



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 07:18 PM UTC

PDB ID : 6JB1 / pdb_00006jb1
EMDB ID : EMD-9787
Title : Structure of pancreatic ATP-sensitive potassium channel bound with repaglinide and ATPgammaS at 3.3Å resolution
Authors : Chen, L.; Ding, D.; Wang, M.; Wu, J.-X.; Kang, Y.
Deposited on : 2019-01-25
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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>.

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

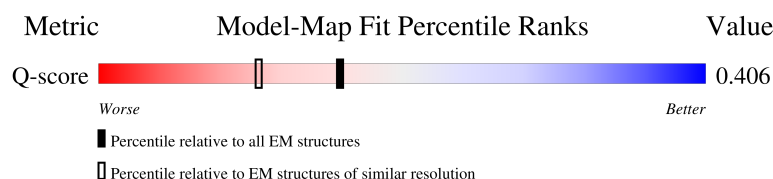
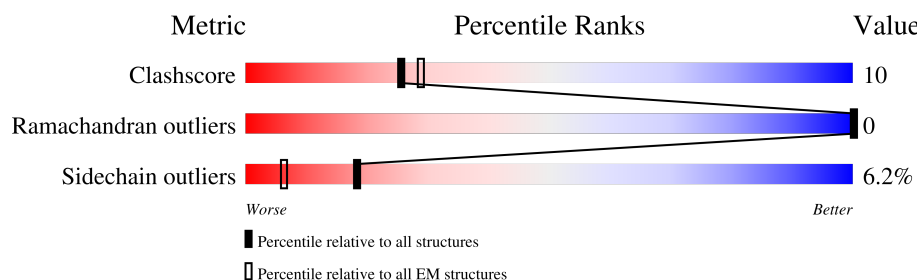
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 ≥ 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	 54% 27% 16%
1	C	390	 54% 27% 16%
1	E	390	 53% 28% 16%
1	G	390	 54% 27% 16%

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Mol	Chain	Length	Quality of chain
2	B	1582	
2	D	1582	
2	F	1582	
2	H	1582	

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	AJP	B	1601	X	-	-	-
5	AJP	D	1601	X	-	-	-
5	AJP	F	1601	X	-	-	-
5	AJP	H	1601	X	-	-	-

2 Entry composition

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
1	A	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		
1	C	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		
1	E	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		
1	G	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		

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

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

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	22	1	7	1	
3	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	B	1	Total	C	N	O	P	0
			25	16	1	7	1	
3	B	1	Total	C	N	O	P	0
			25	16	1	7	1	
3	B	1	Total	C	O			0
			28	23	5			
3	C	1	Total	C	N	O	P	0
			31	22	1	7	1	
3	D	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	D	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	D	1	Total	C	N	O	P	0
			41	31	1	8	1	

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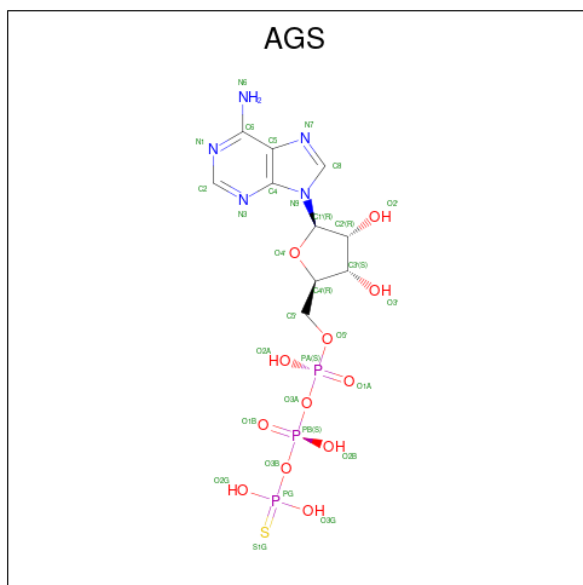
Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	D	1	Total	C	N	O	P	0
			25	16	1	7	1	
3	D	1	Total	C	N	O	P	0
			25	16	1	7	1	
3	D	1	Total	C	O			0
			28	23	5			
3	E	1	Total	C	N	O	P	0
			31	22	1	7	1	
3	F	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	F	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	F	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	F	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	F	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	F	1	Total	C	N	O	P	0
			25	16	1	7	1	
3	F	1	Total	C	N	O	P	0
			25	16	1	7	1	
3	F	1	Total	C	O			0
			28	23	5			
3	G	1	Total	C	N	O	P	0
			31	22	1	7	1	
3	H	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	H	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	H	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	H	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	H	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	H	1	Total	C	N	O	P	0
			25	16	1	7	1	
3	H	1	Total	C	N	O	P	0
			25	16	1	7	1	

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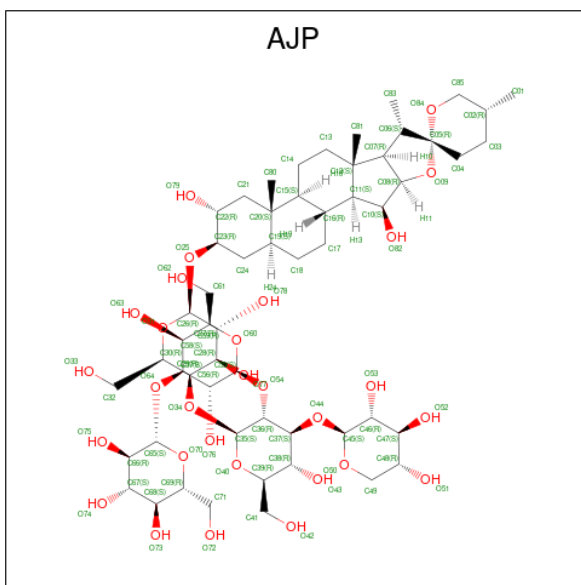
Mol	Chain	Residues	Atoms			AltConf
3	H	1	Total	C	O	0
			28	23	5	

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



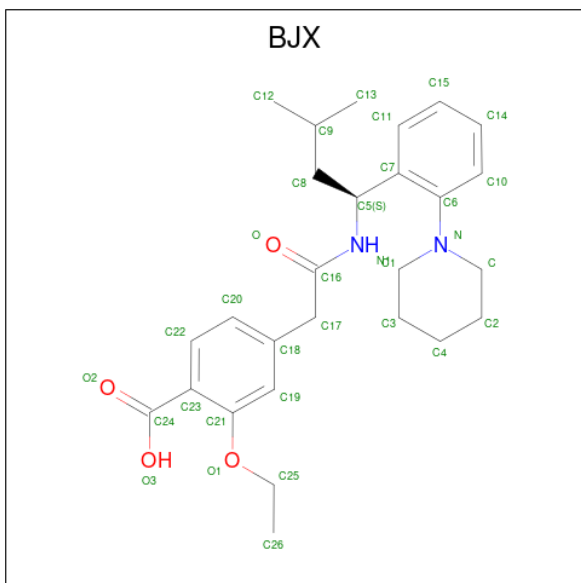
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	G	1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

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



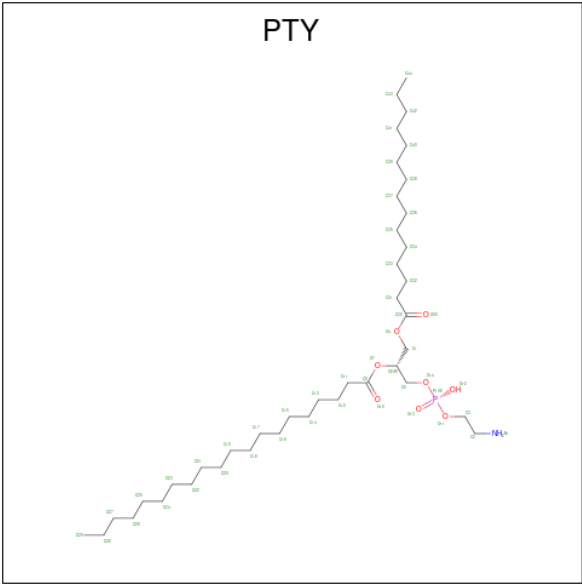
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			74	50	24	
5	D	1	Total	C	O	0
			74	50	24	
5	F	1	Total	C	O	0
			74	50	24	
5	H	1	Total	C	O	0
			74	50	24	

- Molecule 6 is Repaglinide (CCD ID: BJX) (formula: $C_{27}H_{36}N_2O_4$).



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

- Molecule 7 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	B	1	Total	C	N	O	P	0
			27	17	1	8	1	
7	B	1	Total	C	N	O	P	0
			22	13	1	7	1	
7	B	1	Total	C	N	O	P	0
			21	13	1	6	1	
7	D	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	D	1	Total	C	N	O	P	0
			27	17	1	8	1	
7	D	1	Total	C	N	O	P	0
			22	13	1	7	1	
7	D	1	Total	C	N	O	P	0
			21	13	1	6	1	

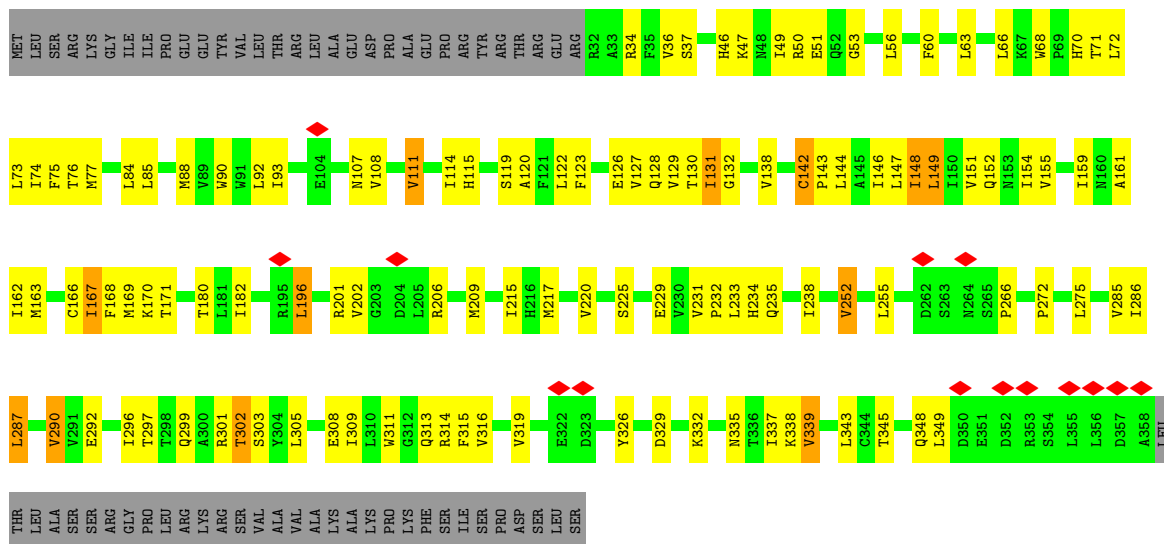
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Mol	Chain	Residues	Atoms					AltConf
7	F	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	F	1	Total	C	N	O	P	0
			27	17	1	8	1	
7	F	1	Total	C	N	O	P	0
			22	13	1	7	1	
7	F	1	Total	C	N	O	P	0
			21	13	1	6	1	
7	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	H	1	Total	C	N	O	P	0
			27	17	1	8	1	
7	H	1	Total	C	N	O	P	0
			22	13	1	7	1	
7	H	1	Total	C	N	O	P	0
			21	13	1	6	1	

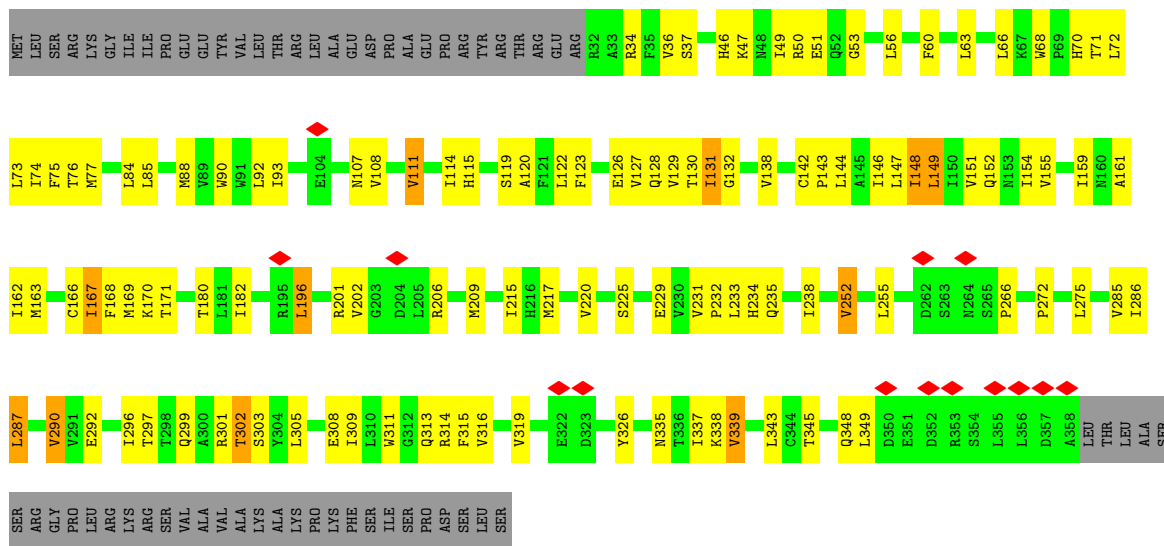
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain E:



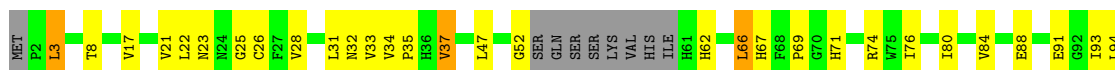
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain G:



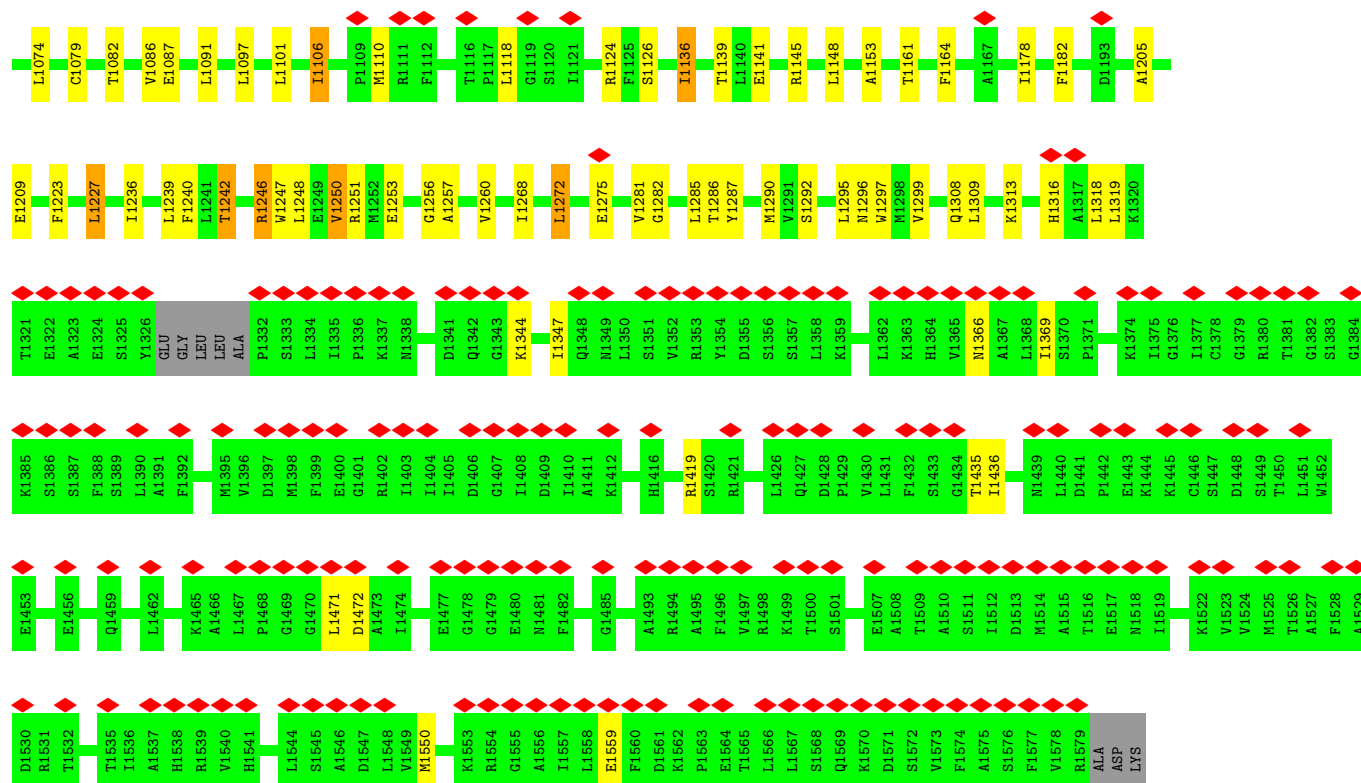
- Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

Chain B:

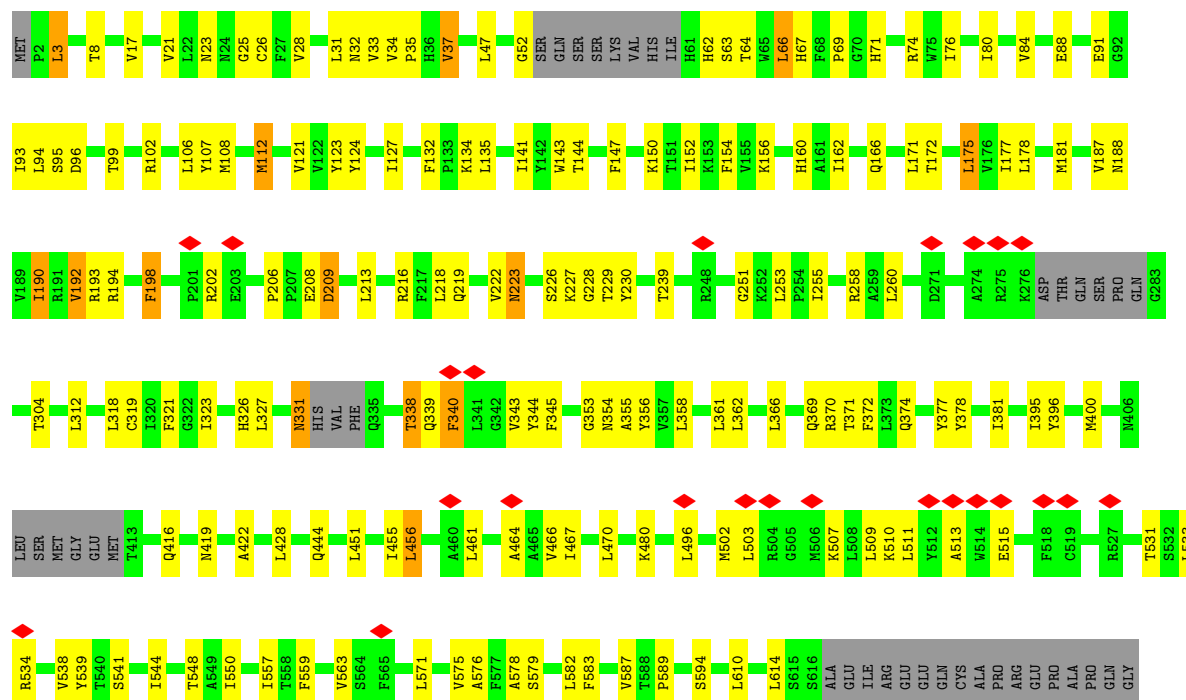


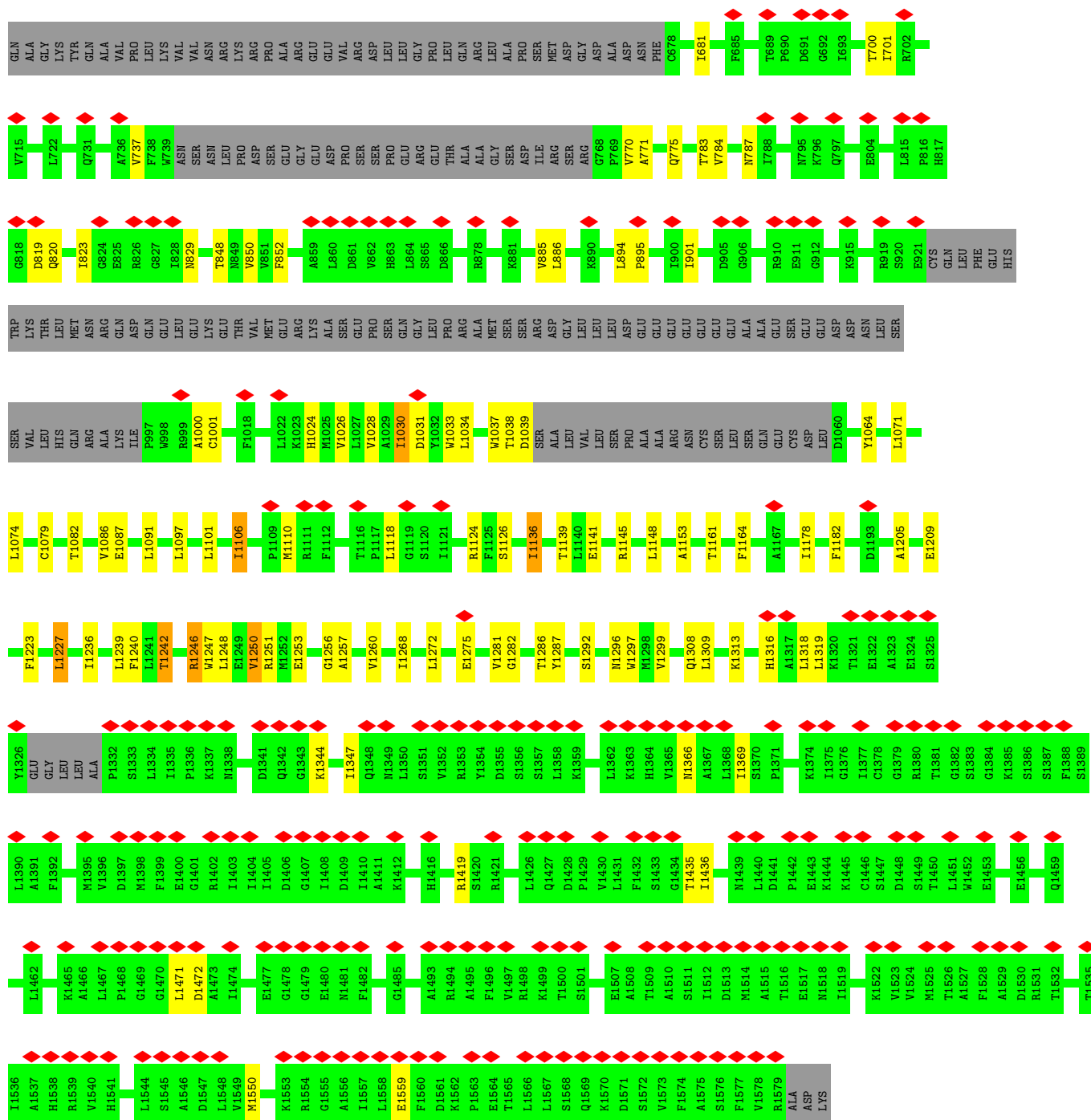




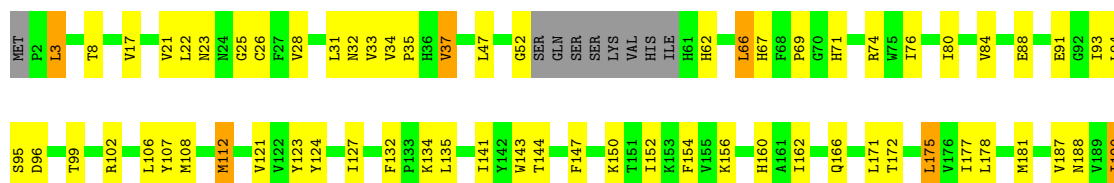


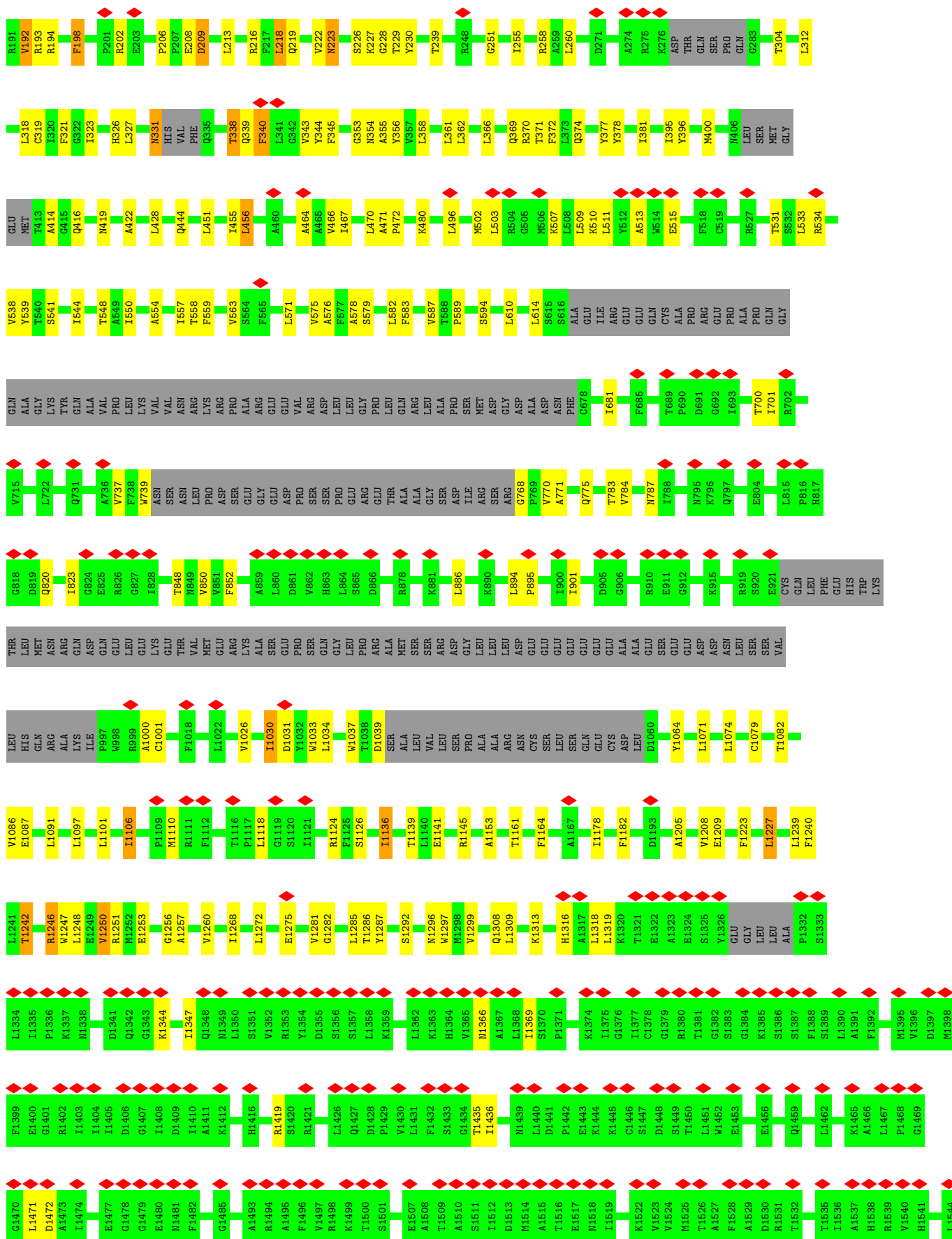
• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2





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





S1545	A1546	D1547	L1548	V1549	K1550	K1553	R1554	G1555	A1556	I1557	L1558	E1559	F1560	D1561	K1562	P1563	E1564	T1565	L1566	L1567	S1568	Q1569	K1570	D1571	S1572	V1573	F1574	A1575	S1576	F1577	V1578	R1579	ALA	ASP	LYS
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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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AJP, BJX, POV, PTY, AGS

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	0.30	0/2600	0.53	1/3535 (0.0%)
1	C	0.30	0/2600	0.53	1/3535 (0.0%)
1	E	0.30	0/2600	0.53	1/3535 (0.0%)
1	G	0.30	0/2600	0.53	1/3535 (0.0%)
2	B	0.18	0/10097	0.36	0/13798
2	D	0.18	0/10097	0.36	0/13798
2	F	0.18	0/10097	0.36	0/13798
2	H	0.18	0/10097	0.36	0/13798
All	All	0.21	0/50788	0.40	4/69332 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	VAL	N-CA-C	-5.14	107.46	112.29
1	C	129	VAL	N-CA-C	-5.14	107.46	112.29
1	E	129	VAL	N-CA-C	-5.14	107.46	112.29
1	G	129	VAL	N-CA-C	-5.14	107.46	112.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	80	0
1	C	2543	0	2571	82	0
1	E	2543	0	2571	81	0
1	G	2543	0	2571	81	0
2	B	9890	0	9397	183	0
2	D	9890	0	9397	185	0
2	F	9890	0	9397	176	0
2	H	9890	0	9397	174	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	1052	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 1052 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
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%)	250 (91%)	26 (9%)	8	30
1	C	276/339 (81%)	250 (91%)	26 (9%)	8	30
1	E	276/339 (81%)	250 (91%)	26 (9%)	8	30
1	G	276/339 (81%)	250 (91%)	26 (9%)	8	30
2	B	931/1371 (68%)	882 (95%)	49 (5%)	20	49
2	D	931/1371 (68%)	882 (95%)	49 (5%)	20	49
2	F	931/1371 (68%)	882 (95%)	49 (5%)	20	49
2	H	931/1371 (68%)	882 (95%)	49 (5%)	20	49
All	All	4828/6840 (71%)	4528 (94%)	300 (6%)	18	45

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	142	CYS
2	H	737	VAL
1	G	196	LEU
2	H	121	VAL
1	C	309	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	846	GLN
2	H	437	ASN
2	F	1308	GLN
1	G	186	HIS
2	H	547	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
4	AGS	H	1602	-	32,33,33	2.08	9 (28%)	45,52,52	1.82	10 (22%)
4	AGS	E	401	-	32,33,33	2.05	9 (28%)	45,52,52	1.78	11 (24%)
7	PTY	H	1612	-	31,31,49	1.25	2 (6%)	34,36,54	1.28	2 (5%)
3	POV	A	401	-	30,30,51	0.98	1 (3%)	35,37,59	1.05	3 (8%)
6	BJX	D	1603	-	35,35,35	1.91	5 (14%)	45,47,47	1.49	7 (15%)
7	PTY	F	1612	-	31,31,49	1.25	2 (6%)	34,36,54	1.28	2 (5%)
4	AGS	F	1602	-	32,33,33	2.08	9 (28%)	45,52,52	1.82	10 (22%)
3	POV	H	1605	-	40,40,51	1.12	2 (5%)	46,48,59	1.04	2 (4%)
6	BJX	H	1603	-	35,35,35	1.91	5 (14%)	45,47,47	1.49	7 (15%)
4	AGS	A	402	-	32,33,33	2.05	9 (28%)	45,52,52	1.78	11 (24%)
7	PTY	B	1615	-	20,20,49	1.22	2 (10%)	22,24,54	1.27	3 (13%)
3	POV	H	1611	-	27,27,51	1.28	2 (7%)	29,29,59	1.25	3 (10%)
3	POV	B	1606	-	39,39,51	1.14	2 (5%)	45,47,59	1.08	2 (4%)
3	POV	B	1608	-	35,35,51	1.20	2 (5%)	41,43,59	1.27	5 (12%)
5	AJP	D	1601	-	83,83,95	0.66	1 (1%)	126,131,149	1.29	14 (11%)
3	POV	D	1604	-	35,35,51	1.18	2 (5%)	41,43,59	1.11	2 (4%)
7	PTY	D	1613	-	26,26,49	1.37	2 (7%)	29,31,54	1.17	2 (6%)
3	POV	B	1609	-	24,24,51	1.08	1 (4%)	29,31,59	1.06	1 (3%)
7	PTY	H	1614	-	21,21,49	1.13	1 (4%)	23,25,54	0.95	1 (4%)
3	POV	F	1608	-	35,35,51	1.20	2 (5%)	41,43,59	1.27	5 (12%)
3	POV	F	1609	-	24,24,51	1.08	1 (4%)	29,31,59	1.06	1 (3%)
7	PTY	F	1614	-	21,21,49	1.13	1 (4%)	23,25,54	0.95	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	B	1610	-	24,24,51	1.04	1 (4%)	29,31,59	1.18	3 (10%)
4	AGS	B	1602	-	32,33,33	2.08	9 (28%)	45,52,52	1.82	10 (22%)
3	POV	B	1604	-	35,35,51	1.18	2 (5%)	41,43,59	1.11	2 (4%)
7	PTY	F	1615	-	20,20,49	1.22	2 (10%)	22,24,54	1.27	3 (13%)
3	POV	D	1608	-	35,35,51	1.20	2 (5%)	41,43,59	1.27	5 (12%)
3	POV	D	1610	-	24,24,51	1.04	1 (4%)	29,31,59	1.18	3 (10%)
5	AJP	H	1601	-	83,83,95	0.66	1 (1%)	126,131,149	1.29	14 (11%)
7	PTY	B	1612	-	31,31,49	1.25	2 (6%)	34,36,54	1.28	2 (5%)
3	POV	F	1605	-	40,40,51	1.12	2 (5%)	46,48,59	1.04	2 (4%)
5	AJP	F	1601	-	83,83,95	0.66	1 (1%)	126,131,149	1.29	14 (11%)
3	POV	G	402	-	30,30,51	0.98	1 (3%)	35,37,59	1.05	3 (8%)
3	POV	D	1606	-	39,39,51	1.14	2 (5%)	45,47,59	1.08	2 (4%)
7	PTY	H	1613	-	26,26,49	1.37	2 (7%)	29,31,54	1.17	2 (6%)
7	PTY	B	1614	-	21,21,49	1.13	1 (4%)	23,25,54	0.95	1 (4%)
3	POV	H	1608	-	35,35,51	1.20	2 (5%)	41,43,59	1.27	5 (12%)
3	POV	B	1605	-	40,40,51	1.12	2 (5%)	46,48,59	1.04	2 (4%)
6	BJX	F	1603	-	35,35,35	1.91	5 (14%)	45,47,47	1.49	7 (15%)
7	PTY	F	1613	-	26,26,49	1.37	2 (7%)	29,31,54	1.17	2 (6%)
3	POV	H	1607	-	40,40,51	1.11	2 (5%)	46,48,59	1.13	4 (8%)
3	POV	D	1607	-	40,40,51	1.11	2 (5%)	46,48,59	1.13	4 (8%)
4	AGS	D	1602	-	32,33,33	2.08	9 (28%)	45,52,52	1.82	10 (22%)
5	AJP	B	1601	-	83,83,95	0.66	1 (1%)	126,131,149	1.29	14 (11%)
3	POV	F	1611	-	27,27,51	1.28	2 (7%)	29,29,59	1.25	3 (10%)
3	POV	E	402	-	30,30,51	0.98	1 (3%)	35,37,59	1.05	3 (8%)
7	PTY	D	1612	-	31,31,49	1.25	2 (6%)	34,36,54	1.28	2 (5%)
3	POV	H	1606	-	39,39,51	1.14	2 (5%)	45,47,59	1.08	2 (4%)
4	AGS	G	401	-	32,33,33	2.05	9 (28%)	45,52,52	1.78	11 (24%)
7	PTY	H	1615	-	20,20,49	1.22	2 (10%)	22,24,54	1.27	3 (13%)
3	POV	C	402	-	30,30,51	0.98	1 (3%)	35,37,59	1.05	3 (8%)
7	PTY	D	1615	-	20,20,49	1.22	2 (10%)	22,24,54	1.27	3 (13%)
3	POV	H	1610	-	24,24,51	1.04	1 (4%)	29,31,59	1.18	3 (10%)
3	POV	D	1611	-	27,27,51	1.28	2 (7%)	29,29,59	1.25	3 (10%)
3	POV	B	1607	-	40,40,51	1.11	2 (5%)	46,48,59	1.13	4 (8%)
3	POV	H	1604	-	35,35,51	1.18	2 (5%)	41,43,59	1.11	2 (4%)
3	POV	F	1607	-	40,40,51	1.11	2 (5%)	46,48,59	1.13	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	H	1609	-	24,24,51	1.08	1 (4%)	29,31,59	1.06	1 (3%)
3	POV	F	1610	-	24,24,51	1.04	1 (4%)	29,31,59	1.18	3 (10%)
3	POV	D	1609	-	24,24,51	1.08	1 (4%)	29,31,59	1.06	1 (3%)
6	BJX	B	1603	-	35,35,35	1.91	5 (14%)	45,47,47	1.49	7 (15%)
3	POV	F	1606	-	39,39,51	1.14	2 (5%)	45,47,59	1.08	2 (4%)
7	PTY	B	1613	-	26,26,49	1.37	2 (7%)	29,31,54	1.17	2 (6%)
3	POV	F	1604	-	35,35,51	1.18	2 (5%)	41,43,59	1.11	2 (4%)
7	PTY	D	1614	-	21,21,49	1.13	1 (4%)	23,25,54	0.95	1 (4%)
3	POV	B	1611	-	27,27,51	1.28	2 (7%)	29,29,59	1.25	3 (10%)
4	AGS	C	401	-	32,33,33	2.05	9 (28%)	45,52,52	1.78	11 (24%)
3	POV	D	1605	-	40,40,51	1.12	2 (5%)	46,48,59	1.04	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	H	1602	-	-	2/21/38/38	0/3/3/3
4	AGS	E	401	-	-	2/21/38/38	0/3/3/3
7	PTY	H	1612	-	-	13/35/35/53	-
3	POV	A	401	-	-	3/33/33/55	-
6	BJX	D	1603	-	-	13/27/35/35	0/3/3/3
7	PTY	F	1612	-	-	13/35/35/53	-
4	AGS	F	1602	-	-	2/21/38/38	0/3/3/3
3	POV	H	1605	-	-	13/44/44/55	-
6	BJX	H	1603	-	-	13/27/35/35	0/3/3/3
4	AGS	A	402	-	-	2/21/38/38	0/3/3/3
7	PTY	B	1615	-	-	13/22/22/53	-
3	POV	H	1611	-	-	9/29/29/55	-
3	POV	B	1606	-	-	15/43/43/55	-
3	POV	B	1608	-	-	12/39/39/55	-
5	AJP	D	1601	-	29/29/33/38	12/22/194/220	0/10/10/11
3	POV	D	1604	-	-	12/39/39/55	-
7	PTY	D	1613	-	-	14/30/30/53	-
3	POV	B	1609	-	-	9/27/27/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PTY	H	1614	-	-	11/23/23/53	-
3	POV	F	1608	-	-	12/39/39/55	-
3	POV	F	1609	-	-	9/27/27/55	-
7	PTY	F	1614	-	-	11/23/23/53	-
3	POV	B	1610	-	-	4/27/27/55	-
4	AGS	B	1602	-	-	2/21/38/38	0/3/3/3
3	POV	B	1604	-	-	12/39/39/55	-
7	PTY	F	1615	-	-	13/22/22/53	-
3	POV	D	1608	-	-	12/39/39/55	-
3	POV	D	1610	-	-	4/27/27/55	-
5	AJP	H	1601	-	29/29/33/38	12/22/194/220	0/10/10/11
7	PTY	B	1612	-	-	13/35/35/53	-
3	POV	F	1605	-	-	13/44/44/55	-
5	AJP	F	1601	-	29/29/33/38	12/22/194/220	0/10/10/11
3	POV	G	402	-	-	3/33/33/55	-
3	POV	D	1606	-	-	15/43/43/55	-
7	PTY	H	1613	-	-	14/30/30/53	-
7	PTY	B	1614	-	-	11/23/23/53	-
3	POV	H	1608	-	-	12/39/39/55	-
3	POV	B	1605	-	-	13/44/44/55	-
6	BJX	F	1603	-	-	13/27/35/35	0/3/3/3
7	PTY	F	1613	-	-	14/30/30/53	-
3	POV	H	1607	-	-	13/44/44/55	-
3	POV	D	1607	-	-	13/44/44/55	-
4	AGS	D	1602	-	-	2/21/38/38	0/3/3/3
5	AJP	B	1601	-	29/29/33/38	12/22/194/220	0/10/10/11
3	POV	F	1611	-	-	9/29/29/55	-
3	POV	E	402	-	-	3/33/33/55	-
7	PTY	D	1612	-	-	13/35/35/53	-
3	POV	H	1606	-	-	15/43/43/55	-
4	AGS	G	401	-	-	2/21/38/38	0/3/3/3
7	PTY	H	1615	-	-	13/22/22/53	-
3	POV	C	402	-	-	3/33/33/55	-
7	PTY	D	1615	-	-	13/22/22/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	H	1610	-	-	4/27/27/55	-
3	POV	D	1611	-	-	9/29/29/55	-
3	POV	B	1607	-	-	13/44/44/55	-
3	POV	H	1604	-	-	12/39/39/55	-
3	POV	F	1607	-	-	13/44/44/55	-
3	POV	H	1609	-	-	9/27/27/55	-
3	POV	F	1610	-	-	4/27/27/55	-
3	POV	D	1609	-	-	9/27/27/55	-
6	BJX	B	1603	-	-	13/27/35/35	0/3/3/3
3	POV	F	1606	-	-	15/43/43/55	-
7	PTY	B	1613	-	-	14/30/30/53	-
3	POV	F	1604	-	-	12/39/39/55	-
7	PTY	D	1614	-	-	11/23/23/53	-
3	POV	B	1611	-	-	9/29/29/55	-
4	AGS	C	401	-	-	2/21/38/38	0/3/3/3
3	POV	D	1605	-	-	13/44/44/55	-

The worst 5 of 184 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1603	BJX	C6-C7	8.62	1.49	1.40
6	D	1603	BJX	C6-C7	8.62	1.49	1.40
6	F	1603	BJX	C6-C7	8.62	1.49	1.40
6	H	1603	BJX	C6-C7	8.62	1.49	1.40
4	A	402	AGS	PG-S1G	8.03	2.08	1.90

The worst 5 of 300 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1602	AGS	C5-C4-N3	-5.74	118.81	126.72
4	D	1602	AGS	C5-C4-N3	-5.74	118.81	126.72
4	F	1602	AGS	C5-C4-N3	-5.74	118.81	126.72
4	H	1602	AGS	C5-C4-N3	-5.74	118.81	126.72
4	A	402	AGS	C5-C4-N3	-5.31	119.41	126.72

5 of 116 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1601	AJP	C15
5	B	1601	AJP	C37
5	B	1601	AJP	C22
5	B	1601	AJP	C16
5	B	1601	AJP	C55

5 of 680 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
4	H	1602	AGS	1	0
4	E	401	AGS	2	0
3	A	401	POV	4	0
6	D	1603	BJX	2	0
4	F	1602	AGS	1	0
3	H	1605	POV	2	0
6	H	1603	BJX	2	0
4	A	402	AGS	2	0
7	B	1615	PTY	2	0
3	H	1611	POV	2	0
3	B	1606	POV	1	0
3	B	1608	POV	8	0
5	D	1601	AJP	1	0
3	D	1604	POV	5	0
7	D	1613	PTY	4	0
3	B	1609	POV	3	0
7	H	1614	PTY	1	0
3	F	1608	POV	7	0
3	F	1609	POV	3	0
7	F	1614	PTY	1	0
4	B	1602	AGS	1	0
3	B	1604	POV	5	0
7	F	1615	PTY	2	0
3	D	1608	POV	8	0

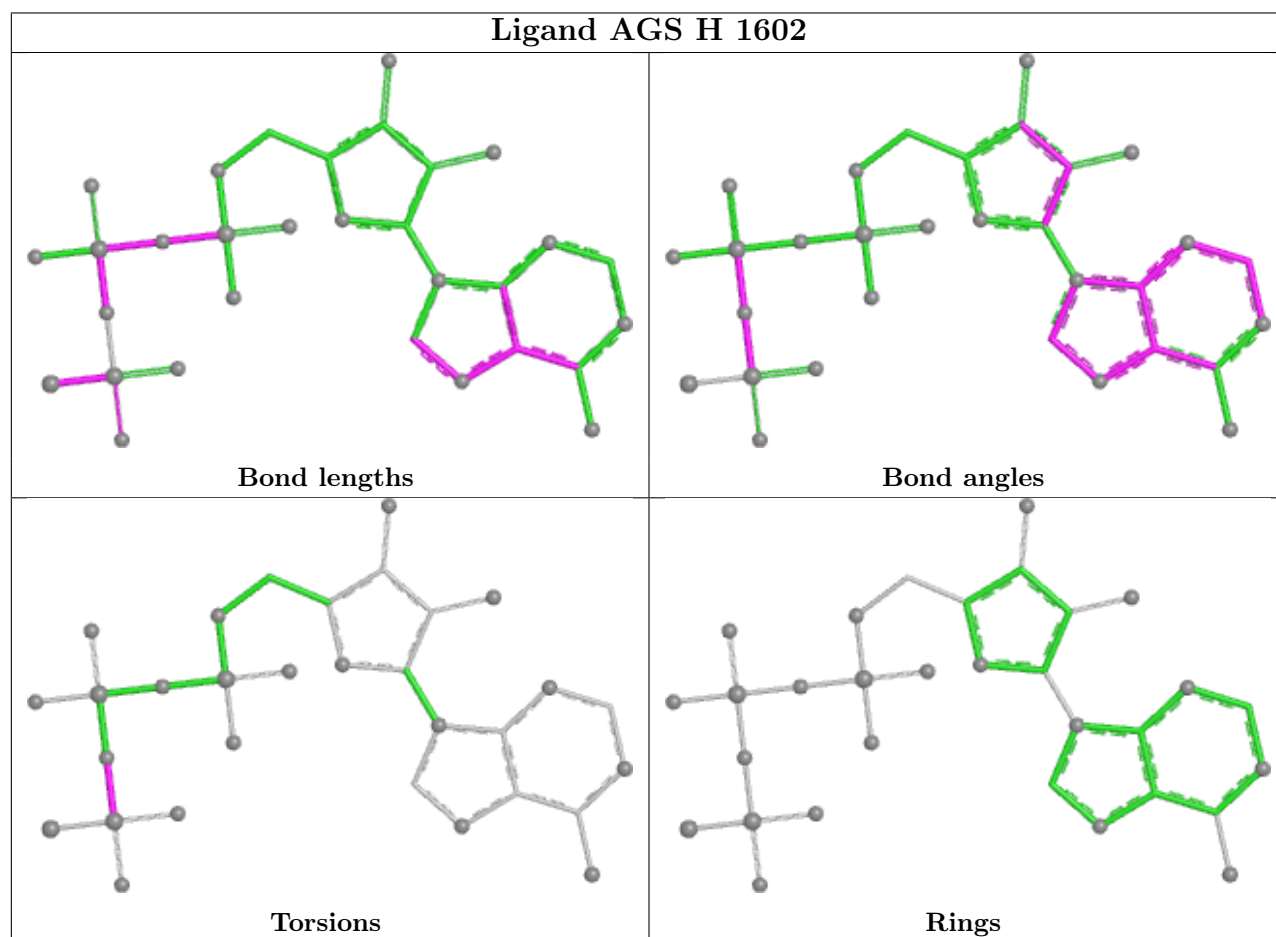
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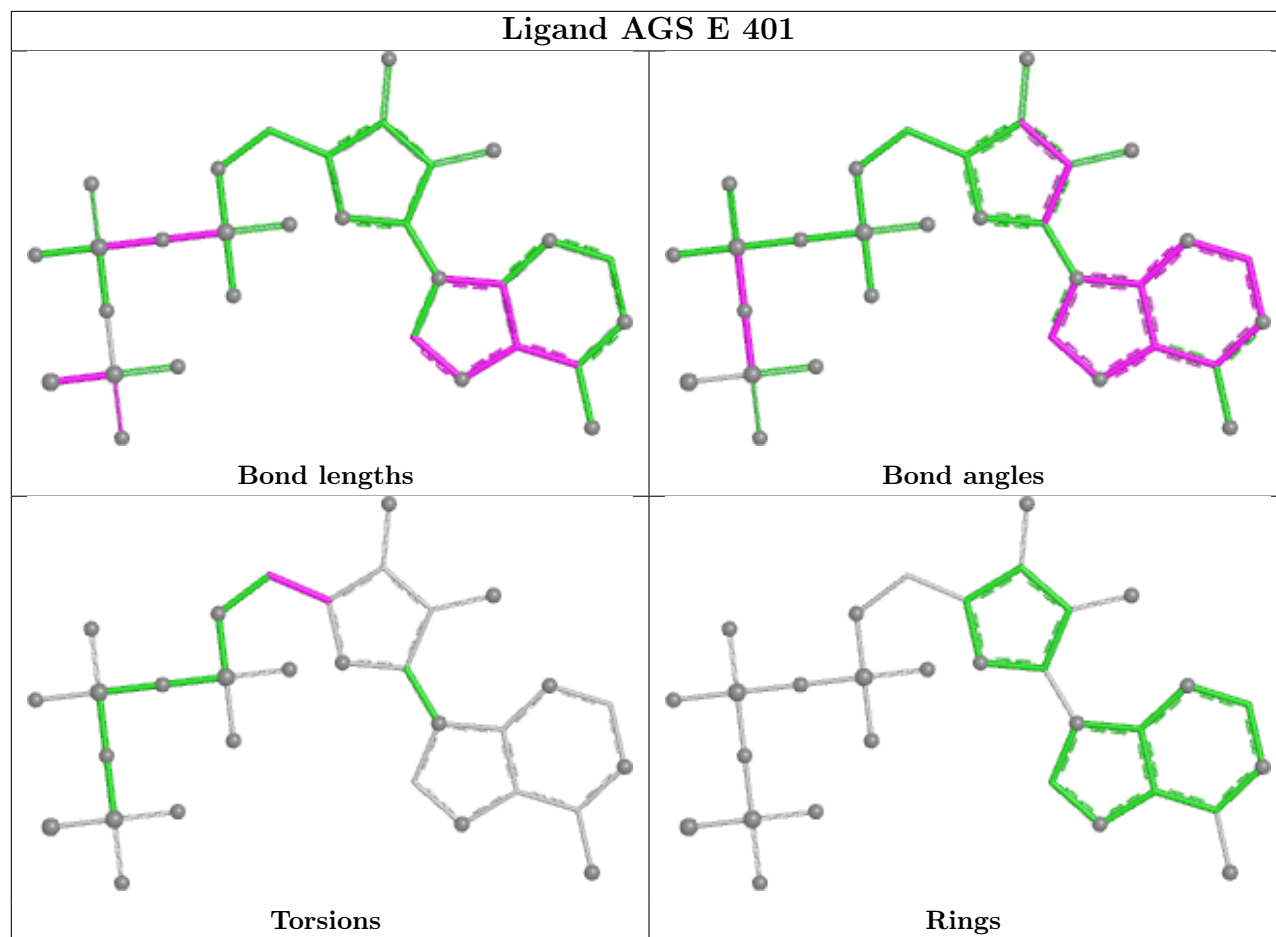
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1601	AJP	1	0
3	F	1605	POV	2	0
5	F	1601	AJP	1	0
3	G	402	POV	4	0
3	D	1606	POV	1	0
7	H	1613	PTY	4	0
7	B	1614	PTY	1	0
3	H	1608	POV	8	0
3	B	1605	POV	3	0
6	F	1603	BJX	2	0
7	F	1613	PTY	4	0
3	H	1607	POV	2	0
3	D	1607	POV	2	0
4	D	1602	AGS	1	0
5	B	1601	AJP	1	0
3	F	1611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

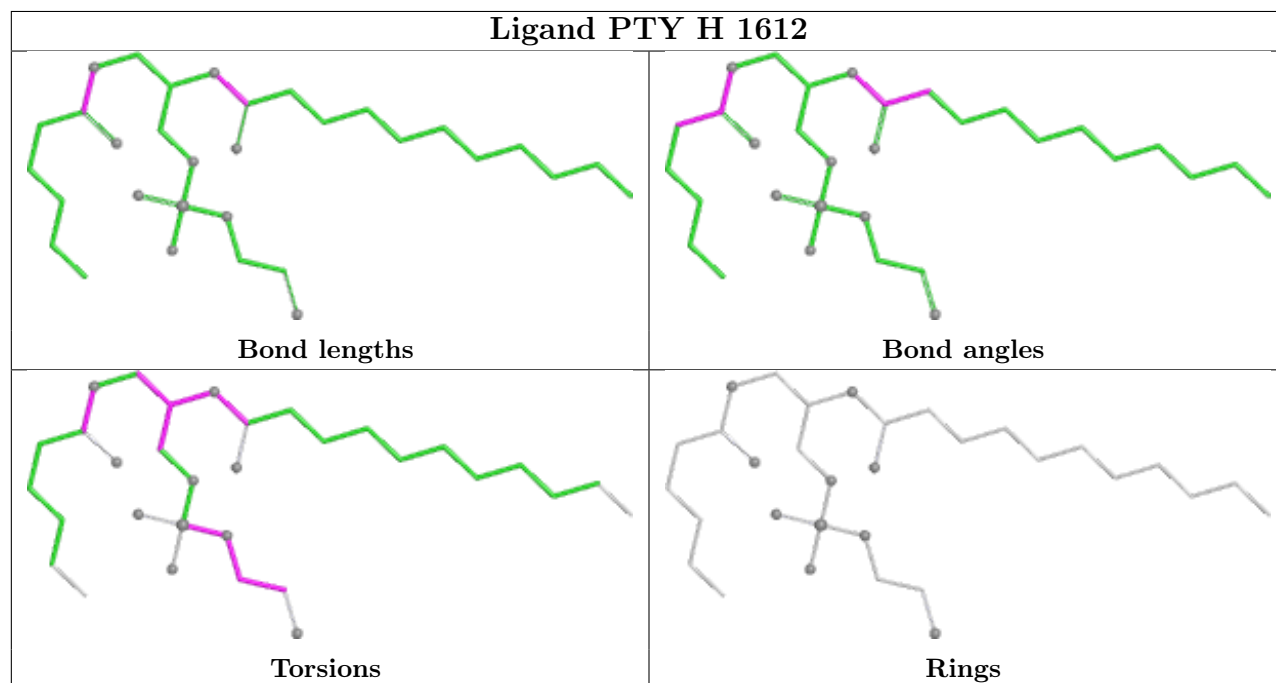
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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

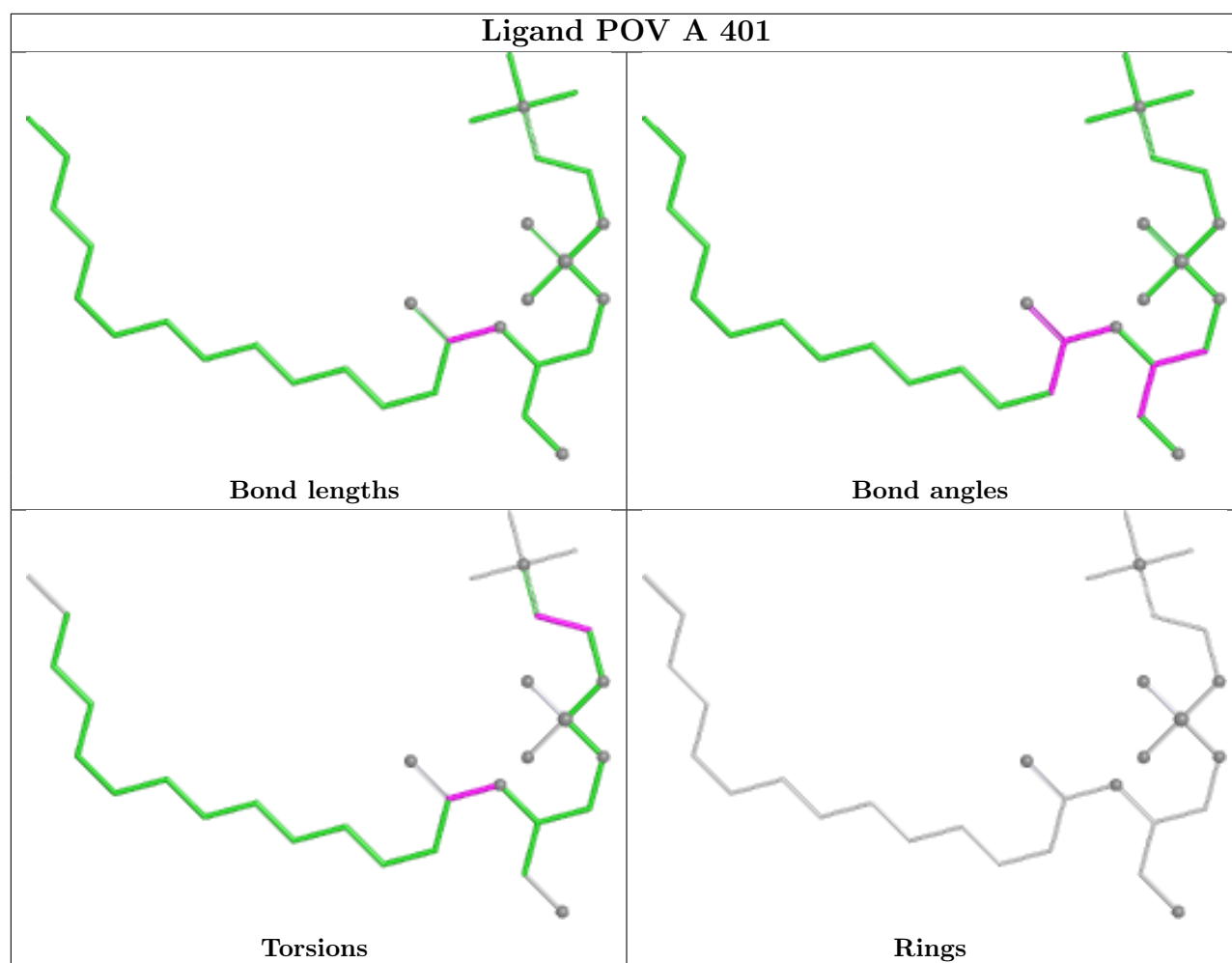


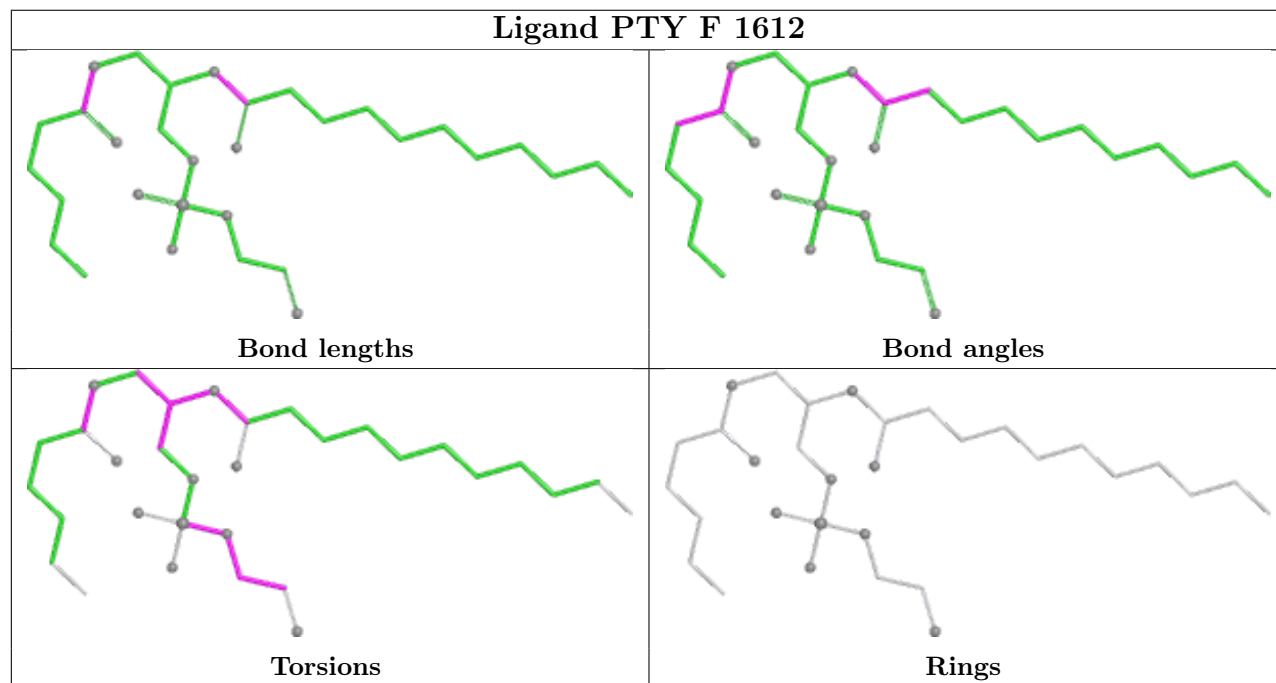
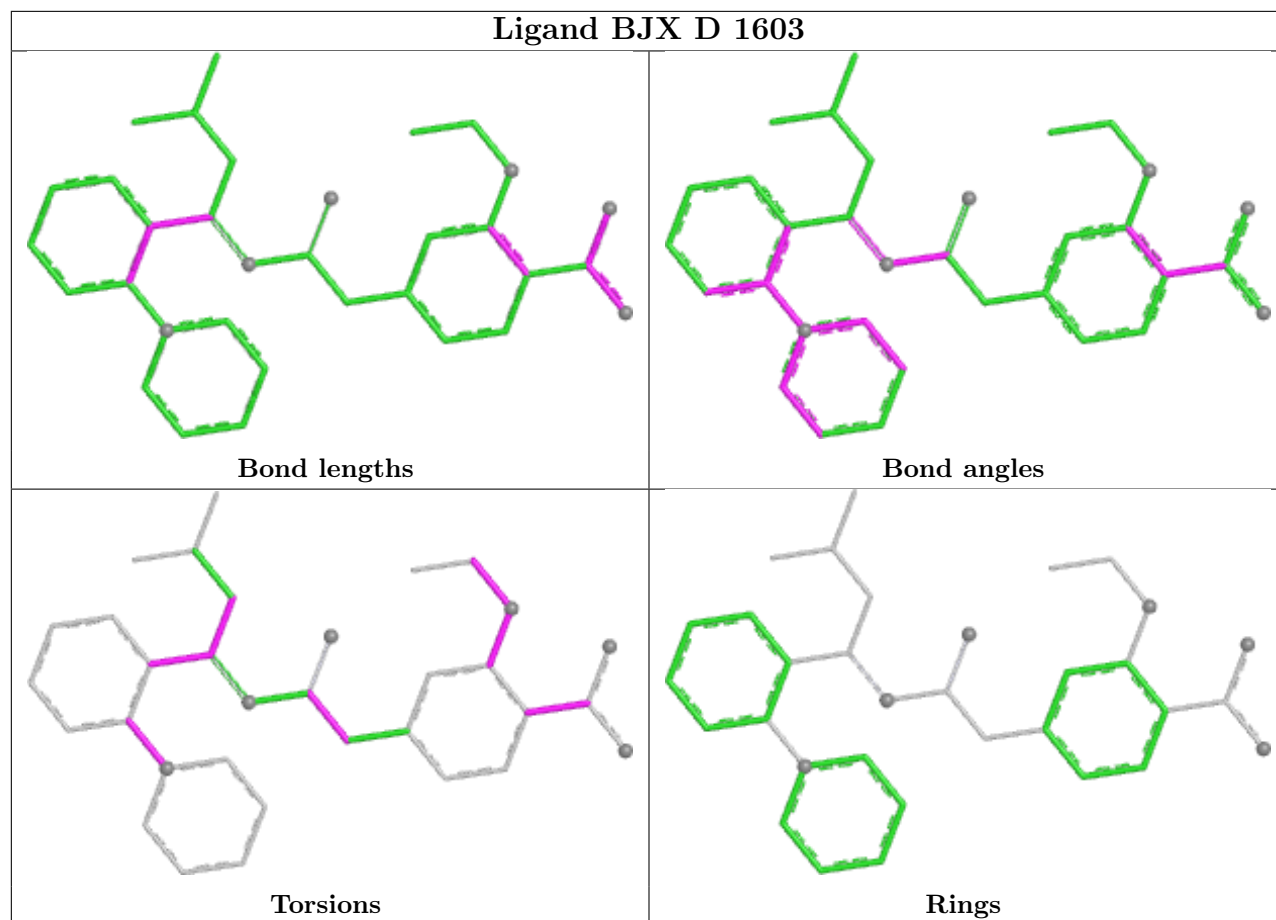
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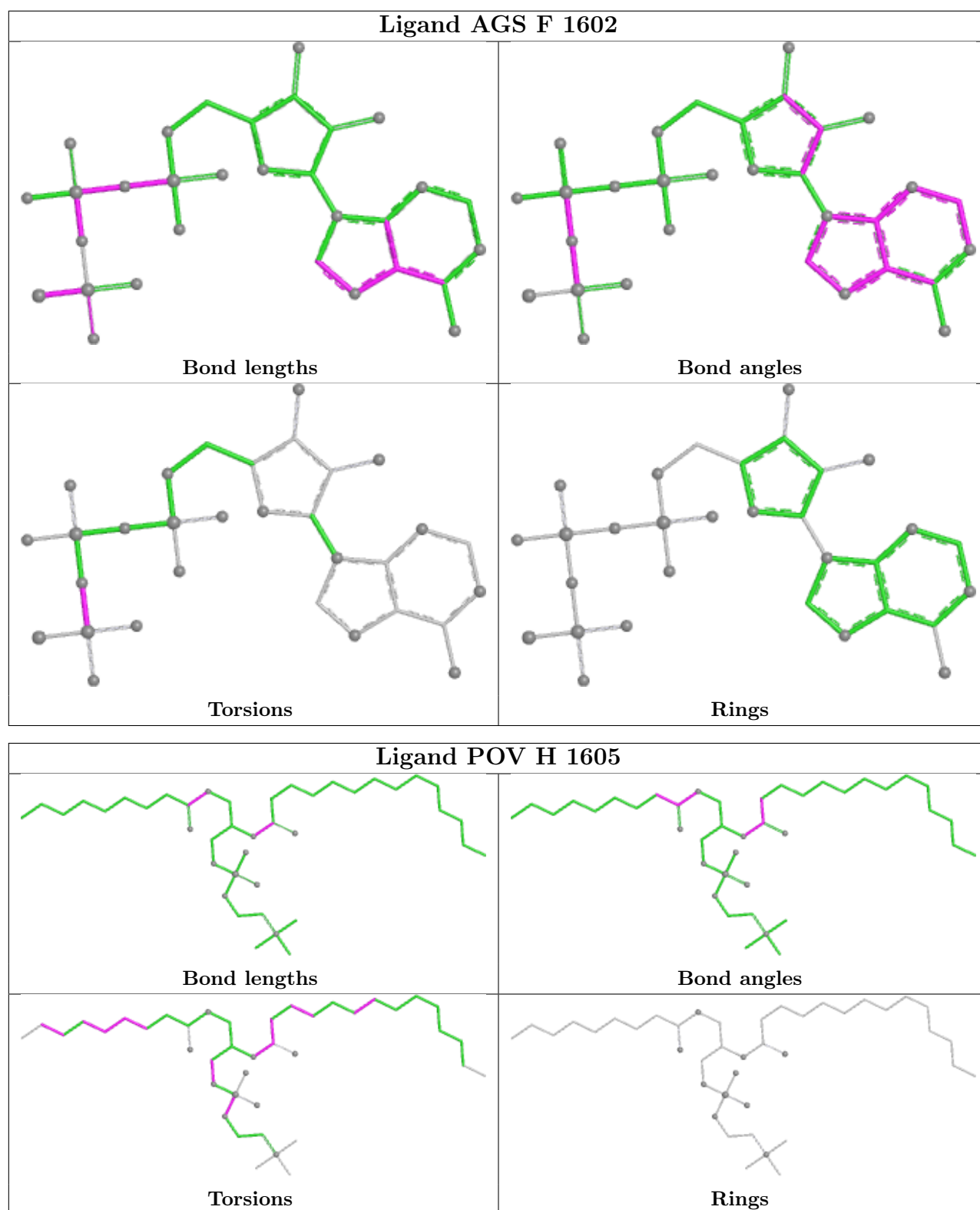


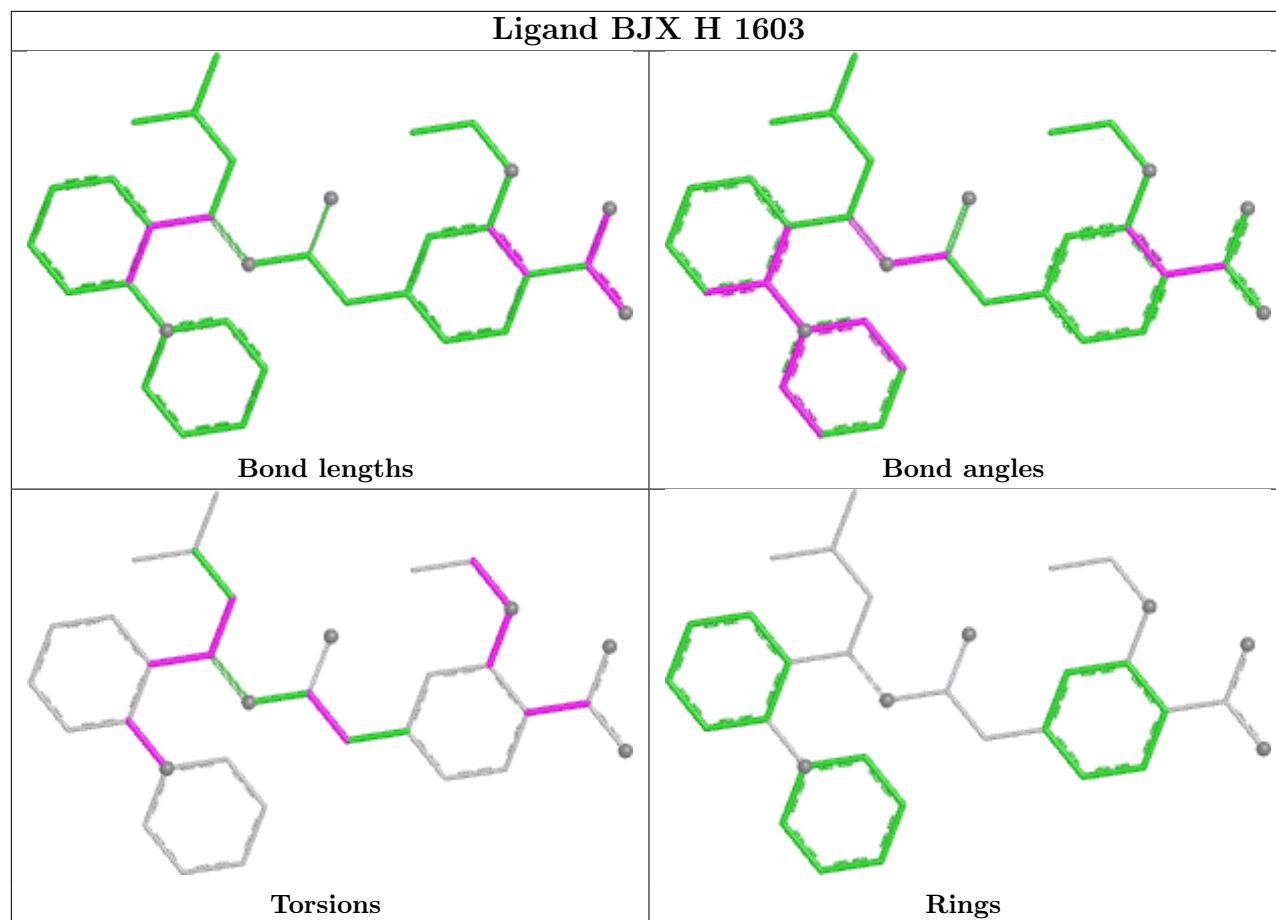
Ligand PTY H 1612

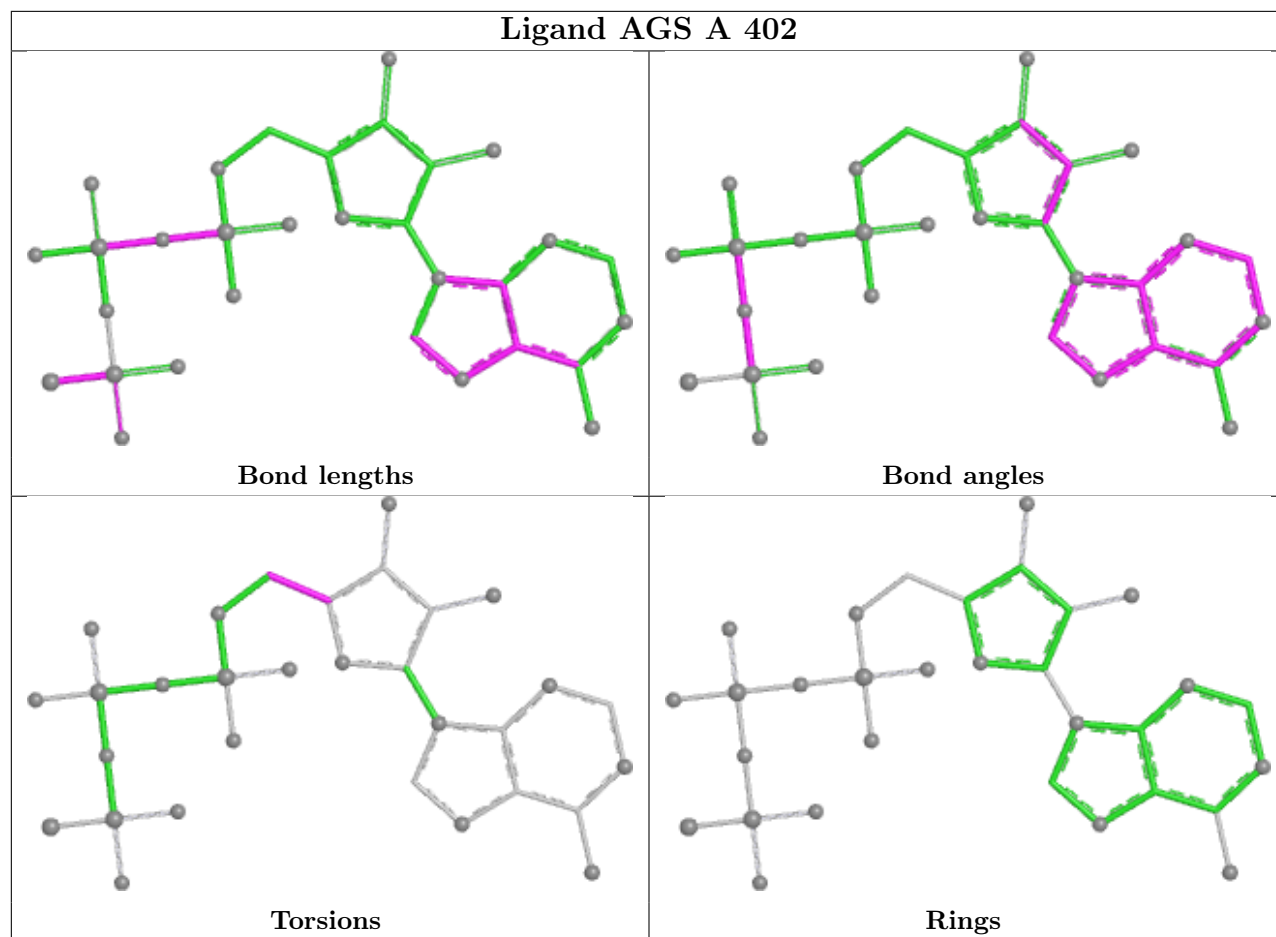


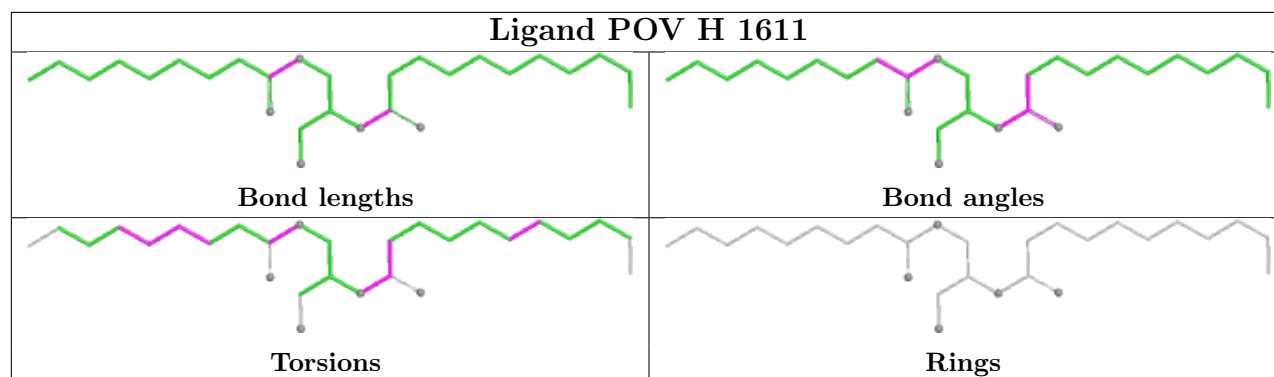
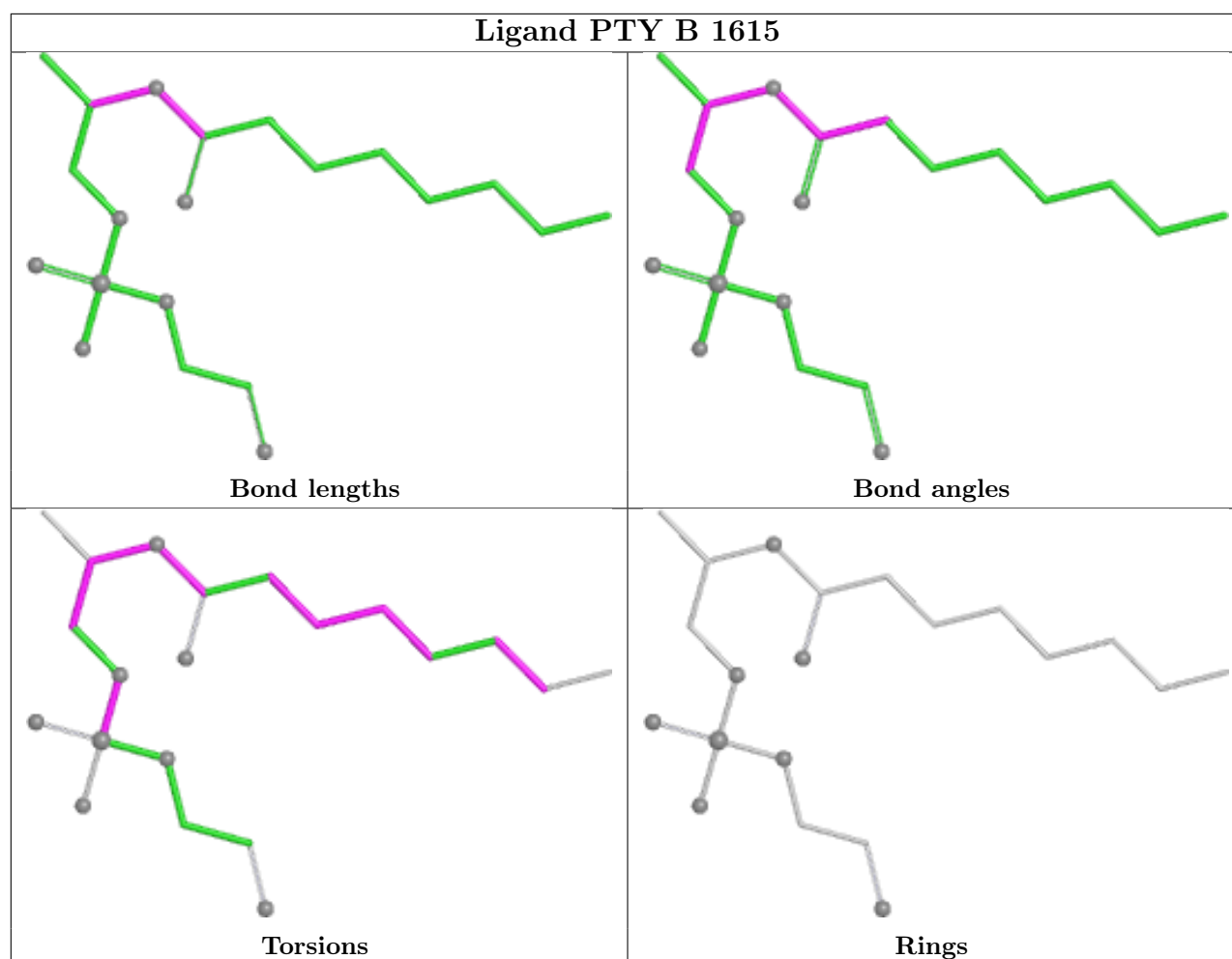


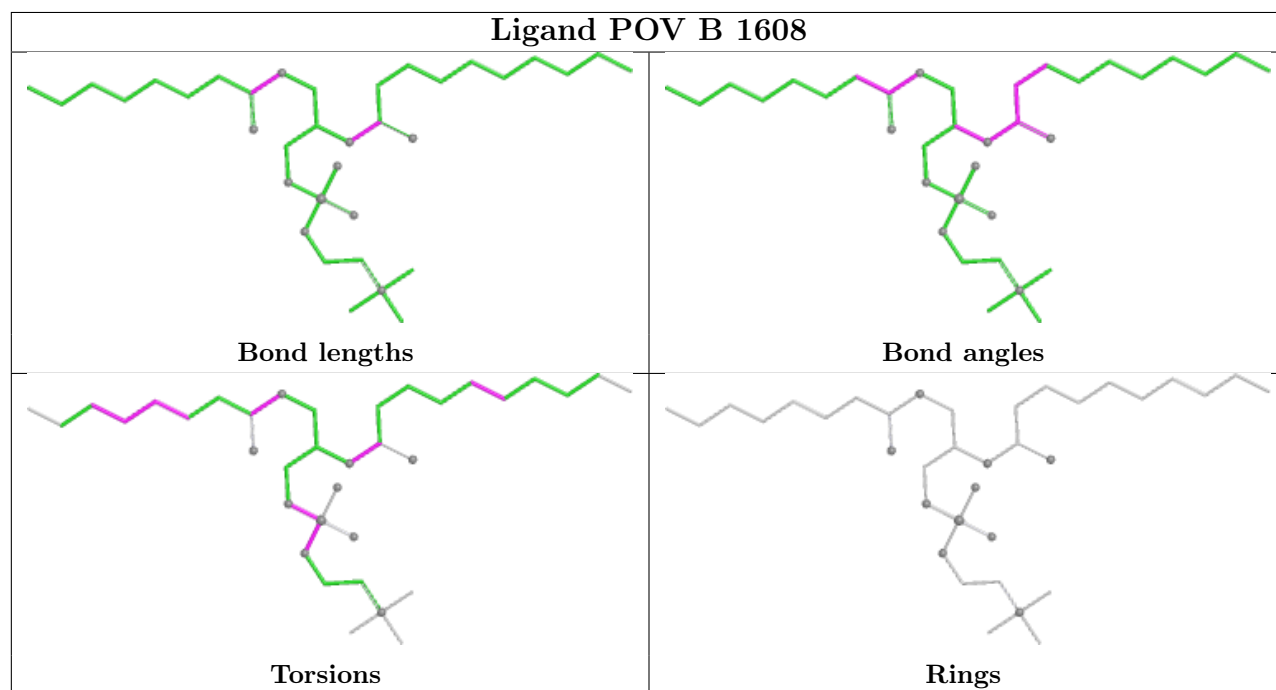
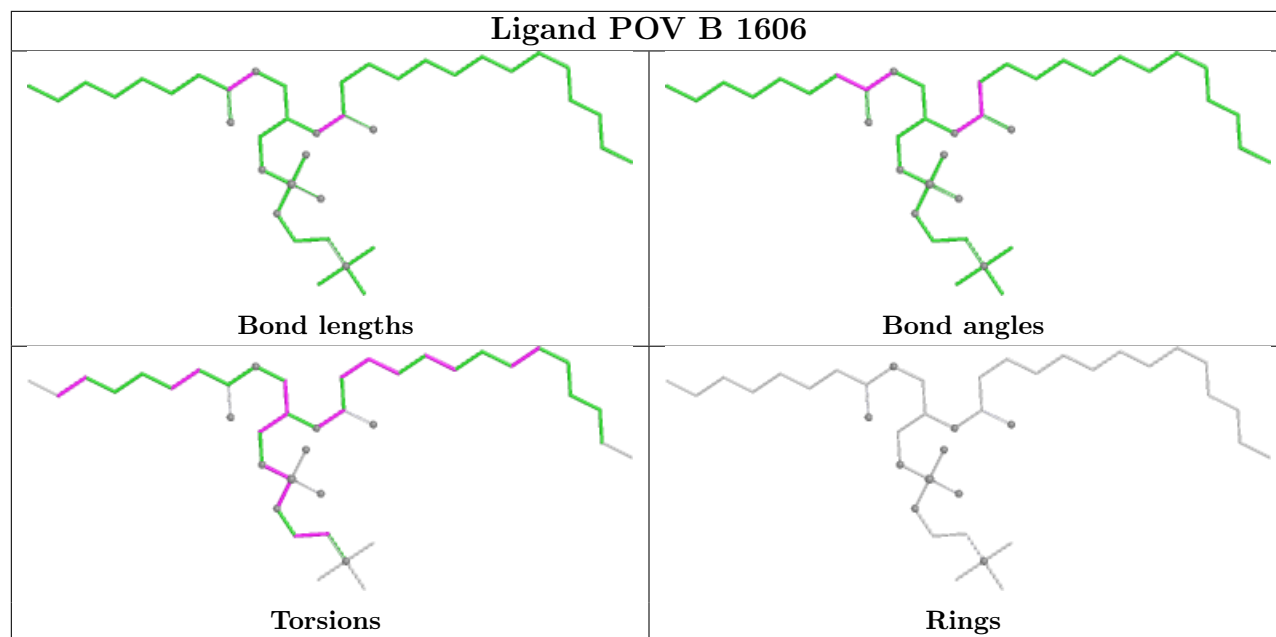


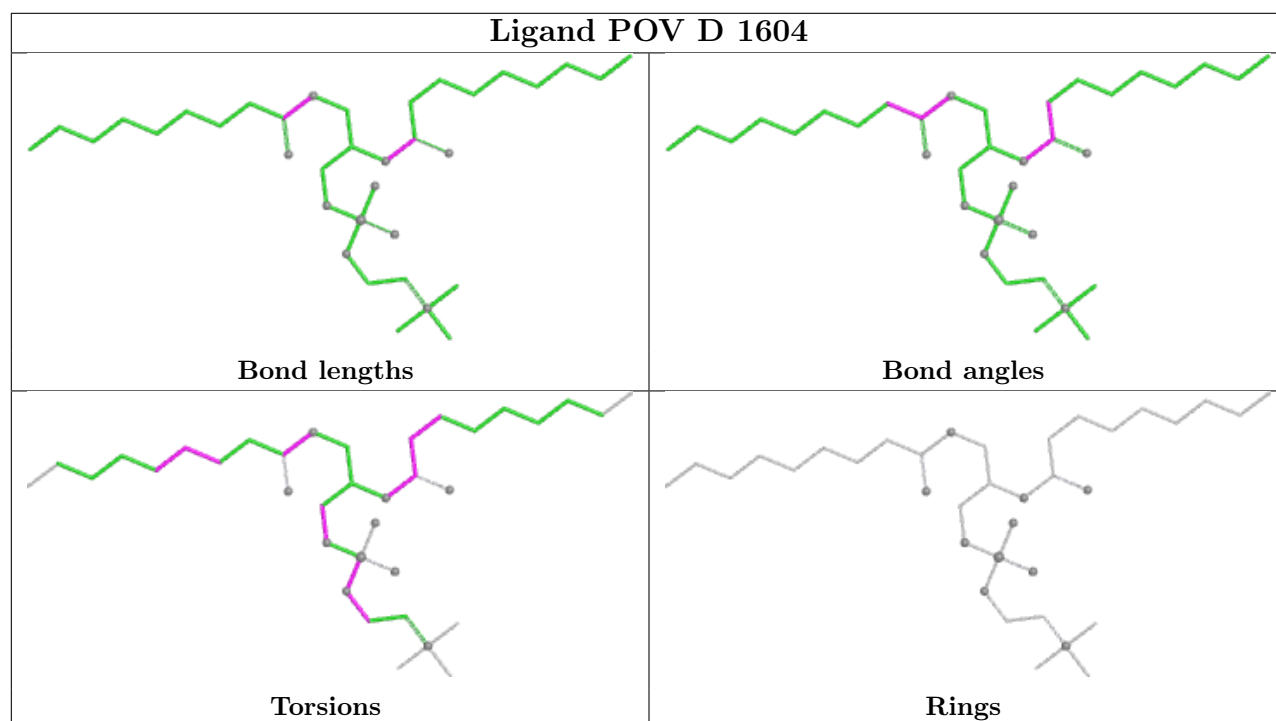
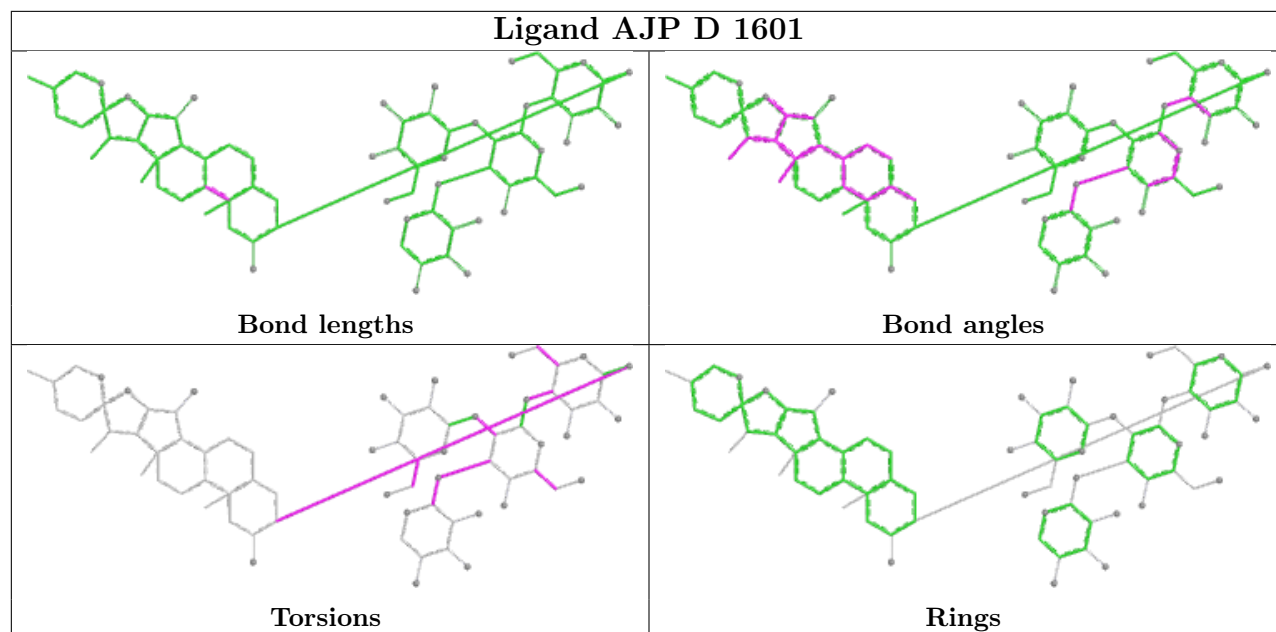


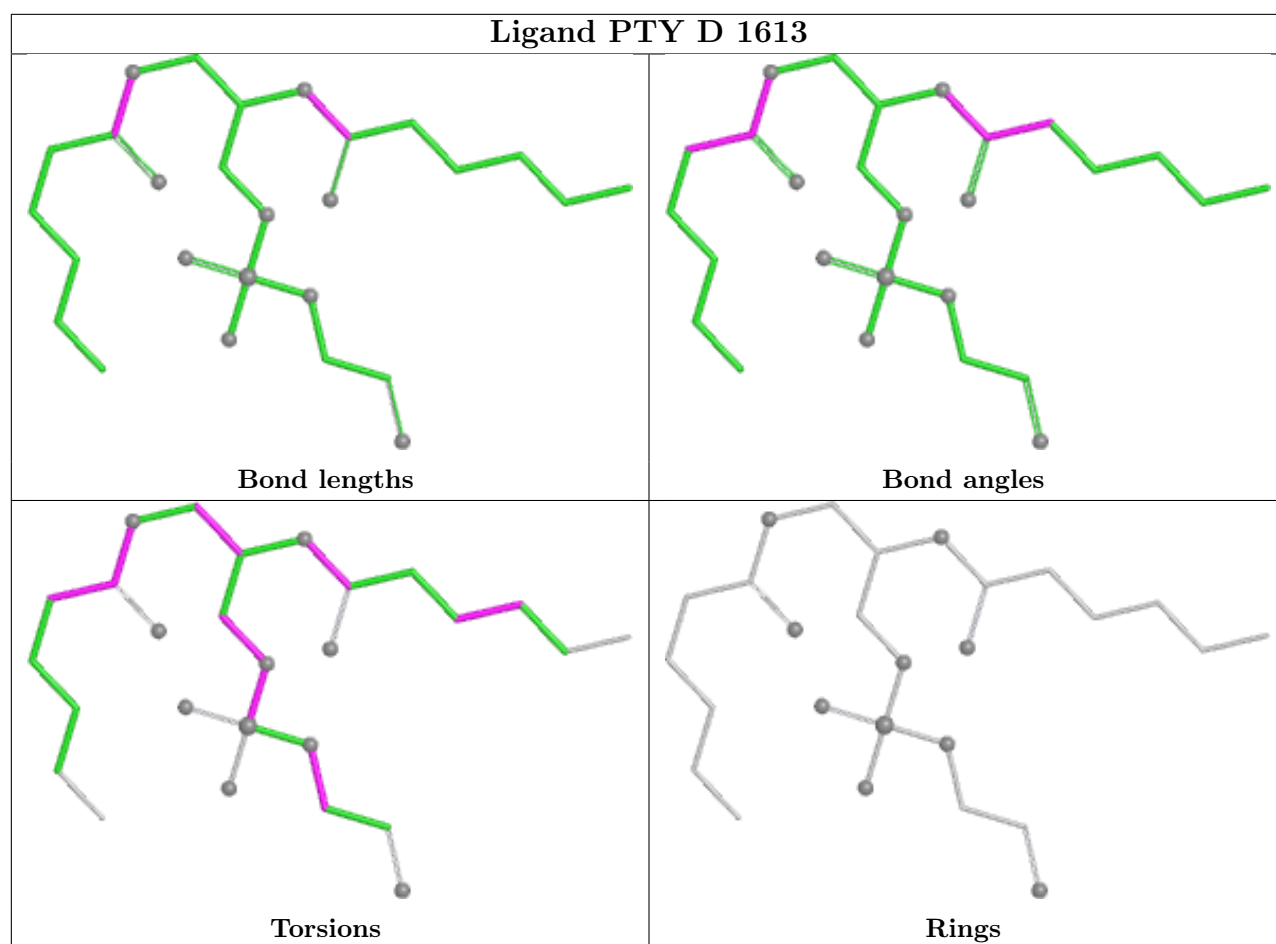


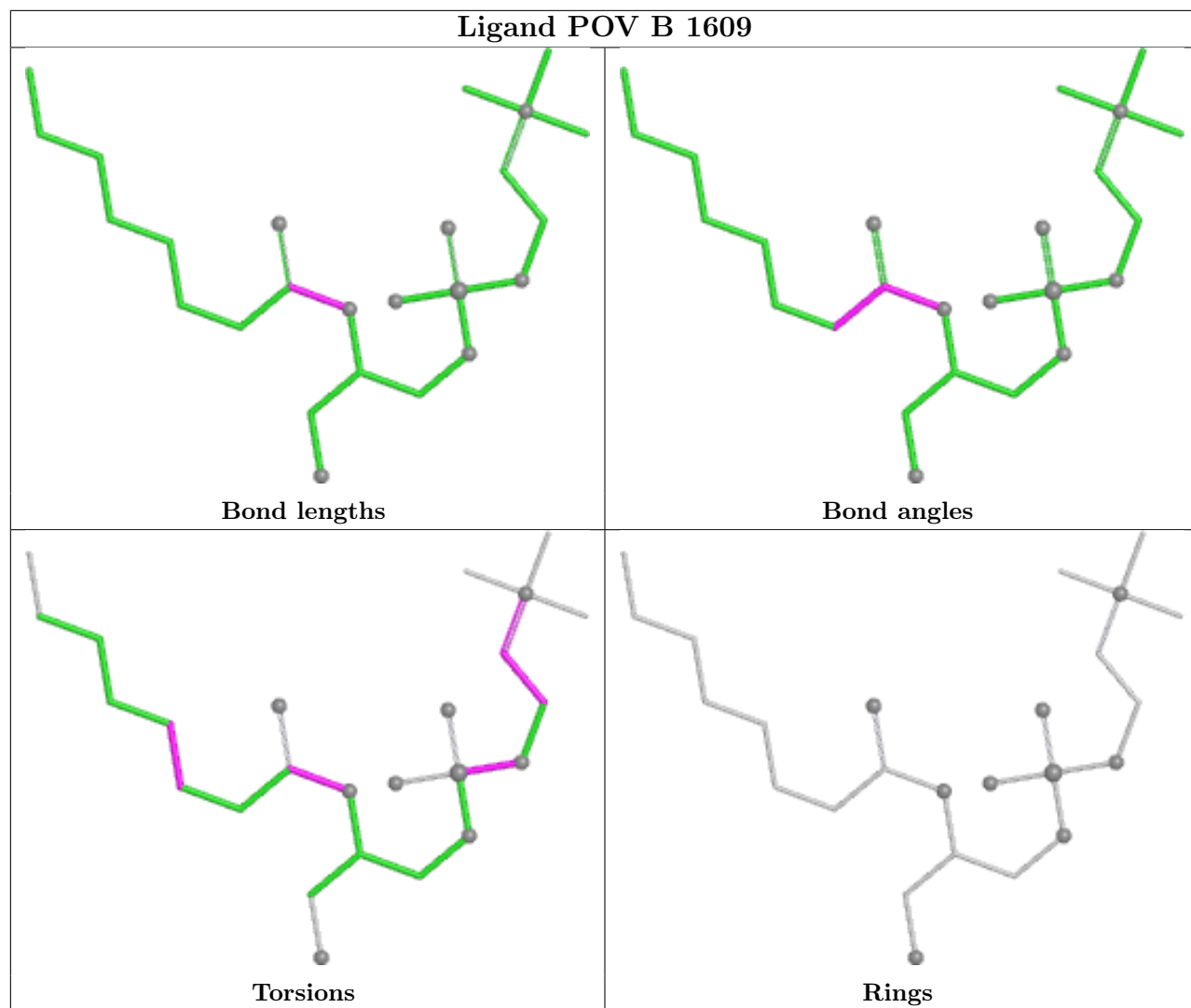


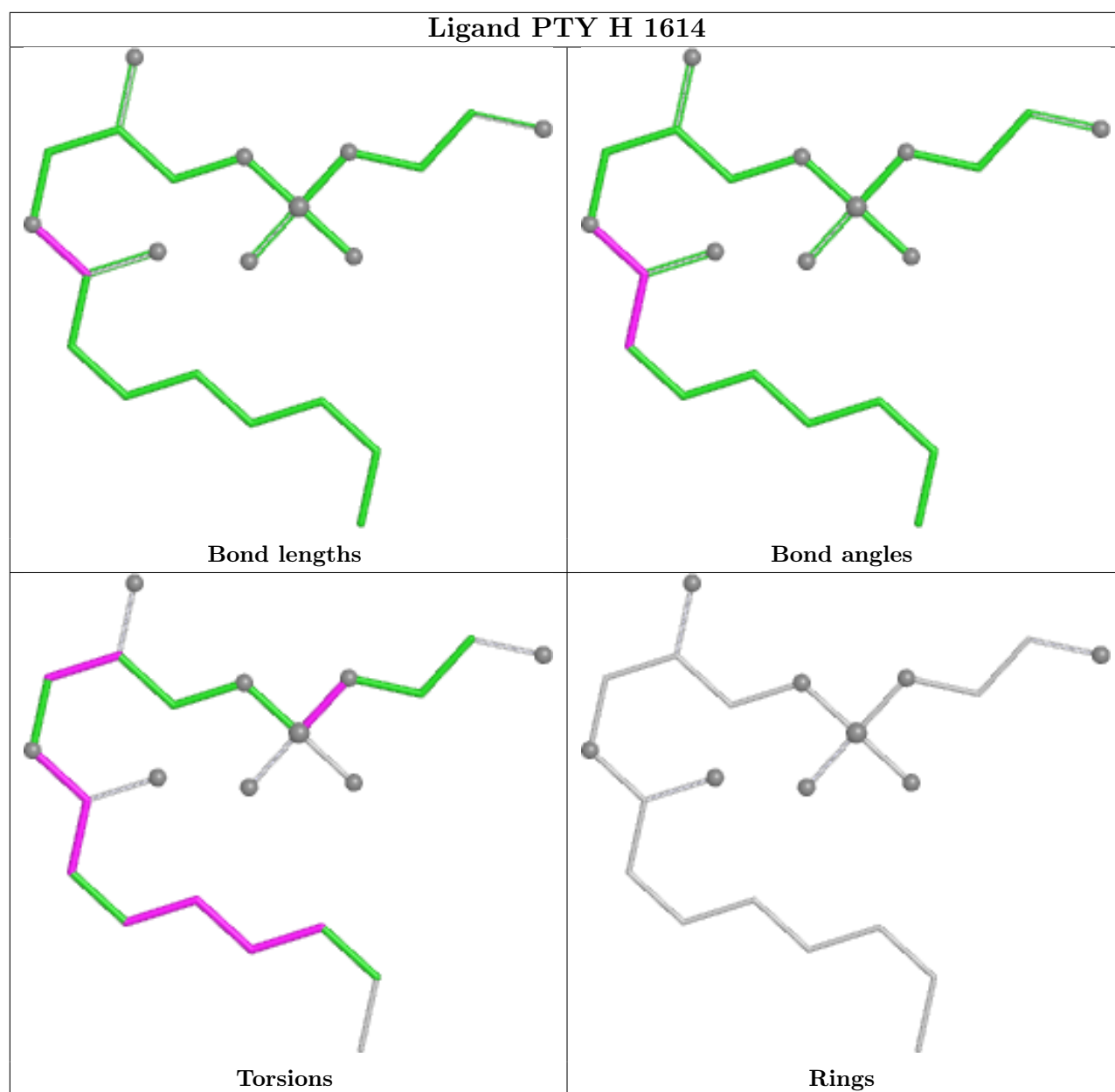


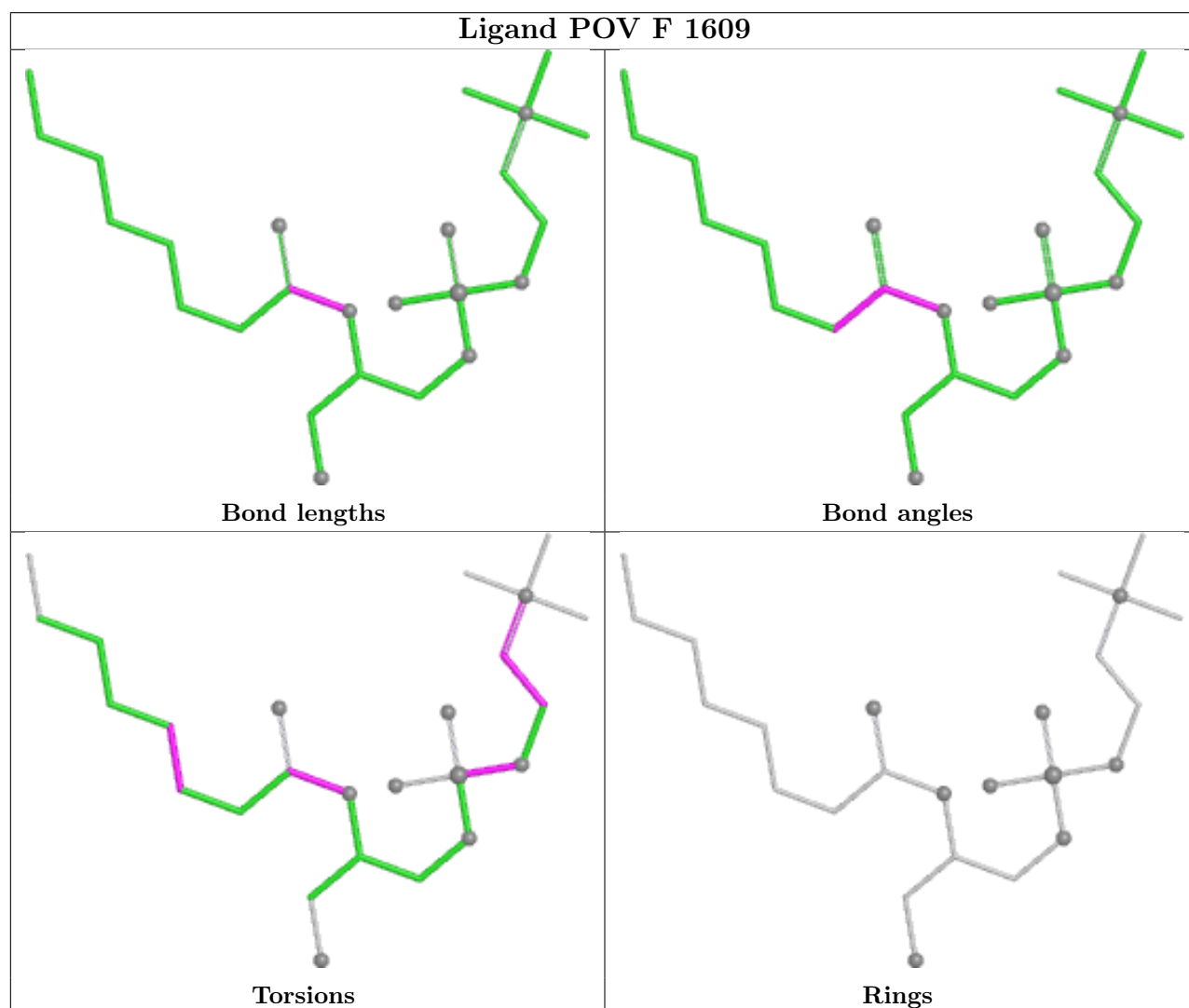
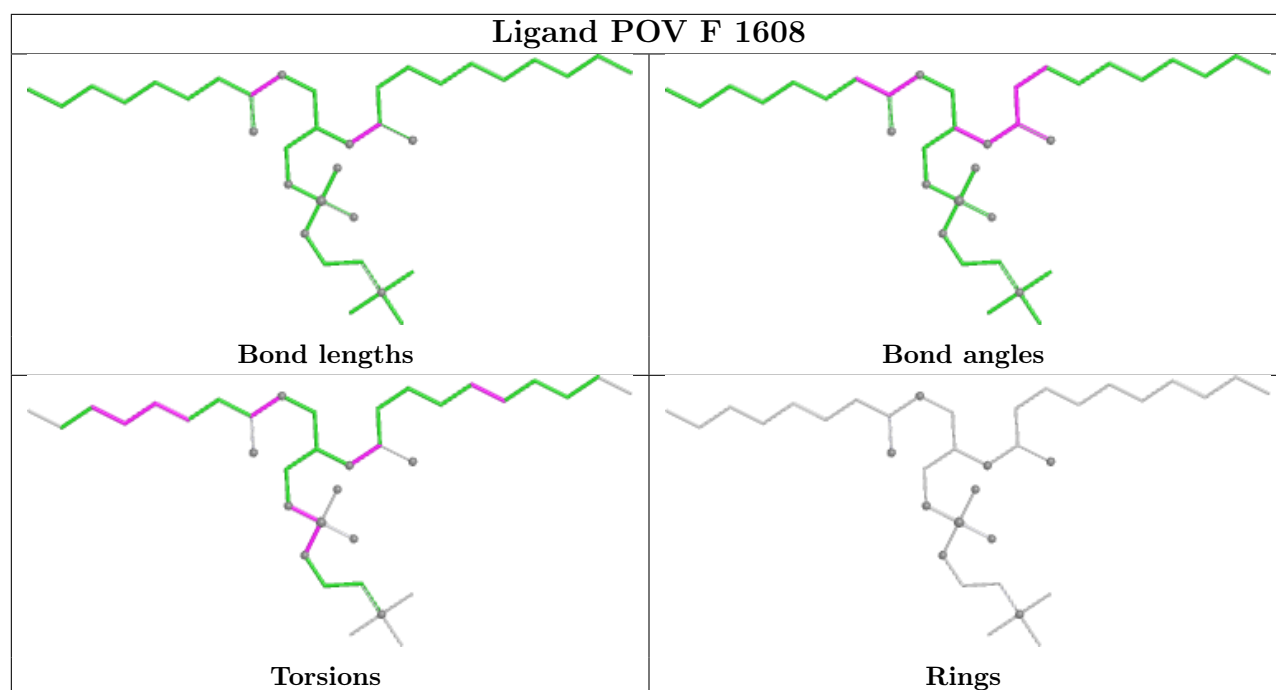


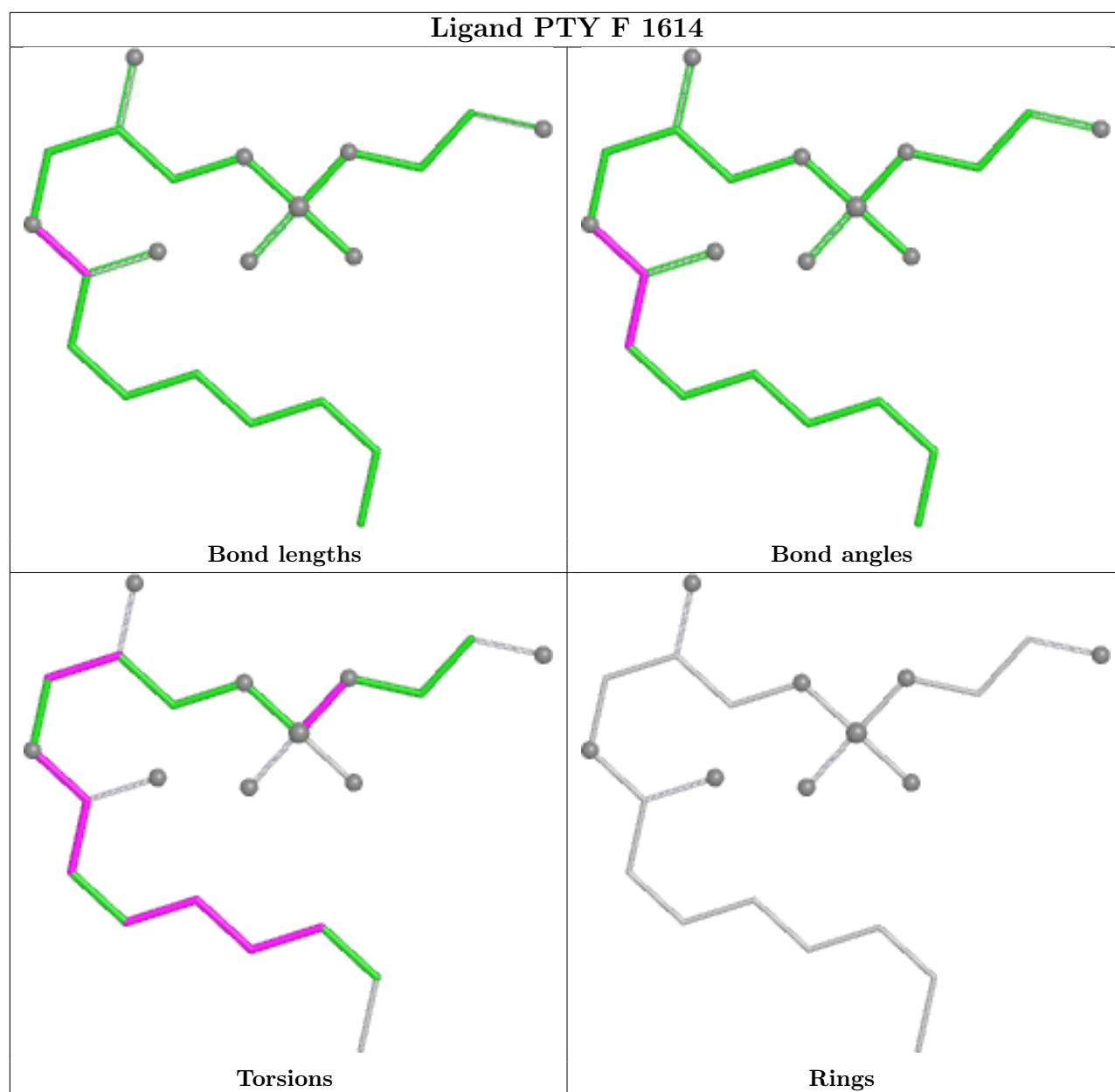


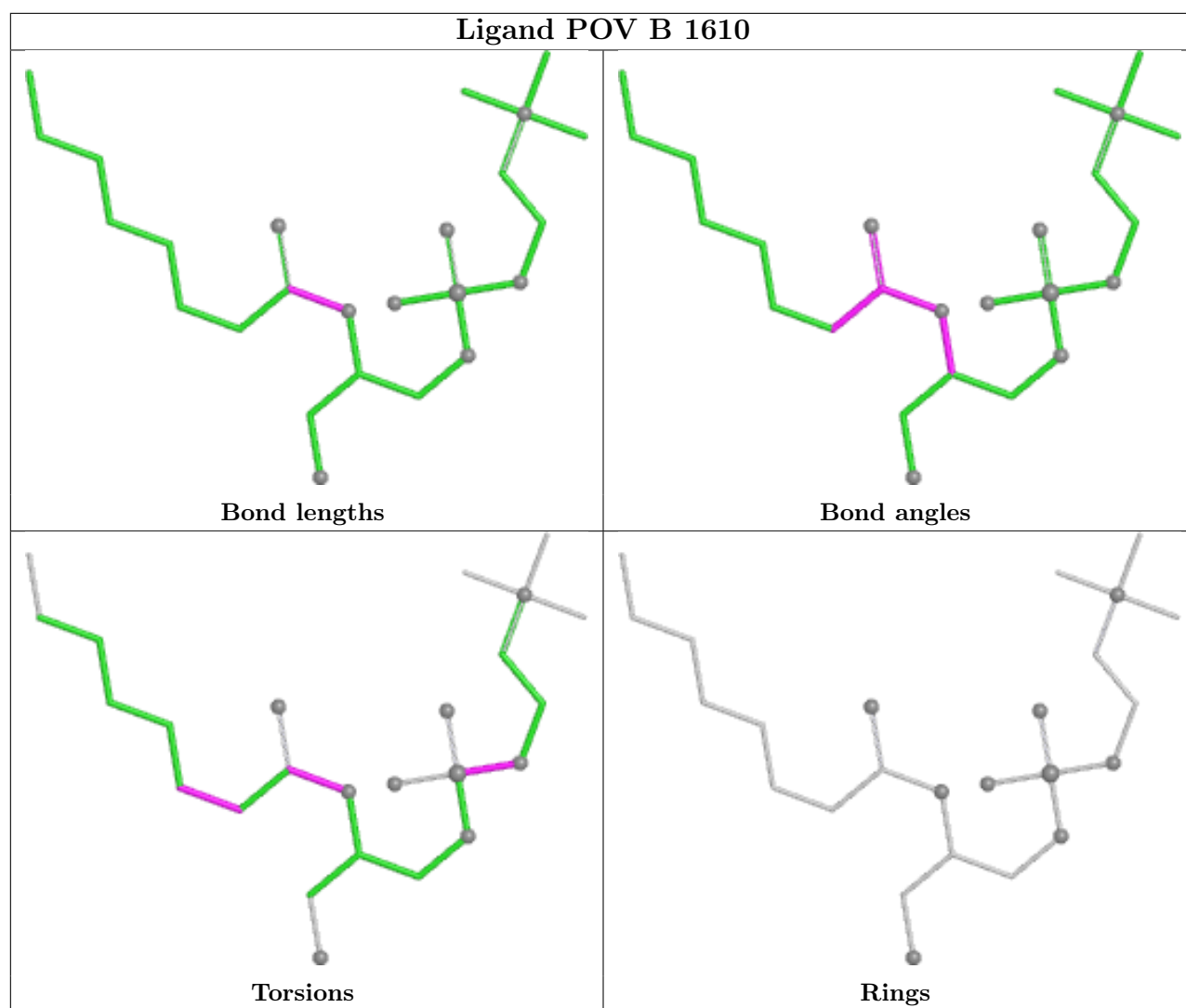


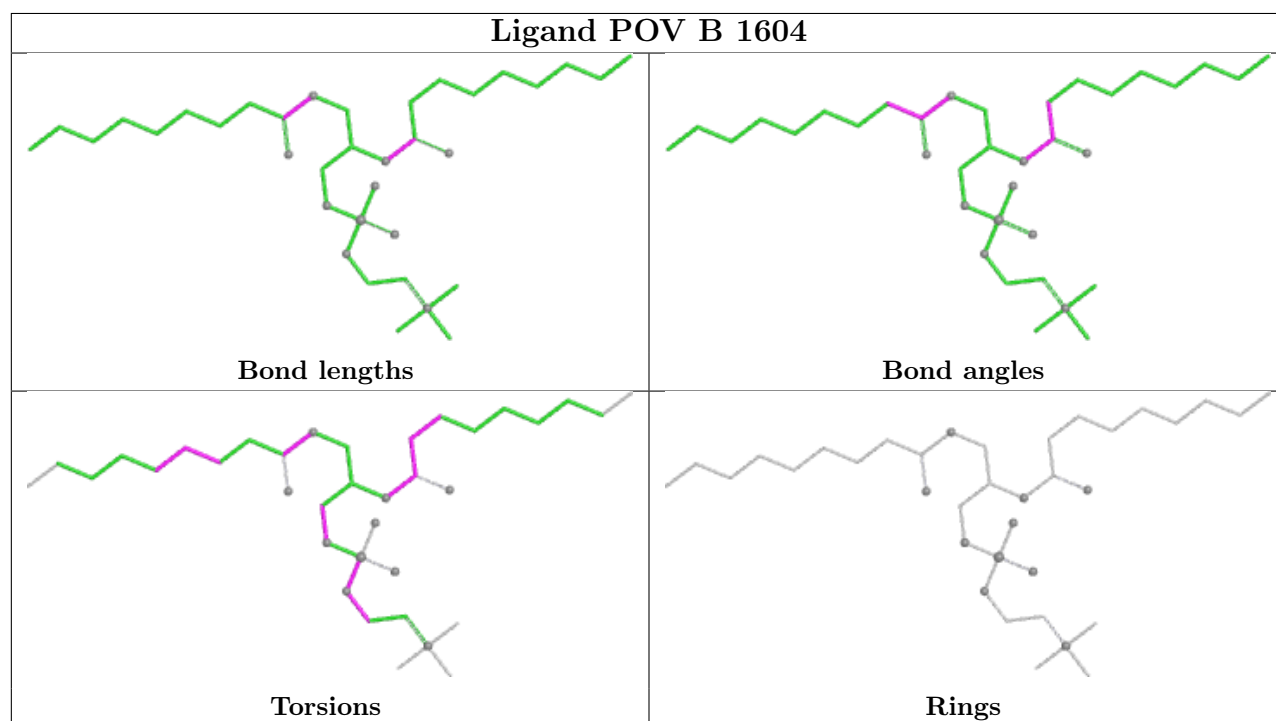
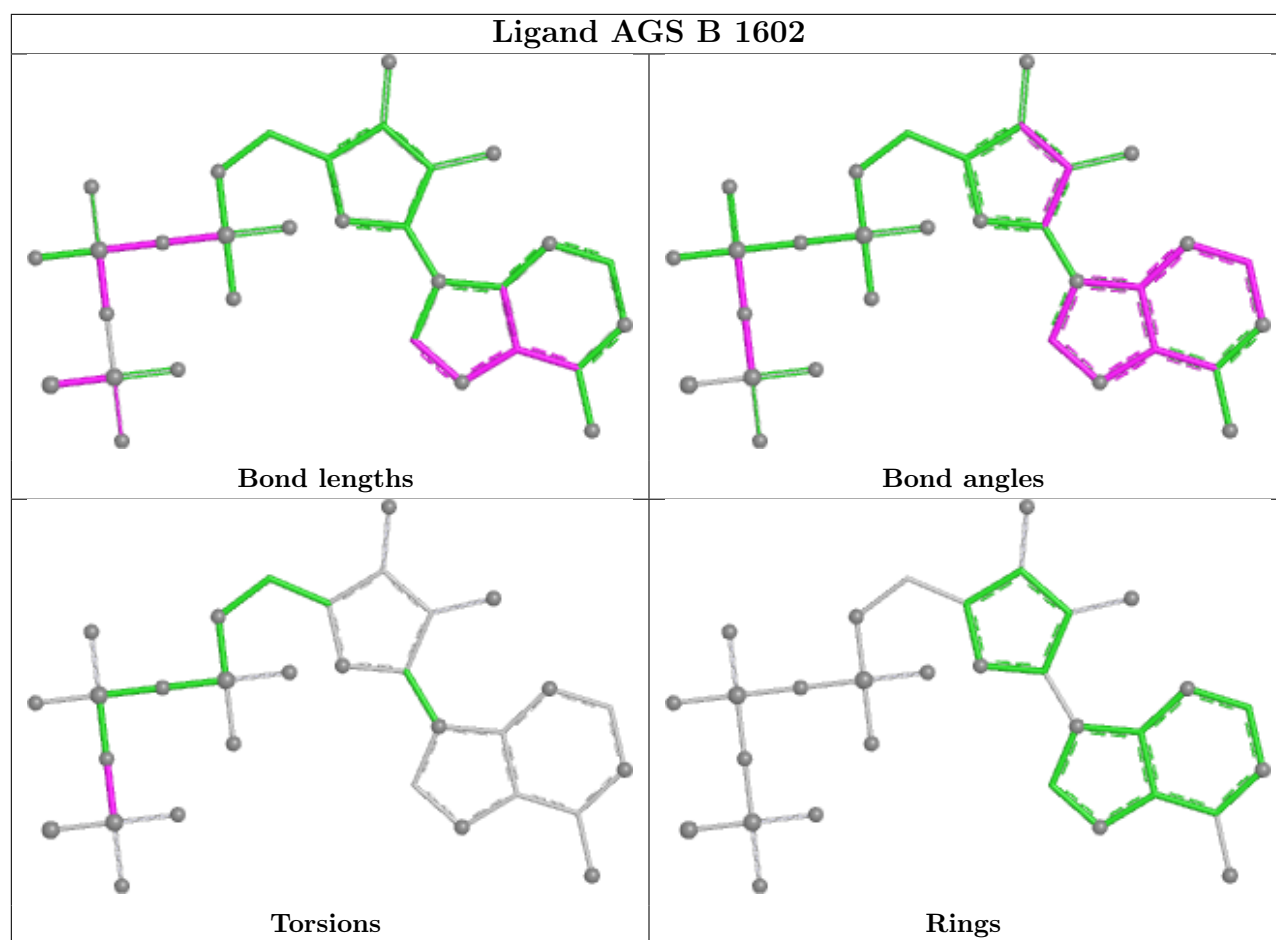


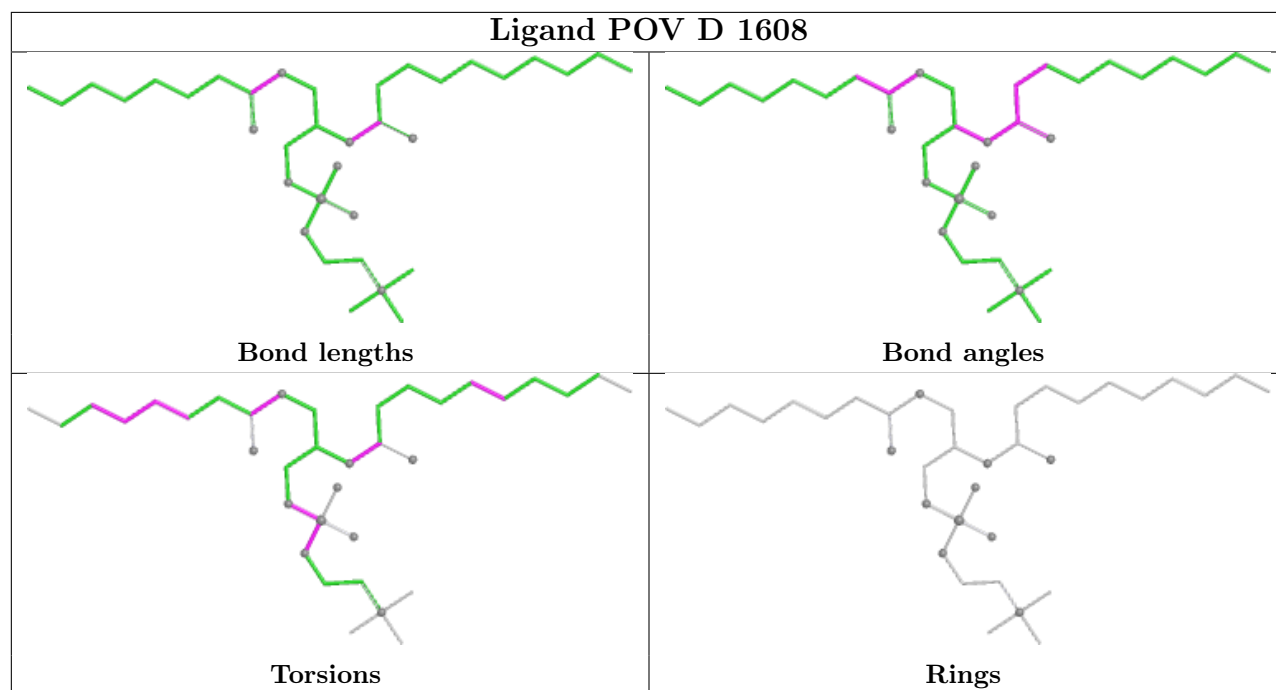
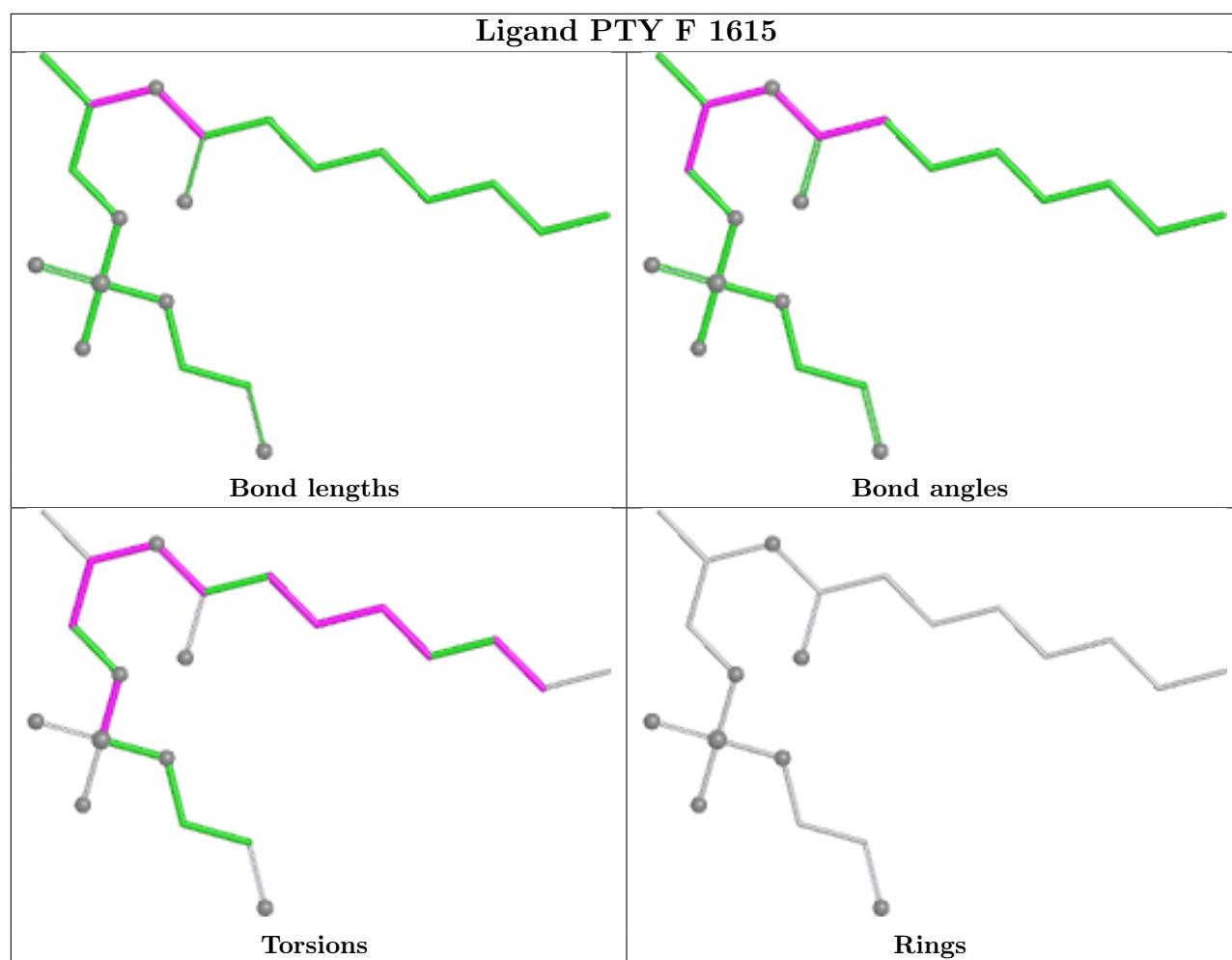


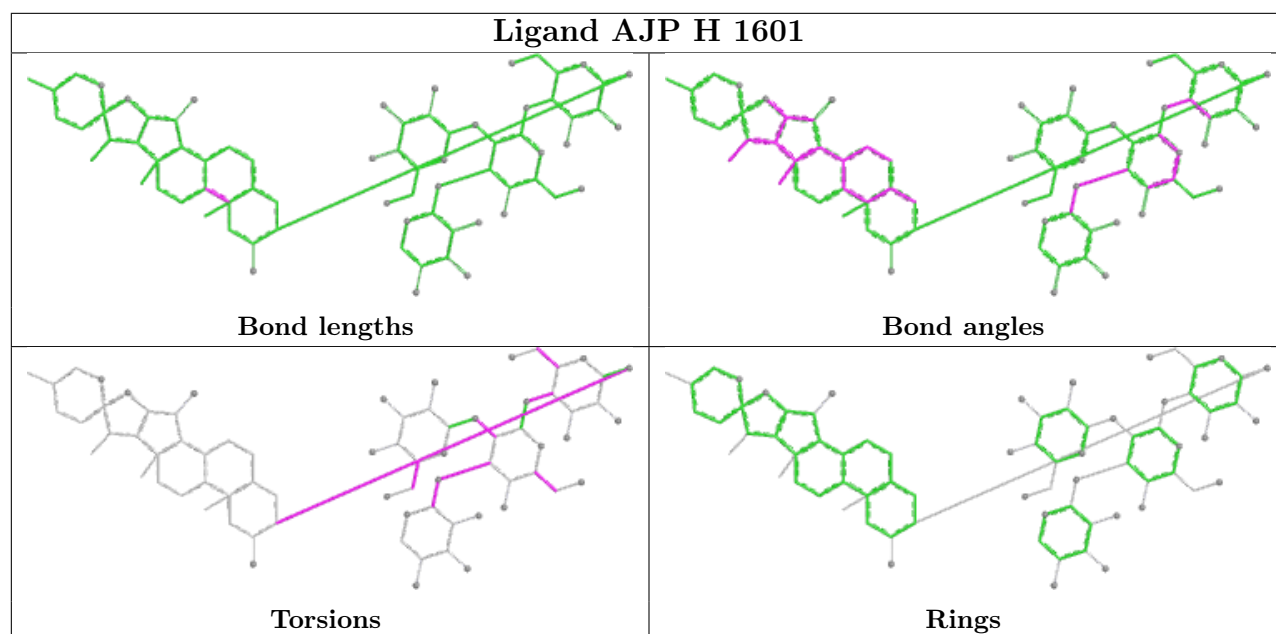
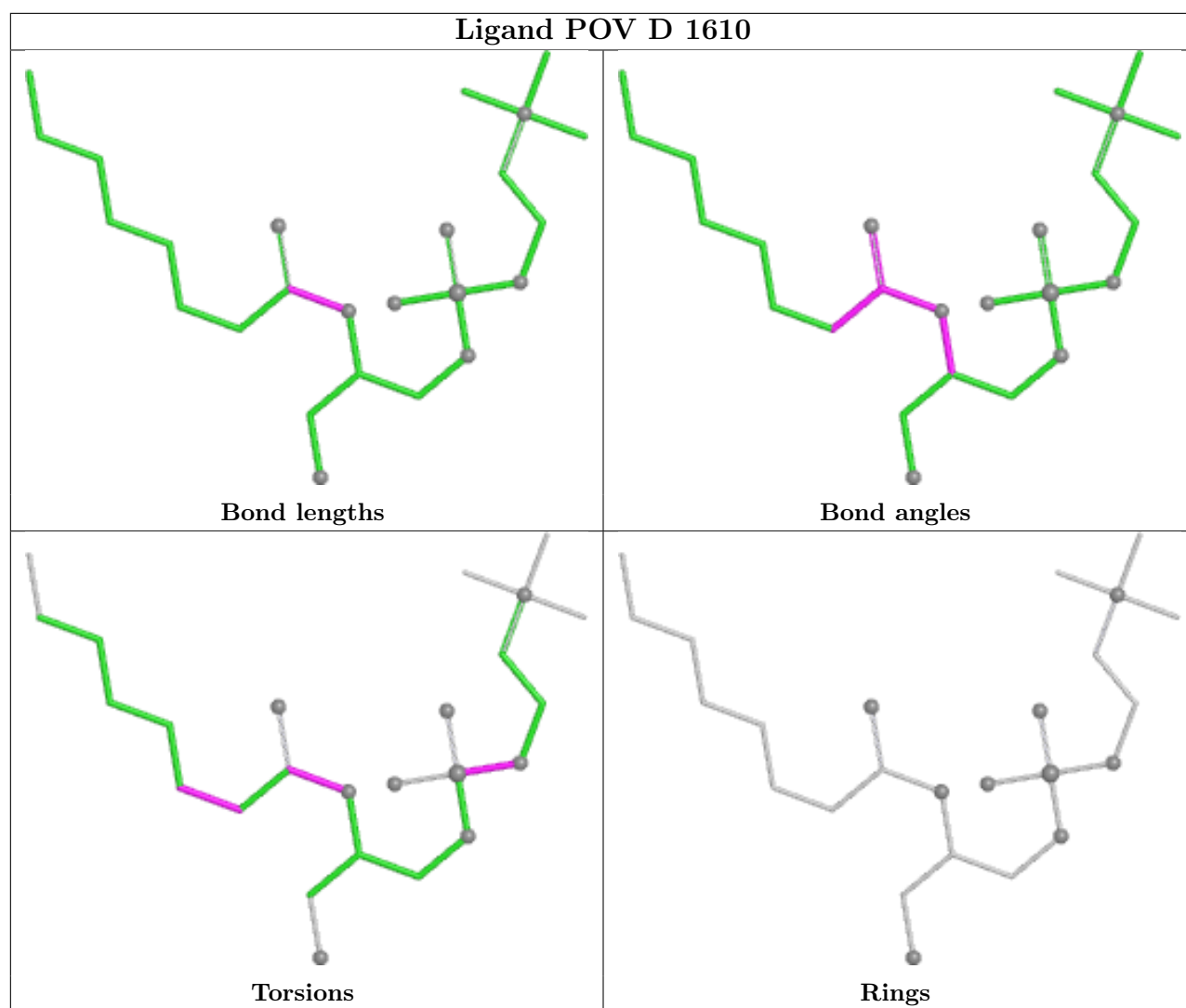


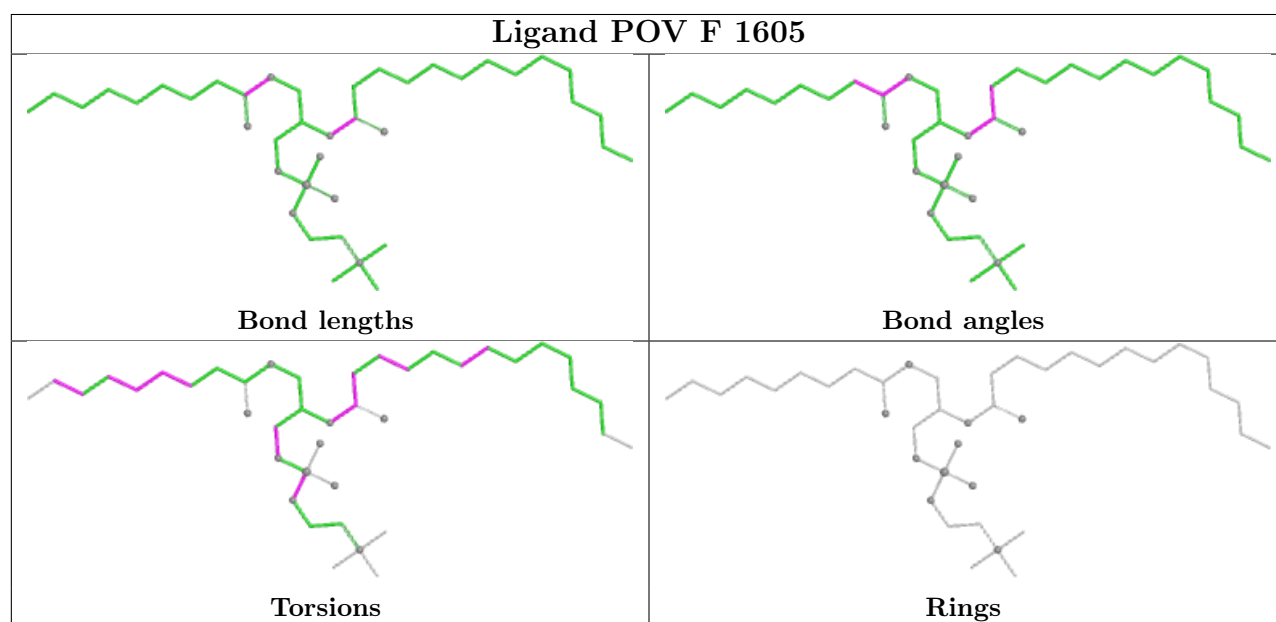
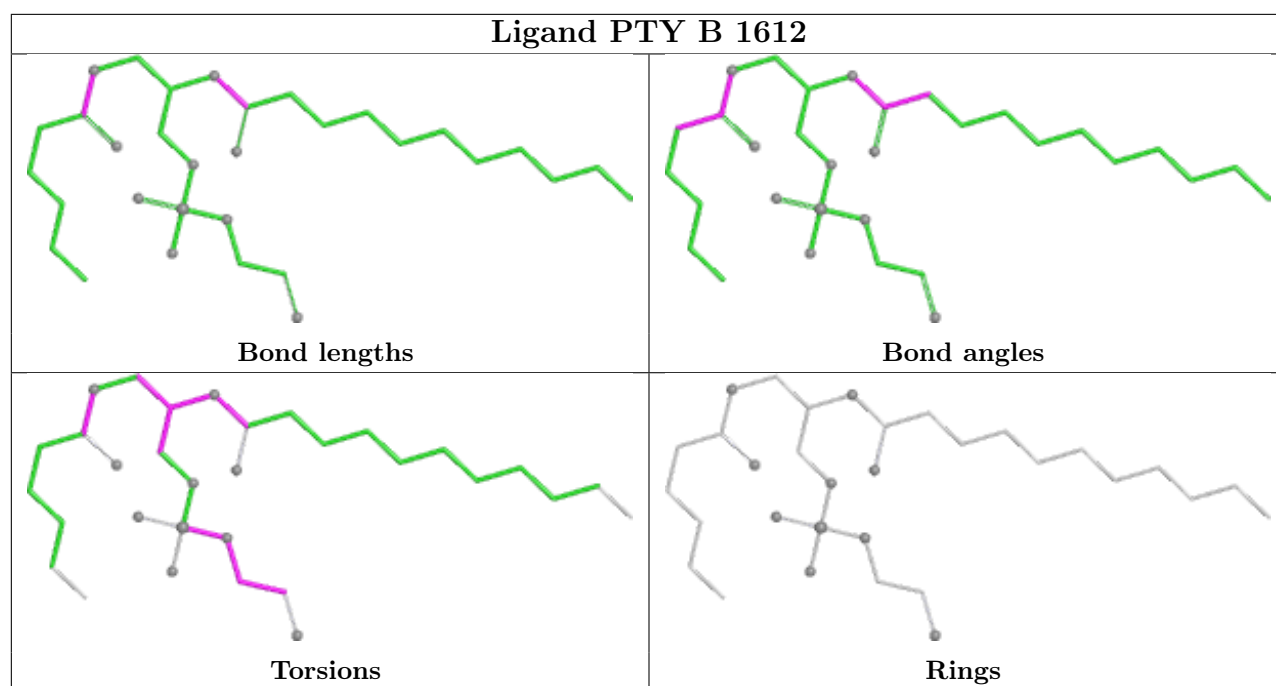


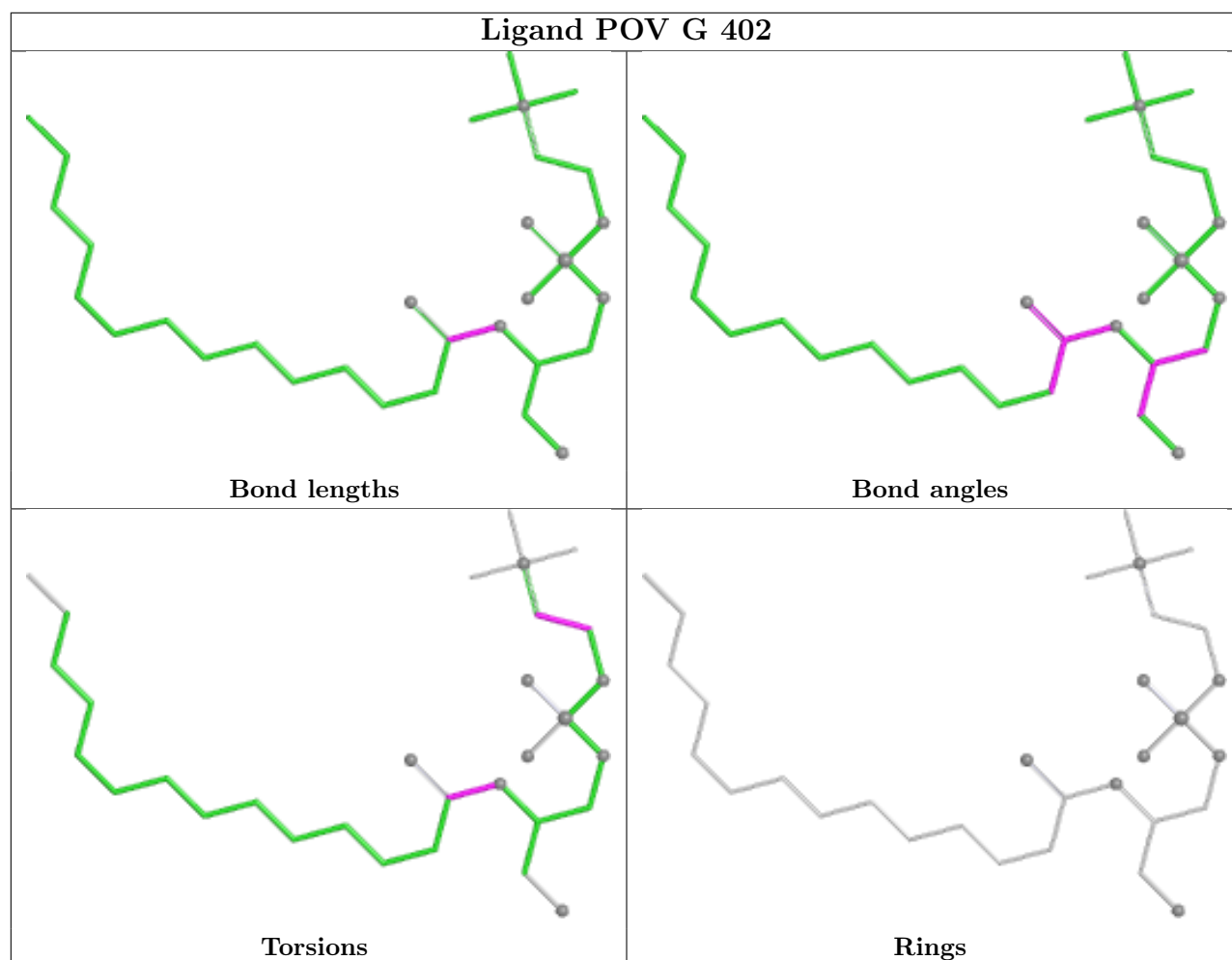
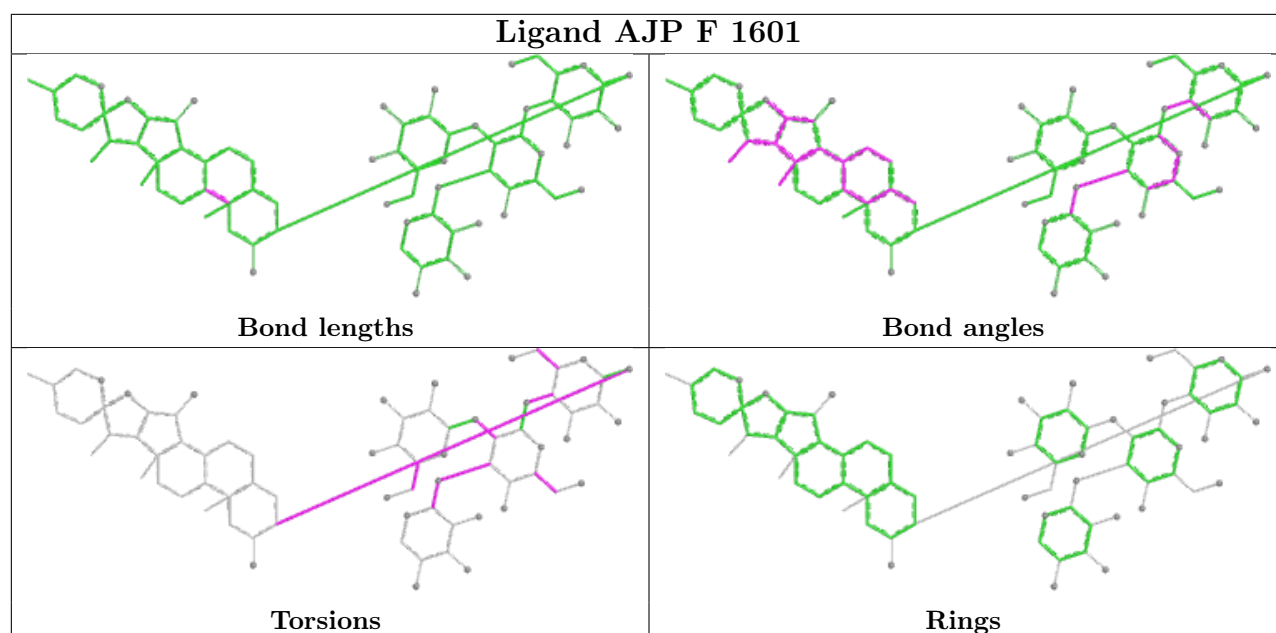


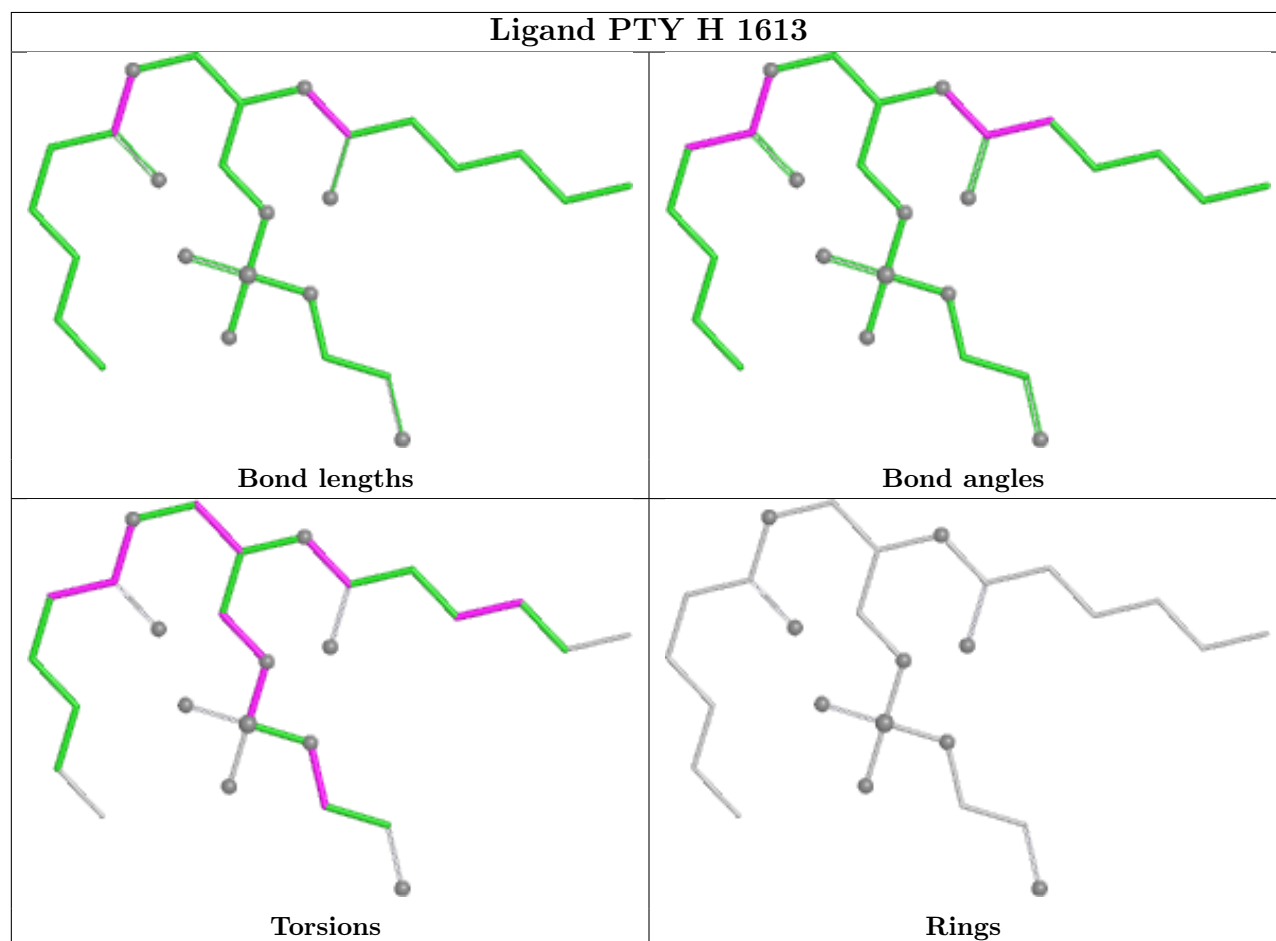
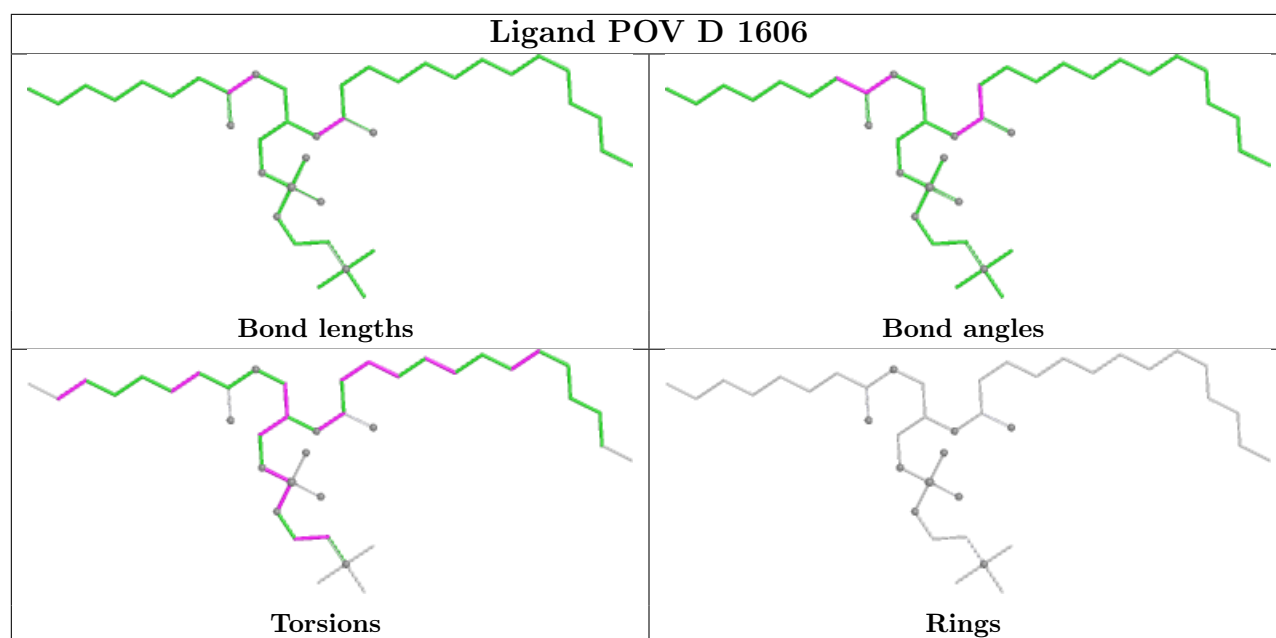


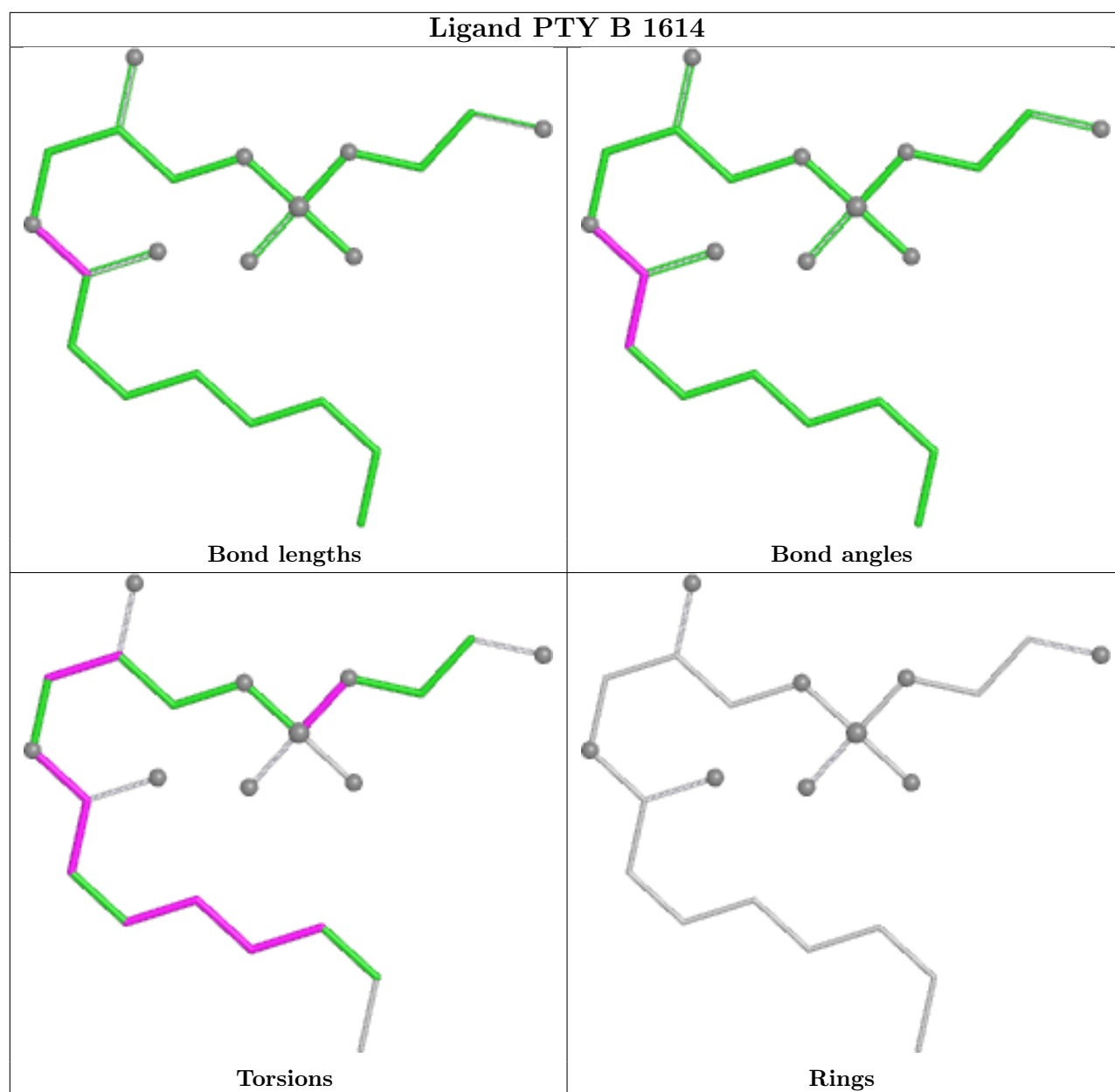


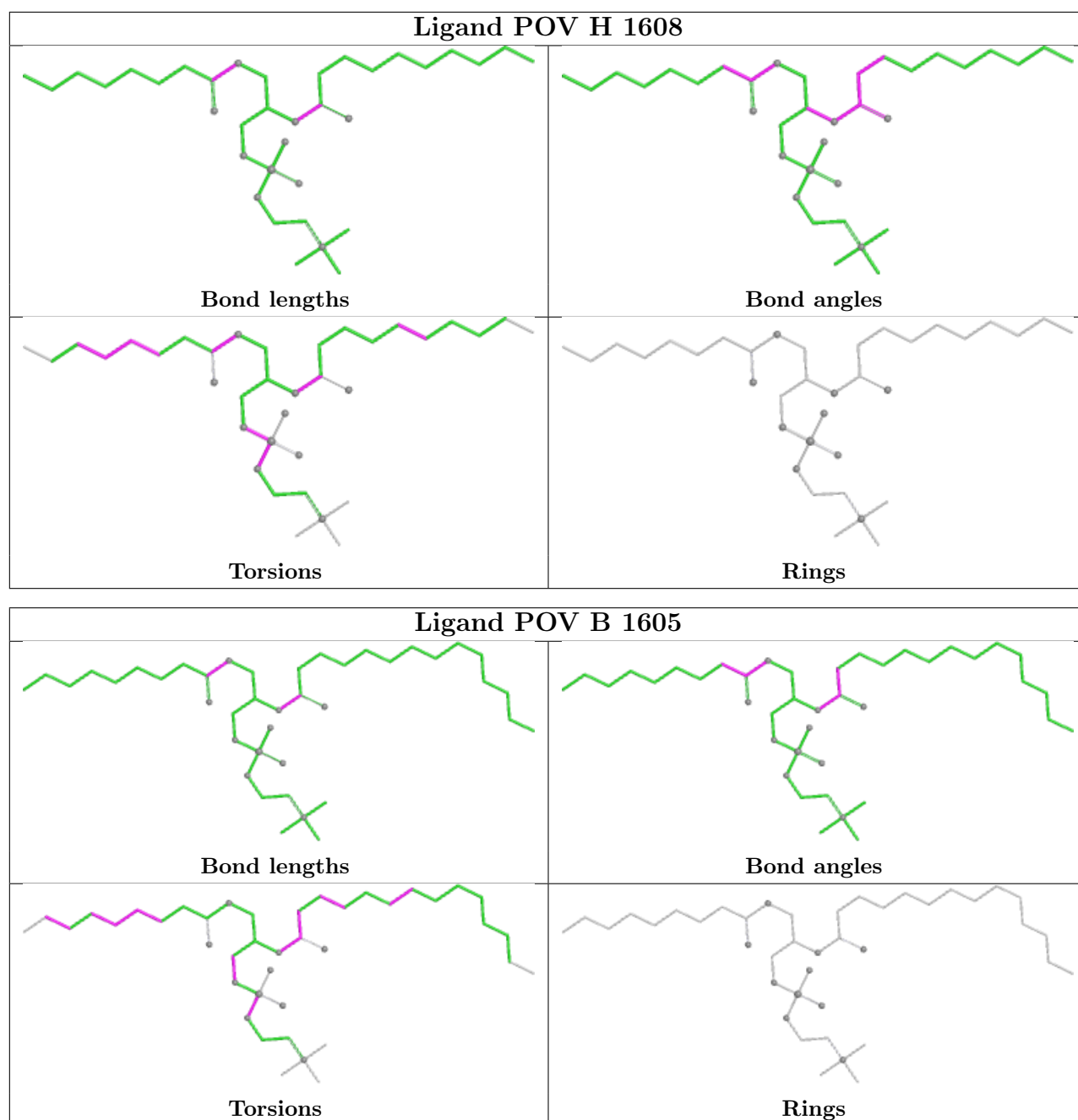


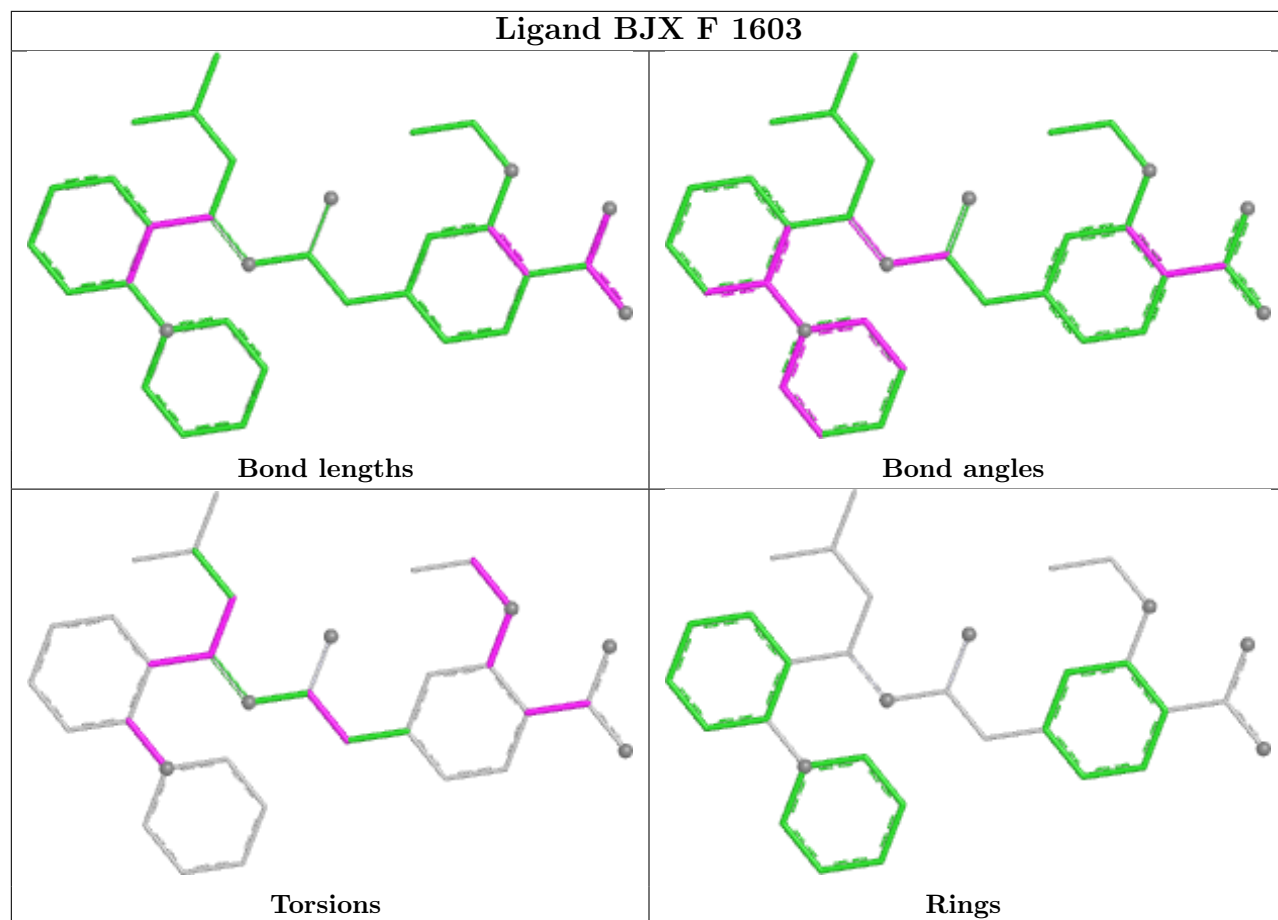


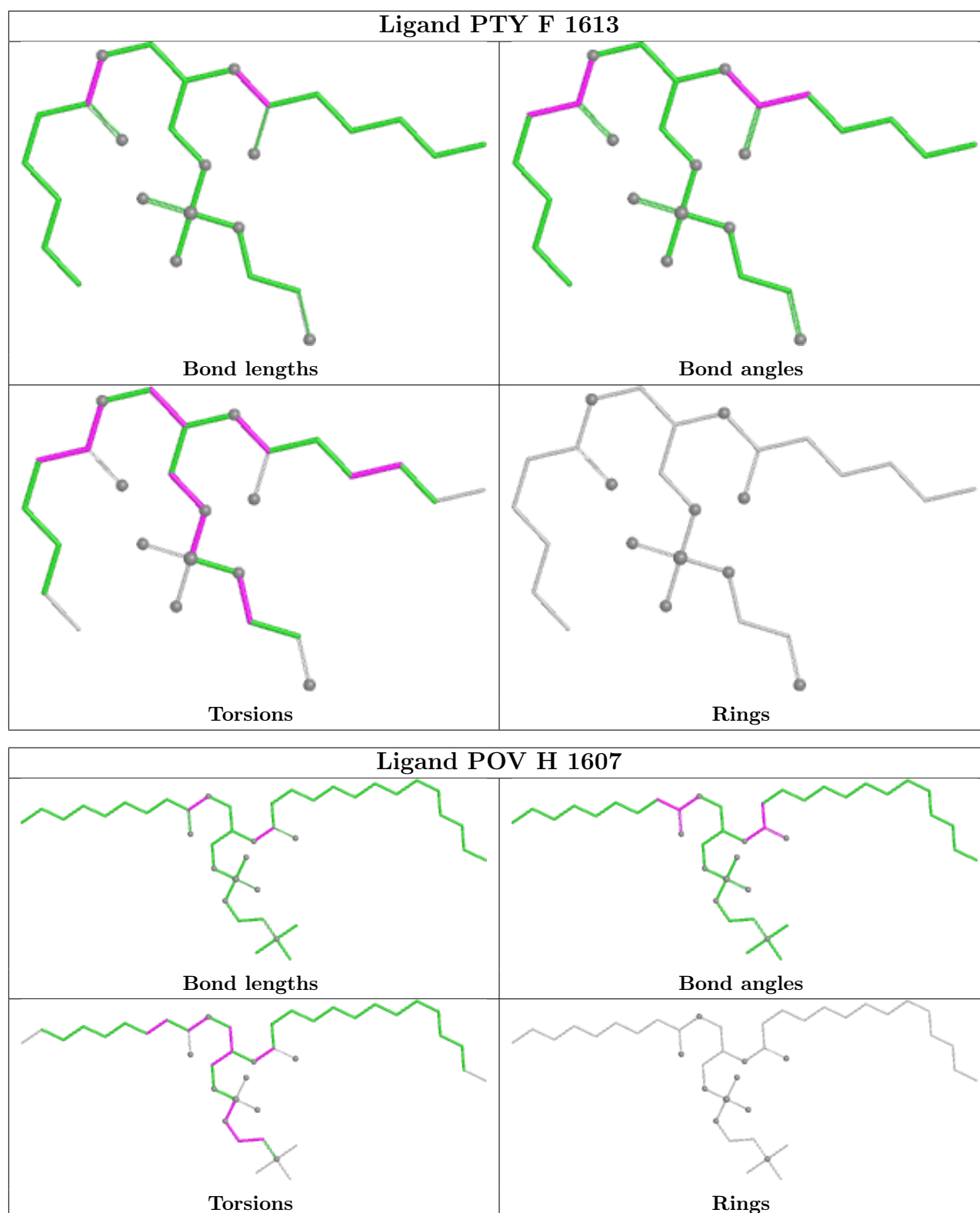


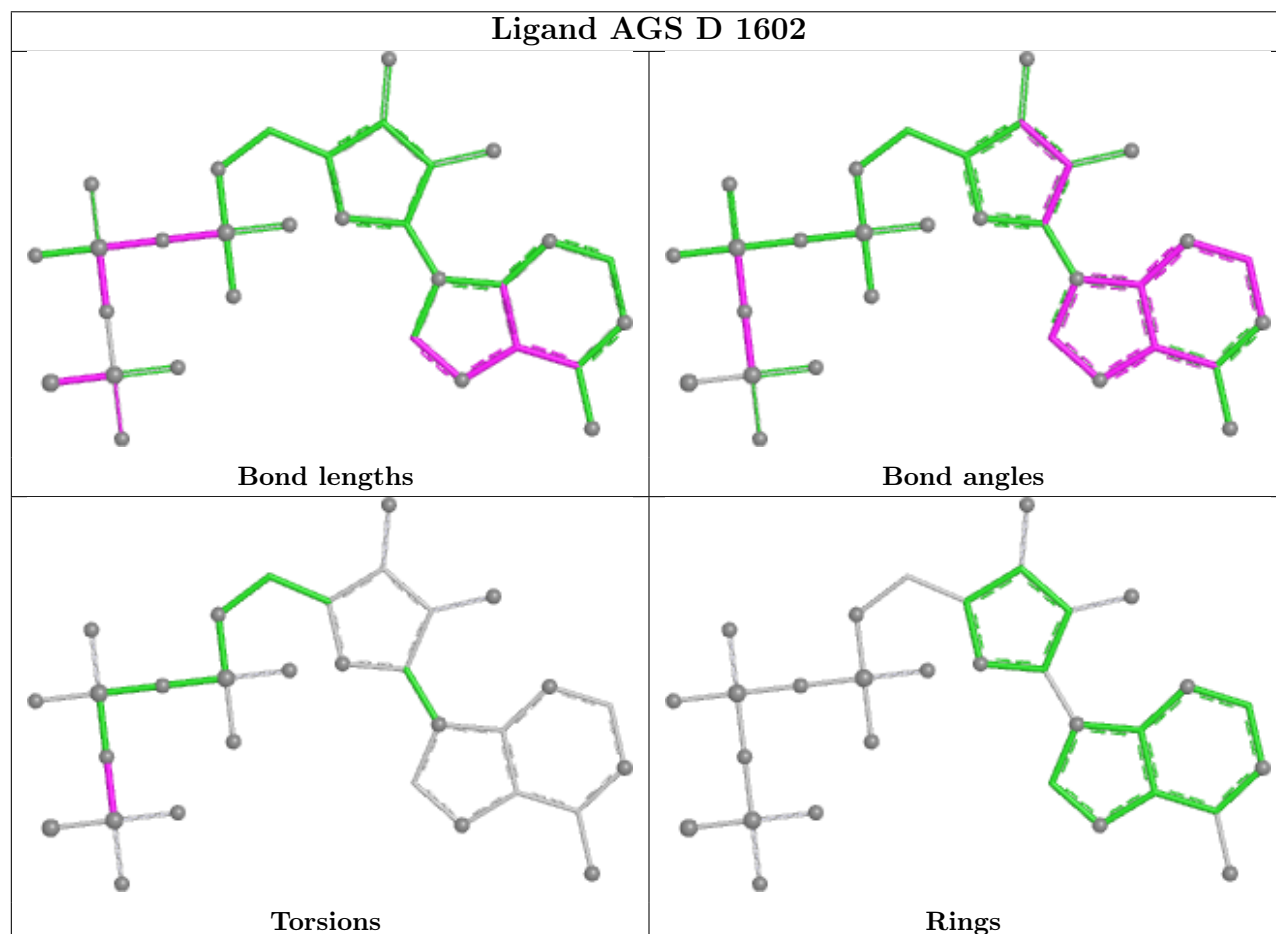
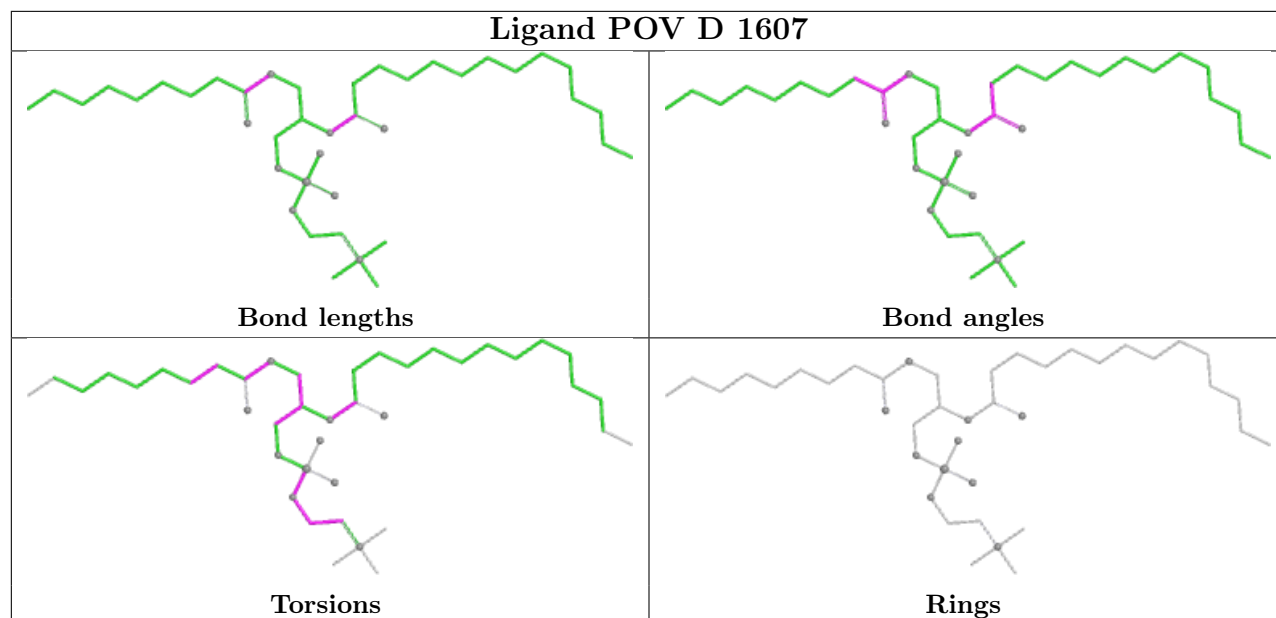


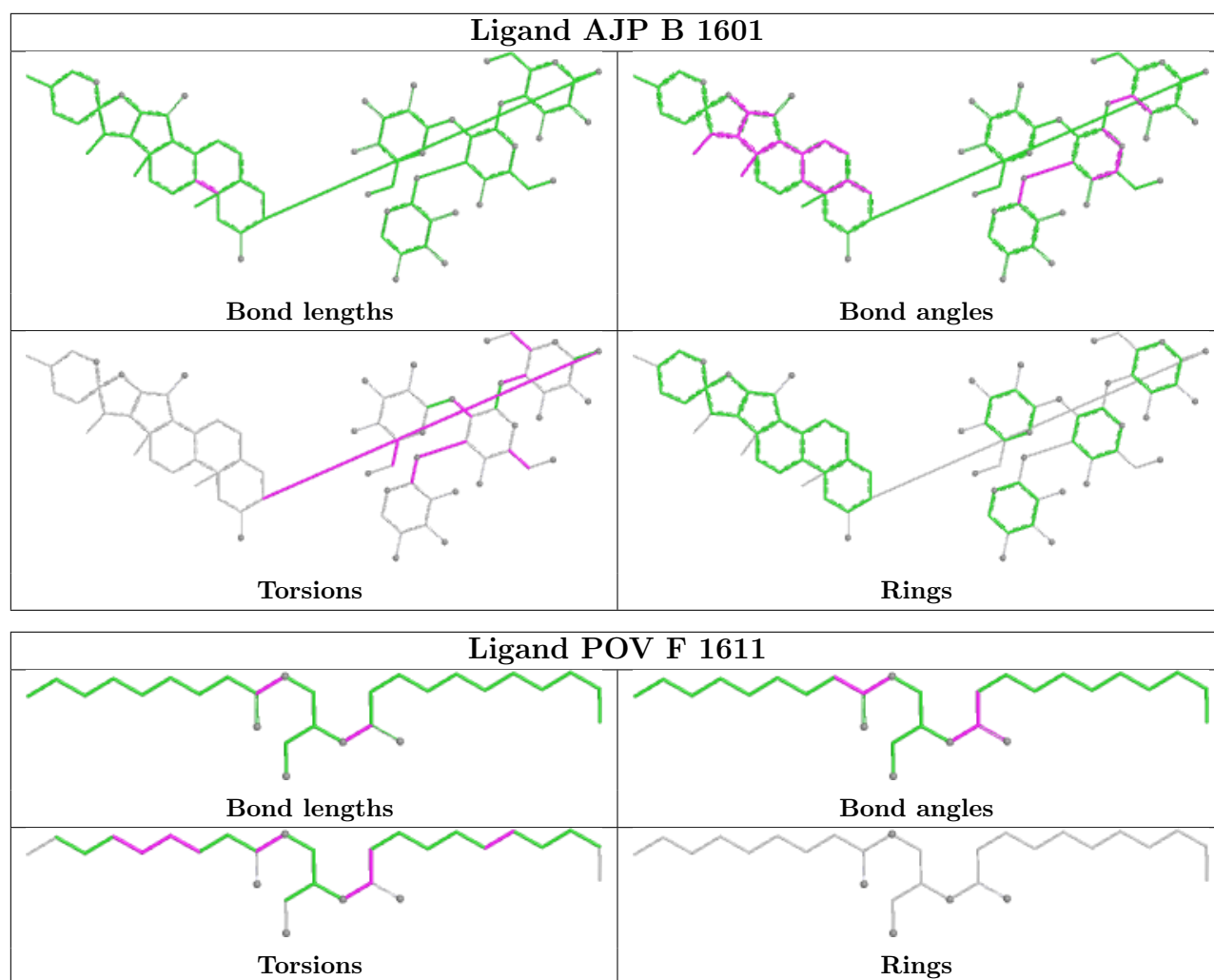


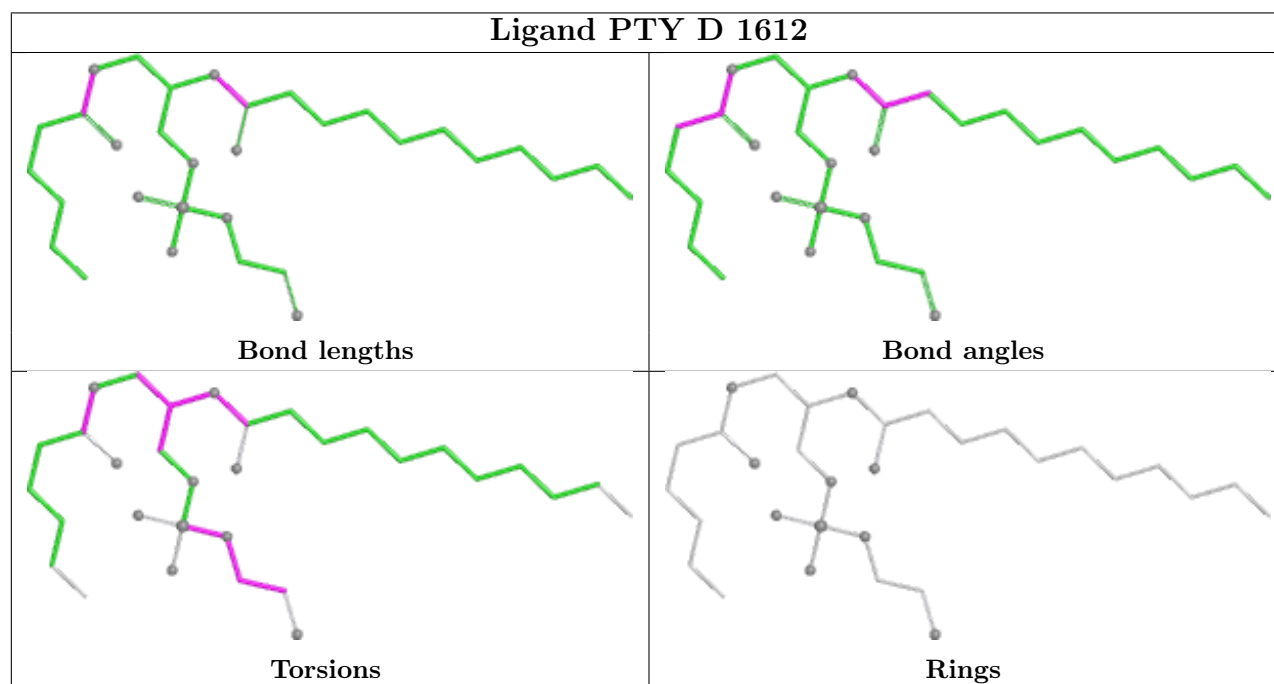
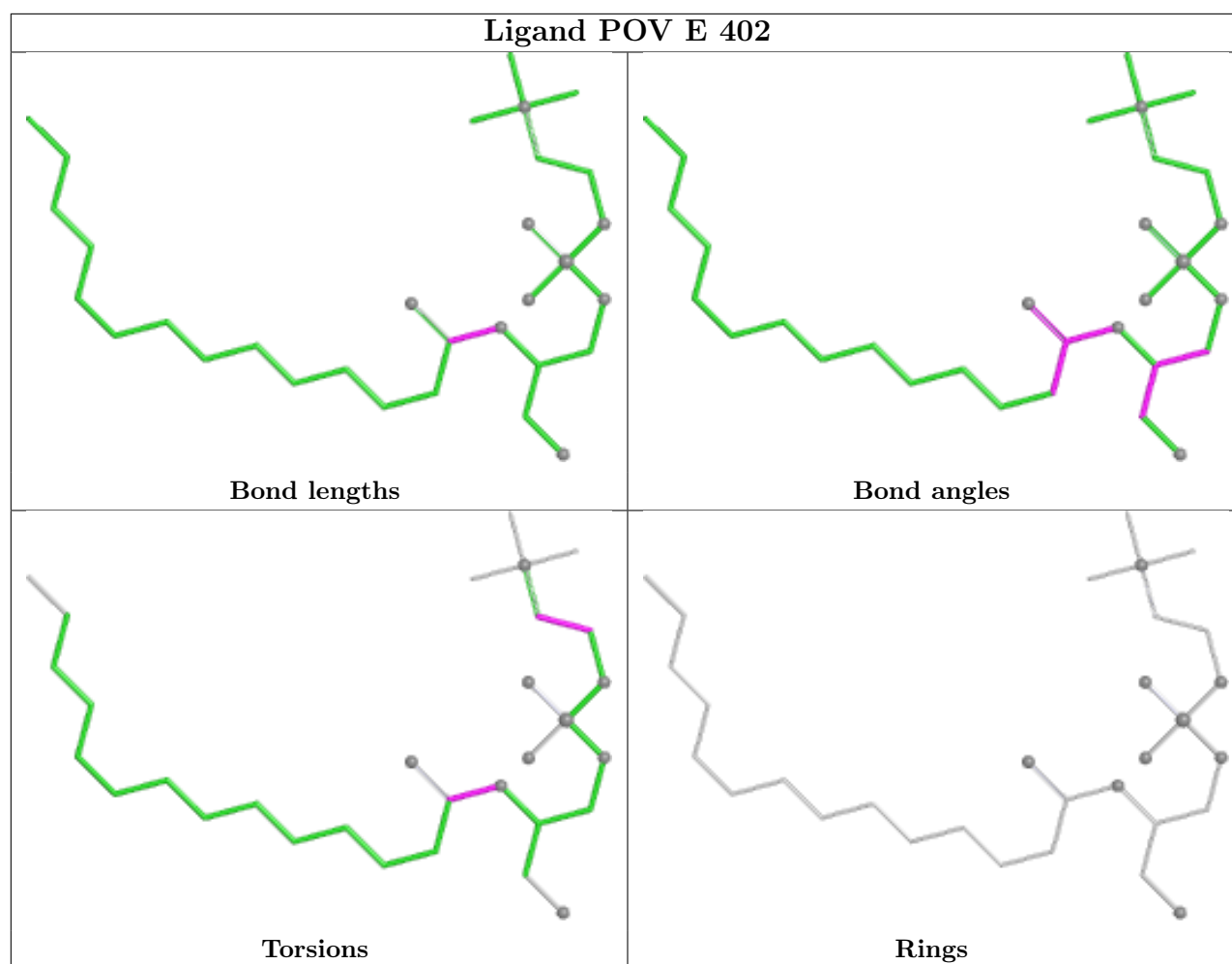


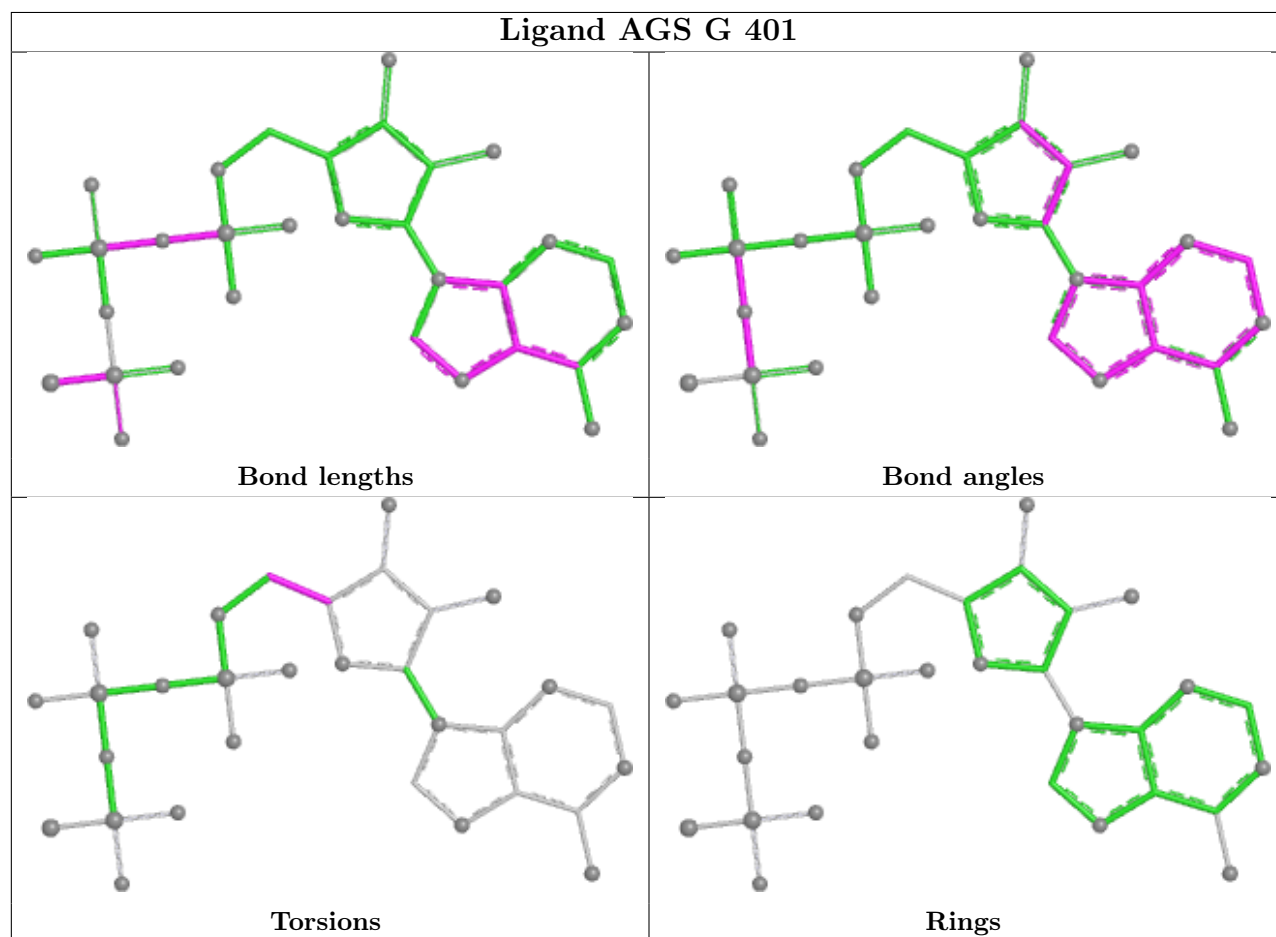
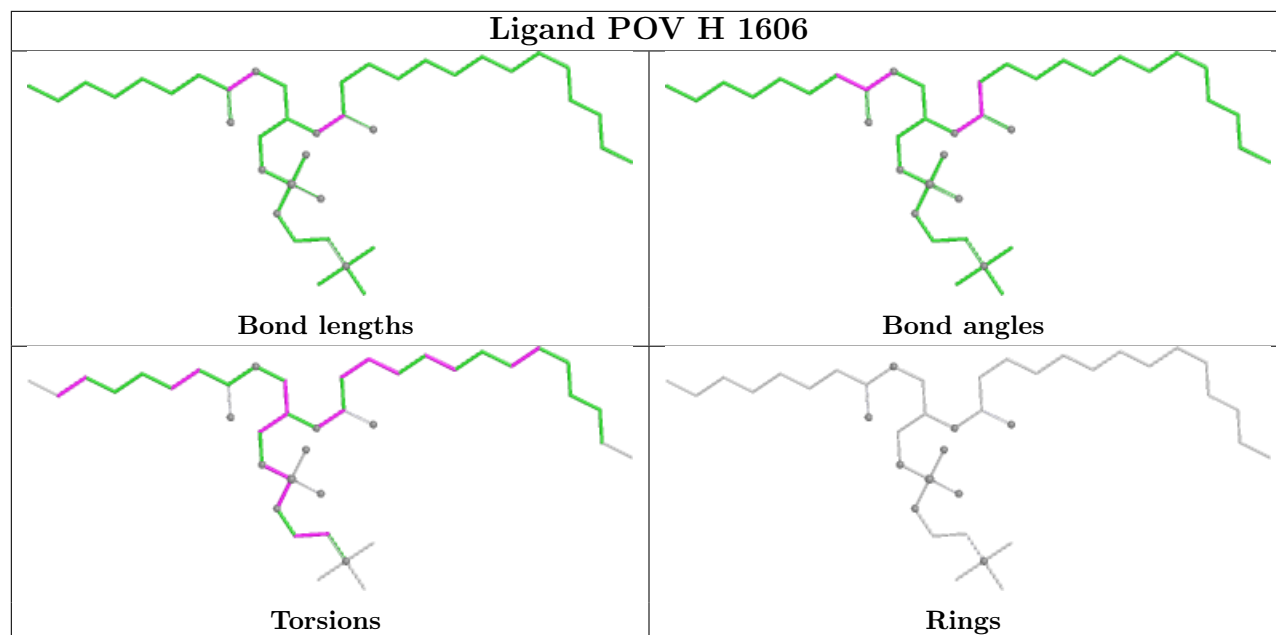


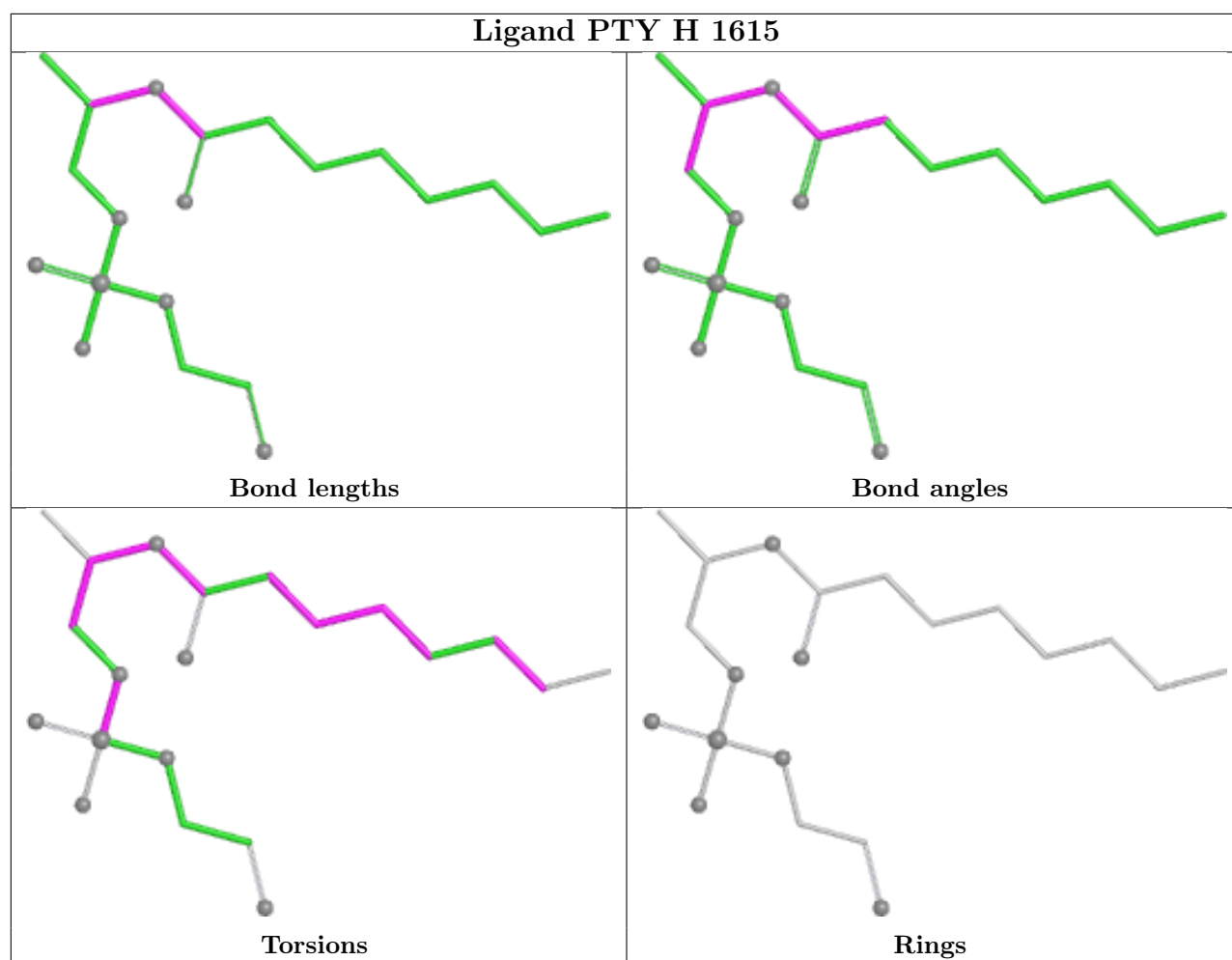


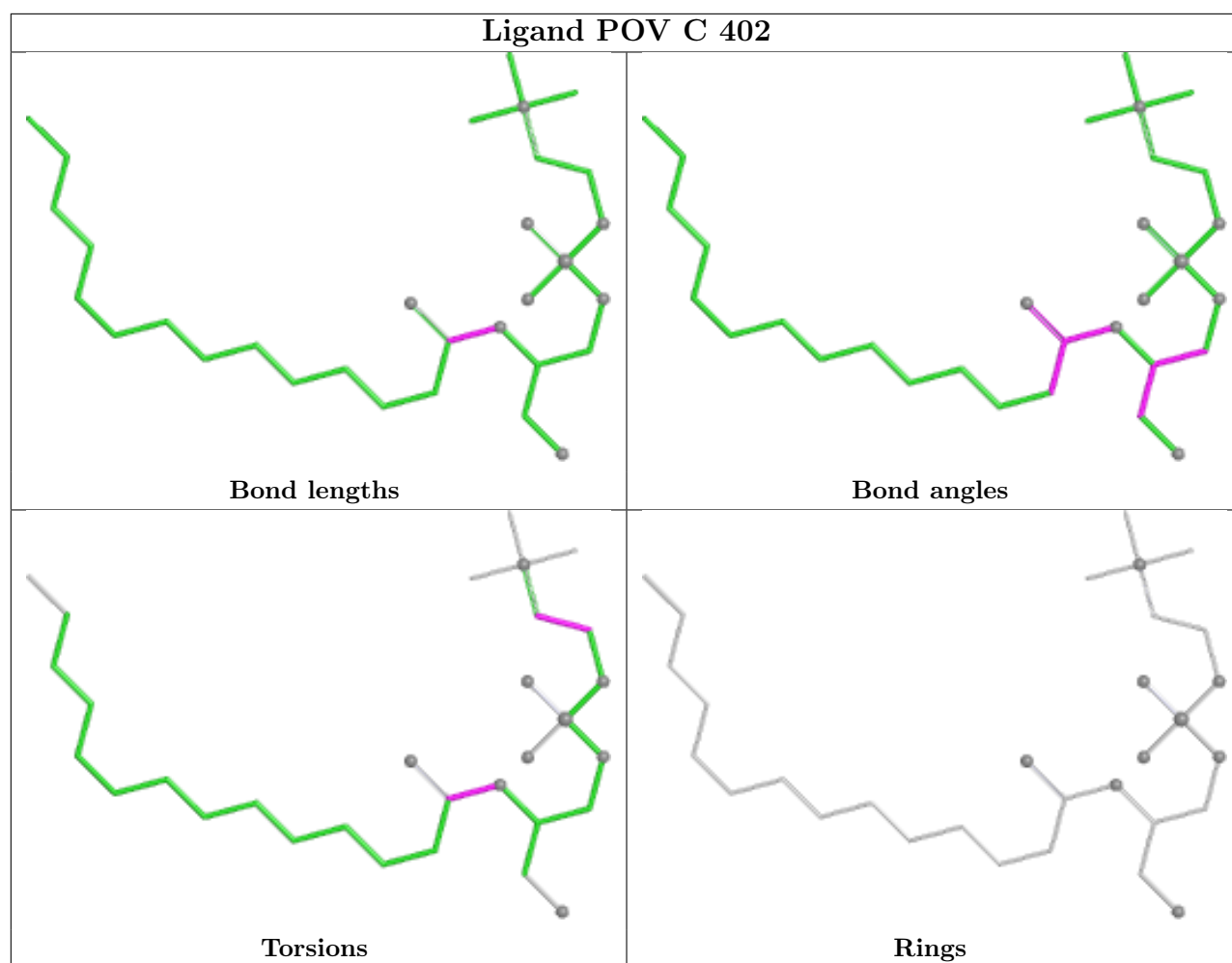


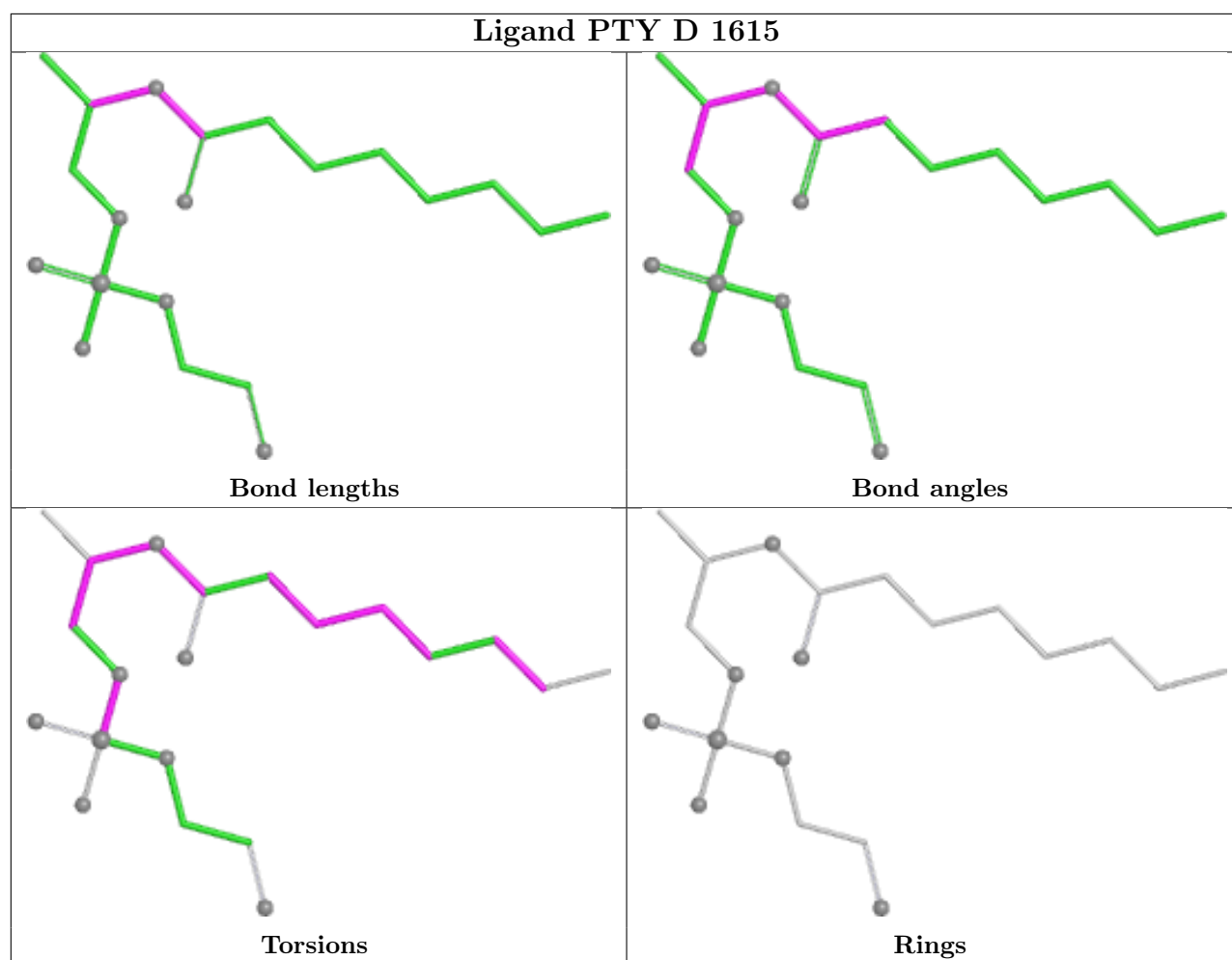


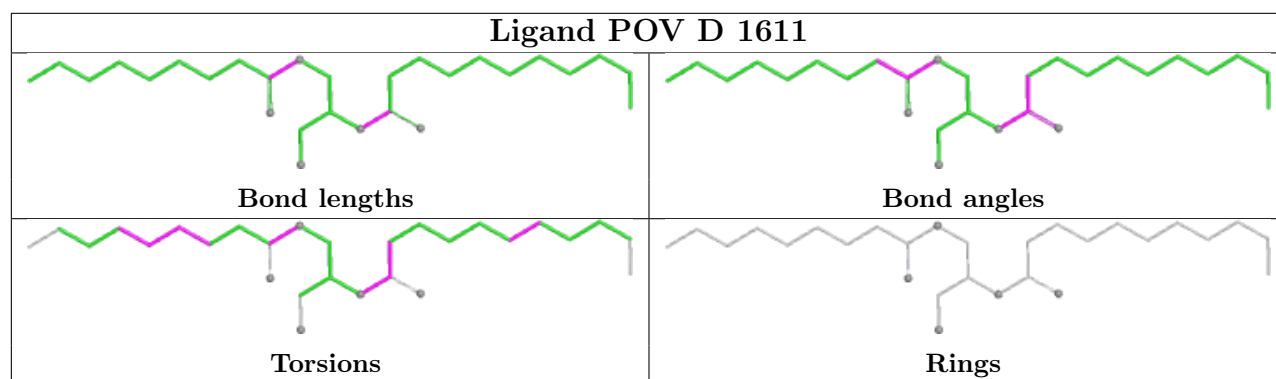
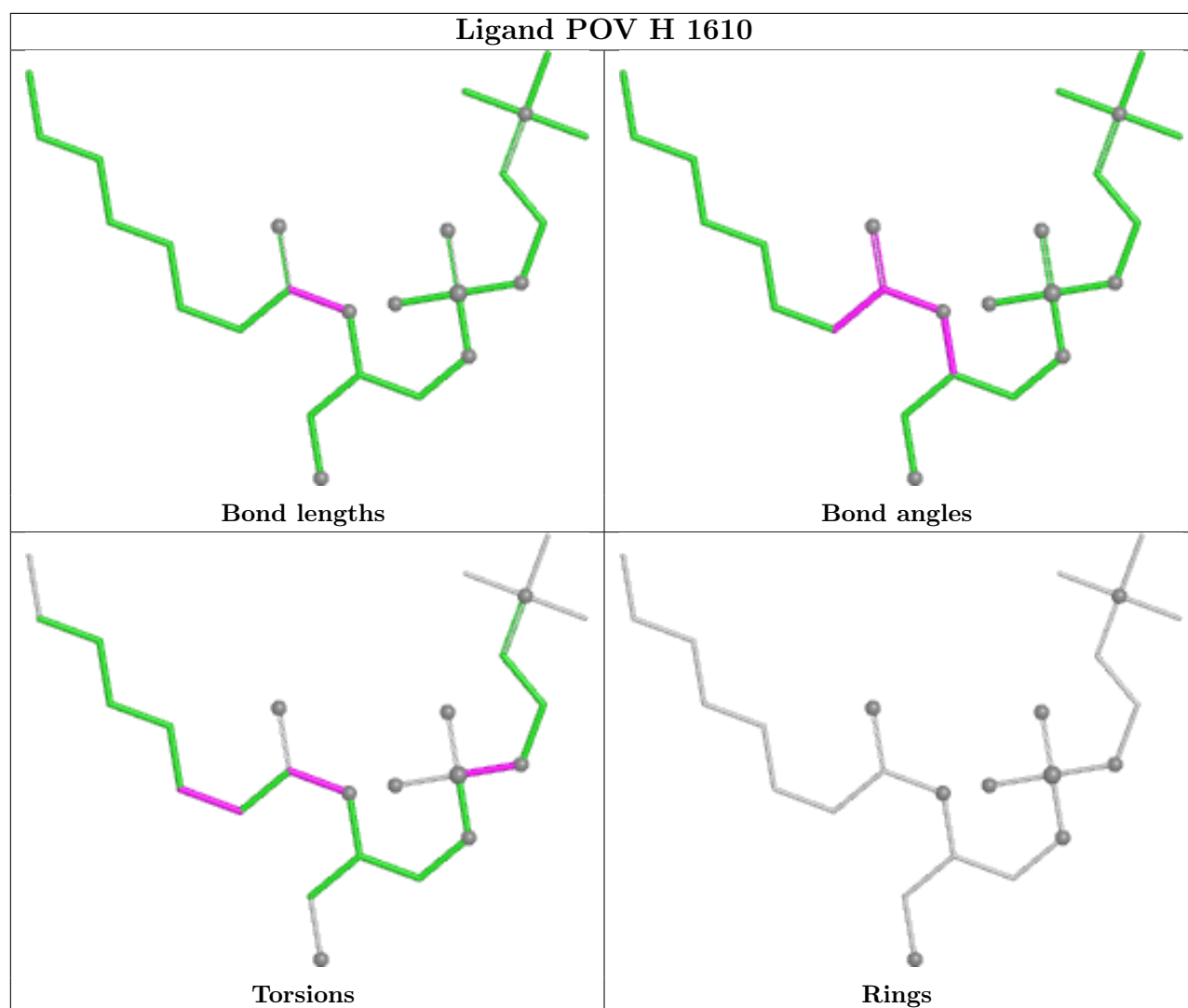


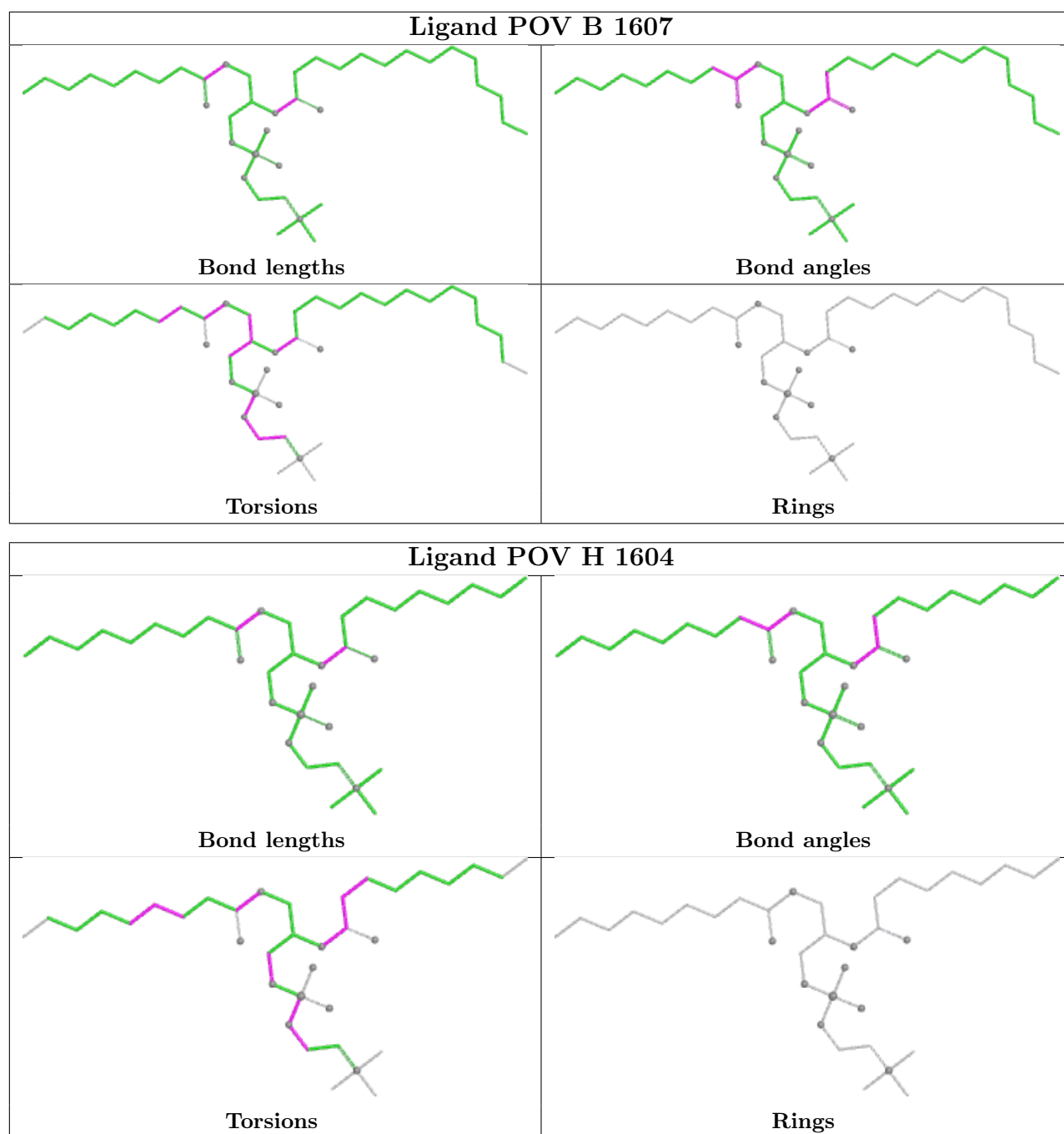


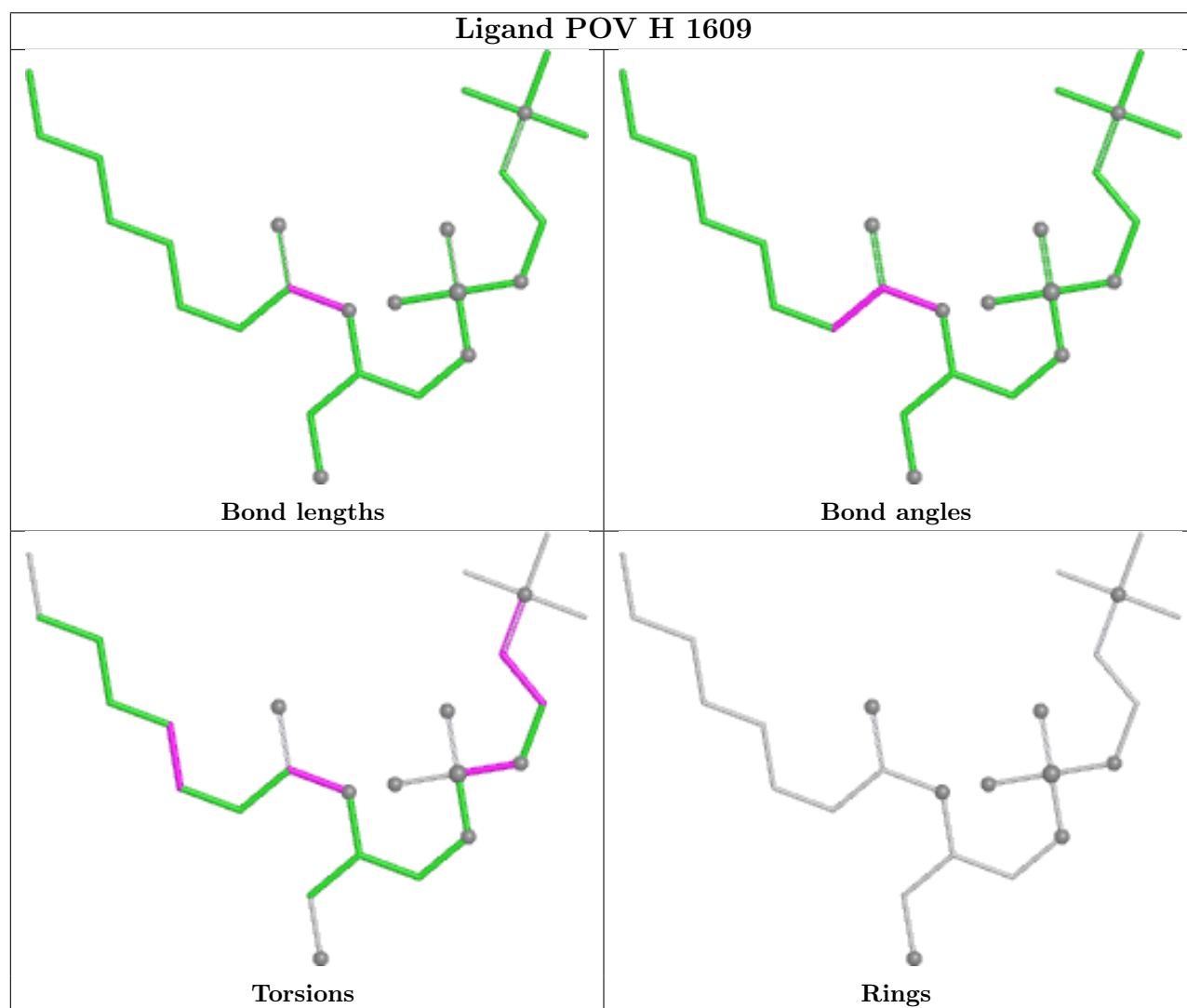
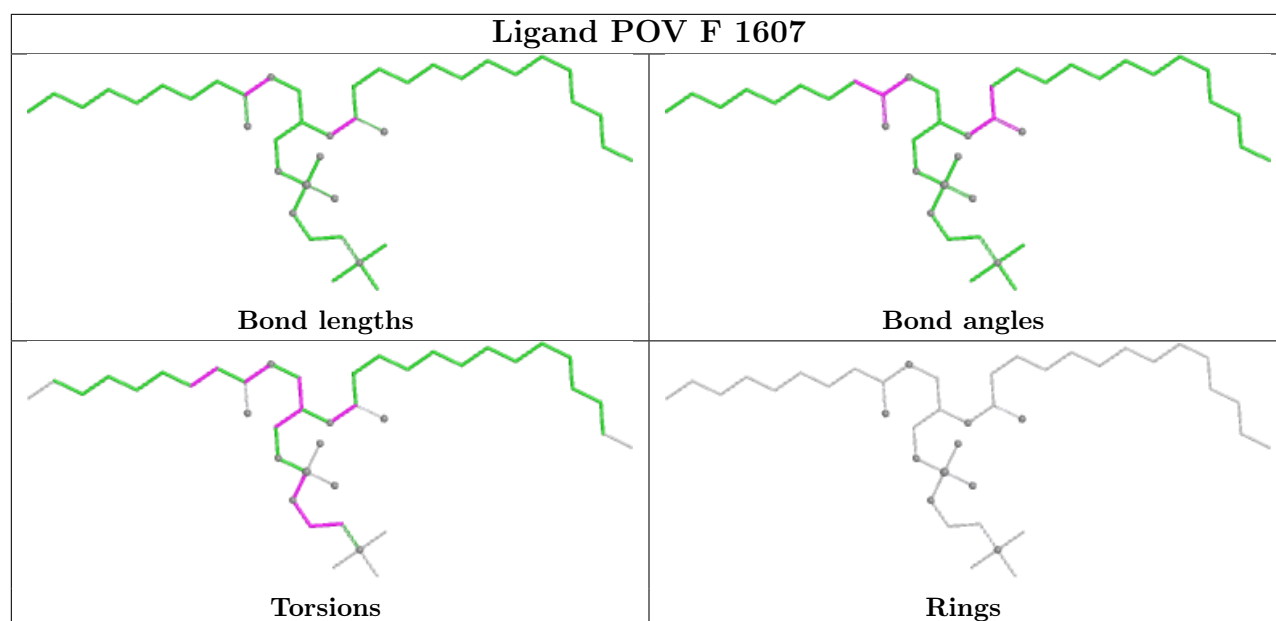


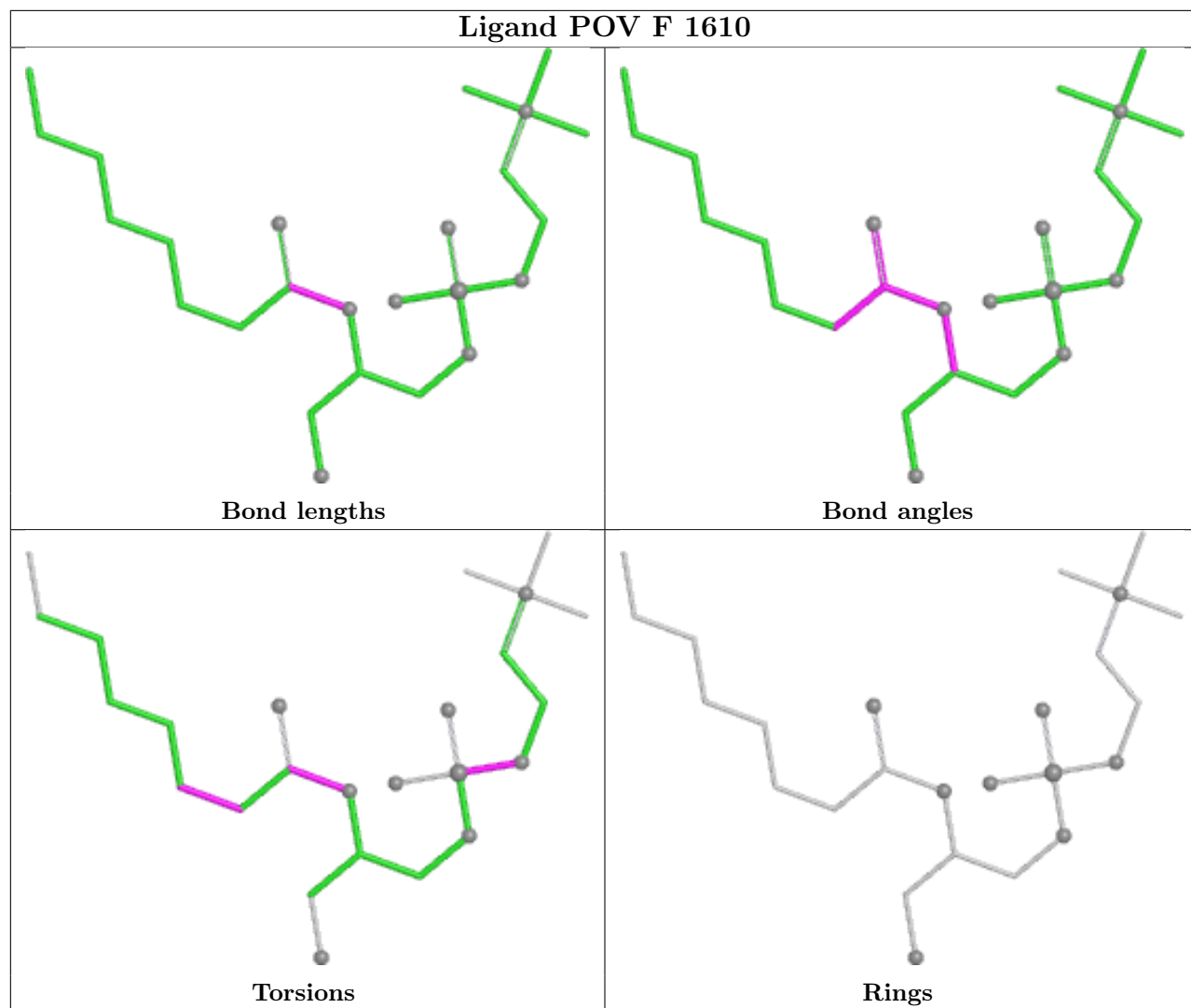


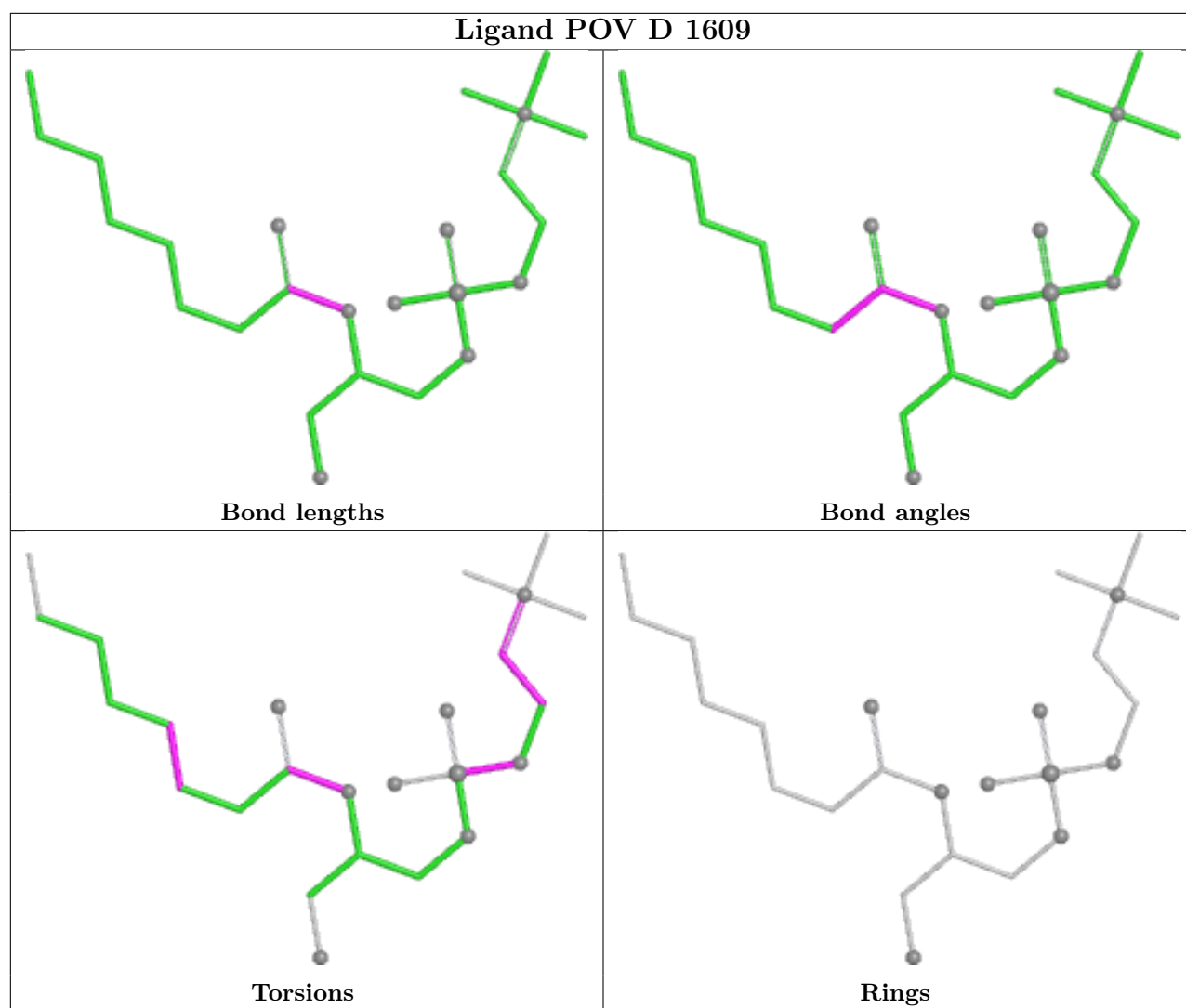


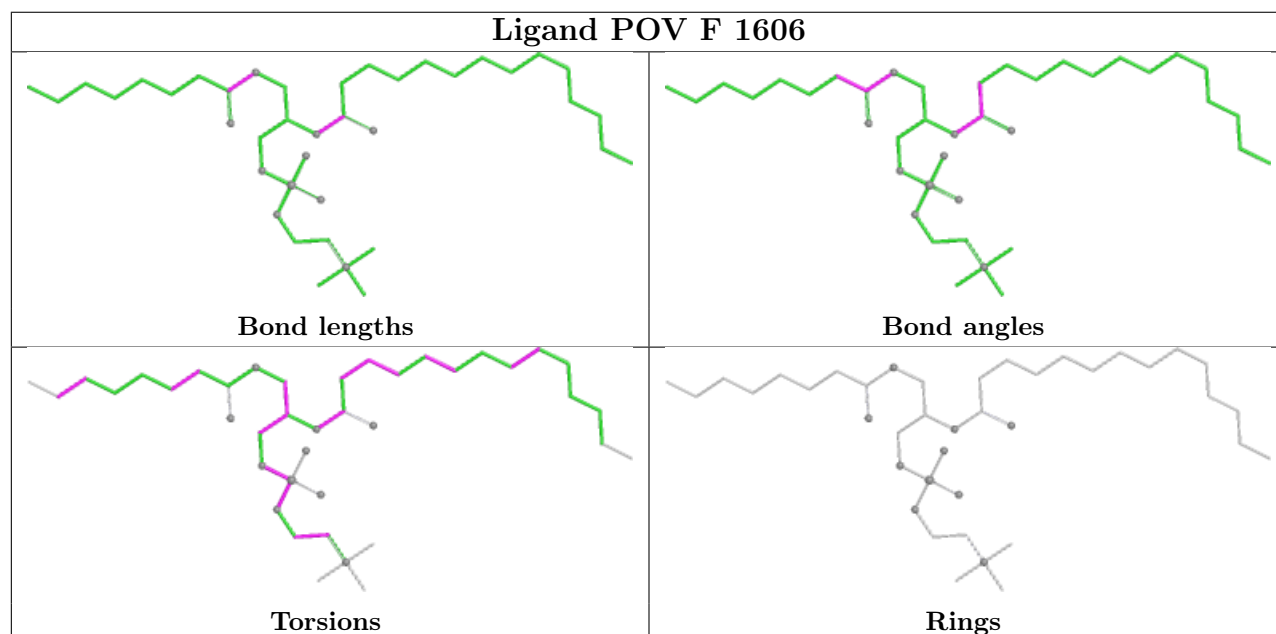
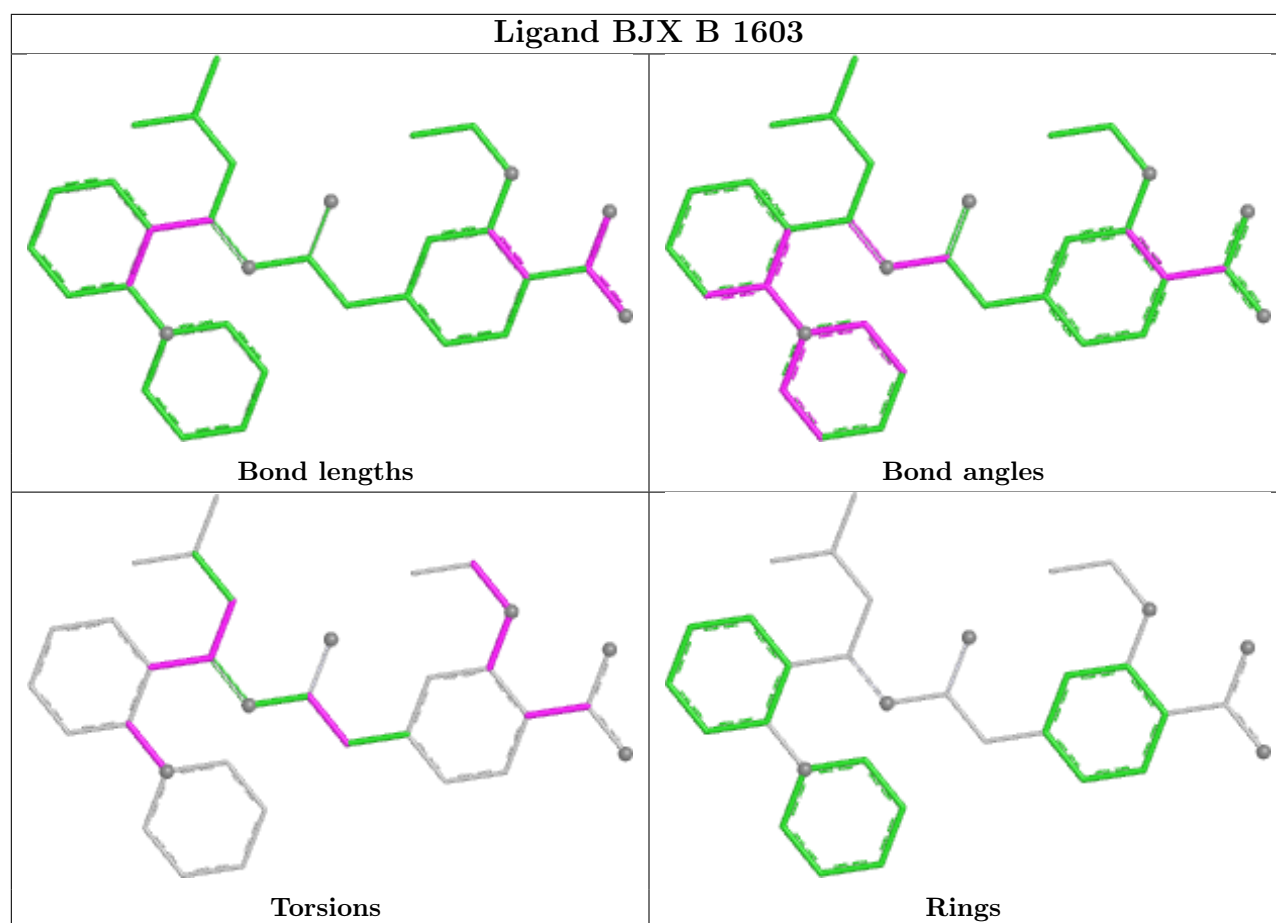


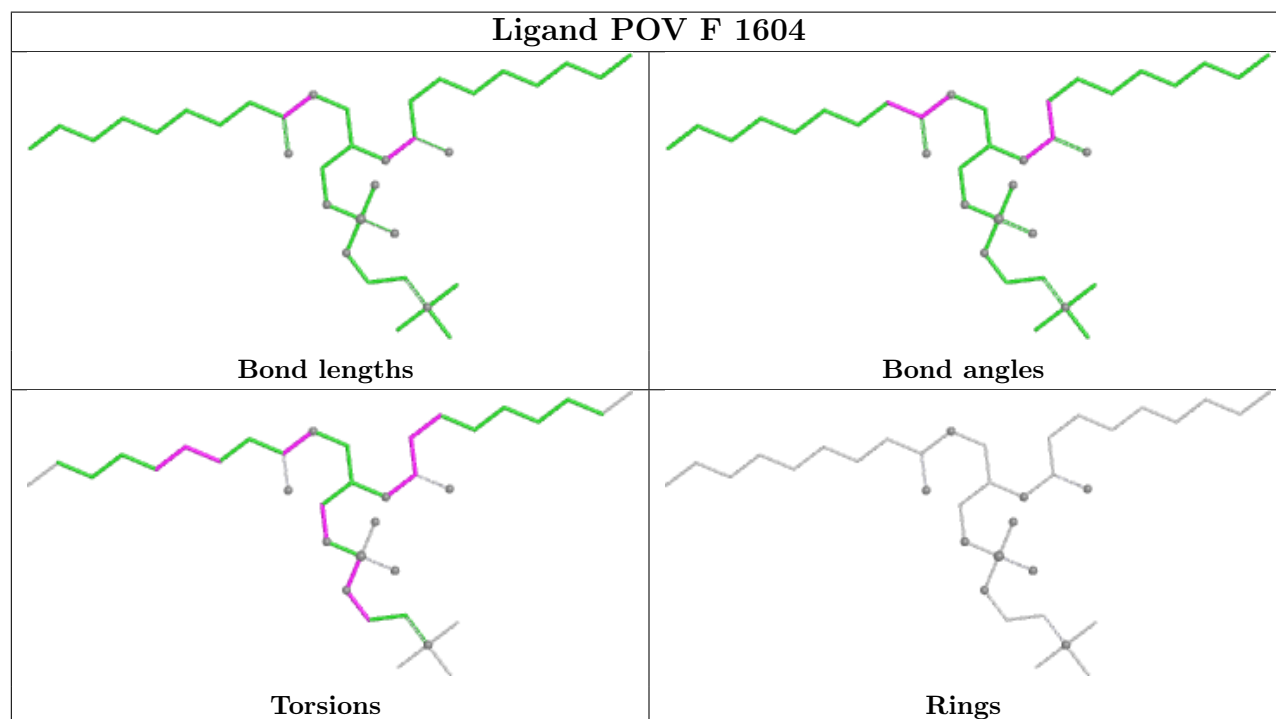
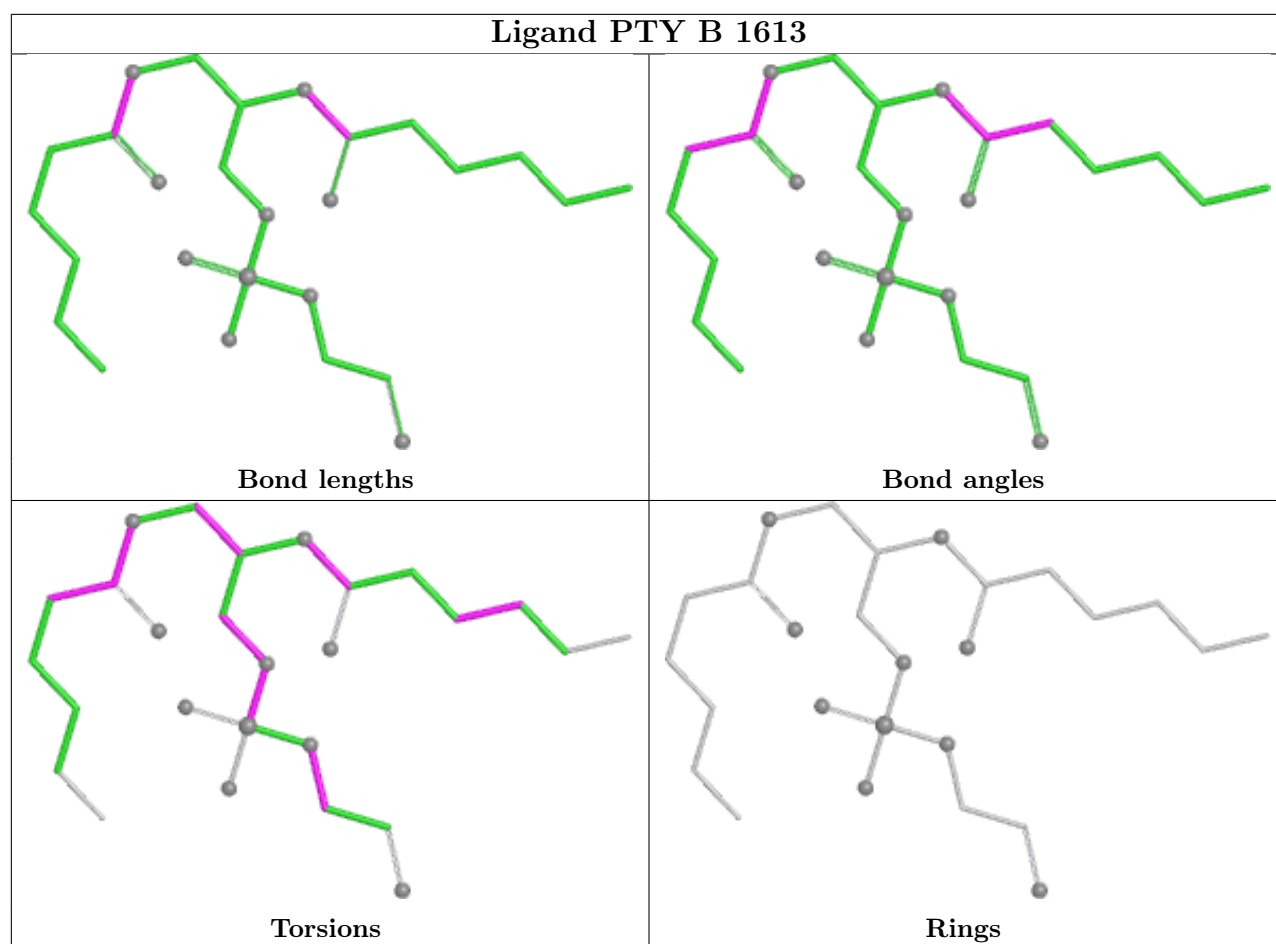


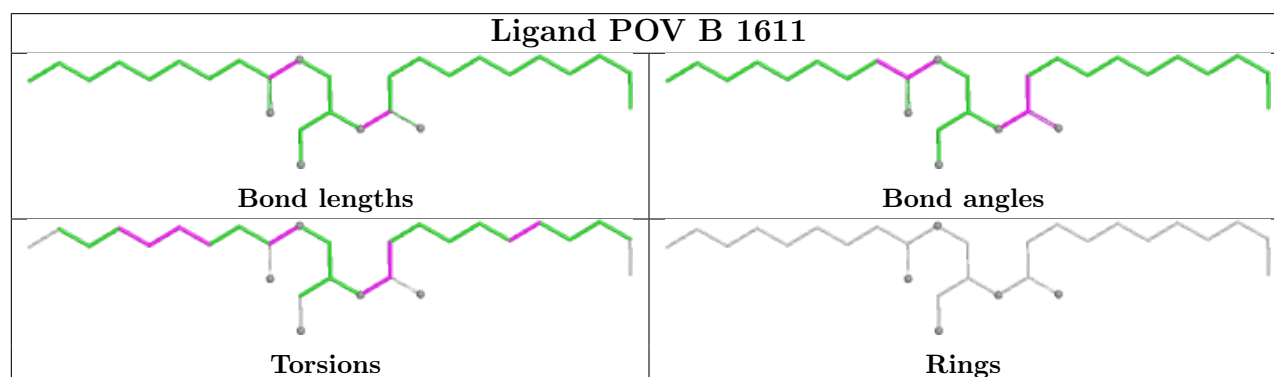
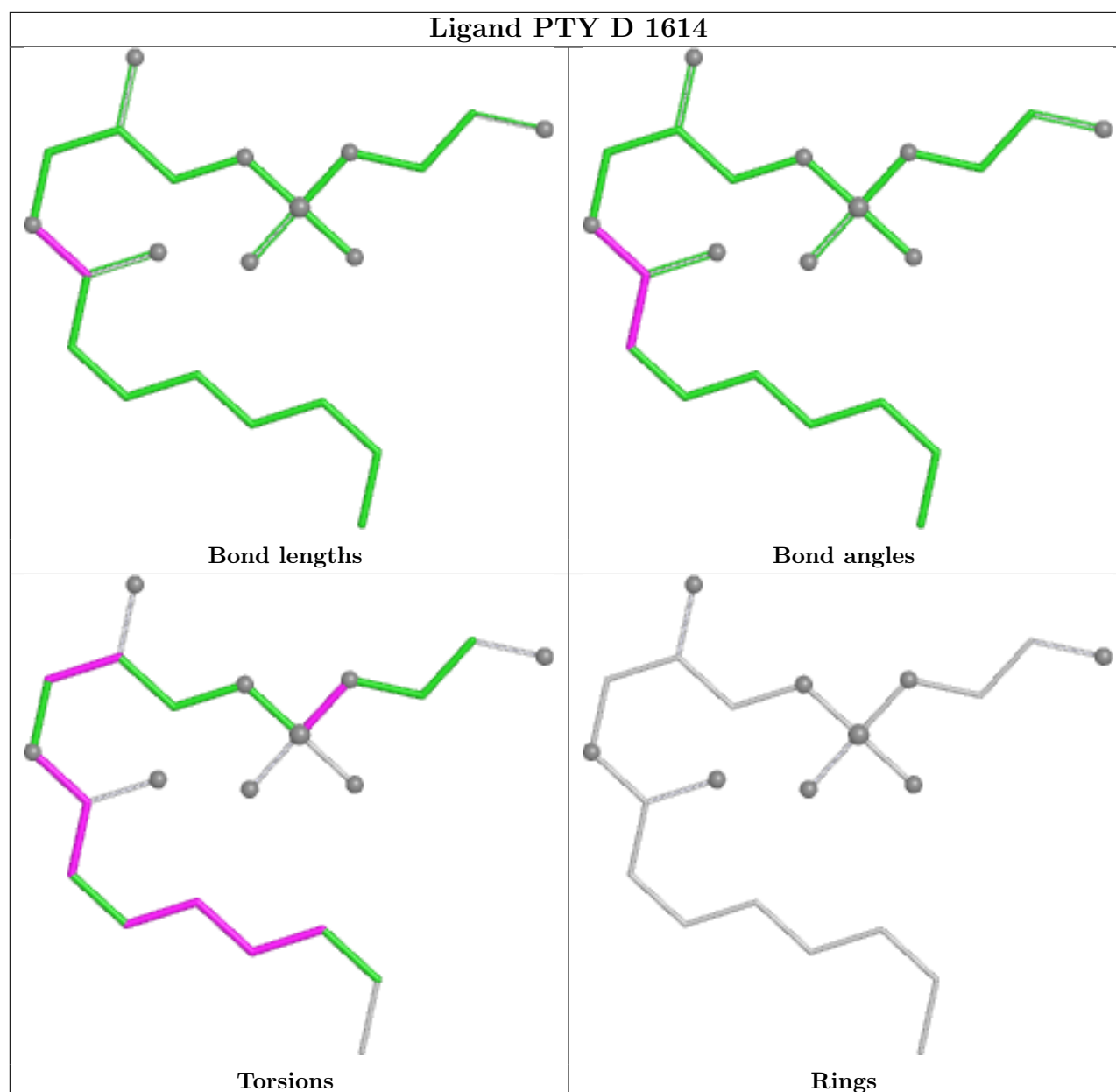


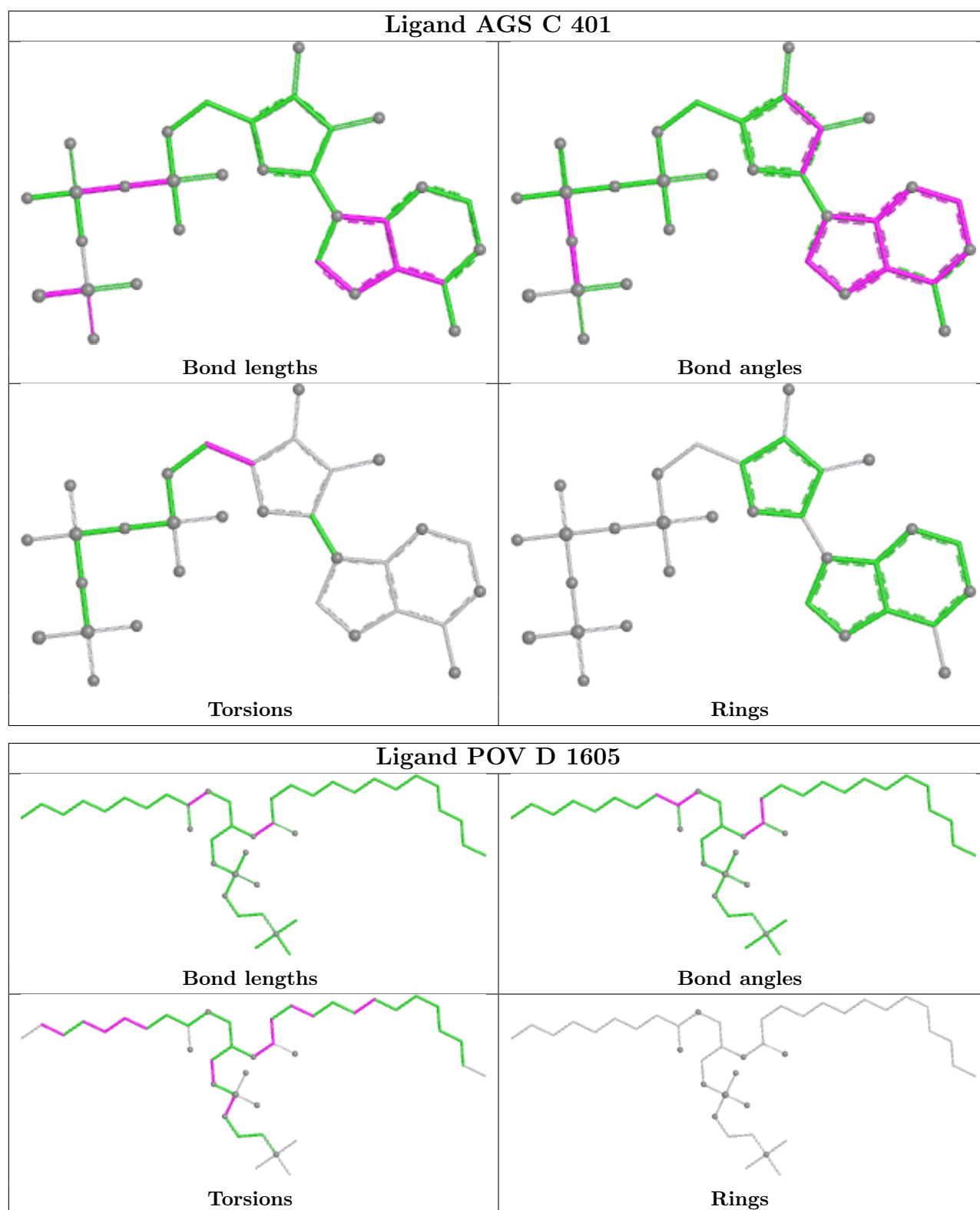












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

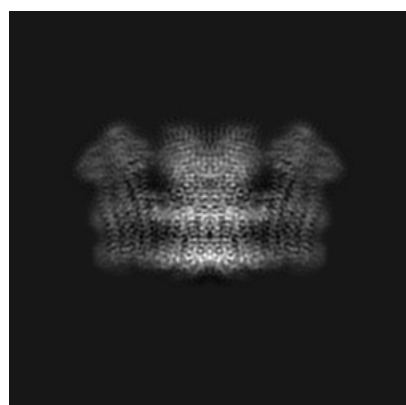
6 Map visualisation [i](#)

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.

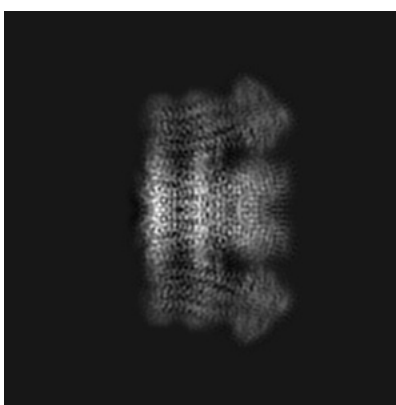
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

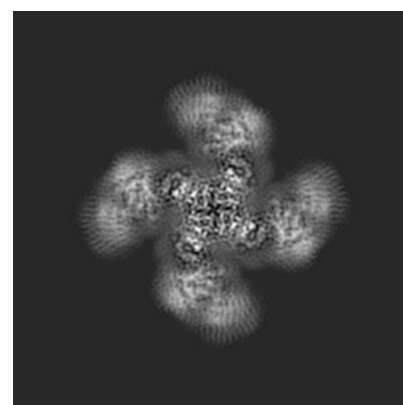
6.1.1 Primary map



X



Y

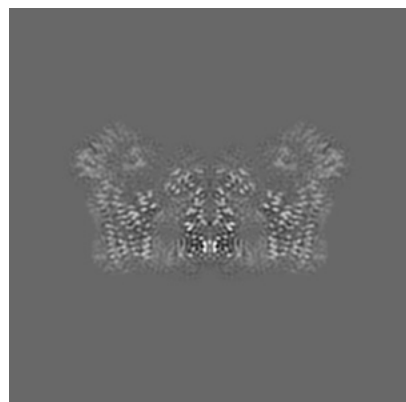


Z

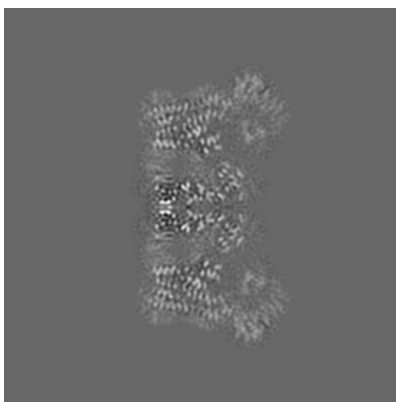
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

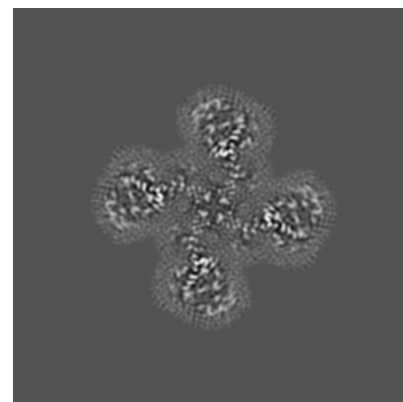
6.2.1 Primary map



X Index: 128



Y Index: 128

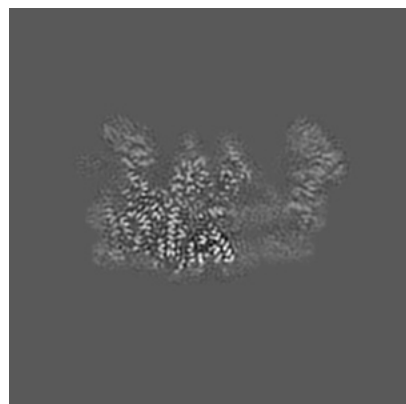


Z Index: 128

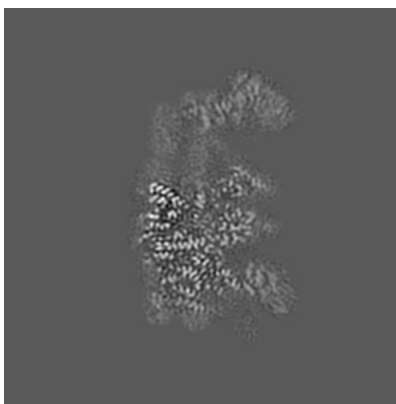
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

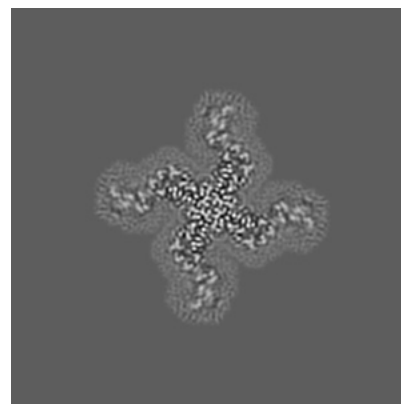
6.3.1 Primary map



X Index: 117



Y Index: 139

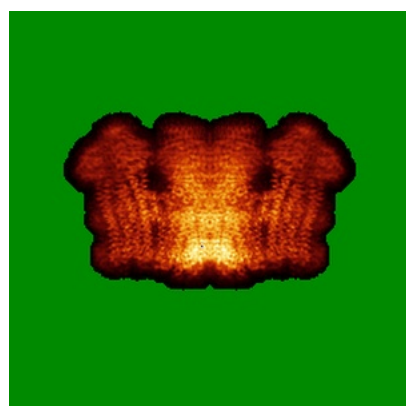


Z Index: 98

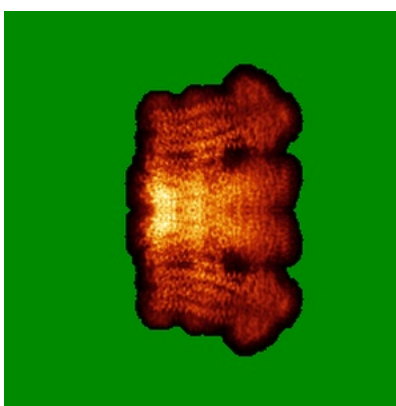
The images above show the largest variance slices of the map in three orthogonal directions.

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

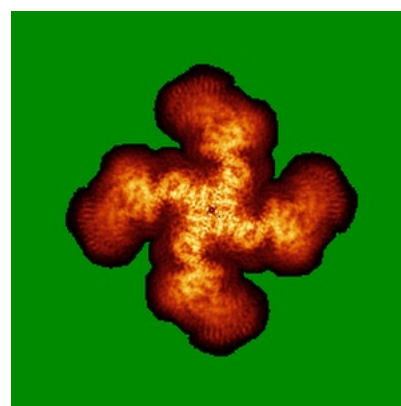
6.4.1 Primary map



X



Y

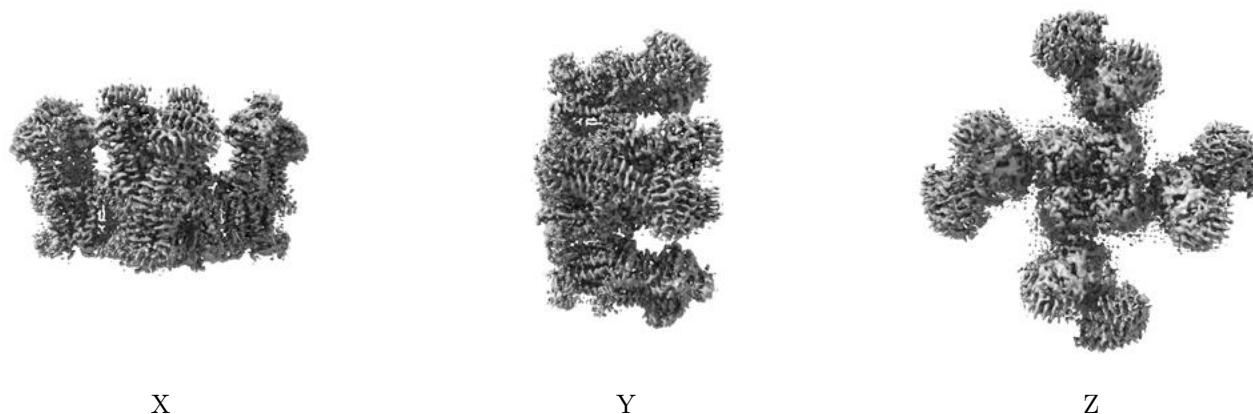


Z

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 3.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

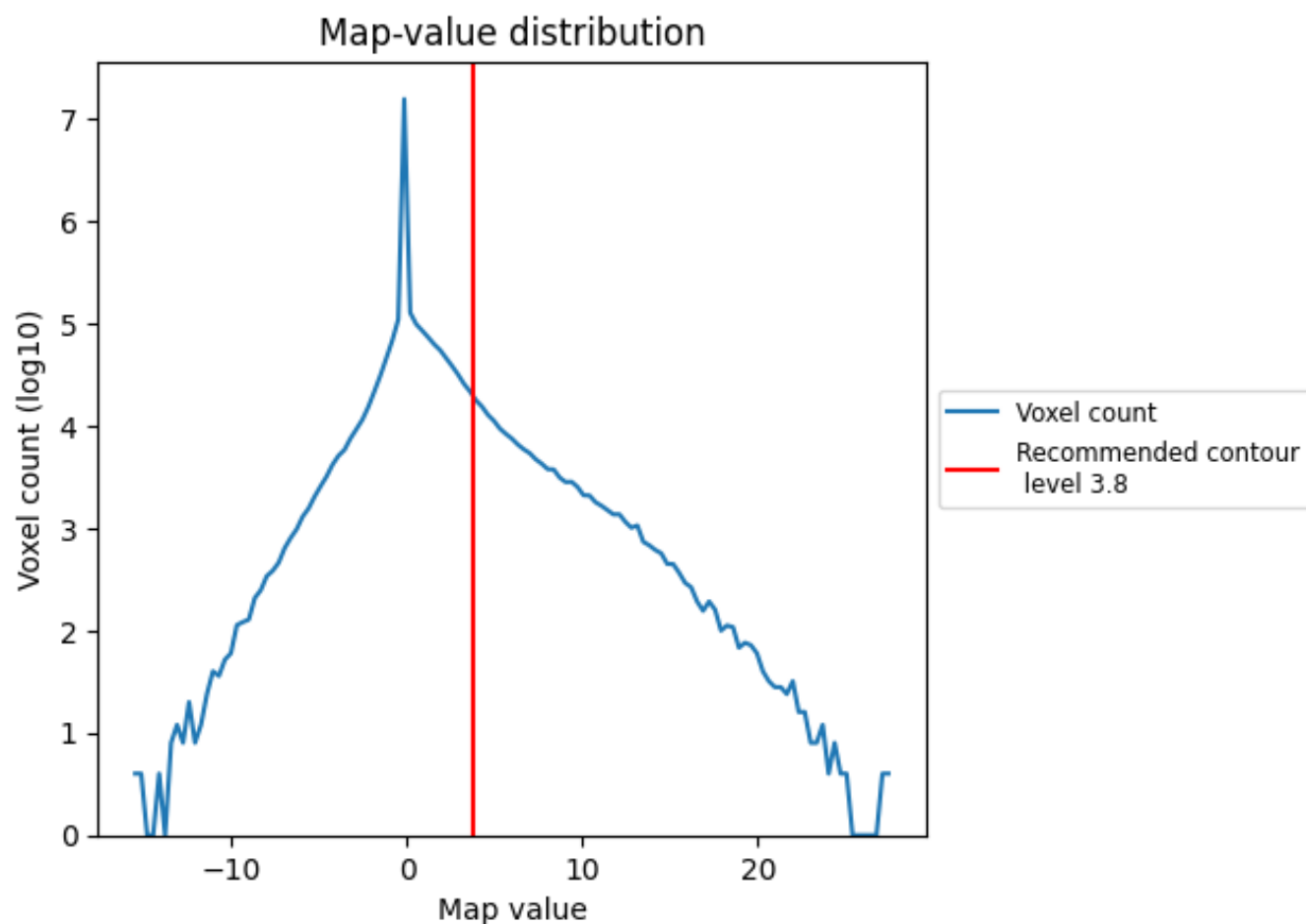
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

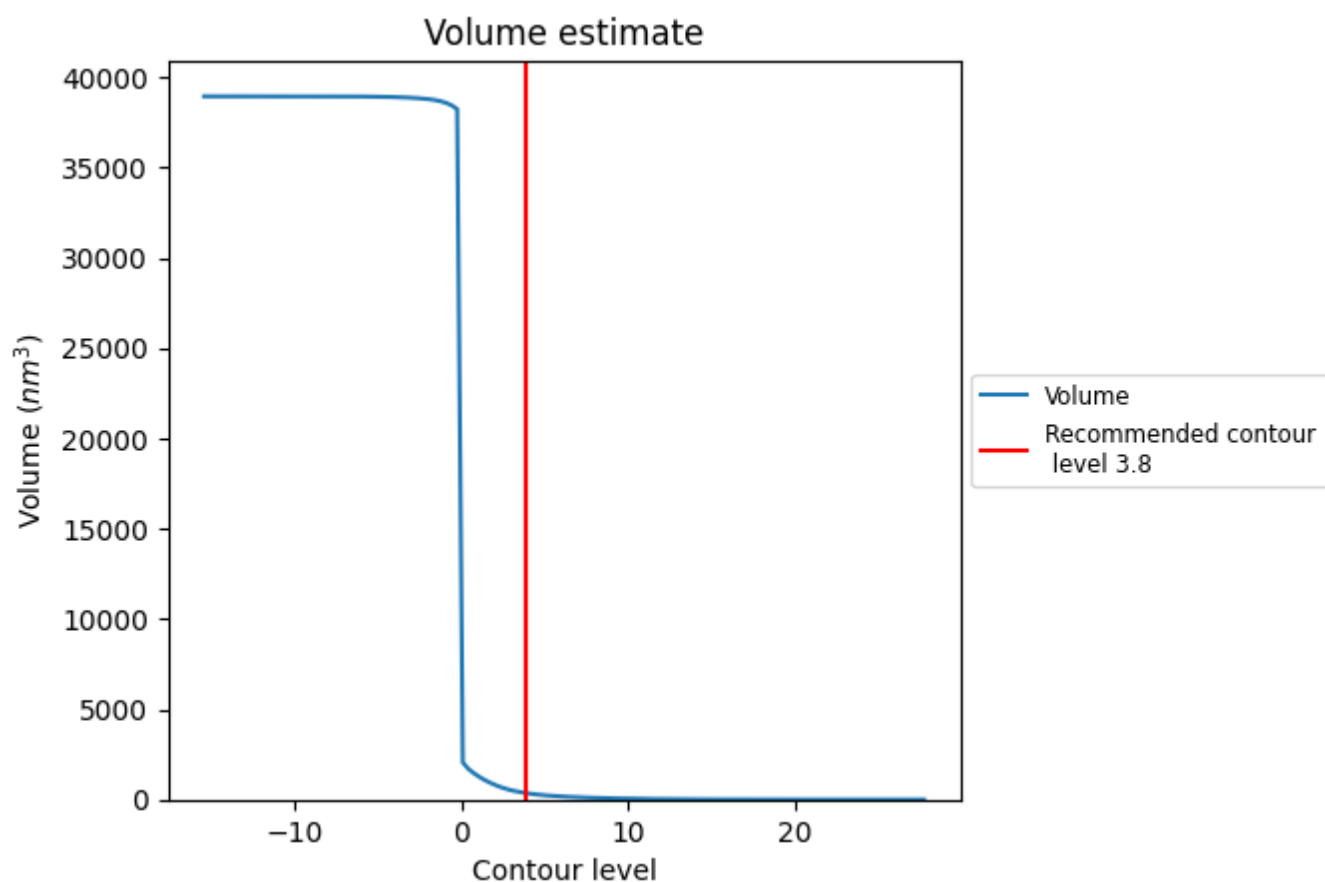
This section contains the results of statistical analysis of the map.

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.

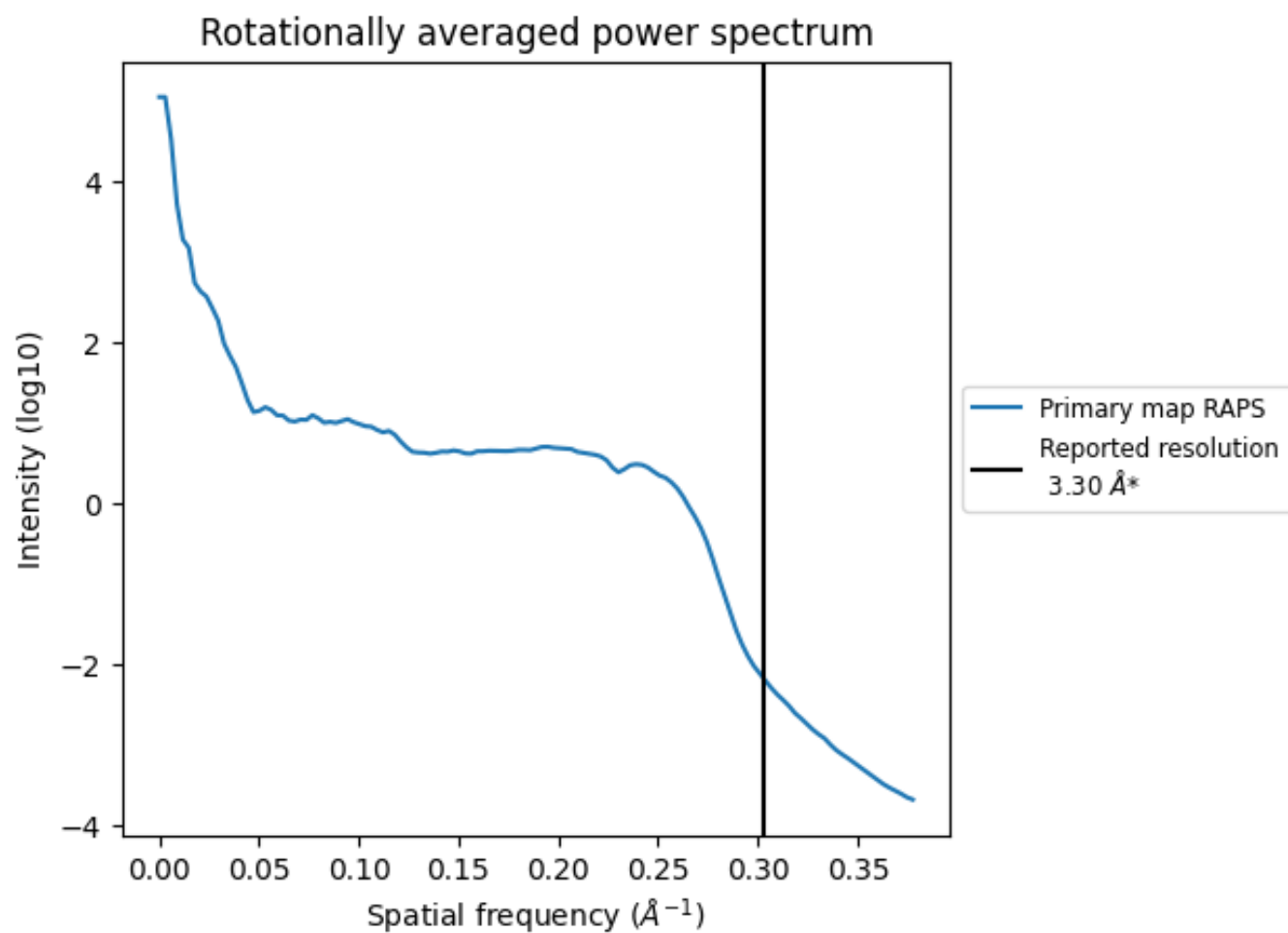
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

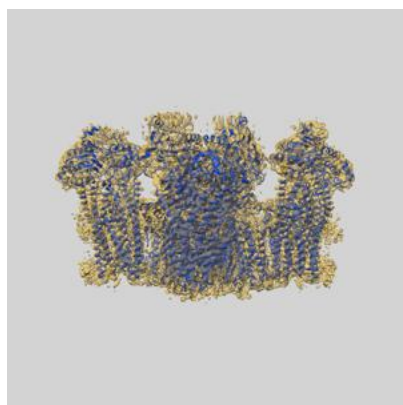
8 Fourier-Shell correlation

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

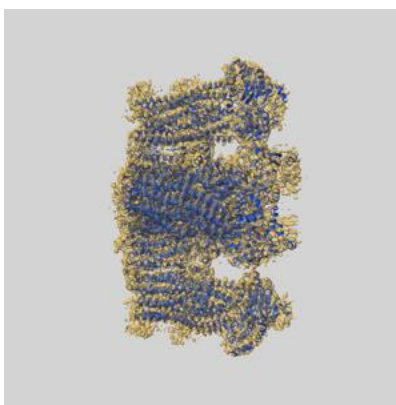
9 Map-model fit [i](#)

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](#).

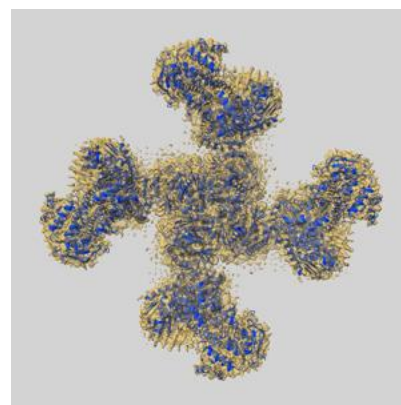
9.1 Map-model overlay [i](#)



X



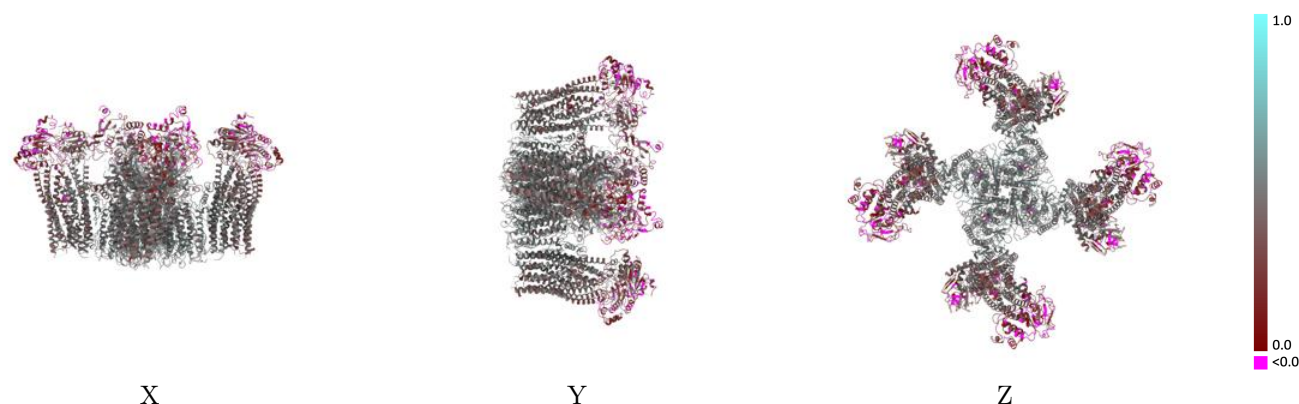
Y



Z

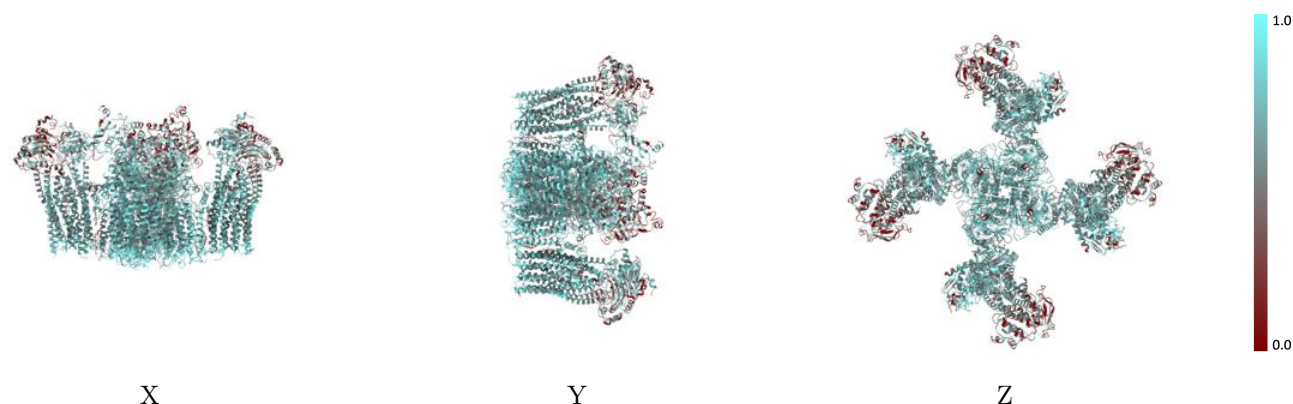
The images above show the 3D surface view of the map at the recommended contour level 3.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



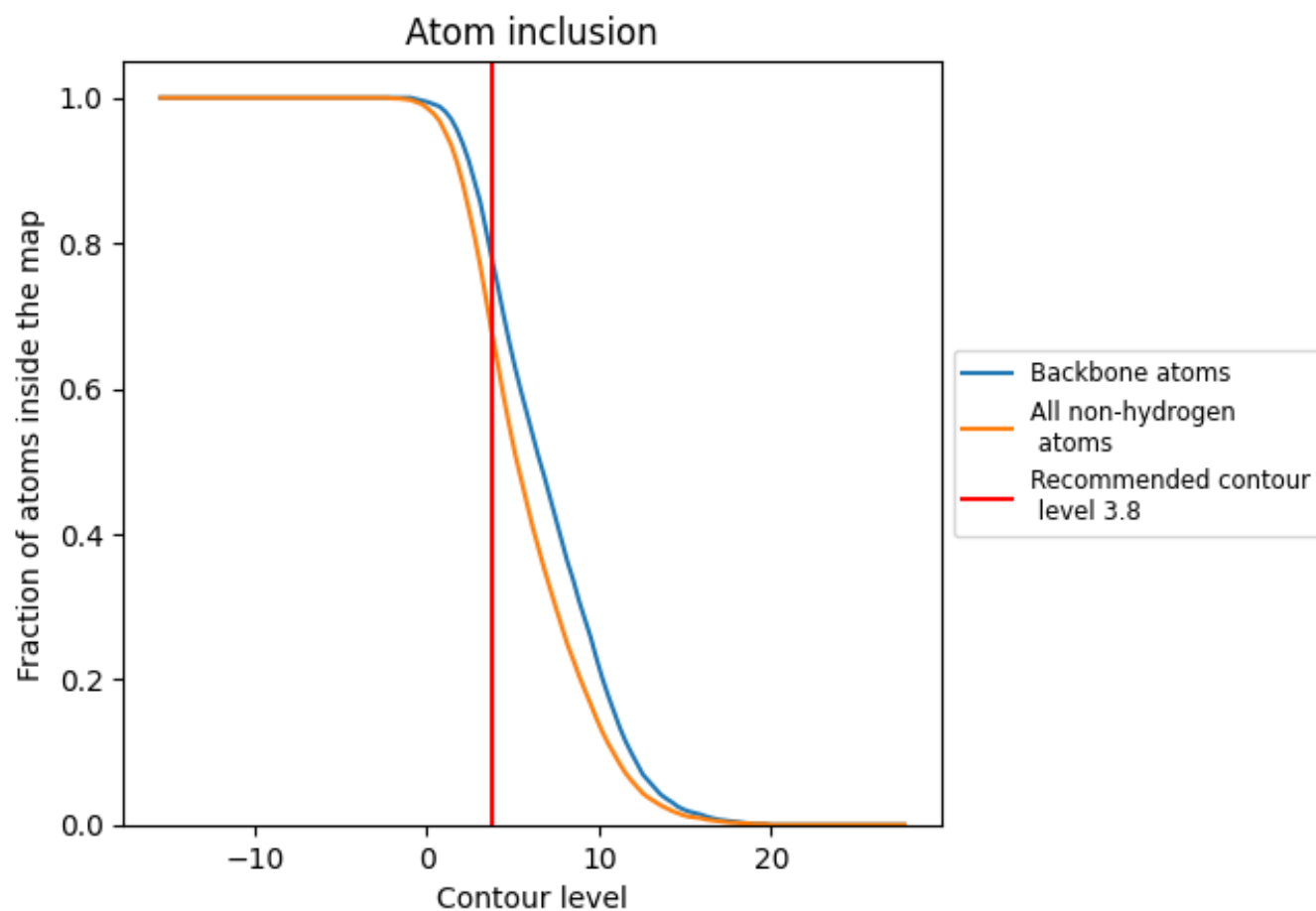
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.6740	0.4060
A	0.7530	0.5010
B	0.6550	0.3820
C	0.7530	0.5000
D	0.6550	0.3820
E	0.7530	0.5010
F	0.6550	0.3830
G	0.7530	0.5000
H	0.6550	0.3820

