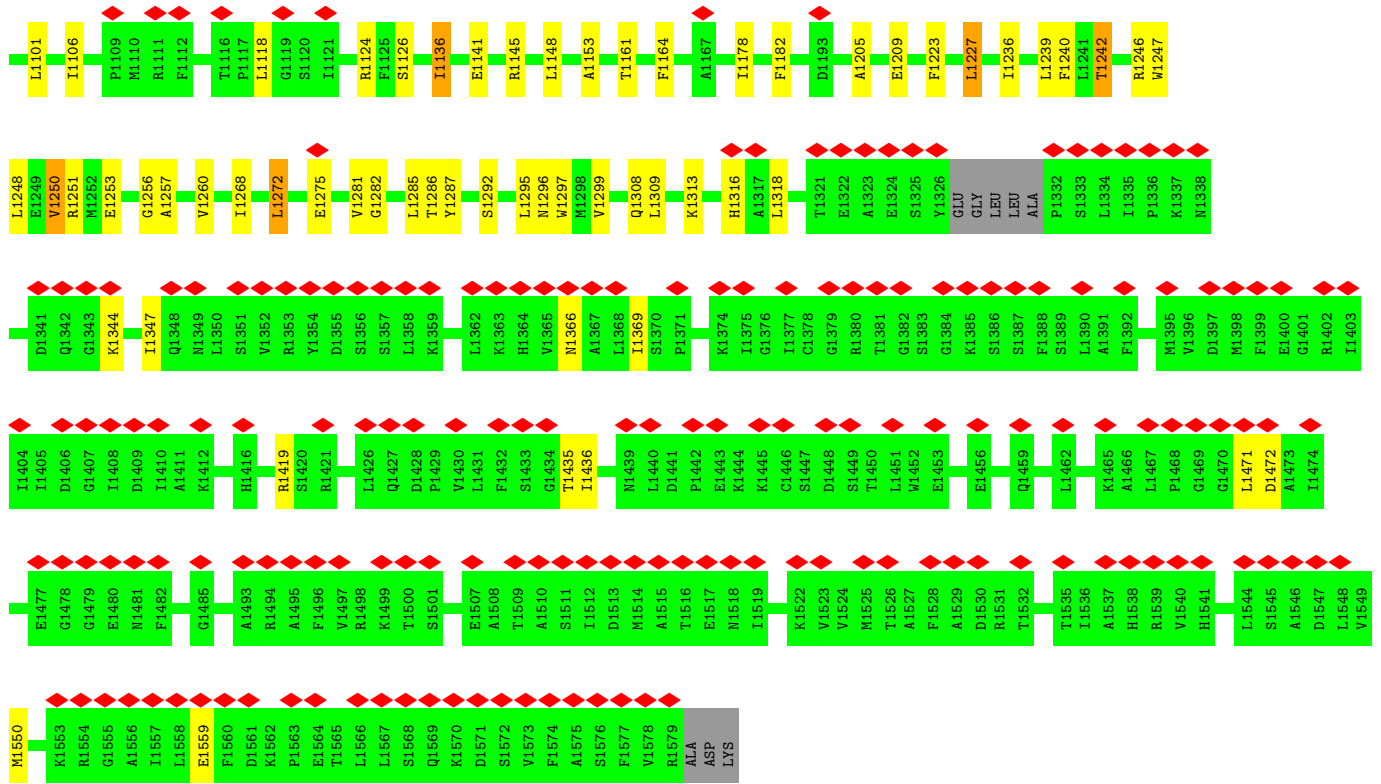




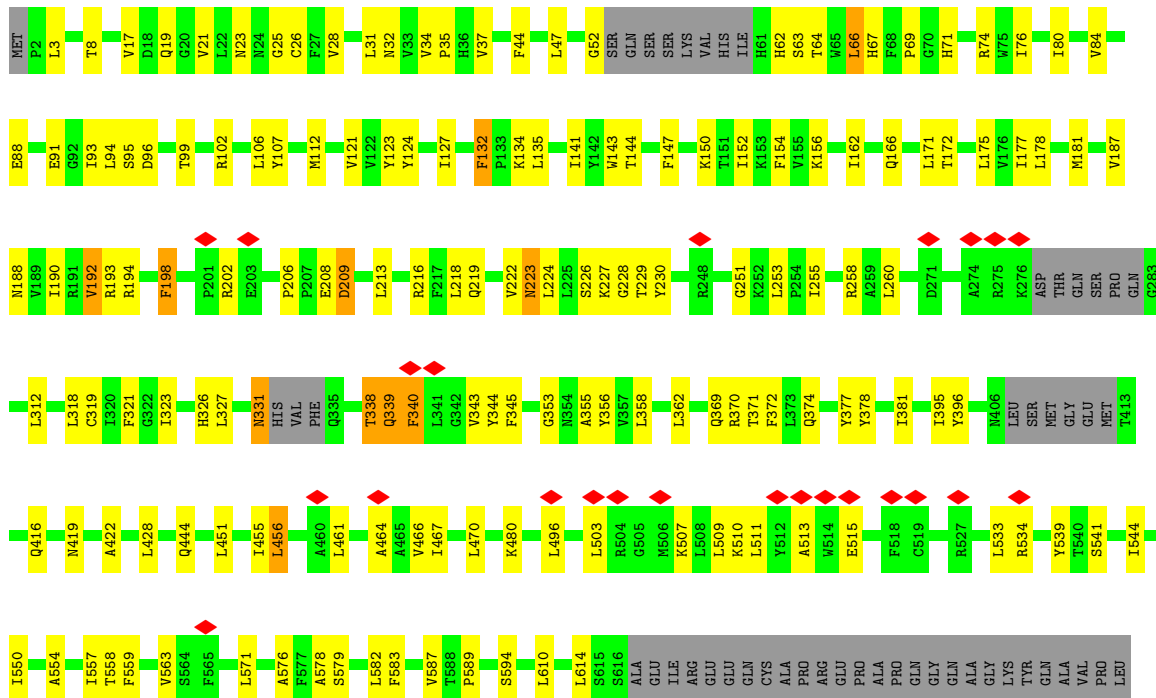


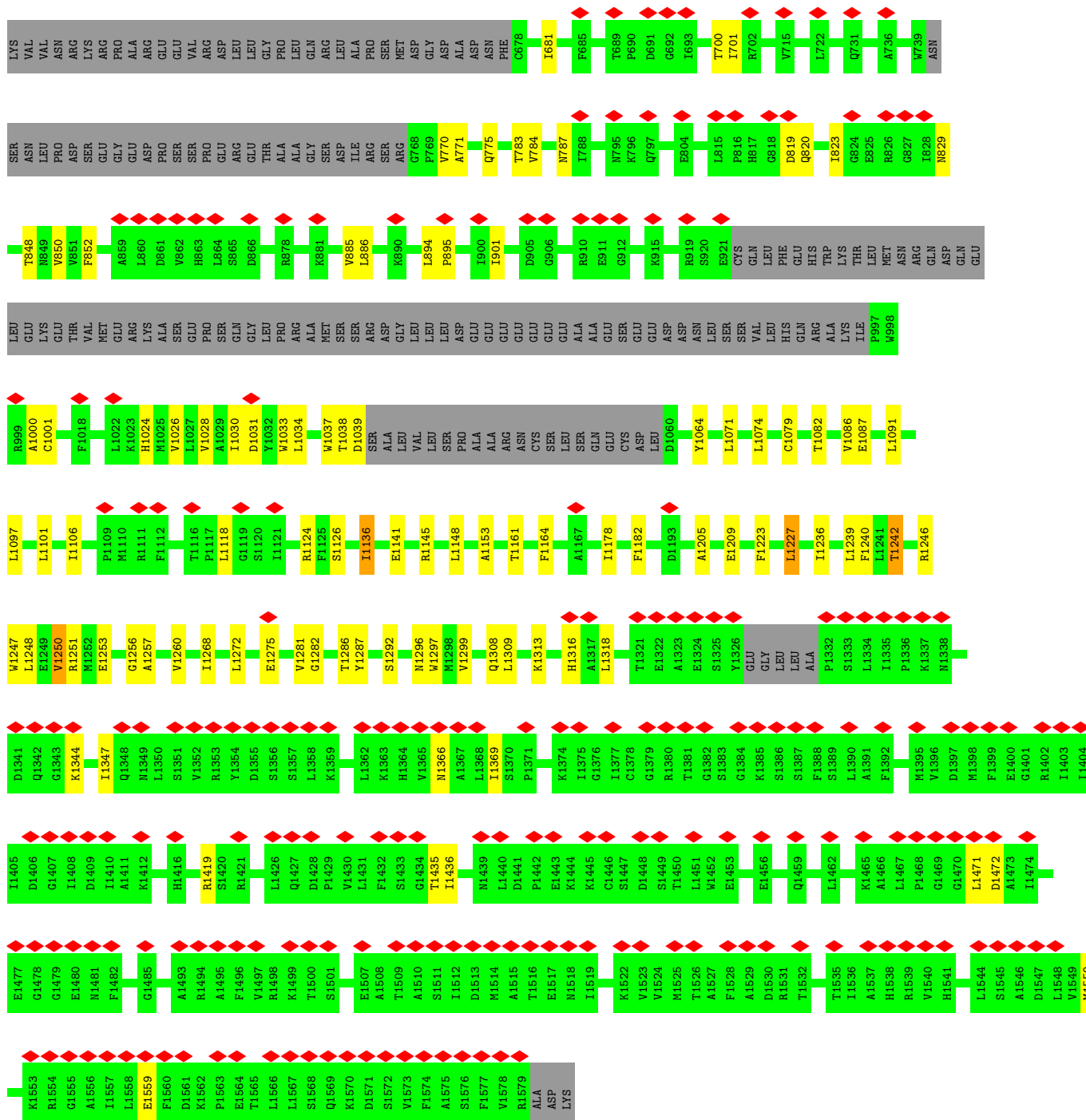
• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2



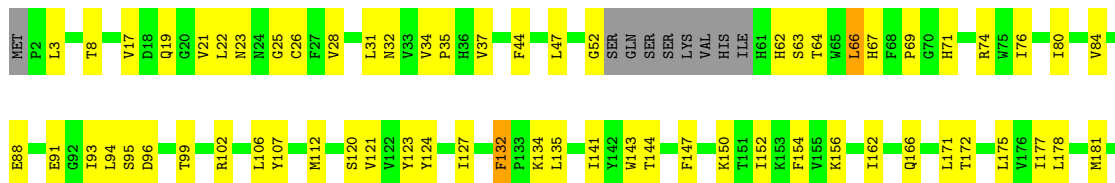


• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

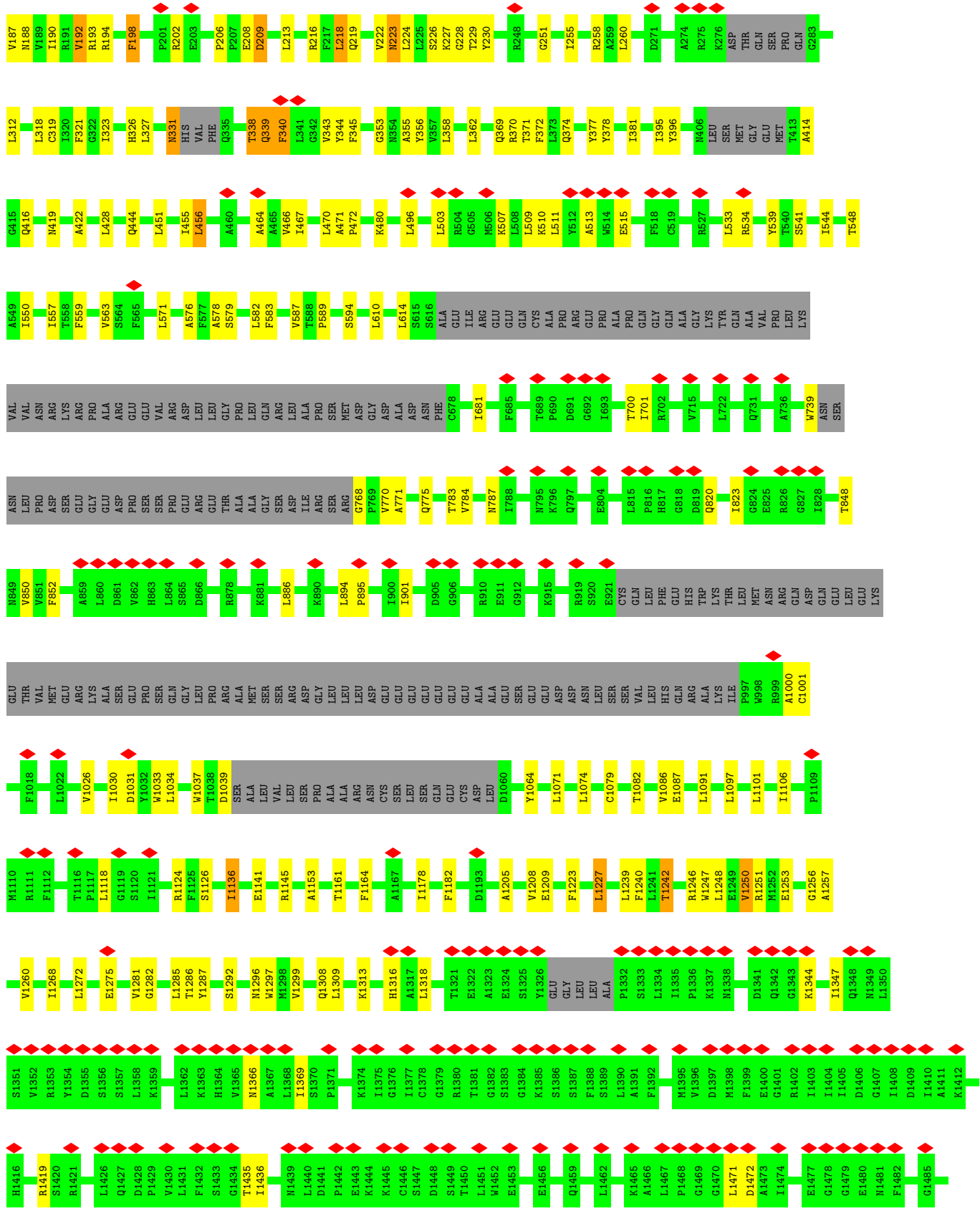


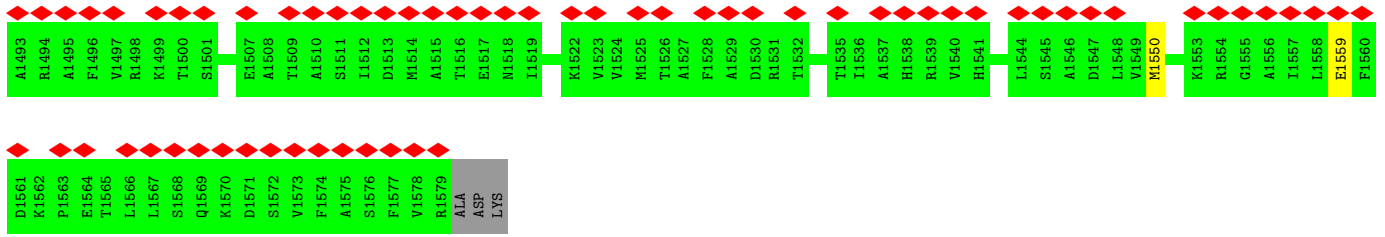


● Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	277548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	27.764	Depositor
Minimum map value	-15.475	Depositor
Average map value	0.095	Depositor
Map value standard deviation	0.834	Depositor
Recommended contour level	3.8	Depositor
Map size ( $\text{\AA}$ )	338.944, 338.944, 338.944	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.324, 1.324, 1.324	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: BJJ, AGS, AJP, POV, PTY

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	0.36	0/2600	0.54	0/3535
1	C	0.36	0/2600	0.54	0/3535
1	E	0.36	0/2600	0.54	0/3535
1	G	0.36	0/2600	0.54	0/3535
2	B	0.28	0/10097	0.43	0/13798
2	D	0.28	0/10097	0.43	0/13798
2	F	0.28	0/10097	0.43	0/13798
2	H	0.28	0/10097	0.43	0/13798
All	All	0.30	0/50788	0.45	0/69332

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2543	0	2571	79	0
1	C	2543	0	2571	80	0
1	E	2543	0	2571	78	0
1	G	2543	0	2571	79	0
2	B	9890	0	9397	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	9890	0	9397	180	0
2	F	9890	0	9397	172	0
2	H	9890	0	9397	170	0
3	A	31	0	40	4	0
3	B	272	0	346	21	0
3	C	31	0	40	3	0
3	D	272	0	346	19	0
3	E	31	0	40	4	0
3	F	272	0	346	18	0
3	G	31	0	40	4	0
3	H	272	0	346	19	0
4	A	31	0	12	2	0
4	B	31	0	12	1	0
4	C	31	0	12	2	0
4	D	31	0	12	1	0
4	E	31	0	12	2	0
4	F	31	0	12	1	0
4	G	31	0	12	2	0
4	H	31	0	12	1	0
5	B	74	0	0	1	0
5	D	74	0	0	1	0
5	F	74	0	0	1	0
5	H	74	0	0	1	0
6	B	33	0	0	2	0
6	D	33	0	0	2	0
6	F	33	0	0	2	0
6	H	33	0	0	2	0
7	B	102	0	108	7	0
7	D	102	0	108	7	0
7	F	102	0	108	7	0
7	H	102	0	108	7	0
All	All	52028	0	49944	1026	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 10.

The worst 5 of 1026 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)
1:A:130:THR:HA	1:G:131:ILE:HG22	1.59	0.85
1:E:131:ILE:HG22	1:G:130:THR:HA	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:HG22	1:C:130:THR:HA	1.59	0.84
1:C:131:ILE:HG22	1:E:130:THR:HA	1.59	0.84
2:F:371:THR:HG21	7:F:1615:PTY:H141	1.63	0.80

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	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
1	C	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
1	E	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
1	G	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
2	B	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
2	D	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
2	F	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
2	H	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
All	All	6684/7888 (85%)	6356 (95%)	328 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	276/339 (81%)	256 (93%)	20 (7%)	14	41
1	C	276/339 (81%)	256 (93%)	20 (7%)	14	41
1	E	276/339 (81%)	256 (93%)	20 (7%)	14	41
1	G	276/339 (81%)	256 (93%)	20 (7%)	14	41
2	B	931/1371 (68%)	896 (96%)	35 (4%)	33	62
2	D	931/1371 (68%)	896 (96%)	35 (4%)	33	62
2	F	931/1371 (68%)	896 (96%)	35 (4%)	33	62
2	H	931/1371 (68%)	896 (96%)	35 (4%)	33	62
All	All	4828/6840 (71%)	4608 (95%)	220 (5%)	31	58

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	88	MET
2	F	218	LEU
2	H	1275	GLU
2	H	223	ASN
1	E	149	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	219	GLN
1	G	299	GLN
1	E	46	HIS
1	G	46	HIS
2	D	437	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](#)

68 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
7	PTY	F	1612	-	31,31,49	1.25	2 (6%)	34,36,54	1.27	2 (5%)
3	POV	F	1609	-	24,24,51	1.08	1 (4%)	29,31,59	1.05	1 (3%)
3	POV	B	1607	-	40,40,51	1.10	2 (5%)	46,48,59	1.12	4 (8%)
3	POV	B	1606	-	39,39,51	1.13	2 (5%)	45,47,59	1.06	2 (4%)
3	POV	D	1608	-	35,35,51	1.19	2 (5%)	41,43,59	1.27	4 (9%)
4	AGS	F	1602	-	26,33,33	1.88	3 (11%)	26,52,52	1.46	4 (15%)
7	PTY	B	1613	-	26,26,49	1.36	2 (7%)	29,31,54	1.16	2 (6%)
7	PTY	B	1614	-	21,21,49	1.12	1 (4%)	23,25,54	0.93	1 (4%)
3	POV	A	401	-	30,30,51	0.98	1 (3%)	35,37,59	1.04	3 (8%)
6	BJX	D	1603	-	35,35,35	1.87	5 (14%)	47,47,47	1.43	7 (14%)
7	PTY	H	1612	-	31,31,49	1.25	2 (6%)	34,36,54	1.27	2 (5%)
5	AJP	H	1601	-	83,83,95	0.64	0	125,131,149	1.31	13 (10%)
3	POV	B	1604	-	35,35,51	1.18	2 (5%)	41,43,59	1.09	2 (4%)
6	BJX	B	1603	-	35,35,35	1.87	5 (14%)	47,47,47	1.43	7 (14%)
3	POV	H	1611	-	27,27,51	1.27	2 (7%)	29,29,59	1.23	2 (6%)
3	POV	B	1608	-	35,35,51	1.19	2 (5%)	41,43,59	1.27	4 (9%)
3	POV	B	1611	-	27,27,51	1.27	2 (7%)	29,29,59	1.23	2 (6%)
7	PTY	B	1615	-	20,20,49	1.22	2 (10%)	22,24,54	1.30	3 (13%)
3	POV	H	1605	-	40,40,51	1.11	2 (5%)	46,48,59	1.02	2 (4%)
6	BJX	F	1603	-	35,35,35	1.87	5 (14%)	47,47,47	1.43	7 (14%)
3	POV	D	1609	-	24,24,51	1.08	1 (4%)	29,31,59	1.05	1 (3%)
4	AGS	D	1602	-	26,33,33	1.88	3 (11%)	26,52,52	1.46	4 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	POV	F	1608	-	35,35,51	1.19	2 (5%)	41,43,59	1.27	4 (9%)
7	PTY	D	1613	-	26,26,49	1.36	2 (7%)	29,31,54	1.16	2 (6%)
3	POV	D	1607	-	40,40,51	1.10	2 (5%)	46,48,59	1.12	4 (8%)
3	POV	D	1604	-	35,35,51	1.18	2 (5%)	41,43,59	1.09	2 (4%)
3	POV	D	1606	-	39,39,51	1.13	2 (5%)	45,47,59	1.06	2 (4%)
4	AGS	E	401	-	26,33,33	1.87	3 (11%)	26,52,52	1.45	5 (19%)
3	POV	D	1610	-	24,24,51	1.03	1 (4%)	29,31,59	1.16	2 (6%)
7	PTY	B	1612	-	31,31,49	1.25	2 (6%)	34,36,54	1.27	2 (5%)
3	POV	F	1607	-	40,40,51	1.10	2 (5%)	46,48,59	1.12	4 (8%)
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3	POV	B	1610	-	24,24,51	1.03	1 (4%)	29,31,59	1.16	2 (6%)
3	POV	H	1608	-	35,35,51	1.19	2 (5%)	41,43,59	1.27	4 (9%)
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4	AGS	B	1602	-	26,33,33	1.88	3 (11%)	26,52,52	1.46	4 (15%)
3	POV	F	1611	-	27,27,51	1.27	2 (7%)	29,29,59	1.23	2 (6%)
3	POV	G	402	-	30,30,51	0.98	1 (3%)	35,37,59	1.04	3 (8%)
3	POV	C	402	-	30,30,51	0.98	1 (3%)	35,37,59	1.04	3 (8%)
3	POV	H	1610	-	24,24,51	1.03	1 (4%)	29,31,59	1.16	2 (6%)
3	POV	F	1605	-	40,40,51	1.11	2 (5%)	46,48,59	1.02	2 (4%)
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3	POV	B	1605	-	40,40,51	1.11	2 (5%)	46,48,59	1.02	2 (4%)
4	AGS	A	402	-	26,33,33	1.87	3 (11%)	26,52,52	1.45	5 (19%)
3	POV	E	402	-	30,30,51	0.98	1 (3%)	35,37,59	1.04	3 (8%)
4	AGS	G	401	-	26,33,33	1.87	3 (11%)	26,52,52	1.45	5 (19%)
4	AGS	H	1602	-	26,33,33	1.88	3 (11%)	26,52,52	1.46	4 (15%)
7	PTY	D	1614	-	21,21,49	1.12	1 (4%)	23,25,54	0.93	1 (4%)
7	PTY	F	1615	-	20,20,49	1.22	2 (10%)	22,24,54	1.30	3 (13%)
3	POV	H	1607	-	40,40,51	1.10	2 (5%)	46,48,59	1.12	4 (8%)
3	POV	H	1604	-	35,35,51	1.18	2 (5%)	41,43,59	1.09	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PTY	H	1613	-	26,26,49	1.36	2 (7%)	29,31,54	1.16	2 (6%)
3	POV	H	1606	-	39,39,51	1.13	2 (5%)	45,47,59	1.06	2 (4%)
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5	AJP	D	1601	-	83,83,95	0.64	0	125,131,149	1.31	13 (10%)
4	AGS	C	401	-	26,33,33	1.87	3 (11%)	26,52,52	1.45	5 (19%)
3	POV	D	1611	-	27,27,51	1.27	2 (7%)	29,29,59	1.23	2 (6%)
3	POV	F	1610	-	24,24,51	1.03	1 (4%)	29,31,59	1.16	2 (6%)
7	PTY	F	1613	-	26,26,49	1.36	2 (7%)	29,31,54	1.16	2 (6%)
5	AJP	F	1601	-	83,83,95	0.64	0	125,131,149	1.31	13 (10%)

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
7	PTY	F	1612	-	-	14/35/35/53	-
3	POV	F	1609	-	-	10/27/27/55	-
3	POV	B	1607	-	-	14/44/44/55	-
3	POV	B	1606	-	-	17/43/43/55	-
3	POV	D	1608	-	-	12/39/39/55	-
4	AGS	F	1602	-	-	2/17/38/38	0/3/3/3
7	PTY	B	1613	-	-	15/30/30/53	-
7	PTY	B	1614	-	-	13/23/23/53	-
3	POV	A	401	-	-	5/33/33/55	-
6	BJX	D	1603	-	-	13/27/35/35	0/3/3/3
7	PTY	H	1612	-	-	14/35/35/53	-
5	AJP	H	1601	-	29/29/33/38	11/22/194/220	0/10/10/11
3	POV	B	1604	-	-	13/39/39/55	-
6	BJX	B	1603	-	-	13/27/35/35	0/3/3/3
3	POV	H	1611	-	-	11/29/29/55	-
3	POV	B	1608	-	-	12/39/39/55	-
3	POV	B	1611	-	-	11/29/29/55	-
7	PTY	B	1615	-	-	14/22/22/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	H	1605	-	-	14/44/44/55	-
6	BJX	F	1603	-	-	13/27/35/35	0/3/3/3
3	POV	D	1609	-	-	10/27/27/55	-
4	AGS	D	1602	-	-	2/17/38/38	0/3/3/3
3	POV	F	1608	-	-	12/39/39/55	-
7	PTY	D	1613	-	-	15/30/30/53	-
3	POV	D	1607	-	-	14/44/44/55	-
3	POV	D	1604	-	-	13/39/39/55	-
3	POV	D	1606	-	-	17/43/43/55	-
4	AGS	E	401	-	-	2/17/38/38	0/3/3/3
3	POV	D	1610	-	-	6/27/27/55	-
7	PTY	B	1612	-	-	14/35/35/53	-
3	POV	F	1607	-	-	14/44/44/55	-
6	BJX	H	1603	-	-	13/27/35/35	0/3/3/3
3	POV	B	1610	-	-	6/27/27/55	-
3	POV	H	1608	-	-	12/39/39/55	-
3	POV	D	1605	-	-	14/44/44/55	-
5	AJP	B	1601	-	29/29/33/38	11/22/194/220	0/10/10/11
7	PTY	D	1612	-	-	14/35/35/53	-
3	POV	F	1604	-	-	13/39/39/55	-
7	PTY	D	1615	-	-	14/22/22/53	-
3	POV	B	1609	-	-	10/27/27/55	-
4	AGS	B	1602	-	-	2/17/38/38	0/3/3/3
3	POV	F	1611	-	-	11/29/29/55	-
3	POV	G	402	-	-	5/33/33/55	-
3	POV	C	402	-	-	5/33/33/55	-
3	POV	H	1610	-	-	6/27/27/55	-
3	POV	F	1605	-	-	14/44/44/55	-
7	PTY	H	1614	-	-	13/23/23/53	-
3	POV	H	1609	-	-	10/27/27/55	-
3	POV	B	1605	-	-	14/44/44/55	-
4	AGS	A	402	-	-	2/17/38/38	0/3/3/3
3	POV	E	402	-	-	5/33/33/55	-
4	AGS	G	401	-	-	2/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	H	1602	-	-	2/17/38/38	0/3/3/3
7	PTY	D	1614	-	-	13/23/23/53	-
7	PTY	F	1615	-	-	14/22/22/53	-
3	POV	H	1607	-	-	14/44/44/55	-
3	POV	H	1604	-	-	13/39/39/55	-
7	PTY	H	1613	-	-	15/30/30/53	-
3	POV	H	1606	-	-	17/43/43/55	-
7	PTY	F	1614	-	-	13/23/23/53	-
3	POV	F	1606	-	-	17/43/43/55	-
7	PTY	H	1615	-	-	14/22/22/53	-
5	AJP	D	1601	-	29/29/33/38	11/22/194/220	0/10/10/11
4	AGS	C	401	-	-	2/17/38/38	0/3/3/3
3	POV	D	1611	-	-	11/29/29/55	-
3	POV	F	1610	-	-	6/27/27/55	-
7	PTY	F	1613	-	-	15/30/30/53	-
5	AJP	F	1601	-	29/29/33/38	11/22/194/220	0/10/10/11

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1603	BJX	C6-C7	8.50	1.49	1.40
6	D	1603	BJX	C6-C7	8.50	1.49	1.40
6	F	1603	BJX	C6-C7	8.50	1.49	1.40
6	H	1603	BJX	C6-C7	8.50	1.49	1.40
4	A	402	AGS	PG-S1G	8.02	2.08	1.90

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1608	POV	O21-C21-C22	5.06	122.41	111.50
3	D	1608	POV	O21-C21-C22	5.06	122.41	111.50
3	F	1608	POV	O21-C21-C22	5.06	122.41	111.50
3	H	1608	POV	O21-C21-C22	5.06	122.41	111.50
5	B	1601	AJP	C12-C07-C08	-5.04	99.43	104.88

5 of 116 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1601	AJP	C12
5	B	1601	AJP	C59
5	B	1601	AJP	C05
5	B	1601	AJP	C45
5	B	1601	AJP	C36

5 of 744 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	POV	C22-C21-O21-C2
3	B	1604	POV	C11-O12-P-O14
3	B	1604	POV	C22-C21-O21-C2
3	B	1605	POV	C11-O12-P-O11
3	B	1605	POV	C11-O12-P-O13

There are no ring outliers.

60 monomers are involved in 137 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1609	POV	3	0
3	B	1607	POV	2	0
3	B	1606	POV	1	0
3	D	1608	POV	8	0
4	F	1602	AGS	1	0
7	B	1613	PTY	4	0
7	B	1614	PTY	1	0
3	A	401	POV	4	0
6	D	1603	BJX	2	0
5	H	1601	AJP	1	0
3	B	1604	POV	5	0
6	B	1603	BJX	2	0
3	H	1611	POV	2	0
3	B	1608	POV	8	0
3	B	1611	POV	2	0
7	B	1615	PTY	2	0
3	H	1605	POV	2	0
6	F	1603	BJX	2	0
3	D	1609	POV	2	0
4	D	1602	AGS	1	0
3	F	1608	POV	7	0
7	D	1613	PTY	4	0
3	D	1607	POV	2	0
3	D	1604	POV	5	0

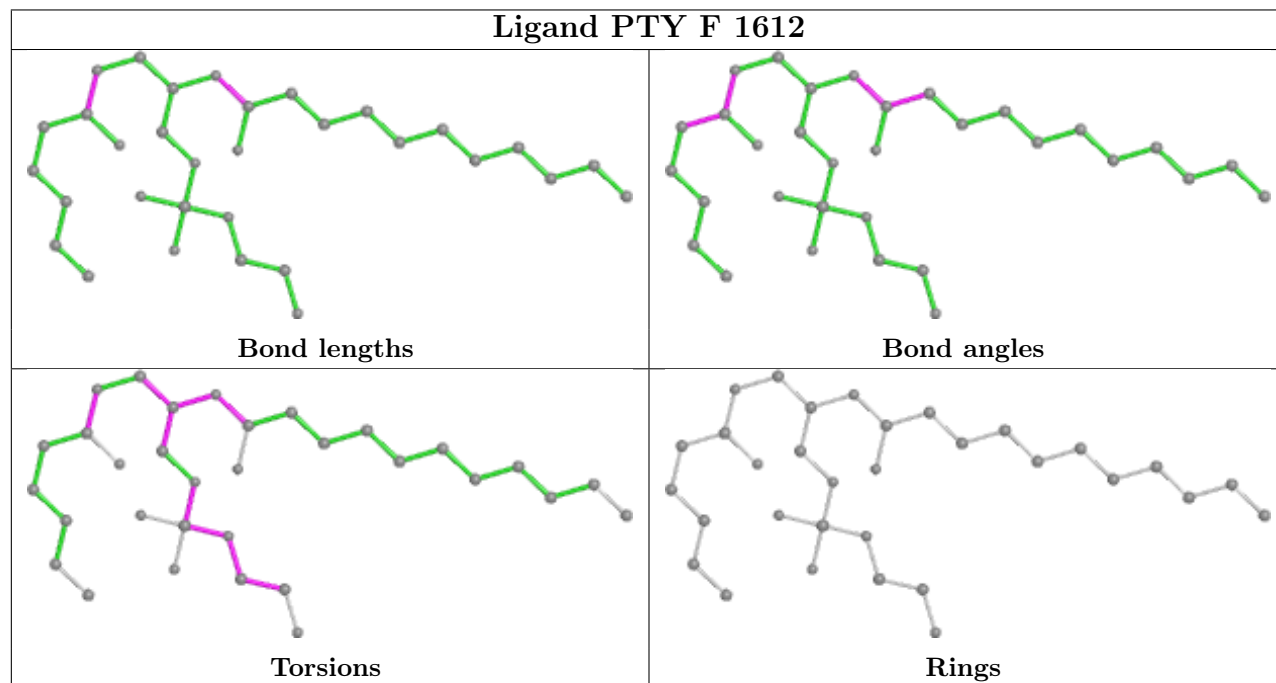
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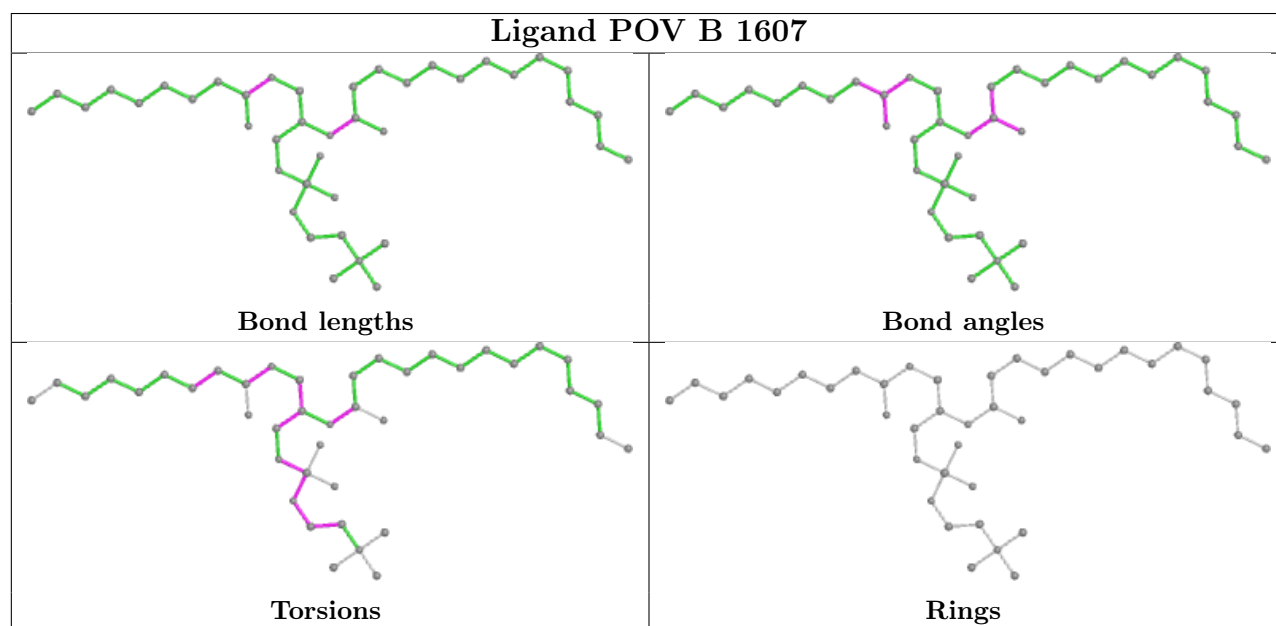
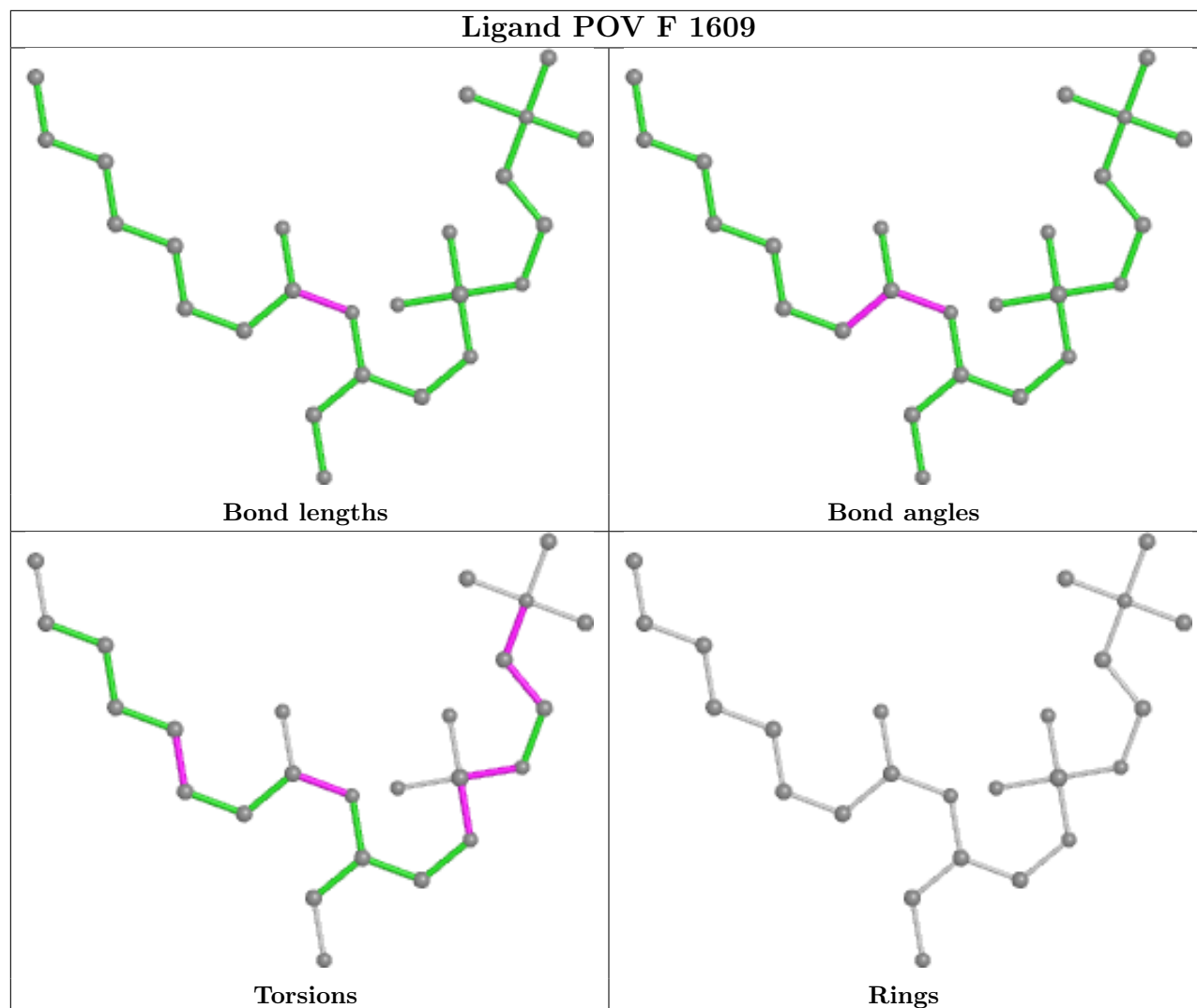
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1606	POV	1	0
4	E	401	AGS	2	0
3	F	1607	POV	2	0
6	H	1603	BJX	2	0
3	H	1608	POV	8	0
3	D	1605	POV	3	0
5	B	1601	AJP	1	0
3	F	1604	POV	4	0
7	D	1615	PTY	2	0
3	B	1609	POV	3	0
4	B	1602	AGS	1	0
3	F	1611	POV	2	0
3	G	402	POV	4	0
3	C	402	POV	3	0
3	F	1605	POV	2	0
7	H	1614	PTY	1	0
3	H	1609	POV	3	0
3	B	1605	POV	3	0
4	A	402	AGS	2	0
3	E	402	POV	4	0
4	G	401	AGS	2	0
4	H	1602	AGS	1	0
7	D	1614	PTY	1	0
7	F	1615	PTY	2	0
3	H	1607	POV	2	0
3	H	1604	POV	4	0
7	H	1613	PTY	4	0
3	H	1606	POV	1	0
7	F	1614	PTY	1	0
3	F	1606	POV	1	0
7	H	1615	PTY	2	0
5	D	1601	AJP	1	0
4	C	401	AGS	2	0
3	D	1611	POV	1	0
7	F	1613	PTY	4	0
5	F	1601	AJP	1	0

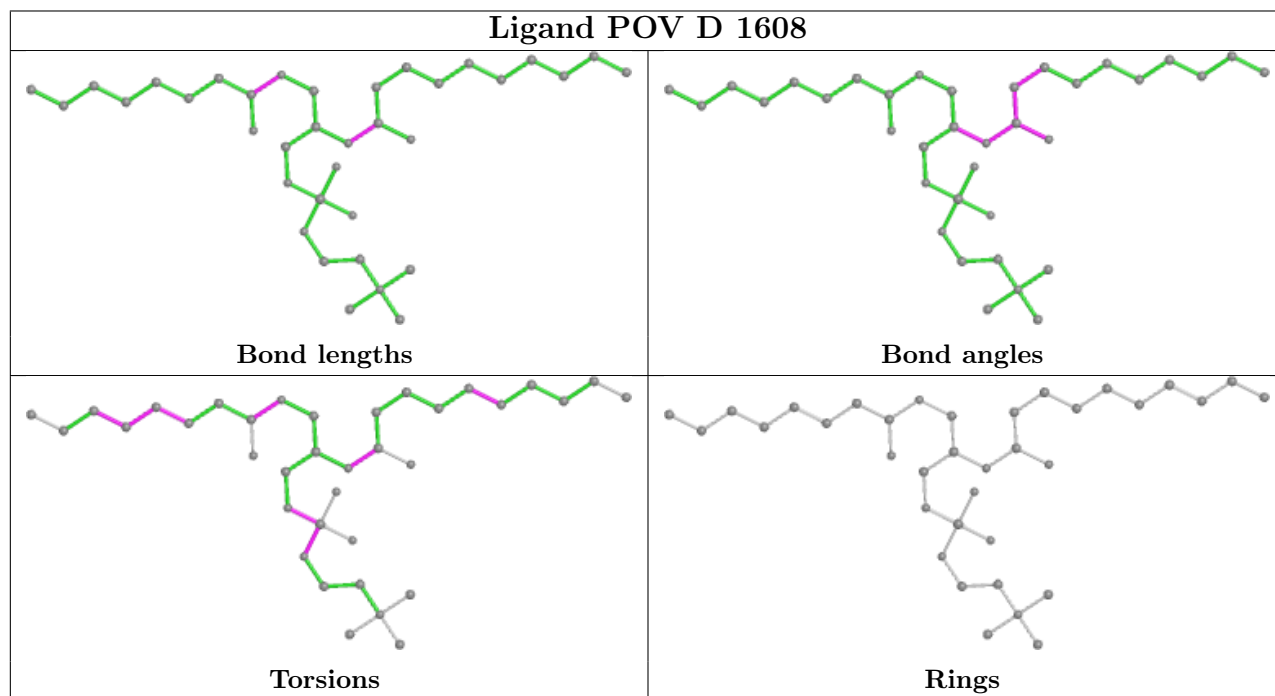
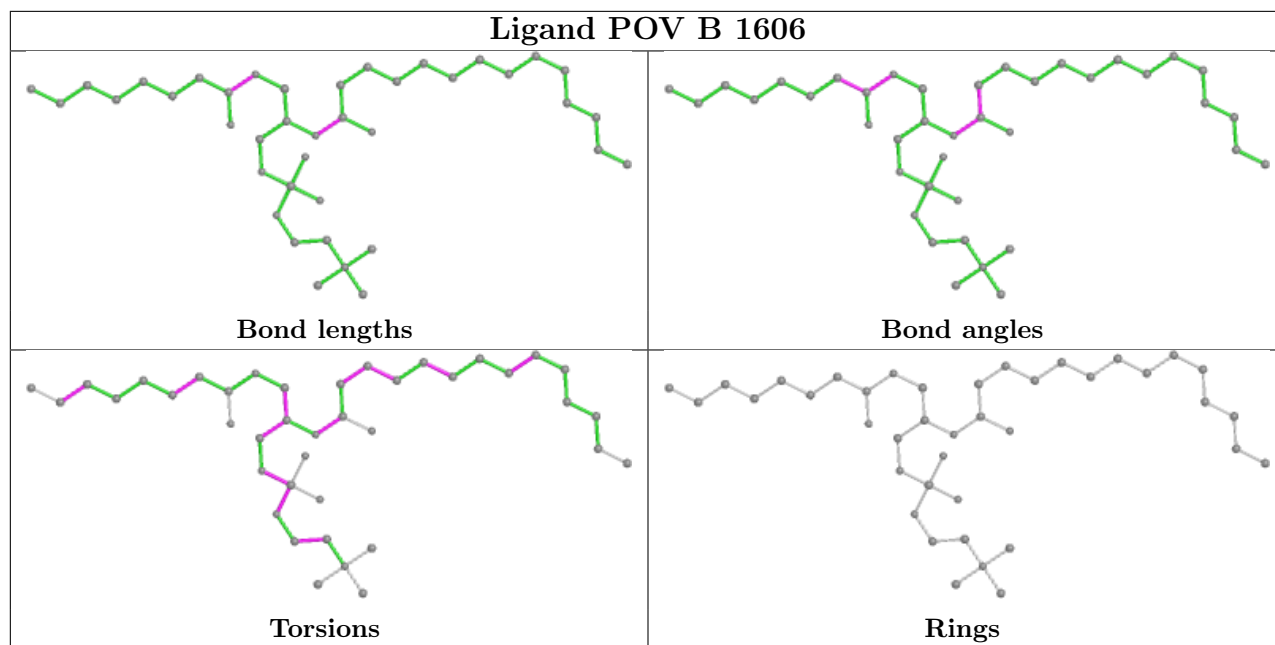
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

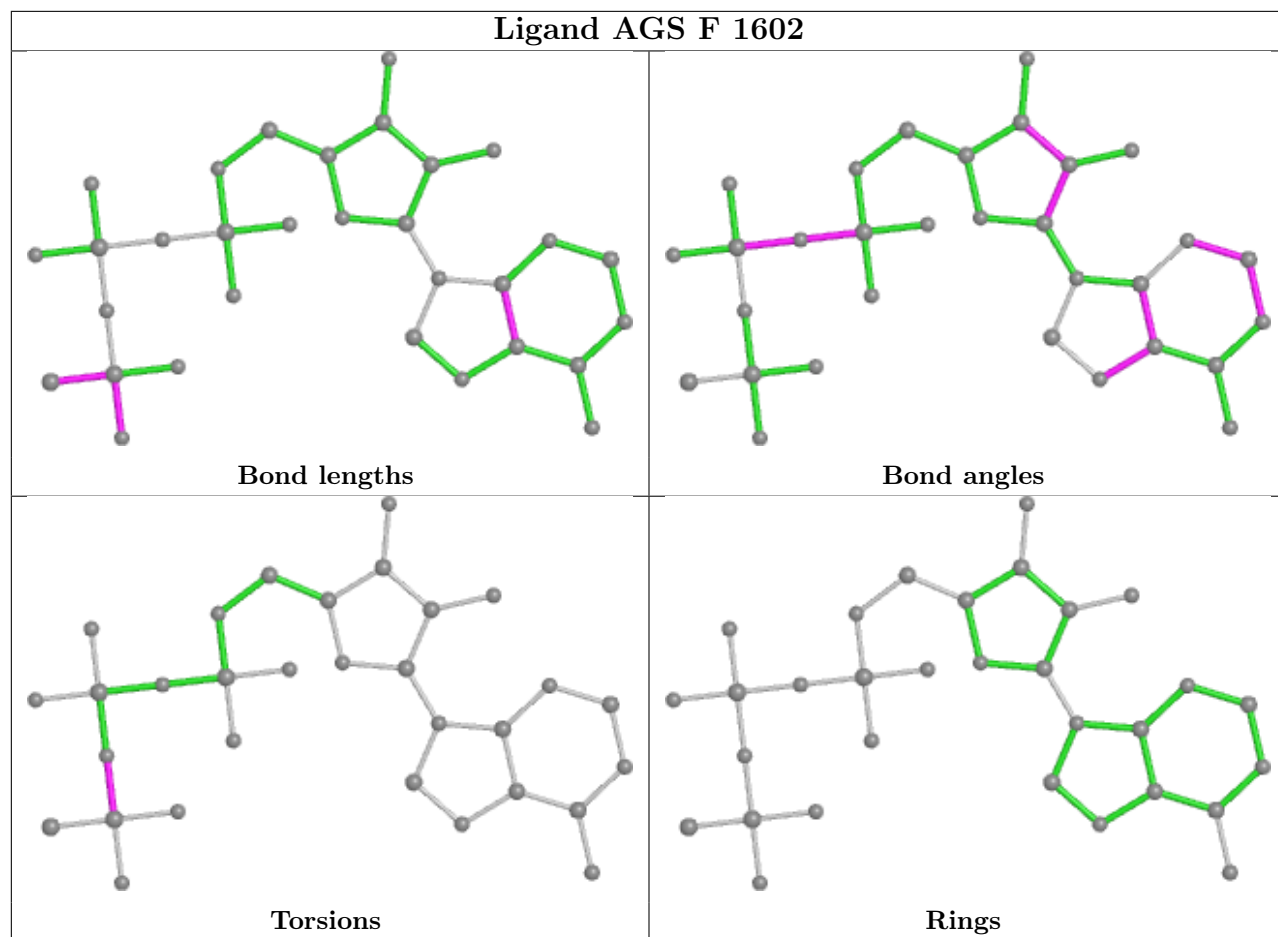
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

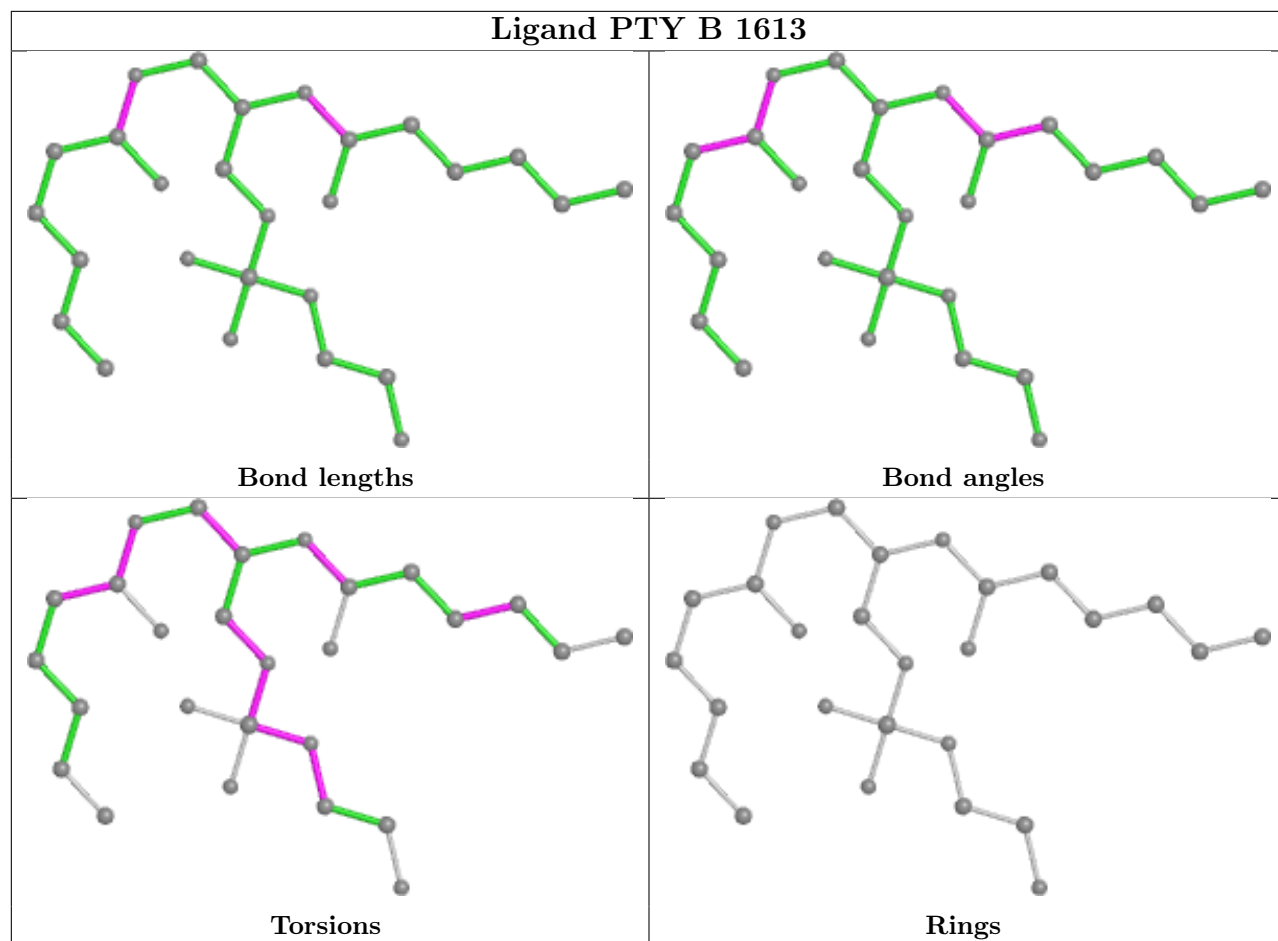


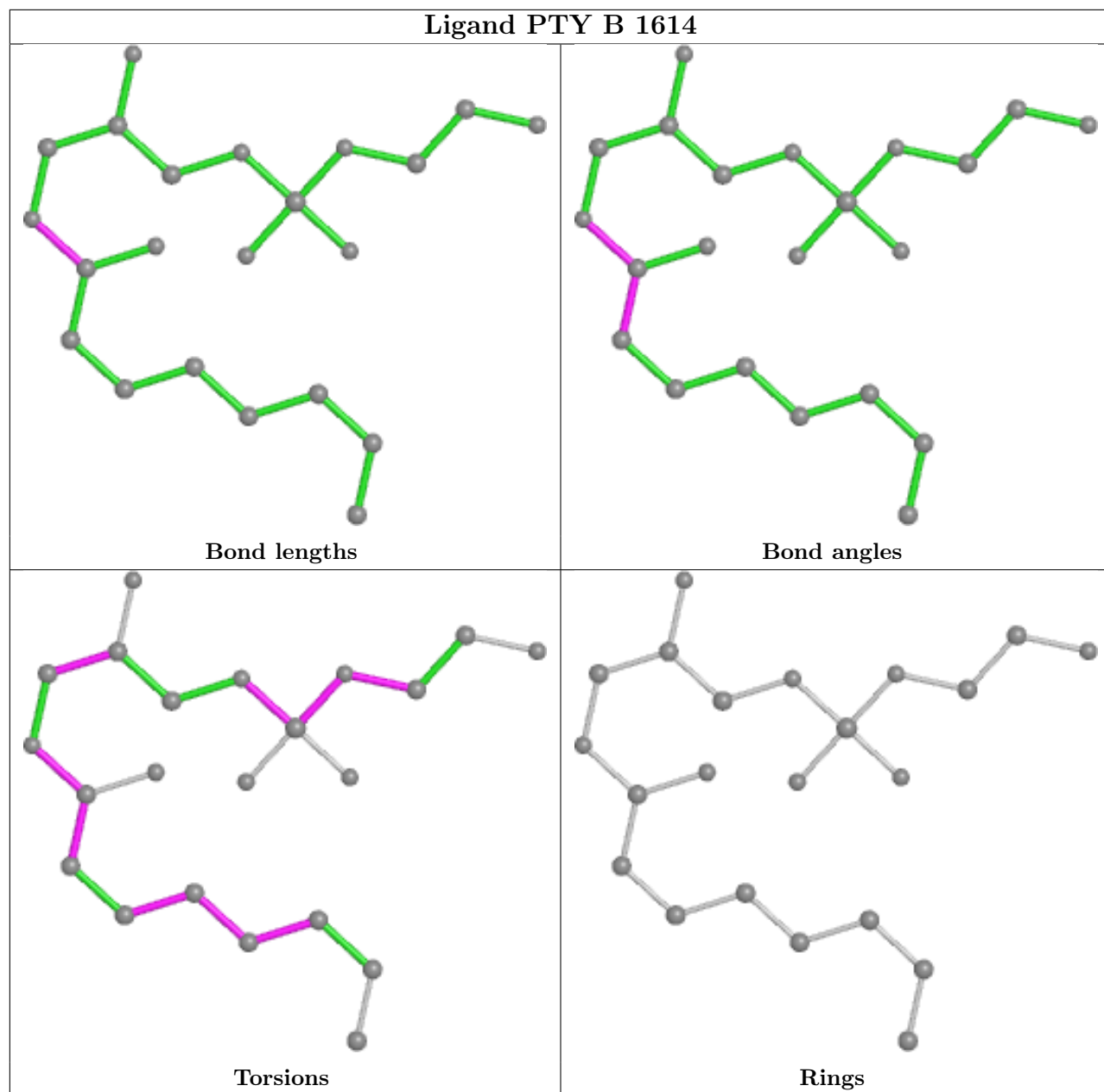


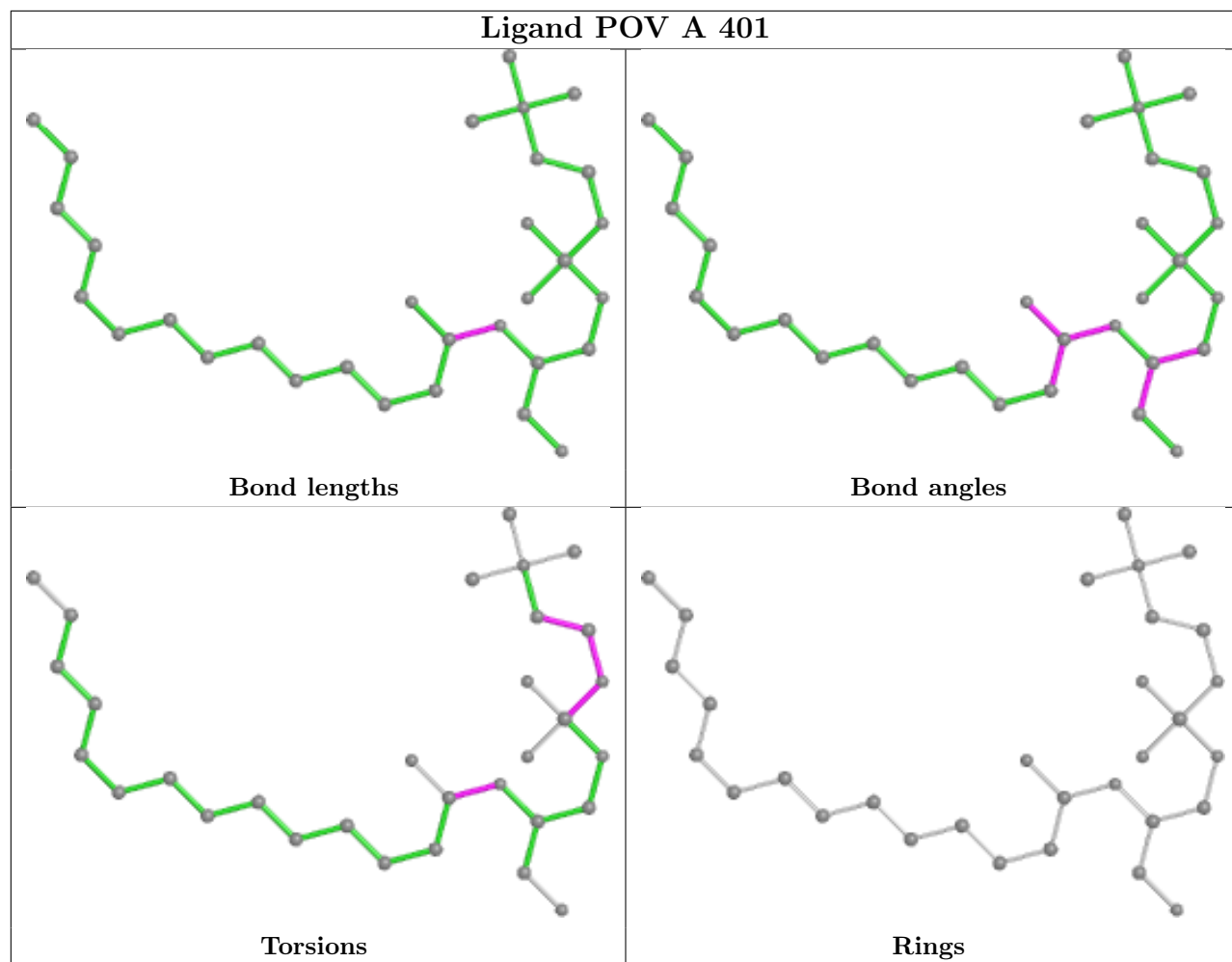


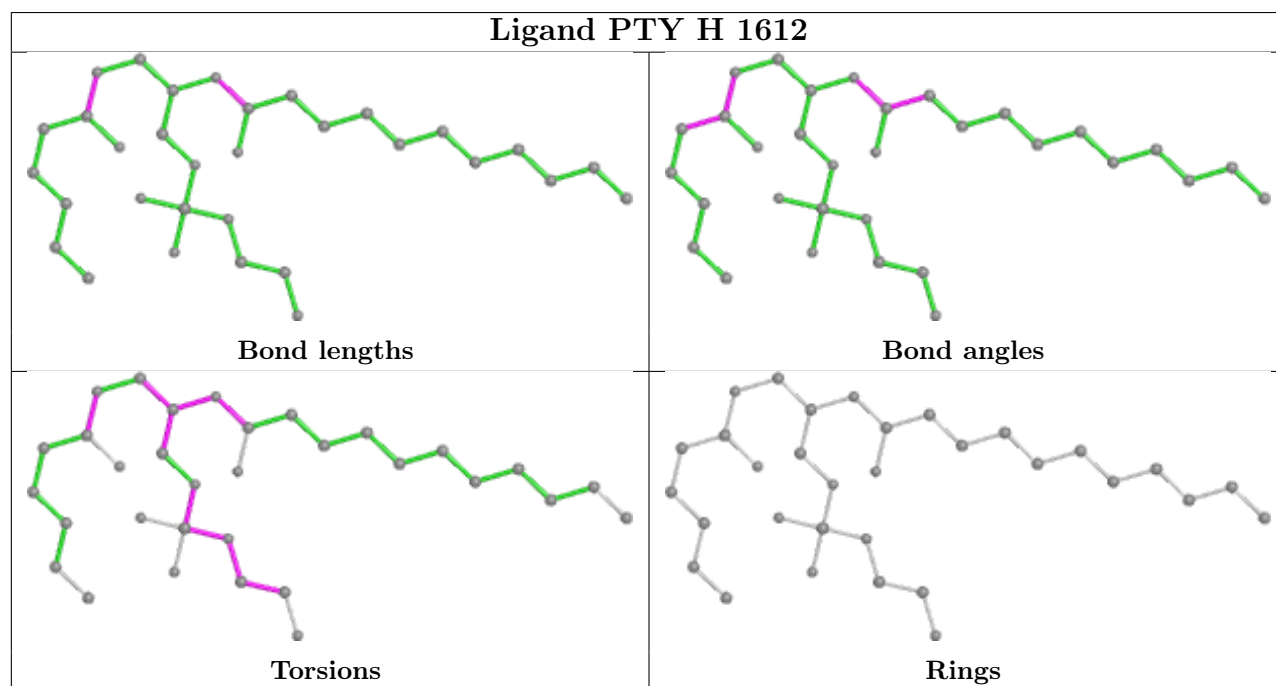
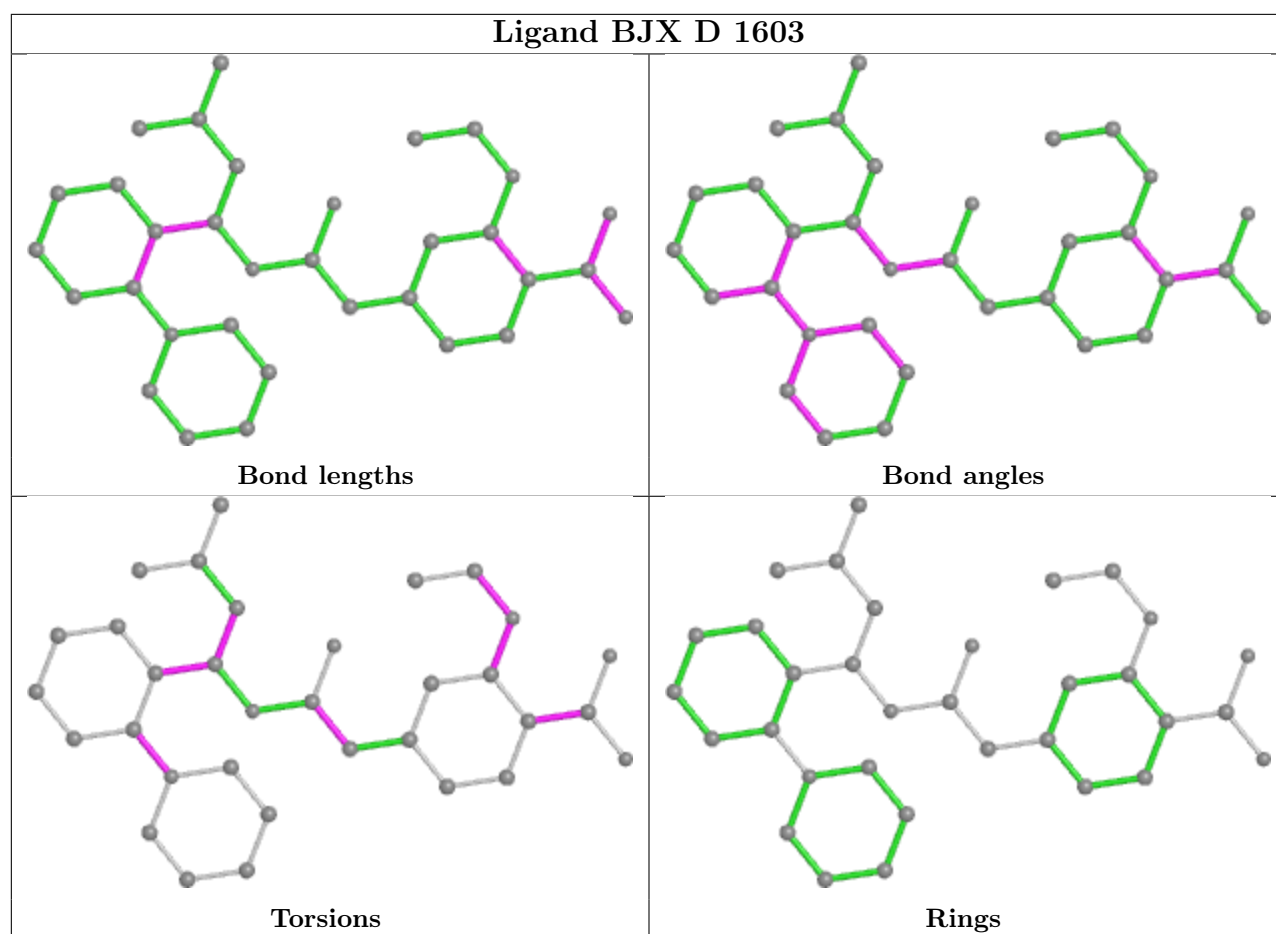


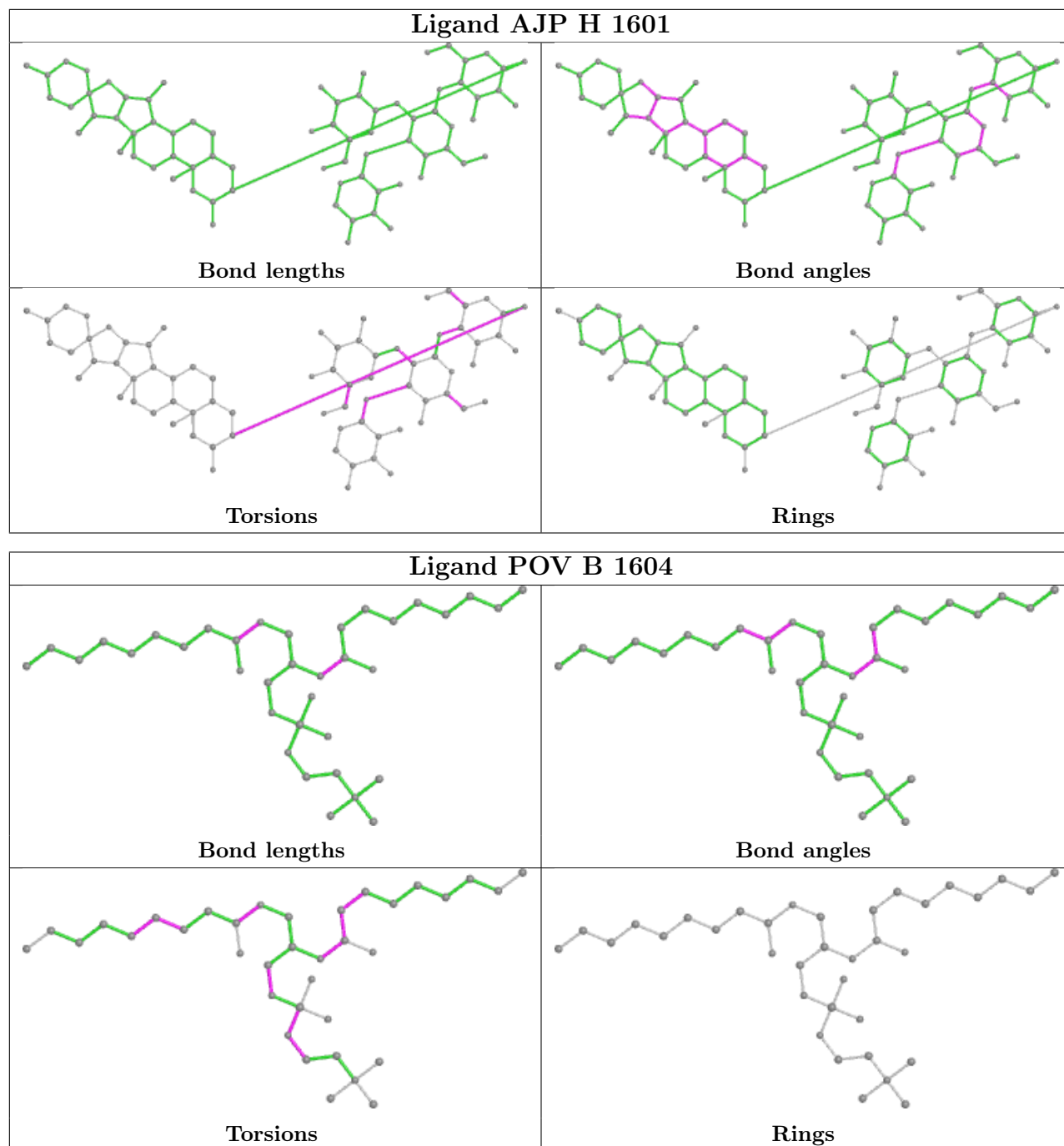


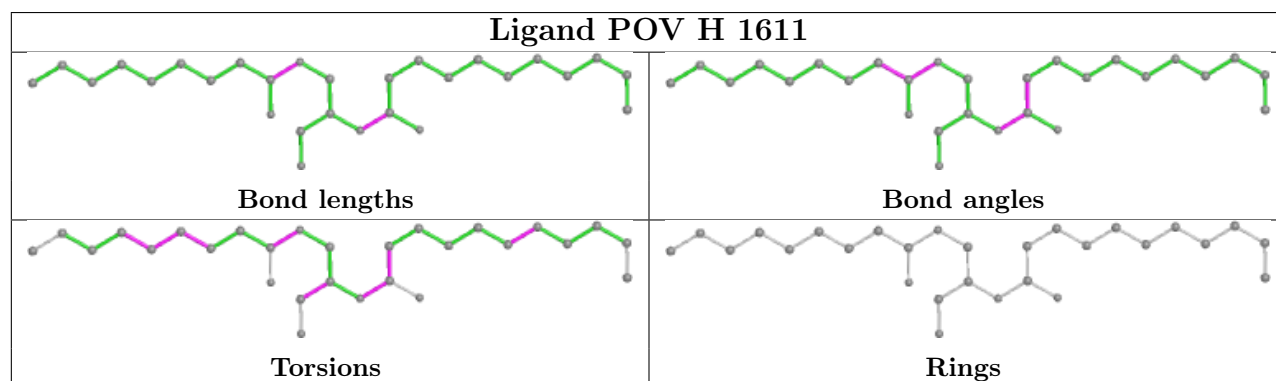
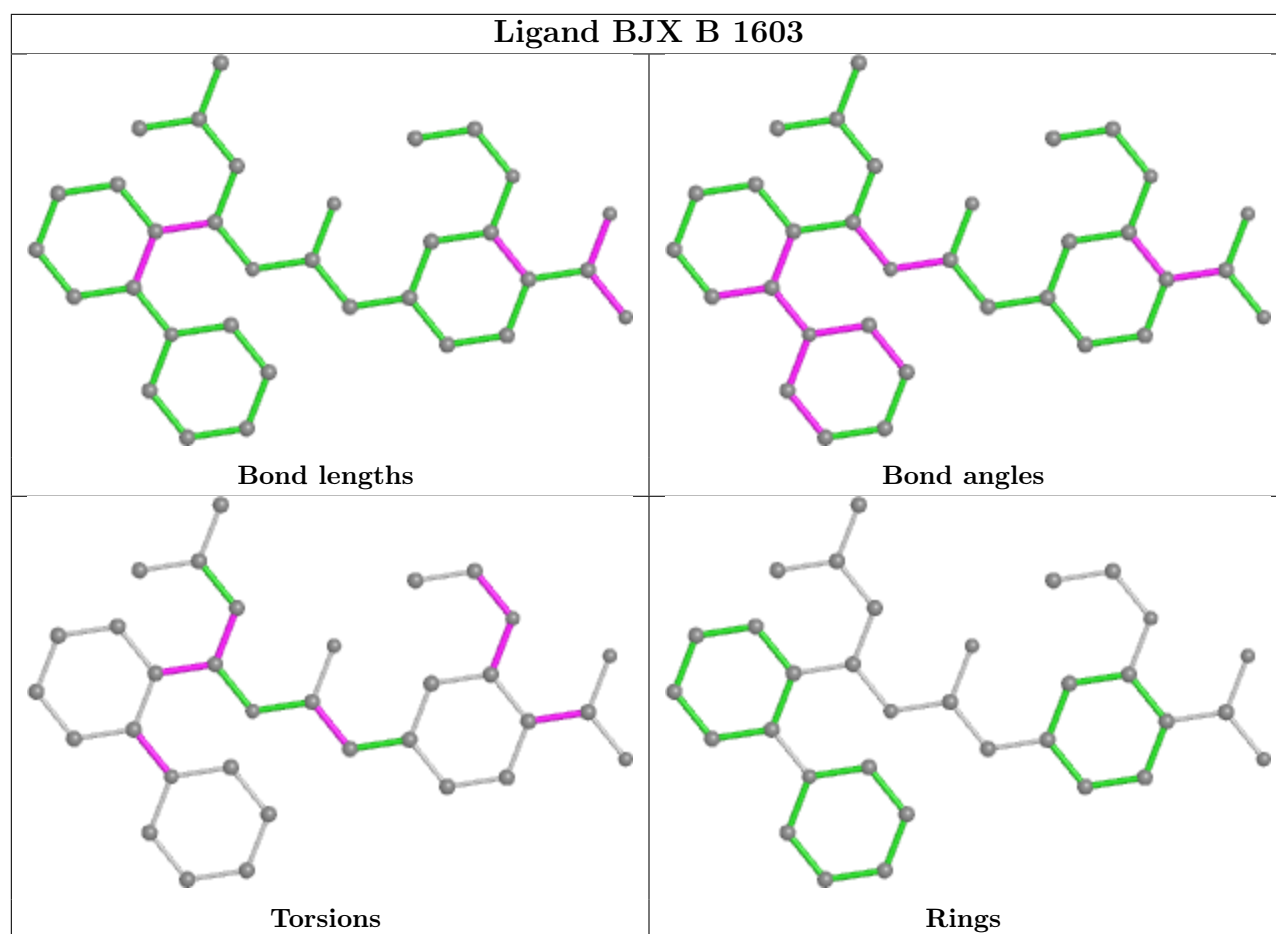




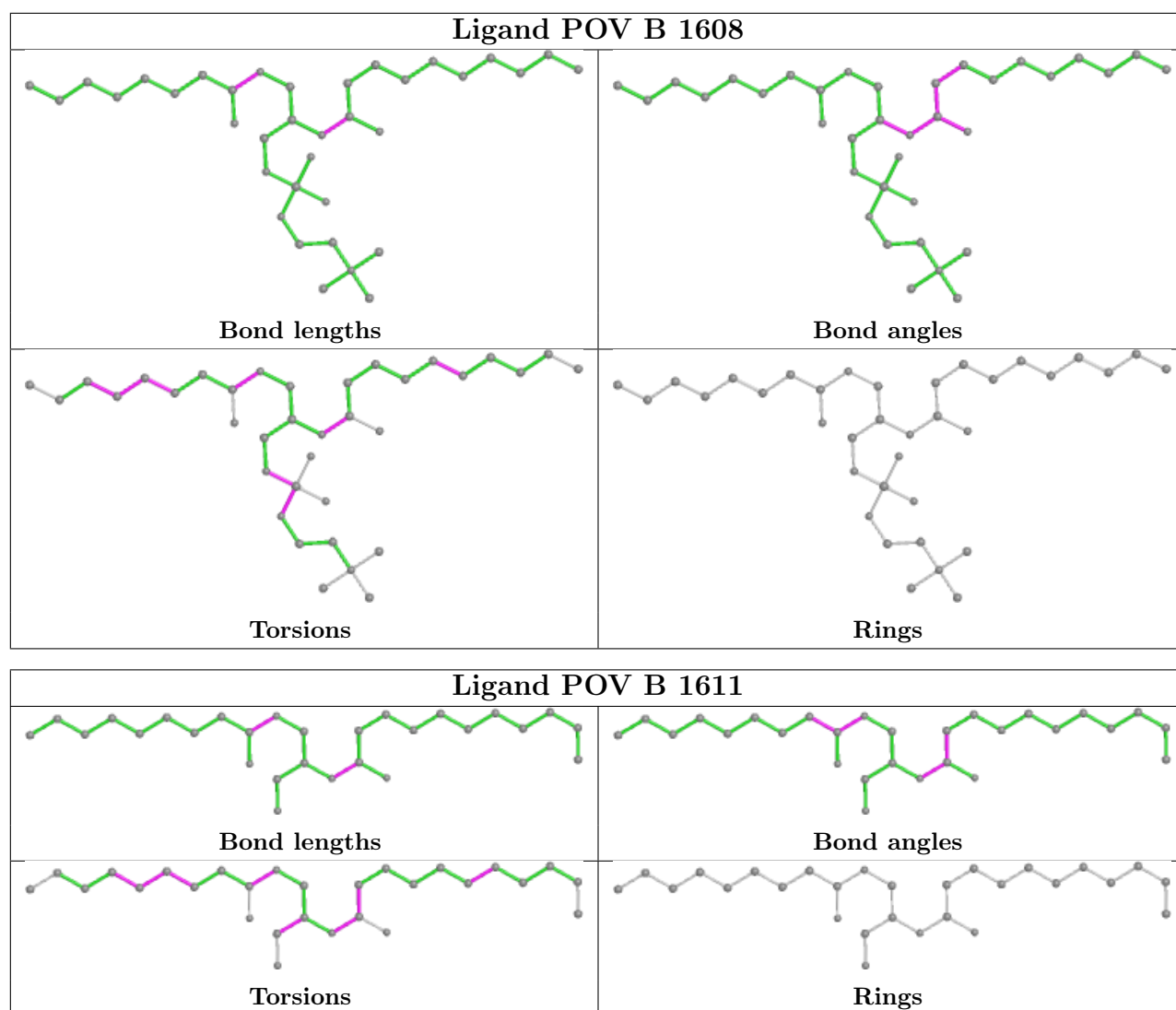


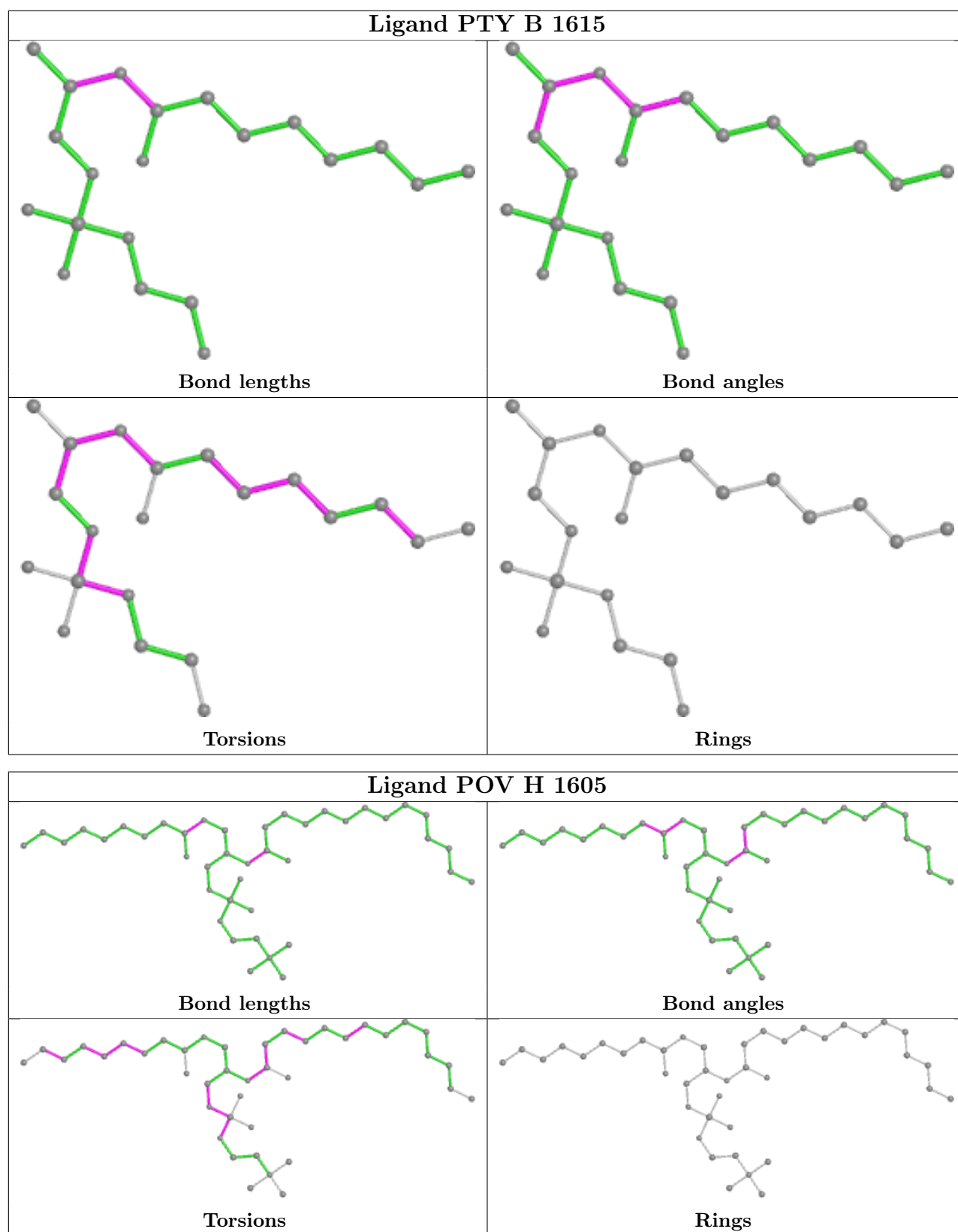


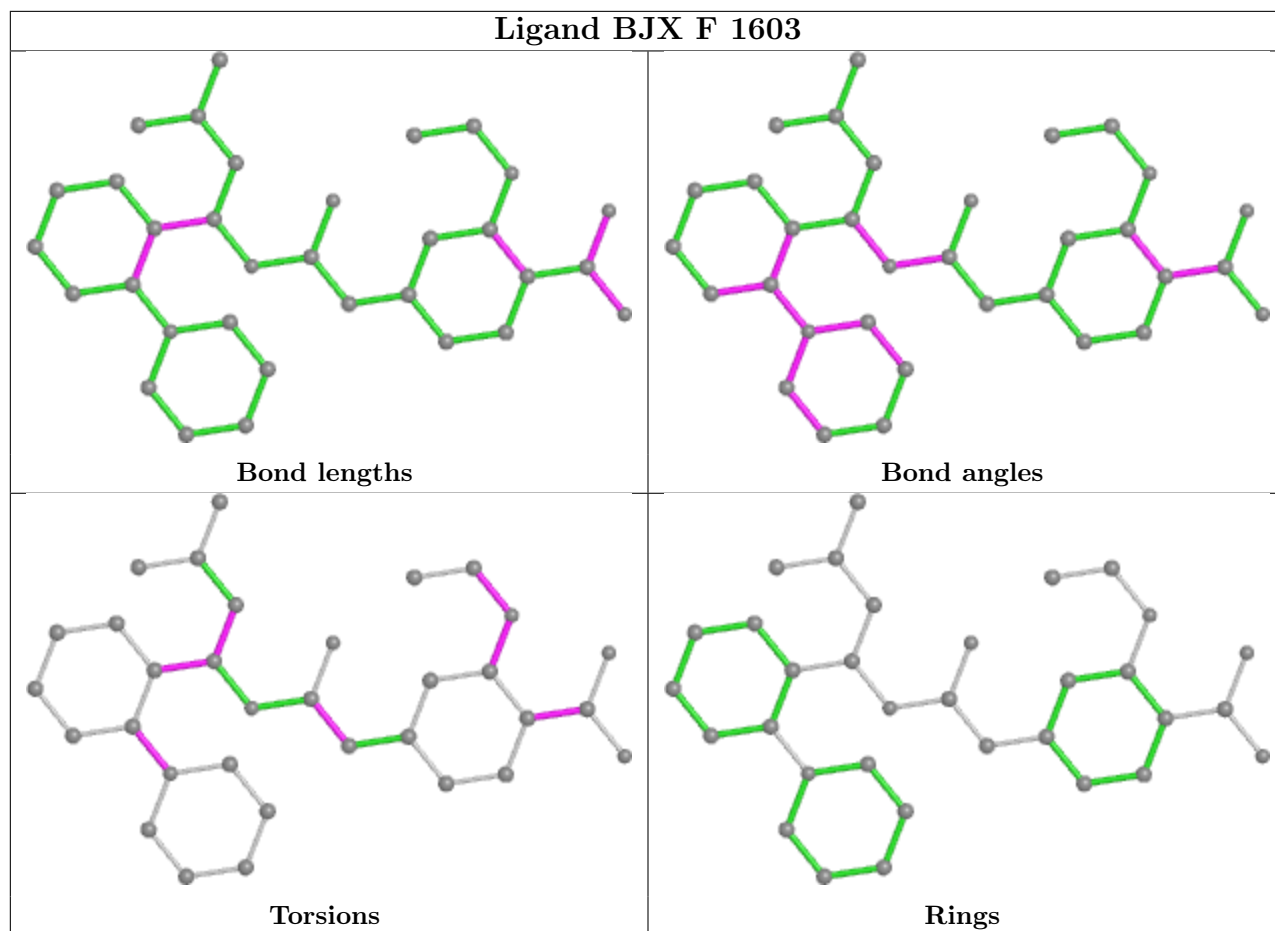


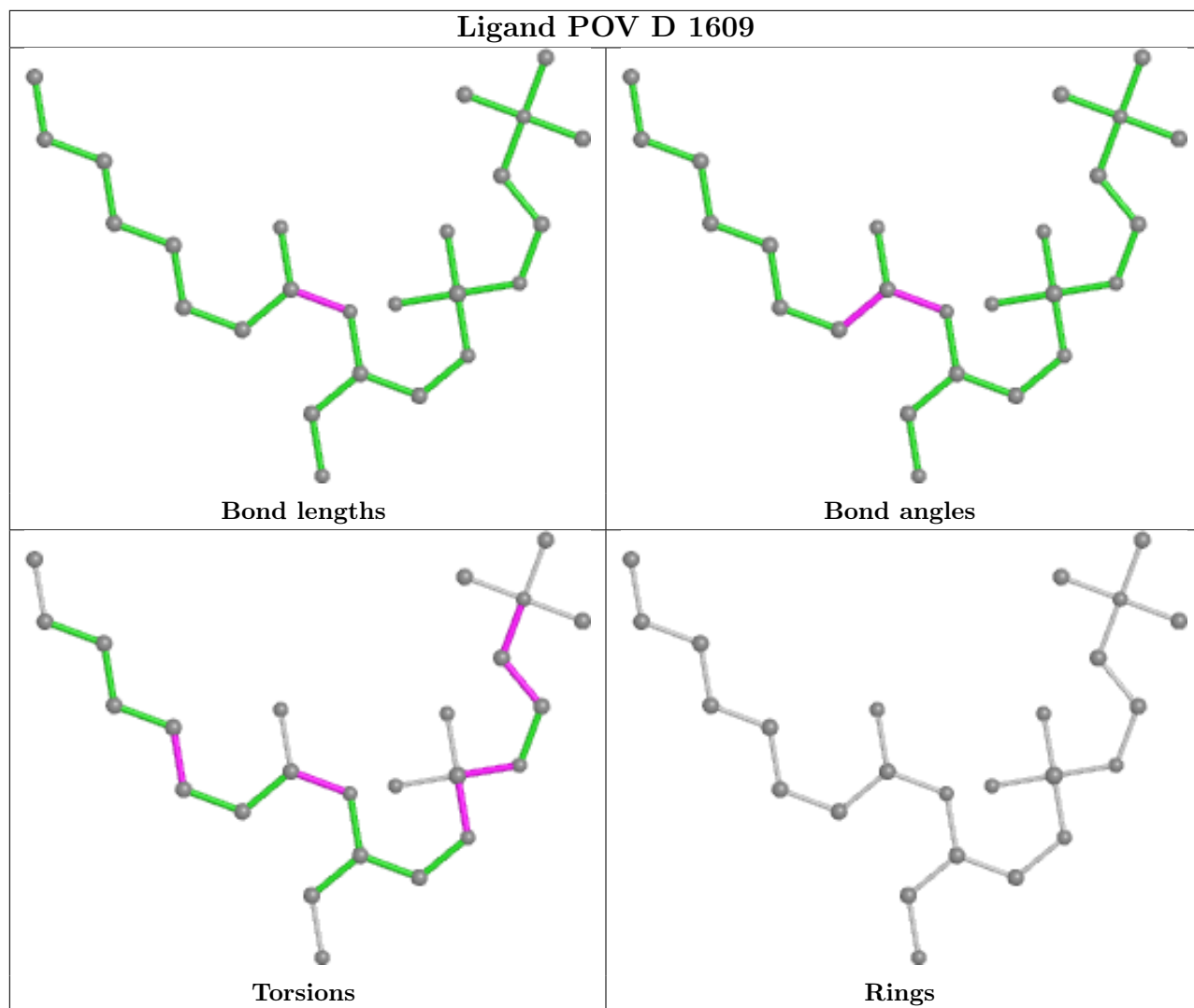


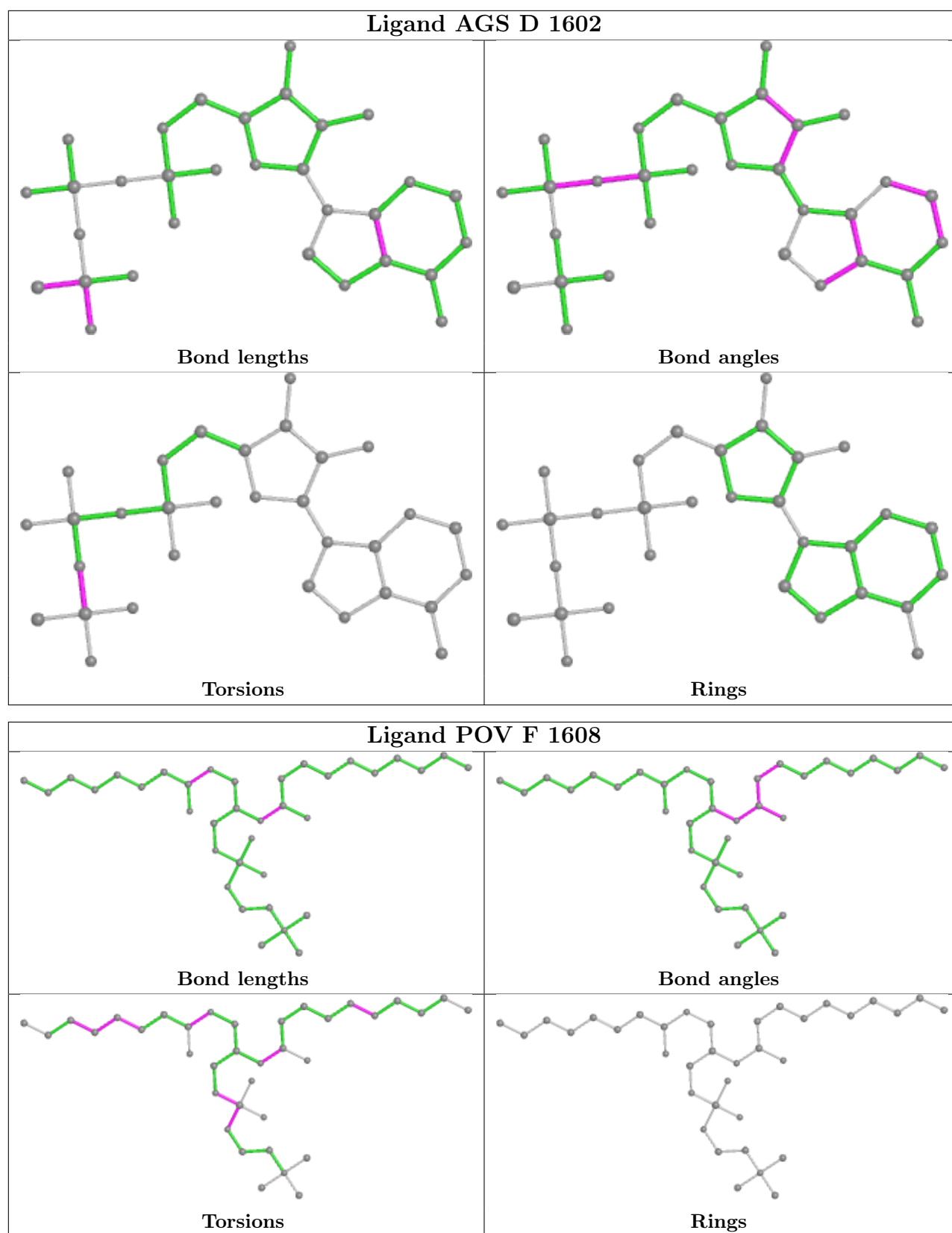


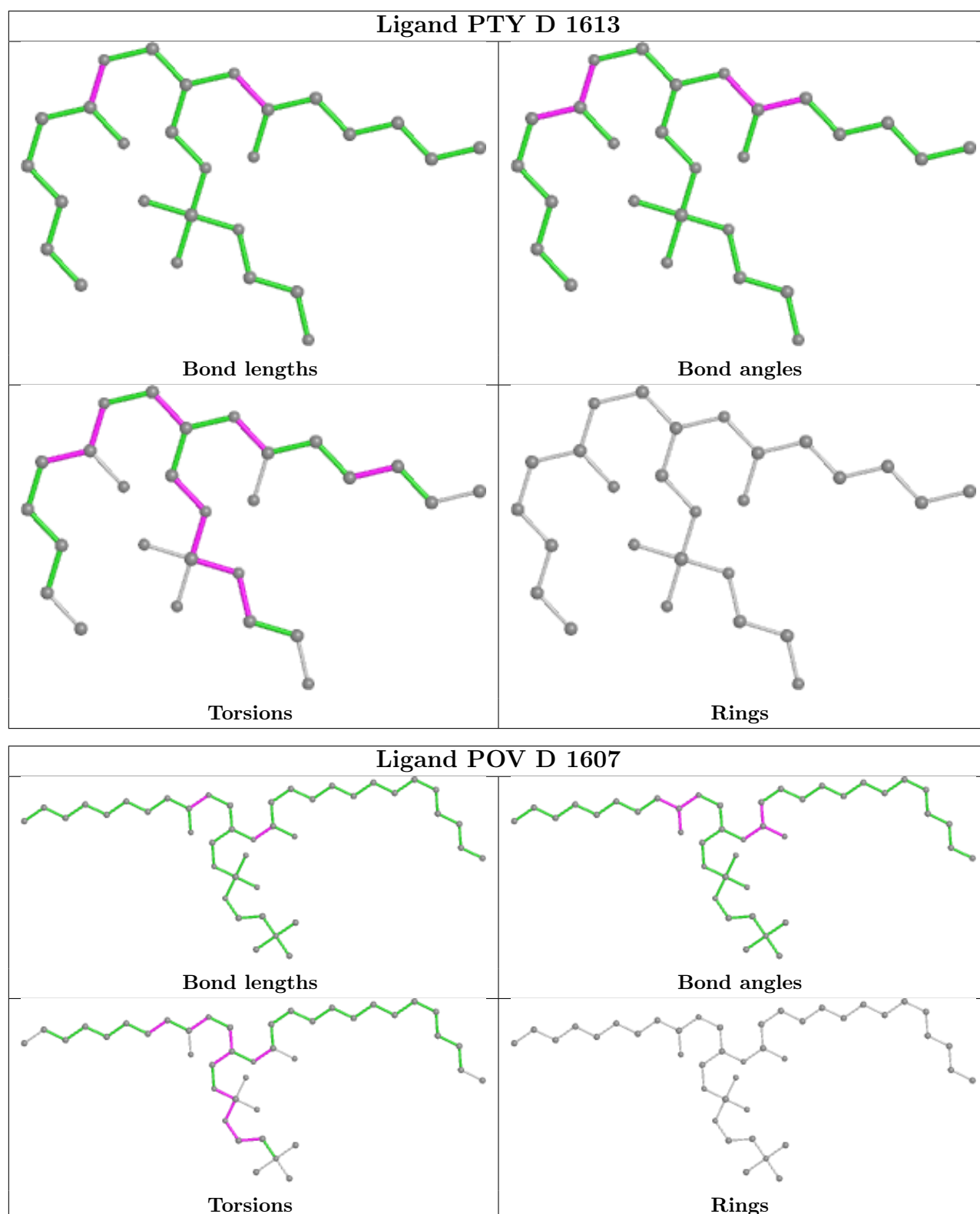


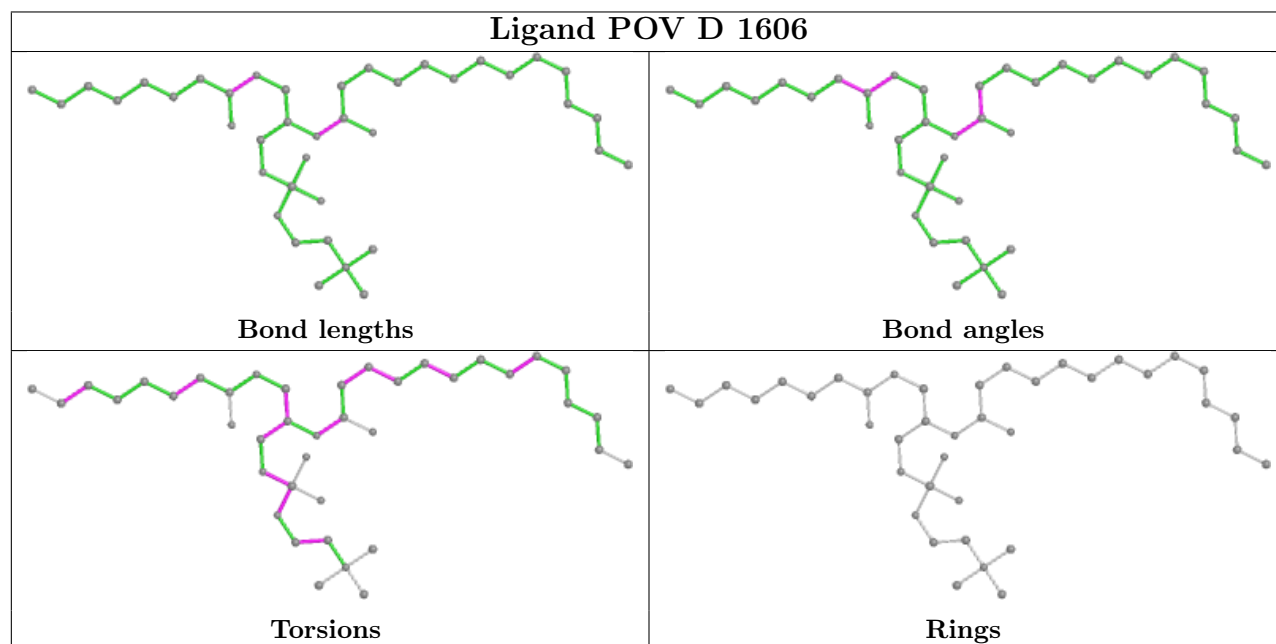
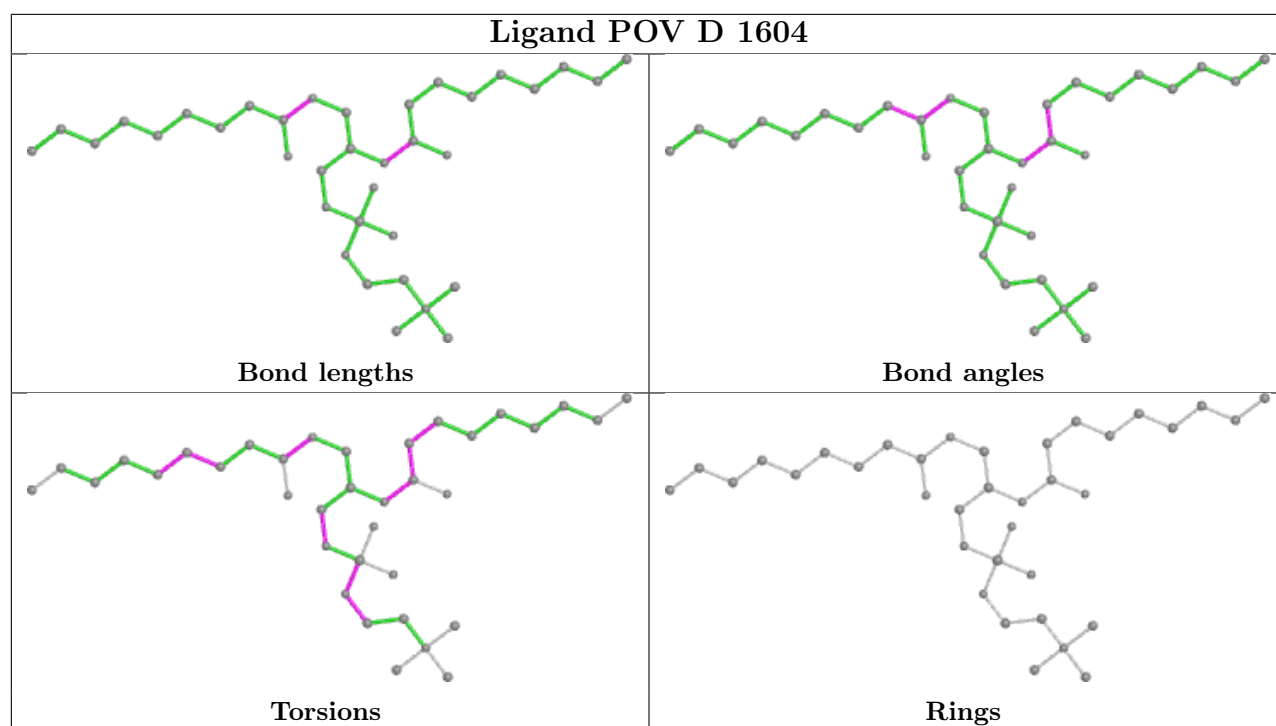


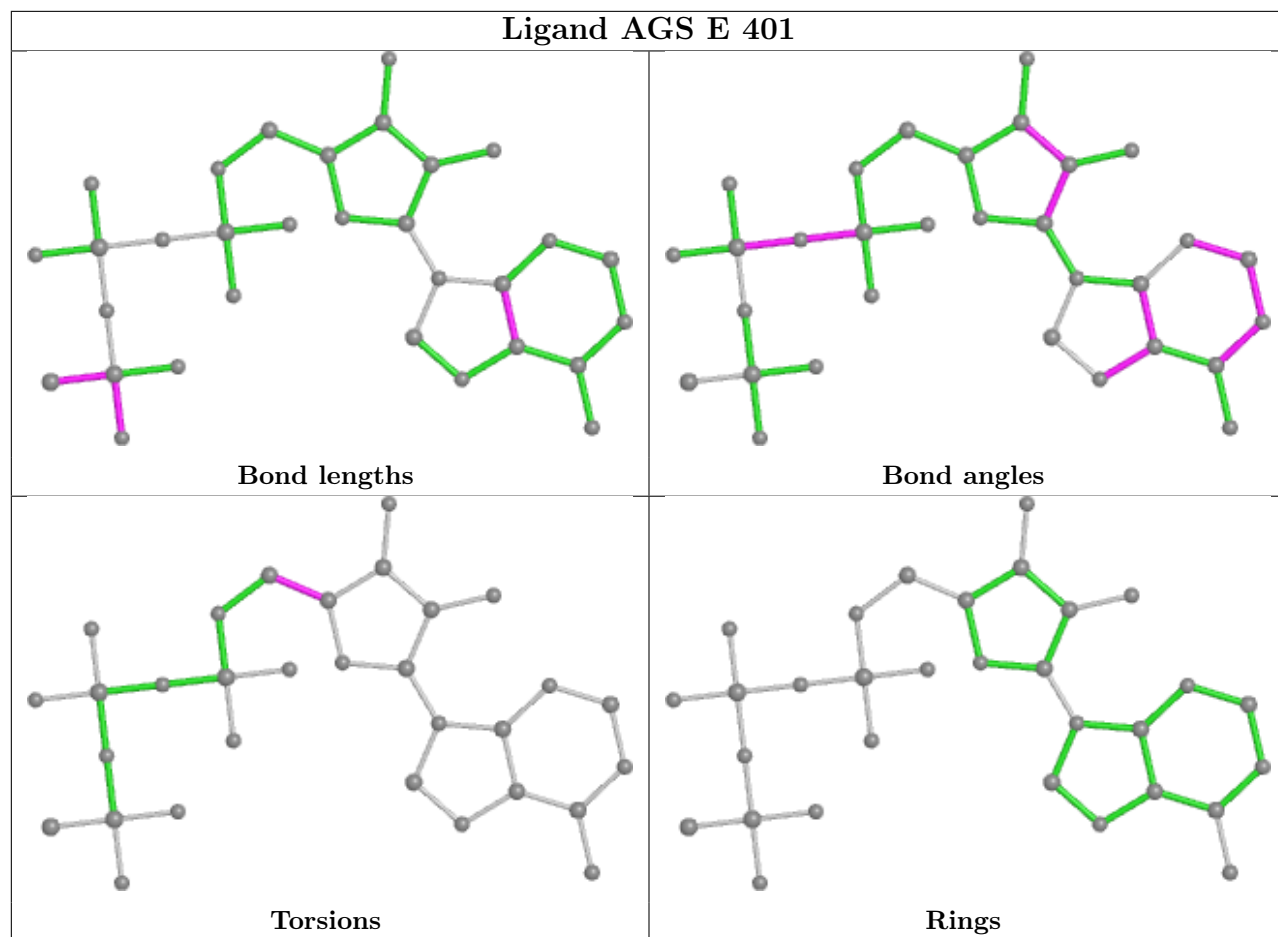




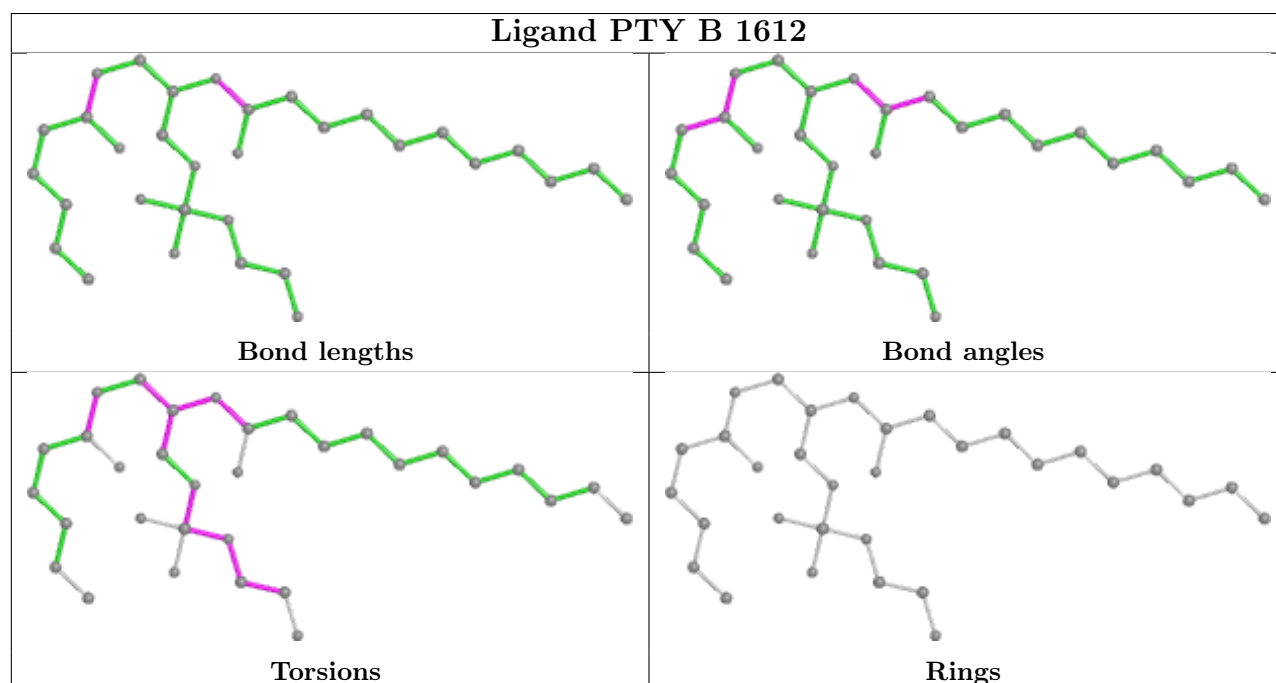
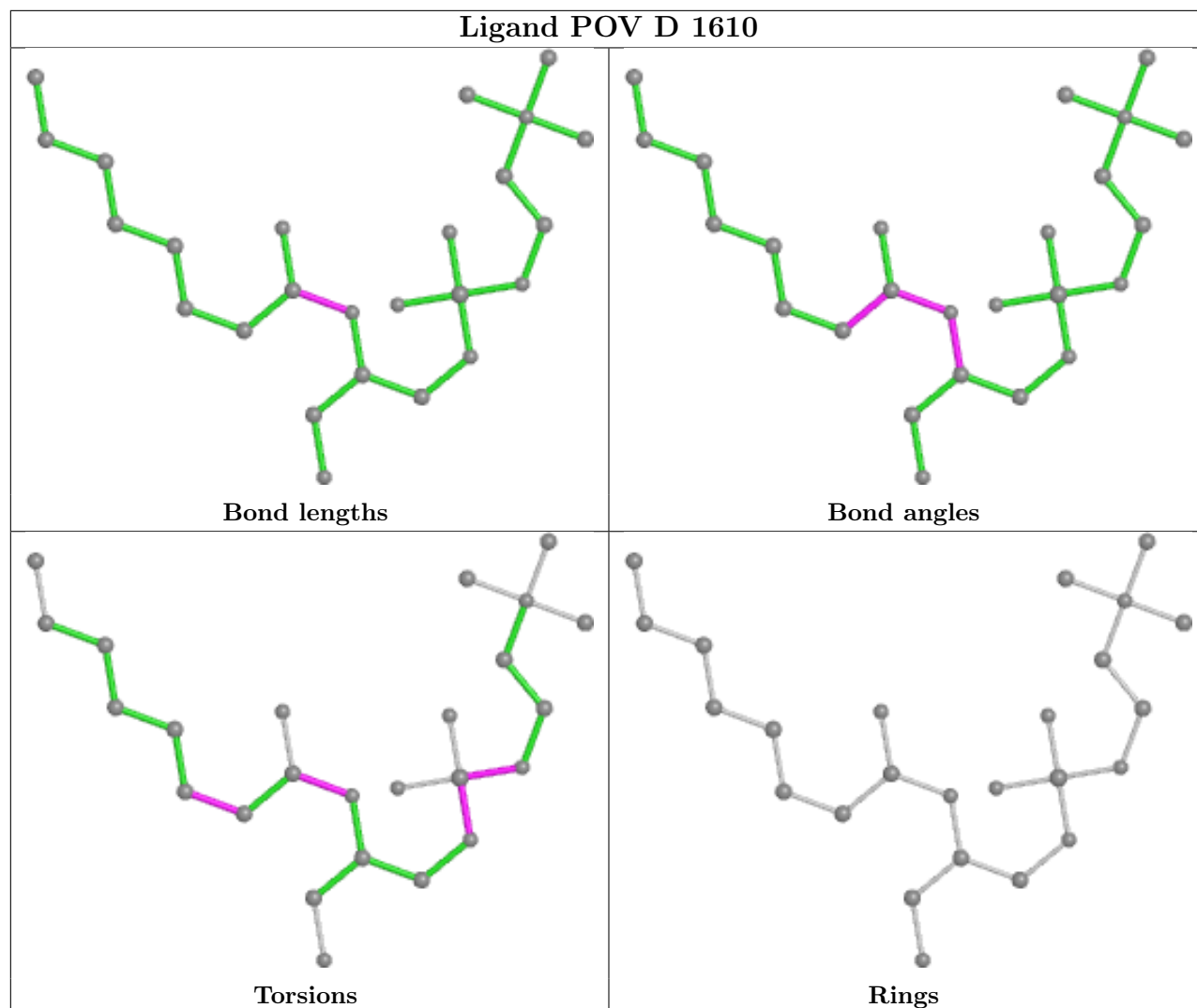


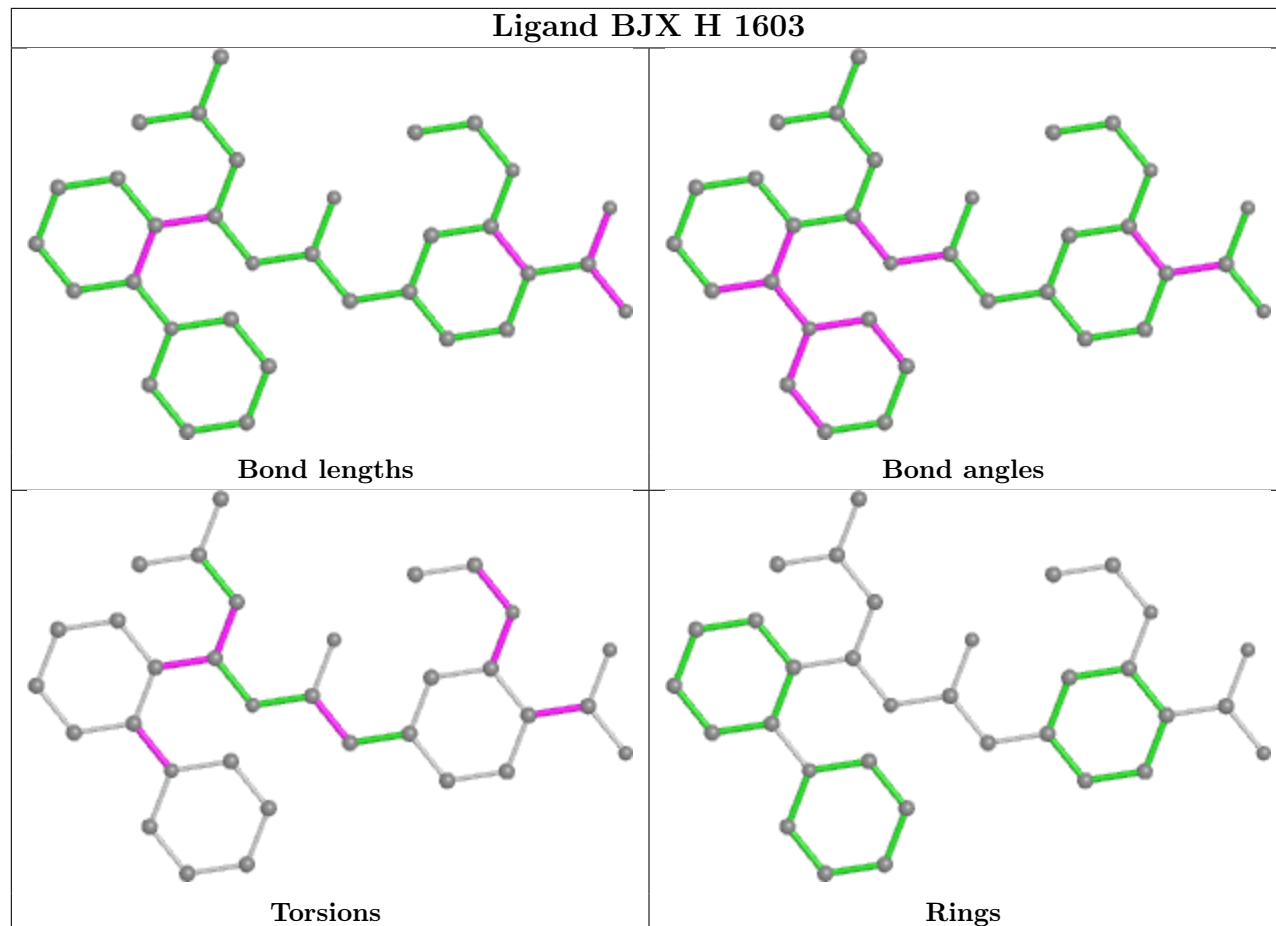
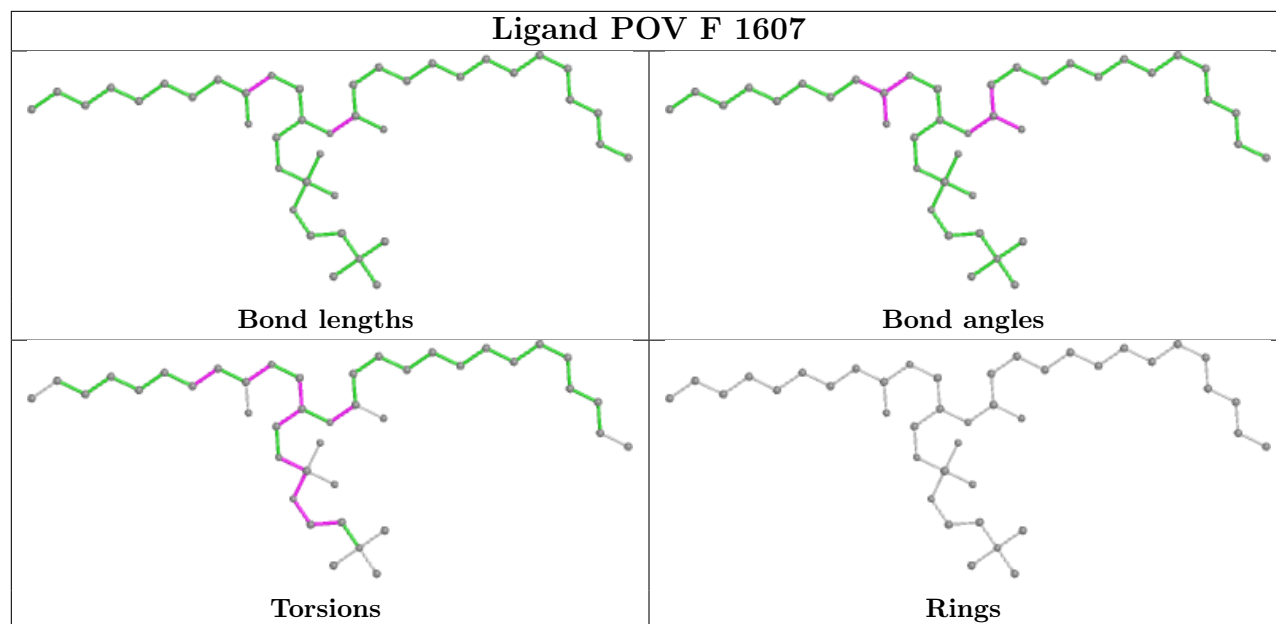


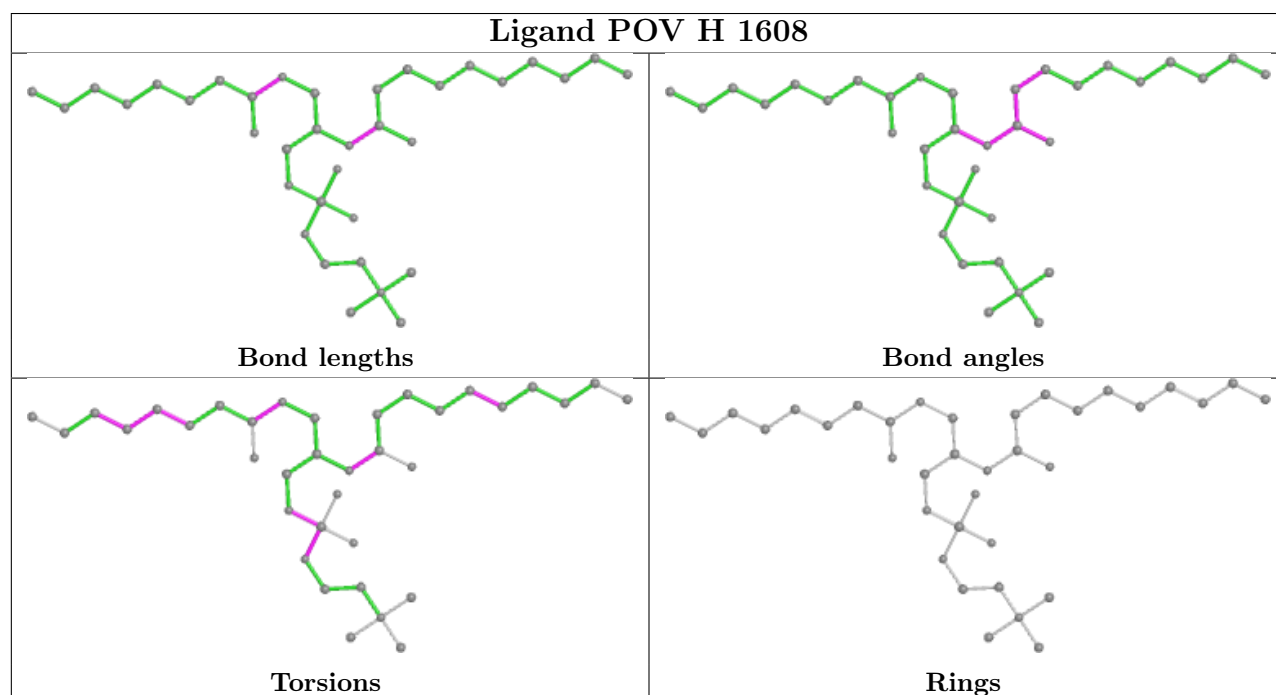
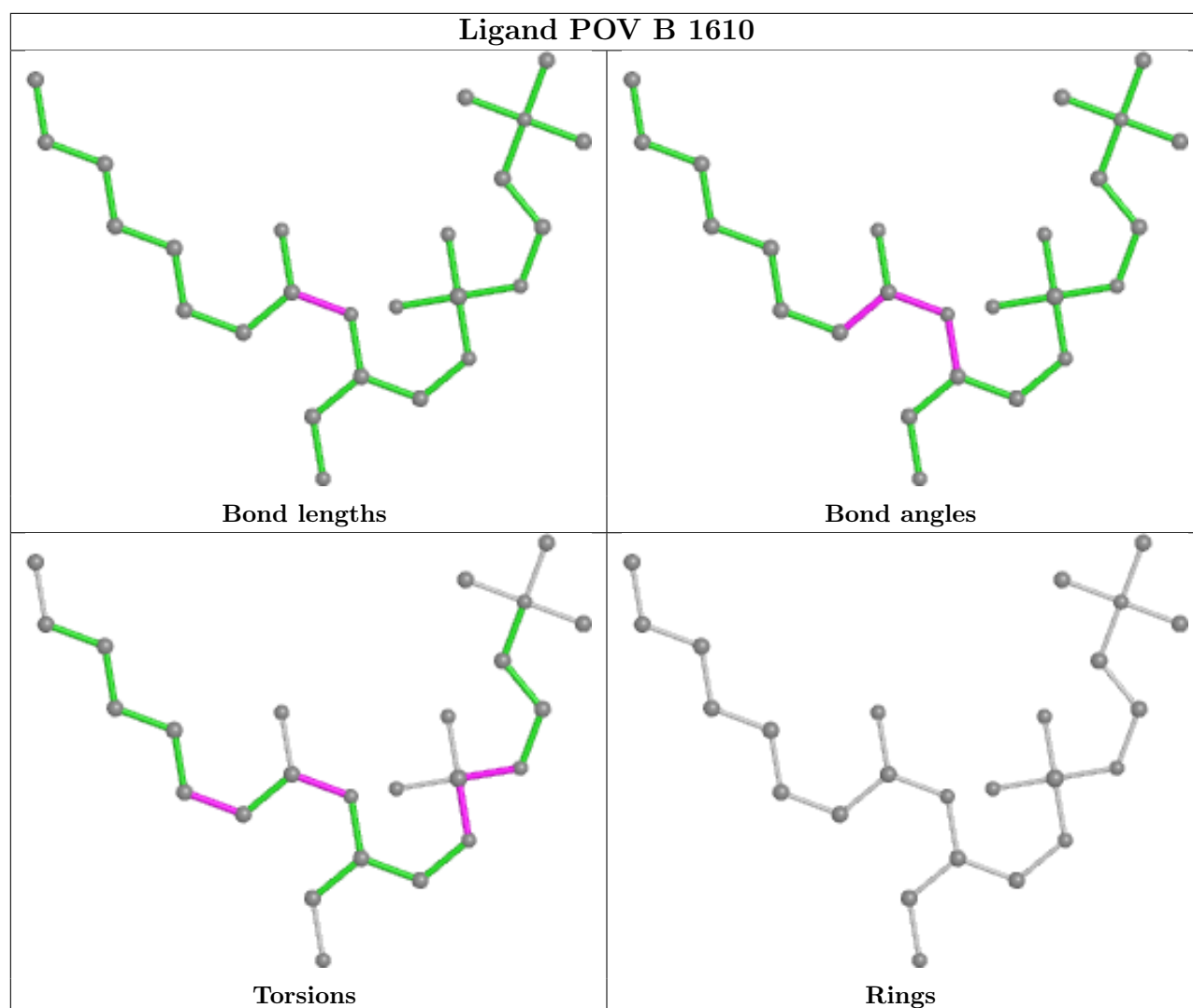


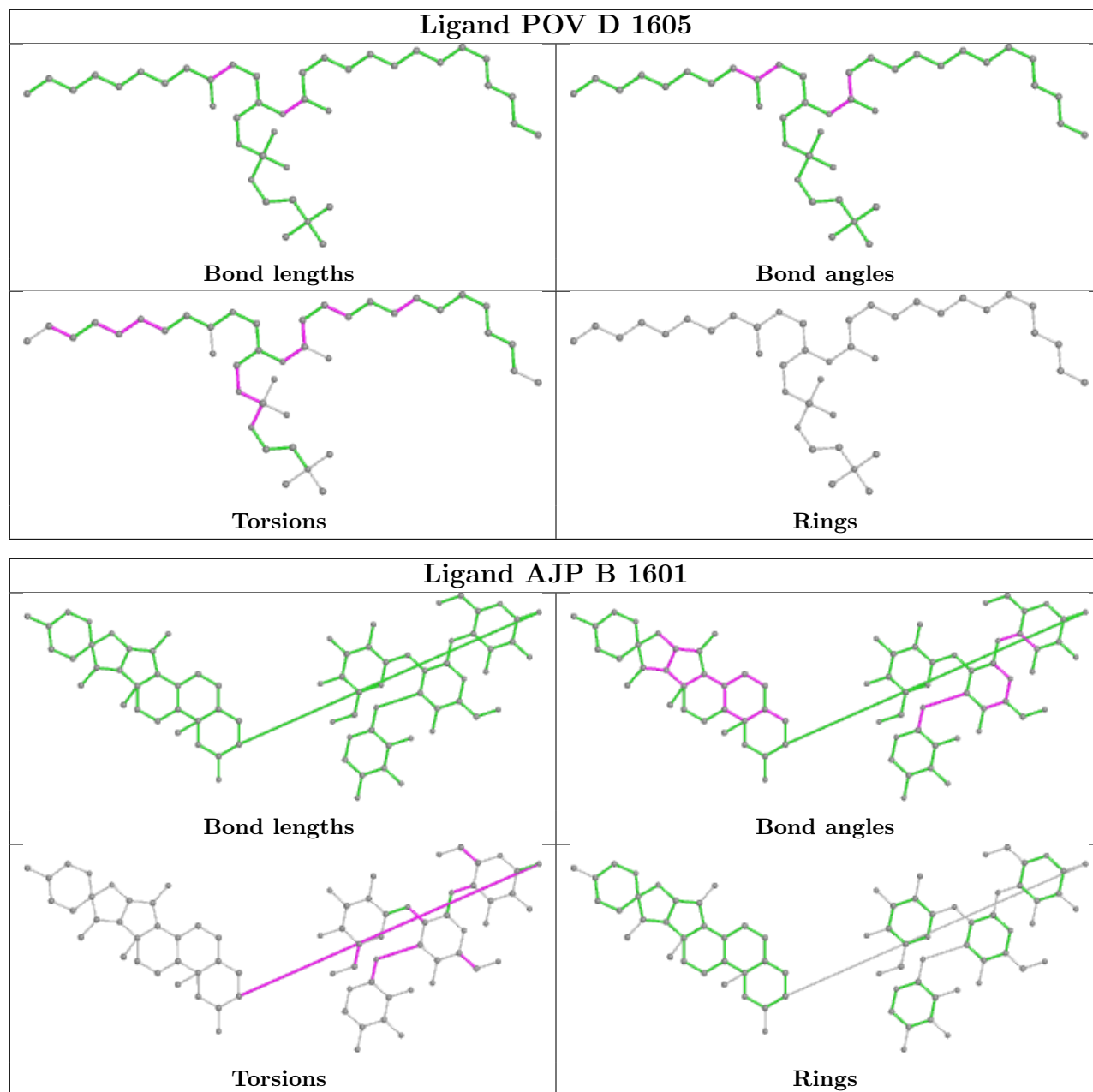


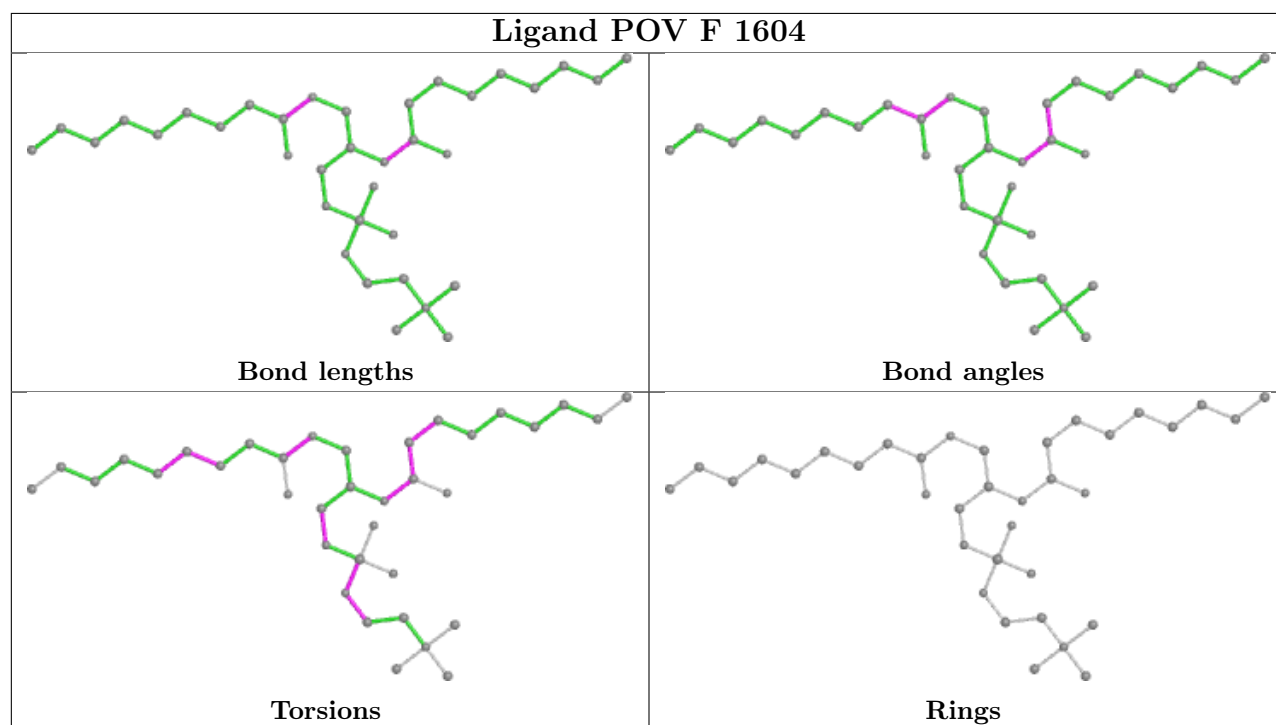
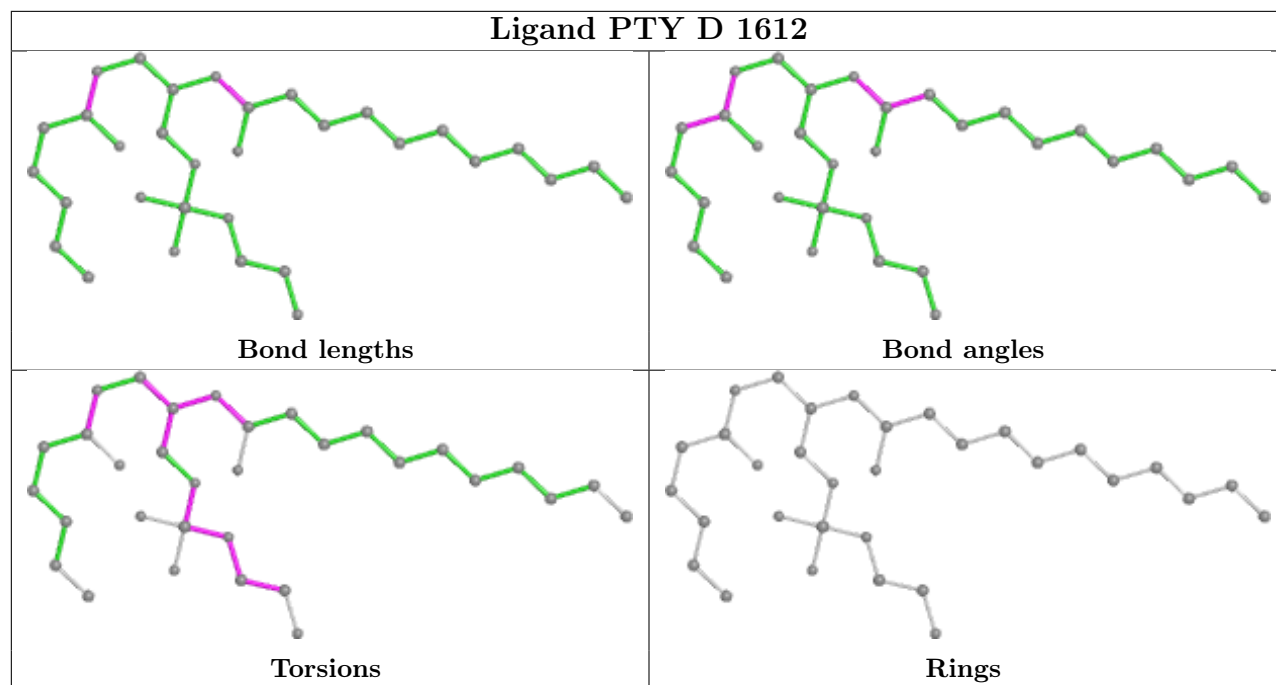


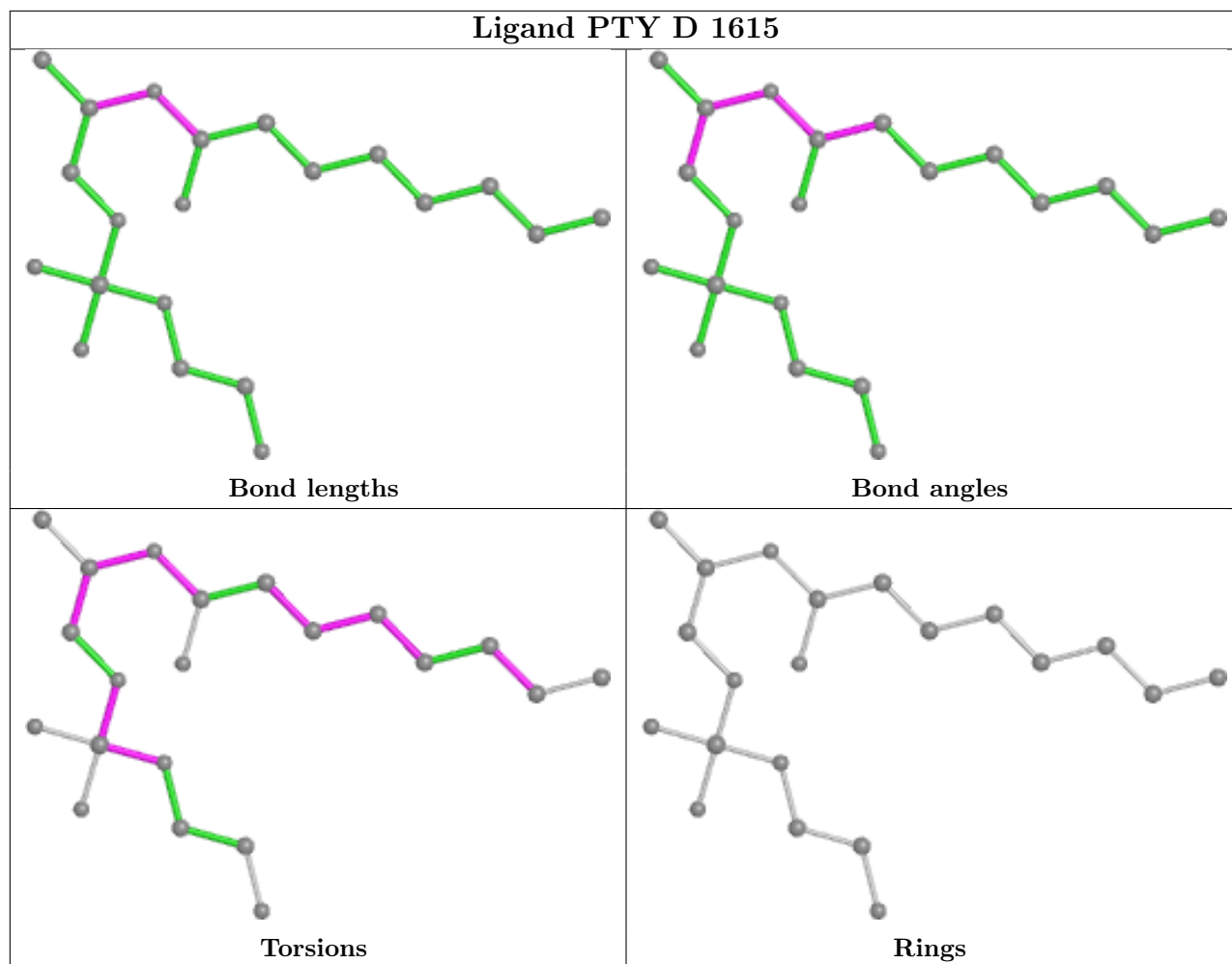


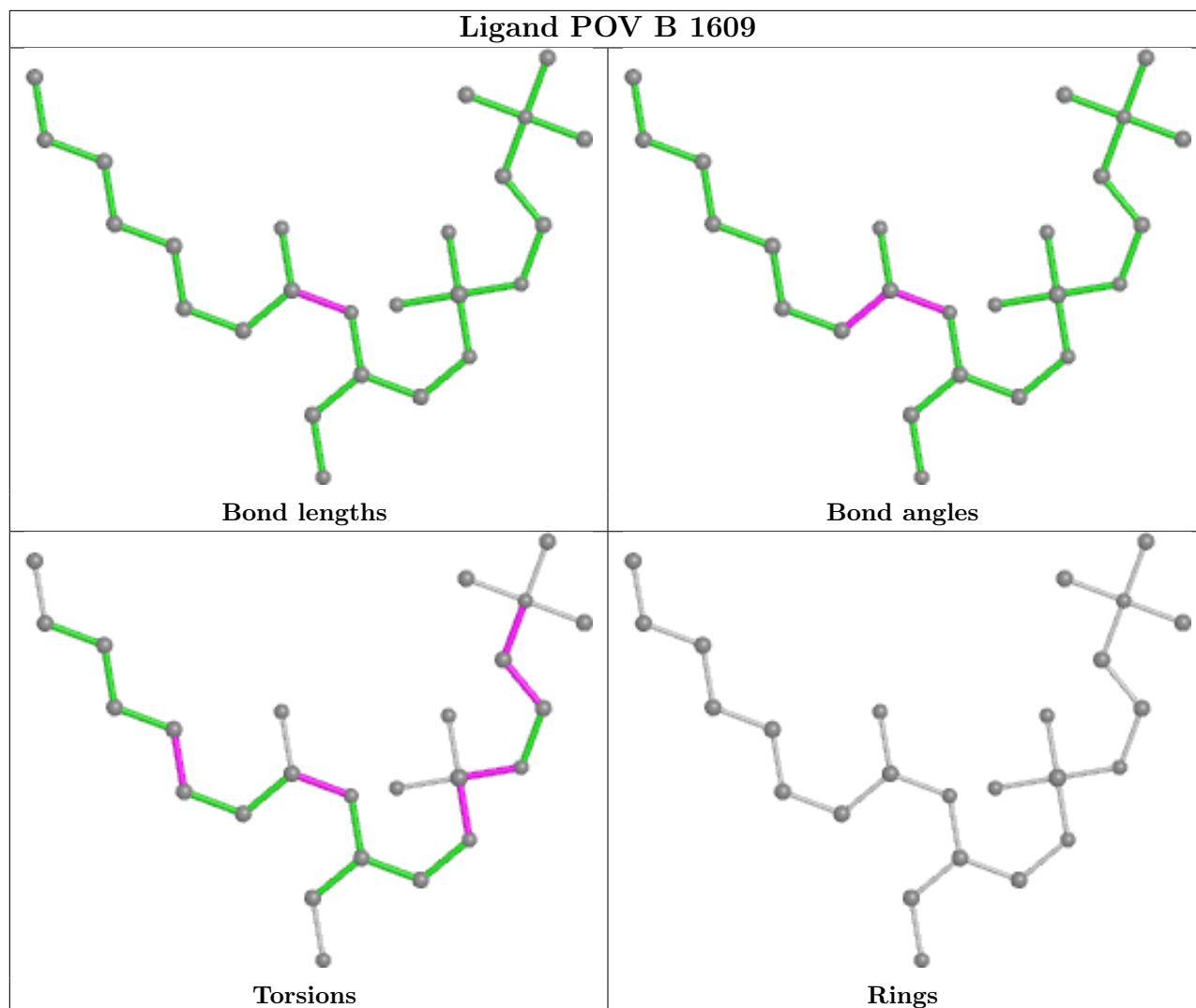


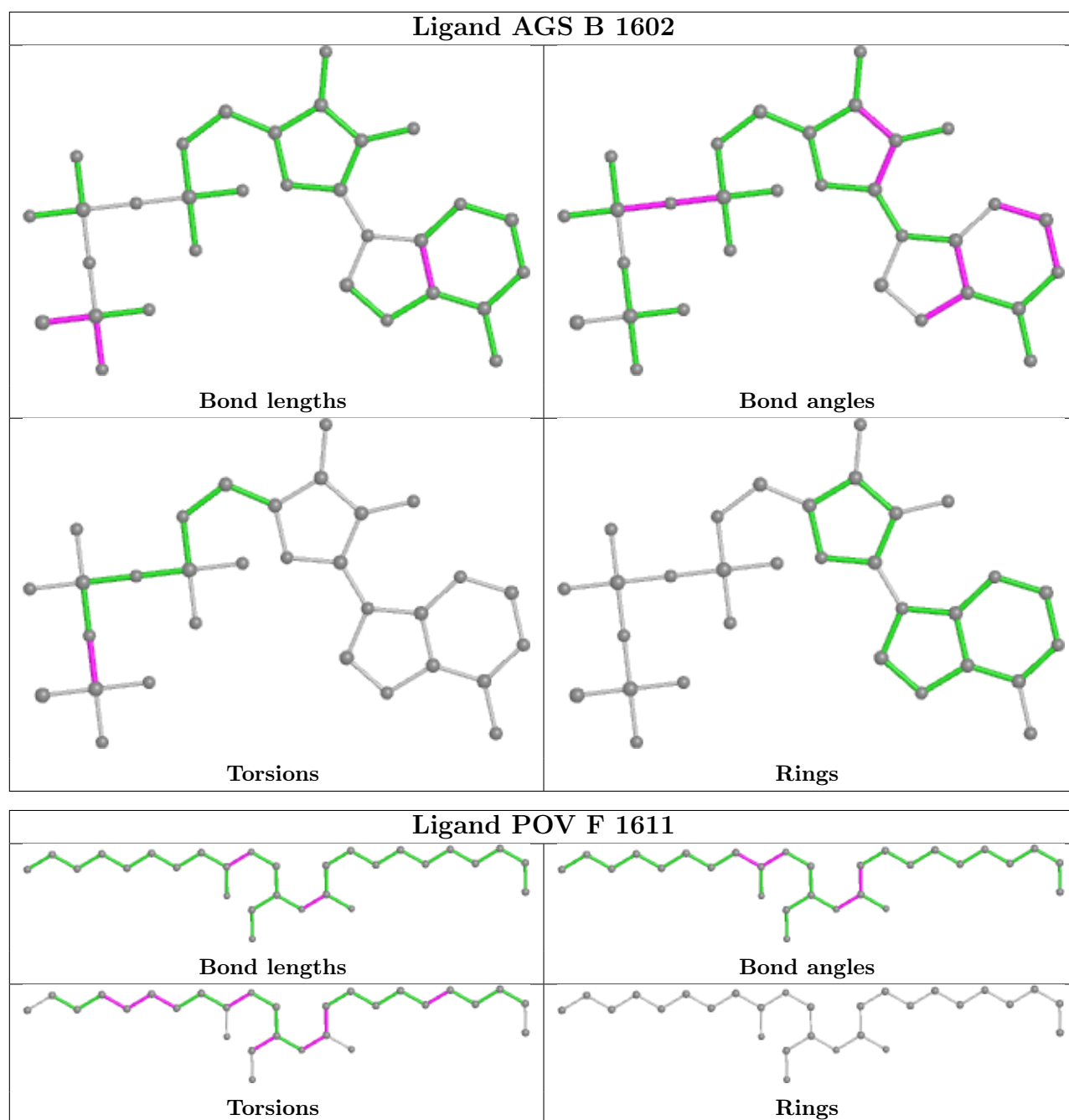




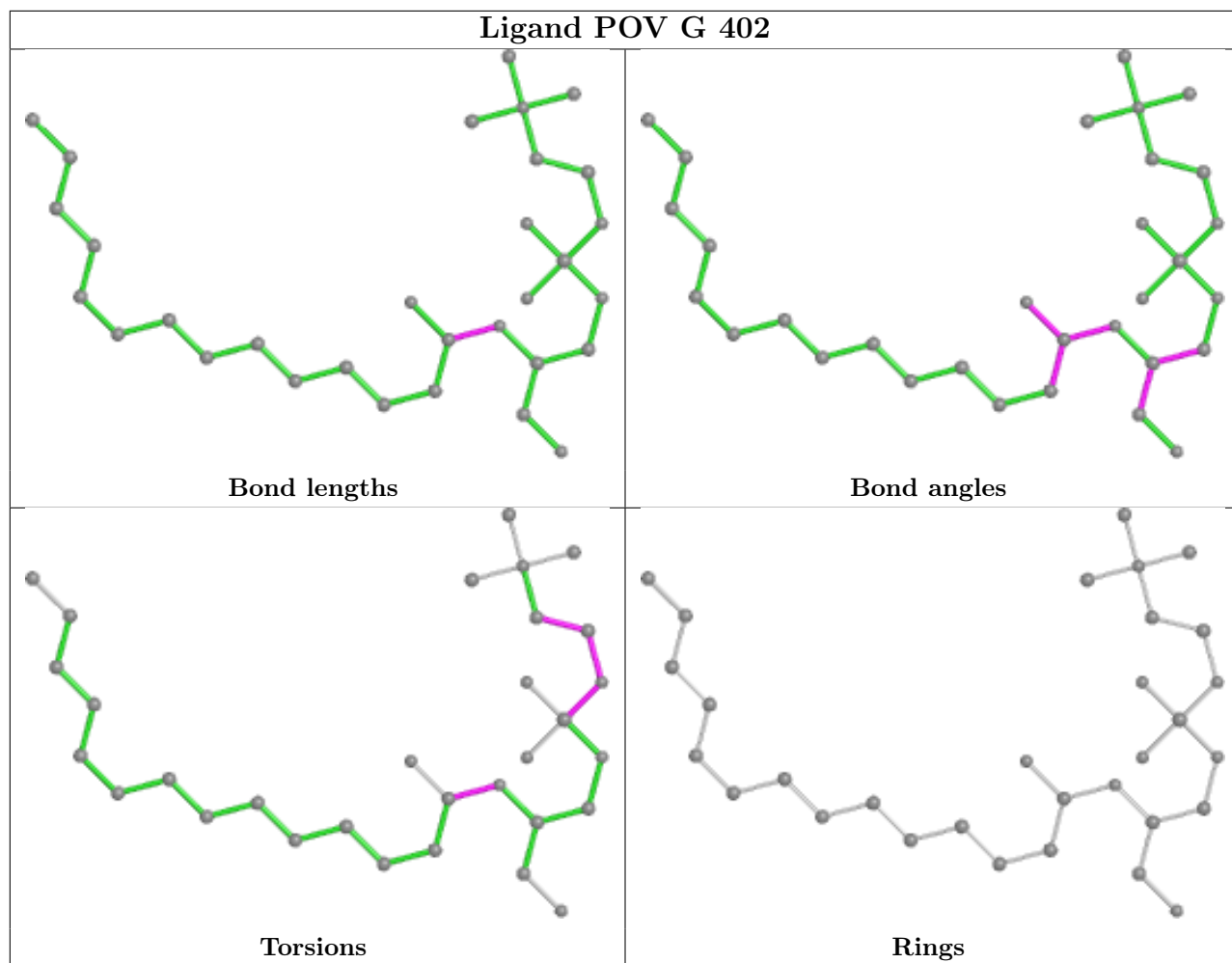


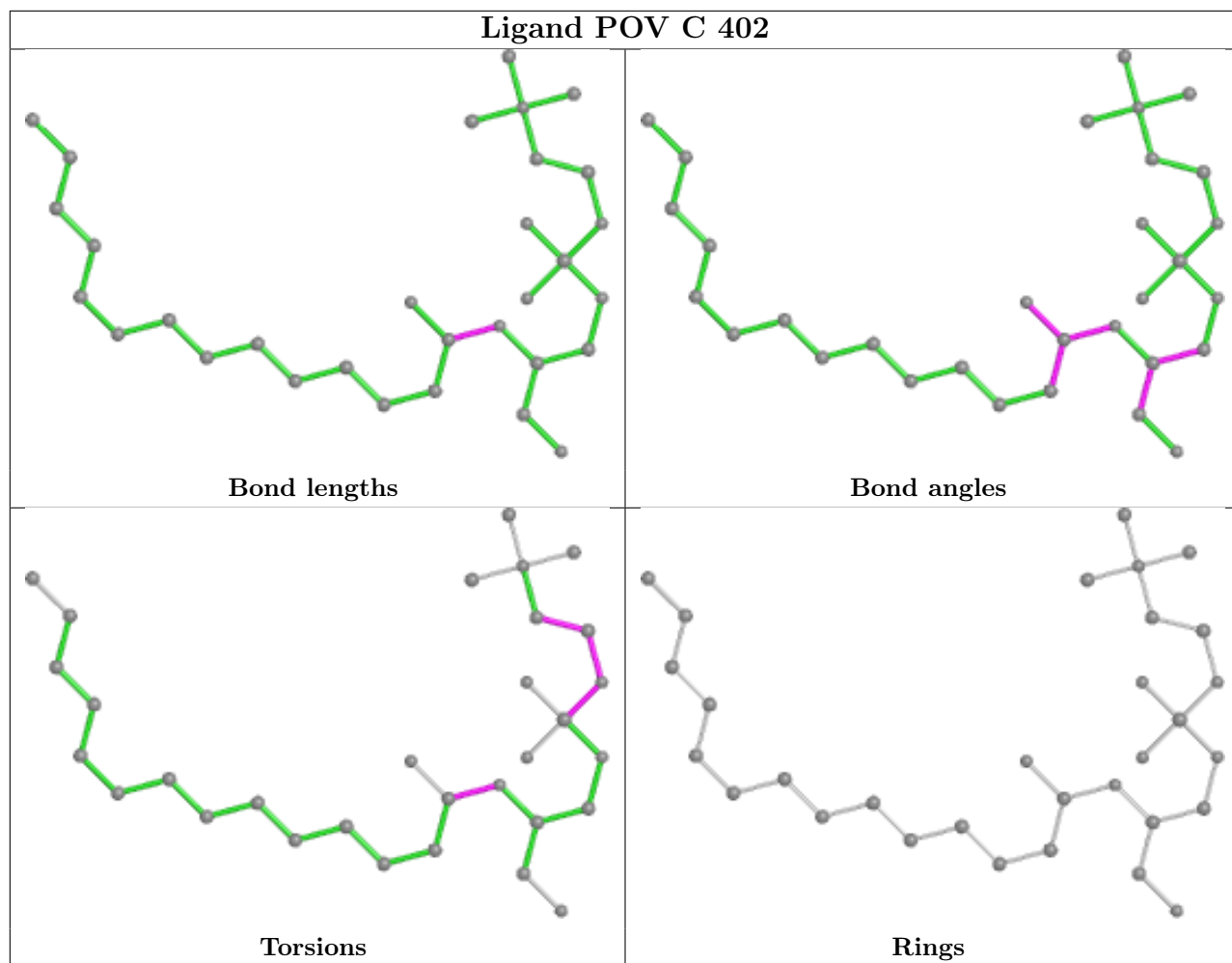


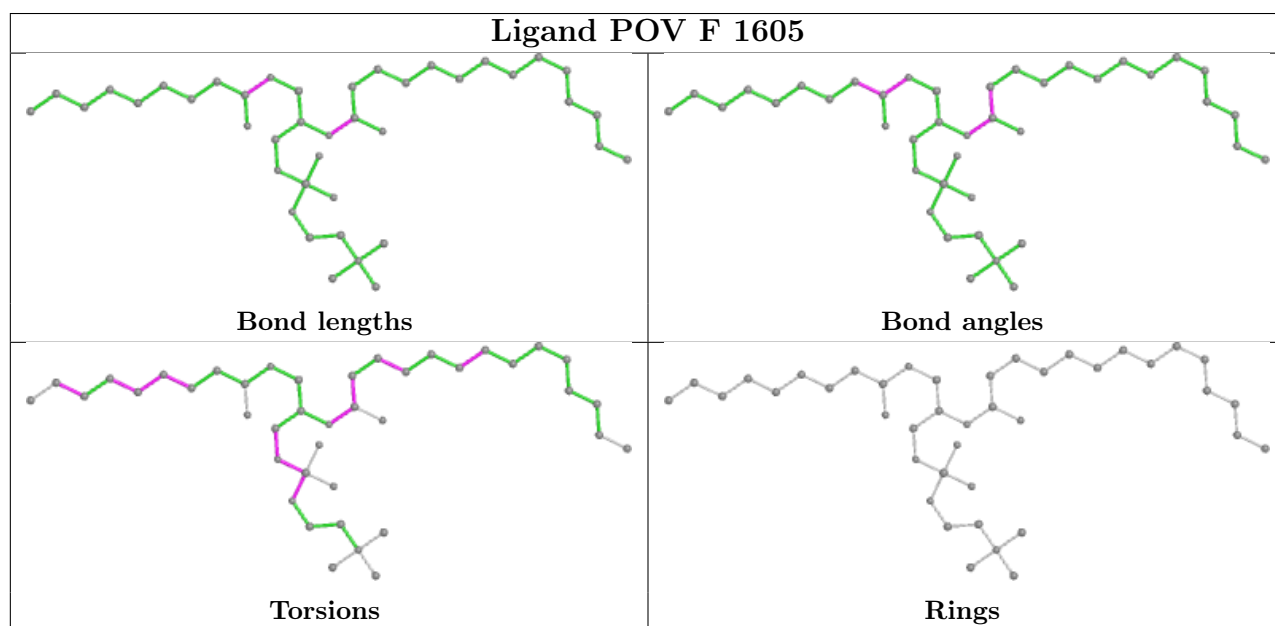
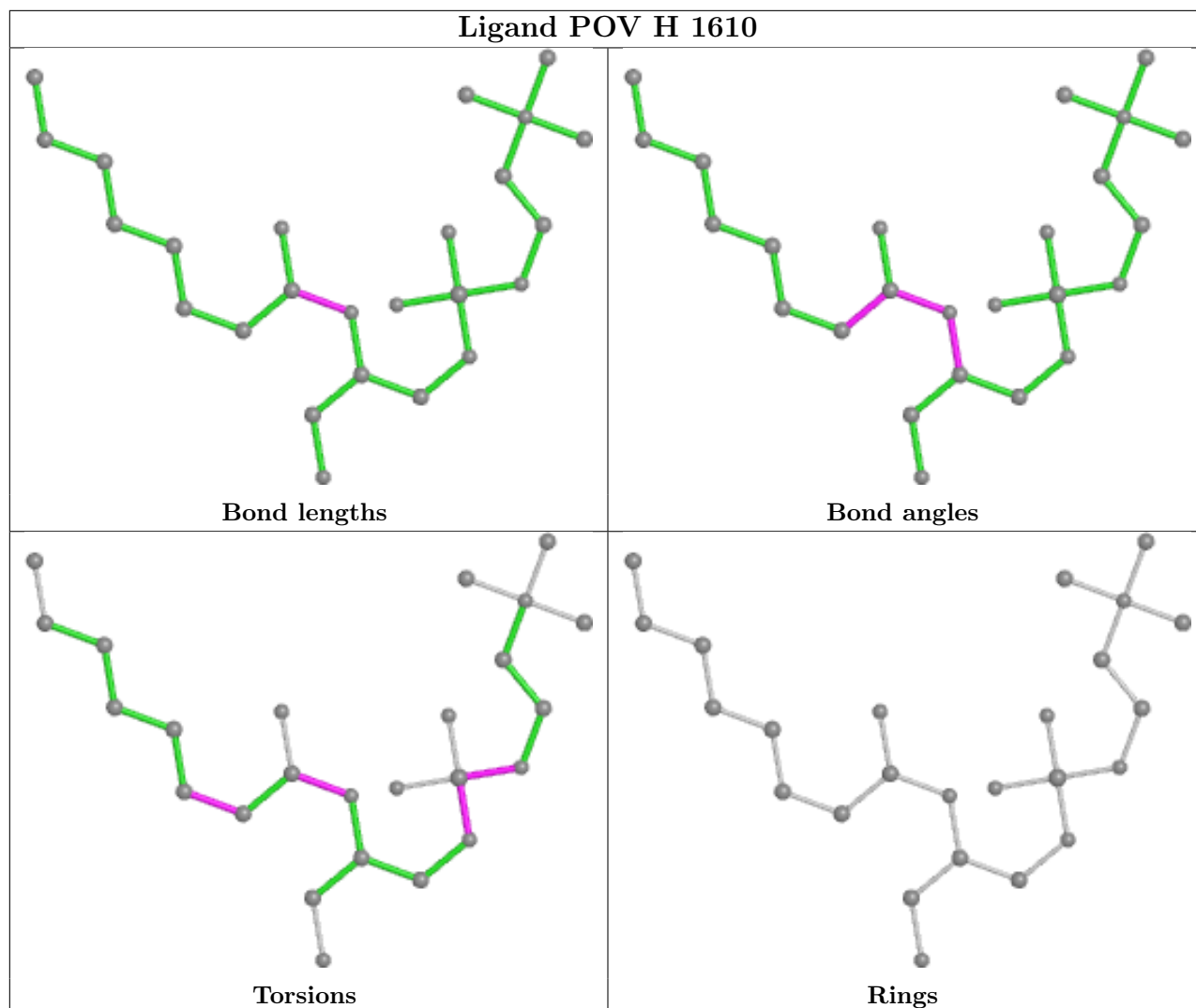


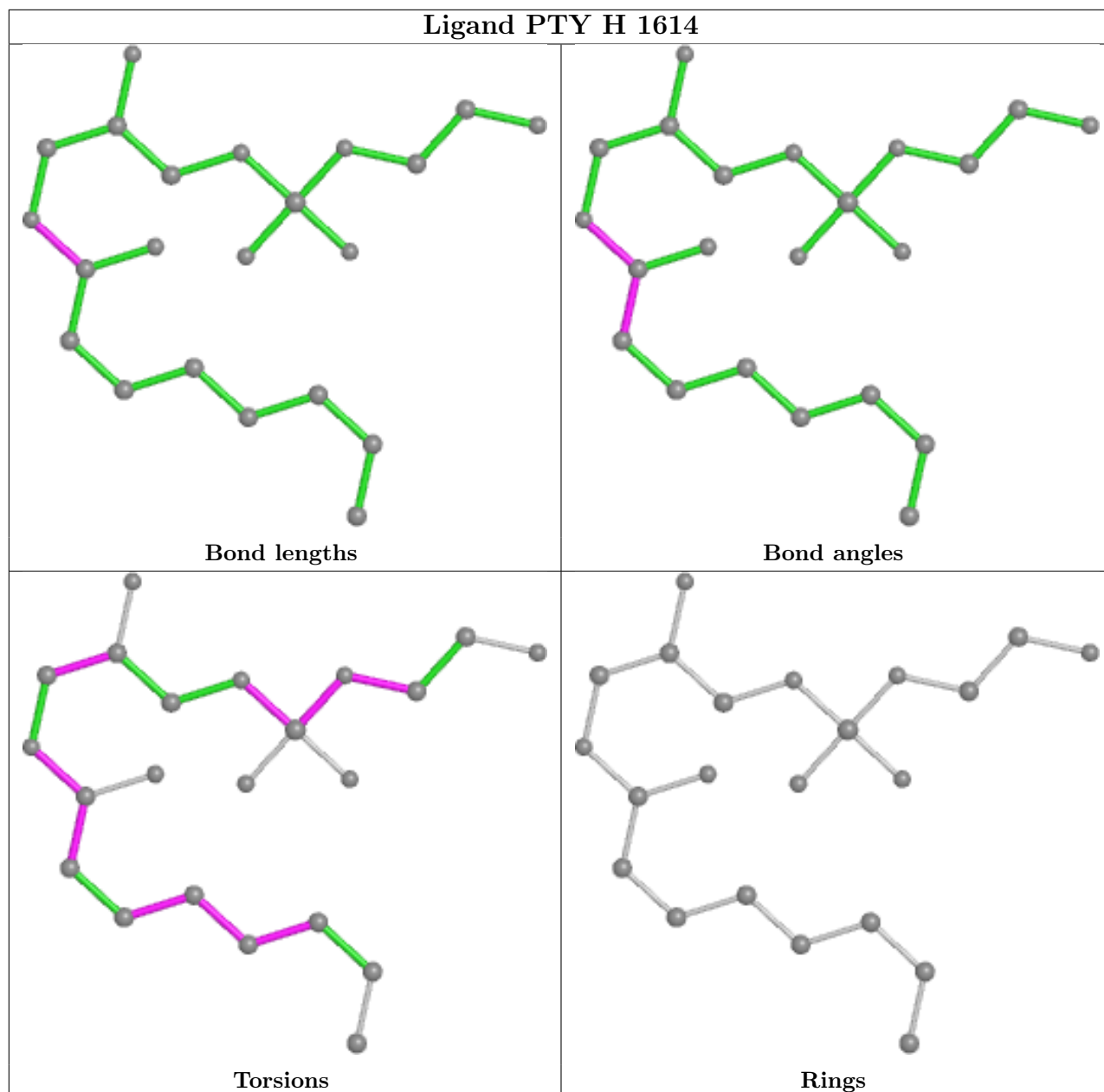


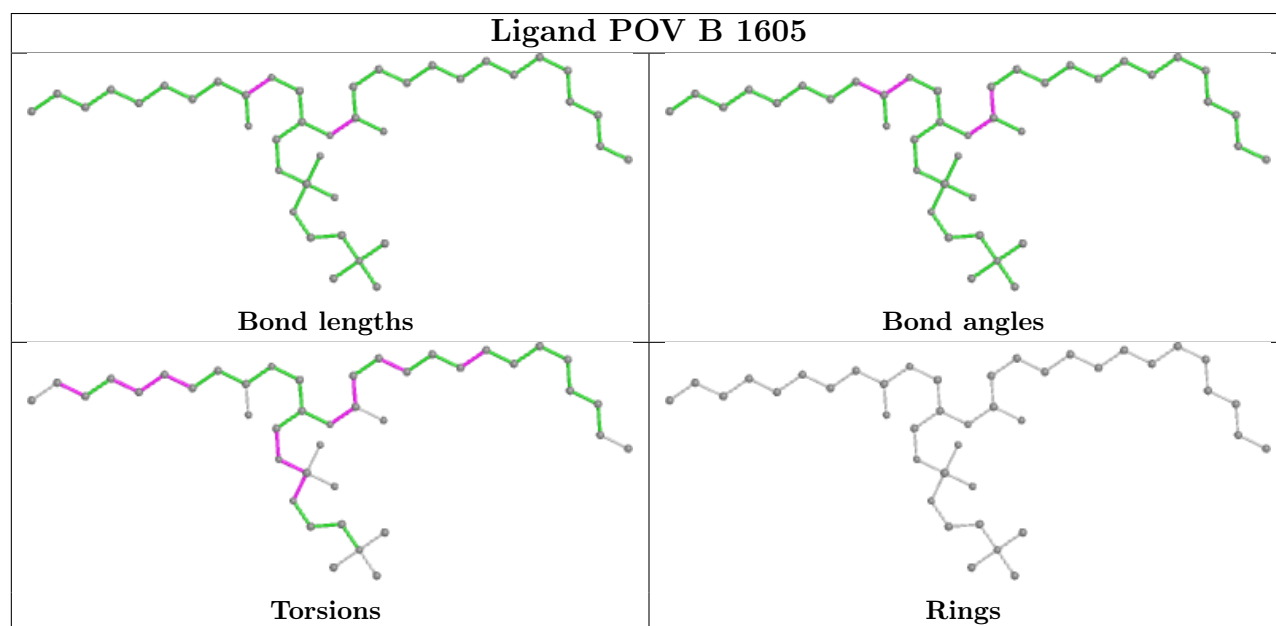
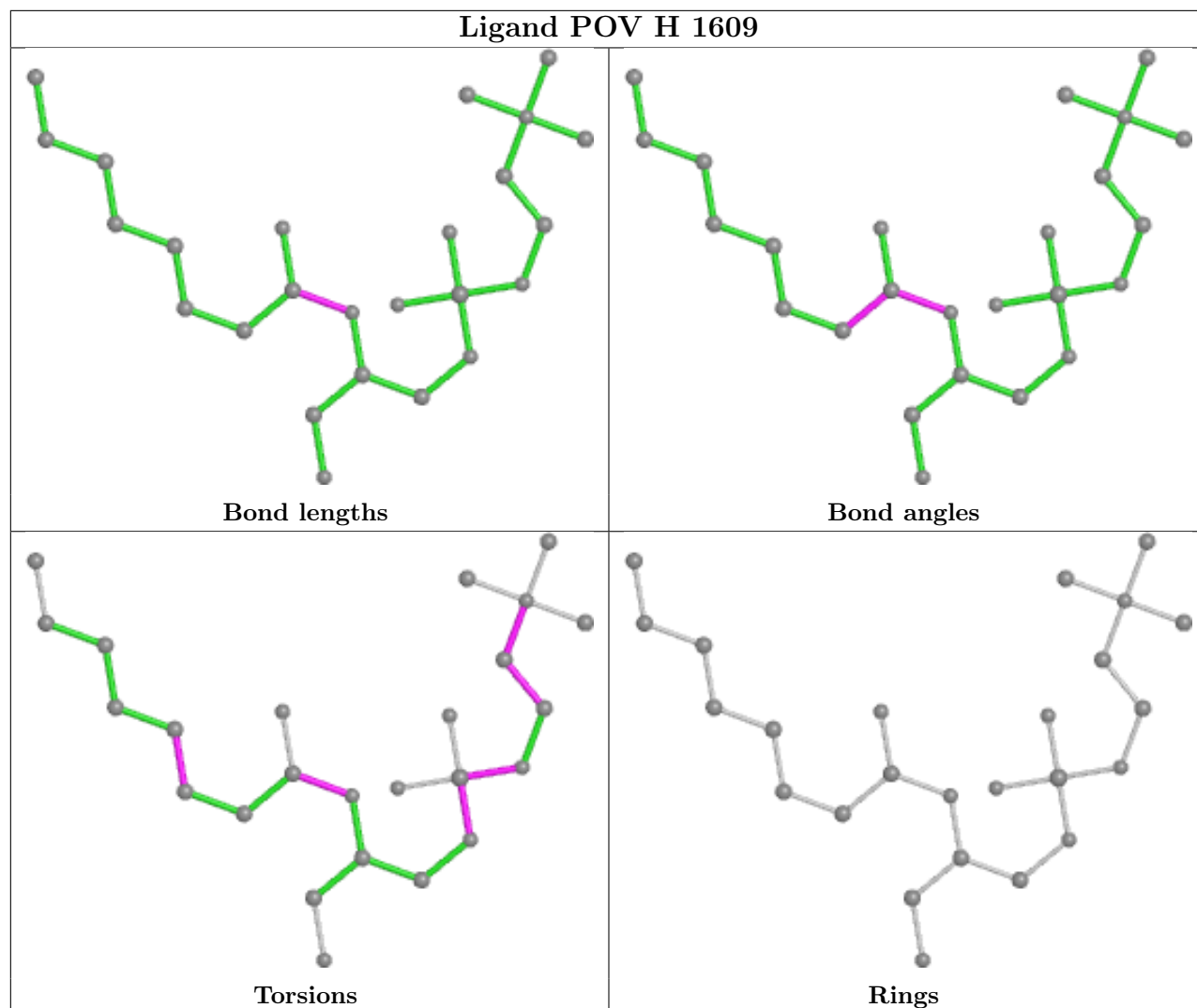


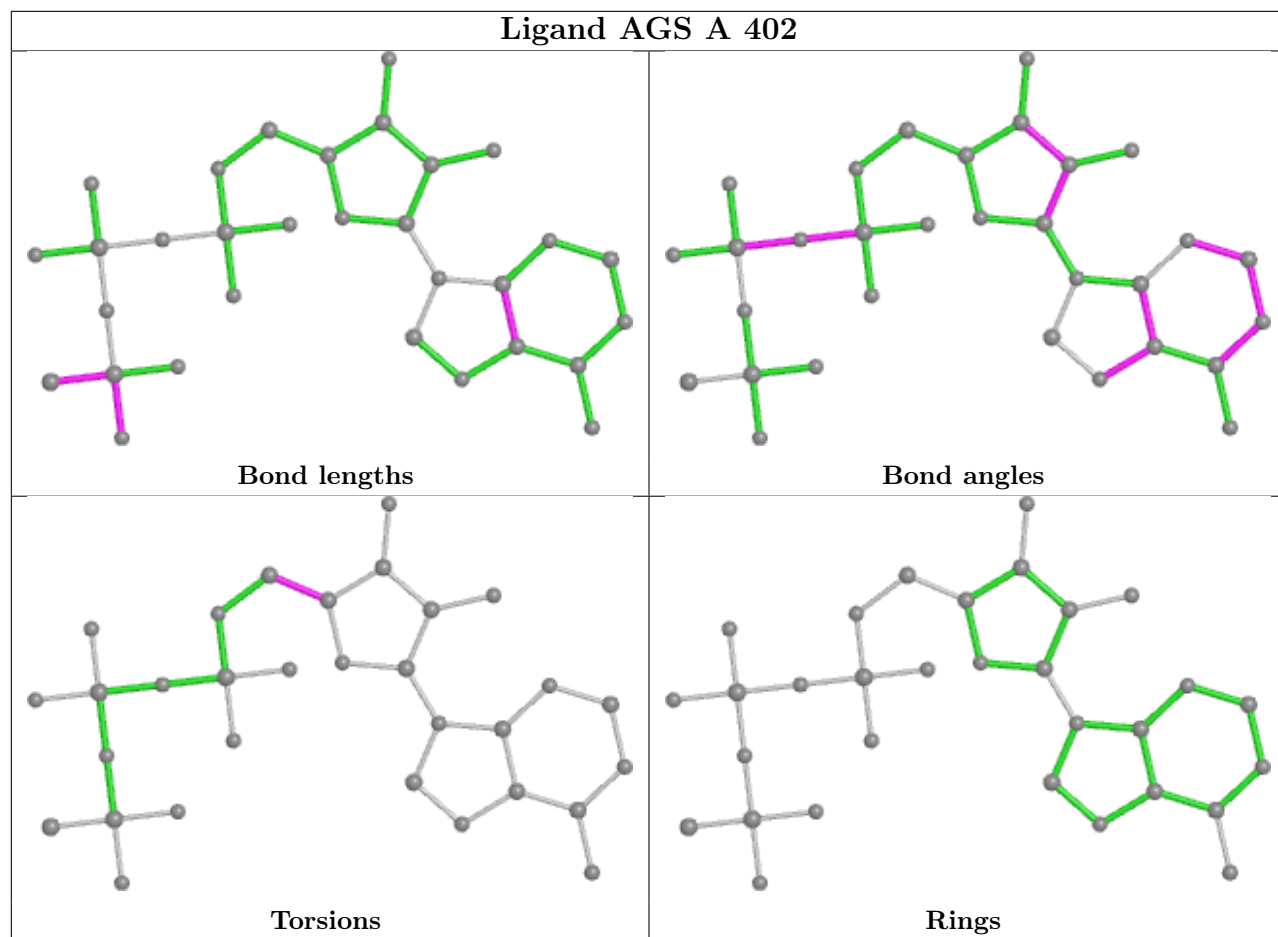


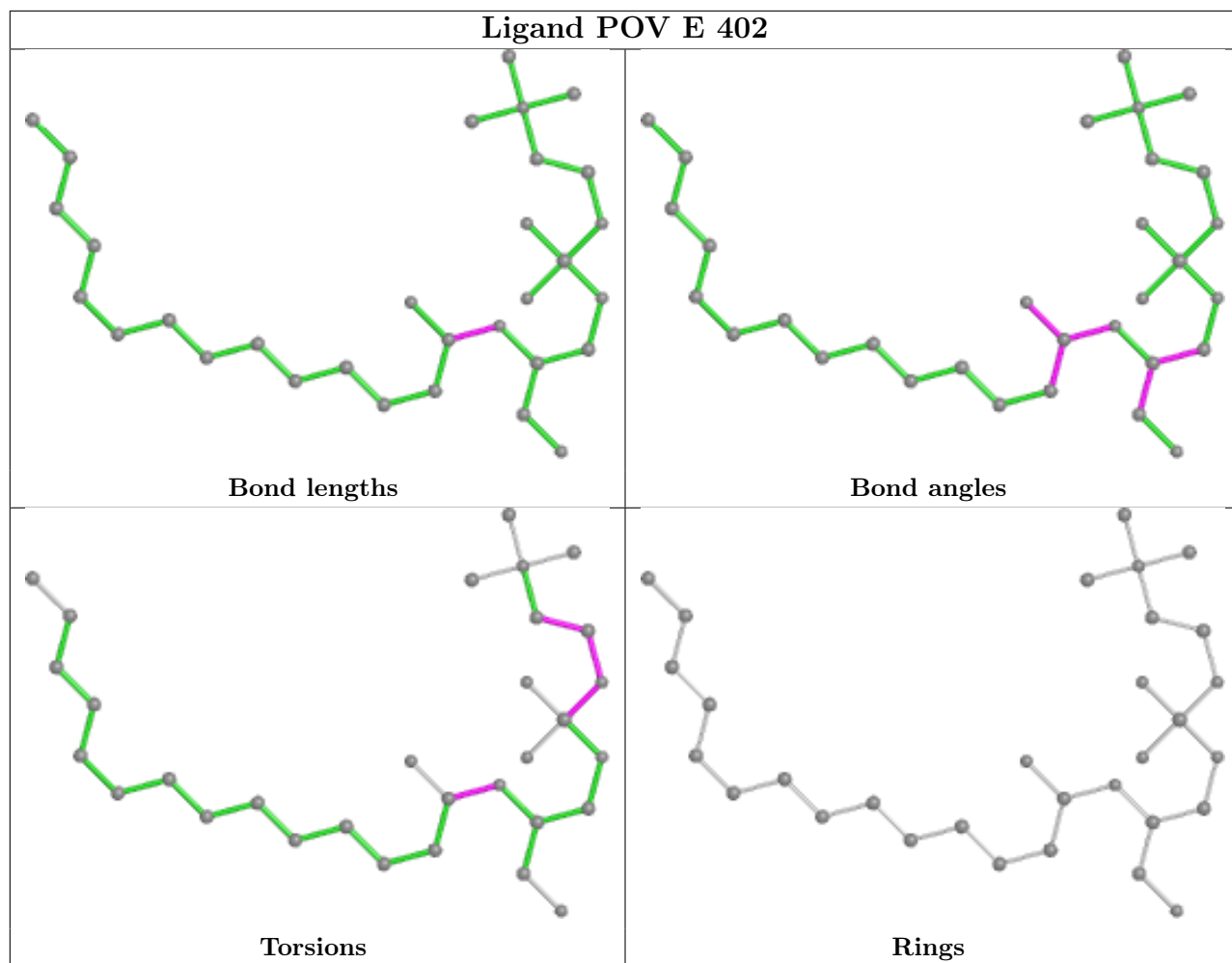


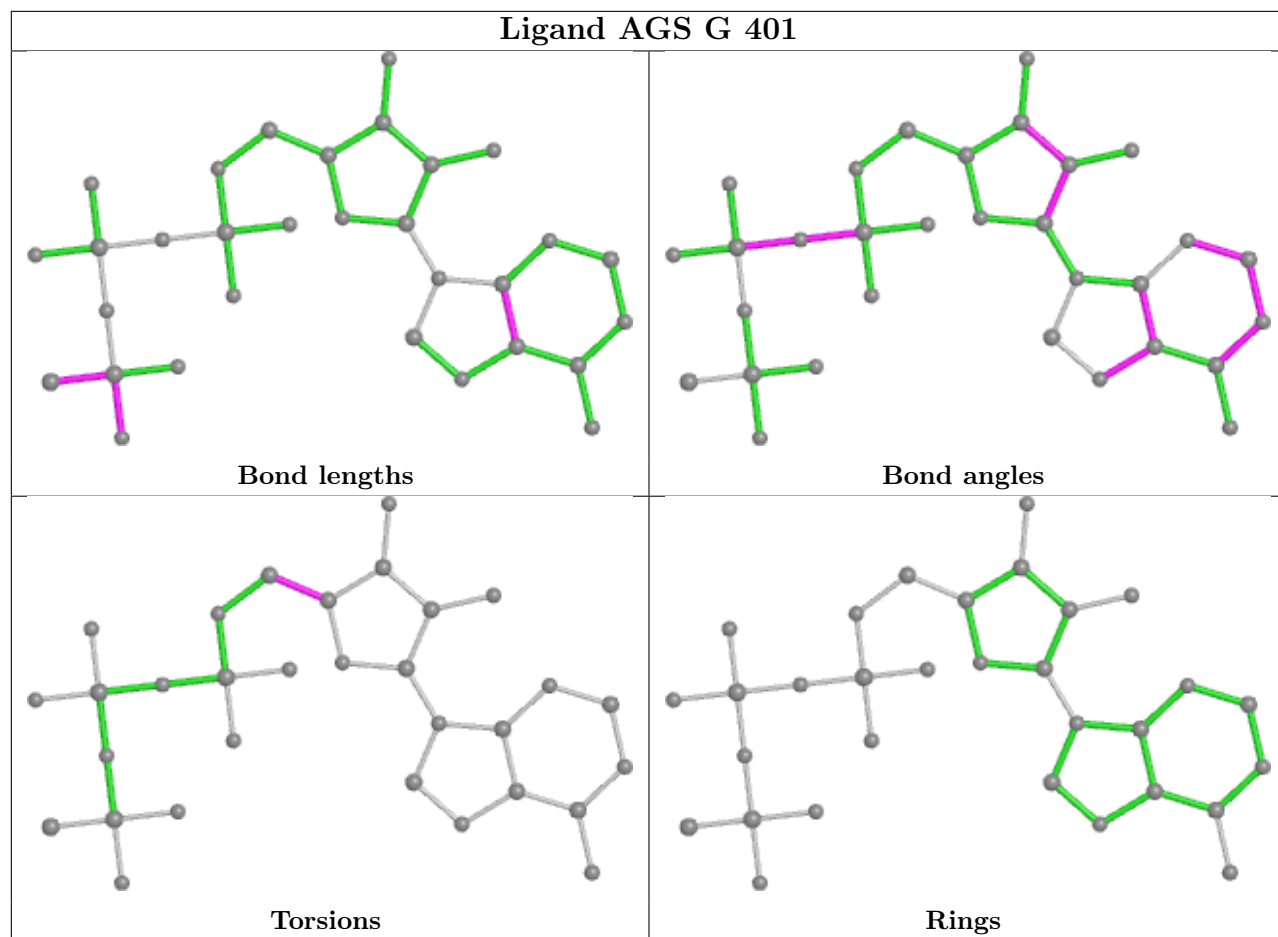




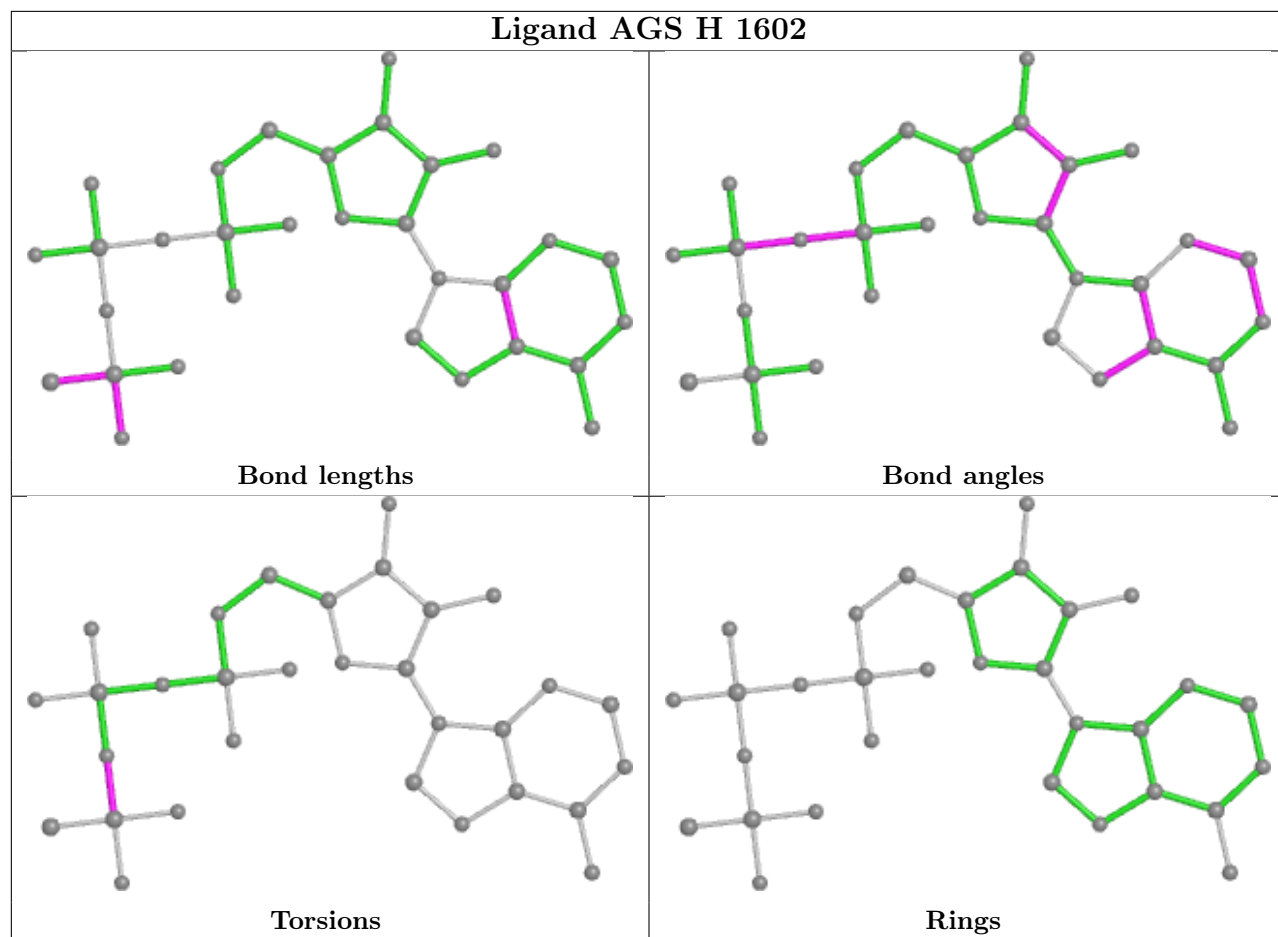


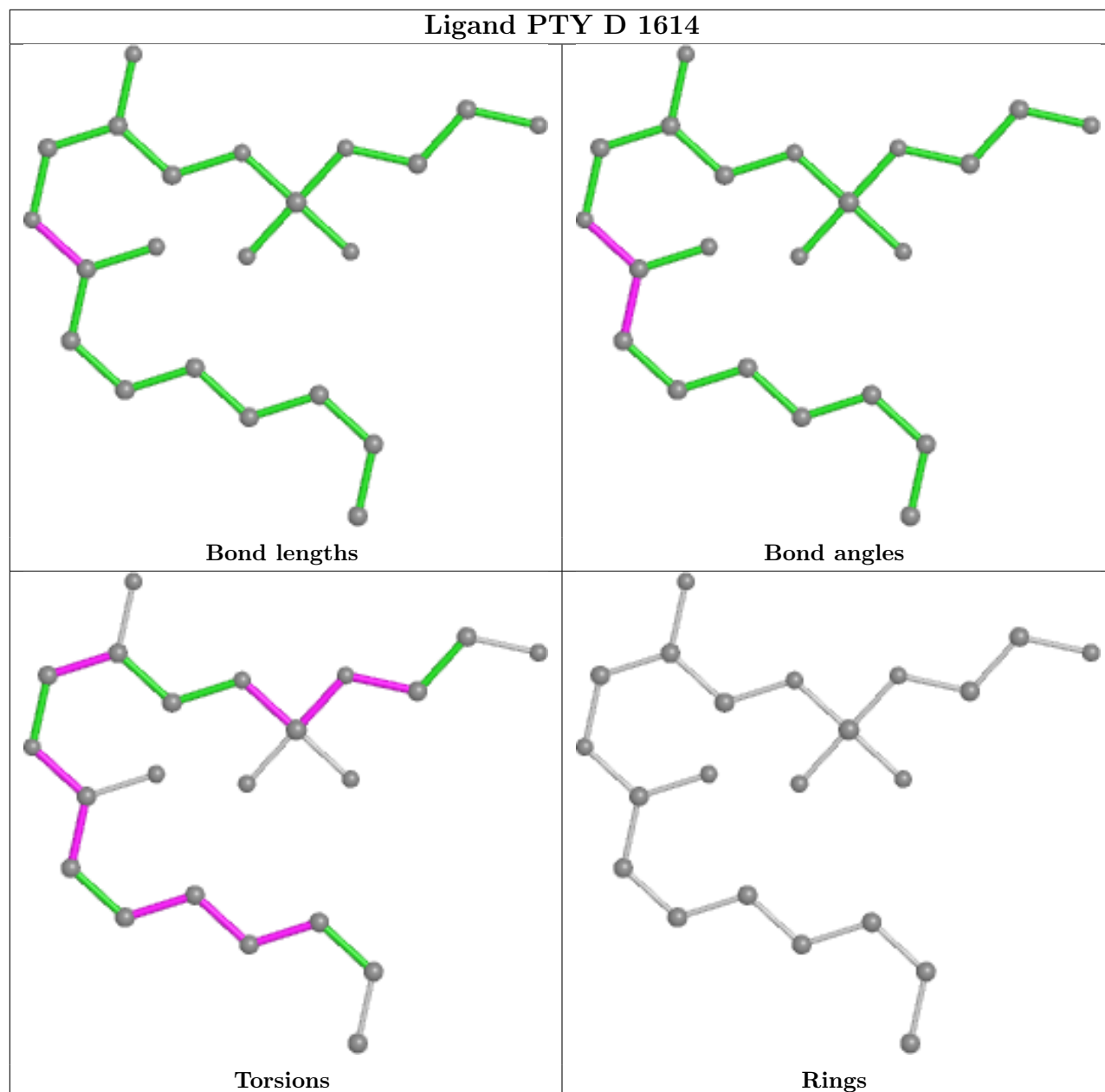


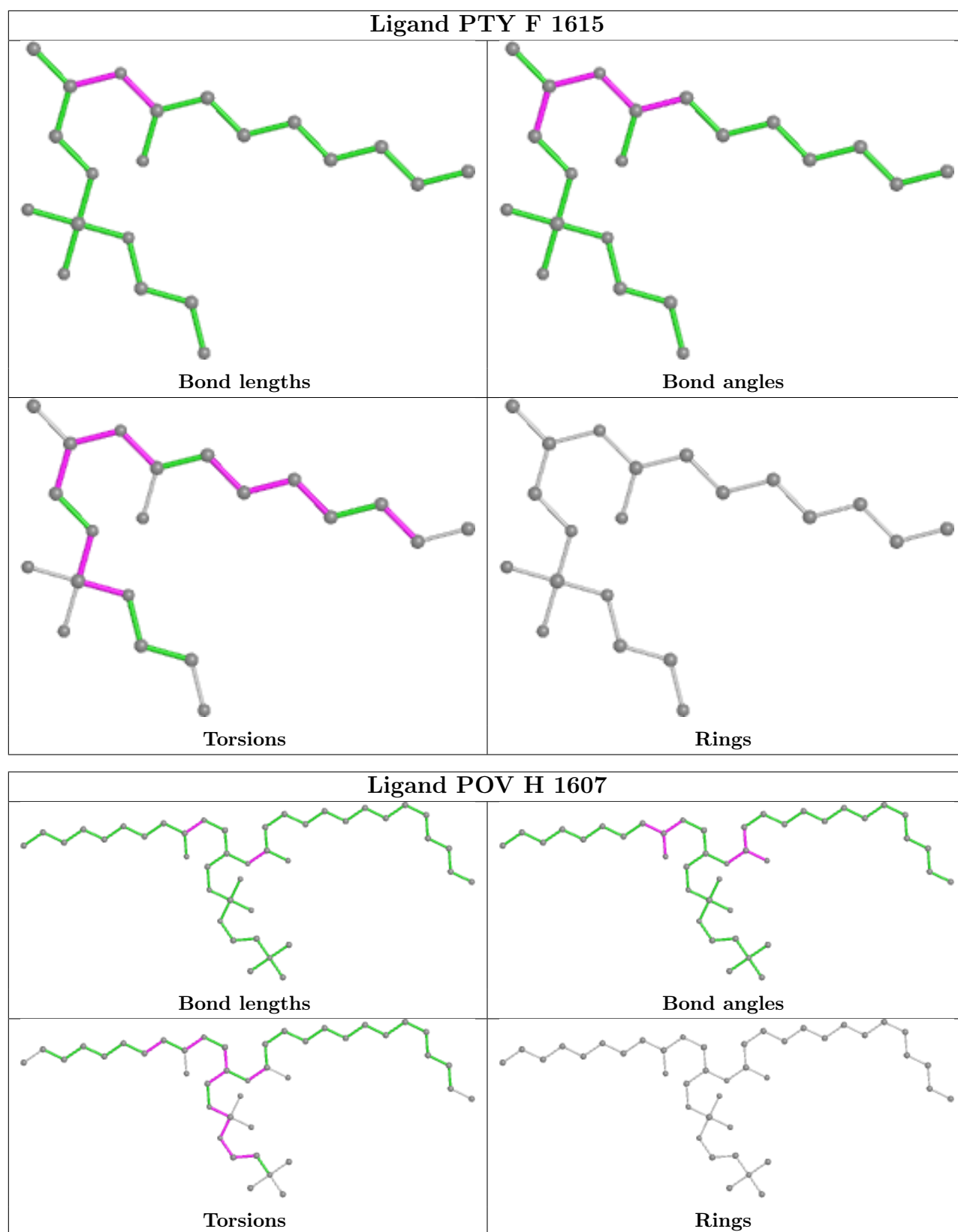


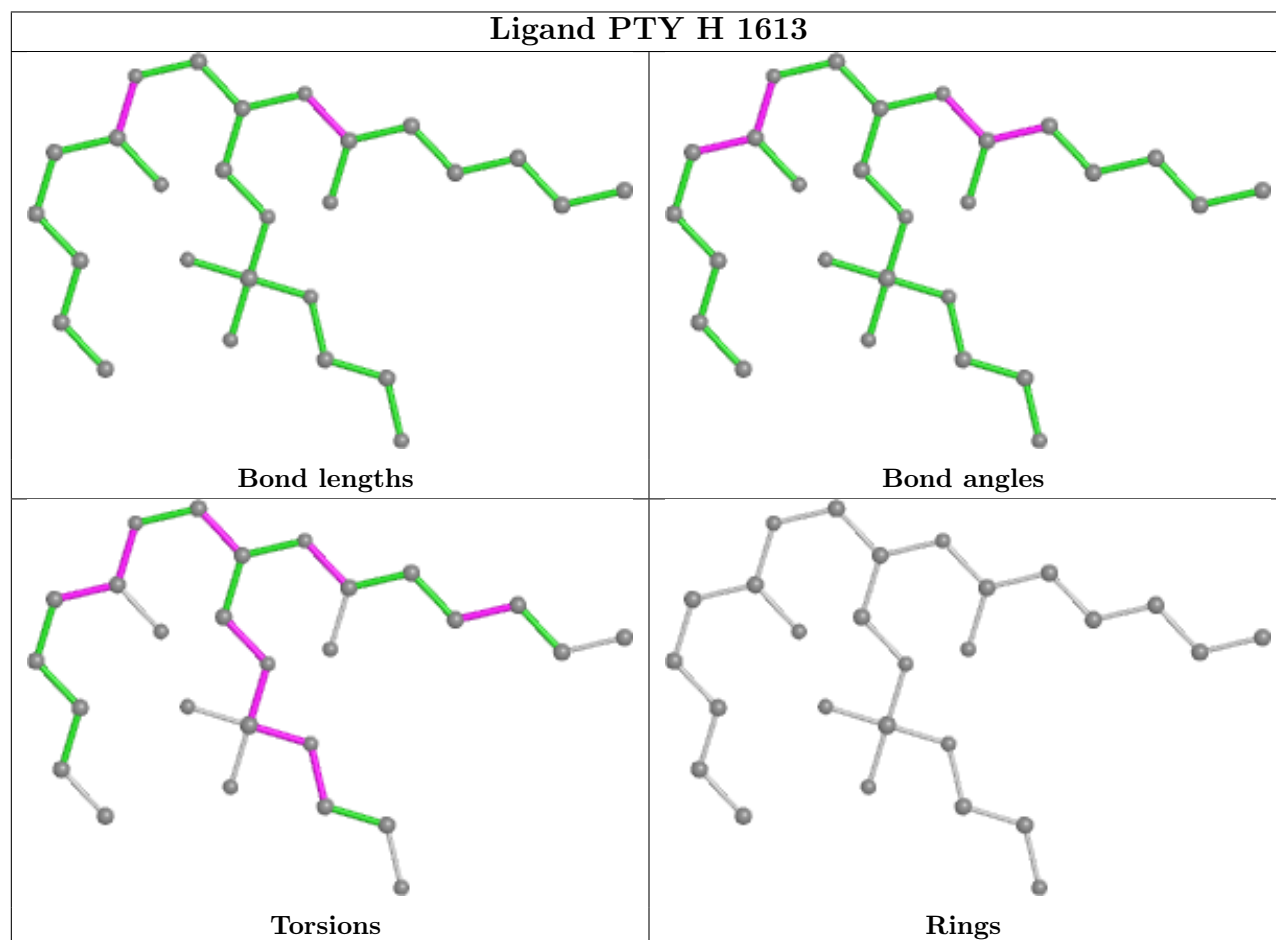
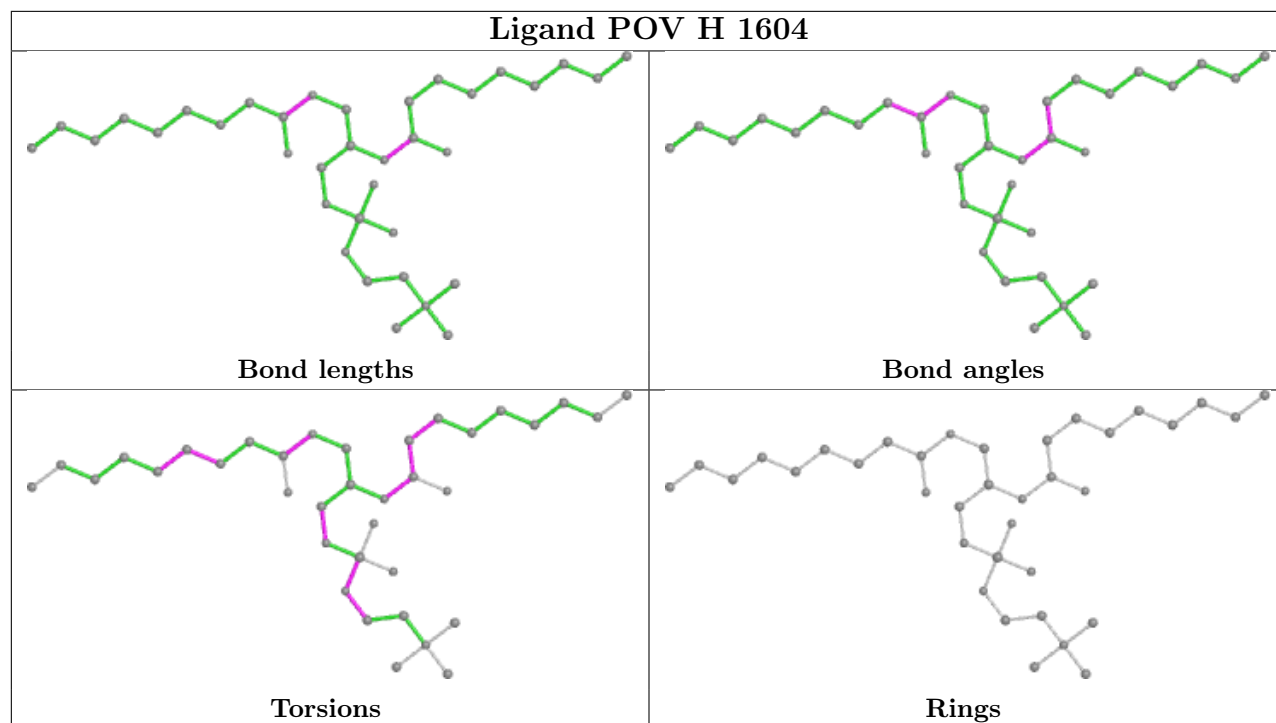


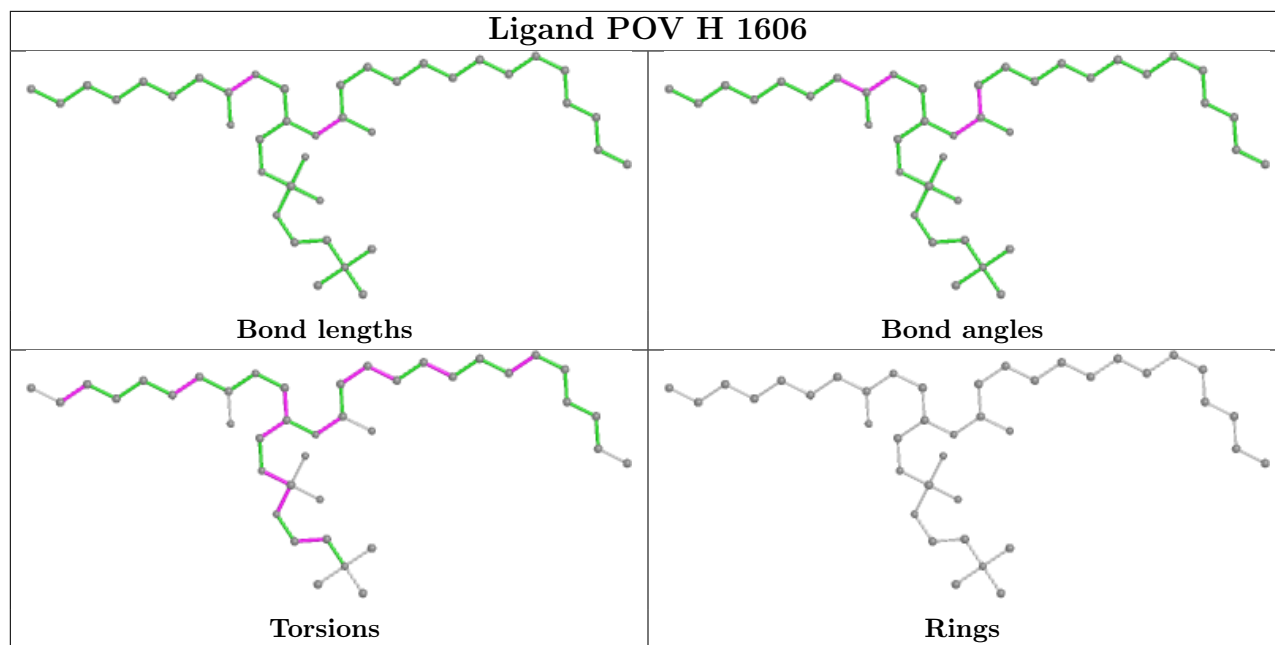


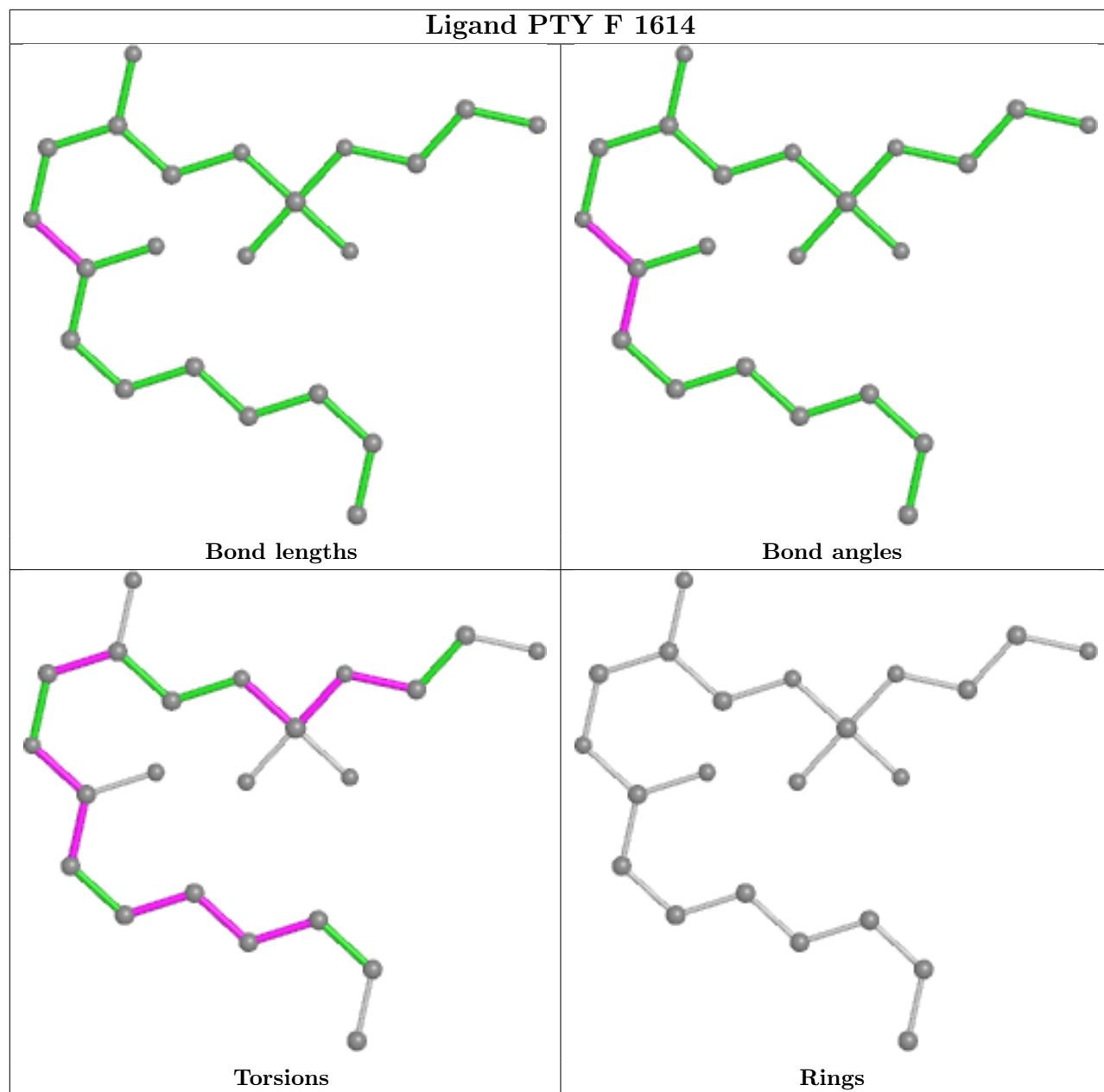


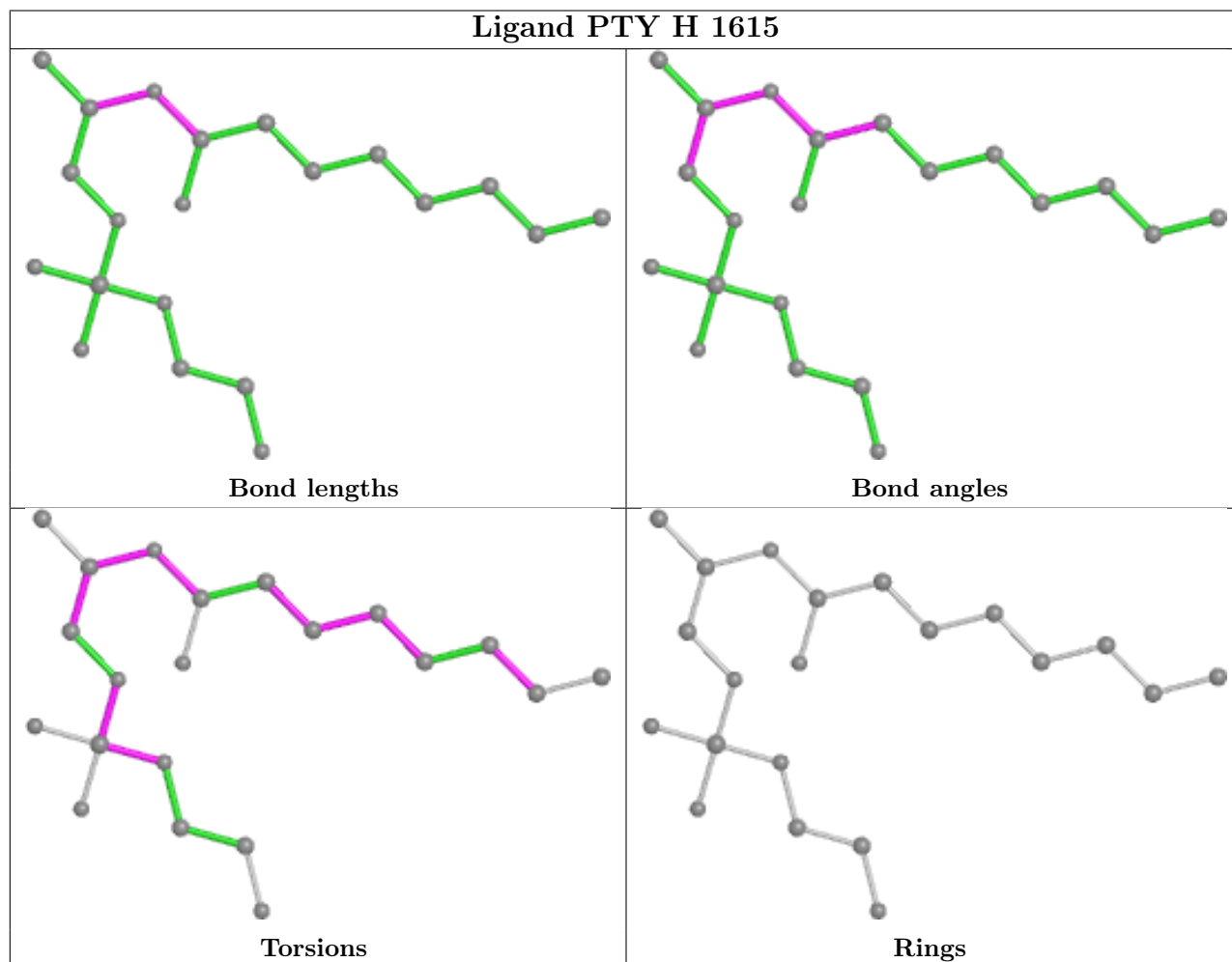
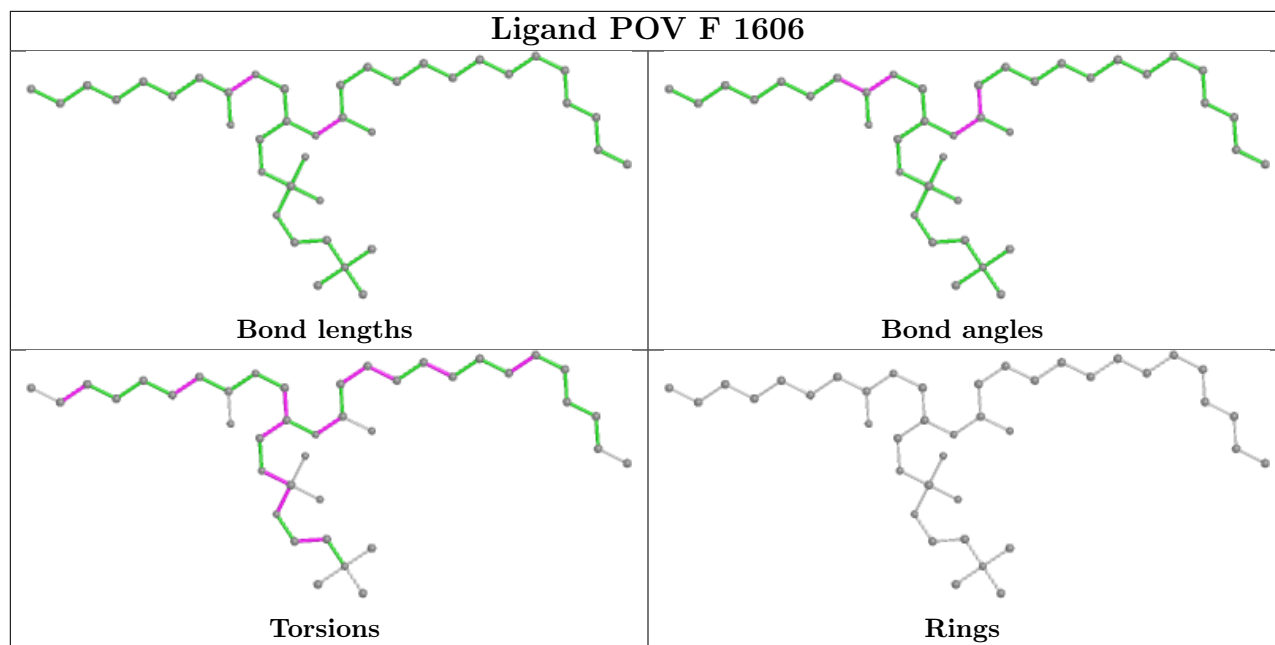


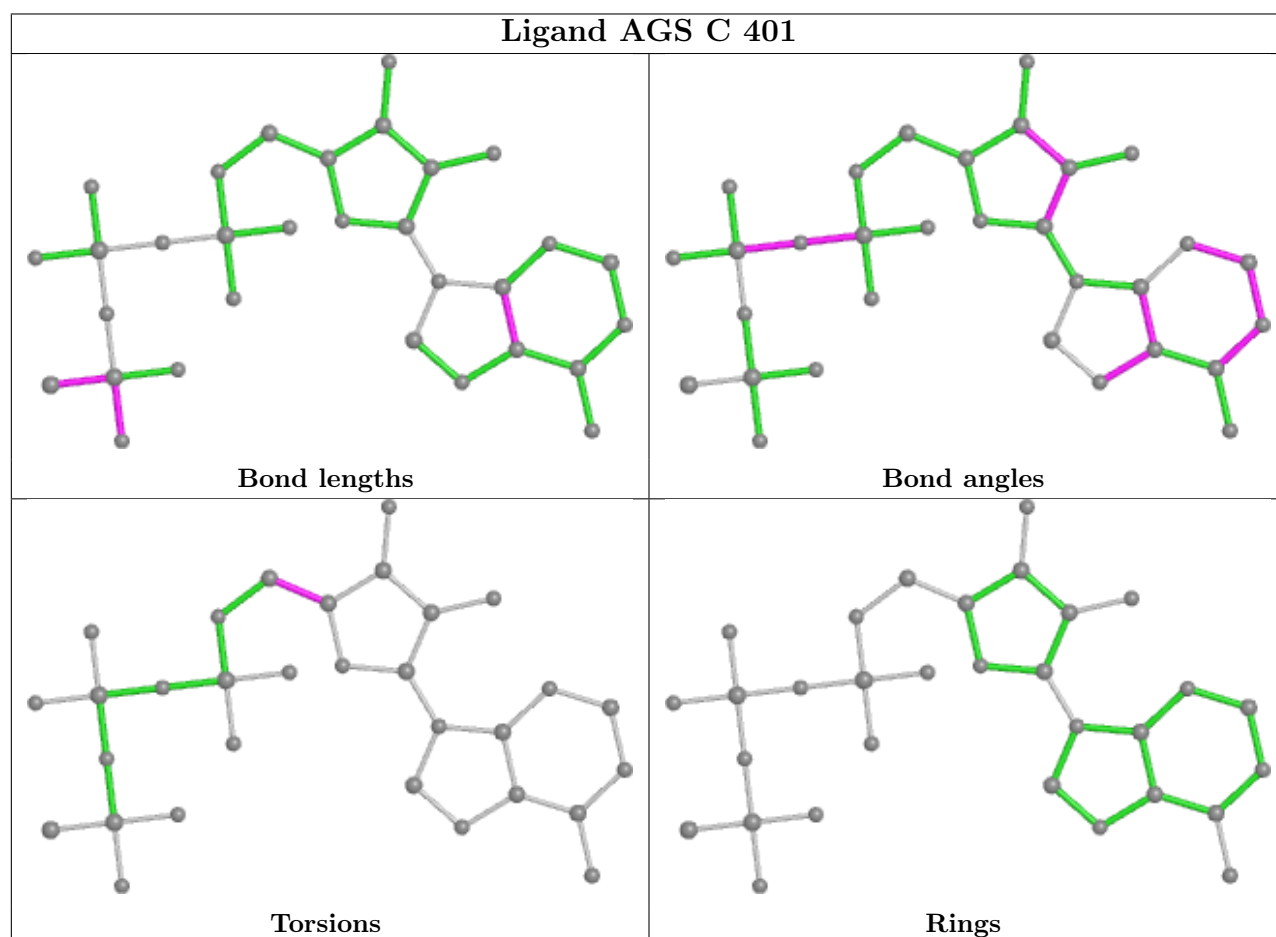
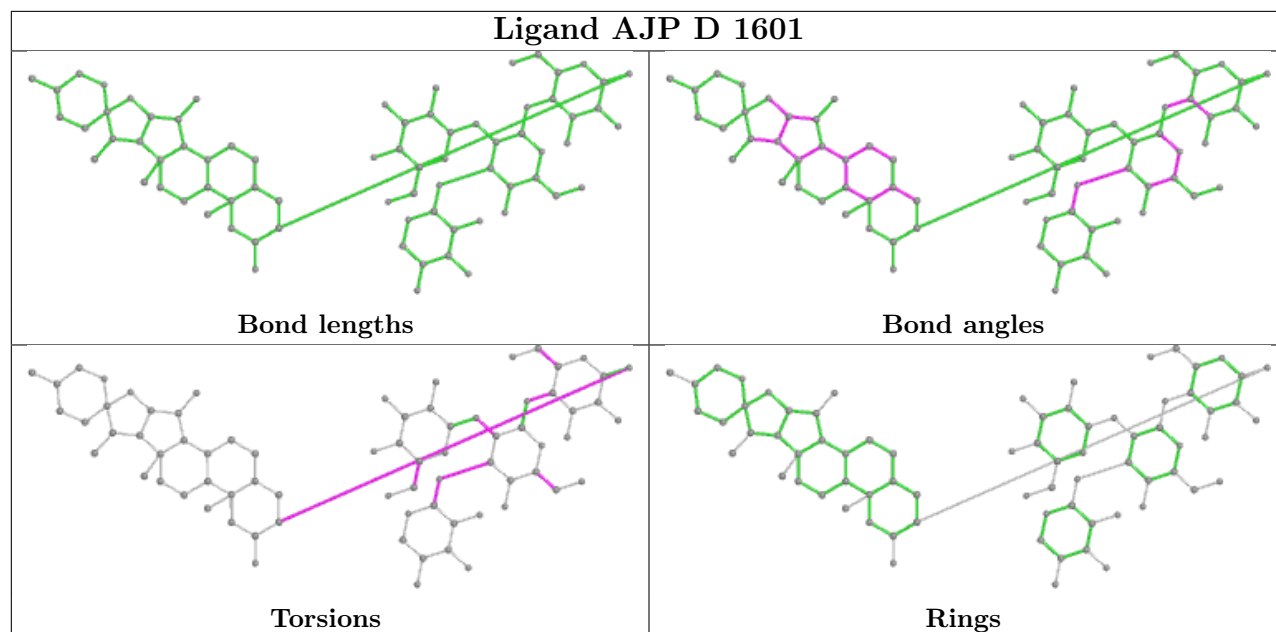




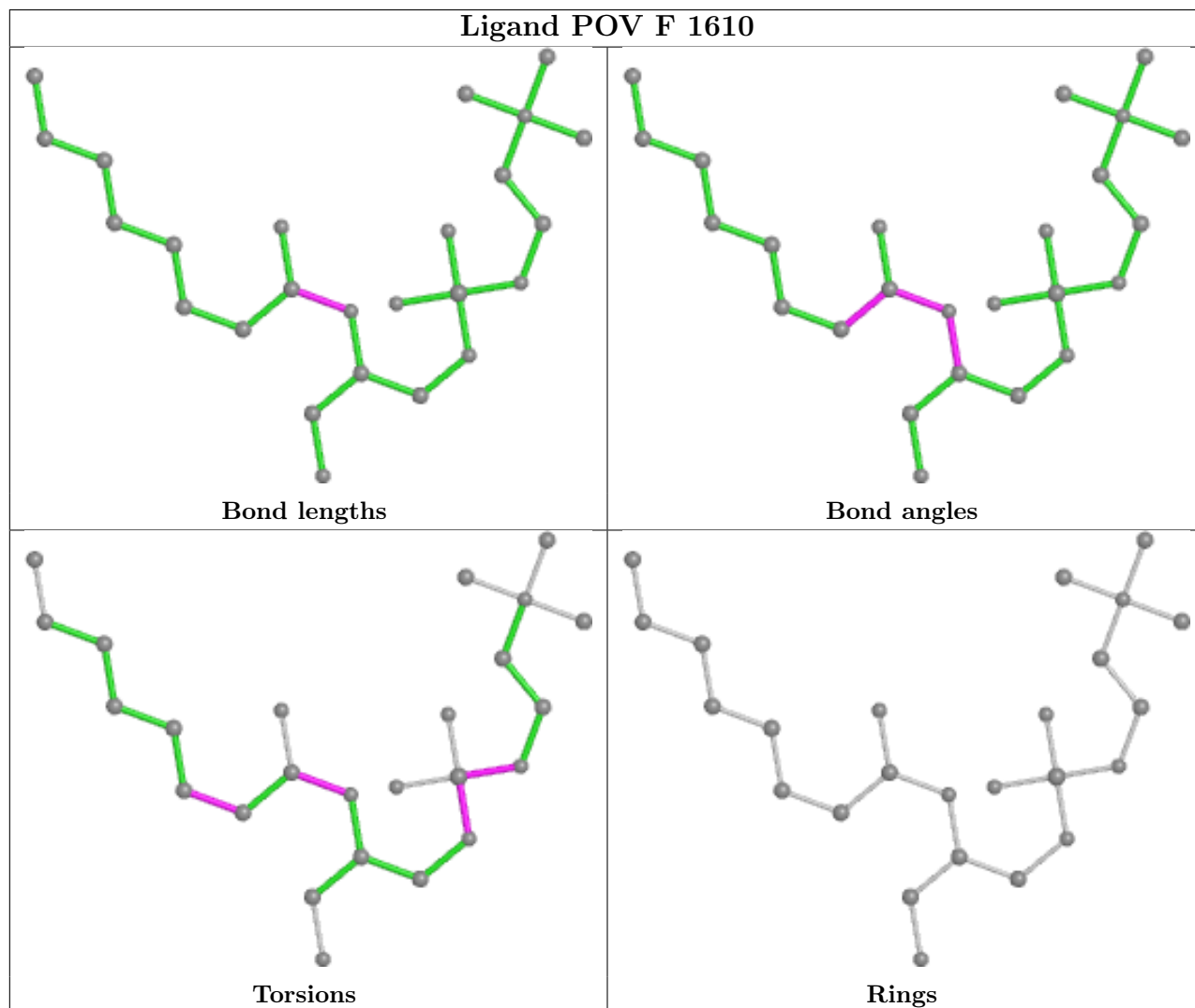
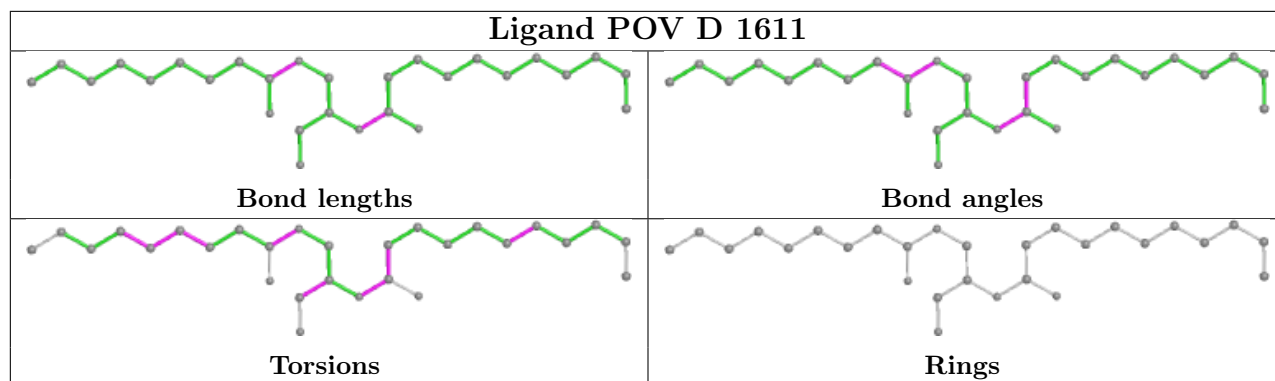


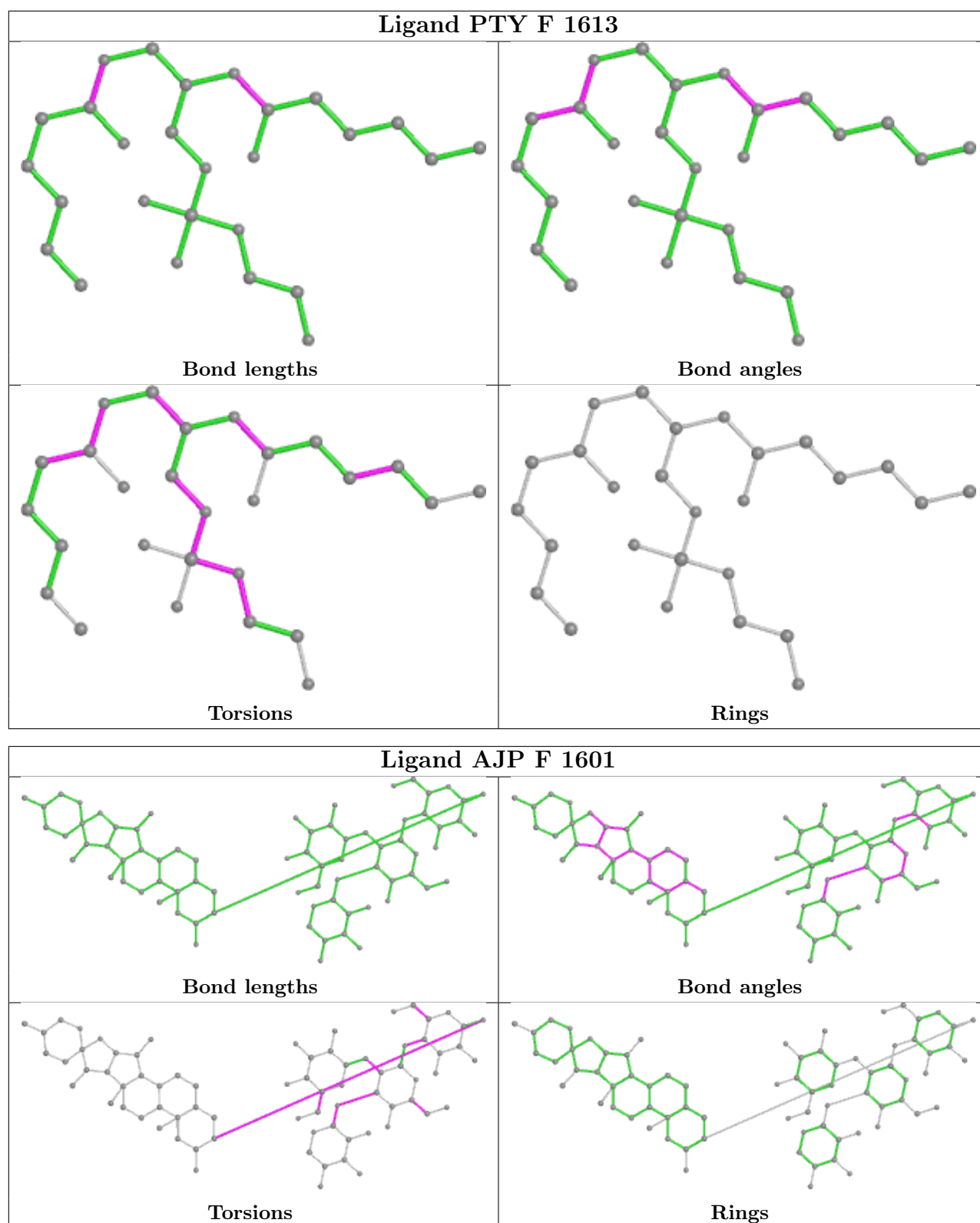












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

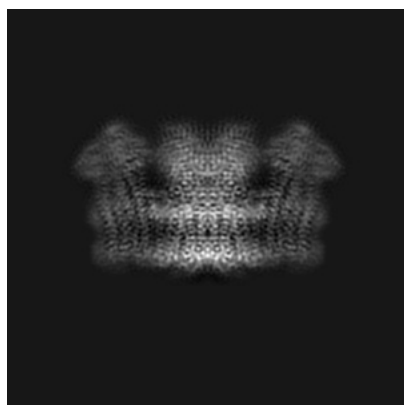
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9787. These allow visual inspection of the internal detail of the map and identification of artifacts.

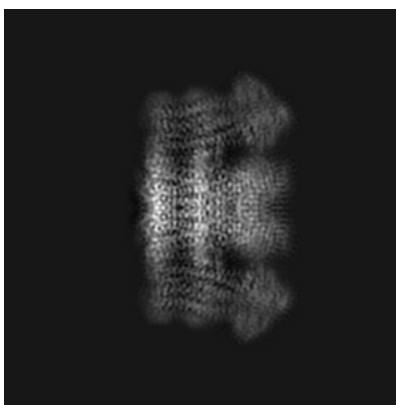
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

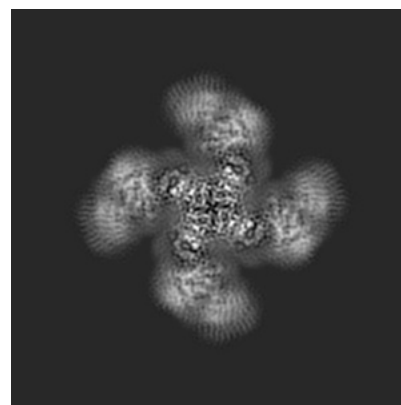
#### 6.1.1 Primary map



X



Y

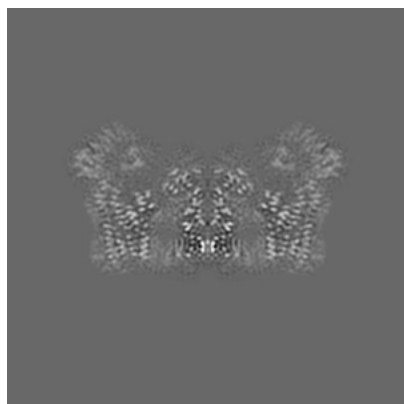


Z

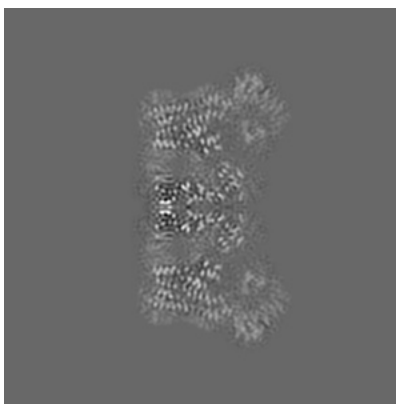
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

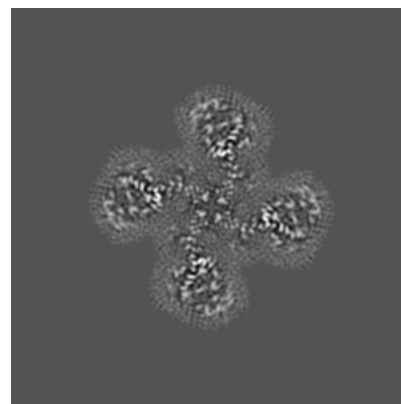
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

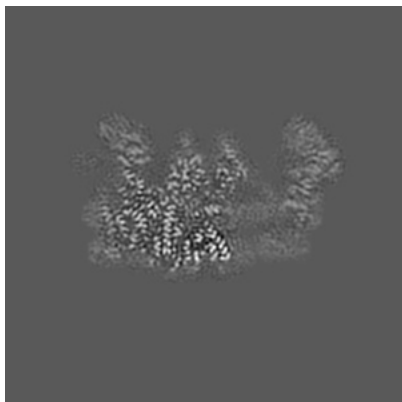


Z Index: 128

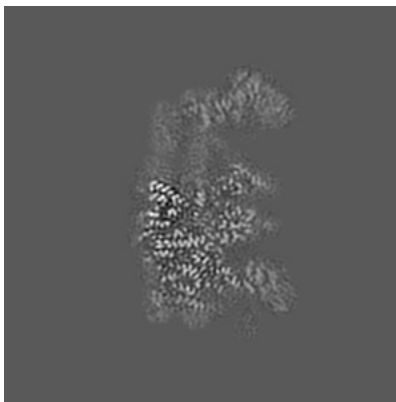
The images above show central slices of the map in three orthogonal directions.

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

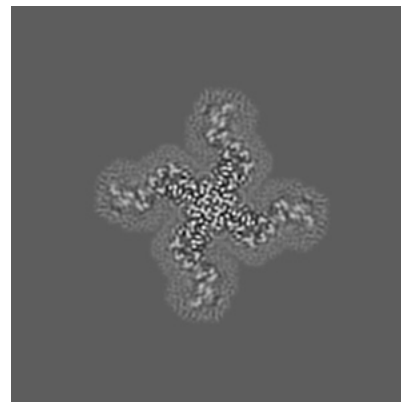
### 6.3.1 Primary map



X Index: 117



Y Index: 139

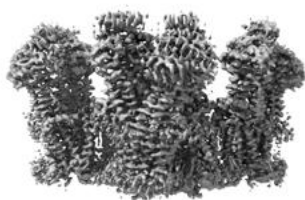


Z Index: 98

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

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

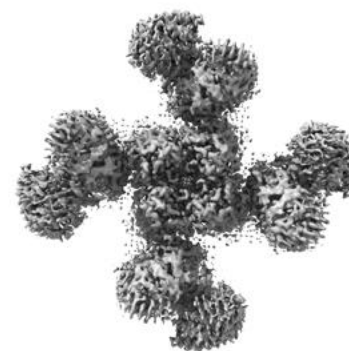
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

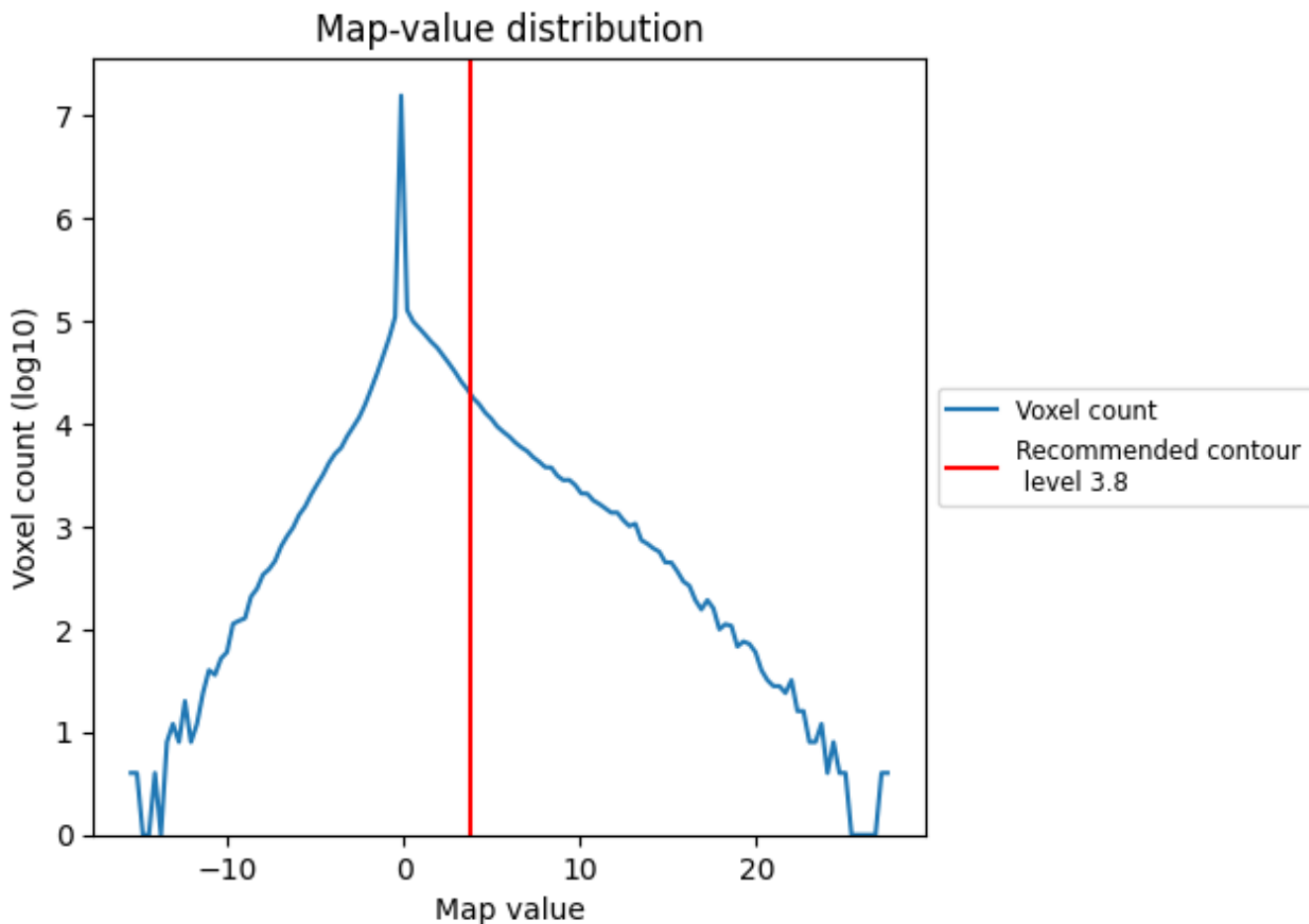
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

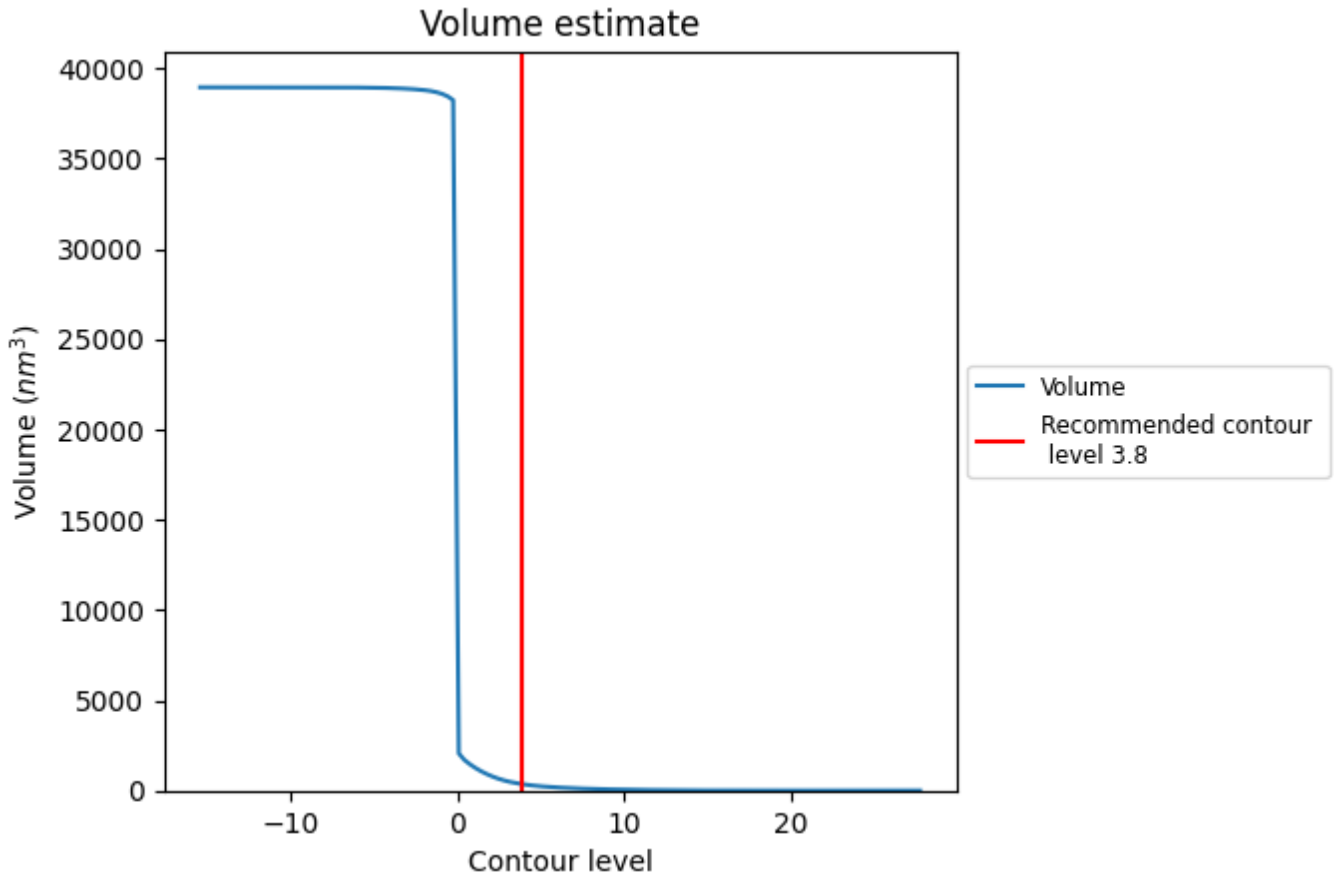
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

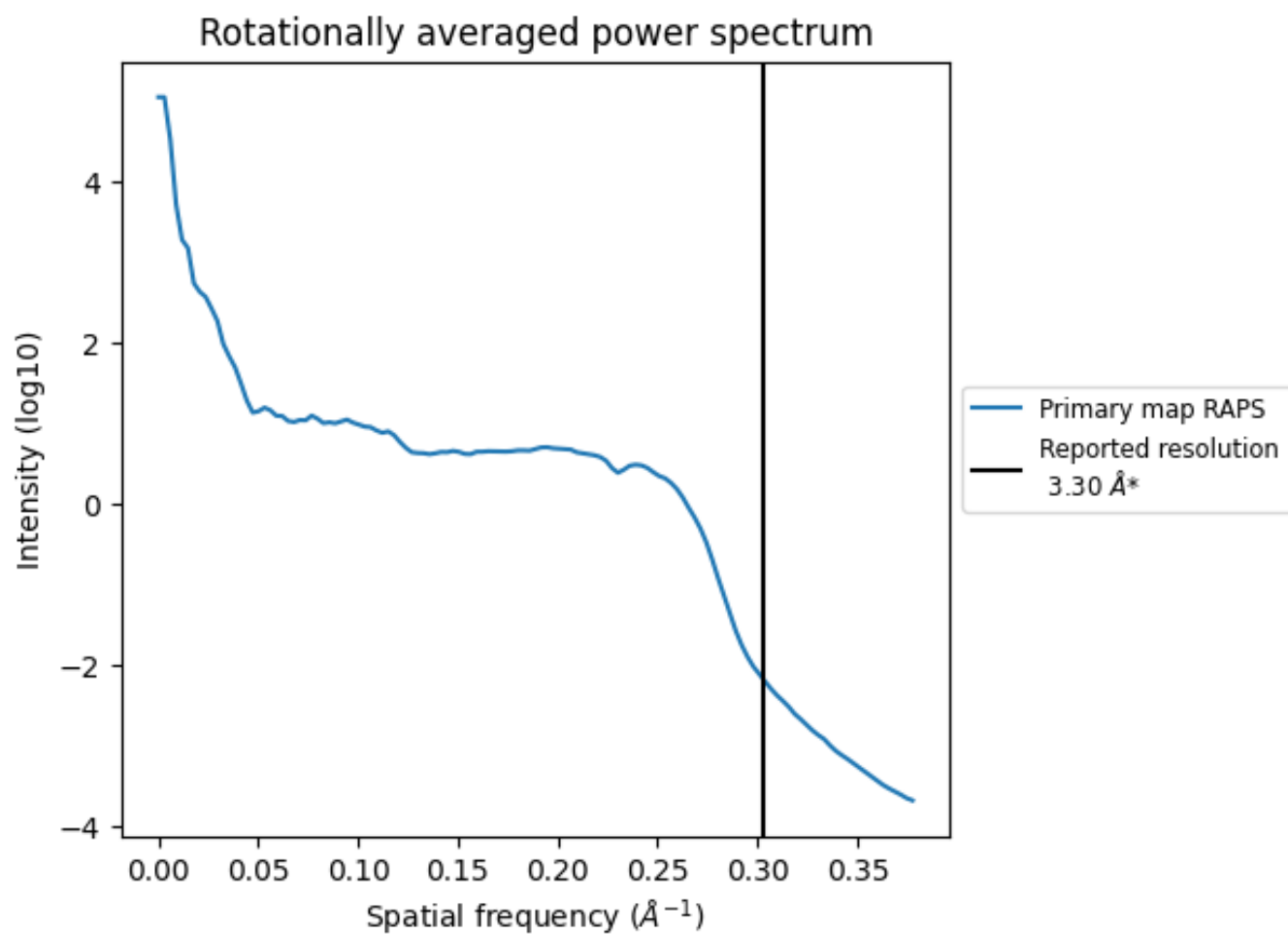


The volume at the recommended contour level is 365 nm<sup>3</sup>; this corresponds to an approximate mass of 330 kDa.

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 0.303 Å<sup>-1</sup>

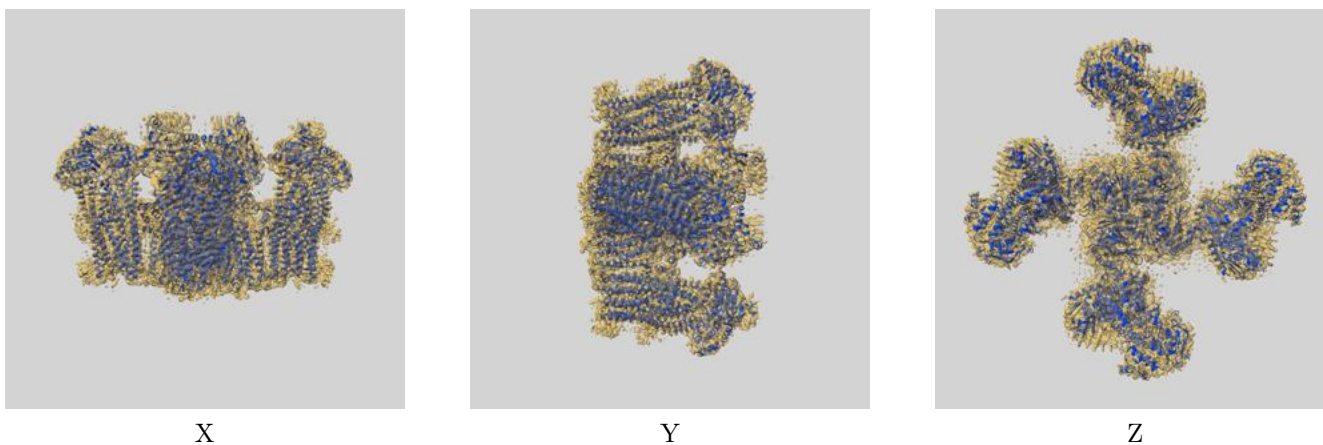
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

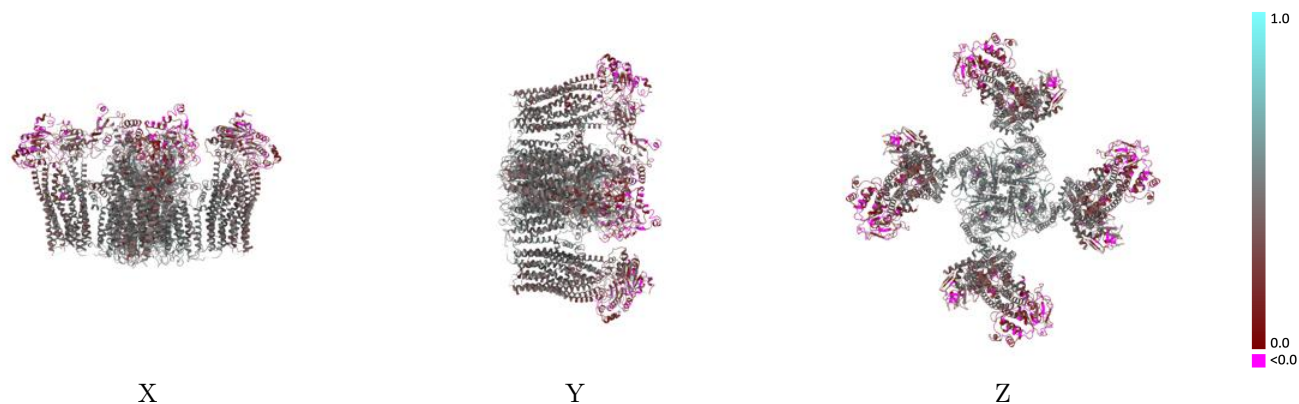
This section contains information regarding the fit between EMDB map EMD-9787 and PDB model 6JB1. Per-residue inclusion information can be found in section 3 on page 11.

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



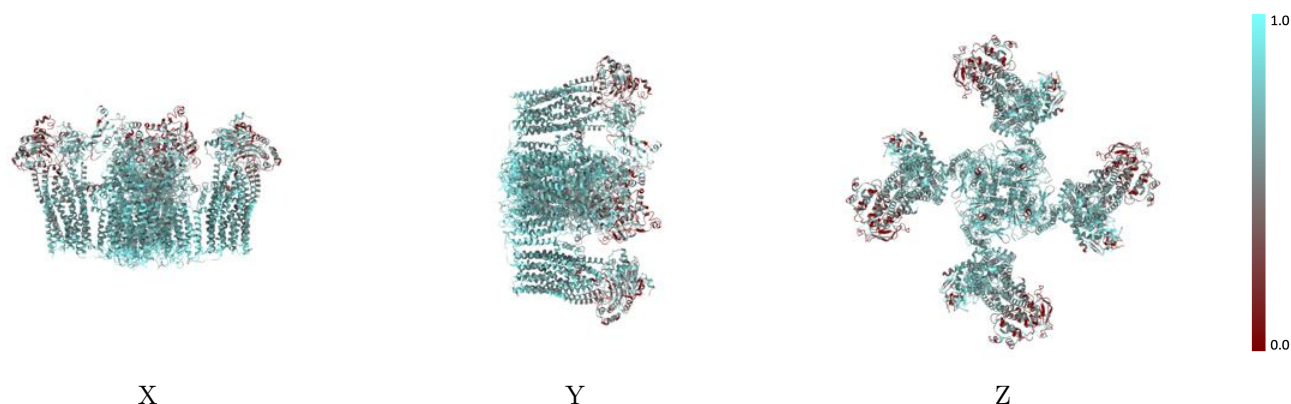
The images above show the 3D surface view of the map at the recommended contour level 3.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



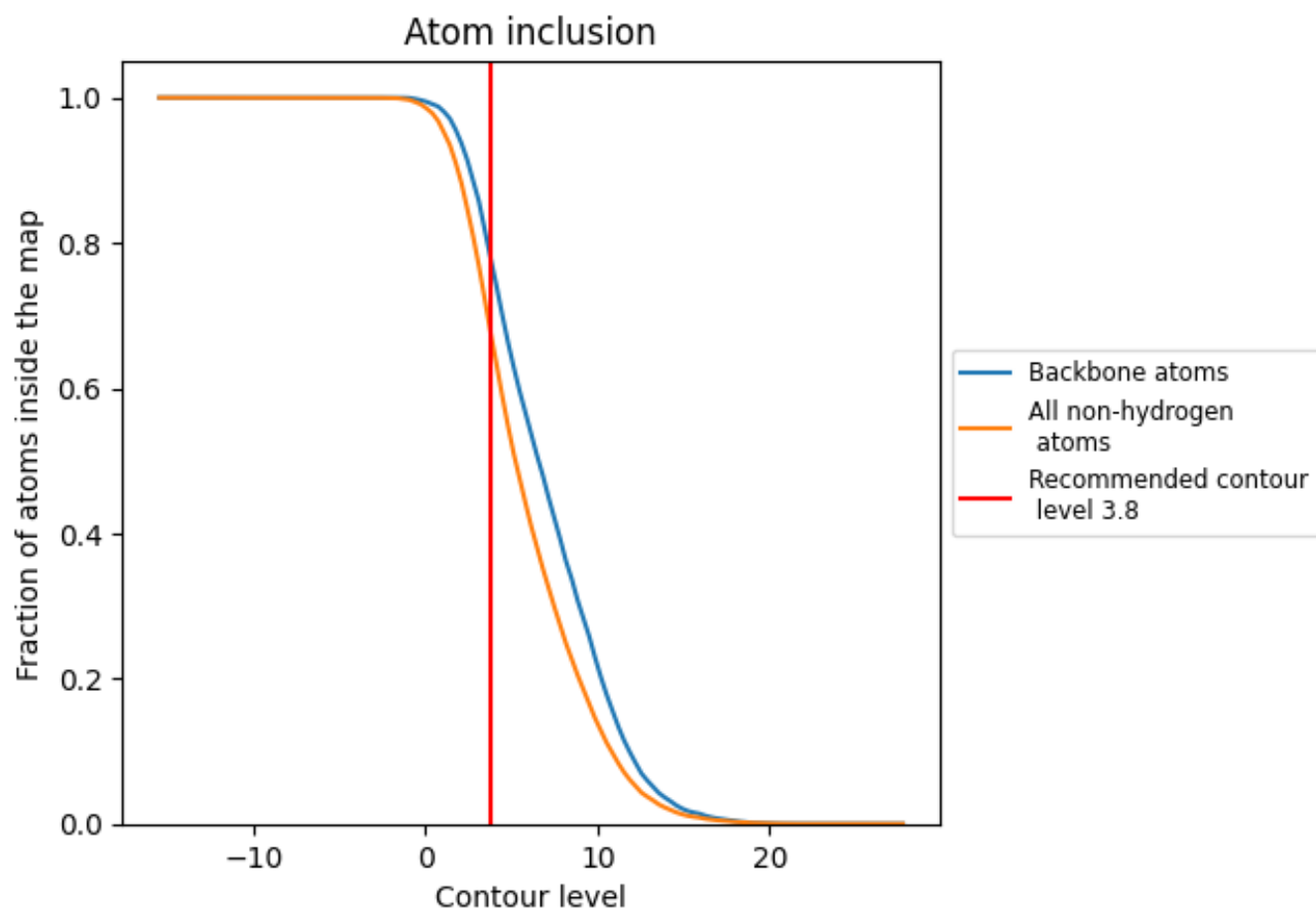
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.8).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6745	 0.4060
A	 0.7532	 0.5010
B	 0.6548	 0.3820
C	 0.7532	 0.5000
D	 0.6548	 0.3820
E	 0.7532	 0.5010
F	 0.6548	 0.3830
G	 0.7532	 0.5000
H	 0.6548	 0.3820

