



Full wwPDB Geometry-Only Validation Report ⓘ

Mar 6, 2026 – 10:05 AM UTC

PDB ID : 3K2S / pdb_00003k2s
Title : Solution structure of double super helix model
Authors : Wu, Z.; Gogonea, V.; Lee, X.; Wagner, M.A.; Li, X.-M.; Huang, Y.; Undurti, A.; May, R.P.; Haertlein, M.; Moulin, M.; Gutsche, I.; Zaccai, G.; Didonato, J.A.; Hazen, L.S.
Deposited on : 2009-09-30
Resolution : Not provided

This is a Full wwPDB Geometry-Only Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

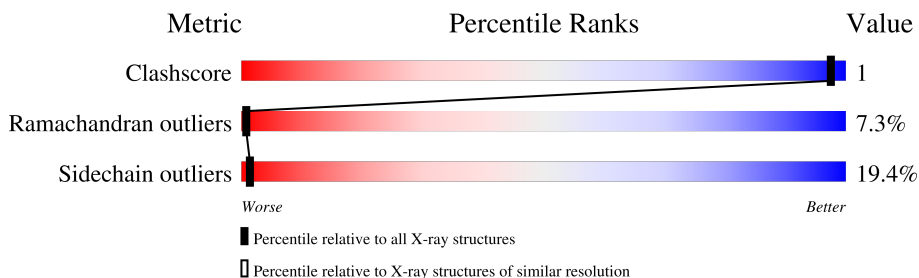
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION SCATTERING

The reported resolution of this entry is unknown.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	-
Ramachandran outliers	187476	-
Sidechain outliers	187428	-

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	243	
1	B	243	

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
2	POV	A	308	X	-	-	-
2	POV	A	316	X	-	-	-
2	POV	A	318	X	-	-	-
2	POV	A	319	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	POV	A	322	X	-	-	-
2	POV	A	326	X	-	-	-
2	POV	A	365	X	-	-	-
2	POV	A	368	X	-	-	-
2	POV	A	378	X	-	-	-
2	POV	A	380	X	-	-	-
2	POV	A	383	X	-	-	-
2	POV	A	385	X	-	-	-
2	POV	A	400	X	-	-	-
2	POV	A	410	X	-	-	-
2	POV	B	303	X	-	-	-
2	POV	B	321	X	-	-	-
2	POV	B	328	X	-	-	-
2	POV	B	329	X	-	-	-
2	POV	B	330	X	-	-	-
2	POV	B	346	X	-	-	-
2	POV	B	347	X	-	-	-
2	POV	B	362	X	-	-	-
2	POV	B	364	X	-	-	-
2	POV	B	367	X	-	-	-

2 Entry composition ⓘ

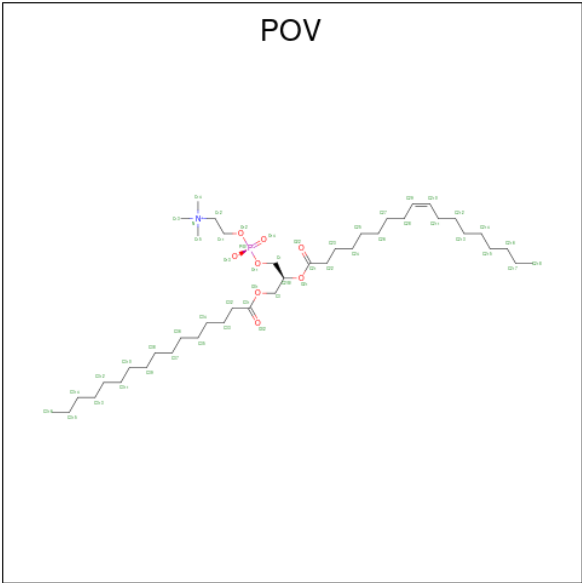
There are 3 unique types of molecules in this entry. The entry contains 14920 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Apolipoprotein A-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1980	1241	347	389	3			
1	B	243	Total	C	N	O	S	0	0	0
			1980	1241	347	389	3			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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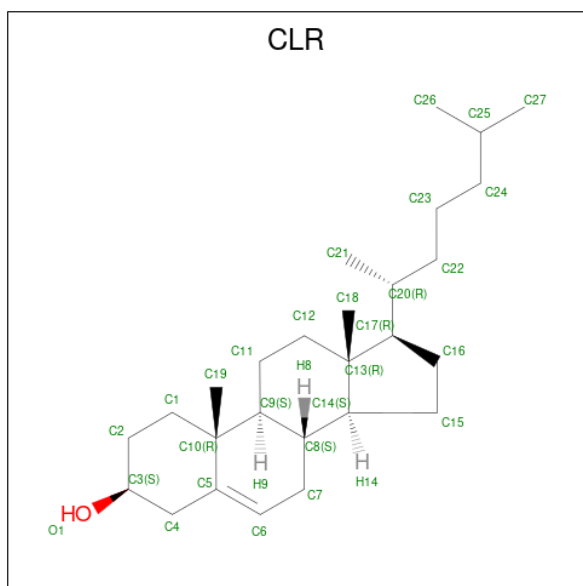
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		
3	B	1	Total	C	O	0	0
			28	27	1		
3	B	1	Total	C	O	0	0
			28	27	1		
3	B	1	Total	C	O	0	0
			28	27	1		
3	B	1	Total	C	O	0	0
			28	27	1		
3	B	1	Total	C	O	0	0
			28	27	1		
3	B	1	Total	C	O	0	0
			28	27	1		
3	B	1	Total	C	O	0	0
			28	27	1		
3	B	1	Total	C	O	0	0
			28	27	1		

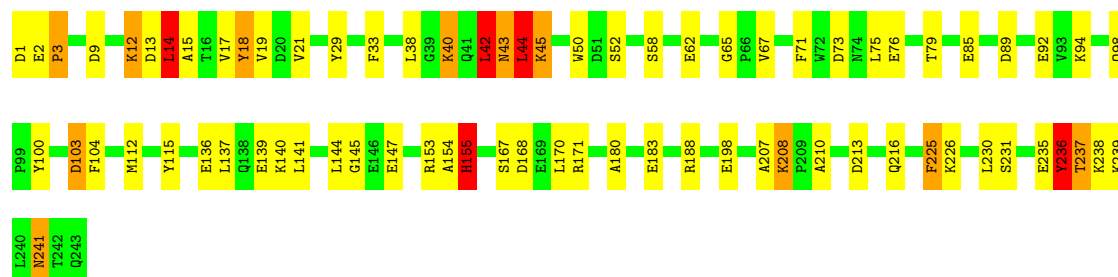
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

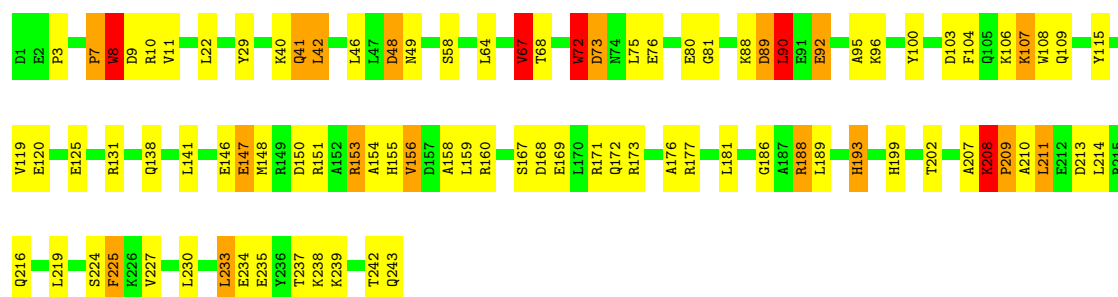
• Molecule 1: Apolipoprotein A-I

Chain A: 



• Molecule 1: Apolipoprotein A-I

Chain B: 



4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, CLR

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	1.08	1/2015 (0.0%)	1.86	48/2714 (1.8%)
1	B	1.07	0/2015	1.84	53/2714 (2.0%)
All	All	1.08	1/4030 (0.0%)	1.85	101/5428 (1.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	9
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	PRO	CA-C	5.52	1.57	1.52

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	PHE	CA-CB-CG	13.91	127.71	113.80
1	A	225	PHE	CA-CB-CG	9.98	123.78	113.80
1	B	8	TRP	O-C-N	-9.28	110.24	122.59
1	A	154	ALA	CA-C-N	8.23	136.52	121.70
1	A	154	ALA	C-N-CA	8.23	136.52	121.70
1	A	2	GLU	CA-C-N	8.03	128.65	120.38
1	A	2	GLU	C-N-CA	8.03	128.65	120.38
1	B	155	HIS	CA-CB-CG	7.39	121.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PRO	N-CA-C	7.37	119.69	110.70
1	A	180	ALA	CA-C-N	7.05	129.72	120.28
1	A	180	ALA	C-N-CA	7.05	129.72	120.28
1	B	76	GLU	CA-C-N	6.84	130.37	120.38
1	B	76	GLU	C-N-CA	6.84	130.37	120.38
1	B	224	SER	CA-C-N	6.79	131.01	120.82
1	B	224	SER	C-N-CA	6.79	131.01	120.82
1	A	236	TYR	CA-CB-CG	6.70	125.95	113.90
1	A	213	ASP	CA-C-N	6.67	129.55	120.54
1	A	213	ASP	C-N-CA	6.67	129.55	120.54
1	B	237	THR	CB-CA-C	6.66	117.74	109.16
1	B	41	GLN	CA-C-N	6.55	133.49	121.70
1	B	41	GLN	C-N-CA	6.55	133.49	121.70
1	B	8	TRP	CB-CG-CD2	6.54	135.96	126.80
1	A	154	ALA	N-CA-C	6.49	124.63	110.80
1	A	103	ASP	CA-CB-CG	6.43	119.03	112.60
1	B	7	PRO	CA-C-N	6.41	133.78	121.54
1	B	7	PRO	C-N-CA	6.41	133.78	121.54
1	A	67	VAL	CA-C-N	6.26	128.67	120.28
1	A	67	VAL	C-N-CA	6.26	128.67	120.28
1	B	209	PRO	CA-C-N	6.19	132.85	121.70
1	B	209	PRO	C-N-CA	6.19	132.85	121.70
1	B	104	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	239	LYS	CA-C-N	6.13	130.44	121.31
1	A	239	LYS	C-N-CA	6.13	130.44	121.31
1	A	33	PHE	CA-CB-CG	6.02	119.82	113.80
1	B	89	ASP	CA-C-N	6.00	133.01	121.54
1	B	89	ASP	C-N-CA	6.00	133.01	121.54
1	B	188	ARG	CA-C-N	6.00	128.32	120.28
1	B	188	ARG	C-N-CA	6.00	128.32	120.28
1	B	95	ALA	CA-C-N	5.98	128.62	120.54
1	B	95	ALA	C-N-CA	5.98	128.62	120.54
1	A	155	HIS	CB-CA-C	5.95	121.40	110.10
1	B	193	HIS	CA-CB-CG	5.94	119.74	113.80
1	B	72	TRP	CA-CB-CG	5.91	124.84	113.60
1	A	238	LYS	CA-C-N	5.87	132.27	121.70
1	A	238	LYS	C-N-CA	5.87	132.27	121.70
1	A	3	PRO	CA-C-N	5.85	127.16	119.84
1	A	3	PRO	C-N-CA	5.85	127.16	119.84
1	B	168	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	8	TRP	CB-CG-CD1	-5.79	118.22	126.90
1	B	210	ALA	CA-C-N	5.77	132.56	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ALA	C-N-CA	5.77	132.56	121.54
1	A	40	LYS	CA-C-N	5.73	131.22	122.11
1	A	40	LYS	C-N-CA	5.73	131.22	122.11
1	B	8	TRP	CA-CB-CG	5.72	124.47	113.60
1	A	230	LEU	N-CA-C	5.64	117.43	111.28
1	A	241	ASN	CA-C-N	5.61	129.07	121.05
1	A	241	ASN	C-N-CA	5.61	129.07	121.05
1	A	71	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	13	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	48	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	137	LEU	CA-C-N	5.53	128.25	120.28
1	A	137	LEU	C-N-CA	5.53	128.25	120.28
1	A	155	HIS	CA-CB-CG	5.50	119.30	113.80
1	A	213	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	85	GLU	CA-C-N	5.49	127.95	120.54
1	A	85	GLU	C-N-CA	5.49	127.95	120.54
1	A	43	ASN	CA-C-N	5.47	131.98	121.54
1	A	43	ASN	C-N-CA	5.47	131.98	121.54
1	A	73	ASP	CA-C-N	5.47	128.15	120.28
1	A	73	ASP	C-N-CA	5.47	128.15	120.28
1	B	171	ARG	CA-C-N	5.47	131.98	121.54
1	B	171	ARG	C-N-CA	5.47	131.98	121.54
1	B	148	MET	CA-C-N	5.45	129.86	121.19
1	B	148	MET	C-N-CA	5.45	129.86	121.19
1	B	64	LEU	CA-C-N	5.41	130.36	121.87
1	B	64	LEU	C-N-CA	5.41	130.36	121.87
1	B	49	ASN	CB-CA-C	5.40	119.61	111.18
1	B	67	VAL	CB-CA-C	5.39	119.75	112.36
1	A	44	LEU	N-CA-C	5.35	122.20	110.80
1	B	233	LEU	N-CA-C	5.31	122.11	110.80
1	B	208	LYS	CB-CA-C	5.27	120.55	110.17
1	B	219	LEU	N-CA-C	5.27	121.46	109.81
1	B	147	GLU	CB-CA-C	5.27	118.81	109.75
1	B	233	LEU	CA-C-N	5.26	131.17	121.70
1	B	233	LEU	C-N-CA	5.26	131.17	121.70
1	B	68	THR	CA-CB-CG2	5.22	119.38	110.50
1	B	227	VAL	CA-C-N	5.20	129.00	120.63
1	B	227	VAL	C-N-CA	5.20	129.00	120.63
1	A	42	LEU	N-CA-C	5.20	115.39	108.38
1	B	158	ALA	CA-C-N	5.18	131.44	121.54
1	B	158	ALA	C-N-CA	5.18	131.44	121.54
1	B	73	ASP	CA-CB-CG	5.17	117.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	LEU	CA-C-N	5.17	127.21	120.28
1	B	22	LEU	C-N-CA	5.17	127.21	120.28
1	A	18	TYR	CA-CB-CG	5.14	123.16	113.90
1	A	52	SER	CA-C-N	5.10	127.45	120.46
1	A	52	SER	C-N-CA	5.10	127.45	120.46
1	A	144	LEU	CA-C-N	5.10	131.40	121.41
1	A	144	LEU	C-N-CA	5.10	131.40	121.41
1	A	238	LYS	N-CA-C	5.02	117.91	110.48
1	B	199	HIS	CA-CB-CG	5.02	118.82	113.80

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ASP	Peptide
1	A	167	SER	Peptide
1	A	168	ASP	Peptide
1	A	236	TYR	Peptide
1	A	237	THR	Peptide
1	B	177	ARG	Sidechain
1	B	239	LYS	Peptide
1	B	67	VAL	Peptide
1	B	7	PRO	Peptide,Mainchain
1	B	8	TRP	Mainchain
1	B	80	GLU	Peptide
1	B	90	LEU	Peptide
1	B	92	GLU	Peptide

4.2 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	1980	0	1968	9	0
1	B	1980	0	1968	10	0
2	A	5772	0	9102	5	0
2	B	4628	0	7298	12	0
3	A	280	0	460	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	280	0	460	1	0
All	All	14920	0	21256	28	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 1.

All (28) 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:12:LYS:HB3	1:A:15:ALA:HB2	1.82	0.62
1:A:44:LEU:HD12	1:A:45:LYS:H	1.67	0.60
1:B:115:TYR:CE1	1:B:119:VAL:HG21	2.37	0.60
1:A:12:LYS:CB	1:A:15:ALA:HB2	2.37	0.54
1:A:210:ALA:HB1	3:A:402:CLR:H181	1.91	0.52
1:B:151:ARG:HA	1:B:154:ALA:HB3	1.92	0.52
1:B:153:ARG:HH21	2:B:388:POV:H22A	1.74	0.52
1:A:42:LEU:CD2	1:A:43:ASN:H	2.24	0.51
2:A:396:POV:H31D	2:B:313:POV:H31G	1.92	0.50
2:A:311:POV:H31H	2:A:311:POV:H31C	1.92	0.50
1:A:236:TYR:HB2	1:A:237:THR:HG23	1.94	0.48
2:B:334:POV:H23	2:B:334:POV:H27A	1.96	0.48
1:A:76:GLU:HA	1:A:79:THR:HG22	1.96	0.47
1:B:11:VAL:HG22	2:B:329:POV:H26A	1.97	0.47
1:B:208:LYS:H	2:B:373:POV:H22A	1.79	0.47
2:A:357:POV:H36	2:B:349:POV:H27	1.98	0.46
3:B:393:CLR:H212	3:B:393:CLR:H121	2.00	0.43
1:B:242:THR:HG21	2:B:314:POV:H2	2.01	0.42
1:A:14:LEU:H	1:A:14:LEU:HD13	1.83	0.42
1:B:103:ASP:OD1	1:B:107:LYS:NZ	2.51	0.42
2:B:339:POV:H22A	2:B:339:POV:H2	1.87	0.42
2:A:412:POV:H13A	2:A:412:POV:H22A	2.01	0.41
1:A:40:LYS:HZ3	1:B:213:ASP:CG	2.28	0.41
2:A:318:POV:H32	2:A:318:POV:H3A	1.90	0.41
2:B:331:POV:H14B	2:B:331:POV:P	2.61	0.41
3:A:402:CLR:C23	2:B:331:POV:H211	2.51	0.41
1:B:131:ARG:HH22	2:B:303:POV:H32A	1.86	0.40
1:B:141:LEU:HD13	2:B:302:POV:H25A	2.03	0.40

There are no symmetry-related clashes.

4.3 Torsion angles

4.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	241/243 (99%)	192 (80%)	37 (15%)	12 (5%)	1	1
1	B	241/243 (99%)	181 (75%)	37 (15%)	23 (10%)	0	0
All	All	482/486 (99%)	373 (77%)	74 (15%)	35 (7%)	1	1

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	B	8	TRP
1	B	10	ARG
1	B	160	ARG
1	B	172	GLN
1	B	176	ALA
1	A	65	GLY
1	A	145	GLY
1	A	155	HIS
1	A	207	ALA
1	A	208	LYS
1	A	241	ASN
1	B	40	LYS
1	B	81	GLY
1	B	89	ASP
1	B	233	LEU
1	A	9	ASP
1	A	45	LYS
1	B	42	LEU
1	B	159	LEU
1	B	207	ALA
1	B	211	LEU
1	A	14	LEU
1	B	9	ASP
1	B	41	GLN

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Mol	Chain	Res	Type
1	A	3	PRO
1	B	3	PRO
1	B	72	TRP
1	B	90	LEU
1	B	146	GLU
1	B	167	SER
1	B	156	VAL
1	A	21	VAL
1	B	186	GLY
1	B	208	LYS

4.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	214/214 (100%)	174 (81%)	40 (19%)	1	1
1	B	214/214 (100%)	171 (80%)	43 (20%)	1	1
All	All	428/428 (100%)	345 (81%)	83 (19%)	1	1

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	14	LEU
1	A	17	VAL
1	A	18	TYR
1	A	19	VAL
1	A	29	TYR
1	A	38	LEU
1	A	42	LEU
1	A	50	TRP
1	A	58	SER
1	A	62	GLU
1	A	75	LEU
1	A	89	ASP

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Mol	Chain	Res	Type
1	A	92	GLU
1	A	94	LYS
1	A	98	GLN
1	A	100	TYR
1	A	103	ASP
1	A	104	PHE
1	A	112	MET
1	A	115	TYR
1	A	136	GLU
1	A	139	GLU
1	A	140	LYS
1	A	141	LEU
1	A	147	GLU
1	A	153	ARG
1	A	155	HIS
1	A	170	LEU
1	A	171	ARG
1	A	183	GLU
1	A	188	ARG
1	A	198	GLU
1	A	208	LYS
1	A	216	GLN
1	A	225	PHE
1	A	226	LYS
1	A	231	SER
1	A	235	GLU
1	A	236	TYR
1	B	8	TRP
1	B	29	TYR
1	B	42	LEU
1	B	46	LEU
1	B	48	ASP
1	B	58	SER
1	B	67	VAL
1	B	72	TRP
1	B	73	ASP
1	B	75	LEU
1	B	88	LYS
1	B	90	LEU
1	B	92	GLU
1	B	96	LYS
1	B	100	TYR

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Mol	Chain	Res	Type
1	B	106	LYS
1	B	107	LYS
1	B	108	TRP
1	B	109	GLN
1	B	120	GLU
1	B	125	GLU
1	B	138	GLN
1	B	147	GLU
1	B	150	ASP
1	B	153	ARG
1	B	156	VAL
1	B	169	GLU
1	B	173	ARG
1	B	181	LEU
1	B	188	ARG
1	B	189	LEU
1	B	193	HIS
1	B	202	THR
1	B	209	PRO
1	B	211	LEU
1	B	214	LEU
1	B	216	GLN
1	B	225	PHE
1	B	230	LEU
1	B	234	GLU
1	B	235	GLU
1	B	238	LYS
1	B	243	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	74	ASN
1	A	84	GLN
1	A	98	GLN
1	A	127	GLN
1	A	184	ASN
1	B	5	GLN
1	B	63	GLN
1	B	105	GLN
1	B	117	GLN

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Mol	Chain	Res	Type
1	B	132	GLN
1	B	138	GLN
1	B	184	ASN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry ⓘ

220 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	$\# Z > 2$
2	POV	B	378	-	51,51,51	0.86	2 (3%)	57,59,59	0.69	1 (1%)
2	POV	B	380	-	51,51,51	0.92	2 (3%)	57,59,59	0.77	2 (3%)
2	POV	A	339	-	51,51,51	0.92	2 (3%)	57,59,59	0.51	0
2	POV	B	343	-	51,51,51	0.94	2 (3%)	57,59,59	0.56	0
2	POV	A	343	-	51,51,51	0.89	2 (3%)	57,59,59	0.69	1 (1%)
2	POV	B	302	-	51,51,51	0.90	2 (3%)	57,59,59	0.73	1 (1%)
2	POV	B	330	-	51,51,51	0.91	2 (3%)	57,59,59	0.51	0
2	POV	A	380	-	51,51,51	0.91	2 (3%)	57,59,59	0.47	0
3	CLR	B	391	-	31,31,31	0.74	0	48,48,48	1.00	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	A	360	-	51,51,51	0.93	2 (3%)	57,59,59	0.55	0
3	CLR	A	421	-	31,31,31	0.74	0	48,48,48	0.99	3 (6%)
2	POV	A	322	-	51,51,51	0.88	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	A	400	-	51,51,51	0.88	2 (3%)	57,59,59	0.58	0
2	POV	A	362	-	51,51,51	0.92	2 (3%)	57,59,59	0.78	1 (1%)
2	POV	A	317	-	51,51,51	0.93	2 (3%)	57,59,59	0.51	0
2	POV	A	327	-	51,51,51	0.93	2 (3%)	57,59,59	0.68	1 (1%)
2	POV	B	327	-	51,51,51	0.93	2 (3%)	57,59,59	0.67	1 (1%)
2	POV	A	389	-	51,51,51	0.91	2 (3%)	57,59,59	0.61	0
2	POV	A	382	-	51,51,51	0.92	2 (3%)	57,59,59	0.50	0
2	POV	B	385	-	51,51,51	0.88	2 (3%)	57,59,59	0.53	0
2	POV	A	324	-	51,51,51	0.92	2 (3%)	57,59,59	0.51	0
2	POV	A	367	-	51,51,51	0.95	2 (3%)	57,59,59	0.56	0
2	POV	B	312	-	51,51,51	0.91	2 (3%)	57,59,59	0.56	0
2	POV	B	350	-	51,51,51	0.93	2 (3%)	57,59,59	0.62	0
3	CLR	A	420	-	31,31,31	0.90	0	48,48,48	1.17	3 (6%)
2	POV	A	323	-	51,51,51	0.92	2 (3%)	57,59,59	0.50	0
2	POV	A	368	-	51,51,51	0.90	2 (3%)	57,59,59	0.49	0
2	POV	B	362	-	51,51,51	0.92	2 (3%)	57,59,59	0.61	0
2	POV	B	319	-	51,51,51	0.93	2 (3%)	57,59,59	0.56	1 (1%)
3	CLR	B	399	-	31,31,31	0.79	0	48,48,48	0.97	3 (6%)
3	CLR	B	390	-	31,31,31	0.69	0	48,48,48	0.97	3 (6%)
2	POV	A	394	-	51,51,51	0.91	2 (3%)	57,59,59	0.50	0
2	POV	B	316	-	51,51,51	0.89	2 (3%)	57,59,59	0.59	0
2	POV	B	310	-	51,51,51	0.94	2 (3%)	57,59,59	0.68	2 (3%)
2	POV	B	367	-	51,51,51	0.91	2 (3%)	57,59,59	0.68	1 (1%)
3	CLR	A	418	-	31,31,31	0.82	0	48,48,48	1.04	2 (4%)
2	POV	B	320	-	51,51,51	0.94	2 (3%)	57,59,59	0.62	1 (1%)
2	POV	B	337	-	51,51,51	0.90	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	A	320	-	51,51,51	0.90	2 (3%)	57,59,59	0.57	0
2	POV	A	332	-	51,51,51	0.87	2 (3%)	57,59,59	0.54	0
2	POV	A	352	-	51,51,51	0.90	2 (3%)	57,59,59	0.70	1 (1%)
2	POV	A	338	-	51,51,51	0.92	2 (3%)	57,59,59	0.49	0
2	POV	A	413	-	51,51,51	0.90	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	A	313	-	51,51,51	0.90	2 (3%)	57,59,59	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	B	361	-	51,51,51	0.92	2 (3%)	57,59,59	0.80	1 (1%)
2	POV	B	305	-	51,51,51	0.89	2 (3%)	57,59,59	0.53	0
2	POV	B	339	-	51,51,51	0.95	2 (3%)	57,59,59	0.85	3 (5%)
2	POV	A	373	-	51,51,51	0.91	2 (3%)	57,59,59	0.51	0
2	POV	A	378	-	51,51,51	0.90	2 (3%)	57,59,59	0.64	2 (3%)
2	POV	B	324	-	51,51,51	0.96	2 (3%)	57,59,59	0.70	1 (1%)
2	POV	B	309	-	51,51,51	0.87	2 (3%)	57,59,59	0.67	0
2	POV	A	333	-	51,51,51	0.92	2 (3%)	57,59,59	0.72	1 (1%)
2	POV	A	399	-	51,51,51	0.94	2 (3%)	57,59,59	0.55	0
2	POV	A	375	-	51,51,51	0.90	2 (3%)	57,59,59	0.52	0
2	POV	A	340	-	51,51,51	0.87	2 (3%)	57,59,59	0.57	0
2	POV	B	336	-	51,51,51	0.89	2 (3%)	57,59,59	0.60	0
2	POV	B	370	-	51,51,51	0.95	2 (3%)	57,59,59	0.59	0
3	CLR	A	406	-	31,31,31	0.84	1 (3%)	48,48,48	0.96	3 (6%)
2	POV	A	369	-	51,51,51	0.91	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	B	374	-	51,51,51	0.93	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	B	328	-	51,51,51	0.92	2 (3%)	57,59,59	0.51	0
2	POV	A	388	-	51,51,51	0.87	2 (3%)	57,59,59	0.49	0
2	POV	B	307	-	51,51,51	0.94	2 (3%)	57,59,59	0.74	1 (1%)
2	POV	A	372	-	51,51,51	0.91	2 (3%)	57,59,59	0.54	0
2	POV	B	340	-	51,51,51	0.90	3 (5%)	57,59,59	0.78	2 (3%)
2	POV	A	303	-	51,51,51	0.91	2 (3%)	57,59,59	0.59	1 (1%)
2	POV	A	334	-	51,51,51	0.98	2 (3%)	57,59,59	0.65	1 (1%)
2	POV	A	359	-	51,51,51	0.87	2 (3%)	57,59,59	0.77	2 (3%)
2	POV	A	312	-	51,51,51	0.95	2 (3%)	57,59,59	0.61	1 (1%)
2	POV	B	306	-	51,51,51	0.92	2 (3%)	57,59,59	0.62	1 (1%)
2	POV	A	396	-	51,51,51	0.84	2 (3%)	57,59,59	0.56	0
2	POV	A	348	-	51,51,51	0.91	2 (3%)	57,59,59	0.55	0
2	POV	B	318	-	51,51,51	0.92	2 (3%)	57,59,59	0.66	1 (1%)
3	CLR	A	405	-	31,31,31	0.81	0	48,48,48	0.88	2 (4%)
2	POV	A	306	-	51,51,51	0.89	2 (3%)	57,59,59	0.49	0
2	POV	A	376	-	51,51,51	0.89	2 (3%)	57,59,59	0.71	1 (1%)
2	POV	A	335	-	51,51,51	0.91	2 (3%)	57,59,59	0.50	0
2	POV	A	392	-	51,51,51	0.91	2 (3%)	57,59,59	0.48	0
2	POV	A	314	-	51,51,51	0.93	2 (3%)	57,59,59	0.61	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	A	316	-	51,51,51	0.88	2 (3%)	57,59,59	0.69	2 (3%)
2	POV	B	347	-	51,51,51	0.88	2 (3%)	57,59,59	0.69	1 (1%)
2	POV	B	377	-	51,51,51	0.83	2 (3%)	57,59,59	0.63	0
2	POV	A	310	-	51,51,51	0.89	2 (3%)	57,59,59	0.65	1 (1%)
2	POV	A	325	-	51,51,51	0.86	2 (3%)	57,59,59	0.66	1 (1%)
2	POV	B	359	-	51,51,51	0.91	2 (3%)	57,59,59	0.55	0
2	POV	B	331	-	51,51,51	0.91	2 (3%)	57,59,59	0.84	3 (5%)
2	POV	A	409	-	51,51,51	0.93	2 (3%)	57,59,59	0.73	1 (1%)
2	POV	B	379	-	51,51,51	0.92	2 (3%)	57,59,59	0.67	1 (1%)
2	POV	B	341	-	51,51,51	0.97	2 (3%)	57,59,59	0.69	1 (1%)
2	POV	A	363	-	51,51,51	0.93	2 (3%)	57,59,59	0.55	0
2	POV	B	358	-	51,51,51	0.87	2 (3%)	57,59,59	0.80	1 (1%)
2	POV	B	360	-	51,51,51	0.89	2 (3%)	57,59,59	0.73	2 (3%)
2	POV	A	361	-	51,51,51	0.89	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	B	372	-	51,51,51	0.86	2 (3%)	57,59,59	0.59	0
2	POV	B	303	-	51,51,51	0.87	2 (3%)	57,59,59	0.50	0
2	POV	A	408	-	51,51,51	0.93	2 (3%)	57,59,59	0.52	0
2	POV	A	358	-	51,51,51	0.88	2 (3%)	57,59,59	0.62	1 (1%)
2	POV	B	386	-	51,51,51	0.95	2 (3%)	57,59,59	0.57	0
2	POV	A	412	-	51,51,51	0.92	2 (3%)	57,59,59	0.62	1 (1%)
2	POV	B	334	-	51,51,51	0.91	2 (3%)	57,59,59	0.77	1 (1%)
3	CLR	A	402	-	31,31,31	0.81	0	48,48,48	1.34	6 (12%)
2	POV	B	371	-	51,51,51	0.93	2 (3%)	57,59,59	0.59	0
2	POV	A	416	-	51,51,51	0.87	2 (3%)	57,59,59	0.51	0
2	POV	B	329	-	51,51,51	0.90	2 (3%)	57,59,59	0.50	0
2	POV	B	344	-	51,51,51	0.89	2 (3%)	57,59,59	0.64	0
2	POV	A	301	-	51,51,51	0.88	2 (3%)	57,59,59	0.53	0
3	CLR	B	398	-	31,31,31	0.79	0	48,48,48	0.95	3 (6%)
2	POV	A	336	-	51,51,51	0.88	2 (3%)	57,59,59	0.67	1 (1%)
2	POV	A	370	-	51,51,51	0.93	2 (3%)	57,59,59	0.54	0
2	POV	B	313	-	51,51,51	0.90	2 (3%)	57,59,59	0.79	2 (3%)
2	POV	B	323	-	51,51,51	0.91	2 (3%)	57,59,59	0.71	2 (3%)
2	POV	B	325	-	51,51,51	0.88	2 (3%)	57,59,59	0.61	0
2	POV	A	321	-	51,51,51	0.93	2 (3%)	57,59,59	0.64	0
2	POV	B	321	-	51,51,51	0.94	2 (3%)	57,59,59	0.68	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	B	348	-	51,51,51	0.89	2 (3%)	57,59,59	0.62	1 (1%)
2	POV	B	366	-	51,51,51	0.89	2 (3%)	57,59,59	0.67	1 (1%)
2	POV	B	365	-	51,51,51	0.88	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	B	301	-	51,51,51	0.93	2 (3%)	57,59,59	0.59	0
2	POV	A	351	-	51,51,51	0.87	2 (3%)	57,59,59	0.60	0
3	CLR	B	394	-	31,31,31	0.89	1 (3%)	48,48,48	1.00	2 (4%)
2	POV	B	311	-	51,51,51	0.98	2 (3%)	57,59,59	0.54	1 (1%)
2	POV	A	328	-	51,51,51	0.91	2 (3%)	57,59,59	0.59	0
2	POV	A	341	-	51,51,51	0.95	2 (3%)	57,59,59	0.70	1 (1%)
2	POV	A	349	-	51,51,51	0.87	2 (3%)	57,59,59	0.61	0
2	POV	A	364	-	51,51,51	0.87	2 (3%)	57,59,59	0.57	0
2	POV	A	355	-	51,51,51	1.00	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	A	337	-	51,51,51	0.89	2 (3%)	57,59,59	0.57	0
2	POV	A	393	-	51,51,51	0.91	2 (3%)	57,59,59	0.55	0
2	POV	B	352	-	51,51,51	0.85	2 (3%)	57,59,59	0.59	1 (1%)
3	CLR	B	397	-	31,31,31	0.83	0	48,48,48	0.92	2 (4%)
2	POV	A	385	-	51,51,51	0.90	2 (3%)	57,59,59	0.51	0
2	POV	A	390	-	51,51,51	0.91	2 (3%)	57,59,59	0.49	0
2	POV	A	347	-	51,51,51	0.88	2 (3%)	57,59,59	0.50	0
2	POV	A	329	-	51,51,51	0.87	2 (3%)	57,59,59	0.78	1 (1%)
2	POV	A	356	-	51,51,51	0.93	2 (3%)	57,59,59	0.60	0
2	POV	A	331	-	51,51,51	0.88	2 (3%)	57,59,59	0.69	2 (3%)
2	POV	A	414	-	51,51,51	0.90	2 (3%)	57,59,59	0.65	0
2	POV	A	319	-	51,51,51	0.89	2 (3%)	57,59,59	0.68	1 (1%)
2	POV	B	333	-	51,51,51	0.90	2 (3%)	57,59,59	0.66	0
2	POV	A	315	-	51,51,51	0.90	2 (3%)	57,59,59	0.66	1 (1%)
2	POV	A	379	-	51,51,51	0.87	2 (3%)	57,59,59	0.51	0
2	POV	B	354	-	51,51,51	0.93	2 (3%)	57,59,59	0.53	0
2	POV	B	317	-	51,51,51	0.88	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	B	355	-	51,51,51	0.87	2 (3%)	57,59,59	0.54	0
2	POV	B	384	-	51,51,51	0.92	2 (3%)	57,59,59	0.57	0
3	CLR	A	404	-	31,31,31	0.86	1 (3%)	48,48,48	1.01	2 (4%)
2	POV	A	395	-	51,51,51	0.92	2 (3%)	57,59,59	0.69	1 (1%)
2	POV	A	410	-	51,51,51	0.89	2 (3%)	57,59,59	0.55	0
2	POV	A	417	-	51,51,51	0.90	2 (3%)	57,59,59	0.67	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	B	356	-	51,51,51	0.92	2 (3%)	57,59,59	0.59	1 (1%)
3	CLR	A	401	-	31,31,31	0.90	0	48,48,48	0.98	1 (2%)
2	POV	B	332	-	51,51,51	0.91	2 (3%)	57,59,59	0.55	0
2	POV	B	349	-	51,51,51	0.90	2 (3%)	57,59,59	0.54	0
2	POV	B	375	-	51,51,51	0.93	2 (3%)	57,59,59	0.47	0
2	POV	B	314	-	51,51,51	0.87	2 (3%)	57,59,59	0.56	0
2	POV	B	364	-	51,51,51	0.89	2 (3%)	57,59,59	0.57	0
3	CLR	B	396	-	31,31,31	0.83	1 (3%)	48,48,48	1.20	5 (10%)
2	POV	A	386	-	51,51,51	0.95	2 (3%)	57,59,59	0.49	0
2	POV	A	391	-	51,51,51	0.92	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	A	344	-	51,51,51	0.96	2 (3%)	57,59,59	0.63	0
2	POV	A	397	-	51,51,51	0.90	2 (3%)	57,59,59	0.54	0
2	POV	A	407	-	51,51,51	0.91	2 (3%)	57,59,59	0.65	1 (1%)
2	POV	B	304	-	51,51,51	0.89	2 (3%)	57,59,59	0.64	1 (1%)
3	CLR	A	403	-	31,31,31	0.83	0	48,48,48	1.02	2 (4%)
2	POV	A	304	-	51,51,51	0.89	2 (3%)	57,59,59	0.54	0
2	POV	B	345	-	51,51,51	0.93	2 (3%)	57,59,59	0.53	0
2	POV	B	338	-	51,51,51	0.90	2 (3%)	57,59,59	0.62	0
3	CLR	A	419	-	31,31,31	0.92	0	48,48,48	1.23	3 (6%)
2	POV	B	346	-	51,51,51	0.90	2 (3%)	57,59,59	0.65	0
3	CLR	B	393	-	31,31,31	0.73	0	48,48,48	1.02	2 (4%)
2	POV	A	350	-	51,51,51	0.90	2 (3%)	57,59,59	0.47	0
2	POV	B	373	-	51,51,51	1.00	2 (3%)	57,59,59	0.77	2 (3%)
2	POV	A	326	-	51,51,51	0.91	2 (3%)	57,59,59	0.55	0
2	POV	A	365	-	51,51,51	0.91	2 (3%)	57,59,59	0.63	0
2	POV	B	383	-	51,51,51	0.90	2 (3%)	57,59,59	0.65	1 (1%)
2	POV	A	387	-	51,51,51	0.91	2 (3%)	57,59,59	0.65	0
2	POV	A	377	-	51,51,51	0.90	2 (3%)	57,59,59	0.55	0
2	POV	B	315	-	51,51,51	0.96	2 (3%)	57,59,59	0.57	0
2	POV	B	335	-	51,51,51	0.92	2 (3%)	57,59,59	0.51	0
2	POV	B	353	-	51,51,51	0.87	2 (3%)	57,59,59	0.76	2 (3%)
2	POV	B	382	-	51,51,51	0.89	2 (3%)	57,59,59	0.68	2 (3%)
2	POV	A	309	-	51,51,51	0.90	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	A	371	-	51,51,51	0.87	2 (3%)	57,59,59	0.56	0
2	POV	B	388	-	51,51,51	0.91	2 (3%)	57,59,59	0.65	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	B	387	-	51,51,51	0.86	2 (3%)	57,59,59	0.55	0
2	POV	B	363	-	51,51,51	0.91	2 (3%)	57,59,59	0.50	0
2	POV	A	366	-	51,51,51	0.88	2 (3%)	57,59,59	0.78	2 (3%)
2	POV	A	346	-	51,51,51	0.90	2 (3%)	57,59,59	0.53	0
2	POV	B	326	-	51,51,51	0.89	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	A	305	-	51,51,51	0.93	2 (3%)	57,59,59	0.66	1 (1%)
2	POV	A	381	-	51,51,51	0.89	2 (3%)	57,59,59	0.46	0
2	POV	B	357	-	51,51,51	0.96	2 (3%)	57,59,59	0.74	1 (1%)
2	POV	B	381	-	51,51,51	0.96	2 (3%)	57,59,59	0.51	0
3	CLR	B	395	-	31,31,31	0.76	0	48,48,48	1.06	4 (8%)
2	POV	A	311	-	51,51,51	0.90	2 (3%)	57,59,59	0.61	1 (1%)
2	POV	A	308	-	51,51,51	0.92	2 (3%)	57,59,59	0.55	0
2	POV	A	374	-	51,51,51	0.92	2 (3%)	57,59,59	0.68	0
2	POV	A	415	-	51,51,51	0.88	3 (5%)	57,59,59	0.54	0
2	POV	B	389	-	51,51,51	0.90	2 (3%)	57,59,59	0.69	1 (1%)
2	POV	A	353	-	51,51,51	0.89	2 (3%)	57,59,59	0.60	1 (1%)
2	POV	B	368	-	51,51,51	0.90	2 (3%)	57,59,59	0.71	1 (1%)
3	CLR	B	392	-	31,31,31	0.76	0	48,48,48	1.28	5 (10%)
2	POV	B	351	-	51,51,51	0.90	2 (3%)	57,59,59	0.66	1 (1%)
2	POV	B	342	-	51,51,51	0.92	2 (3%)	57,59,59	0.57	0
2	POV	A	307	-	51,51,51	0.89	2 (3%)	57,59,59	0.52	0
2	POV	A	411	-	51,51,51	0.93	2 (3%)	57,59,59	0.72	2 (3%)
2	POV	A	342	-	51,51,51	0.88	2 (3%)	57,59,59	0.59	0
2	POV	A	354	-	51,51,51	0.93	2 (3%)	57,59,59	0.63	0
2	POV	A	318	-	51,51,51	0.93	2 (3%)	57,59,59	0.70	1 (1%)
2	POV	A	398	-	51,51,51	0.92	2 (3%)	57,59,59	0.60	0
2	POV	B	376	-	51,51,51	0.89	2 (3%)	57,59,59	0.52	0
2	POV	B	322	-	51,51,51	0.93	2 (3%)	57,59,59	0.49	0
2	POV	A	384	-	51,51,51	0.92	2 (3%)	57,59,59	0.80	2 (3%)
2	POV	B	308	-	51,51,51	0.86	2 (3%)	57,59,59	0.50	0
2	POV	A	330	-	51,51,51	0.87	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	B	369	-	51,51,51	0.90	2 (3%)	57,59,59	0.59	0
2	POV	A	383	-	51,51,51	0.93	2 (3%)	57,59,59	0.51	0
2	POV	A	302	-	51,51,51	0.87	2 (3%)	57,59,59	0.62	1 (1%)
2	POV	A	357	-	51,51,51	0.92	2 (3%)	57,59,59	0.67	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	A	345	-	51,51,51	0.92	2 (3%)	57,59,59	0.67	1 (1%)

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
2	POV	B	378	-	-	16/55/55/55	-
2	POV	B	380	-	-	9/55/55/55	-
2	POV	A	339	-	-	12/55/55/55	-
2	POV	B	343	-	-	13/55/55/55	-
2	POV	A	343	-	-	8/55/55/55	-
2	POV	B	302	-	-	15/55/55/55	-
2	POV	B	330	-	1/1/5/7	12/55/55/55	-
2	POV	A	380	-	1/1/5/7	11/55/55/55	-
3	CLR	B	391	-	-	0/10/68/68	0/4/4/4
2	POV	A	360	-	-	9/55/55/55	-
3	CLR	A	421	-	-	2/10/68/68	0/4/4/4
2	POV	A	322	-	1/1/5/7	12/55/55/55	-
2	POV	A	400	-	1/1/5/7	8/55/55/55	-
2	POV	A	362	-	-	11/55/55/55	-
2	POV	A	317	-	-	12/55/55/55	-
2	POV	A	327	-	-	15/55/55/55	-
2	POV	B	327	-	-	10/55/55/55	-
2	POV	A	389	-	-	14/55/55/55	-
2	POV	A	382	-	-	10/55/55/55	-
2	POV	B	385	-	-	8/55/55/55	-
2	POV	A	324	-	-	11/55/55/55	-
2	POV	A	367	-	-	4/55/55/55	-
2	POV	B	312	-	-	10/55/55/55	-
2	POV	B	350	-	-	8/55/55/55	-
3	CLR	A	420	-	-	1/10/68/68	0/4/4/4
2	POV	A	368	-	1/1/5/7	8/55/55/55	-
2	POV	A	323	-	-	9/55/55/55	-
2	POV	B	362	-	1/1/5/7	11/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	319	-	-	11/55/55/55	-
3	CLR	B	399	-	-	4/10/68/68	0/4/4/4
3	CLR	B	390	-	-	2/10/68/68	0/4/4/4
2	POV	A	394	-	-	12/55/55/55	-
2	POV	B	316	-	-	6/55/55/55	-
2	POV	B	310	-	-	7/55/55/55	-
2	POV	B	367	-	1/1/5/7	10/55/55/55	-
3	CLR	A	418	-	-	2/10/68/68	0/4/4/4
2	POV	B	320	-	-	11/55/55/55	-
2	POV	B	337	-	-	2/55/55/55	-
2	POV	A	320	-	-	8/55/55/55	-
2	POV	A	332	-	-	9/55/55/55	-
2	POV	A	352	-	-	13/55/55/55	-
2	POV	A	338	-	-	11/55/55/55	-
2	POV	A	413	-	-	8/55/55/55	-
2	POV	A	313	-	-	16/55/55/55	-
2	POV	B	361	-	-	14/55/55/55	-
2	POV	B	305	-	-	8/55/55/55	-
2	POV	B	339	-	-	11/55/55/55	-
2	POV	A	373	-	-	6/55/55/55	-
2	POV	A	378	-	1/1/5/7	16/55/55/55	-
2	POV	B	324	-	-	10/55/55/55	-
2	POV	B	309	-	-	6/55/55/55	-
2	POV	A	333	-	-	6/55/55/55	-
2	POV	A	399	-	-	12/55/55/55	-
2	POV	A	375	-	-	7/55/55/55	-
2	POV	A	340	-	-	9/55/55/55	-
2	POV	B	336	-	-	12/55/55/55	-
2	POV	B	370	-	-	11/55/55/55	-
3	CLR	A	406	-	-	0/10/68/68	0/4/4/4
2	POV	A	369	-	-	9/55/55/55	-
2	POV	B	374	-	-	18/55/55/55	-
2	POV	B	328	-	1/1/5/7	7/55/55/55	-
2	POV	A	388	-	-	6/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	307	-	-	14/55/55/55	-
2	POV	A	372	-	-	8/55/55/55	-
2	POV	B	340	-	-	11/55/55/55	-
2	POV	A	303	-	-	10/55/55/55	-
2	POV	A	334	-	-	13/55/55/55	-
2	POV	A	359	-	-	15/55/55/55	-
2	POV	A	312	-	-	9/55/55/55	-
2	POV	B	306	-	-	10/55/55/55	-
2	POV	A	396	-	-	11/55/55/55	-
2	POV	A	348	-	-	12/55/55/55	-
2	POV	B	318	-	-	11/55/55/55	-
3	CLR	A	405	-	-	2/10/68/68	0/4/4/4
2	POV	A	306	-	-	5/55/55/55	-
2	POV	A	376	-	-	13/55/55/55	-
2	POV	A	335	-	-	8/55/55/55	-
2	POV	B	347	-	1/1/5/7	13/55/55/55	-
2	POV	A	316	-	1/1/5/7	4/55/55/55	-
2	POV	A	314	-	-	8/55/55/55	-
2	POV	A	392	-	-	8/55/55/55	-
2	POV	B	377	-	-	6/55/55/55	-
2	POV	A	310	-	-	12/55/55/55	-
2	POV	A	325	-	-	14/55/55/55	-
2	POV	B	359	-	-	8/55/55/55	-
2	POV	B	331	-	-	13/55/55/55	-
2	POV	A	409	-	-	11/55/55/55	-
2	POV	B	379	-	-	14/55/55/55	-
2	POV	B	341	-	-	14/55/55/55	-
2	POV	A	363	-	-	14/55/55/55	-
2	POV	B	358	-	-	16/55/55/55	-
2	POV	B	360	-	-	13/55/55/55	-
2	POV	A	361	-	-	5/55/55/55	-
2	POV	B	372	-	-	7/55/55/55	-
2	POV	B	303	-	1/1/5/7	8/55/55/55	-
2	POV	A	408	-	-	13/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	358	-	-	6/55/55/55	-
2	POV	B	386	-	-	7/55/55/55	-
2	POV	A	412	-	-	6/55/55/55	-
2	POV	B	334	-	-	11/55/55/55	-
3	CLR	A	402	-	-	4/10/68/68	0/4/4/4
2	POV	B	371	-	-	11/55/55/55	-
2	POV	A	416	-	-	8/55/55/55	-
2	POV	B	329	-	1/1/5/7	5/55/55/55	-
2	POV	B	344	-	-	9/55/55/55	-
2	POV	A	301	-	-	11/55/55/55	-
3	CLR	B	398	-	-	1/10/68/68	0/4/4/4
2	POV	A	336	-	-	12/55/55/55	-
2	POV	A	370	-	-	11/55/55/55	-
2	POV	B	313	-	-	9/55/55/55	-
2	POV	B	323	-	-	11/55/55/55	-
2	POV	B	325	-	-	5/55/55/55	-
2	POV	A	321	-	-	11/55/55/55	-
2	POV	B	321	-	1/1/5/7	9/55/55/55	-
2	POV	B	348	-	-	8/55/55/55	-
2	POV	B	366	-	-	9/55/55/55	-
2	POV	B	365	-	-	8/55/55/55	-
2	POV	B	301	-	-	7/55/55/55	-
2	POV	A	351	-	-	9/55/55/55	-
3	CLR	B	394	-	-	0/10/68/68	0/4/4/4
2	POV	B	311	-	-	13/55/55/55	-
2	POV	A	328	-	-	8/55/55/55	-
2	POV	A	341	-	-	11/55/55/55	-
2	POV	A	349	-	-	9/55/55/55	-
2	POV	A	364	-	-	10/55/55/55	-
2	POV	A	355	-	-	6/55/55/55	-
2	POV	A	337	-	-	4/55/55/55	-
2	POV	A	393	-	-	17/55/55/55	-
2	POV	B	352	-	-	8/55/55/55	-
3	CLR	B	397	-	-	0/10/68/68	0/4/4/4
2	POV	A	385	-	1/1/5/7	8/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	390	-	-	11/55/55/55	-
2	POV	A	347	-	-	14/55/55/55	-
2	POV	A	329	-	-	9/55/55/55	-
2	POV	A	356	-	-	10/55/55/55	-
2	POV	A	331	-	-	15/55/55/55	-
2	POV	A	414	-	-	5/55/55/55	-
2	POV	A	319	-	1/1/5/7	11/55/55/55	-
2	POV	B	333	-	-	9/55/55/55	-
2	POV	A	315	-	-	13/55/55/55	-
2	POV	A	379	-	-	5/55/55/55	-
2	POV	B	354	-	-	10/55/55/55	-
2	POV	B	317	-	-	10/55/55/55	-
2	POV	B	355	-	-	10/55/55/55	-
2	POV	B	384	-	-	11/55/55/55	-
3	CLR	A	404	-	-	3/10/68/68	0/4/4/4
2	POV	A	395	-	-	14/55/55/55	-
2	POV	A	410	-	1/1/5/7	8/55/55/55	-
2	POV	A	417	-	-	6/55/55/55	-
2	POV	B	356	-	-	5/55/55/55	-
3	CLR	A	401	-	-	0/10/68/68	0/4/4/4
2	POV	B	332	-	-	11/55/55/55	-
2	POV	B	349	-	-	10/55/55/55	-
2	POV	B	375	-	-	6/55/55/55	-
2	POV	B	314	-	-	8/55/55/55	-
2	POV	B	364	-	1/1/5/7	9/55/55/55	-
3	CLR	B	396	-	-	5/10/68/68	0/4/4/4
2	POV	A	386	-	-	8/55/55/55	-
2	POV	A	391	-	-	5/55/55/55	-
2	POV	A	344	-	-	8/55/55/55	-
2	POV	A	397	-	-	9/55/55/55	-
2	POV	A	407	-	-	7/55/55/55	-
2	POV	B	304	-	-	11/55/55/55	-
3	CLR	A	403	-	-	0/10/68/68	0/4/4/4
2	POV	A	304	-	-	9/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	345	-	-	12/55/55/55	-
2	POV	B	338	-	-	10/55/55/55	-
3	CLR	A	419	-	-	1/10/68/68	0/4/4/4
2	POV	B	346	-	1/1/5/7	13/55/55/55	-
3	CLR	B	393	-	-	0/10/68/68	0/4/4/4
2	POV	A	350	-	-	9/55/55/55	-
2	POV	B	373	-	-	12/55/55/55	-
2	POV	A	326	-	1/1/5/7	8/55/55/55	-
2	POV	A	365	-	1/1/5/7	11/55/55/55	-
2	POV	B	383	-	-	12/55/55/55	-
2	POV	A	387	-	-	9/55/55/55	-
2	POV	A	377	-	-	6/55/55/55	-
2	POV	B	315	-	-	4/55/55/55	-
2	POV	B	335	-	-	6/55/55/55	-
2	POV	B	353	-	-	5/55/55/55	-
2	POV	B	382	-	-	14/55/55/55	-
2	POV	A	309	-	-	4/55/55/55	-
2	POV	A	371	-	-	10/55/55/55	-
2	POV	B	388	-	-	10/55/55/55	-
2	POV	B	387	-	-	9/55/55/55	-
2	POV	B	363	-	-	2/55/55/55	-
2	POV	A	366	-	-	9/55/55/55	-
2	POV	A	346	-	-	9/55/55/55	-
2	POV	B	326	-	-	10/55/55/55	-
2	POV	A	305	-	-	8/55/55/55	-
2	POV	A	381	-	-	8/55/55/55	-
2	POV	B	357	-	-	12/55/55/55	-
2	POV	B	381	-	-	15/55/55/55	-
3	CLR	B	395	-	-	0/10/68/68	0/4/4/4
2	POV	A	311	-	-	16/55/55/55	-
2	POV	A	308	-	1/1/5/7	7/55/55/55	-
2	POV	A	374	-	-	6/55/55/55	-
2	POV	A	415	-	-	13/55/55/55	-
2	POV	B	389	-	-	8/55/55/55	-
2	POV	A	353	-	-	13/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	368	-	-	8/55/55/55	-
3	CLR	B	392	-	-	4/10/68/68	0/4/4/4
2	POV	B	351	-	-	6/55/55/55	-
2	POV	B	342	-	-	6/55/55/55	-
2	POV	A	307	-	-	6/55/55/55	-
2	POV	A	411	-	-	15/55/55/55	-
2	POV	A	342	-	-	7/55/55/55	-
2	POV	A	354	-	-	16/55/55/55	-
2	POV	A	318	-	1/1/5/7	11/55/55/55	-
2	POV	A	398	-	-	8/55/55/55	-
2	POV	B	376	-	-	7/55/55/55	-
2	POV	B	322	-	-	10/55/55/55	-
2	POV	A	384	-	-	16/55/55/55	-
2	POV	B	308	-	-	5/55/55/55	-
2	POV	A	330	-	-	6/55/55/55	-
2	POV	B	369	-	-	11/55/55/55	-
2	POV	A	383	-	1/1/5/7	8/55/55/55	-
2	POV	A	302	-	-	8/55/55/55	-
2	POV	A	357	-	-	8/55/55/55	-
2	POV	A	345	-	-	8/55/55/55	-

All (406) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	POV	O21-C2	-3.76	1.37	1.46
2	A	317	POV	O21-C2	-3.76	1.37	1.46
2	B	341	POV	O21-C2	-3.74	1.37	1.46
2	B	362	POV	O21-C2	-3.72	1.37	1.46
2	B	324	POV	O21-C2	-3.71	1.37	1.46
2	A	308	POV	O21-C2	-3.69	1.37	1.46
2	A	387	POV	O21-C2	-3.68	1.37	1.46
2	A	344	POV	O31-C3	-3.64	1.37	1.45
2	A	314	POV	O21-C2	-3.64	1.38	1.46
2	A	355	POV	O21-C2	-3.64	1.38	1.46
2	B	311	POV	O21-C2	-3.63	1.38	1.46
2	B	370	POV	O31-C3	-3.62	1.37	1.45
2	A	408	POV	O21-C2	-3.58	1.38	1.46
2	A	386	POV	O21-C2	-3.58	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	334	POV	O21-C2	-3.54	1.38	1.46
2	B	339	POV	O21-C2	-3.54	1.38	1.46
2	A	365	POV	O31-C3	-3.53	1.37	1.45
2	B	373	POV	O21-C2	-3.52	1.38	1.46
2	A	383	POV	O21-C2	-3.51	1.38	1.46
2	A	373	POV	O21-C2	-3.50	1.38	1.46
2	A	411	POV	O21-C2	-3.50	1.38	1.46
2	B	335	POV	O21-C2	-3.49	1.38	1.46
2	B	306	POV	O21-C2	-3.49	1.38	1.46
2	B	343	POV	O21-C2	-3.49	1.38	1.46
2	B	346	POV	O21-C2	-3.49	1.38	1.46
2	A	357	POV	O21-C2	-3.49	1.38	1.46
2	B	369	POV	O21-C2	-3.48	1.38	1.46
2	A	333	POV	O21-C2	-3.47	1.38	1.46
2	B	320	POV	O21-C2	-3.47	1.38	1.46
2	A	409	POV	O21-C2	-3.45	1.38	1.46
2	A	348	POV	O31-C3	-3.45	1.37	1.45
2	B	354	POV	O21-C2	-3.44	1.38	1.46
2	B	350	POV	O21-C2	-3.44	1.38	1.46
2	B	321	POV	O31-C3	-3.44	1.37	1.45
2	A	368	POV	O21-C2	-3.44	1.38	1.46
2	A	303	POV	O21-C2	-3.44	1.38	1.46
2	B	367	POV	O21-C2	-3.44	1.38	1.46
2	B	356	POV	O21-C2	-3.43	1.38	1.46
2	A	382	POV	O21-C2	-3.43	1.38	1.46
2	A	391	POV	O21-C2	-3.43	1.38	1.46
2	B	372	POV	O21-C2	-3.43	1.38	1.46
2	A	312	POV	O21-C2	-3.42	1.38	1.46
2	A	377	POV	O31-C3	-3.42	1.37	1.45
2	B	337	POV	O21-C2	-3.42	1.38	1.46
2	A	354	POV	O21-C2	-3.41	1.38	1.46
2	A	324	POV	O21-C2	-3.41	1.38	1.46
2	A	413	POV	O21-C2	-3.41	1.38	1.46
2	A	311	POV	O21-C2	-3.41	1.38	1.46
2	A	327	POV	O21-C2	-3.41	1.38	1.46
2	B	331	POV	O21-C2	-3.41	1.38	1.46
2	B	323	POV	O31-C3	-3.40	1.37	1.45
2	A	397	POV	O21-C2	-3.40	1.38	1.46
2	A	326	POV	O21-C2	-3.40	1.38	1.46
2	B	342	POV	O31-C3	-3.40	1.37	1.45
2	B	330	POV	O21-C2	-3.39	1.38	1.46
2	B	386	POV	O21-C2	-3.39	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	342	POV	O21-C2	-3.39	1.38	1.46
2	B	381	POV	O31-C3	-3.39	1.37	1.45
2	A	361	POV	O21-C2	-3.39	1.38	1.46
2	B	301	POV	O21-C2	-3.39	1.38	1.46
2	B	322	POV	O21-C2	-3.39	1.38	1.46
2	A	383	POV	O31-C3	-3.38	1.37	1.45
2	A	339	POV	O31-C3	-3.37	1.37	1.45
2	B	321	POV	O21-C2	-3.37	1.38	1.46
2	B	375	POV	O31-C3	-3.37	1.37	1.45
2	B	389	POV	O31-C3	-3.37	1.37	1.45
2	A	336	POV	O21-C2	-3.37	1.38	1.46
2	B	363	POV	O21-C2	-3.37	1.38	1.46
2	B	364	POV	O21-C2	-3.37	1.38	1.46
2	B	329	POV	O21-C2	-3.37	1.38	1.46
2	A	389	POV	O21-C2	-3.36	1.38	1.46
2	A	393	POV	O21-C2	-3.36	1.38	1.46
2	A	350	POV	O21-C2	-3.36	1.38	1.46
2	B	345	POV	O21-C2	-3.36	1.38	1.46
2	A	390	POV	O31-C3	-3.36	1.37	1.45
2	A	369	POV	O21-C2	-3.35	1.38	1.46
2	A	412	POV	O21-C2	-3.35	1.38	1.46
2	A	384	POV	O21-C2	-3.34	1.38	1.46
2	A	344	POV	O21-C2	-3.34	1.38	1.46
2	B	376	POV	O21-C2	-3.34	1.38	1.46
2	A	338	POV	O21-C2	-3.34	1.38	1.46
2	A	360	POV	O21-C2	-3.34	1.38	1.46
2	A	312	POV	O31-C3	-3.33	1.37	1.45
2	A	334	POV	O31-C3	-3.33	1.37	1.45
2	A	392	POV	O31-C3	-3.33	1.37	1.45
2	B	371	POV	O31-C3	-3.33	1.37	1.45
2	B	338	POV	O21-C2	-3.33	1.38	1.46
2	A	362	POV	O21-C2	-3.33	1.38	1.46
2	B	304	POV	O21-C2	-3.33	1.38	1.46
2	A	395	POV	O31-C3	-3.33	1.37	1.45
2	A	398	POV	O21-C2	-3.33	1.38	1.46
2	B	342	POV	O21-C2	-3.33	1.38	1.46
2	A	333	POV	O31-C3	-3.32	1.37	1.45
2	B	311	POV	O31-C3	-3.32	1.37	1.45
2	B	327	POV	O31-C3	-3.32	1.37	1.45
2	B	388	POV	O31-C3	-3.32	1.37	1.45
2	A	355	POV	O31-C3	-3.32	1.37	1.45
2	B	315	POV	O31-C3	-3.31	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	358	POV	O21-C2	-3.31	1.38	1.46
2	A	328	POV	O31-C3	-3.31	1.37	1.45
2	B	381	POV	O21-C2	-3.31	1.38	1.46
2	A	360	POV	O31-C3	-3.31	1.37	1.45
2	B	359	POV	O31-C3	-3.31	1.37	1.45
2	A	301	POV	O21-C2	-3.31	1.38	1.46
2	B	350	POV	O31-C3	-3.31	1.37	1.45
2	A	332	POV	O21-C2	-3.30	1.38	1.46
2	B	370	POV	O21-C2	-3.30	1.38	1.46
2	B	322	POV	O31-C3	-3.30	1.37	1.45
2	A	327	POV	O31-C3	-3.30	1.37	1.45
2	A	367	POV	O31-C3	-3.30	1.37	1.45
2	A	376	POV	O31-C3	-3.30	1.37	1.45
2	B	326	POV	O21-C2	-3.29	1.38	1.46
2	B	373	POV	O31-C3	-3.29	1.37	1.45
2	A	316	POV	O21-C2	-3.29	1.38	1.46
2	A	329	POV	O21-C2	-3.29	1.38	1.46
2	B	308	POV	O21-C2	-3.29	1.38	1.46
2	B	348	POV	O21-C2	-3.29	1.38	1.46
2	B	380	POV	O21-C2	-3.29	1.38	1.46
2	A	377	POV	O21-C2	-3.28	1.38	1.46
2	B	365	POV	O21-C2	-3.28	1.38	1.46
2	A	400	POV	O21-C2	-3.28	1.38	1.46
2	B	355	POV	O21-C2	-3.28	1.38	1.46
2	A	328	POV	O21-C2	-3.28	1.38	1.46
2	A	375	POV	O21-C2	-3.28	1.38	1.46
2	B	332	POV	O31-C3	-3.28	1.37	1.45
2	A	363	POV	O21-C2	-3.28	1.38	1.46
2	B	316	POV	O21-C2	-3.28	1.38	1.46
2	A	350	POV	O31-C3	-3.28	1.37	1.45
2	A	399	POV	O31-C3	-3.28	1.37	1.45
2	B	324	POV	O31-C3	-3.28	1.37	1.45
2	A	341	POV	O21-C2	-3.27	1.38	1.46
2	A	323	POV	O31-C3	-3.27	1.37	1.45
2	B	307	POV	O31-C3	-3.27	1.37	1.45
2	B	385	POV	O31-C3	-3.27	1.37	1.45
2	A	326	POV	O31-C3	-3.27	1.37	1.45
2	A	416	POV	O21-C2	-3.27	1.38	1.46
2	B	331	POV	O31-C3	-3.26	1.37	1.45
2	A	349	POV	O21-C2	-3.26	1.38	1.46
2	B	333	POV	O21-C2	-3.25	1.38	1.46
2	B	306	POV	O31-C3	-3.25	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	345	POV	O31-C3	-3.25	1.37	1.45
2	B	327	POV	O21-C2	-3.25	1.39	1.46
2	A	338	POV	O31-C3	-3.25	1.37	1.45
2	B	336	POV	O21-C2	-3.24	1.39	1.46
2	A	305	POV	O21-C2	-3.24	1.39	1.46
2	A	367	POV	O21-C2	-3.24	1.39	1.46
2	A	414	POV	O21-C2	-3.23	1.39	1.46
2	B	320	POV	O31-C3	-3.23	1.37	1.45
2	B	312	POV	O21-C2	-3.23	1.39	1.46
2	A	335	POV	O21-C2	-3.23	1.39	1.46
2	A	304	POV	O21-C2	-3.23	1.39	1.46
2	B	346	POV	O31-C3	-3.22	1.38	1.45
2	A	319	POV	O21-C2	-3.22	1.39	1.46
2	B	383	POV	O31-C3	-3.22	1.38	1.45
2	A	356	POV	O21-C2	-3.22	1.39	1.46
2	A	318	POV	O21-C2	-3.22	1.39	1.46
2	B	383	POV	O21-C2	-3.21	1.39	1.46
2	B	371	POV	O21-C2	-3.21	1.39	1.46
2	A	320	POV	O21-C2	-3.21	1.39	1.46
2	B	358	POV	O21-C2	-3.21	1.39	1.46
2	A	324	POV	O31-C3	-3.21	1.38	1.45
2	B	310	POV	O31-C3	-3.21	1.38	1.45
2	A	315	POV	O31-C3	-3.20	1.38	1.45
2	A	323	POV	O21-C2	-3.20	1.39	1.46
2	A	359	POV	O21-C2	-3.20	1.39	1.46
2	A	396	POV	O21-C2	-3.20	1.39	1.46
2	B	375	POV	O21-C2	-3.20	1.39	1.46
2	A	341	POV	O31-C3	-3.20	1.38	1.45
2	A	372	POV	O21-C2	-3.20	1.39	1.46
2	A	301	POV	O31-C3	-3.20	1.38	1.45
2	A	337	POV	O31-C3	-3.20	1.38	1.45
2	B	329	POV	O31-C3	-3.20	1.38	1.45
2	B	351	POV	O21-C2	-3.19	1.39	1.46
2	A	399	POV	O21-C2	-3.19	1.39	1.46
2	A	379	POV	O31-C3	-3.19	1.38	1.45
2	B	319	POV	O31-C3	-3.19	1.38	1.45
2	B	344	POV	O21-C2	-3.19	1.39	1.46
2	A	321	POV	O21-C2	-3.19	1.39	1.46
2	A	306	POV	O21-C2	-3.18	1.39	1.46
2	A	348	POV	O21-C2	-3.18	1.39	1.46
2	B	319	POV	O21-C2	-3.18	1.39	1.46
2	A	343	POV	O21-C2	-3.18	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	364	POV	O21-C2	-3.18	1.39	1.46
2	B	359	POV	O21-C2	-3.18	1.39	1.46
2	B	353	POV	O31-C3	-3.18	1.38	1.45
2	A	415	POV	O21-C2	-3.17	1.39	1.46
2	B	347	POV	O21-C2	-3.17	1.39	1.46
2	A	309	POV	O31-C3	-3.17	1.38	1.45
2	B	376	POV	O31-C3	-3.17	1.38	1.45
2	A	366	POV	O21-C2	-3.17	1.39	1.46
2	B	340	POV	O21-C2	-3.17	1.39	1.46
2	A	363	POV	O31-C3	-3.16	1.38	1.45
2	A	382	POV	O31-C3	-3.16	1.38	1.45
2	B	328	POV	O31-C3	-3.16	1.38	1.45
2	A	310	POV	O21-C2	-3.16	1.39	1.46
2	A	352	POV	O31-C3	-3.16	1.38	1.45
2	A	361	POV	O31-C3	-3.16	1.38	1.45
2	A	378	POV	O31-C3	-3.16	1.38	1.45
2	A	385	POV	O21-C2	-3.16	1.39	1.46
2	B	323	POV	O21-C2	-3.16	1.39	1.46
2	B	379	POV	O21-C2	-3.16	1.39	1.46
2	A	390	POV	O21-C2	-3.16	1.39	1.46
2	B	325	POV	O21-C2	-3.16	1.39	1.46
2	B	344	POV	O31-C3	-3.16	1.38	1.45
2	A	305	POV	O31-C3	-3.15	1.38	1.45
2	B	354	POV	O31-C3	-3.15	1.38	1.45
2	A	347	POV	O21-C2	-3.15	1.39	1.46
2	A	381	POV	O21-C2	-3.15	1.39	1.46
2	B	303	POV	O21-C2	-3.15	1.39	1.46
2	B	332	POV	O21-C2	-3.15	1.39	1.46
2	A	307	POV	O31-C3	-3.15	1.38	1.45
2	A	308	POV	O31-C3	-3.15	1.38	1.45
2	B	345	POV	O31-C3	-3.15	1.38	1.45
2	A	378	POV	O21-C2	-3.15	1.39	1.46
2	B	357	POV	O21-C2	-3.15	1.39	1.46
2	B	335	POV	O31-C3	-3.15	1.38	1.45
2	B	361	POV	O31-C3	-3.15	1.38	1.45
2	A	395	POV	O21-C2	-3.15	1.39	1.46
2	B	389	POV	O21-C2	-3.14	1.39	1.46
2	A	346	POV	O21-C2	-3.14	1.39	1.46
2	B	378	POV	O21-C2	-3.14	1.39	1.46
2	A	369	POV	O31-C3	-3.14	1.38	1.45
2	A	331	POV	O31-C3	-3.14	1.38	1.45
2	B	386	POV	O31-C3	-3.14	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	366	POV	O21-C2	-3.14	1.39	1.46
2	A	302	POV	O21-C2	-3.14	1.39	1.46
2	B	318	POV	O21-C2	-3.14	1.39	1.46
2	A	356	POV	O31-C3	-3.14	1.38	1.45
2	A	398	POV	O31-C3	-3.13	1.38	1.45
2	A	407	POV	O31-C3	-3.13	1.38	1.45
2	A	413	POV	O31-C3	-3.13	1.38	1.45
2	A	313	POV	O21-C2	-3.13	1.39	1.46
2	A	370	POV	O21-C2	-3.13	1.39	1.46
2	A	368	POV	O31-C3	-3.13	1.38	1.45
2	A	380	POV	O31-C3	-3.13	1.38	1.45
2	A	394	POV	O31-C3	-3.13	1.38	1.45
2	B	328	POV	O21-C2	-3.12	1.39	1.46
2	A	304	POV	O31-C3	-3.12	1.38	1.45
2	A	362	POV	O31-C3	-3.12	1.38	1.45
2	A	417	POV	O31-C3	-3.12	1.38	1.45
2	B	310	POV	O21-C2	-3.12	1.39	1.46
2	B	374	POV	O21-C2	-3.12	1.39	1.46
2	A	394	POV	O21-C2	-3.12	1.39	1.46
2	A	320	POV	O31-C3	-3.12	1.38	1.45
2	A	410	POV	O21-C2	-3.12	1.39	1.46
2	B	334	POV	O21-C2	-3.12	1.39	1.46
2	A	364	POV	O31-C3	-3.11	1.38	1.45
2	B	316	POV	O31-C3	-3.11	1.38	1.45
2	A	345	POV	O21-C2	-3.11	1.39	1.46
2	A	371	POV	O21-C2	-3.11	1.39	1.46
2	B	349	POV	O21-C2	-3.11	1.39	1.46
2	A	303	POV	O31-C3	-3.11	1.38	1.45
2	B	317	POV	O21-C2	-3.11	1.39	1.46
2	A	353	POV	O21-C2	-3.11	1.39	1.46
2	B	365	POV	O31-C3	-3.10	1.38	1.45
2	B	314	POV	O21-C2	-3.10	1.39	1.46
2	B	385	POV	O21-C2	-3.10	1.39	1.46
2	B	305	POV	O21-C2	-3.10	1.39	1.46
2	A	410	POV	O31-C3	-3.10	1.38	1.45
2	A	412	POV	O31-C3	-3.10	1.38	1.45
2	B	366	POV	O31-C3	-3.09	1.38	1.45
2	B	352	POV	O21-C2	-3.09	1.39	1.46
2	A	357	POV	O31-C3	-3.09	1.38	1.45
2	B	356	POV	O31-C3	-3.09	1.38	1.45
2	B	367	POV	O31-C3	-3.08	1.38	1.45
2	A	388	POV	O21-C2	-3.08	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	341	POV	O31-C3	-3.08	1.38	1.45
2	A	343	POV	O31-C3	-3.08	1.38	1.45
2	B	330	POV	O31-C3	-3.08	1.38	1.45
2	B	333	POV	O31-C3	-3.08	1.38	1.45
2	A	319	POV	O31-C3	-3.08	1.38	1.45
2	A	392	POV	O21-C2	-3.07	1.39	1.46
2	A	393	POV	O31-C3	-3.07	1.38	1.45
2	A	340	POV	O21-C2	-3.07	1.39	1.46
2	B	307	POV	O21-C2	-3.07	1.39	1.46
2	A	370	POV	O31-C3	-3.07	1.38	1.45
2	A	354	POV	O31-C3	-3.07	1.38	1.45
2	B	384	POV	O21-C2	-3.07	1.39	1.46
2	A	387	POV	O31-C3	-3.06	1.38	1.45
2	A	358	POV	O31-C3	-3.06	1.38	1.45
2	A	384	POV	O31-C3	-3.06	1.38	1.45
2	A	409	POV	O31-C3	-3.05	1.38	1.45
2	A	339	POV	O21-C2	-3.05	1.39	1.46
2	A	336	POV	O31-C3	-3.05	1.38	1.45
2	A	322	POV	O21-C2	-3.04	1.39	1.46
2	A	331	POV	O21-C2	-3.04	1.39	1.46
2	B	360	POV	O31-C3	-3.04	1.38	1.45
2	A	380	POV	O21-C2	-3.04	1.39	1.46
2	B	347	POV	O31-C3	-3.04	1.38	1.45
2	B	363	POV	O31-C3	-3.04	1.38	1.45
2	A	376	POV	O21-C2	-3.03	1.39	1.46
2	A	352	POV	O21-C2	-3.03	1.39	1.46
2	B	384	POV	O31-C3	-3.03	1.38	1.45
2	A	330	POV	O21-C2	-3.02	1.39	1.46
2	A	314	POV	O31-C3	-3.02	1.38	1.45
2	A	375	POV	O31-C3	-3.02	1.38	1.45
2	A	397	POV	O31-C3	-3.02	1.38	1.45
2	A	309	POV	O21-C2	-3.02	1.39	1.46
2	B	360	POV	O21-C2	-3.01	1.39	1.46
2	A	407	POV	O21-C2	-3.01	1.39	1.46
2	A	408	POV	O31-C3	-3.01	1.38	1.45
2	A	313	POV	O31-C3	-3.01	1.38	1.45
2	B	317	POV	O31-C3	-3.01	1.38	1.45
2	B	351	POV	O31-C3	-3.01	1.38	1.45
2	A	381	POV	O31-C3	-3.00	1.38	1.45
2	A	322	POV	O31-C3	-3.00	1.38	1.45
2	A	307	POV	O21-C2	-3.00	1.39	1.46
2	A	347	POV	O31-C3	-3.00	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	308	POV	O31-C3	-3.00	1.38	1.45
2	A	400	POV	O31-C3	-3.00	1.38	1.45
2	B	301	POV	O31-C3	-3.00	1.38	1.45
2	B	313	POV	O21-C2	-3.00	1.39	1.46
2	B	388	POV	O21-C2	-2.99	1.39	1.46
2	A	386	POV	O31-C3	-2.99	1.38	1.45
2	A	411	POV	O31-C3	-2.99	1.38	1.45
2	A	374	POV	O31-C3	-2.98	1.38	1.45
2	B	374	POV	O31-C3	-2.98	1.38	1.45
2	A	317	POV	O31-C3	-2.98	1.38	1.45
2	B	382	POV	O31-C3	-2.98	1.38	1.45
2	A	332	POV	O31-C3	-2.98	1.38	1.45
2	A	388	POV	O31-C3	-2.98	1.38	1.45
2	B	305	POV	O31-C3	-2.98	1.38	1.45
2	A	321	POV	O31-C3	-2.97	1.38	1.45
2	B	325	POV	O31-C3	-2.97	1.38	1.45
2	B	302	POV	O21-C2	-2.97	1.39	1.46
2	B	349	POV	O31-C3	-2.96	1.38	1.45
2	B	355	POV	O31-C3	-2.96	1.38	1.45
2	B	357	POV	O31-C3	-2.96	1.38	1.45
2	B	339	POV	O31-C3	-2.96	1.38	1.45
2	B	369	POV	O31-C3	-2.96	1.38	1.45
2	A	302	POV	O31-C3	-2.95	1.38	1.45
2	A	365	POV	O21-C2	-2.95	1.39	1.46
2	B	368	POV	O21-C2	-2.95	1.39	1.46
2	A	306	POV	O31-C3	-2.95	1.38	1.45
2	A	366	POV	O31-C3	-2.94	1.38	1.45
2	B	318	POV	O31-C3	-2.94	1.38	1.45
2	B	313	POV	O31-C3	-2.93	1.38	1.45
2	B	358	POV	O31-C3	-2.93	1.38	1.45
2	A	414	POV	O31-C3	-2.93	1.38	1.45
2	A	351	POV	O21-C2	-2.93	1.39	1.46
2	B	353	POV	O21-C2	-2.93	1.39	1.46
2	B	382	POV	O21-C2	-2.93	1.39	1.46
2	B	343	POV	O31-C3	-2.93	1.38	1.45
2	A	417	POV	O21-C2	-2.93	1.39	1.46
2	B	364	POV	O31-C3	-2.92	1.38	1.45
2	A	337	POV	O21-C2	-2.92	1.39	1.46
2	A	349	POV	O31-C3	-2.91	1.38	1.45
2	B	368	POV	O31-C3	-2.91	1.38	1.45
2	B	372	POV	O31-C3	-2.91	1.38	1.45
2	B	348	POV	O31-C3	-2.90	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	318	POV	O31-C3	-2.90	1.38	1.45
2	A	416	POV	O31-C3	-2.90	1.38	1.45
2	B	302	POV	O31-C3	-2.90	1.38	1.45
2	A	340	POV	O31-C3	-2.90	1.38	1.45
2	A	346	POV	O31-C3	-2.89	1.38	1.45
2	A	391	POV	O31-C3	-2.89	1.38	1.45
2	B	326	POV	O31-C3	-2.89	1.38	1.45
2	B	387	POV	O31-C3	-2.89	1.38	1.45
2	B	338	POV	O31-C3	-2.88	1.38	1.45
2	A	396	POV	O31-C3	-2.87	1.38	1.45
2	A	379	POV	O21-C2	-2.87	1.39	1.46
2	B	309	POV	O21-C2	-2.87	1.39	1.46
2	A	389	POV	O31-C3	-2.86	1.38	1.45
2	A	315	POV	O21-C2	-2.85	1.39	1.46
2	B	377	POV	O21-C2	-2.85	1.39	1.46
2	B	387	POV	O21-C2	-2.84	1.39	1.46
2	A	353	POV	O31-C3	-2.84	1.38	1.45
2	A	372	POV	O31-C3	-2.84	1.38	1.45
2	B	361	POV	O21-C2	-2.83	1.39	1.46
2	A	311	POV	O31-C3	-2.83	1.38	1.45
2	B	309	POV	O31-C3	-2.83	1.38	1.45
2	B	303	POV	O31-C3	-2.83	1.38	1.45
2	B	377	POV	O31-C3	-2.82	1.38	1.45
2	A	335	POV	O31-C3	-2.81	1.38	1.45
2	B	304	POV	O31-C3	-2.81	1.38	1.45
2	B	312	POV	O31-C3	-2.80	1.38	1.45
2	B	378	POV	O31-C3	-2.80	1.38	1.45
2	B	314	POV	O31-C3	-2.80	1.38	1.45
2	B	379	POV	O31-C3	-2.80	1.38	1.45
2	B	337	POV	O31-C3	-2.79	1.38	1.45
2	A	415	POV	O31-C3	-2.78	1.38	1.45
2	A	373	POV	O31-C3	-2.77	1.39	1.45
2	A	374	POV	O21-C2	-2.73	1.40	1.46
2	A	385	POV	O31-C3	-2.73	1.39	1.45
2	B	352	POV	O31-C3	-2.73	1.39	1.45
2	A	325	POV	O21-C2	-2.73	1.40	1.46
2	B	336	POV	O31-C3	-2.72	1.39	1.45
2	A	371	POV	O31-C3	-2.72	1.39	1.45
2	B	362	POV	O31-C3	-2.71	1.39	1.45
2	A	325	POV	O31-C3	-2.70	1.39	1.45
2	A	351	POV	O31-C3	-2.69	1.39	1.45
2	A	342	POV	O31-C3	-2.66	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	380	POV	O31-C3	-2.66	1.39	1.45
2	B	334	POV	O31-C3	-2.63	1.39	1.45
2	A	310	POV	O31-C3	-2.63	1.39	1.45
2	A	359	POV	O31-C3	-2.62	1.39	1.45
2	A	316	POV	O31-C3	-2.61	1.39	1.45
2	A	330	POV	O31-C3	-2.60	1.39	1.45
2	A	329	POV	O31-C3	-2.59	1.39	1.45
2	B	340	POV	O31-C3	-2.49	1.39	1.45
3	B	396	CLR	C11-C9	2.24	1.57	1.53
3	B	394	CLR	C11-C9	2.21	1.57	1.53
3	A	404	CLR	C11-C9	2.15	1.57	1.53
2	B	340	POV	C3-C2	2.08	1.57	1.50
3	A	406	CLR	C11-C9	2.07	1.57	1.53
2	A	415	POV	C1-C2	2.02	1.57	1.50

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	392	CLR	C16-C17-C20	4.81	119.46	112.18
2	A	362	POV	O31-C3-C2	4.15	120.36	108.40
3	B	399	CLR	C4-C5-C10	4.07	121.63	116.42
2	B	361	POV	O21-C2-C1	4.02	122.78	108.34
2	B	334	POV	C26-C27-C28	3.97	132.94	113.86
3	A	418	CLR	C4-C5-C10	3.91	121.43	116.42
3	A	420	CLR	C4-C5-C10	3.91	121.42	116.42
2	A	352	POV	O31-C3-C2	3.85	119.48	108.40
3	B	393	CLR	C4-C5-C10	3.81	121.30	116.42
3	A	402	CLR	C4-C5-C10	3.80	121.29	116.42
3	A	421	CLR	C4-C5-C10	3.79	121.28	116.42
3	B	397	CLR	C4-C5-C10	3.78	121.27	116.42
3	A	406	CLR	C4-C5-C10	3.73	121.20	116.42
3	B	398	CLR	C4-C5-C10	3.73	121.19	116.42
3	B	396	CLR	C4-C5-C10	3.72	121.19	116.42
3	B	391	CLR	C4-C5-C10	3.71	121.17	116.42
3	B	395	CLR	C4-C5-C10	3.65	121.09	116.42
3	A	403	CLR	C4-C5-C10	3.63	121.07	116.42
3	B	394	CLR	C4-C5-C10	3.57	120.99	116.42
3	A	419	CLR	C4-C5-C10	3.56	120.97	116.42
2	A	333	POV	O31-C3-C2	3.54	118.59	108.40
2	B	358	POV	O31-C3-C2	3.53	118.59	108.40
3	A	402	CLR	C22-C20-C17	3.52	117.62	110.33
2	A	329	POV	O31-C3-C2	3.49	118.45	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	340	POV	O31-C3-C2	3.45	118.35	108.40
3	B	396	CLR	C16-C17-C20	3.45	117.40	112.18
3	B	390	CLR	C4-C5-C10	3.37	120.74	116.42
2	A	417	POV	C314-C313-C312	3.36	131.37	114.37
3	A	405	CLR	C4-C5-C10	3.36	120.72	116.42
3	A	401	CLR	C4-C5-C10	3.30	120.65	116.42
2	A	318	POV	O31-C3-C2	3.28	117.85	108.40
2	A	359	POV	O31-C3-C2	3.28	117.85	108.40
3	B	392	CLR	C4-C5-C10	3.22	120.55	116.42
3	B	395	CLR	C3-C4-C5	-3.14	107.06	112.05
3	A	404	CLR	C4-C5-C10	3.11	120.41	116.42
2	A	316	POV	O31-C3-C2	2.96	116.94	108.40
2	B	353	POV	O21-C2-C1	2.94	118.90	108.34
2	A	315	POV	O21-C2-C1	2.92	118.83	108.34
2	B	313	POV	O31-C3-C2	2.91	116.79	108.40
2	B	307	POV	O31-C3-C2	2.90	116.74	108.40
2	A	345	POV	O31-C3-C2	2.89	116.74	108.40
2	B	323	POV	O31-C3-C2	2.89	116.72	108.40
2	B	339	POV	C2-O21-C21	2.84	124.60	117.80
2	A	341	POV	O31-C3-C2	2.83	116.55	108.40
2	B	331	POV	O21-C2-C1	2.83	118.48	108.34
2	A	411	POV	O21-C21-C22	2.81	117.55	111.48
2	A	331	POV	O21-C2-C1	2.80	118.39	108.34
2	A	376	POV	O31-C3-C2	2.77	116.37	108.40
2	A	305	POV	O31-C3-C2	2.76	116.34	108.40
2	B	313	POV	O21-C2-C1	2.75	118.23	108.34
2	A	361	POV	O31-C3-C2	2.74	116.29	108.40
2	B	382	POV	O21-C2-C3	2.73	118.13	108.34
3	A	418	CLR	C4-C5-C6	-2.73	116.87	120.57
2	B	317	POV	O31-C3-C2	2.72	116.25	108.40
2	B	339	POV	O31-C3-C2	2.69	116.16	108.40
2	A	384	POV	O21-C2-C1	2.69	117.98	108.34
2	A	384	POV	O31-C3-C2	2.68	116.14	108.40
3	B	396	CLR	C4-C5-C6	-2.67	116.95	120.57
2	B	321	POV	O21-C21-C22	2.67	117.25	111.48
3	B	390	CLR	C3-C4-C5	-2.66	107.82	112.05
3	B	391	CLR	C4-C5-C6	-2.66	116.97	120.57
2	A	378	POV	O21-C21-C22	-2.63	105.78	111.48
2	B	339	POV	O21-C21-C22	2.63	117.18	111.48
3	B	392	CLR	C21-C20-C17	-2.63	108.94	112.88
2	A	314	POV	O21-C21-C22	-2.62	105.80	111.48
2	A	412	POV	O31-C3-C2	2.62	115.95	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	304	POV	O31-C3-C2	2.62	115.94	108.40
2	B	380	POV	O31-C3-C2	2.61	115.93	108.40
2	A	322	POV	O21-C21-C22	-2.61	105.83	111.48
2	B	340	POV	O21-C2-C3	2.60	117.69	108.34
2	B	373	POV	O21-C21-C22	-2.60	105.85	111.48
2	A	357	POV	O31-C3-C2	2.60	115.90	108.40
2	A	353	POV	O31-C3-C2	2.60	115.88	108.40
2	B	360	POV	O21-C2-C3	2.59	117.62	108.34
3	B	397	CLR	C4-C5-C6	-2.58	117.08	120.57
2	B	326	POV	O31-C3-C2	2.57	115.81	108.40
3	A	402	CLR	C4-C5-C6	-2.57	117.09	120.57
2	B	337	POV	O31-C3-C2	2.56	115.77	108.40
2	A	355	POV	O31-C3-C2	2.55	115.75	108.40
2	B	351	POV	O31-C3-C2	2.54	115.70	108.40
2	B	365	POV	O21-C21-C22	-2.52	106.04	111.48
2	A	310	POV	O31-C3-C2	2.51	115.62	108.40
2	A	409	POV	O21-C2-C3	2.49	117.29	108.34
2	B	302	POV	O21-C2-C1	2.49	117.29	108.34
2	A	358	POV	O31-C3-C2	2.49	115.57	108.40
2	B	331	POV	O21-C21-C22	-2.49	106.10	111.48
3	A	402	CLR	C21-C20-C17	-2.48	109.16	112.88
3	B	399	CLR	C4-C5-C6	-2.45	117.25	120.57
2	A	366	POV	O21-C2-C1	2.44	117.10	108.34
3	B	396	CLR	C15-C14-C13	2.43	106.70	103.84
3	B	391	CLR	C3-C4-C5	-2.43	108.19	112.05
2	B	327	POV	O21-C2-C3	2.42	117.04	108.34
2	A	343	POV	O31-C3-C2	2.42	115.38	108.40
2	B	378	POV	O21-C2-C3	2.41	116.98	108.34
3	A	420	CLR	C22-C20-C17	2.40	115.31	110.33
2	A	395	POV	O21-C21-C22	-2.39	106.30	111.48
2	B	356	POV	O31-C3-C2	2.39	115.28	108.40
3	A	419	CLR	C21-C20-C22	2.36	114.00	110.34
2	B	323	POV	O21-C2-C1	2.36	116.82	108.34
2	B	318	POV	O31-C3-C2	2.34	115.15	108.40
2	B	310	POV	O21-C2-C1	2.34	116.74	108.34
2	A	319	POV	O21-C21-C22	-2.34	106.43	111.48
2	A	336	POV	O21-C2-C3	2.32	116.65	108.34
2	A	407	POV	O31-C3-C2	2.31	115.07	108.40
2	A	369	POV	O21-C21-C22	-2.31	106.48	111.48
2	B	352	POV	O31-C3-C2	2.31	115.04	108.40
2	B	320	POV	O31-C3-C2	2.30	115.04	108.40
2	B	357	POV	O21-C2-C1	2.30	116.59	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	391	POV	O31-C3-C2	2.29	115.01	108.40
3	B	390	CLR	C4-C5-C6	-2.29	117.47	120.57
2	A	316	POV	C3-C2-C1	-2.29	106.45	111.78
2	B	348	POV	O21-C2-C3	2.29	116.54	108.34
3	B	398	CLR	C3-C4-C5	-2.28	108.42	112.05
3	A	406	CLR	C4-C5-C6	-2.28	117.48	120.57
2	A	312	POV	O31-C3-C2	2.27	114.94	108.40
3	A	403	CLR	C4-C5-C6	-2.27	117.50	120.57
3	B	393	CLR	C7-C8-C9	-2.26	107.10	109.72
2	B	353	POV	O31-C3-C2	2.26	114.92	108.40
3	B	396	CLR	C3-C4-C5	-2.24	108.48	112.05
2	A	302	POV	O21-C2-C3	2.24	116.38	108.34
3	A	420	CLR	C1-C10-C5	-2.23	104.90	108.74
2	B	347	POV	O21-C2-C1	2.23	116.34	108.34
2	A	411	POV	C2-O21-C21	2.21	123.09	117.80
2	B	383	POV	O31-C3-C2	2.20	114.75	108.40
3	A	419	CLR	C4-C5-C6	-2.20	117.58	120.57
3	A	402	CLR	C16-C17-C20	2.20	115.50	112.18
2	B	374	POV	O21-C2-C1	2.18	116.18	108.34
3	B	398	CLR	C4-C5-C6	-2.18	117.61	120.57
2	B	380	POV	C2-O21-C21	2.17	123.00	117.80
2	A	309	POV	O31-C3-C2	2.17	114.65	108.40
3	A	405	CLR	C4-C5-C6	-2.17	117.63	120.57
3	B	394	CLR	C4-C5-C6	-2.16	117.64	120.57
3	A	421	CLR	C21-C20-C22	-2.16	107.00	110.34
3	A	404	CLR	C4-C5-C6	-2.16	117.65	120.57
2	B	382	POV	O31-C31-C32	-2.15	105.27	111.83
2	B	368	POV	O21-C2-C1	2.15	116.07	108.34
2	B	388	POV	O21-C21-C22	-2.15	106.82	111.48
2	A	327	POV	O21-C2-C1	2.15	116.06	108.34
3	A	406	CLR	C3-C4-C5	-2.15	108.63	112.05
2	A	325	POV	O21-C2-C3	2.14	116.02	108.34
2	B	324	POV	O21-C21-O22	-2.14	118.71	123.70
3	B	395	CLR	C9-C10-C5	2.13	112.77	109.65
2	A	303	POV	O31-C3-C2	2.12	114.52	108.40
2	B	310	POV	O31-C3-C2	2.10	114.46	108.40
2	A	413	POV	O21-C21-C22	-2.10	106.94	111.48
3	B	392	CLR	C13-C17-C20	-2.09	116.26	119.50
2	B	373	POV	O31-C31-C32	2.09	118.21	111.83
2	A	311	POV	O31-C3-C2	2.09	114.42	108.40
2	B	367	POV	O31-C3-C2	2.09	114.42	108.40
2	A	334	POV	O21-C21-C22	-2.08	106.98	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	CLR	C15-C14-C13	2.07	106.27	103.84
2	A	359	POV	O21-C2-C3	2.06	115.74	108.34
2	B	360	POV	O21-C2-C1	2.05	115.72	108.34
3	B	392	CLR	C22-C20-C17	2.05	114.58	110.33
2	A	366	POV	O31-C3-C2	2.05	114.30	108.40
2	B	341	POV	O31-C3-C2	2.05	114.30	108.40
2	A	378	POV	O31-C3-C2	2.04	114.29	108.40
3	B	395	CLR	C4-C5-C6	-2.03	117.81	120.57
2	B	306	POV	O31-C31-C32	-2.03	105.63	111.83
3	B	399	CLR	C3-C4-C5	-2.03	108.82	112.05
2	B	379	POV	O31-C3-C2	2.02	114.23	108.40
2	B	366	POV	O31-C3-C2	2.02	114.22	108.40
2	B	311	POV	O21-C21-C22	-2.02	107.11	111.48
3	A	421	CLR	C4-C5-C6	-2.02	117.83	120.57
2	B	321	POV	C2-O21-C21	2.01	122.62	117.80
2	B	319	POV	O31-C3-C2	2.01	114.20	108.40
2	A	330	POV	O31-C3-C2	2.01	114.20	108.40
2	B	331	POV	O21-C2-C3	2.01	115.57	108.34
2	B	389	POV	O31-C31-C32	-2.01	105.70	111.83
2	A	331	POV	O21-C21-C22	-2.01	107.14	111.48

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	308	POV	C2
2	A	316	POV	C2
2	A	318	POV	C2
2	A	319	POV	C2
2	A	322	POV	C2
2	A	326	POV	C2
2	A	365	POV	C2
2	A	368	POV	C2
2	A	378	POV	C2
2	A	380	POV	C2
2	A	383	POV	C2
2	A	385	POV	C2
2	A	400	POV	C2
2	A	410	POV	C2
2	B	303	POV	C2
2	B	321	POV	C2
2	B	328	POV	C2
2	B	329	POV	C2

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Mol	Chain	Res	Type	Atom
2	B	330	POV	C2
2	B	346	POV	C2
2	B	347	POV	C2
2	B	362	POV	C2
2	B	364	POV	C2
2	B	367	POV	C2

All (1964) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	POV	C11-O12-P-O11
2	A	301	POV	C11-O12-P-O13
2	A	301	POV	C11-O12-P-O14
2	A	301	POV	O12-C11-C12-N
2	A	305	POV	C11-O12-P-O14
2	A	307	POV	C32-C31-O31-C3
2	A	307	POV	O32-C31-O31-C3
2	A	309	POV	C32-C31-O31-C3
2	A	309	POV	O32-C31-O31-C3
2	A	310	POV	C11-O12-P-O11
2	A	310	POV	C11-O12-P-O13
2	A	310	POV	C2-C1-O11-P
2	A	310	POV	O32-C31-O31-C3
2	A	311	POV	C11-O12-P-O11
2	A	311	POV	C11-O12-P-O14
2	A	312	POV	C1-O11-P-O12
2	A	312	POV	C1-O11-P-O14
2	A	313	POV	C1-O11-P-O13
2	A	313	POV	C2-C1-O11-P
2	A	314	POV	C1-O11-P-O12
2	A	314	POV	C1-O11-P-O13
2	A	315	POV	C1-O11-P-O12
2	A	315	POV	C1-O11-P-O13
2	A	315	POV	C1-O11-P-O14
2	A	315	POV	C11-O12-P-O11
2	A	315	POV	C11-O12-P-O13
2	A	315	POV	C11-O12-P-O14
2	A	315	POV	C2-C1-O11-P
2	A	316	POV	C2-C1-O11-P
2	A	317	POV	C1-O11-P-O12
2	A	317	POV	C1-O11-P-O13
2	A	318	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
2	A	318	POV	C1-O11-P-O14
2	A	318	POV	O32-C31-O31-C3
2	A	319	POV	C1-O11-P-O14
2	A	321	POV	O32-C31-O31-C3
2	A	322	POV	C1-O11-P-O12
2	A	322	POV	C1-O11-P-O13
2	A	322	POV	C1-O11-P-O14
2	A	322	POV	C12-C11-O12-P
2	A	324	POV	C1-O11-P-O12
2	A	324	POV	C1-O11-P-O14
2	A	325	POV	C1-O11-P-O13
2	A	325	POV	C11-O12-P-O11
2	A	325	POV	C12-C11-O12-P
2	A	326	POV	C11-O12-P-O11
2	A	326	POV	C11-O12-P-O13
2	A	326	POV	O22-C21-O21-C2
2	A	327	POV	C1-O11-P-O14
2	A	327	POV	C12-C11-O12-P
2	A	327	POV	C22-C21-O21-C2
2	A	330	POV	C1-O11-P-O14
2	A	330	POV	O32-C31-O31-C3
2	A	331	POV	C11-O12-P-O14
2	A	334	POV	C1-O11-P-O12
2	A	334	POV	O32-C31-O31-C3
2	A	335	POV	C11-O12-P-O14
2	A	336	POV	C1-O11-P-O14
2	A	338	POV	C11-O12-P-O11
2	A	338	POV	C11-O12-P-O13
2	A	338	POV	C11-O12-P-O14
2	A	339	POV	C11-O12-P-O14
2	A	339	POV	O12-C11-C12-N
2	A	339	POV	C22-C21-O21-C2
2	A	339	POV	O22-C21-O21-C2
2	A	340	POV	C11-O12-P-O14
2	A	340	POV	O12-C11-C12-N
2	A	341	POV	C1-O11-P-O13
2	A	341	POV	O12-C11-C12-N
2	A	341	POV	O22-C21-O21-C2
2	A	343	POV	C22-C21-O21-C2
2	A	343	POV	O22-C21-O21-C2
2	A	344	POV	C1-O11-P-O14
2	A	344	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
2	A	344	POV	O22-C21-O21-C2
2	A	345	POV	C22-C21-O21-C2
2	A	345	POV	O22-C21-O21-C2
2	A	347	POV	C1-O11-P-O12
2	A	347	POV	C1-O11-P-O14
2	A	348	POV	C1-O11-P-O13
2	A	348	POV	C11-O12-P-O14
2	A	350	POV	C11-O12-P-O14
2	A	353	POV	C1-O11-P-O14
2	A	354	POV	C1-O11-P-O12
2	A	354	POV	C1-O11-P-O13
2	A	354	POV	C1-O11-P-O14
2	A	354	POV	O12-C11-C12-N
2	A	354	POV	C32-C31-O31-C3
2	A	354	POV	O32-C31-O31-C3
2	A	360	POV	C1-O11-P-O14
2	A	360	POV	O22-C21-O21-C2
2	A	361	POV	C2-C1-O11-P
2	A	362	POV	C1-O11-P-O12
2	A	362	POV	C1-O11-P-O13
2	A	362	POV	C1-O11-P-O14
2	A	362	POV	C2-C1-O11-P
2	A	363	POV	C1-O11-P-O12
2	A	363	POV	C1-O11-P-O13
2	A	363	POV	C11-O12-P-O14
2	A	363	POV	C2-C1-O11-P
2	A	363	POV	C12-C11-O12-P
2	A	364	POV	C11-O12-P-O14
2	A	365	POV	C2-C1-O11-P
2	A	366	POV	C1-O11-P-O12
2	A	369	POV	C22-C21-O21-C2
2	A	369	POV	O22-C21-O21-C2
2	A	369	POV	O32-C31-O31-C3
2	A	370	POV	C2-C1-O11-P
2	A	370	POV	O12-C11-C12-N
2	A	371	POV	C11-O12-P-O14
2	A	372	POV	O32-C31-O31-C3
2	A	374	POV	C11-O12-P-O14
2	A	374	POV	C32-C31-O31-C3
2	A	374	POV	O32-C31-O31-C3
2	A	375	POV	C1-O11-P-O12
2	A	375	POV	C12-C11-O12-P

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Mol	Chain	Res	Type	Atoms
2	A	376	POV	C11-O12-P-O11
2	A	376	POV	C11-O12-P-O13
2	A	376	POV	C11-O12-P-O14
2	A	377	POV	C22-C21-O21-C2
2	A	377	POV	O22-C21-O21-C2
2	A	378	POV	C11-O12-P-O11
2	A	378	POV	C11-O12-P-O13
2	A	378	POV	C11-O12-P-O14
2	A	380	POV	C1-O11-P-O14
2	A	380	POV	C11-O12-P-O11
2	A	380	POV	C11-O12-P-O13
2	A	380	POV	C11-O12-P-O14
2	A	380	POV	C2-C1-O11-P
2	A	380	POV	C12-C11-O12-P
2	A	382	POV	C11-O12-P-O14
2	A	384	POV	C1-O11-P-O14
2	A	386	POV	C1-O11-P-O14
2	A	386	POV	C2-C1-O11-P
2	A	387	POV	C1-O11-P-O12
2	A	388	POV	O22-C21-O21-C2
2	A	389	POV	C11-O12-P-O11
2	A	389	POV	C11-O12-P-O13
2	A	389	POV	C11-O12-P-O14
2	A	389	POV	O22-C21-O21-C2
2	A	390	POV	C11-O12-P-O11
2	A	390	POV	C11-O12-P-O13
2	A	391	POV	O32-C31-O31-C3
2	A	394	POV	C1-O11-P-O12
2	A	398	POV	C12-C11-O12-P
2	A	398	POV	O32-C31-O31-C3
2	A	399	POV	O12-C11-C12-N
2	A	399	POV	O32-C31-O31-C3
2	A	393	POV	C1-O11-P-O12
2	A	393	POV	C1-O11-P-O13
2	A	400	POV	C2-C1-O11-P
2	A	400	POV	O12-C11-C12-N
2	A	395	POV	C1-O11-P-O12
2	A	395	POV	O32-C31-O31-C3
2	A	397	POV	C11-O12-P-O11
2	A	409	POV	O12-C11-C12-N
2	A	410	POV	C32-C31-O31-C3
2	A	410	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	A	411	POV	C1-O11-P-O12
2	A	411	POV	C1-O11-P-O13
2	A	411	POV	C22-C21-O21-C2
2	A	411	POV	O22-C21-O21-C2
2	A	413	POV	C2-C1-O11-P
2	A	414	POV	C12-C11-O12-P
2	A	415	POV	C1-O11-P-O14
2	A	415	POV	C2-C1-O11-P
2	A	417	POV	C11-O12-P-O11
2	A	417	POV	C11-O12-P-O13
2	B	301	POV	C11-O12-P-O11
2	B	301	POV	C11-O12-P-O13
2	B	301	POV	C11-O12-P-O14
2	B	301	POV	C22-C21-O21-C2
2	B	301	POV	O22-C21-O21-C2
2	B	302	POV	O32-C31-O31-C3
2	B	305	POV	C2-C1-O11-P
2	B	306	POV	C1-O11-P-O14
2	B	306	POV	C11-O12-P-O11
2	B	306	POV	C11-O12-P-O14
2	B	306	POV	C2-C1-O11-P
2	B	306	POV	C12-C11-O12-P
2	B	307	POV	C1-O11-P-O12
2	B	307	POV	C22-C21-O21-C2
2	B	307	POV	O22-C21-O21-C2
2	B	308	POV	C2-C1-O11-P
2	B	311	POV	O12-C11-C12-N
2	B	312	POV	O32-C31-O31-C3
2	B	314	POV	C1-O11-P-O14
2	B	316	POV	C2-C1-O11-P
2	B	317	POV	C1-O11-P-O14
2	B	318	POV	C1-O11-P-O12
2	B	318	POV	C1-O11-P-O13
2	B	318	POV	O32-C31-O31-C3
2	B	319	POV	C1-O11-P-O12
2	B	319	POV	C1-O11-P-O13
2	B	319	POV	C1-O11-P-O14
2	B	320	POV	C11-O12-P-O13
2	B	321	POV	C1-O11-P-O12
2	B	321	POV	C1-O11-P-O13
2	B	321	POV	C22-C21-O21-C2
2	B	321	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
2	B	322	POV	C1-O11-P-O12
2	B	322	POV	C1-O11-P-O13
2	B	322	POV	C1-O11-P-O14
2	B	323	POV	C2-C1-O11-P
2	B	324	POV	C11-O12-P-O11
2	B	324	POV	C22-C21-O21-C2
2	B	324	POV	O22-C21-O21-C2
2	B	326	POV	C1-O11-P-O14
2	B	326	POV	C11-O12-P-O11
2	B	326	POV	C11-O12-P-O13
2	B	326	POV	O32-C31-O31-C3
2	B	328	POV	C2-C1-O11-P
2	B	328	POV	O12-C11-C12-N
2	B	330	POV	O12-C11-C12-N
2	B	330	POV	O32-C31-O31-C3
2	B	331	POV	C11-O12-P-O13
2	B	332	POV	C1-O11-P-O12
2	B	332	POV	C1-O11-P-O14
2	B	333	POV	C11-O12-P-O14
2	B	334	POV	O12-C11-C12-N
2	B	335	POV	O12-C11-C12-N
2	B	336	POV	C1-O11-P-O14
2	B	336	POV	O22-C21-O21-C2
2	B	337	POV	C11-O12-P-O11
2	B	337	POV	C11-O12-P-O14
2	B	338	POV	C1-O11-P-O13
2	B	339	POV	C1-O11-P-O12
2	B	339	POV	C22-C21-O21-C2
2	B	339	POV	O22-C21-O21-C2
2	B	341	POV	C1-O11-P-O14
2	B	341	POV	O32-C31-O31-C3
2	B	342	POV	C2-C1-O11-P
2	B	343	POV	C1-O11-P-O14
2	B	343	POV	O12-C11-C12-N
2	B	344	POV	C1-O11-P-O12
2	B	345	POV	C1-O11-P-O12
2	B	345	POV	C1-O11-P-O13
2	B	345	POV	C12-C11-O12-P
2	B	345	POV	O32-C31-O31-C3
2	B	347	POV	C1-O11-P-O12
2	B	347	POV	C1-O11-P-O13
2	B	350	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
2	B	350	POV	C11-O12-P-O13
2	B	351	POV	C1-O11-P-O12
2	B	351	POV	C1-O11-P-O14
2	B	354	POV	C2-C1-O11-P
2	B	355	POV	C1-O11-P-O14
2	B	355	POV	C11-O12-P-O11
2	B	355	POV	C11-O12-P-O13
2	B	357	POV	O12-C11-C12-N
2	B	357	POV	C32-C31-O31-C3
2	B	357	POV	O32-C31-O31-C3
2	B	358	POV	O12-C11-C12-N
2	B	358	POV	O22-C21-O21-C2
2	B	359	POV	C1-O11-P-O12
2	B	359	POV	C1-O11-P-O13
2	B	359	POV	C1-O11-P-O14
2	B	360	POV	C1-O11-P-O12
2	B	360	POV	C1-O11-P-O14
2	B	361	POV	C1-O11-P-O14
2	B	361	POV	C11-O12-P-O14
2	B	364	POV	C1-O11-P-O12
2	B	364	POV	C1-O11-P-O13
2	B	364	POV	C11-O12-P-O13
2	B	369	POV	O12-C11-C12-N
2	B	370	POV	C11-O12-P-O11
2	B	370	POV	C11-O12-P-O13
2	B	370	POV	C2-C1-O11-P
2	B	372	POV	C11-O12-P-O11
2	B	372	POV	C11-O12-P-O14
2	B	373	POV	C32-C31-O31-C3
2	B	373	POV	O32-C31-O31-C3
2	B	374	POV	C1-O11-P-O12
2	B	374	POV	C1-O11-P-O13
2	B	374	POV	C2-C1-O11-P
2	B	374	POV	C12-C11-O12-P
2	B	376	POV	C11-O12-P-O14
2	B	377	POV	C11-O12-P-O14
2	B	378	POV	C11-O12-P-O11
2	B	378	POV	C11-O12-P-O14
2	B	379	POV	C1-O11-P-O12
2	B	379	POV	C1-O11-P-O13
2	B	379	POV	C1-O11-P-O14
2	B	379	POV	C11-O12-P-O13

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Mol	Chain	Res	Type	Atoms
2	B	379	POV	C2-C1-O11-P
2	B	380	POV	O12-C11-C12-N
2	B	380	POV	C22-C21-O21-C2
2	B	380	POV	O22-C21-O21-C2
2	B	381	POV	C11-O12-P-O11
2	B	381	POV	C11-O12-P-O13
2	B	381	POV	C11-O12-P-O14
2	B	381	POV	C12-C11-O12-P
2	B	382	POV	C1-O11-P-O12
2	B	382	POV	C1-O11-P-O14
2	B	382	POV	C11-O12-P-O11
2	B	382	POV	C11-O12-P-O13
2	B	382	POV	C11-O12-P-O14
2	B	382	POV	O12-C11-C12-N
2	B	383	POV	C11-O12-P-O11
2	B	383	POV	C11-O12-P-O13
2	B	384	POV	C11-O12-P-O11
2	B	384	POV	C11-O12-P-O14
2	B	384	POV	C32-C31-O31-C3
2	B	384	POV	O32-C31-O31-C3
2	B	385	POV	C1-O11-P-O14
2	B	385	POV	C11-O12-P-O11
2	B	385	POV	C11-O12-P-O14
2	B	386	POV	C1-O11-P-O14
2	B	386	POV	C32-C31-O31-C3
2	B	386	POV	O32-C31-O31-C3
2	B	387	POV	C11-O12-P-O11
2	B	387	POV	C11-O12-P-O13
2	B	388	POV	C1-O11-P-O14
2	B	388	POV	C32-C31-O31-C3
2	B	388	POV	O32-C31-O31-C3
2	B	389	POV	O22-C21-O21-C2
2	A	311	POV	O32-C31-O31-C3
2	A	349	POV	O32-C31-O31-C3
2	A	400	POV	O32-C31-O31-C3
2	A	408	POV	O32-C31-O31-C3
2	B	319	POV	O32-C31-O31-C3
2	B	328	POV	O32-C31-O31-C3
2	B	343	POV	O32-C31-O31-C3
2	B	355	POV	O32-C31-O31-C3
2	B	361	POV	O32-C31-O31-C3
2	B	366	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	B	370	POV	O32-C31-O31-C3
2	B	378	POV	O32-C31-O31-C3
2	B	379	POV	O32-C31-O31-C3
2	A	310	POV	C32-C31-O31-C3
2	A	321	POV	C32-C31-O31-C3
2	A	369	POV	C32-C31-O31-C3
2	A	372	POV	C32-C31-O31-C3
2	A	400	POV	C32-C31-O31-C3
2	B	312	POV	C32-C31-O31-C3
2	B	318	POV	C32-C31-O31-C3
2	B	341	POV	C32-C31-O31-C3
2	B	361	POV	C32-C31-O31-C3
2	B	379	POV	C32-C31-O31-C3
2	A	365	POV	O32-C31-O31-C3
2	B	309	POV	O32-C31-O31-C3
2	B	320	POV	O32-C31-O31-C3
2	B	383	POV	O32-C31-O31-C3
3	B	392	CLR	C13-C17-C20-C22
2	A	327	POV	O22-C21-O21-C2
2	A	331	POV	O22-C21-O21-C2
2	A	332	POV	O22-C21-O21-C2
2	A	395	POV	O22-C21-O21-C2
2	B	331	POV	O22-C21-O21-C2
2	B	348	POV	O22-C21-O21-C2
2	B	367	POV	O22-C21-O21-C2
2	A	318	POV	C32-C31-O31-C3
2	A	330	POV	C32-C31-O31-C3
2	A	334	POV	C32-C31-O31-C3
2	A	349	POV	C32-C31-O31-C3
2	A	391	POV	C32-C31-O31-C3
2	A	398	POV	C32-C31-O31-C3
2	A	395	POV	C32-C31-O31-C3
2	A	408	POV	C32-C31-O31-C3
2	B	320	POV	C32-C31-O31-C3
2	B	326	POV	C32-C31-O31-C3
2	B	328	POV	C32-C31-O31-C3
2	B	330	POV	C32-C31-O31-C3
2	B	343	POV	C32-C31-O31-C3
2	B	345	POV	C32-C31-O31-C3
2	B	355	POV	C32-C31-O31-C3
2	B	366	POV	C32-C31-O31-C3
2	A	326	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
2	A	341	POV	C22-C21-O21-C2
2	A	360	POV	C22-C21-O21-C2
2	A	388	POV	C22-C21-O21-C2
2	A	389	POV	C22-C21-O21-C2
2	B	336	POV	C22-C21-O21-C2
2	B	348	POV	C22-C21-O21-C2
2	B	358	POV	C22-C21-O21-C2
2	B	389	POV	C22-C21-O21-C2
3	B	392	CLR	C16-C17-C20-C21
2	A	311	POV	C32-C31-O31-C3
2	A	399	POV	C32-C31-O31-C3
2	B	302	POV	C32-C31-O31-C3
2	B	309	POV	C32-C31-O31-C3
2	B	319	POV	C32-C31-O31-C3
2	B	378	POV	C32-C31-O31-C3
2	B	383	POV	C32-C31-O31-C3
2	A	329	POV	O32-C31-O31-C3
2	A	359	POV	O32-C31-O31-C3
2	B	327	POV	O22-C21-O21-C2
2	A	352	POV	C2-C3-O31-C31
3	B	392	CLR	C13-C17-C20-C21
3	B	396	CLR	C13-C17-C20-C21
2	B	370	POV	C32-C31-O31-C3
2	B	349	POV	O32-C31-O31-C3
2	A	321	POV	C2-C1-O11-P
2	A	356	POV	C2-C1-O11-P
2	B	311	POV	C2-C1-O11-P
2	B	359	POV	C2-C1-O11-P
2	B	363	POV	C2-C1-O11-P
2	B	364	POV	C2-C1-O11-P
2	B	388	POV	C2-C1-O11-P
2	B	389	POV	C2-C1-O11-P
2	B	340	POV	O32-C31-O31-C3
3	B	396	CLR	C16-C17-C20-C21
3	B	396	CLR	C13-C17-C20-C22
3	A	405	CLR	C17-C20-C22-C23
2	A	417	POV	C312-C313-C314-C315
2	B	383	POV	C25-C26-C27-C28
2	A	352	POV	O32-C31-O31-C3
2	A	329	POV	C32-C31-O31-C3
2	A	365	POV	C32-C31-O31-C3
3	A	405	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
2	B	304	POV	C31-C32-C33-C34
2	B	340	POV	C31-C32-C33-C34
3	B	392	CLR	C16-C17-C20-C22
2	A	305	POV	O21-C2-C3-O31
3	A	402	CLR	C13-C17-C20-C22
3	B	399	CLR	C17-C20-C22-C23
2	B	340	POV	C2-C3-O31-C31
2	B	306	POV	C11-C12-N-C13
2	A	348	POV	C21-C22-C23-C24
2	A	396	POV	C21-C22-C23-C24
2	B	314	POV	C31-C32-C33-C34
2	B	362	POV	C31-C32-C33-C34
2	A	395	POV	C22-C21-O21-C2
3	B	396	CLR	C16-C17-C20-C22
2	A	359	POV	C32-C31-O31-C3
2	A	311	POV	C2-C1-O11-P
2	A	345	POV	C2-C1-O11-P
2	A	348	POV	C2-C1-O11-P
2	A	350	POV	C2-C1-O11-P
2	A	378	POV	C2-C1-O11-P
2	B	304	POV	C2-C1-O11-P
2	B	353	POV	C2-C1-O11-P
2	B	368	POV	C2-C1-O11-P
2	B	373	POV	C2-C1-O11-P
3	B	399	CLR	C21-C20-C22-C23
2	A	323	POV	C31-C32-C33-C34
2	A	335	POV	C21-C22-C23-C24
2	A	382	POV	C31-C32-C33-C34
2	A	395	POV	C21-C22-C23-C24
2	B	388	POV	C31-C32-C33-C34
2	B	323	POV	C21-C22-C23-C24
2	B	338	POV	C21-C22-C23-C24
2	B	349	POV	C32-C31-O31-C3
2	B	341	POV	C31-C32-C33-C34
2	A	319	POV	C31-C32-C33-C34
2	A	353	POV	C31-C32-C33-C34
2	A	315	POV	O22-C21-O21-C2
2	B	340	POV	O22-C21-O21-C2
2	A	362	POV	C32-C31-O31-C3
3	A	402	CLR	C13-C17-C20-C21
3	B	396	CLR	C20-C22-C23-C24
3	B	398	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
2	B	327	POV	C22-C21-O21-C2
2	B	331	POV	C22-C21-O21-C2
3	A	402	CLR	C16-C17-C20-C21
2	A	370	POV	C31-C32-C33-C34
2	A	371	POV	C2-C1-O11-P
2	A	384	POV	C2-C1-O11-P
2	A	388	POV	C2-C1-O11-P
2	B	331	POV	C2-C1-O11-P
2	B	326	POV	C312-C313-C314-C315
2	A	349	POV	C21-C22-C23-C24
3	A	404	CLR	C17-C20-C22-C23
2	B	388	POV	C22-C21-O21-C2
2	B	358	POV	C32-C31-O31-C3
2	A	354	POV	C213-C214-C215-C216
2	A	324	POV	C311-C310-C39-C38
2	A	408	POV	C37-C38-C39-C310
2	B	302	POV	C311-C312-C313-C314
2	B	328	POV	C37-C38-C39-C310
2	B	327	POV	C311-C312-C313-C314
2	B	368	POV	O32-C31-O31-C3
2	B	371	POV	C32-C31-O31-C3
2	A	323	POV	C311-C312-C313-C314
2	A	328	POV	C310-C311-C312-C313
2	B	311	POV	C25-C26-C27-C28
2	B	323	POV	C34-C35-C36-C37
2	B	332	POV	C22-C23-C24-C25
2	A	353	POV	C25-C26-C27-C28
2	A	393	POV	C310-C311-C312-C313
2	A	415	POV	C212-C213-C214-C215
2	B	374	POV	C33-C34-C35-C36
2	A	349	POV	C26-C27-C28-C29
3	A	404	CLR	C22-C23-C24-C25
2	A	314	POV	C22-C21-O21-C2
2	B	347	POV	C22-C21-O21-C2
2	A	338	POV	C23-C24-C25-C26
2	A	328	POV	C211-C212-C213-C214
2	A	329	POV	C35-C36-C37-C38
2	B	366	POV	C211-C212-C213-C214
2	A	359	POV	C31-C32-C33-C34
2	A	408	POV	C21-C22-C23-C24
2	B	367	POV	C21-C22-C23-C24
2	A	304	POV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
2	A	326	POV	C213-C214-C215-C216
2	A	413	POV	C211-C212-C213-C214
2	B	316	POV	C212-C213-C214-C215
2	A	310	POV	C2-C3-O31-C31
2	B	333	POV	C31-C32-C33-C34
2	A	323	POV	C36-C37-C38-C39
2	A	352	POV	C33-C34-C35-C36
2	A	390	POV	O32-C31-O31-C3
2	A	396	POV	C311-C312-C313-C314
2	A	314	POV	C311-C312-C313-C314
2	B	354	POV	C25-C26-C27-C28
2	B	373	POV	C32-C33-C34-C35
2	A	346	POV	C32-C31-O31-C3
2	A	409	POV	C1-C2-C3-O31
2	A	396	POV	C212-C213-C214-C215
2	A	411	POV	C24-C25-C26-C27
2	A	325	POV	C31-C32-C33-C34
2	A	362	POV	C21-C22-C23-C24
2	A	317	POV	C311-C312-C313-C314
2	A	332	POV	C24-C25-C26-C27
2	A	344	POV	C211-C212-C213-C214
2	A	354	POV	C311-C310-C39-C38
2	A	389	POV	C32-C33-C34-C35
2	A	397	POV	C33-C34-C35-C36
2	B	308	POV	C311-C312-C313-C314
2	B	343	POV	C24-C25-C26-C27
2	B	345	POV	C312-C313-C314-C315
2	A	359	POV	C310-C311-C312-C313
2	A	359	POV	C24-C25-C26-C27
2	A	373	POV	C34-C35-C36-C37
2	A	393	POV	C34-C35-C36-C37
2	A	413	POV	C34-C35-C36-C37
2	B	343	POV	C311-C312-C313-C314
2	B	352	POV	C34-C35-C36-C37
2	A	357	POV	C214-C215-C216-C217
2	B	306	POV	C11-C12-N-C14
2	B	306	POV	C11-C12-N-C15
2	A	386	POV	C310-C311-C312-C313
2	B	372	POV	C22-C23-C24-C25
2	B	346	POV	C21-C22-C23-C24
2	B	364	POV	C21-C22-C23-C24
2	B	385	POV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	A	360	POV	C39-C310-C311-C312
2	A	367	POV	C213-C214-C215-C216
2	B	338	POV	C24-C25-C26-C27
2	B	323	POV	C22-C21-O21-C2
2	B	367	POV	C22-C21-O21-C2
2	B	387	POV	C22-C21-O21-C2
2	A	417	POV	C26-C27-C28-C29
2	B	354	POV	C26-C27-C28-C29
2	A	319	POV	C2-C1-O11-P
2	B	324	POV	C2-C1-O11-P
2	A	311	POV	C213-C214-C215-C216
2	B	361	POV	C32-C33-C34-C35
2	B	373	POV	C36-C37-C38-C39
2	B	357	POV	C25-C26-C27-C28
2	A	302	POV	C31-C32-C33-C34
2	A	321	POV	C21-C22-C23-C24
2	A	342	POV	C212-C213-C214-C215
2	A	399	POV	C23-C24-C25-C26
2	B	371	POV	C214-C215-C216-C217
2	A	313	POV	C213-C214-C215-C216
2	A	362	POV	C311-C310-C39-C38
2	A	372	POV	C211-C212-C213-C214
2	A	390	POV	C36-C37-C38-C39
2	B	340	POV	C32-C31-O31-C3
2	B	360	POV	C32-C31-O31-C3
2	B	382	POV	C32-C31-O31-C3
2	B	354	POV	C311-C310-C39-C38
2	B	381	POV	C311-C312-C313-C314
2	A	378	POV	C33-C34-C35-C36
2	B	307	POV	C32-C33-C34-C35
2	B	334	POV	C23-C24-C25-C26
2	A	380	POV	C310-C311-C312-C313
2	B	312	POV	C213-C214-C215-C216
2	B	366	POV	C31-C32-C33-C34
2	A	357	POV	C37-C38-C39-C310
2	B	347	POV	C39-C310-C311-C312
2	A	302	POV	C22-C21-O21-C2
2	A	319	POV	C22-C21-O21-C2
2	A	331	POV	C22-C21-O21-C2
2	A	332	POV	C22-C21-O21-C2
2	A	378	POV	C22-C21-O21-C2
2	A	380	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
2	A	393	POV	C22-C21-O21-C2
2	A	400	POV	C22-C21-O21-C2
2	B	352	POV	C22-C21-O21-C2
2	B	378	POV	C22-C21-O21-C2
2	B	386	POV	C22-C21-O21-C2
2	A	415	POV	C31-C32-C33-C34
2	B	382	POV	O22-C21-O21-C2
2	A	314	POV	C25-C26-C27-C28
2	A	314	POV	C26-C27-C28-C29
2	B	371	POV	C210-C211-C212-C213
2	B	373	POV	C210-C211-C212-C213
2	B	381	POV	C26-C27-C28-C29
2	B	305	POV	C37-C38-C39-C310
2	B	360	POV	C31-C32-C33-C34
2	A	334	POV	C33-C34-C35-C36
2	A	415	POV	C32-C31-O31-C3
2	A	354	POV	C32-C33-C34-C35
2	B	371	POV	C23-C24-C25-C26
2	B	317	POV	C22-C23-C24-C25
2	B	335	POV	C25-C26-C27-C28
2	A	351	POV	C214-C215-C216-C217
2	B	329	POV	C310-C311-C312-C313
2	B	308	POV	C211-C212-C213-C214
2	B	369	POV	C311-C312-C313-C314
2	A	358	POV	O22-C21-O21-C2
2	A	393	POV	C37-C38-C39-C310
2	B	375	POV	C22-C23-C24-C25
2	A	417	POV	C22-C21-O21-C2
2	A	302	POV	C23-C24-C25-C26
2	A	303	POV	C311-C312-C313-C314
2	A	306	POV	C31-C32-C33-C34
2	A	379	POV	C31-C32-C33-C34
2	A	389	POV	C31-C32-C33-C34
2	B	302	POV	C21-C22-C23-C24
2	B	358	POV	C210-C211-C212-C213
2	B	360	POV	C34-C35-C36-C37
2	A	325	POV	C32-C31-O31-C3
2	B	317	POV	C213-C214-C215-C216
3	A	419	CLR	C21-C20-C22-C23
2	A	311	POV	C35-C36-C37-C38
2	A	414	POV	C25-C26-C27-C28
2	B	311	POV	C211-C212-C213-C214

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Mol	Chain	Res	Type	Atoms
2	A	306	POV	C2-C1-O11-P
2	A	354	POV	C2-C1-O11-P
2	A	387	POV	C2-C1-O11-P
2	A	394	POV	C2-C1-O11-P
2	B	303	POV	C2-C1-O11-P
2	A	393	POV	C23-C24-C25-C26
2	A	391	POV	C31-C32-C33-C34
2	A	329	POV	C32-C33-C34-C35
2	A	351	POV	C39-C310-C311-C312
2	B	381	POV	C212-C213-C214-C215
2	B	359	POV	C32-C31-O31-C3
2	A	417	POV	C311-C312-C313-C314
2	A	341	POV	C311-C312-C313-C314
2	A	334	POV	C22-C21-O21-C2
2	B	318	POV	C22-C21-O21-C2
2	B	340	POV	C22-C21-O21-C2
2	B	361	POV	C22-C21-O21-C2
2	B	362	POV	C22-C21-O21-C2
2	A	313	POV	C33-C34-C35-C36
2	A	335	POV	C34-C35-C36-C37
2	A	377	POV	C36-C37-C38-C39
2	B	333	POV	C312-C313-C314-C315
2	B	333	POV	C25-C26-C27-C28
2	B	366	POV	C39-C310-C311-C312
2	B	327	POV	C22-C23-C24-C25
2	A	388	POV	C210-C211-C212-C213
2	B	354	POV	C210-C211-C212-C213
2	B	360	POV	C26-C27-C28-C29
2	B	367	POV	C26-C27-C28-C29
2	B	356	POV	C24-C25-C26-C27
2	A	319	POV	O11-C1-C2-C3
2	A	356	POV	O11-C1-C2-C3
2	A	359	POV	O11-C1-C2-C3
2	A	364	POV	O11-C1-C2-C3
2	B	372	POV	O11-C1-C2-C3
3	A	404	CLR	C21-C20-C22-C23
2	A	415	POV	C311-C312-C313-C314
2	A	313	POV	C31-C32-C33-C34
2	A	411	POV	C25-C26-C27-C28
2	B	369	POV	C34-C35-C36-C37
2	B	358	POV	C24-C25-C26-C27
2	B	317	POV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
2	A	408	POV	C31-C32-C33-C34
2	A	383	POV	C211-C212-C213-C214
2	A	379	POV	C22-C21-O21-C2
2	B	346	POV	C22-C21-O21-C2
2	A	326	POV	C33-C34-C35-C36
2	B	331	POV	C310-C311-C312-C313
2	A	411	POV	C31-C32-C33-C34
2	A	311	POV	C211-C212-C213-C214
2	B	307	POV	C23-C24-C25-C26
2	B	334	POV	C32-C31-O31-C3
2	A	305	POV	C1-C2-C3-O31
2	A	321	POV	C1-C2-C3-O31
2	A	326	POV	C1-C2-C3-O31
2	A	352	POV	C1-C2-C3-O31
2	A	353	POV	C1-C2-C3-O31
2	A	353	POV	C36-C37-C38-C39
2	A	336	POV	C26-C27-C28-C29
2	A	384	POV	C26-C27-C28-C29
2	B	313	POV	C210-C211-C212-C213
2	B	324	POV	C26-C27-C28-C29
2	B	332	POV	C26-C27-C28-C29
2	B	368	POV	C312-C313-C314-C315
2	A	352	POV	C312-C313-C314-C315
2	A	368	POV	C24-C25-C26-C27
2	B	343	POV	C23-C24-C25-C26
2	B	348	POV	C214-C215-C216-C217
2	B	323	POV	C32-C31-O31-C3
2	A	335	POV	C22-C23-C24-C25
2	B	349	POV	C32-C33-C34-C35
2	A	346	POV	C25-C26-C27-C28
2	A	359	POV	C37-C38-C39-C310
2	B	322	POV	C213-C214-C215-C216
2	B	378	POV	C313-C314-C315-C316
2	A	325	POV	C23-C24-C25-C26
2	A	363	POV	C33-C34-C35-C36
2	B	345	POV	C310-C311-C312-C313
3	B	399	CLR	C20-C22-C23-C24
2	A	339	POV	C2-C1-O11-P
2	A	338	POV	C311-C310-C39-C38
2	A	346	POV	C34-C35-C36-C37
2	B	313	POV	C211-C212-C213-C214
2	B	307	POV	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	B	387	POV	C32-C31-O31-C3
2	B	302	POV	C33-C34-C35-C36
2	B	344	POV	C33-C34-C35-C36
3	A	420	CLR	C22-C23-C24-C25
2	A	324	POV	C24-C25-C26-C27
2	A	373	POV	C21-C22-C23-C24
2	A	351	POV	O11-C1-C2-O21
2	A	413	POV	O11-C1-C2-O21
2	B	372	POV	O11-C1-C2-O21
2	A	301	POV	C32-C31-O31-C3
2	A	362	POV	C22-C21-O21-C2
2	A	339	POV	C25-C26-C27-C28
2	A	301	POV	C34-C35-C36-C37
2	A	346	POV	C312-C313-C314-C315
2	A	385	POV	C311-C310-C39-C38
2	A	397	POV	C211-C212-C213-C214
2	B	386	POV	C32-C33-C34-C35
2	B	378	POV	C310-C311-C312-C313
2	A	331	POV	O21-C2-C3-O31
2	A	310	POV	C311-C310-C39-C38
2	A	363	POV	C24-C25-C26-C27
2	A	385	POV	C37-C38-C39-C310
2	B	331	POV	C211-C212-C213-C214
2	B	336	POV	C214-C215-C216-C217
2	B	323	POV	O31-C31-C32-C33
2	B	329	POV	C23-C24-C25-C26
2	B	339	POV	C35-C36-C37-C38
2	A	384	POV	C210-C211-C212-C213
2	B	318	POV	C26-C27-C28-C29
2	A	346	POV	C21-C22-C23-C24
2	B	362	POV	C312-C313-C314-C315
2	A	320	POV	C32-C31-O31-C3
2	A	359	POV	C2-C3-O31-C31
2	B	329	POV	C22-C21-O21-C2
2	B	349	POV	C22-C21-O21-C2
2	A	380	POV	C34-C35-C36-C37
2	A	416	POV	C32-C33-C34-C35
2	A	329	POV	C21-C22-C23-C24
2	B	357	POV	C31-C32-C33-C34
2	A	336	POV	C22-C23-C24-C25
2	B	322	POV	C39-C310-C311-C312
2	A	385	POV	C313-C314-C315-C316

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Mol	Chain	Res	Type	Atoms
2	B	347	POV	C32-C31-O31-C3
2	B	325	POV	C21-C22-C23-C24
2	A	312	POV	C34-C35-C36-C37
2	A	412	POV	C22-C23-C24-C25
2	A	384	POV	C29-C210-C211-C212
2	B	317	POV	C27-C28-C29-C210
3	B	390	CLR	C17-C20-C22-C23
2	A	385	POV	C25-C26-C27-C28
2	A	408	POV	C25-C26-C27-C28
2	B	334	POV	C35-C36-C37-C38
2	A	307	POV	C2-C1-O11-P
2	A	309	POV	C2-C1-O11-P
2	A	317	POV	C2-C1-O11-P
2	A	373	POV	C2-C1-O11-P
2	A	391	POV	C2-C1-O11-P
2	B	313	POV	C2-C1-O11-P
2	B	320	POV	C2-C1-O11-P
2	B	332	POV	C2-C1-O11-P
2	B	345	POV	C2-C1-O11-P
2	B	351	POV	C2-C1-O11-P
2	B	387	POV	C2-C1-O11-P
2	A	320	POV	C24-C25-C26-C27
2	A	378	POV	C212-C213-C214-C215
2	B	311	POV	C35-C36-C37-C38
2	A	324	POV	C22-C23-C24-C25
2	B	306	POV	C32-C33-C34-C35
2	B	303	POV	C31-C32-C33-C34
2	A	301	POV	C215-C216-C217-C218
2	A	317	POV	O11-C1-C2-C3
2	A	357	POV	O11-C1-C2-C3
2	A	382	POV	O11-C1-C2-C3
2	A	392	POV	O11-C1-C2-C3
2	B	303	POV	O11-C1-C2-C3
2	B	325	POV	O11-C1-C2-C3
2	A	381	POV	C22-C21-O21-C2
2	A	345	POV	C37-C38-C39-C310
2	A	356	POV	C24-C25-C26-C27
2	A	360	POV	C311-C312-C313-C314
2	A	365	POV	C313-C314-C315-C316
2	A	327	POV	C11-C12-N-C14
2	B	342	POV	C35-C36-C37-C38
2	A	361	POV	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	B	317	POV	C23-C24-C25-C26
2	A	375	POV	C27-C28-C29-C210
2	A	318	POV	C214-C215-C216-C217
2	B	303	POV	O32-C31-O31-C3
2	A	381	POV	C36-C37-C38-C39
2	A	351	POV	C33-C34-C35-C36
2	A	395	POV	C37-C38-C39-C310
2	B	378	POV	C36-C37-C38-C39
2	A	322	POV	C31-C32-C33-C34
2	A	399	POV	C313-C314-C315-C316
2	A	412	POV	C313-C314-C315-C316
2	B	304	POV	C23-C24-C25-C26
2	B	357	POV	C310-C311-C312-C313
2	A	389	POV	C1-C2-C3-O31
2	B	304	POV	C1-C2-C3-O31
2	B	360	POV	C1-C2-C3-O31
2	B	382	POV	C1-C2-C3-O31
2	A	360	POV	C32-C33-C34-C35
2	B	326	POV	C313-C314-C315-C316
2	A	393	POV	C212-C213-C214-C215
2	B	302	POV	C211-C212-C213-C214
2	B	321	POV	C39-C310-C311-C312
2	B	322	POV	C212-C213-C214-C215
2	B	333	POV	C311-C312-C313-C314
2	A	335	POV	C35-C36-C37-C38
2	B	310	POV	O31-C31-C32-C33
2	B	361	POV	C312-C313-C314-C315
2	A	322	POV	C37-C38-C39-C310
2	A	376	POV	C211-C212-C213-C214
2	B	338	POV	C312-C313-C314-C315
2	B	310	POV	C31-C32-C33-C34
2	A	306	POV	O11-C1-C2-O21
2	A	319	POV	O11-C1-C2-O21
2	A	359	POV	O11-C1-C2-O21
2	A	363	POV	O11-C1-C2-O21
2	A	382	POV	O11-C1-C2-O21
2	A	394	POV	O11-C1-C2-O21
2	B	304	POV	O11-C1-C2-O21
2	B	381	POV	O11-C1-C2-O21
2	A	323	POV	C39-C310-C311-C312
2	A	359	POV	C22-C23-C24-C25
2	B	371	POV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
2	B	346	POV	C29-C210-C211-C212
2	B	339	POV	C26-C27-C28-C29
2	B	381	POV	C32-C31-O31-C3
2	A	325	POV	C2-C1-O11-P
2	A	347	POV	C2-C1-O11-P
2	A	351	POV	C2-C1-O11-P
2	A	359	POV	C2-C1-O11-P
2	A	385	POV	C2-C1-O11-P
2	A	390	POV	C2-C1-O11-P
2	A	414	POV	C2-C1-O11-P
2	B	307	POV	C2-C1-O11-P
2	B	340	POV	C2-C1-O11-P
2	A	388	POV	C21-C22-C23-C24
2	A	382	POV	C212-C213-C214-C215
3	A	421	CLR	C21-C20-C22-C23
2	B	326	POV	C36-C37-C38-C39
2	B	332	POV	C39-C310-C311-C312
2	A	371	POV	C311-C310-C39-C38
2	A	399	POV	C312-C313-C314-C315
2	B	319	POV	C212-C213-C214-C215
2	B	361	POV	C34-C35-C36-C37
2	A	382	POV	O21-C21-C22-C23
2	A	371	POV	O21-C2-C3-O31
2	A	378	POV	O21-C2-C3-O31
2	A	387	POV	O21-C2-C3-O31
2	A	412	POV	O21-C2-C3-O31
2	B	307	POV	O21-C2-C3-O31
2	B	369	POV	C23-C24-C25-C26
2	A	303	POV	C21-C22-C23-C24
2	A	335	POV	C31-C32-C33-C34
2	A	381	POV	C31-C32-C33-C34
2	B	320	POV	C31-C32-C33-C34
2	A	357	POV	C311-C310-C39-C38
2	B	334	POV	C211-C212-C213-C214
2	B	341	POV	C310-C311-C312-C313
2	B	302	POV	C23-C24-C25-C26
2	B	344	POV	C31-C32-C33-C34
2	A	356	POV	C32-C31-O31-C3
2	A	367	POV	C32-C31-O31-C3
2	A	409	POV	C23-C24-C25-C26
2	B	305	POV	C210-C211-C212-C213
2	A	318	POV	C215-C216-C217-C218

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Mol	Chain	Res	Type	Atoms
2	A	384	POV	C215-C216-C217-C218
2	B	315	POV	C25-C26-C27-C28
2	B	342	POV	C27-C28-C29-C210
2	B	306	POV	C31-C32-C33-C34
2	B	316	POV	C31-C32-C33-C34
2	A	356	POV	C23-C24-C25-C26
2	A	315	POV	C22-C21-O21-C2
2	A	315	POV	C32-C33-C34-C35
2	B	311	POV	C212-C213-C214-C215
2	A	311	POV	C2-C3-O31-C31
3	B	390	CLR	C21-C20-C22-C23
2	B	375	POV	C211-C212-C213-C214
2	A	355	POV	C32-C31-O31-C3
2	B	351	POV	C32-C31-O31-C3
2	A	313	POV	O11-C1-C2-C3
2	A	368	POV	O11-C1-C2-C3
2	A	371	POV	O11-C1-C2-C3
2	A	384	POV	O11-C1-C2-C3
2	A	394	POV	O11-C1-C2-C3
2	B	318	POV	C29-C210-C211-C212
2	B	355	POV	C2-C1-O11-P
2	A	379	POV	C25-C26-C27-C28
2	A	397	POV	C32-C33-C34-C35
2	B	307	POV	C22-C23-C24-C25
2	B	362	POV	C21-C22-C23-C24
2	A	376	POV	C212-C213-C214-C215
2	A	387	POV	C22-C23-C24-C25
2	A	394	POV	C212-C213-C214-C215
2	B	339	POV	C22-C23-C24-C25
2	B	369	POV	C310-C311-C312-C313
2	A	375	POV	C32-C33-C34-C35
2	B	381	POV	C32-C33-C34-C35
2	A	368	POV	O22-C21-O21-C2
2	A	357	POV	C34-C35-C36-C37
2	B	319	POV	C33-C34-C35-C36
2	B	324	POV	C311-C310-C39-C38
2	A	411	POV	C33-C34-C35-C36
2	B	329	POV	C34-C35-C36-C37
2	B	334	POV	C26-C27-C28-C29
2	B	322	POV	C35-C36-C37-C38
2	B	334	POV	C25-C26-C27-C28
2	A	416	POV	C313-C314-C315-C316

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Mol	Chain	Res	Type	Atoms
2	A	376	POV	C32-C31-O31-C3
2	A	313	POV	O11-C1-C2-O21
2	A	317	POV	O11-C1-C2-O21
2	A	356	POV	O11-C1-C2-O21
2	A	364	POV	O11-C1-C2-O21
2	A	370	POV	O11-C1-C2-O21
2	A	415	POV	O11-C1-C2-O21
2	B	303	POV	O11-C1-C2-O21
2	B	360	POV	O11-C1-C2-O21
2	A	376	POV	C35-C36-C37-C38
2	A	412	POV	C1-C2-C3-O31
2	B	362	POV	C213-C214-C215-C216
2	A	387	POV	C39-C310-C311-C312
2	B	340	POV	C35-C36-C37-C38
2	B	347	POV	C211-C212-C213-C214
2	B	369	POV	C213-C214-C215-C216
2	A	384	POV	C212-C213-C214-C215
2	A	370	POV	C37-C38-C39-C310
2	B	302	POV	C37-C38-C39-C310
2	B	303	POV	C24-C25-C26-C27
2	A	301	POV	C12-C11-O12-P
2	A	305	POV	C12-C11-O12-P
2	A	312	POV	C12-C11-O12-P
2	A	321	POV	C12-C11-O12-P
2	A	323	POV	C12-C11-O12-P
2	A	324	POV	C12-C11-O12-P
2	A	328	POV	C12-C11-O12-P
2	A	330	POV	C12-C11-O12-P
2	A	331	POV	C12-C11-O12-P
2	A	334	POV	C12-C11-O12-P
2	A	340	POV	C12-C11-O12-P
2	A	345	POV	C12-C11-O12-P
2	A	347	POV	C12-C11-O12-P
2	A	351	POV	C12-C11-O12-P
2	A	352	POV	C12-C11-O12-P
2	A	354	POV	C12-C11-O12-P
2	A	356	POV	C12-C11-O12-P
2	A	359	POV	C12-C11-O12-P
2	A	364	POV	C12-C11-O12-P
2	A	369	POV	C12-C11-O12-P
2	A	370	POV	C12-C11-O12-P
2	A	378	POV	C12-C11-O12-P

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Mol	Chain	Res	Type	Atoms
2	A	379	POV	C12-C11-O12-P
2	A	384	POV	C12-C11-O12-P
2	A	389	POV	C12-C11-O12-P
2	A	390	POV	C12-C11-O12-P
2	A	393	POV	C12-C11-O12-P
2	A	407	POV	C12-C11-O12-P
2	A	409	POV	C12-C11-O12-P
2	A	413	POV	C12-C11-O12-P
2	B	309	POV	C12-C11-O12-P
2	B	312	POV	C12-C11-O12-P
2	B	314	POV	C12-C11-O12-P
2	B	315	POV	C12-C11-O12-P
2	B	316	POV	C12-C11-O12-P
2	B	318	POV	C12-C11-O12-P
2	B	321	POV	C12-C11-O12-P
2	B	324	POV	C12-C11-O12-P
2	B	328	POV	C12-C11-O12-P
2	B	333	POV	C12-C11-O12-P
2	B	335	POV	C12-C11-O12-P
2	B	336	POV	C12-C11-O12-P
2	B	338	POV	C12-C11-O12-P
2	B	341	POV	C12-C11-O12-P
2	B	347	POV	C12-C11-O12-P
2	B	357	POV	C12-C11-O12-P
2	B	360	POV	C12-C11-O12-P
2	B	361	POV	C12-C11-O12-P
2	B	364	POV	C12-C11-O12-P
2	B	367	POV	C12-C11-O12-P
2	B	368	POV	C12-C11-O12-P
2	B	369	POV	C12-C11-O12-P
2	B	373	POV	C12-C11-O12-P
2	B	379	POV	C12-C11-O12-P
2	B	382	POV	C12-C11-O12-P
2	B	388	POV	C12-C11-O12-P
2	B	336	POV	C31-C32-C33-C34
2	A	313	POV	O21-C2-C3-O31
2	A	352	POV	O21-C2-C3-O31
2	A	353	POV	O21-C2-C3-O31
2	A	355	POV	O21-C2-C3-O31
2	A	365	POV	O21-C2-C3-O31
2	B	304	POV	O21-C2-C3-O31
2	B	333	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	B	371	POV	O21-C2-C3-O31
2	B	374	POV	O21-C2-C3-O31
2	A	411	POV	C36-C37-C38-C39
2	B	345	POV	C213-C214-C215-C216
2	A	337	POV	O32-C31-O31-C3
2	A	313	POV	C313-C314-C315-C316
2	A	378	POV	C36-C37-C38-C39
2	B	348	POV	O32-C31-O31-C3
2	B	312	POV	C212-C213-C214-C215
2	B	365	POV	C22-C21-O21-C2
2	B	352	POV	C2-C1-O11-P
2	B	387	POV	C32-C33-C34-C35
2	A	372	POV	C310-C311-C312-C313
2	A	386	POV	C212-C213-C214-C215
2	A	330	POV	O12-C11-C12-N
2	A	331	POV	O12-C11-C12-N
2	A	338	POV	O12-C11-C12-N
2	A	343	POV	O12-C11-C12-N
2	A	344	POV	O12-C11-C12-N
2	A	352	POV	O12-C11-C12-N
2	A	375	POV	O12-C11-C12-N
2	A	379	POV	O12-C11-C12-N
2	A	390	POV	O12-C11-C12-N
2	A	397	POV	O12-C11-C12-N
2	A	412	POV	O12-C11-C12-N
2	A	415	POV	O12-C11-C12-N
2	B	332	POV	O12-C11-C12-N
2	B	336	POV	O12-C11-C12-N
2	B	356	POV	O12-C11-C12-N
2	B	359	POV	O12-C11-C12-N
2	B	364	POV	O12-C11-C12-N
2	B	374	POV	O12-C11-C12-N
2	B	379	POV	O12-C11-C12-N
2	B	384	POV	O12-C11-C12-N
2	A	372	POV	C214-C215-C216-C217
2	A	416	POV	C37-C38-C39-C310
2	A	315	POV	C310-C311-C312-C313
2	A	378	POV	C21-C22-C23-C24
2	A	381	POV	C213-C214-C215-C216
2	B	327	POV	C211-C212-C213-C214
2	B	348	POV	C213-C214-C215-C216
2	B	365	POV	C213-C214-C215-C216

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Mol	Chain	Res	Type	Atoms
2	B	373	POV	C34-C35-C36-C37
2	A	394	POV	C29-C210-C211-C212
2	B	361	POV	C27-C28-C29-C210
2	A	305	POV	C22-C23-C24-C25
2	A	352	POV	C32-C31-O31-C3
2	A	348	POV	C22-C21-O21-C2
2	A	321	POV	C2-C3-O31-C31
2	A	304	POV	C214-C215-C216-C217
2	B	326	POV	C35-C36-C37-C38
2	A	343	POV	C32-C31-O31-C3
2	B	317	POV	C32-C31-O31-C3
2	A	302	POV	C37-C38-C39-C310
2	B	335	POV	C37-C38-C39-C310
2	A	343	POV	O31-C31-C32-C33
2	A	324	POV	C32-C33-C34-C35
2	B	330	POV	C310-C311-C312-C313
2	B	339	POV	C312-C313-C314-C315
2	B	343	POV	C213-C214-C215-C216
2	A	387	POV	C2-C3-O31-C31
2	B	305	POV	C311-C312-C313-C314
2	A	308	POV	C210-C211-C212-C213
2	A	306	POV	O11-C1-C2-C3
2	A	331	POV	O11-C1-C2-C3
2	A	363	POV	O11-C1-C2-C3
2	A	413	POV	O11-C1-C2-C3
2	B	381	POV	O11-C1-C2-C3
2	B	332	POV	C311-C310-C39-C38
2	A	336	POV	C21-C22-C23-C24
2	B	311	POV	C311-C310-C39-C38
2	A	302	POV	C33-C34-C35-C36
2	A	396	POV	C25-C26-C27-C28
2	B	379	POV	C311-C310-C39-C38
2	B	376	POV	C311-C310-C39-C38
2	A	373	POV	C23-C24-C25-C26
2	B	324	POV	C37-C38-C39-C310
2	A	410	POV	C313-C314-C315-C316
2	A	341	POV	C27-C28-C29-C210
2	A	304	POV	C24-C25-C26-C27
2	A	381	POV	C22-C23-C24-C25
2	A	304	POV	C2-C1-O11-P
2	A	305	POV	C2-C1-O11-P
2	A	308	POV	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
2	A	336	POV	C2-C1-O11-P
2	A	393	POV	C2-C1-O11-P
2	B	312	POV	C2-C1-O11-P
2	B	336	POV	C2-C1-O11-P
2	B	358	POV	C33-C34-C35-C36
2	A	331	POV	O11-C1-C2-O21
2	A	357	POV	O11-C1-C2-O21
2	A	366	POV	O11-C1-C2-O21
2	A	392	POV	O11-C1-C2-O21
2	B	325	POV	O11-C1-C2-O21
2	A	303	POV	C31-C32-C33-C34
2	A	356	POV	C22-C21-O21-C2
2	A	327	POV	C11-C12-N-C15
2	A	334	POV	C11-C12-N-C13
2	B	347	POV	C11-C12-N-C13
2	A	348	POV	C25-C26-C27-C28
2	B	363	POV	O31-C31-C32-C33
2	A	411	POV	C311-C312-C313-C314
2	B	339	POV	C37-C38-C39-C310
2	B	356	POV	C211-C212-C213-C214
2	A	413	POV	C35-C36-C37-C38
2	B	385	POV	C313-C314-C315-C316
2	A	378	POV	C27-C28-C29-C210
2	A	308	POV	C33-C34-C35-C36
2	A	393	POV	C32-C33-C34-C35
2	A	321	POV	O21-C2-C3-O31
2	A	325	POV	O21-C2-C3-O31
2	A	389	POV	O21-C2-C3-O31
2	A	398	POV	O21-C2-C3-O31
2	A	408	POV	O21-C2-C3-O31
2	B	302	POV	O21-C2-C3-O31
2	B	343	POV	O21-C2-C3-O31
2	B	381	POV	O21-C2-C3-O31
2	B	382	POV	O21-C2-C3-O31
2	A	321	POV	C37-C38-C39-C310
2	A	323	POV	C311-C310-C39-C38
2	A	310	POV	C1-C2-C3-O31
2	A	408	POV	C1-C2-C3-O31
2	B	307	POV	C1-C2-C3-O31
2	B	343	POV	C1-C2-C3-O31
2	B	371	POV	C1-C2-C3-O31
2	B	377	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	B	346	POV	C310-C311-C312-C313
2	A	313	POV	C311-C310-C39-C38
2	B	344	POV	C36-C37-C38-C39
2	A	399	POV	C32-C33-C34-C35
2	A	347	POV	C34-C35-C36-C37
2	A	347	POV	C35-C36-C37-C38
2	A	302	POV	C1-O11-P-O14
2	A	303	POV	C11-O12-P-O14
2	A	304	POV	C11-O12-P-O14
2	A	308	POV	C11-O12-P-O14
2	A	310	POV	C11-O12-P-O14
2	A	312	POV	C1-O11-P-O13
2	A	313	POV	C1-O11-P-O12
2	A	313	POV	C1-O11-P-O14
2	A	320	POV	C11-O12-P-O14
2	A	322	POV	C11-O12-P-O14
2	A	324	POV	C1-O11-P-O13
2	A	325	POV	C11-O12-P-O14
2	A	327	POV	C11-C12-N-C13
2	A	327	POV	C1-O11-P-O12
2	A	334	POV	C1-O11-P-O14
2	A	339	POV	C1-O11-P-O14
2	A	339	POV	C11-O12-P-O11
2	A	340	POV	C11-O12-P-O11
2	A	340	POV	C11-O12-P-O13
2	A	341	POV	C1-O11-P-O12
2	A	342	POV	C11-O12-P-O14
2	A	346	POV	C11-O12-P-O14
2	A	347	POV	C1-O11-P-O13
2	A	353	POV	C1-O11-P-O12
2	A	359	POV	C11-O12-P-O14
2	A	360	POV	C1-O11-P-O12
2	A	358	POV	C11-O12-P-O14
2	A	365	POV	C11-O12-P-O14
2	A	366	POV	C1-O11-P-O14
2	A	368	POV	C11-O12-P-O11
2	A	368	POV	C11-O12-P-O13
2	A	375	POV	C1-O11-P-O14
2	A	377	POV	C1-O11-P-O12
2	A	377	POV	C1-O11-P-O13
2	A	380	POV	C1-O11-P-O12
2	A	383	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
2	A	387	POV	C1-O11-P-O14
2	A	390	POV	C11-O12-P-O14
2	A	394	POV	C1-O11-P-O14
2	A	396	POV	C11-O12-P-O14
2	A	395	POV	C1-O11-P-O14
2	A	397	POV	C11-O12-P-O14
2	A	407	POV	C1-O11-P-O14
2	A	407	POV	C11-O12-P-O14
2	A	412	POV	C1-O11-P-O14
2	A	414	POV	C1-O11-P-O13
2	B	302	POV	C1-O11-P-O14
2	B	303	POV	C11-O12-P-O14
2	B	307	POV	C1-O11-P-O14
2	B	308	POV	C11-O12-P-O14
2	B	309	POV	C1-O11-P-O14
2	B	310	POV	C11-O12-P-O14
2	B	314	POV	C11-O12-P-O14
2	B	316	POV	C1-O11-P-O14
2	B	320	POV	C11-O12-P-O11
2	B	321	POV	C11-O12-P-O14
2	B	323	POV	C11-O12-P-O14
2	B	324	POV	C11-O12-P-O14
2	B	327	POV	C11-O12-P-O14
2	B	329	POV	C1-O11-P-O14
2	B	330	POV	C1-O11-P-O14
2	B	331	POV	C11-O12-P-O11
2	B	336	POV	C1-O11-P-O12
2	B	336	POV	C1-O11-P-O13
2	B	338	POV	C1-O11-P-O12
2	B	339	POV	C1-O11-P-O14
2	B	339	POV	C11-O12-P-O14
2	B	341	POV	C11-O12-P-O14
2	B	344	POV	C1-O11-P-O14
2	B	344	POV	C11-O12-P-O14
2	B	347	POV	C11-C12-N-C14
2	B	349	POV	C11-O12-P-O11
2	B	349	POV	C11-O12-P-O13
2	B	352	POV	C11-O12-P-O14
2	B	358	POV	C1-O11-P-O14
2	B	358	POV	C11-O12-P-O14
2	B	359	POV	C11-O12-P-O14
2	B	362	POV	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
2	B	362	POV	C11-O12-P-O14
2	B	368	POV	C1-O11-P-O14
2	B	369	POV	C1-O11-P-O14
2	B	372	POV	C11-O12-P-O13
2	B	374	POV	C1-O11-P-O14
2	B	375	POV	C11-O12-P-O14
2	B	376	POV	C11-O12-P-O11
2	B	379	POV	C11-O12-P-O11
2	B	382	POV	C1-O11-P-O13
2	B	384	POV	C11-O12-P-O13
2	B	385	POV	C11-O12-P-O13
2	B	388	POV	C11-O12-P-O14
2	B	389	POV	C1-O11-P-O13
2	A	392	POV	C312-C313-C314-C315
2	B	365	POV	O32-C31-O31-C3
2	B	304	POV	C33-C34-C35-C36
2	A	311	POV	C310-C311-C312-C313
2	A	316	POV	C22-C21-O21-C2
2	A	322	POV	C22-C21-O21-C2
2	B	383	POV	C29-C210-C211-C212
2	A	301	POV	C35-C36-C37-C38
2	A	322	POV	C21-C22-C23-C24
2	B	379	POV	C210-C211-C212-C213
2	A	323	POV	C2-C1-O11-P
2	A	331	POV	C2-C1-O11-P
2	A	342	POV	C2-C1-O11-P
2	A	352	POV	C2-C1-O11-P
2	A	364	POV	C2-C1-O11-P
2	A	372	POV	C2-C1-O11-P
2	A	392	POV	C2-C1-O11-P
2	A	407	POV	C2-C1-O11-P
2	A	409	POV	C2-C1-O11-P
2	A	416	POV	C2-C1-O11-P
2	B	314	POV	C2-C1-O11-P
2	B	315	POV	C2-C1-O11-P
2	B	317	POV	C2-C1-O11-P
2	B	318	POV	C2-C1-O11-P
2	B	341	POV	C2-C1-O11-P
2	A	317	POV	C37-C38-C39-C310
2	B	371	POV	C310-C311-C312-C313
2	A	409	POV	C22-C23-C24-C25
2	A	338	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
3	A	402	CLR	C16-C17-C20-C22
2	A	320	POV	C39-C310-C311-C312
2	B	317	POV	C21-C22-C23-C24
2	B	319	POV	C21-C22-C23-C24
2	B	360	POV	C21-C22-C23-C24
2	A	358	POV	C35-C36-C37-C38
2	B	331	POV	C39-C310-C311-C312
2	A	384	POV	C1-C2-O21-C21
2	B	307	POV	C1-C2-O21-C21
2	B	313	POV	C1-C2-O21-C21
2	B	353	POV	C1-C2-O21-C21
2	B	360	POV	C3-C2-O21-C21
2	B	361	POV	C1-C2-O21-C21
2	A	320	POV	C311-C312-C313-C314
2	A	347	POV	C23-C24-C25-C26
2	A	353	POV	C213-C214-C215-C216
2	A	353	POV	C35-C36-C37-C38
2	B	373	POV	C35-C36-C37-C38
2	B	338	POV	C33-C34-C35-C36
2	A	318	POV	C36-C37-C38-C39
2	A	393	POV	O11-C1-C2-C3
2	B	304	POV	O11-C1-C2-C3
2	B	357	POV	O11-C1-C2-C3
2	A	407	POV	C36-C37-C38-C39
2	A	313	POV	C32-C31-O31-C3
2	A	416	POV	C32-C31-O31-C3
2	B	384	POV	C32-C33-C34-C35
2	B	314	POV	C29-C210-C211-C212
2	A	347	POV	C21-C22-C23-C24
2	B	387	POV	C31-C32-C33-C34
2	A	348	POV	O11-C1-C2-O21
2	A	368	POV	O11-C1-C2-O21
2	A	371	POV	O11-C1-C2-O21
2	A	370	POV	C25-C26-C27-C28
2	B	368	POV	C33-C34-C35-C36
2	A	388	POV	C211-C212-C213-C214
2	B	311	POV	C36-C37-C38-C39
2	A	344	POV	C310-C311-C312-C313
2	A	400	POV	C36-C37-C38-C39
2	B	373	POV	C33-C34-C35-C36
2	A	365	POV	C32-C33-C34-C35
2	B	352	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	A	350	POV	C311-C310-C39-C38
2	A	310	POV	O21-C2-C3-O31
2	A	326	POV	O21-C2-C3-O31
2	B	305	POV	O21-C2-C3-O31
2	A	350	POV	C31-C32-C33-C34
2	A	390	POV	C23-C24-C25-C26
2	B	382	POV	C35-C36-C37-C38
2	A	333	POV	C22-C21-O21-C2
2	A	372	POV	C22-C21-O21-C2
2	A	390	POV	C22-C21-O21-C2
2	B	389	POV	C21-C22-C23-C24
2	A	410	POV	C214-C215-C216-C217
2	A	315	POV	C26-C27-C28-C29
2	A	342	POV	C26-C27-C28-C29
2	B	336	POV	C26-C27-C28-C29
2	B	377	POV	C22-C23-C24-C25
2	B	313	POV	C1-C2-C3-O31
2	A	337	POV	C33-C34-C35-C36
2	A	370	POV	C311-C312-C313-C314
2	A	339	POV	C32-C33-C34-C35
2	A	391	POV	C211-C212-C213-C214
2	B	380	POV	C25-C26-C27-C28
2	B	321	POV	C27-C28-C29-C210
2	B	323	POV	C29-C210-C211-C212
2	B	346	POV	C27-C28-C29-C210
2	A	409	POV	C21-C22-C23-C24
2	B	344	POV	C311-C312-C313-C314
3	A	418	CLR	C23-C24-C25-C26
2	B	384	POV	C21-C22-C23-C24
2	A	357	POV	C26-C27-C28-C29
2	A	365	POV	O21-C21-C22-C23
2	A	376	POV	O31-C31-C32-C33
2	A	334	POV	C11-C12-N-C15
2	A	303	POV	C212-C213-C214-C215
2	B	319	POV	C31-C32-C33-C34
2	A	381	POV	C37-C38-C39-C310
2	A	346	POV	C33-C34-C35-C36
2	B	335	POV	C34-C35-C36-C37
2	B	380	POV	C32-C33-C34-C35
2	A	353	POV	C32-C31-O31-C3
2	B	383	POV	C36-C37-C38-C39
2	A	314	POV	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
2	A	370	POV	C312-C313-C314-C315
2	B	309	POV	C22-C23-C24-C25
2	A	345	POV	C36-C37-C38-C39
2	A	365	POV	O22-C21-C22-C23
2	A	339	POV	O31-C31-C32-C33
2	A	393	POV	C24-C25-C26-C27
2	B	341	POV	O11-C1-C2-O21
2	A	316	POV	C27-C28-C29-C210
2	B	322	POV	C36-C37-C38-C39
2	A	370	POV	O11-C1-C2-C3
2	A	311	POV	C34-C35-C36-C37
2	A	362	POV	C23-C24-C25-C26
2	A	396	POV	C22-C21-O21-C2
2	A	366	POV	C35-C36-C37-C38
2	A	392	POV	C33-C34-C35-C36
2	A	378	POV	C213-C214-C215-C216
2	A	317	POV	O32-C31-O31-C3
2	B	347	POV	C11-C12-N-C15
2	A	399	POV	C211-C212-C213-C214
2	B	346	POV	C35-C36-C37-C38
2	A	304	POV	C211-C212-C213-C214
2	B	336	POV	C25-C26-C27-C28
2	B	338	POV	C214-C215-C216-C217
2	B	362	POV	C211-C212-C213-C214
2	B	377	POV	C21-C22-C23-C24
2	A	411	POV	C310-C311-C312-C313
2	B	362	POV	C212-C213-C214-C215
2	A	320	POV	O21-C2-C3-O31
2	A	395	POV	O21-C2-C3-O31
2	A	415	POV	O21-C2-C3-O31
2	A	394	POV	C22-C23-C24-C25
2	A	411	POV	C32-C33-C34-C35
2	A	376	POV	C311-C310-C39-C38
2	A	376	POV	C23-C24-C25-C26
2	A	311	POV	C31-C32-C33-C34
2	A	309	POV	C2-C3-O31-C31
2	B	358	POV	C32-C33-C34-C35
2	A	364	POV	C24-C25-C26-C27
2	B	311	POV	C310-C311-C312-C313
2	A	310	POV	C21-C22-C23-C24
2	B	388	POV	C311-C312-C313-C314
2	B	301	POV	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
2	B	327	POV	C2-C1-O11-P
2	B	346	POV	C2-C1-O11-P
2	B	378	POV	C2-C1-O11-P
2	B	381	POV	C2-C1-O11-P
2	A	383	POV	C36-C37-C38-C39
2	A	324	POV	C25-C26-C27-C28
2	B	307	POV	C34-C35-C36-C37
2	A	334	POV	C11-C12-N-C14
2	B	374	POV	C24-C25-C26-C27
2	B	358	POV	C2-C3-O31-C31
2	B	302	POV	C35-C36-C37-C38
2	A	336	POV	C1-C2-C3-O31
2	B	350	POV	C1-C2-C3-O31
2	B	381	POV	C1-C2-C3-O31
2	A	336	POV	C311-C312-C313-C314
2	B	355	POV	C213-C214-C215-C216
2	A	317	POV	C35-C36-C37-C38
2	A	383	POV	C311-C310-C39-C38
2	A	408	POV	C23-C24-C25-C26
2	A	410	POV	C33-C34-C35-C36
2	A	315	POV	C1-C2-O21-C21
2	A	325	POV	C3-C2-O21-C21
2	A	327	POV	C1-C2-O21-C21
2	A	327	POV	C3-C2-O21-C21
2	A	331	POV	C1-C2-O21-C21
2	A	366	POV	C1-C2-O21-C21
2	A	389	POV	C1-C2-O21-C21
2	A	389	POV	C3-C2-O21-C21
2	A	415	POV	C3-C2-O21-C21
2	B	325	POV	C3-C2-O21-C21
2	B	331	POV	C3-C2-O21-C21
2	B	333	POV	C3-C2-O21-C21
2	B	340	POV	C3-C2-O21-C21
2	B	348	POV	C3-C2-O21-C21
2	B	368	POV	C1-C2-O21-C21
2	B	382	POV	C3-C2-O21-C21
2	B	324	POV	C23-C24-C25-C26
2	A	345	POV	C34-C35-C36-C37
2	B	384	POV	C33-C34-C35-C36
2	A	328	POV	C212-C213-C214-C215
2	A	395	POV	C36-C37-C38-C39
2	A	327	POV	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
2	A	304	POV	C32-C33-C34-C35
2	A	355	POV	C311-C312-C313-C314
2	A	332	POV	O31-C31-C32-C33
2	B	383	POV	O21-C21-C22-C23
2	A	342	POV	C214-C215-C216-C217
2	A	378	POV	C311-C310-C39-C38
2	A	393	POV	C211-C212-C213-C214
2	B	341	POV	C2-C3-O31-C31
2	B	332	POV	C211-C212-C213-C214
2	A	357	POV	C27-C28-C29-C210
2	A	396	POV	C32-C31-O31-C3
2	A	340	POV	C2-C1-O11-P
2	A	398	POV	C2-C1-O11-P
2	A	397	POV	C39-C310-C311-C312
2	B	354	POV	O11-C1-C2-C3
2	B	305	POV	C311-C310-C39-C38
2	A	348	POV	C214-C215-C216-C217
2	A	373	POV	C310-C311-C312-C313
2	B	330	POV	C27-C28-C29-C210
2	B	352	POV	C27-C28-C29-C210
2	A	383	POV	C313-C314-C315-C316
2	A	374	POV	C36-C37-C38-C39
2	B	313	POV	C312-C313-C314-C315
2	B	357	POV	C213-C214-C215-C216
2	A	345	POV	C212-C213-C214-C215
2	B	380	POV	C212-C213-C214-C215
2	B	312	POV	C210-C211-C212-C213
2	B	378	POV	C26-C27-C28-C29
2	A	313	POV	C214-C215-C216-C217
2	B	349	POV	C36-C37-C38-C39
2	A	375	POV	C211-C212-C213-C214
2	A	354	POV	C37-C38-C39-C310
2	A	332	POV	C32-C31-O31-C3
2	A	305	POV	O31-C31-C32-C33
2	B	371	POV	C34-C35-C36-C37
2	B	365	POV	C21-C22-C23-C24
2	A	328	POV	C22-C21-O21-C2
2	B	344	POV	C22-C21-O21-C2
2	B	374	POV	C22-C21-O21-C2
2	B	313	POV	C311-C312-C313-C314
2	B	345	POV	C211-C212-C213-C214
2	B	383	POV	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	B	304	POV	C24-C25-C26-C27
2	B	364	POV	C212-C213-C214-C215
2	B	343	POV	C313-C314-C315-C316
2	A	325	POV	C39-C310-C311-C312
2	A	394	POV	C312-C313-C314-C315
2	B	320	POV	C311-C310-C39-C38
2	B	323	POV	C311-C312-C313-C314
2	A	338	POV	C210-C211-C212-C213
2	B	369	POV	C26-C27-C28-C29
3	A	421	CLR	C20-C22-C23-C24
2	A	328	POV	C2-C1-O11-P
2	A	367	POV	C2-C1-O11-P
2	A	369	POV	C23-C24-C25-C26
2	B	345	POV	C25-C26-C27-C28
2	A	323	POV	C37-C38-C39-C310
2	B	349	POV	C35-C36-C37-C38
2	B	371	POV	C213-C214-C215-C216
2	A	354	POV	C1-C2-C3-O31
2	A	350	POV	C311-C312-C313-C314
2	A	303	POV	C23-C24-C25-C26
2	A	323	POV	C211-C212-C213-C214
2	A	416	POV	C35-C36-C37-C38
2	A	317	POV	C24-C25-C26-C27
2	B	321	POV	O31-C31-C32-C33
2	B	356	POV	O21-C21-C22-C23
2	B	362	POV	O21-C21-C22-C23
2	A	384	POV	C25-C26-C27-C28
2	B	385	POV	O32-C31-O31-C3
2	A	344	POV	C212-C213-C214-C215
2	A	332	POV	C212-C213-C214-C215
2	B	387	POV	C27-C28-C29-C210
2	A	322	POV	C32-C31-O31-C3
2	A	321	POV	C211-C212-C213-C214
2	A	303	POV	C36-C37-C38-C39
2	A	327	POV	C212-C213-C214-C215
2	A	394	POV	C37-C38-C39-C310
2	A	328	POV	C39-C310-C311-C312
2	A	376	POV	C22-C23-C24-C25
2	A	318	POV	O21-C21-C22-C23
2	A	327	POV	O32-C31-C32-C33
2	A	414	POV	C312-C313-C314-C315
2	A	415	POV	C311-C310-C39-C38

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Mol	Chain	Res	Type	Atoms
2	A	342	POV	O11-C1-C2-C3
2	A	351	POV	O11-C1-C2-C3
2	B	331	POV	O11-C1-C2-C3
2	B	340	POV	O11-C1-C2-C3
2	B	366	POV	O11-C1-C2-C3
2	B	378	POV	O11-C1-C2-C3
2	A	311	POV	C312-C313-C314-C315
2	A	389	POV	C35-C36-C37-C38
2	B	311	POV	O21-C2-C3-O31
2	B	358	POV	O21-C2-C3-O31
2	A	351	POV	O31-C31-C32-C33
2	A	394	POV	O21-C21-C22-C23
2	A	327	POV	C27-C28-C29-C210
2	A	352	POV	C29-C210-C211-C212
2	A	320	POV	C2-C1-O11-P
2	A	303	POV	C311-C310-C39-C38
2	A	332	POV	C213-C214-C215-C216
2	B	311	POV	C214-C215-C216-C217
2	B	322	POV	C214-C215-C216-C217
2	B	322	POV	C311-C310-C39-C38
2	B	370	POV	O21-C21-C22-C23
2	A	313	POV	C211-C212-C213-C214
2	A	383	POV	C212-C213-C214-C215
2	B	312	POV	C211-C212-C213-C214
2	B	375	POV	C39-C310-C311-C312
2	A	369	POV	C211-C212-C213-C214
2	B	379	POV	C311-C312-C313-C314
2	B	320	POV	O31-C31-C32-C33
2	A	390	POV	C29-C210-C211-C212
2	B	331	POV	C29-C210-C211-C212
2	B	357	POV	C29-C210-C211-C212
2	B	359	POV	C27-C28-C29-C210
2	B	367	POV	C29-C210-C211-C212
2	B	376	POV	C29-C210-C211-C212
2	B	358	POV	C39-C310-C311-C312
2	B	376	POV	C212-C213-C214-C215
2	A	385	POV	O21-C21-C22-C23
2	A	386	POV	C313-C314-C315-C316
2	A	399	POV	C24-C25-C26-C27
2	A	333	POV	O31-C31-C32-C33
2	B	366	POV	C33-C34-C35-C36
2	A	360	POV	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
2	A	395	POV	C1-C2-O21-C21
2	B	302	POV	C3-C2-O21-C21
2	B	310	POV	C1-C2-O21-C21
2	B	342	POV	C3-C2-O21-C21
2	B	348	POV	C1-C2-O21-C21
2	B	384	POV	C1-C2-O21-C21
2	A	301	POV	C25-C26-C27-C28
2	A	348	POV	C212-C213-C214-C215
2	A	321	POV	C27-C28-C29-C210
2	A	347	POV	C29-C210-C211-C212
2	A	348	POV	C27-C28-C29-C210
2	A	350	POV	C27-C28-C29-C210
2	A	409	POV	C29-C210-C211-C212
2	B	374	POV	C29-C210-C211-C212
2	A	312	POV	C213-C214-C215-C216
2	A	344	POV	C26-C27-C28-C29
2	A	314	POV	C212-C213-C214-C215
2	A	364	POV	C214-C215-C216-C217
2	A	331	POV	C27-C28-C29-C210
2	A	349	POV	C29-C210-C211-C212
2	B	325	POV	C27-C28-C29-C210
2	B	365	POV	C29-C210-C211-C212
2	A	330	POV	C2-C1-O11-P
2	A	411	POV	C2-C1-O11-P
2	B	383	POV	C33-C34-C35-C36
2	A	397	POV	C32-C31-O31-C3
2	A	343	POV	C24-C25-C26-C27
2	A	416	POV	C311-C312-C313-C314
2	A	331	POV	C210-C211-C212-C213
2	A	355	POV	C1-C2-C3-O31
2	A	371	POV	C1-C2-C3-O31
2	B	305	POV	C1-C2-C3-O31
2	B	353	POV	C1-C2-C3-O31
2	A	304	POV	C212-C213-C214-C215
2	A	317	POV	C33-C34-C35-C36
2	B	367	POV	C34-C35-C36-C37
2	A	366	POV	C32-C31-O31-C3
2	A	305	POV	C29-C210-C211-C212
2	A	350	POV	C29-C210-C211-C212
2	B	311	POV	C29-C210-C211-C212
2	B	358	POV	C27-C28-C29-C210
2	B	383	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
2	A	400	POV	C39-C310-C311-C312
2	B	366	POV	C214-C215-C216-C217
2	A	338	POV	C12-C11-O12-P
2	B	330	POV	C12-C11-O12-P
2	B	354	POV	C12-C11-O12-P
3	A	418	CLR	C23-C24-C25-C27
2	A	366	POV	C215-C216-C217-C218
2	A	340	POV	C35-C36-C37-C38
2	A	349	POV	C32-C33-C34-C35
2	B	378	POV	C311-C310-C39-C38
2	A	336	POV	O21-C21-C22-C23
2	A	382	POV	O31-C31-C32-C33
2	A	410	POV	O21-C21-C22-C23
2	B	348	POV	C34-C35-C36-C37
2	B	316	POV	C311-C310-C39-C38
2	B	356	POV	O22-C21-C22-C23
2	B	334	POV	O21-C2-C3-O31
2	B	365	POV	O21-C2-C3-O31
2	A	318	POV	C312-C313-C314-C315
2	A	329	POV	C27-C28-C29-C210
2	A	339	POV	C27-C28-C29-C210
2	A	352	POV	C27-C28-C29-C210
2	A	353	POV	C27-C28-C29-C210
2	A	383	POV	C29-C210-C211-C212
2	A	396	POV	C29-C210-C211-C212
2	B	307	POV	C29-C210-C211-C212
2	B	389	POV	C27-C28-C29-C210
2	A	317	POV	C22-C23-C24-C25
2	B	305	POV	C36-C37-C38-C39
2	A	364	POV	O21-C21-C22-C23
2	A	369	POV	O21-C21-C22-C23
2	B	342	POV	O21-C21-C22-C23
2	B	368	POV	O31-C31-C32-C33
2	B	380	POV	O21-C21-C22-C23
2	B	388	POV	O31-C31-C32-C33
2	A	415	POV	O11-C1-C2-C3
2	B	341	POV	O11-C1-C2-C3
2	B	320	POV	C39-C310-C311-C312
2	B	350	POV	C11-C12-N-C13
2	A	415	POV	O21-C21-C22-C23
2	B	355	POV	O31-C31-C32-C33
2	B	310	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
2	A	361	POV	C22-C21-O21-C2
2	B	377	POV	C22-C21-O21-C2
2	A	322	POV	O31-C31-C32-C33
2	A	329	POV	O31-C31-C32-C33
2	A	411	POV	O21-C21-C22-C23
2	B	352	POV	O31-C31-C32-C33
2	A	319	POV	C27-C28-C29-C210
2	A	367	POV	C29-C210-C211-C212
2	B	358	POV	C311-C312-C313-C314
2	B	389	POV	C213-C214-C215-C216
2	B	317	POV	C214-C215-C216-C217
2	B	374	POV	C34-C35-C36-C37
2	B	353	POV	C34-C35-C36-C37
2	A	318	POV	O31-C31-C32-C33
2	A	325	POV	O21-C21-C22-C23
2	B	355	POV	O21-C21-C22-C23
2	A	304	POV	C35-C36-C37-C38
2	A	371	POV	C39-C310-C311-C312
2	A	374	POV	C34-C35-C36-C37
2	A	348	POV	O21-C21-C22-C23
2	A	356	POV	O21-C21-C22-C23
2	A	371	POV	O21-C21-C22-C23
2	B	338	POV	O31-C31-C32-C33
2	B	360	POV	O31-C31-C32-C33
2	B	373	POV	O21-C21-C22-C23
2	B	374	POV	O21-C21-C22-C23
2	A	358	POV	C29-C210-C211-C212
2	A	399	POV	C27-C28-C29-C210
2	B	318	POV	C211-C212-C213-C214
2	B	345	POV	C22-C21-O21-C2
2	B	354	POV	C22-C21-O21-C2
2	A	398	POV	C37-C38-C39-C310
2	B	302	POV	C2-C3-O31-C31
2	A	306	POV	O32-C31-O31-C3
2	A	312	POV	O21-C21-C22-C23
2	A	346	POV	O31-C31-C32-C33
2	A	381	POV	O31-C31-C32-C33
2	B	338	POV	O21-C21-C22-C23
2	B	341	POV	O31-C31-C32-C33
2	B	358	POV	O31-C31-C32-C33
2	A	362	POV	C310-C311-C312-C313
2	A	349	POV	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
2	A	363	POV	C11-C12-N-C15
2	B	350	POV	C11-C12-N-C14
2	B	346	POV	C313-C314-C315-C316
2	A	322	POV	O21-C21-C22-C23
2	A	399	POV	O21-C21-C22-C23
2	A	393	POV	O21-C21-C22-C23
2	B	304	POV	O31-C31-C32-C33
2	B	330	POV	C34-C35-C36-C37
2	A	343	POV	C31-C32-C33-C34
2	A	311	POV	C36-C37-C38-C39
2	A	393	POV	O11-C1-C2-O21
2	B	378	POV	O11-C1-C2-O21
2	A	313	POV	O21-C21-C22-C23
2	A	396	POV	O31-C31-C32-C33
2	B	327	POV	O21-C21-C22-C23
2	B	376	POV	O31-C31-C32-C33
2	B	389	POV	O21-C21-C22-C23
2	A	353	POV	C2-C3-O31-C31
2	A	371	POV	C32-C33-C34-C35
2	A	334	POV	C24-C25-C26-C27
2	A	408	POV	C39-C310-C311-C312
2	B	373	POV	C310-C311-C312-C313
2	A	376	POV	C33-C34-C35-C36
2	A	333	POV	C212-C213-C214-C215
2	B	320	POV	C36-C37-C38-C39
2	A	353	POV	C212-C213-C214-C215
2	B	311	POV	C39-C310-C311-C312
2	A	338	POV	O31-C31-C32-C33
2	A	380	POV	O31-C31-C32-C33
2	A	407	POV	O31-C31-C32-C33
2	A	410	POV	O31-C31-C32-C33
2	B	302	POV	O31-C31-C32-C33
2	B	350	POV	O31-C31-C32-C33
2	B	361	POV	O31-C31-C32-C33
2	B	362	POV	O31-C31-C32-C33
2	B	365	POV	O21-C21-C22-C23
2	B	367	POV	O31-C31-C32-C33
2	A	316	POV	C36-C37-C38-C39
2	B	313	POV	C34-C35-C36-C37
2	A	320	POV	C1-C2-C3-O31
2	A	378	POV	C1-C2-C3-O31
2	A	398	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	B	334	POV	C1-C2-C3-O31
2	B	351	POV	C1-C2-C3-O31
2	B	374	POV	C1-C2-C3-O31
2	A	349	POV	C11-C12-N-C13
2	B	350	POV	C11-C12-N-C15
2	A	308	POV	C34-C35-C36-C37
2	A	312	POV	C32-C33-C34-C35
2	B	374	POV	C215-C216-C217-C218
2	B	304	POV	C211-C212-C213-C214
2	B	309	POV	C23-C24-C25-C26
2	B	379	POV	C35-C36-C37-C38
2	B	377	POV	C214-C215-C216-C217
2	A	338	POV	O21-C21-C22-C23
2	A	384	POV	O31-C31-C32-C33
2	A	385	POV	O31-C31-C32-C33
2	B	334	POV	O31-C31-C32-C33
2	B	335	POV	O31-C31-C32-C33
2	B	381	POV	O31-C31-C32-C33
2	B	387	POV	O31-C31-C32-C33
2	A	354	POV	O21-C2-C3-O31
2	B	351	POV	O21-C2-C3-O31
2	B	313	POV	C23-C24-C25-C26
2	A	351	POV	C32-C33-C34-C35
2	B	370	POV	O22-C21-C22-C23
2	B	330	POV	C24-C25-C26-C27
2	B	341	POV	C35-C36-C37-C38
2	A	386	POV	C213-C214-C215-C216
2	B	330	POV	C23-C24-C25-C26
2	A	303	POV	O31-C31-C32-C33
2	A	337	POV	O31-C31-C32-C33
2	A	400	POV	O31-C31-C32-C33
2	A	395	POV	O21-C21-C22-C23
2	B	314	POV	O21-C21-C22-C23
2	B	332	POV	O31-C31-C32-C33
2	A	319	POV	C213-C214-C215-C216
2	A	396	POV	C26-C27-C28-C29
2	A	409	POV	C26-C27-C28-C29
2	A	341	POV	C312-C313-C314-C315
2	A	381	POV	C39-C310-C311-C312
2	A	382	POV	C35-C36-C37-C38
2	A	307	POV	O31-C31-C32-C33
2	A	324	POV	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	A	354	POV	O31-C31-C32-C33
2	A	384	POV	O21-C21-C22-C23
2	A	392	POV	O21-C21-C22-C23
2	A	396	POV	O21-C21-C22-C23
2	B	323	POV	O21-C21-C22-C23
2	B	330	POV	O31-C31-C32-C33
2	B	346	POV	O31-C31-C32-C33
2	B	367	POV	O21-C21-C22-C23
2	A	386	POV	C211-C212-C213-C214
2	A	335	POV	C211-C212-C213-C214
2	B	365	POV	C36-C37-C38-C39
2	A	392	POV	C27-C28-C29-C210
2	A	413	POV	O21-C21-C22-C23
2	A	408	POV	C312-C313-C314-C315
2	A	331	POV	C215-C216-C217-C218
2	A	370	POV	C34-C35-C36-C37
2	A	302	POV	C1-C2-O21-C21
2	A	319	POV	C1-C2-O21-C21
2	A	337	POV	C3-C2-O21-C21
2	A	340	POV	C3-C2-O21-C21
2	A	354	POV	C3-C2-O21-C21
2	A	355	POV	C3-C2-O21-C21
2	A	359	POV	C3-C2-O21-C21
2	A	365	POV	C3-C2-O21-C21
2	A	407	POV	C1-C2-O21-C21
2	B	327	POV	C3-C2-O21-C21
2	B	347	POV	C1-C2-O21-C21
2	B	374	POV	C3-C2-O21-C21
2	B	378	POV	C3-C2-O21-C21
2	B	380	POV	C1-C2-O21-C21
2	B	380	POV	C3-C2-O21-C21
2	B	357	POV	C37-C38-C39-C310
2	B	374	POV	C310-C311-C312-C313
2	A	378	POV	C39-C310-C311-C312
2	A	348	POV	C210-C211-C212-C213
2	B	302	POV	C26-C27-C28-C29
2	B	343	POV	C210-C211-C212-C213
2	A	318	POV	C2-C3-O31-C31
2	A	362	POV	C2-C3-O31-C31
2	A	347	POV	O31-C31-C32-C33
2	A	311	POV	C214-C215-C216-C217
2	A	382	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	B	332	POV	C213-C214-C215-C216
2	A	384	POV	C22-C23-C24-C25
2	B	369	POV	O22-C21-O21-C2
2	A	331	POV	C212-C213-C214-C215
2	A	333	POV	C36-C37-C38-C39
2	A	384	POV	C23-C24-C25-C26
2	B	334	POV	C24-C25-C26-C27
2	B	346	POV	C34-C35-C36-C37
2	B	352	POV	C311-C312-C313-C314
2	B	347	POV	C34-C35-C36-C37
2	A	307	POV	O21-C21-C22-C23
2	B	375	POV	O31-C31-C32-C33
2	A	340	POV	O32-C31-C32-C33
2	B	370	POV	O32-C31-C32-C33
2	B	370	POV	C27-C28-C29-C210
2	B	323	POV	C2-C3-O31-C31
2	A	368	POV	C2-C1-O11-P
2	B	347	POV	C2-C1-O11-P
2	A	308	POV	O22-C21-C22-C23
2	B	371	POV	O32-C31-C32-C33
2	B	346	POV	O32-C31-O31-C3
2	A	335	POV	O21-C21-C22-C23
2	A	336	POV	O31-C31-C32-C33
2	A	352	POV	O31-C31-C32-C33
2	A	386	POV	O31-C31-C32-C33
2	A	393	POV	O31-C31-C32-C33
2	A	395	POV	O31-C31-C32-C33
2	B	349	POV	C21-C22-C23-C24
2	B	349	POV	C310-C311-C312-C313
2	B	326	POV	C2-C3-O31-C31
2	A	332	POV	C37-C38-C39-C310
2	B	310	POV	C311-C312-C313-C314
2	A	358	POV	O22-C21-C22-C23
2	A	376	POV	O32-C31-C32-C33
2	B	303	POV	O22-C21-C22-C23
2	B	360	POV	O22-C21-C22-C23
2	A	324	POV	C34-C35-C36-C37
2	B	341	POV	C33-C34-C35-C36
2	A	360	POV	O21-C21-C22-C23
2	B	330	POV	O21-C21-C22-C23
2	B	340	POV	O31-C31-C32-C33
2	A	364	POV	C29-C210-C211-C212

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Mol	Chain	Res	Type	Atoms
2	B	355	POV	C29-C210-C211-C212
2	A	333	POV	O22-C21-C22-C23
2	A	334	POV	O22-C21-C22-C23
2	A	399	POV	O22-C21-C22-C23
2	B	354	POV	O22-C21-C22-C23
2	A	363	POV	C11-C12-N-C13
2	A	363	POV	C11-C12-N-C14
2	A	350	POV	C310-C311-C312-C313
2	B	314	POV	O22-C21-C22-C23
2	B	386	POV	O32-C31-C32-C33
2	B	312	POV	C310-C311-C312-C313
2	A	347	POV	C39-C310-C311-C312
2	B	374	POV	C39-C310-C311-C312
2	A	312	POV	O22-C21-C22-C23
2	A	361	POV	O32-C31-C32-C33
2	A	387	POV	O22-C21-C22-C23
2	A	398	POV	O22-C21-C22-C23
2	B	331	POV	O22-C21-C22-C23
2	B	344	POV	O22-C21-C22-C23
2	B	331	POV	C37-C38-C39-C310
2	B	353	POV	O31-C31-C32-C33
2	B	361	POV	C29-C210-C211-C212
2	A	325	POV	O32-C31-C32-C33
2	A	328	POV	O22-C21-C22-C23
2	A	329	POV	O22-C21-C22-C23
2	A	365	POV	C311-C310-C39-C38
2	A	366	POV	C310-C311-C312-C313
2	A	372	POV	C25-C26-C27-C28
2	A	366	POV	C213-C214-C215-C216
2	A	383	POV	C33-C34-C35-C36
2	B	308	POV	C25-C26-C27-C28
2	A	319	POV	C35-C36-C37-C38
2	A	385	POV	C33-C34-C35-C36
2	A	394	POV	O31-C31-C32-C33
2	A	325	POV	C212-C213-C214-C215
2	A	301	POV	O32-C31-C32-C33
2	A	347	POV	O32-C31-C32-C33
2	A	363	POV	O22-C21-C22-C23
2	A	408	POV	O32-C31-C32-C33
2	A	410	POV	O22-C21-C22-C23
2	A	411	POV	O22-C21-C22-C23
2	B	346	POV	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
2	B	378	POV	O22-C21-C22-C23
2	A	389	POV	C37-C38-C39-C310
2	B	376	POV	C25-C26-C27-C28
2	A	333	POV	O21-C2-C3-O31
2	A	302	POV	O32-C31-C32-C33
2	A	336	POV	O22-C21-C22-C23
2	A	355	POV	O22-C21-C22-C23
2	B	301	POV	O22-C21-C22-C23
2	B	339	POV	O22-C21-C22-C23
2	B	366	POV	O32-C31-C32-C33
2	A	329	POV	O21-C21-C22-C23
2	A	416	POV	O31-C31-C32-C33
2	B	318	POV	O21-C21-C22-C23
2	B	369	POV	O21-C21-C22-C23
2	A	392	POV	C32-C33-C34-C35
2	A	408	POV	C213-C214-C215-C216
2	A	334	POV	C27-C28-C29-C210
2	B	328	POV	C29-C210-C211-C212
2	B	361	POV	C1-C2-C3-O31
2	A	307	POV	O32-C31-C32-C33
2	A	361	POV	O22-C21-C22-C23
2	A	369	POV	O32-C31-C32-C33
2	B	327	POV	O32-C31-C32-C33
2	B	383	POV	O32-C31-C32-C33
2	A	332	POV	C2-C1-O11-P
2	A	374	POV	C2-C1-O11-P
2	A	368	POV	O21-C21-C22-C23
2	A	387	POV	O21-C21-C22-C23
2	B	350	POV	O21-C21-C22-C23
2	B	386	POV	O31-C31-C32-C33
2	A	336	POV	C11-C12-N-C13
2	A	336	POV	C11-C12-N-C14
2	A	359	POV	C11-C12-N-C13
2	A	327	POV	C214-C215-C216-C217
2	A	319	POV	O22-C21-C22-C23
2	A	341	POV	O21-C21-C22-C23
2	B	315	POV	O21-C21-C22-C23
2	B	367	POV	C25-C26-C27-C28
3	B	399	CLR	C22-C23-C24-C25
2	A	331	POV	C23-C24-C25-C26
2	A	350	POV	C32-C33-C34-C35
2	B	346	POV	C213-C214-C215-C216

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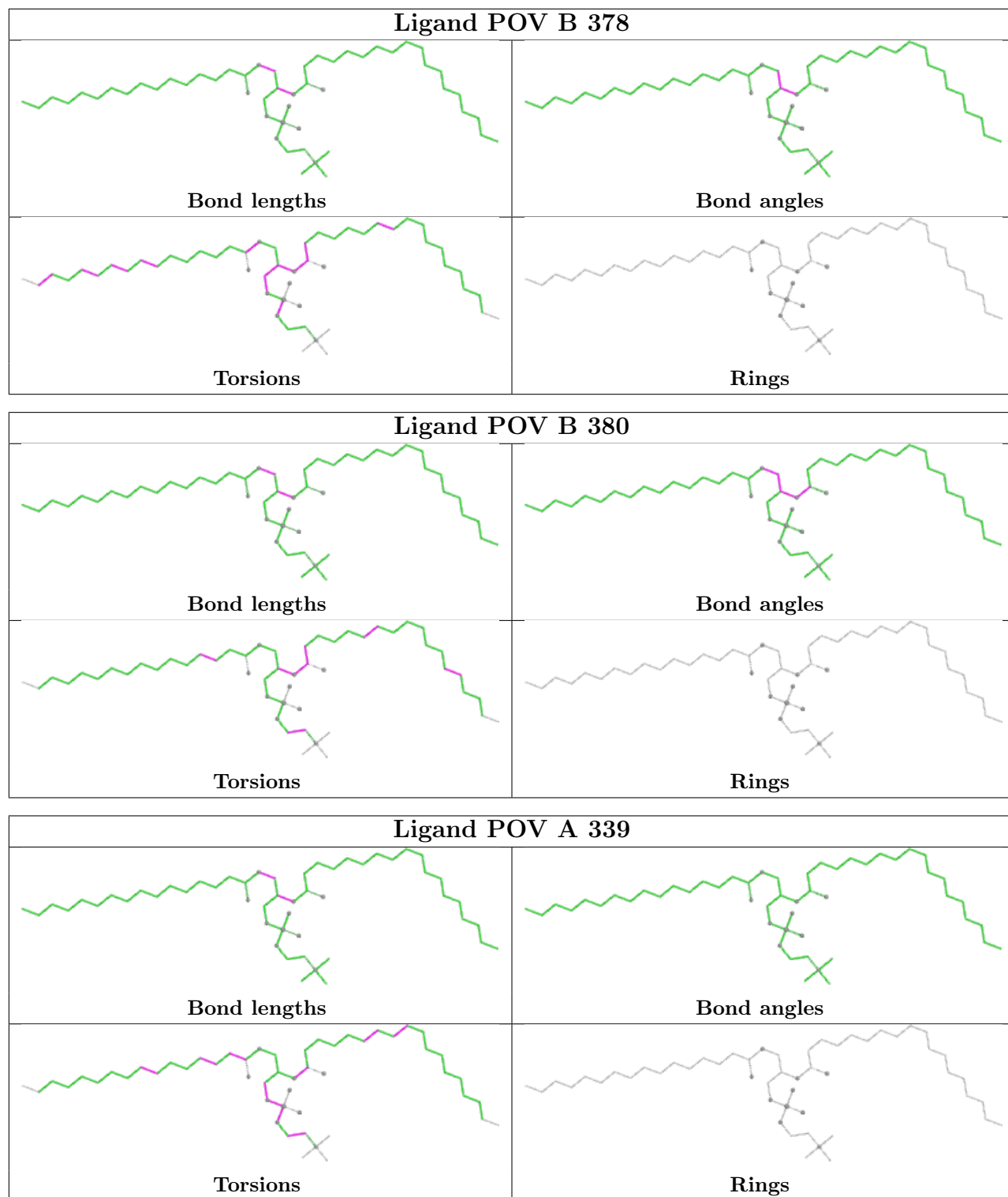
Mol	Chain	Res	Type	Atoms
2	B	319	POV	C211-C212-C213-C214
2	B	320	POV	C32-C33-C34-C35
2	B	333	POV	C27-C28-C29-C210
2	B	370	POV	C25-C26-C27-C28
2	A	377	POV	O22-C21-C22-C23
2	A	384	POV	O32-C31-C32-C33
2	A	364	POV	O31-C31-C32-C33
2	B	385	POV	O31-C31-C32-C33
2	A	347	POV	C311-C310-C39-C38
2	B	384	POV	C34-C35-C36-C37
2	B	364	POV	C25-C26-C27-C28
2	B	372	POV	C34-C35-C36-C37
2	A	310	POV	C32-C33-C34-C35
2	A	339	POV	C36-C37-C38-C39
2	A	342	POV	C37-C38-C39-C310
2	A	358	POV	C311-C312-C313-C314
2	A	382	POV	C39-C310-C311-C312
2	A	373	POV	O31-C31-C32-C33
2	A	409	POV	O31-C31-C32-C33
2	B	378	POV	O21-C21-C22-C23
2	B	310	POV	C34-C35-C36-C37
2	A	341	POV	C310-C311-C312-C313
2	B	370	POV	C22-C21-O21-C2
2	A	303	POV	O32-C31-C32-C33
2	A	409	POV	O32-C31-C32-C33
2	B	312	POV	O32-C31-C32-C33
2	B	357	POV	O32-C31-C32-C33
2	B	375	POV	C34-C35-C36-C37
2	A	395	POV	C311-C310-C39-C38
2	A	346	POV	C311-C312-C313-C314
2	A	308	POV	O21-C21-C22-C23
2	A	341	POV	O31-C31-C32-C33
2	A	343	POV	O21-C21-C22-C23
2	A	349	POV	O31-C31-C32-C33
2	A	356	POV	O31-C31-C32-C33
2	A	363	POV	O21-C21-C22-C23
2	B	343	POV	C33-C34-C35-C36
2	A	311	POV	O32-C31-C32-C33
2	A	397	POV	O22-C21-C22-C23
2	B	342	POV	O22-C21-C22-C23
2	B	319	POV	C214-C215-C216-C217
2	B	354	POV	C34-C35-C36-C37

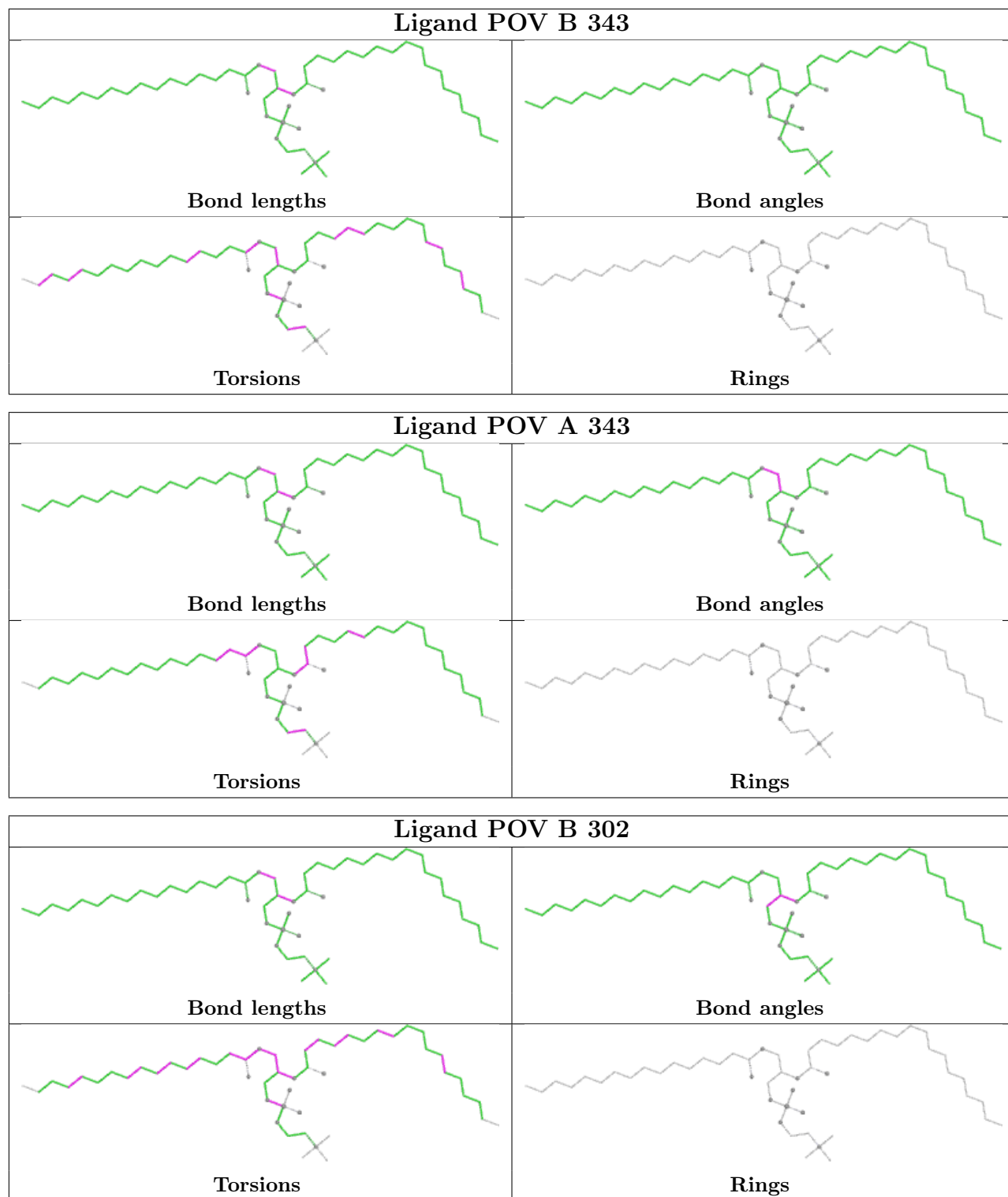
There are no ring outliers.

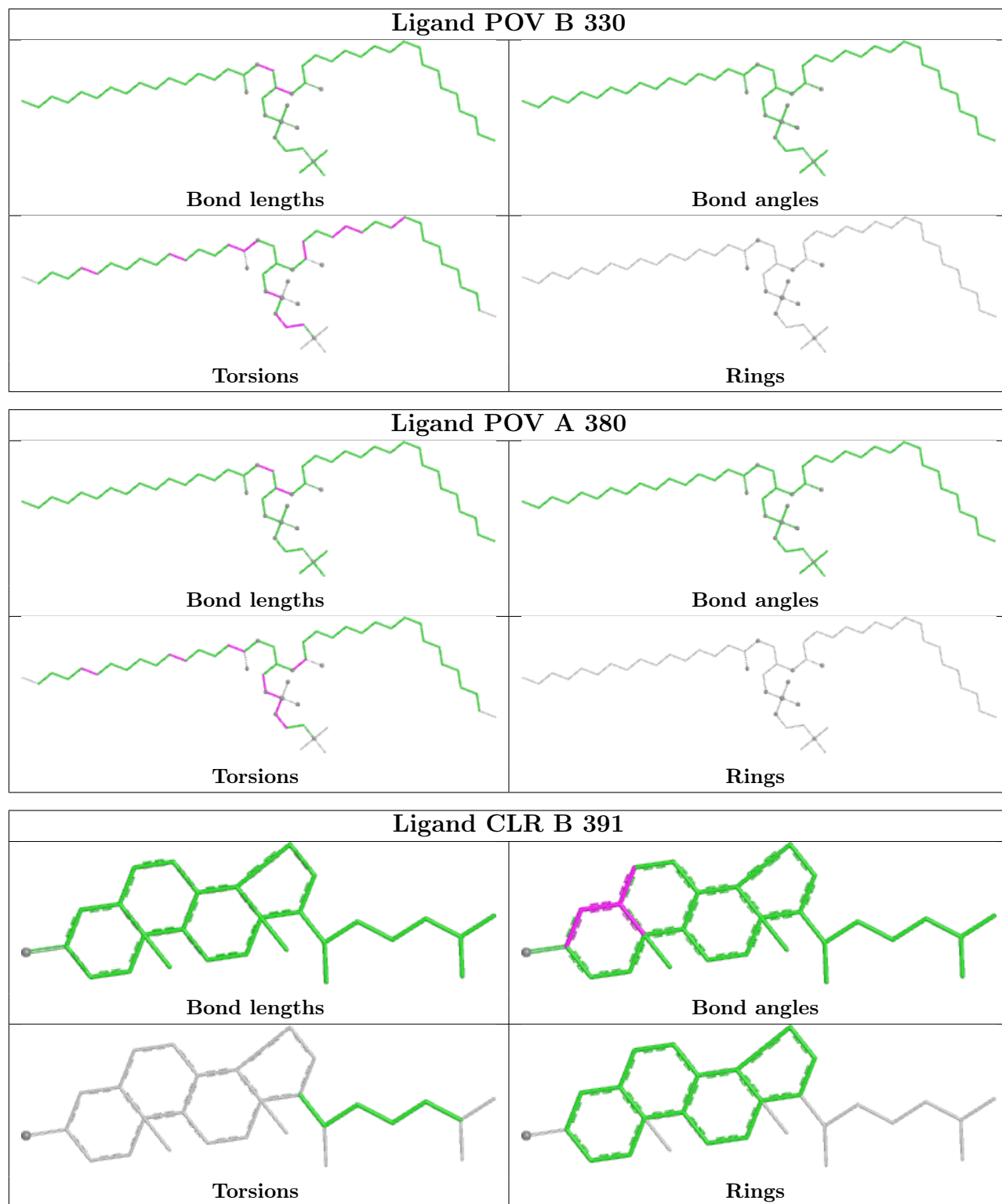
18 monomers are involved in 17 short contacts:

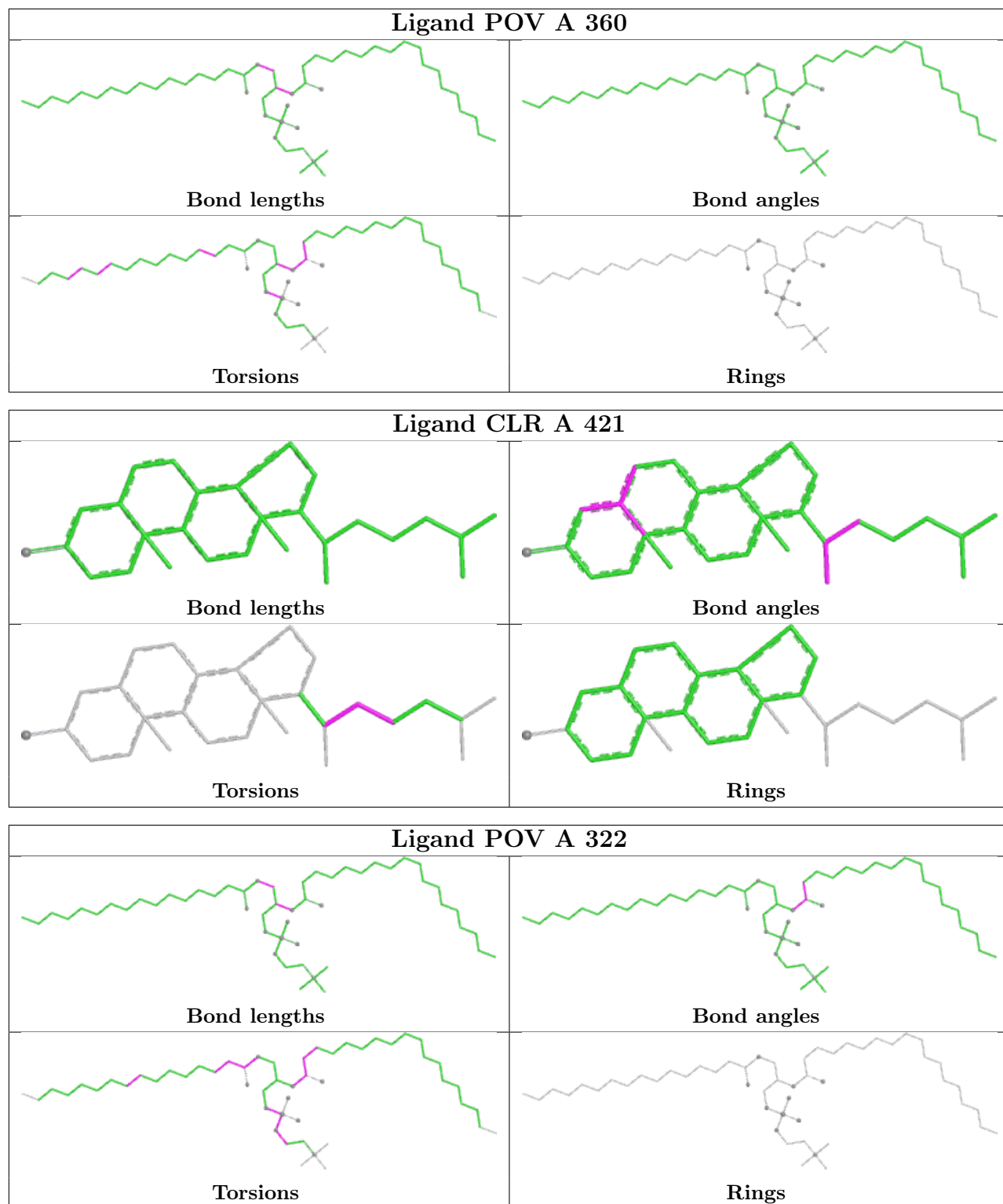
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	POV	1	0
2	B	339	POV	1	0
2	A	396	POV	1	0
2	B	331	POV	2	0
2	B	303	POV	1	0
2	A	412	POV	1	0
2	B	334	POV	1	0
3	A	402	CLR	2	0
2	B	329	POV	1	0
2	B	313	POV	1	0
2	B	349	POV	1	0
2	B	314	POV	1	0
3	B	393	CLR	1	0
2	B	373	POV	1	0
2	B	388	POV	1	0
2	A	311	POV	1	0
2	A	318	POV	1	0
2	A	357	POV	1	0

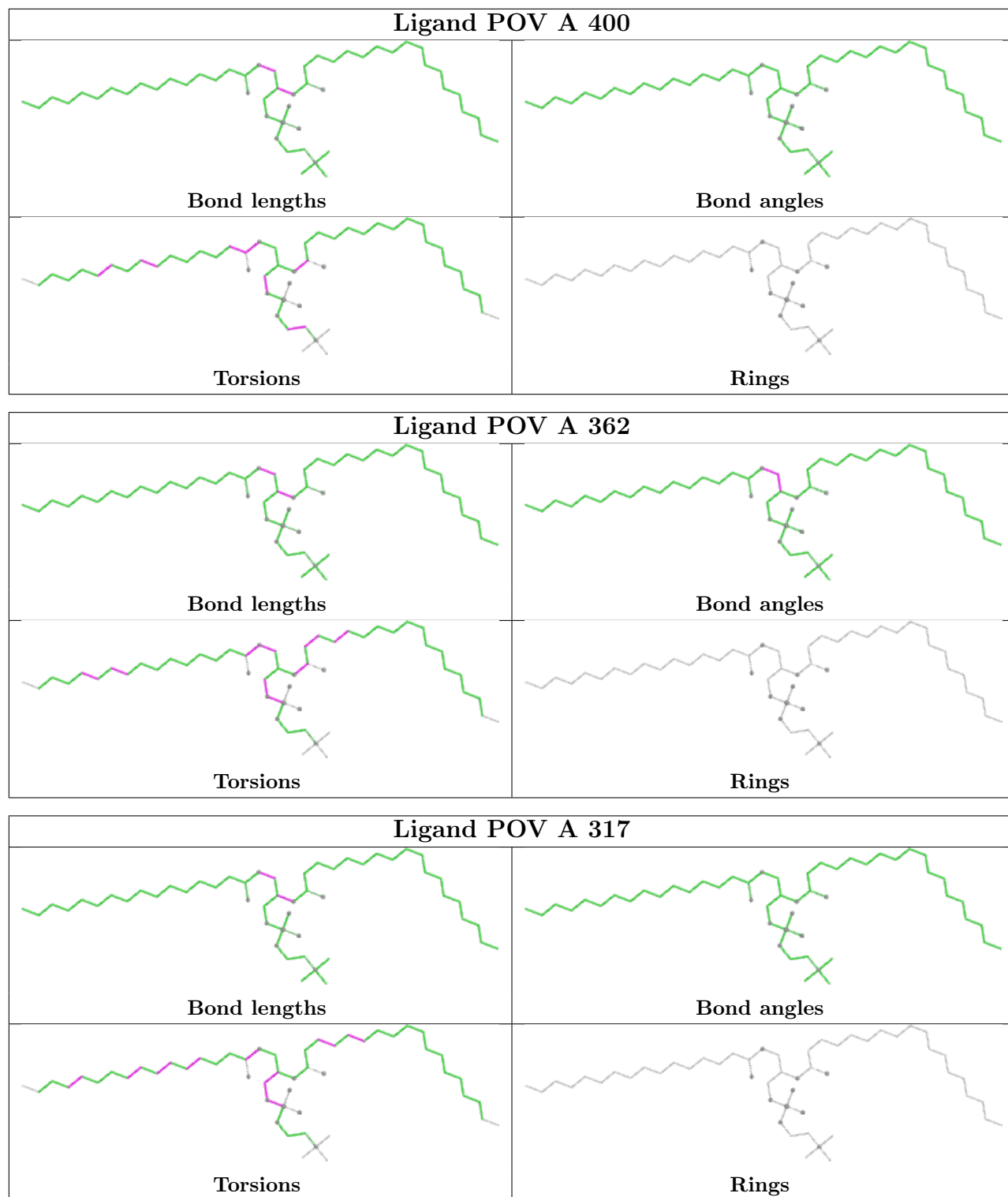
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

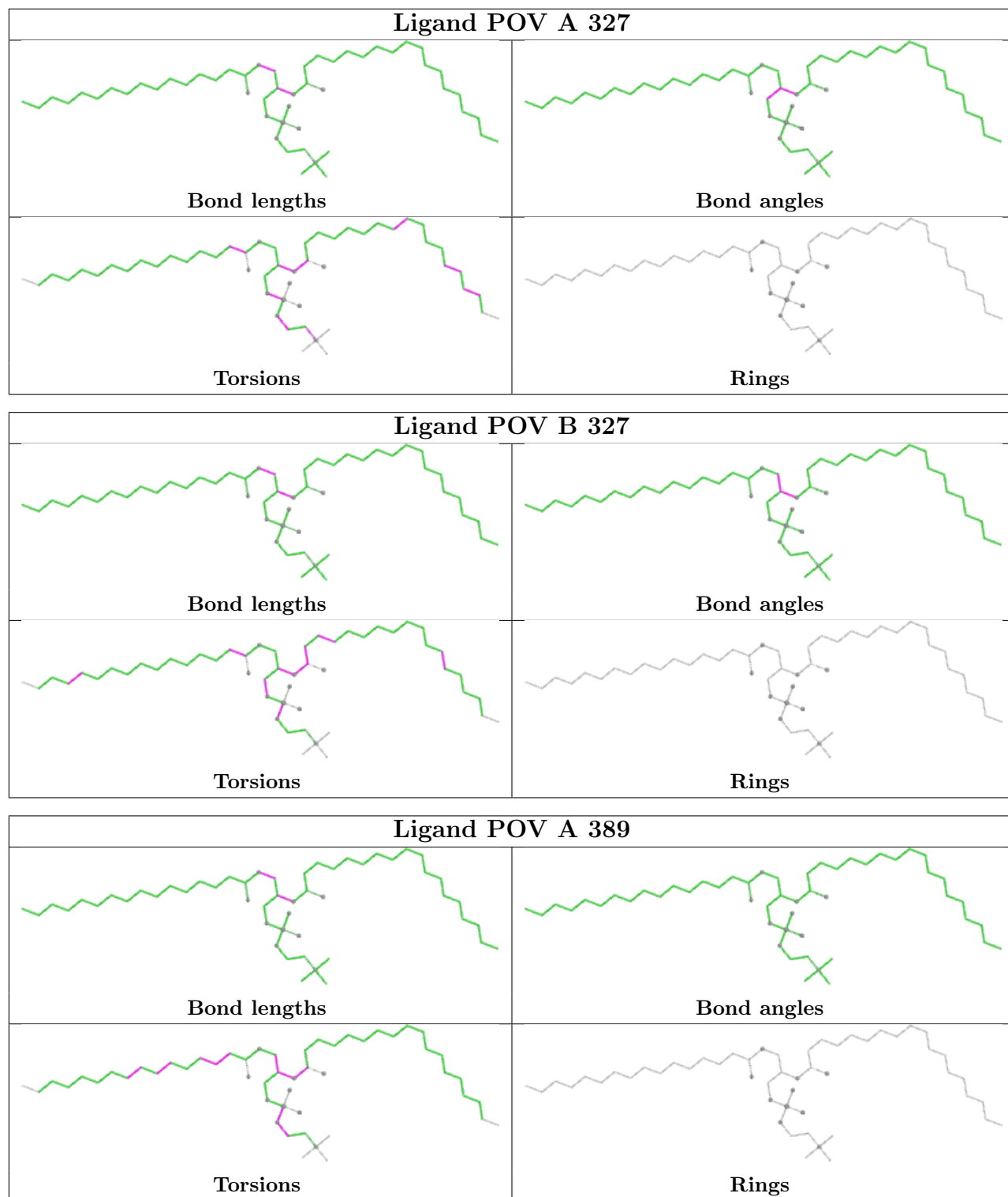


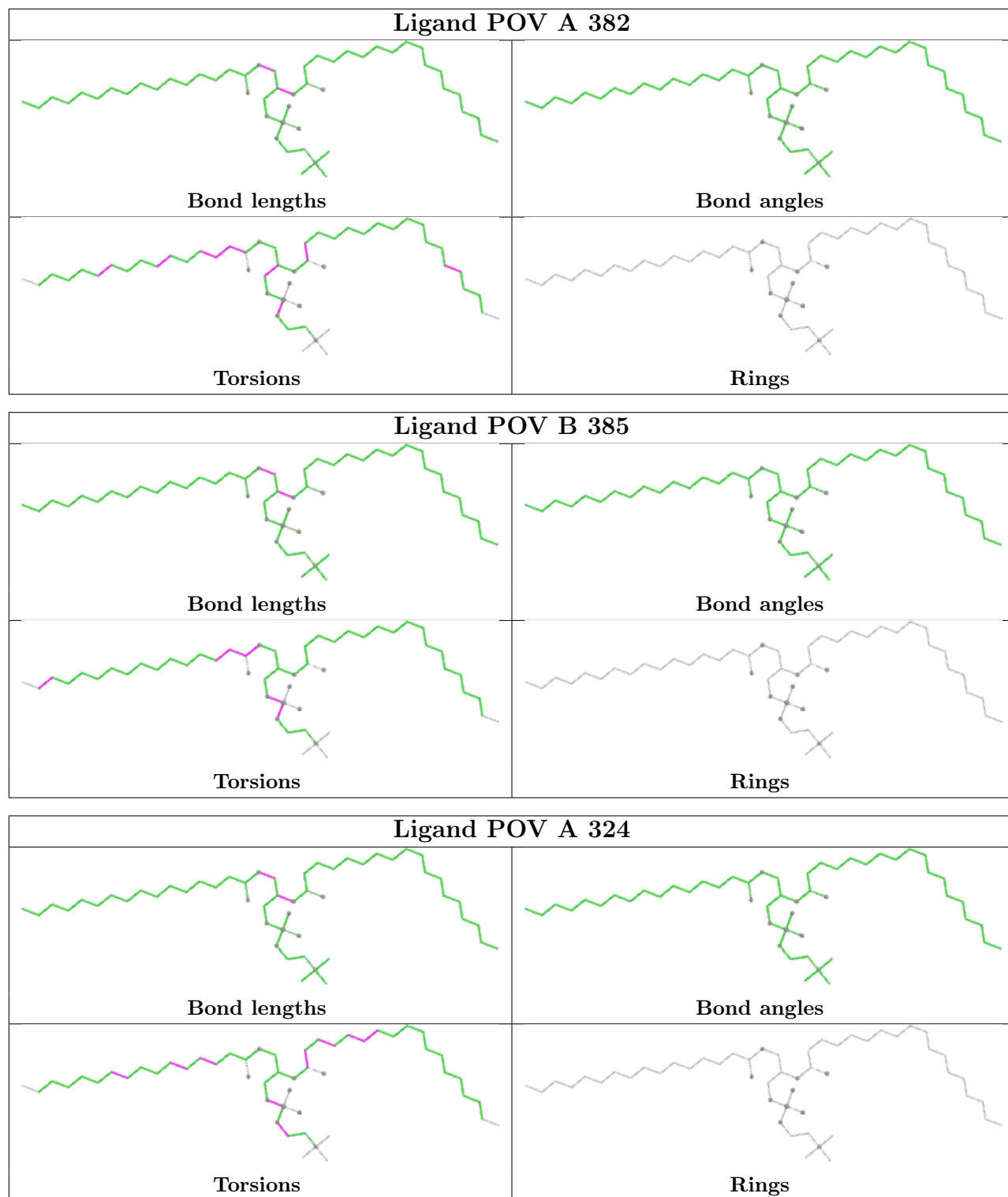


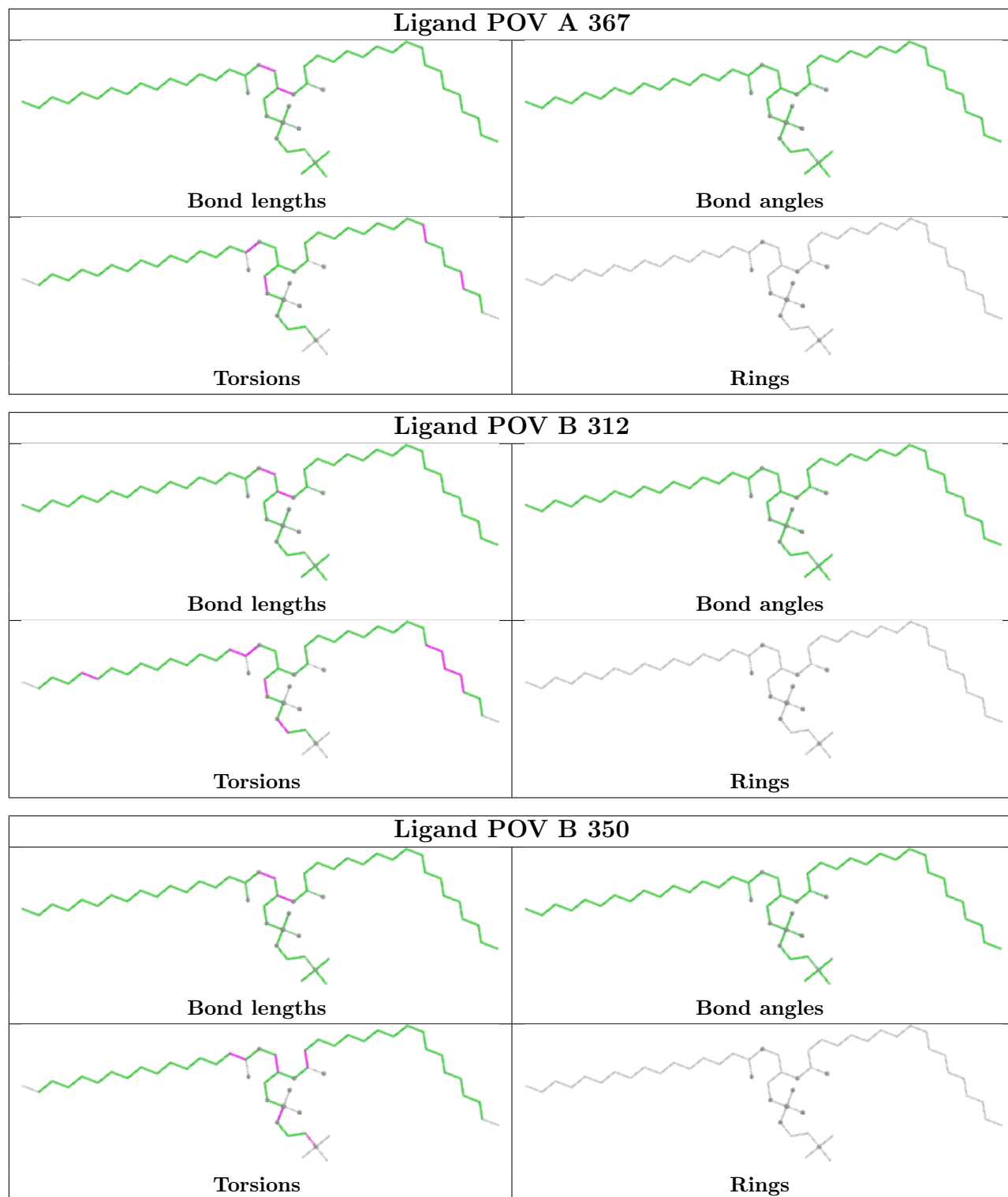


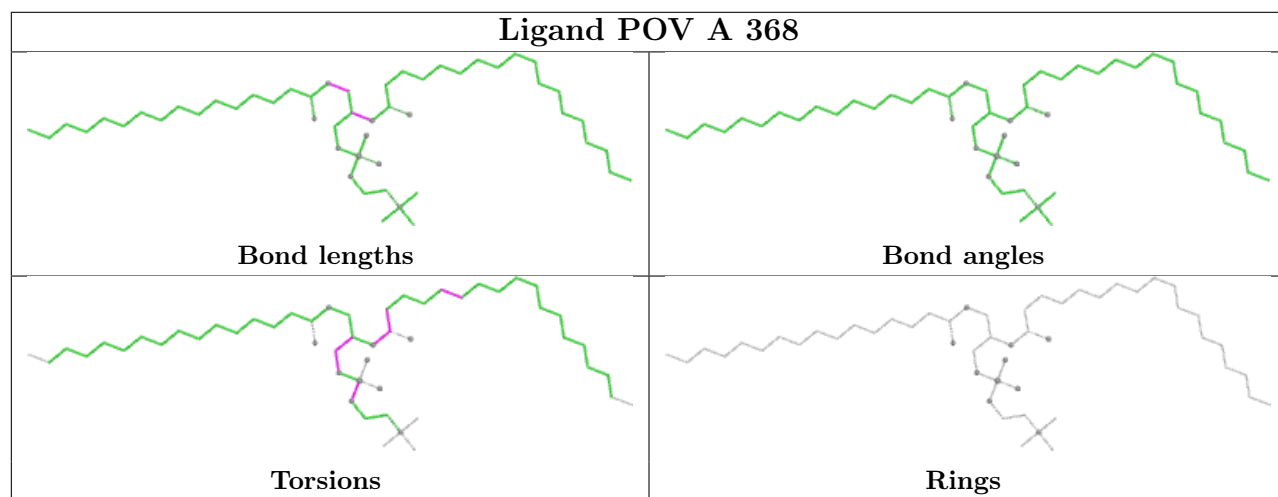
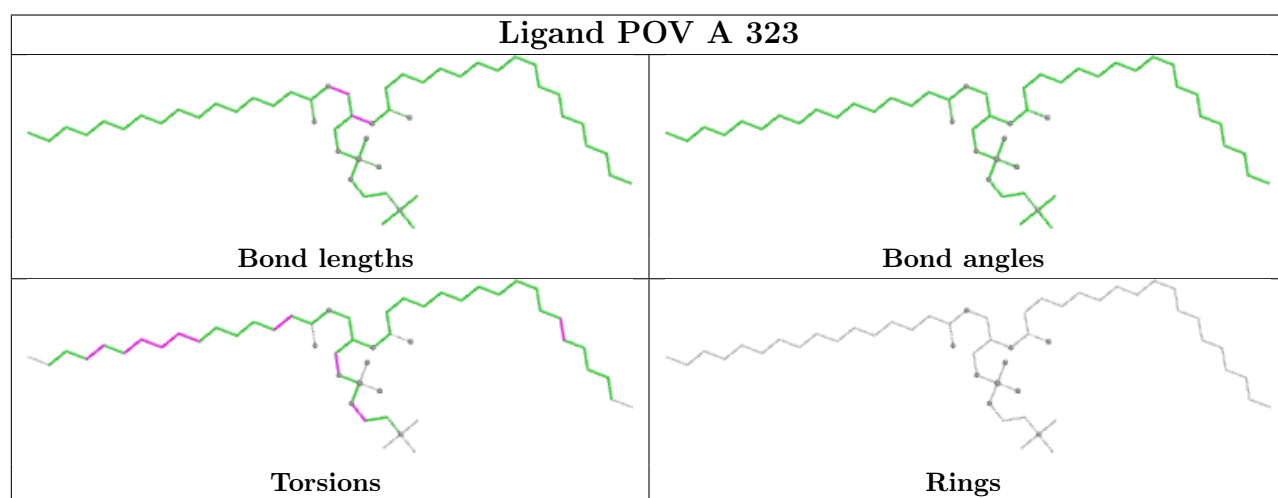
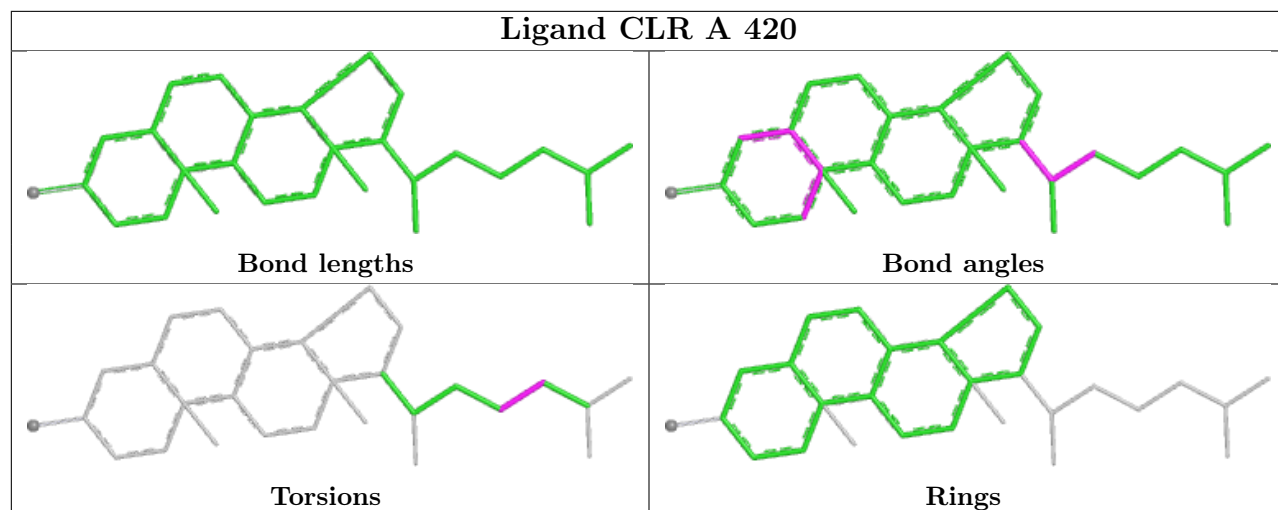


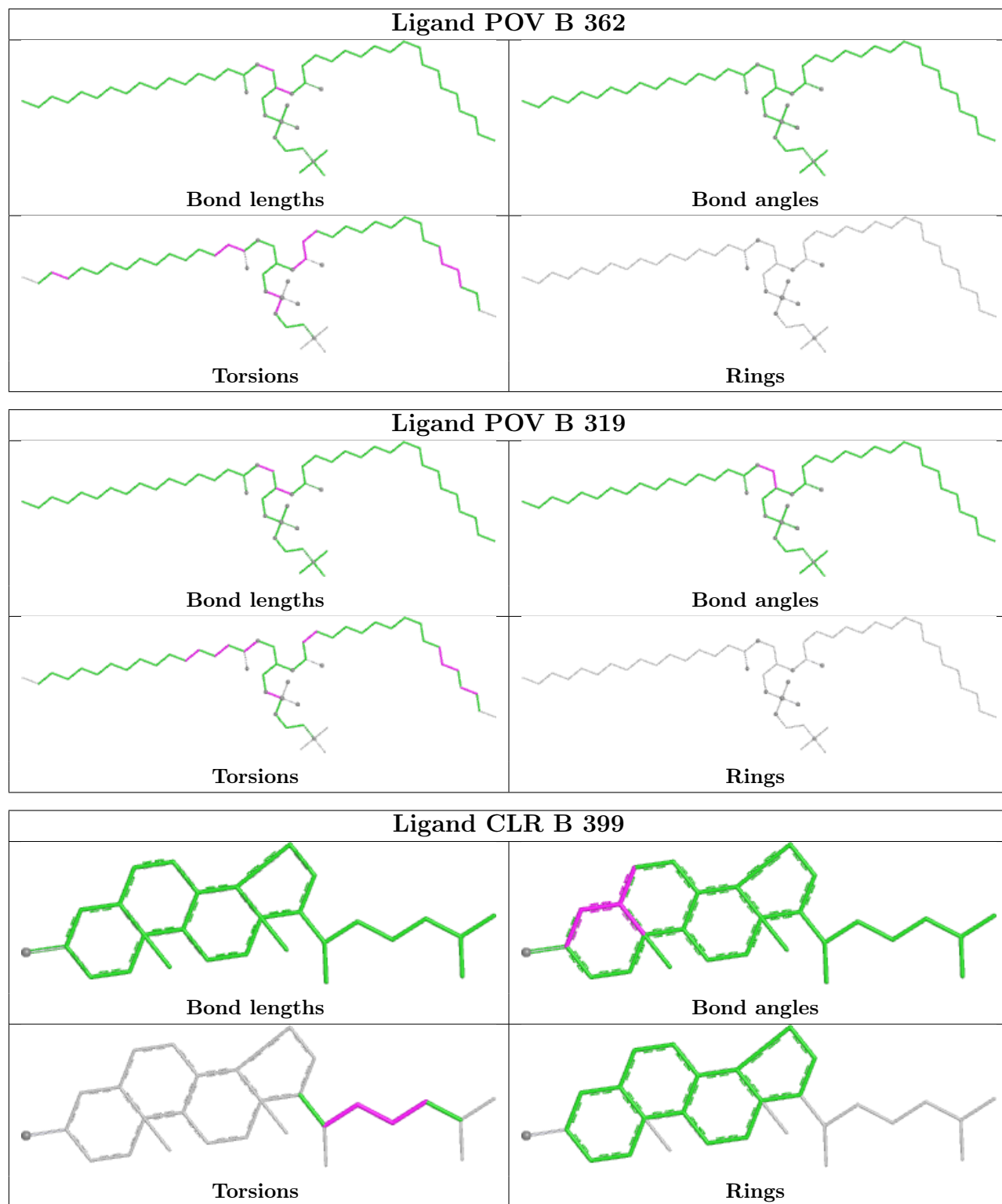


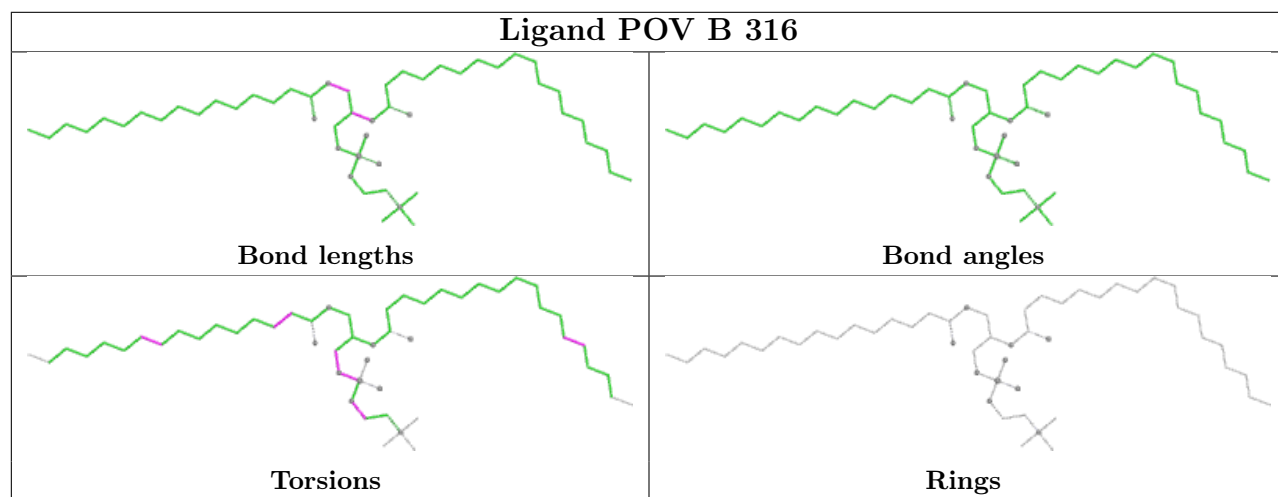
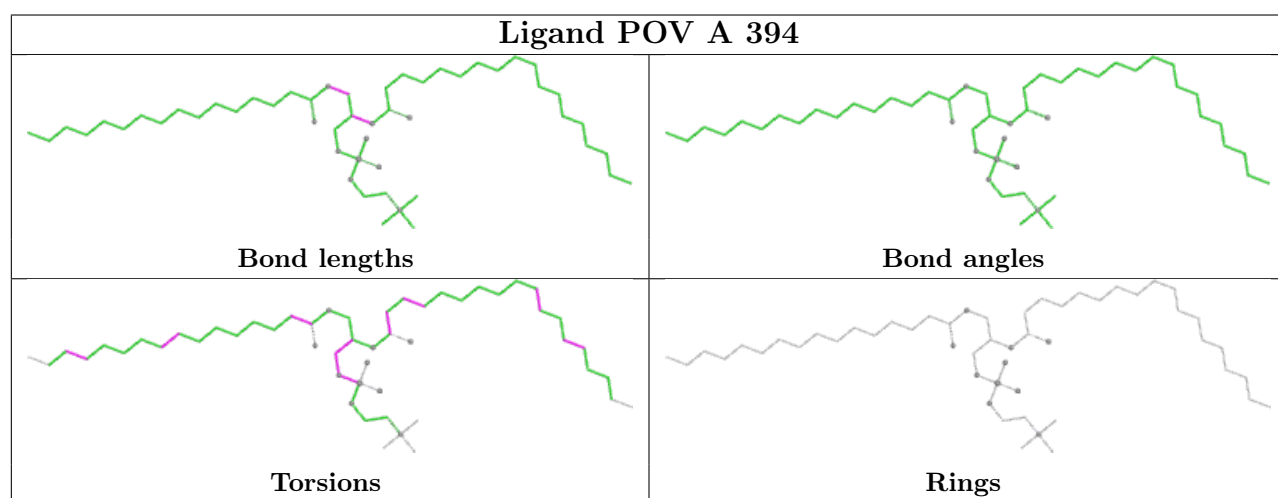
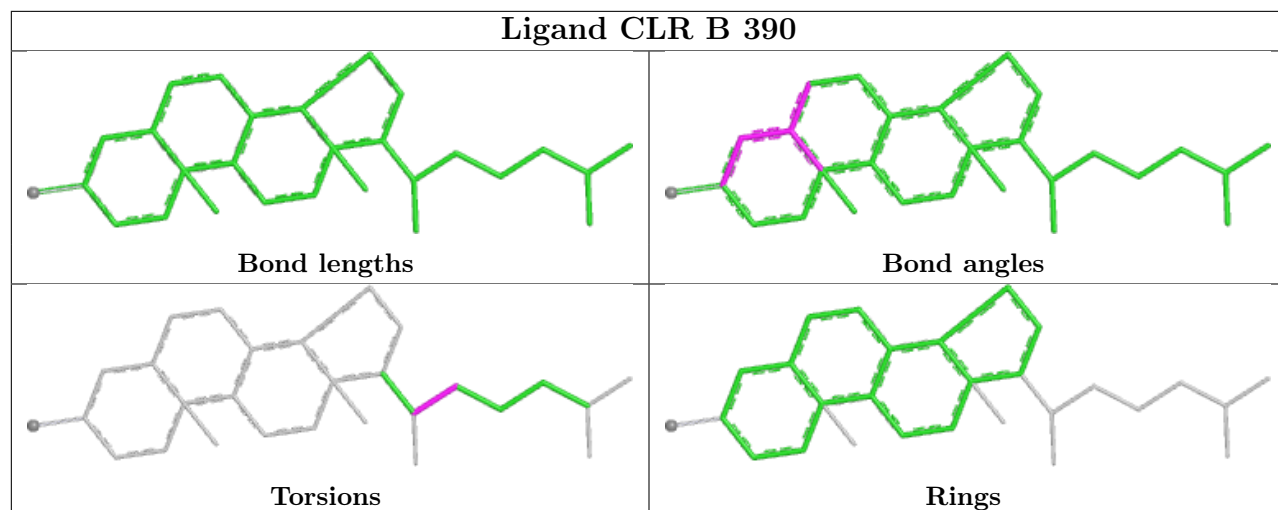


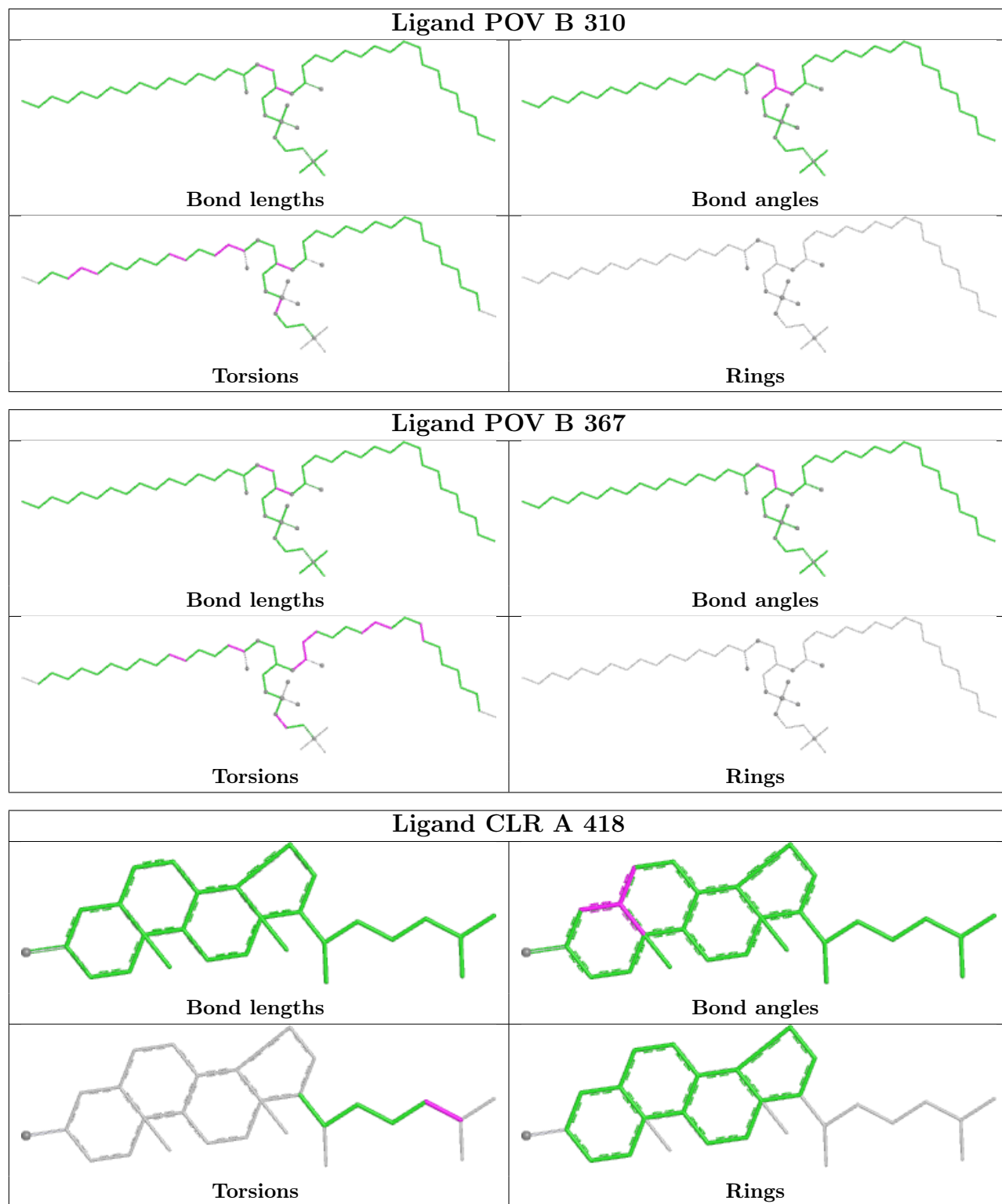


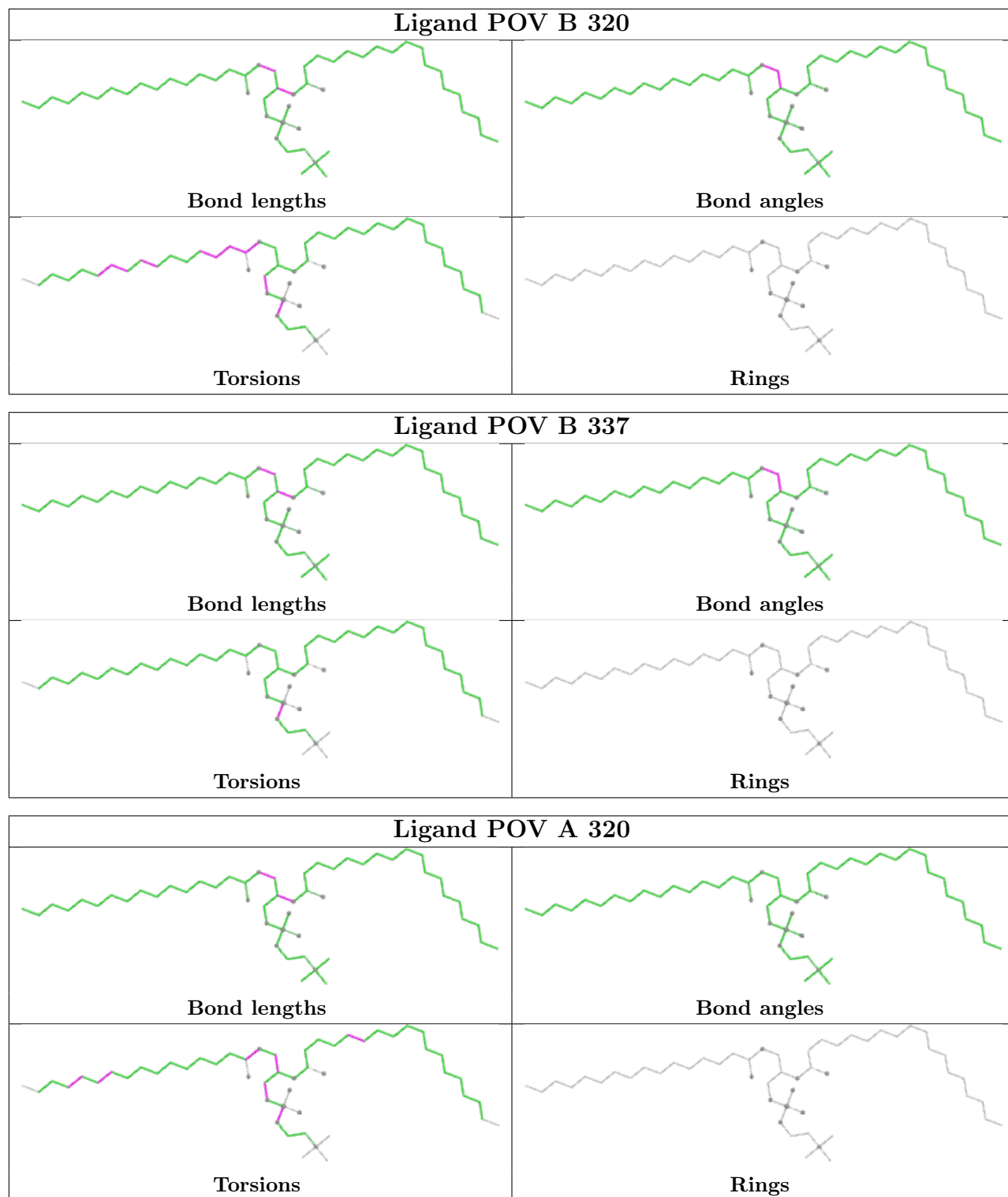


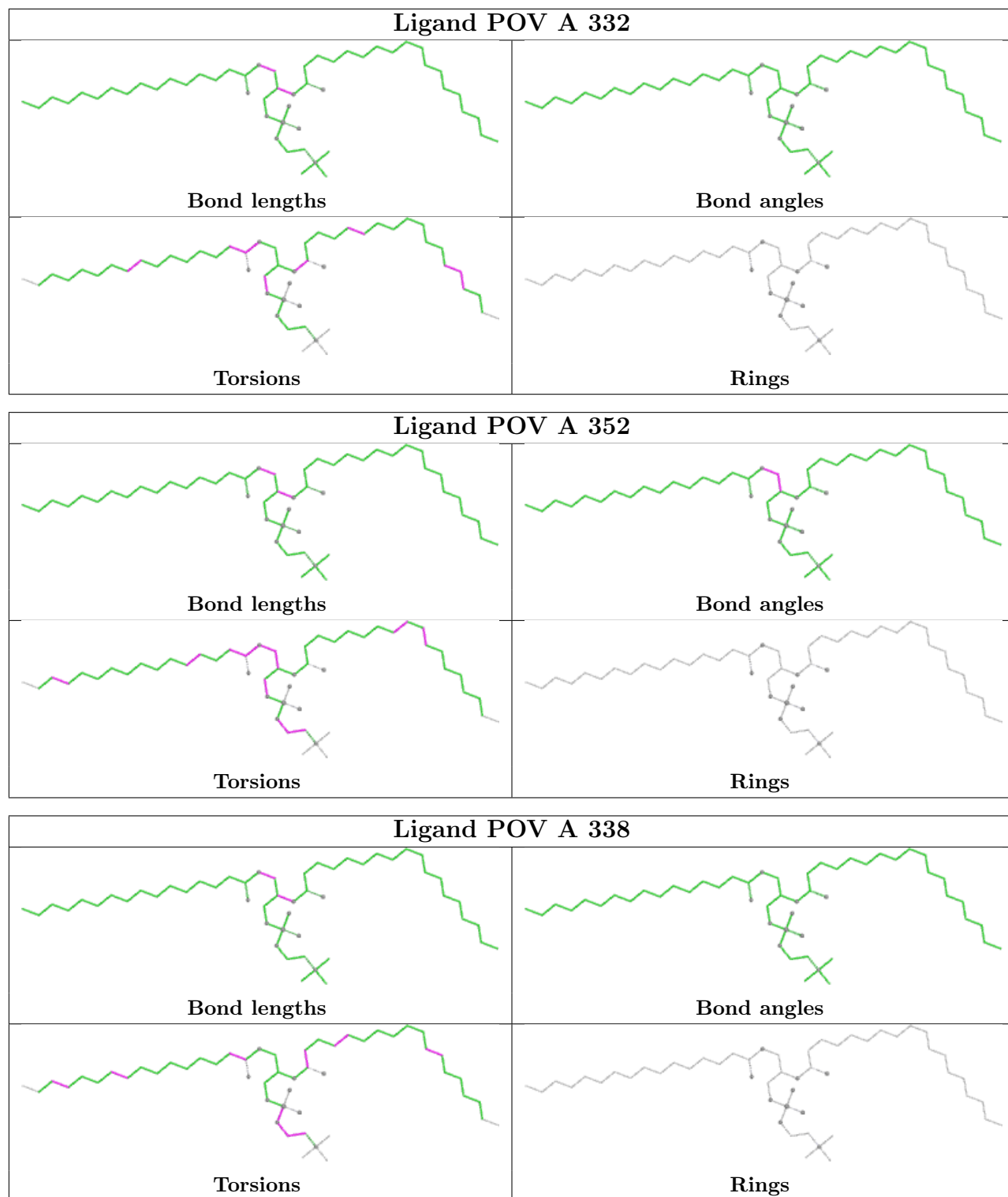


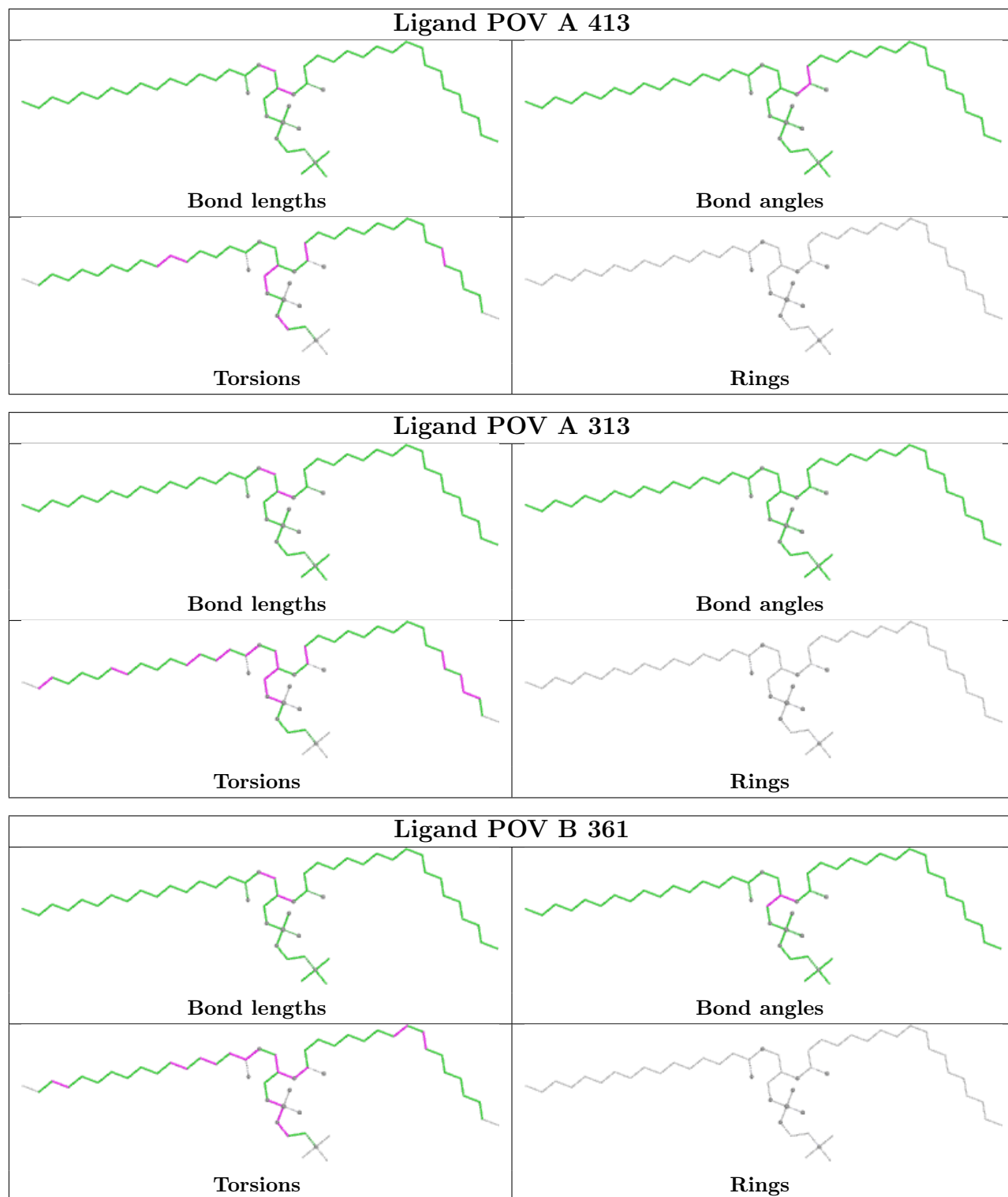


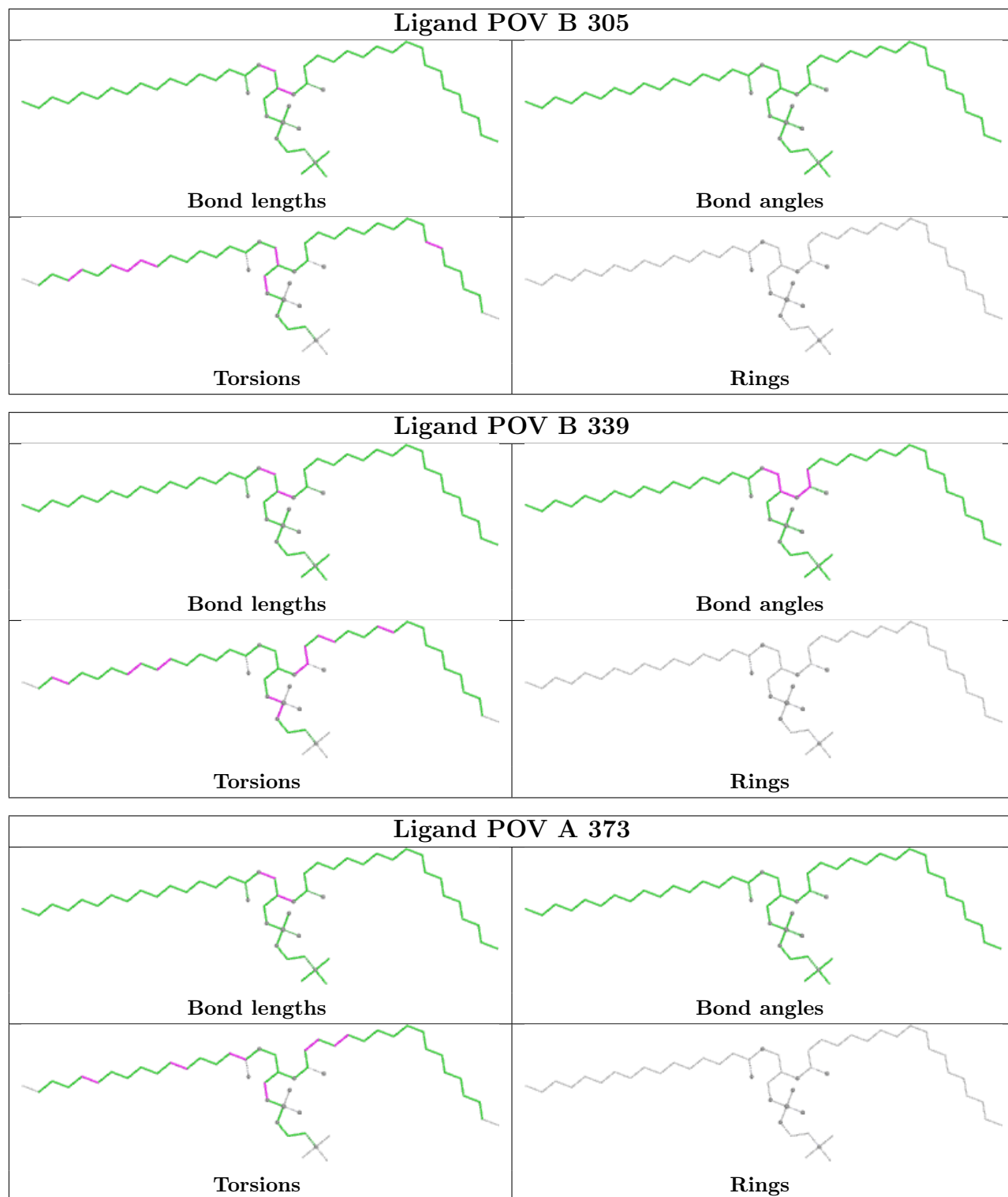


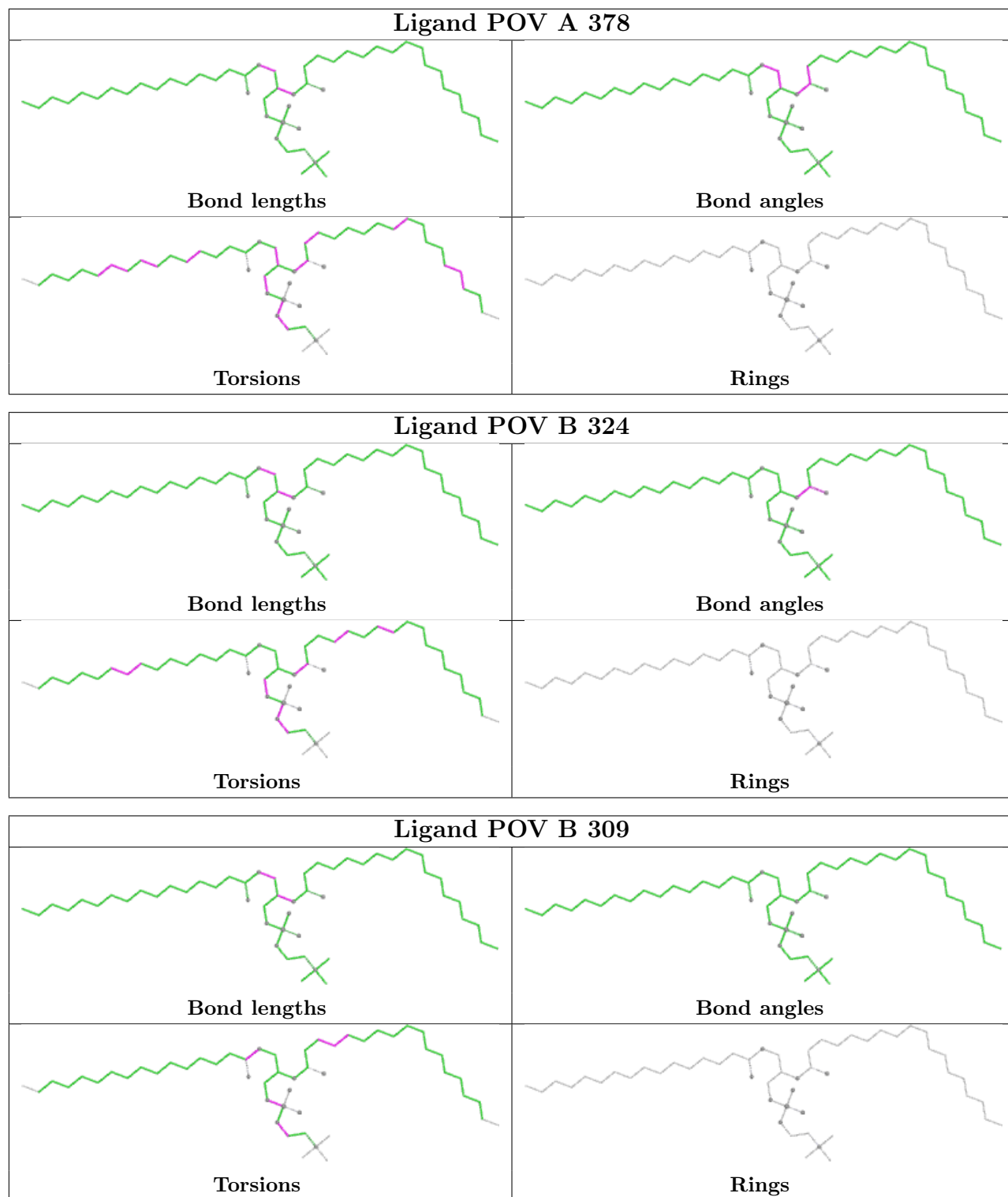


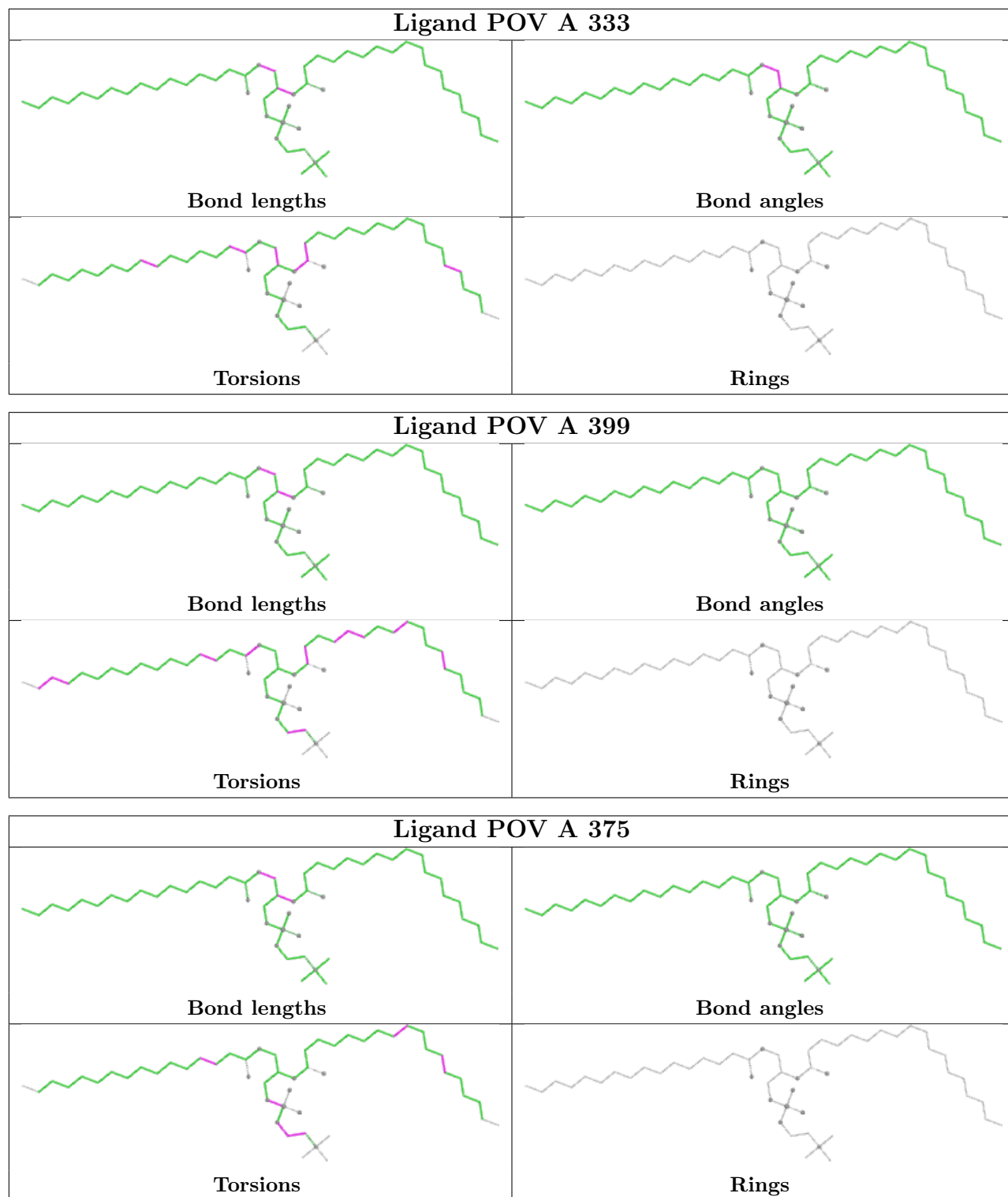


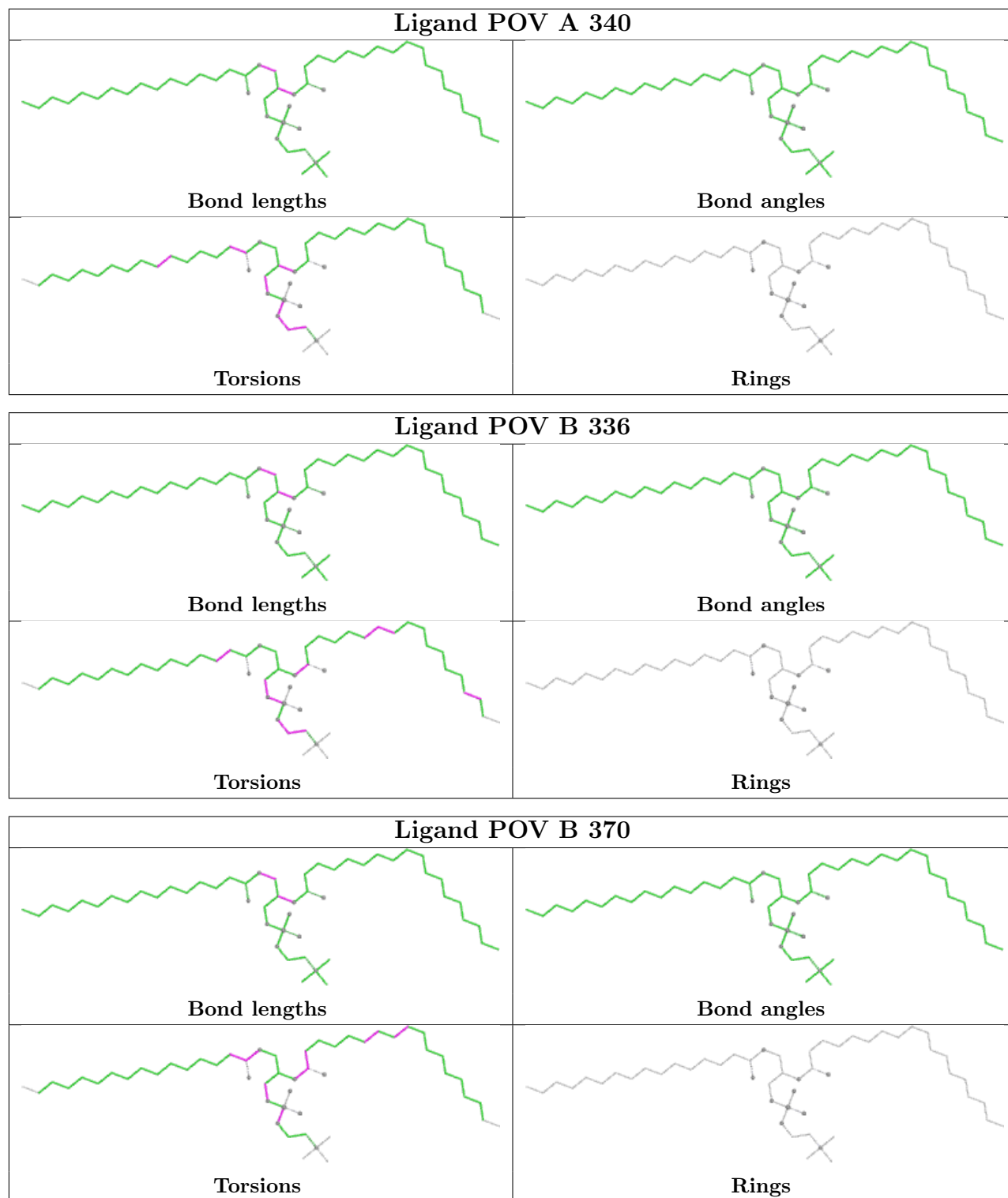


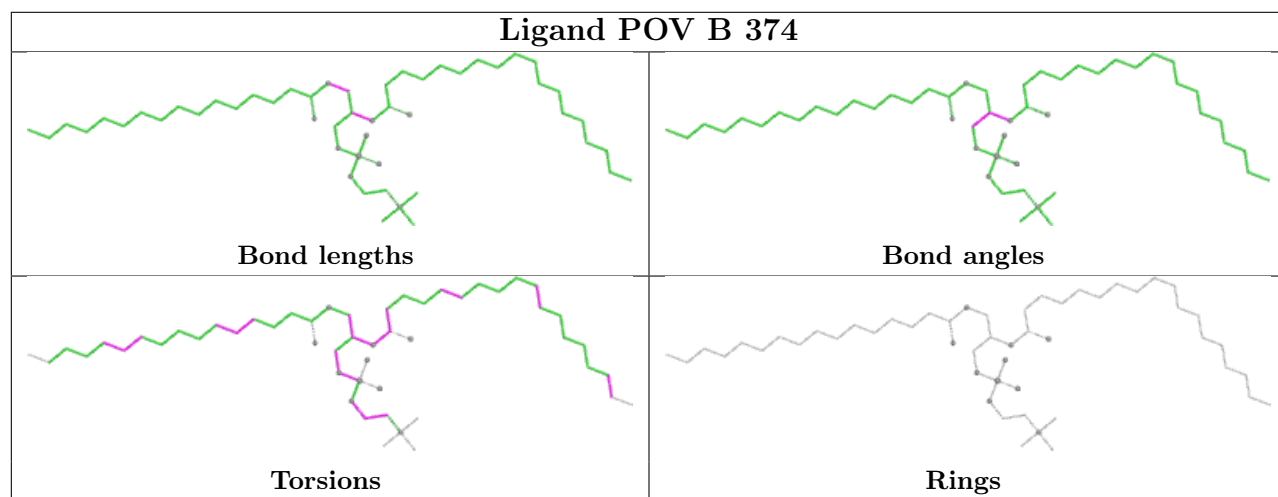
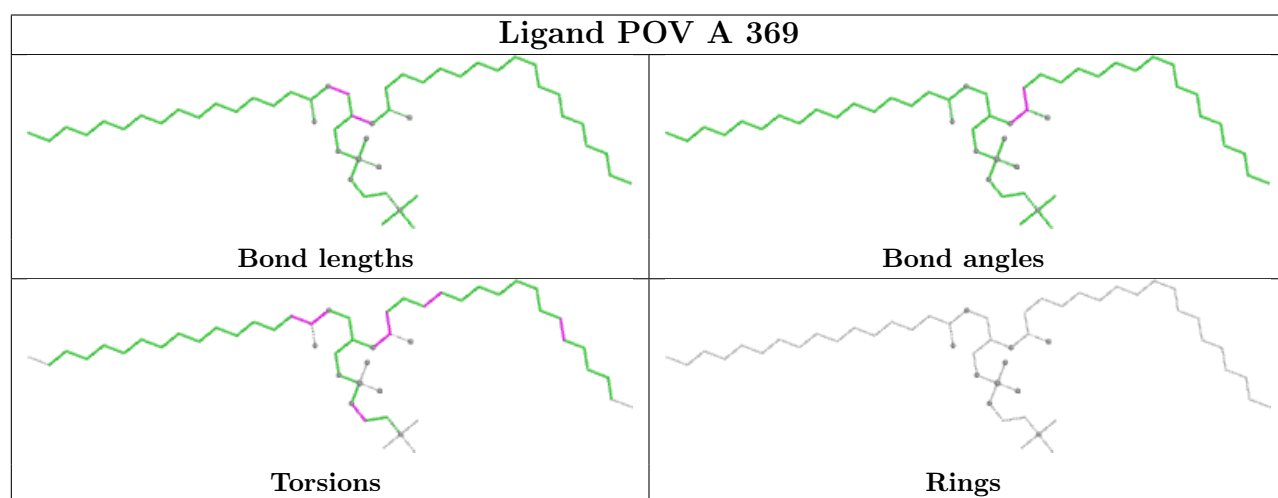
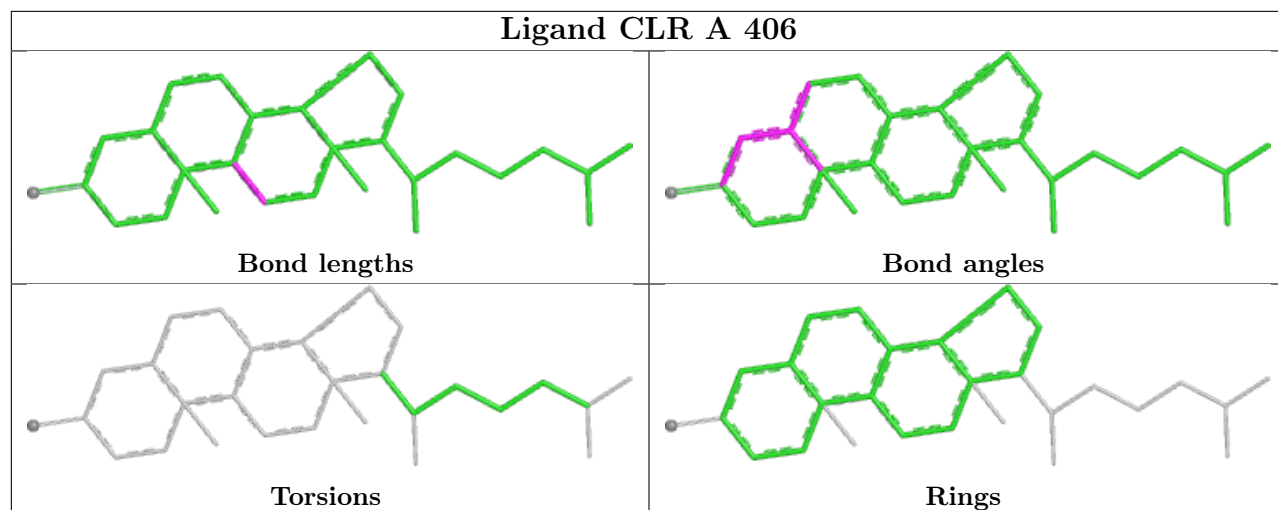


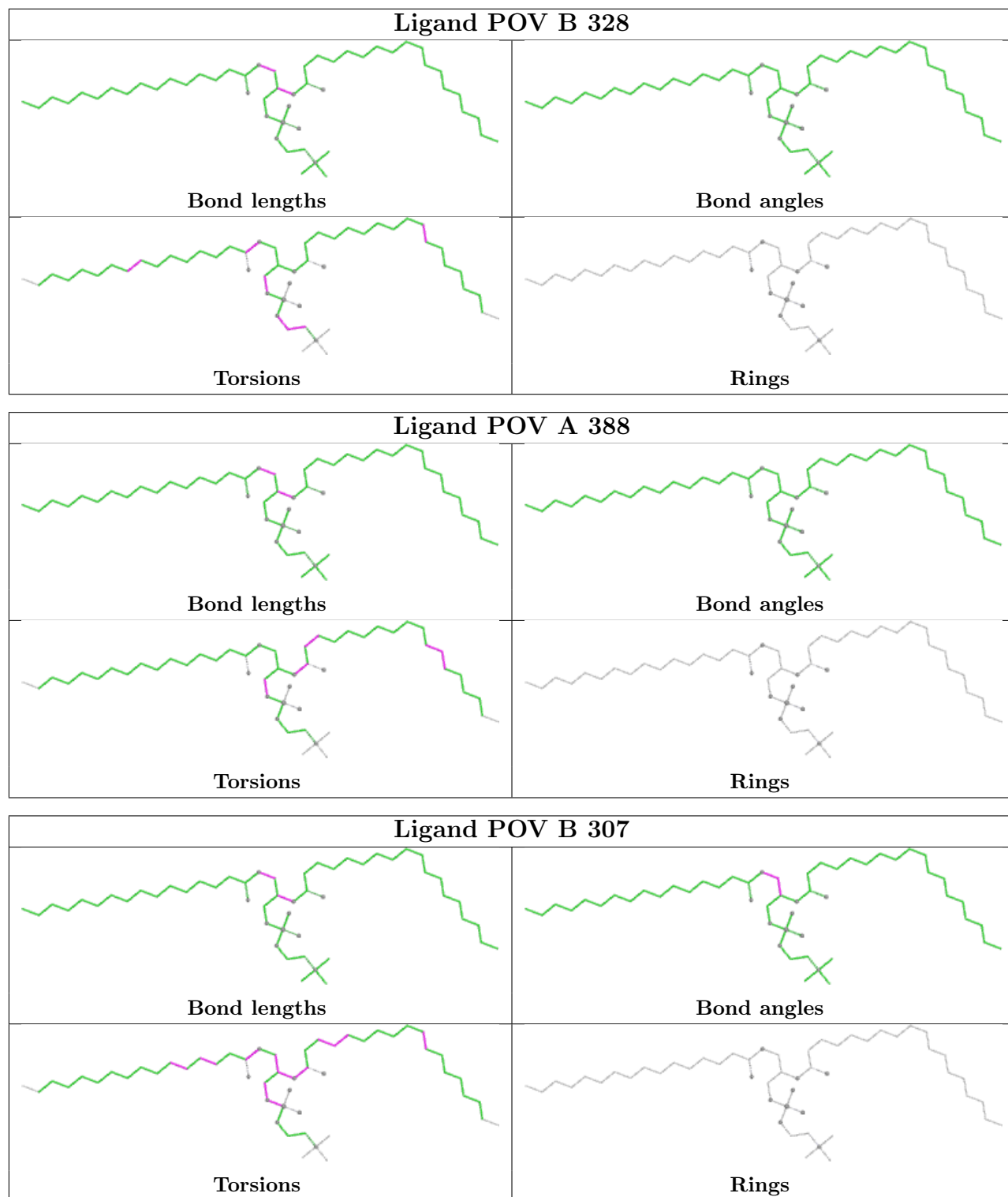


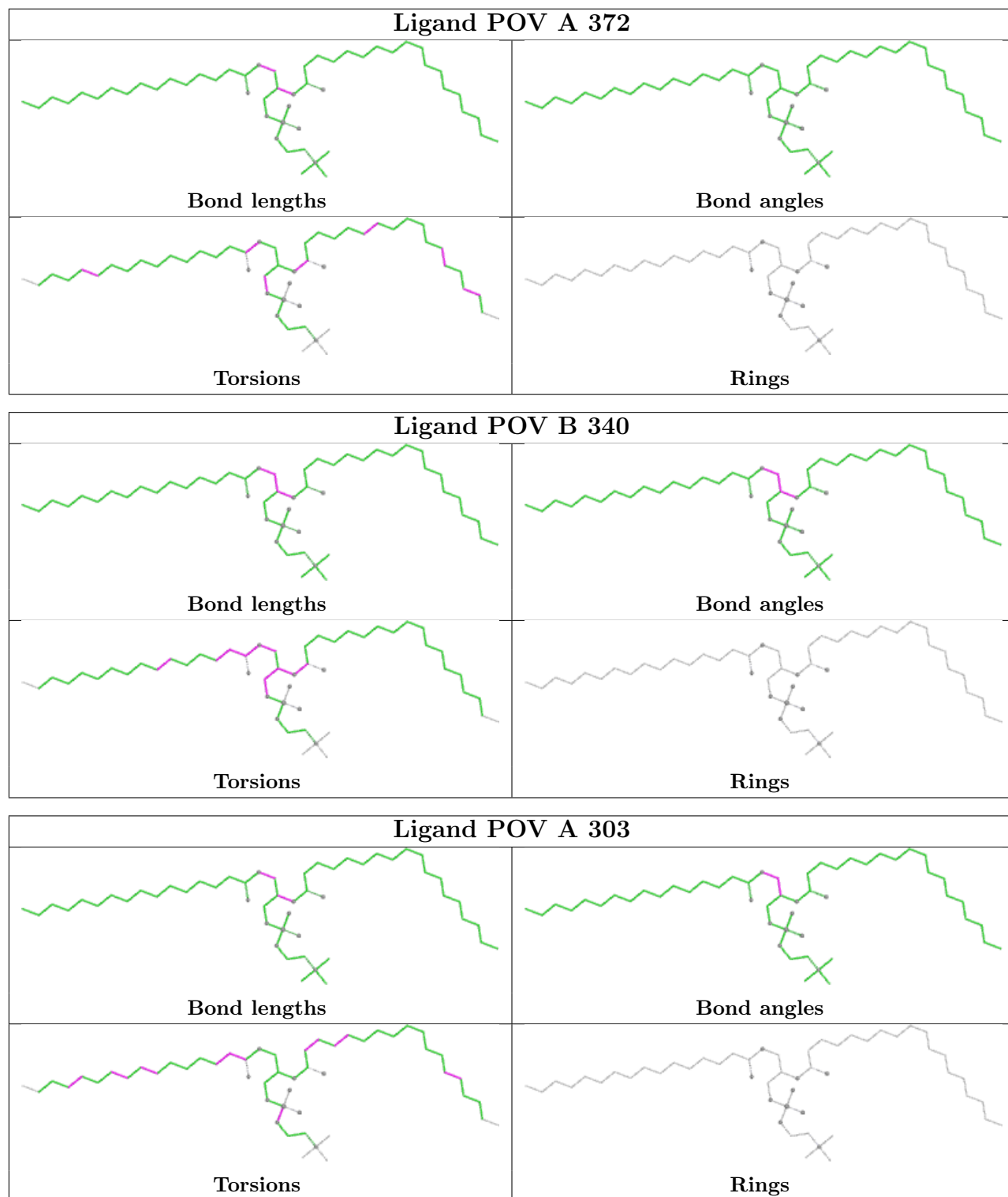


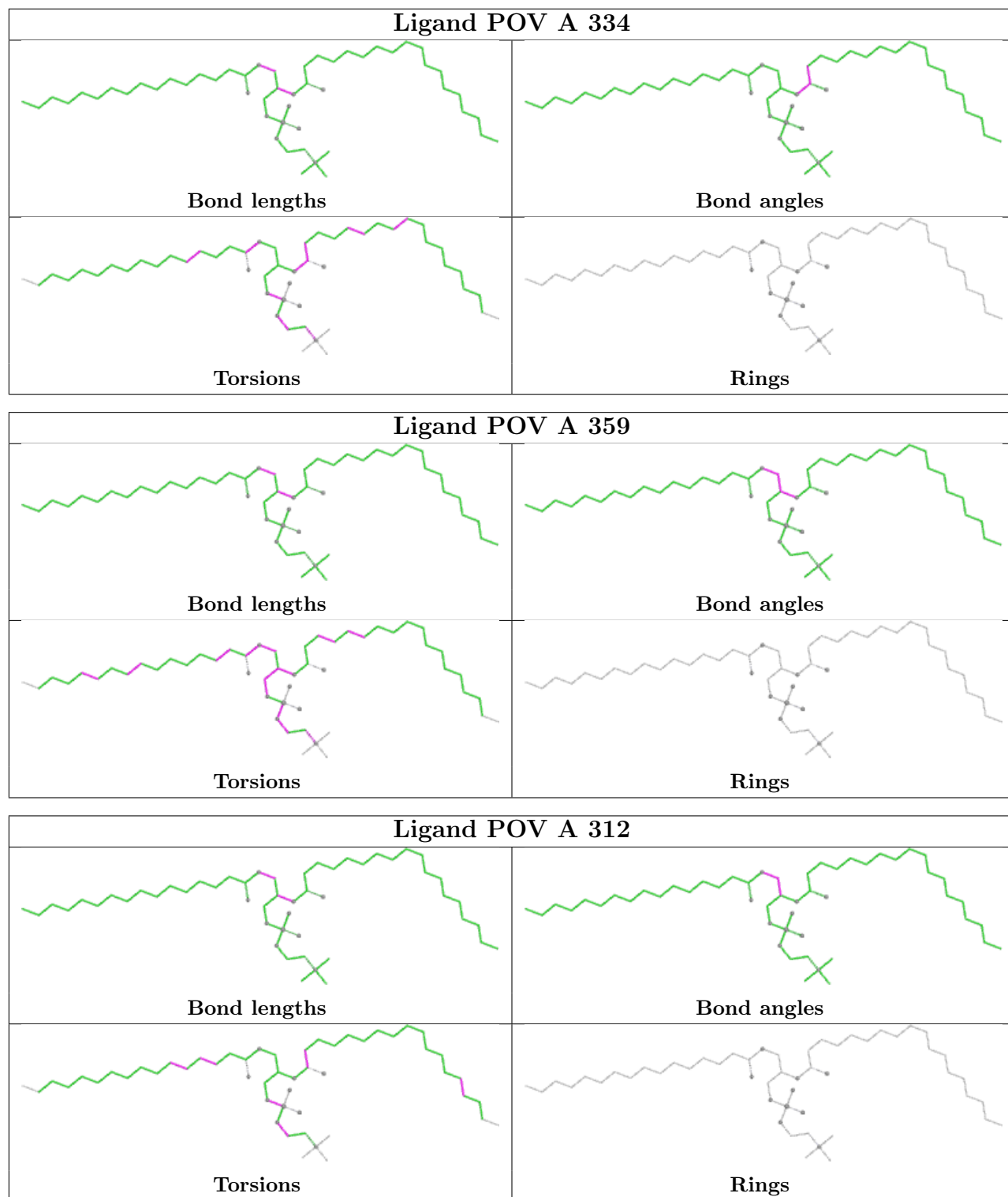


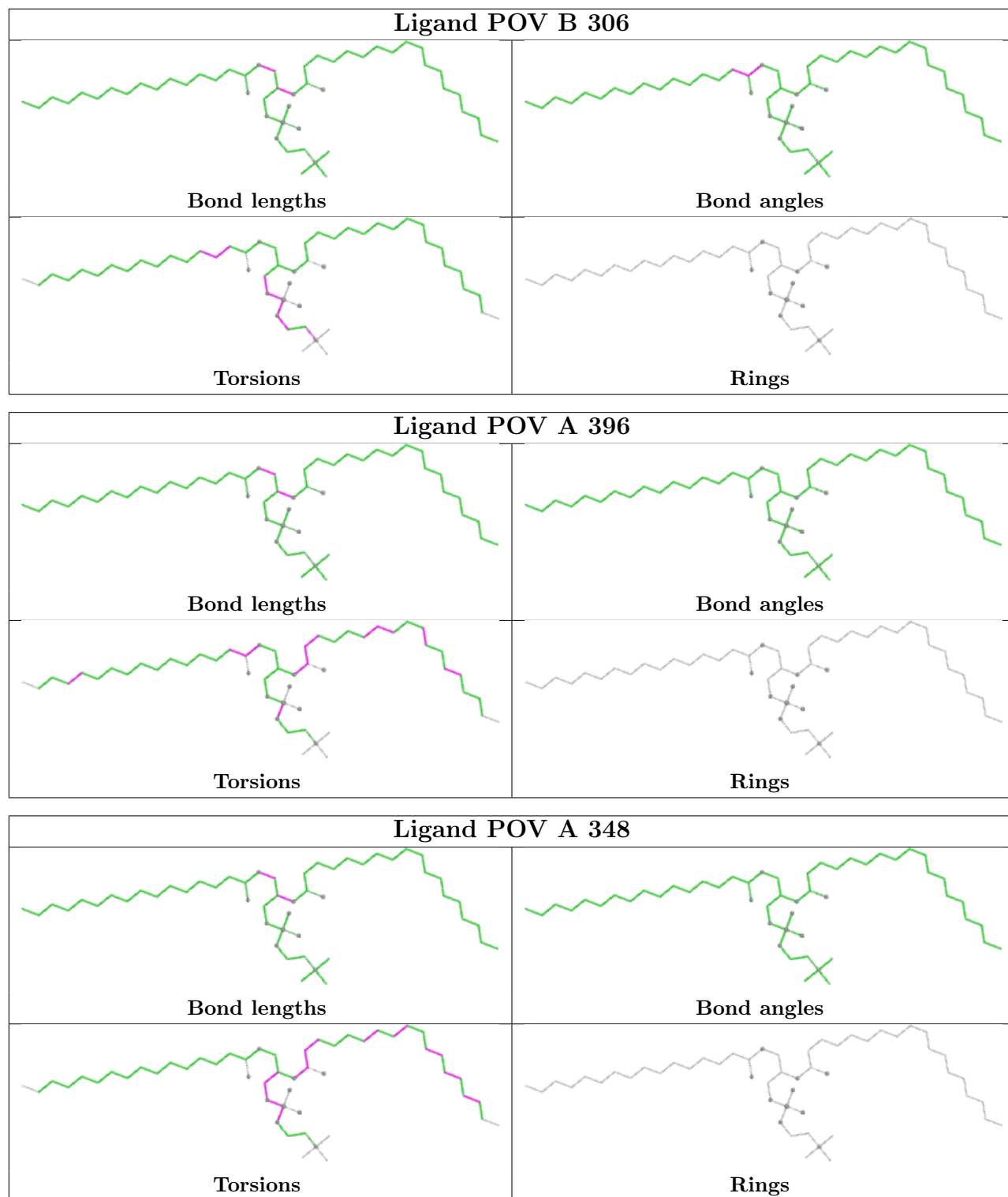


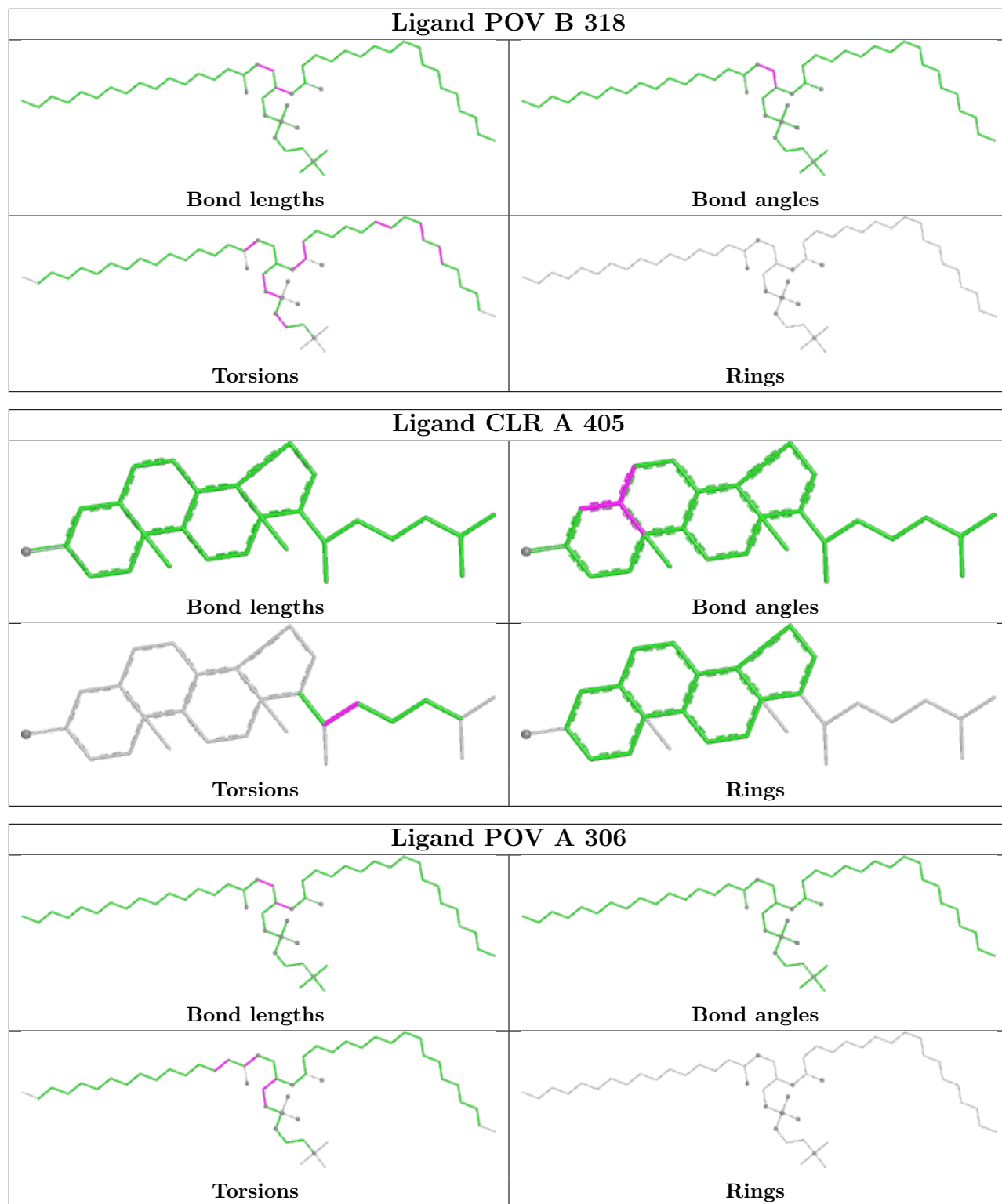


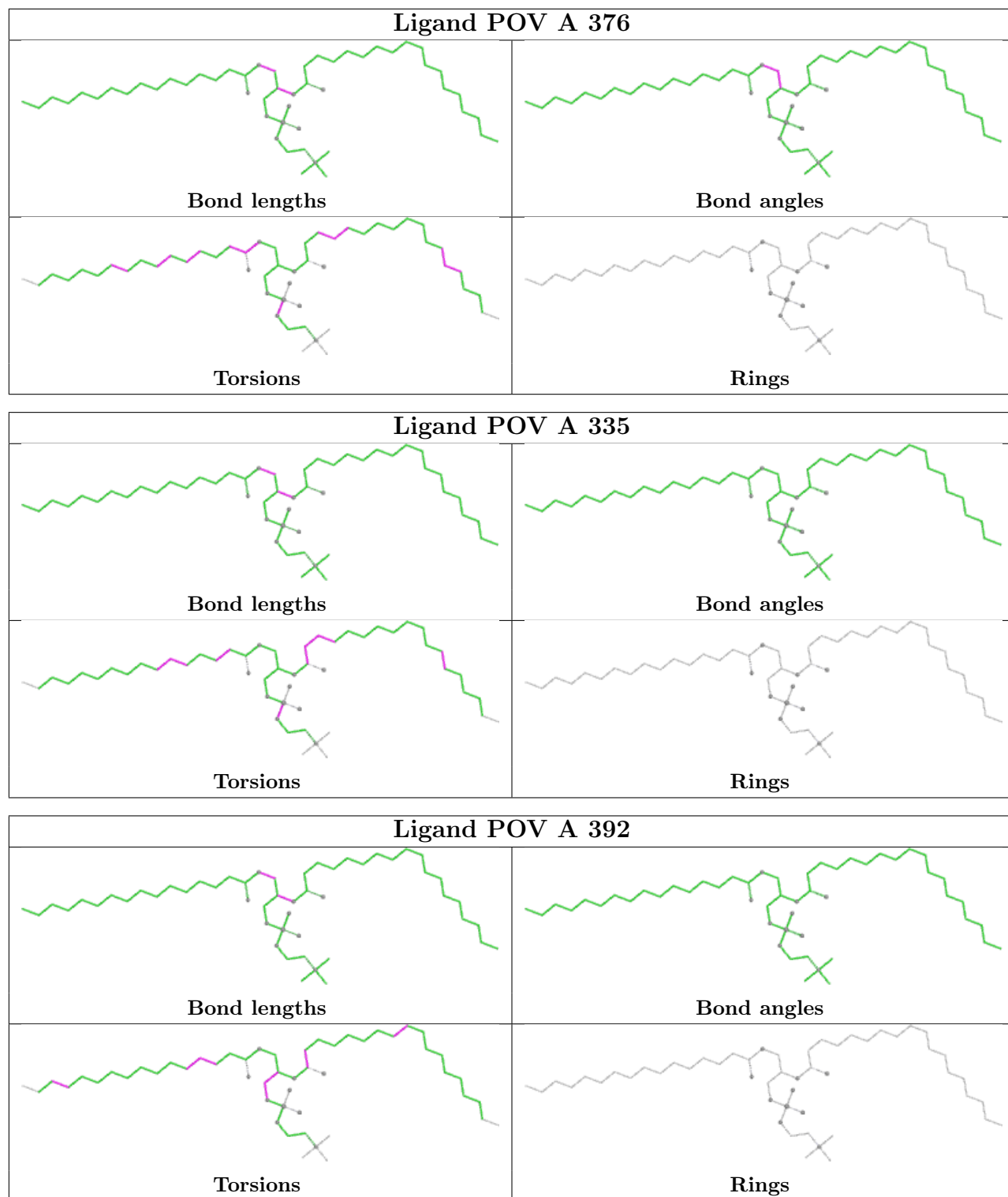


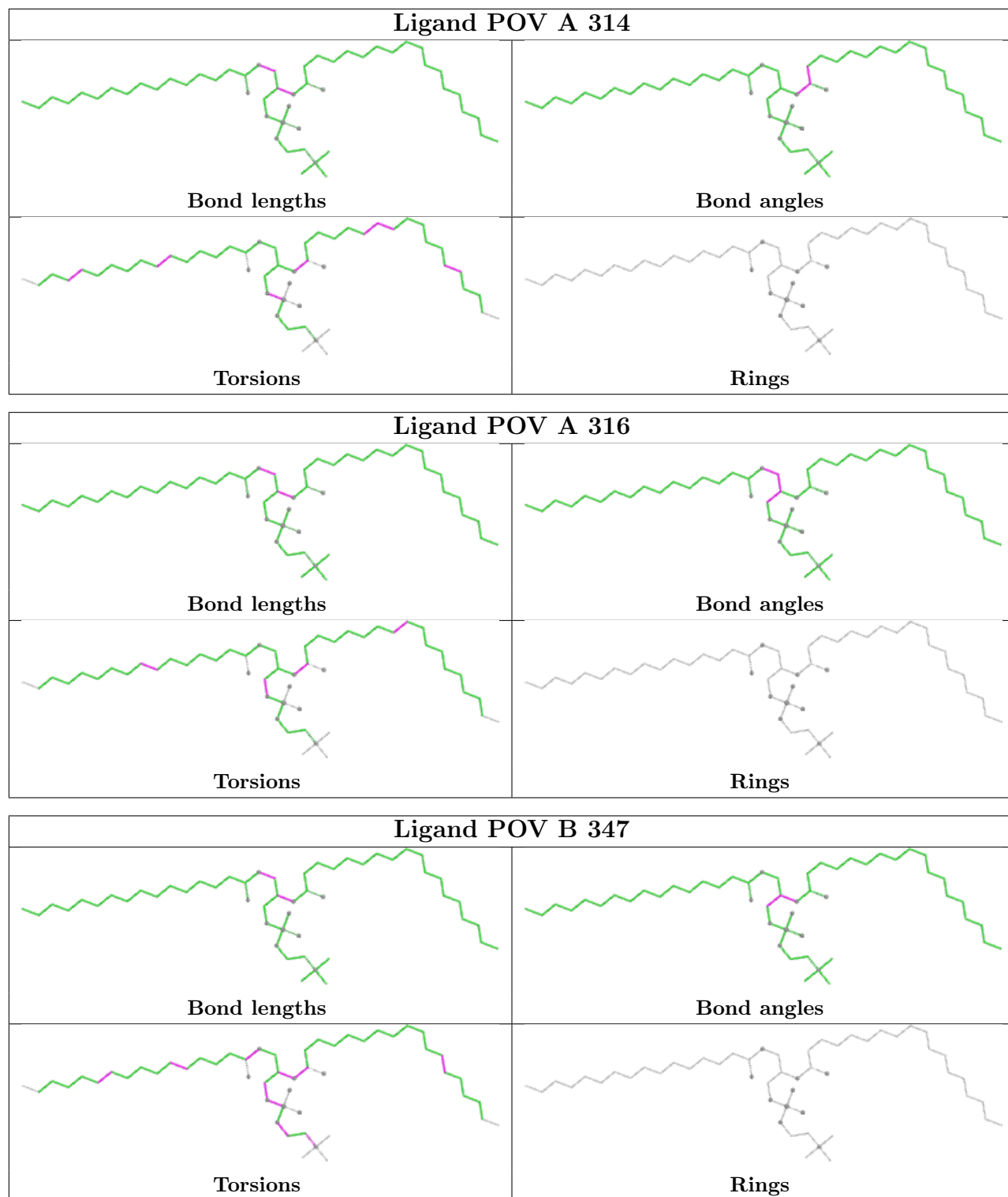


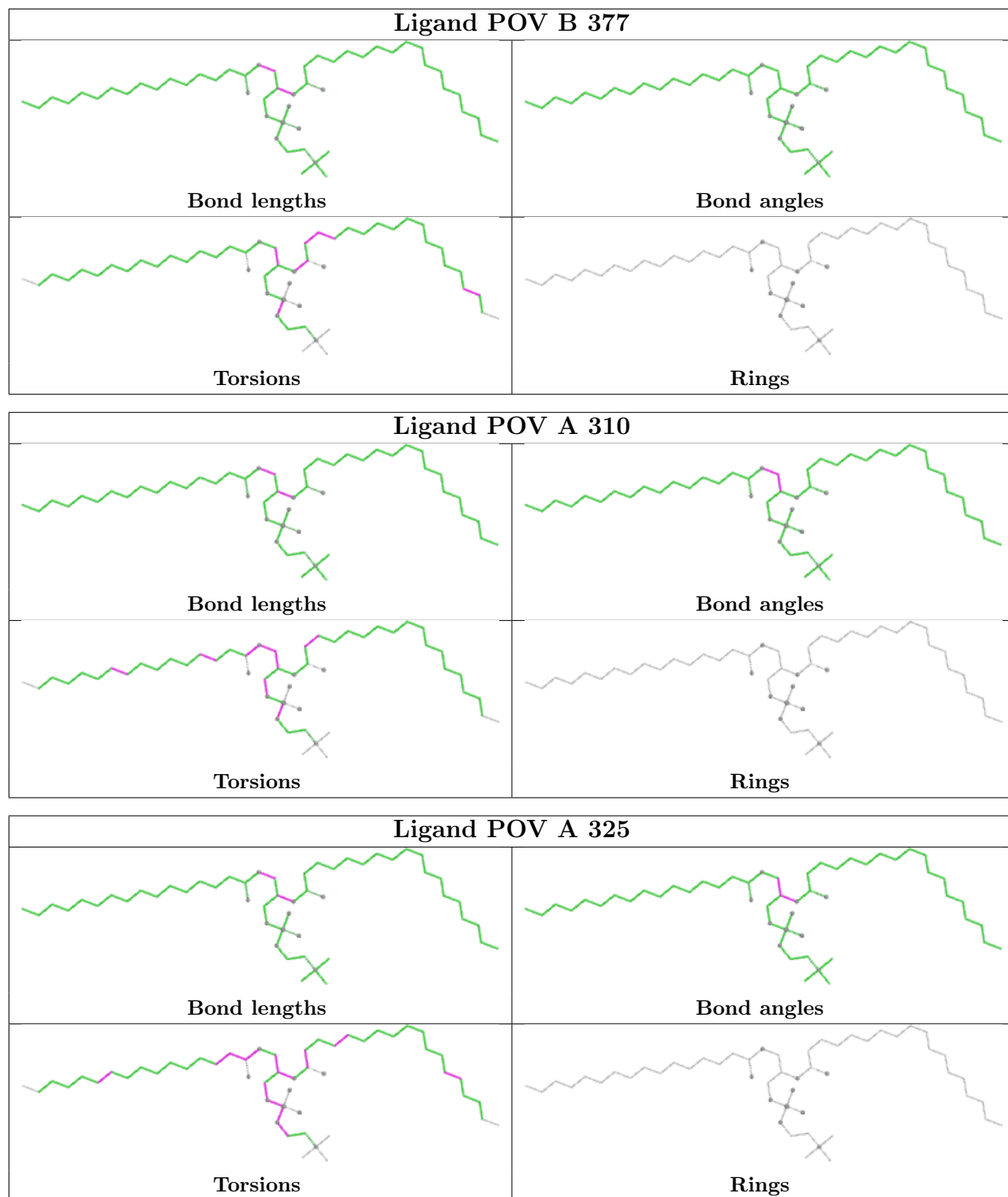


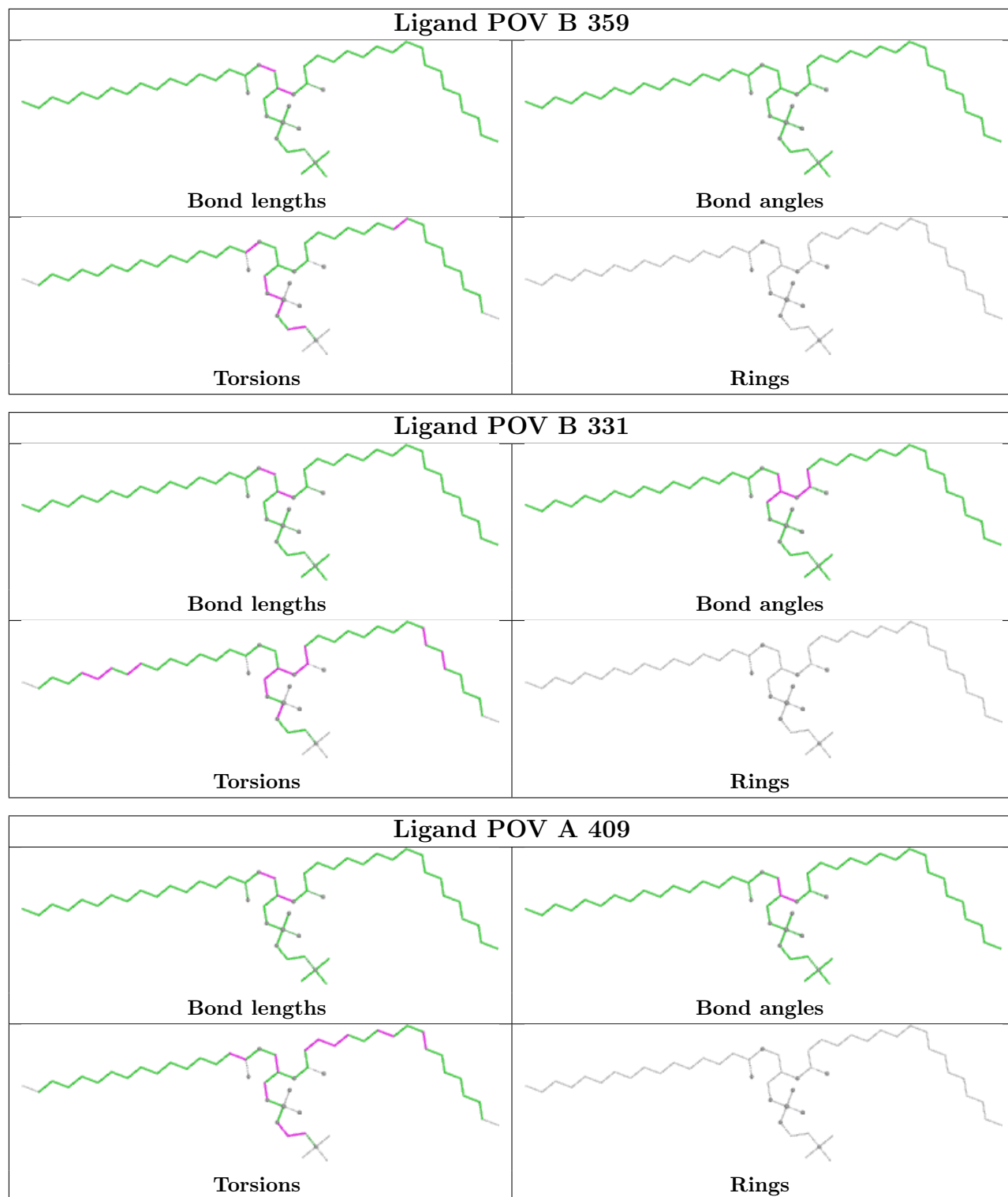


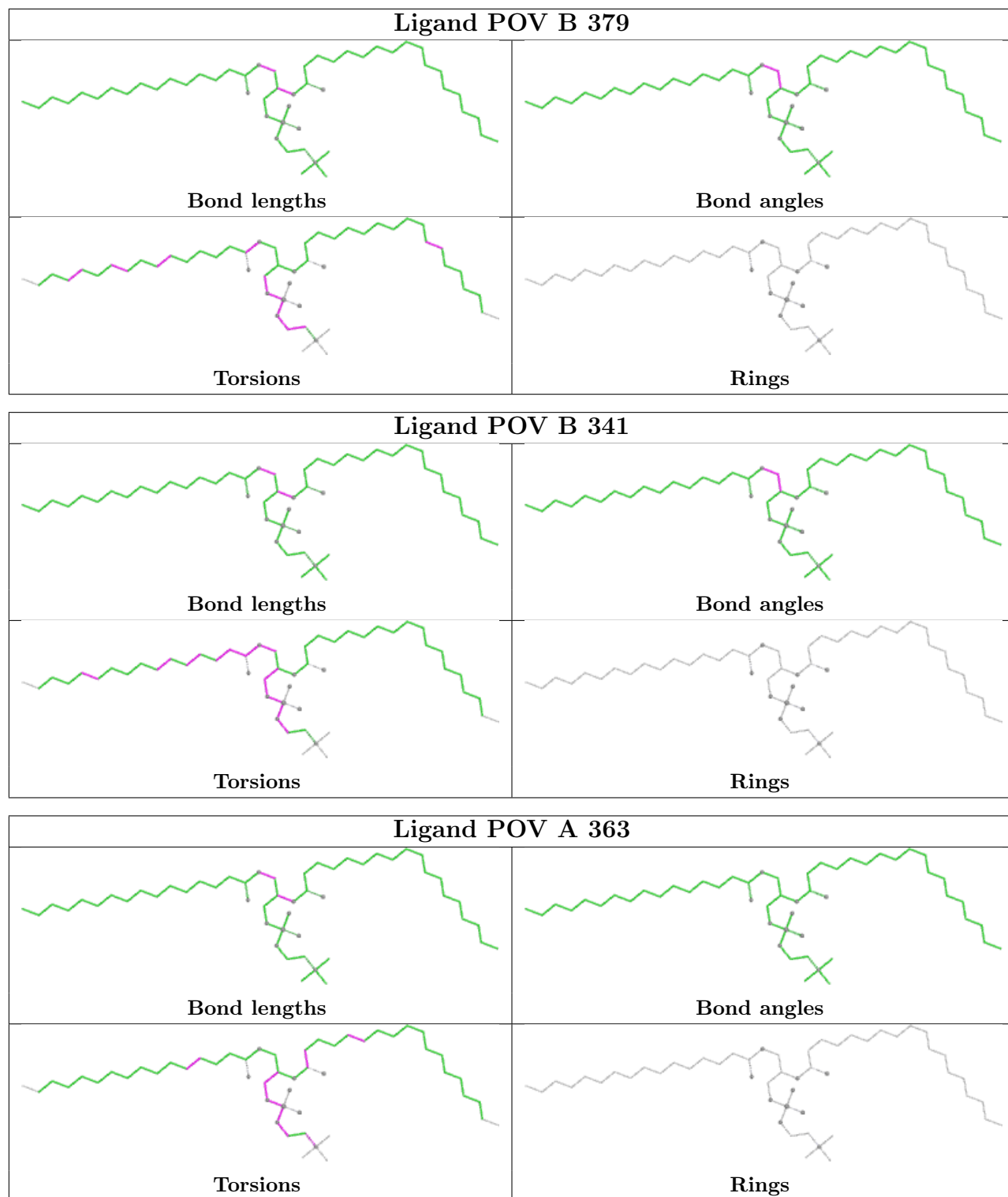


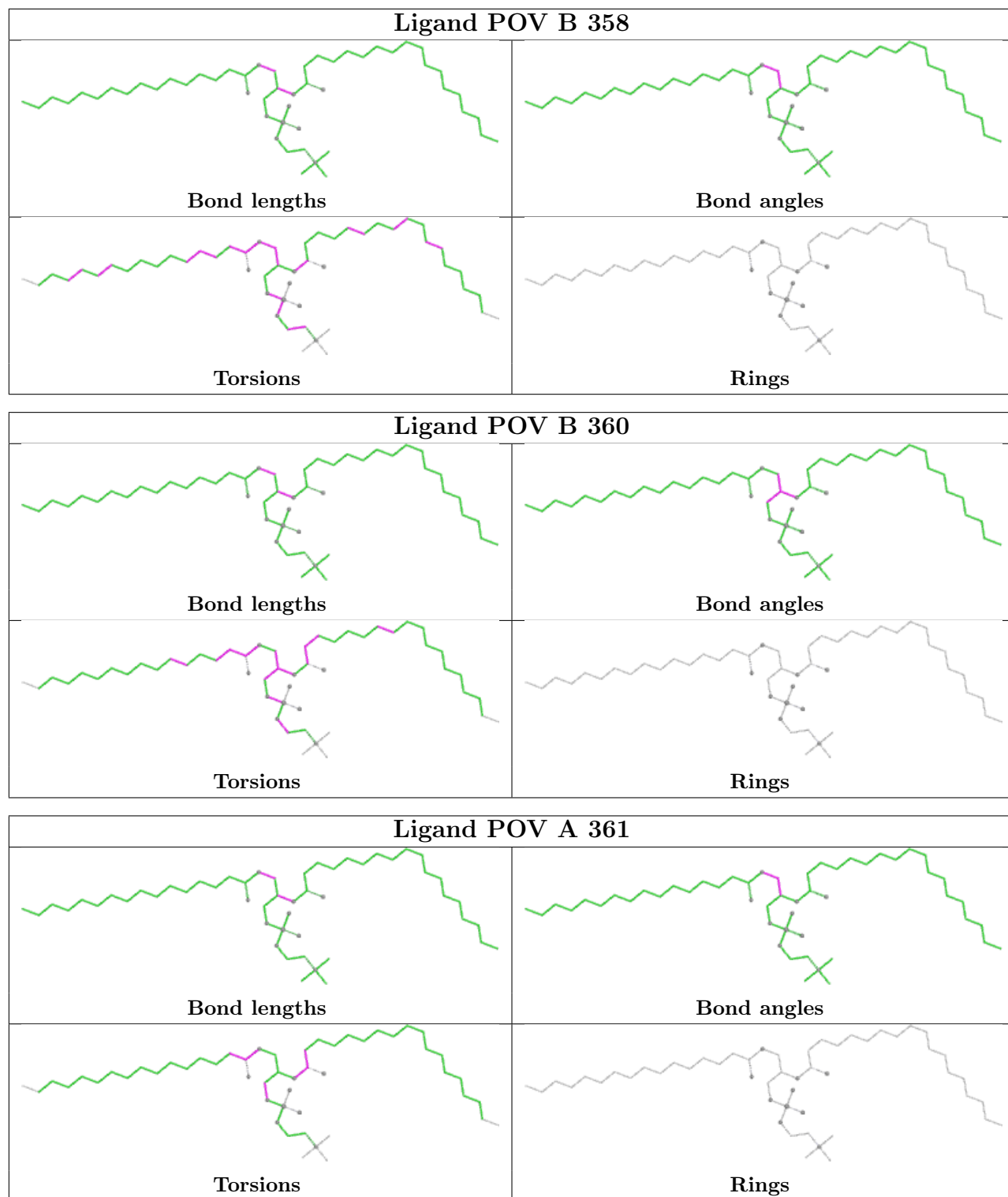


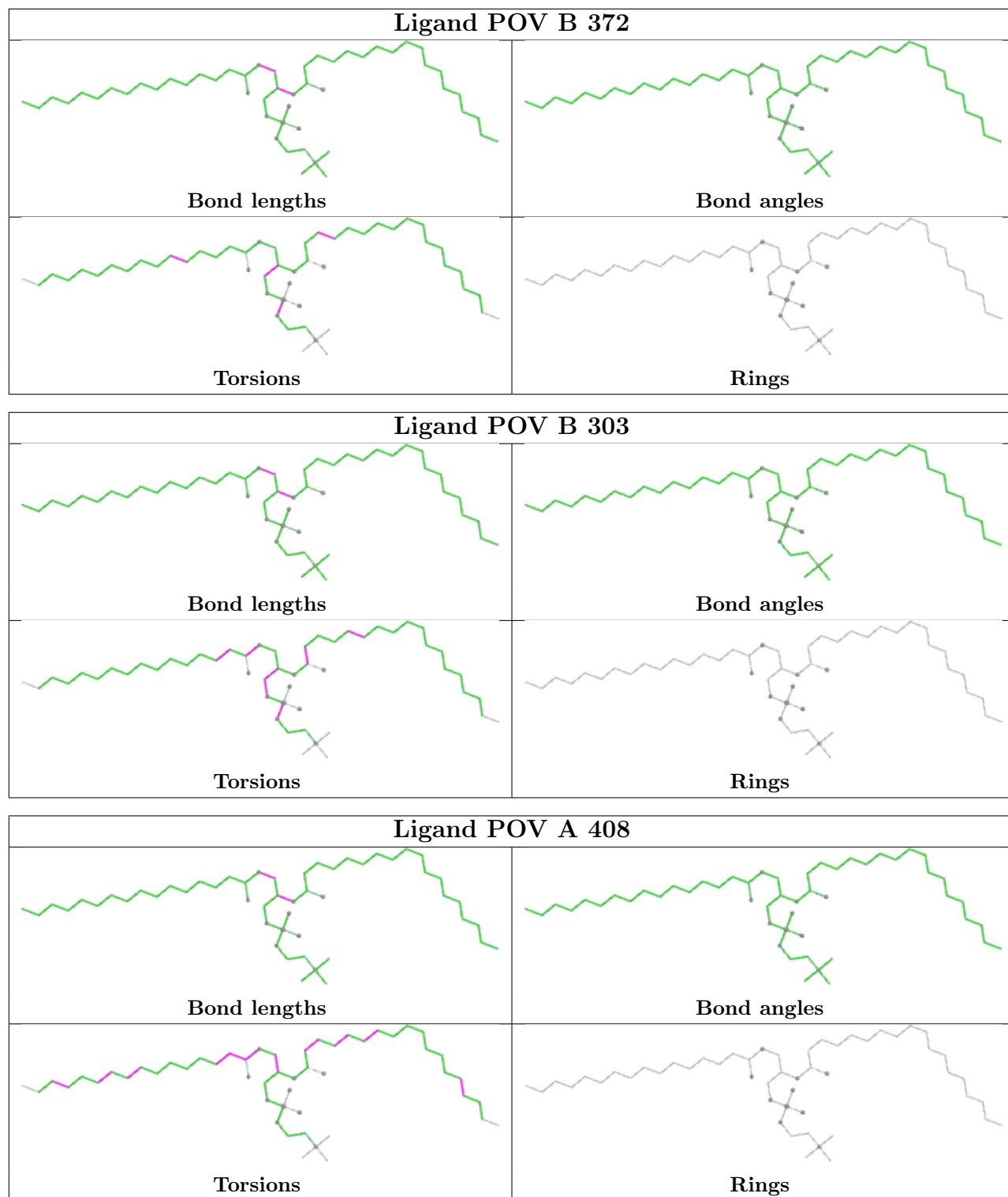


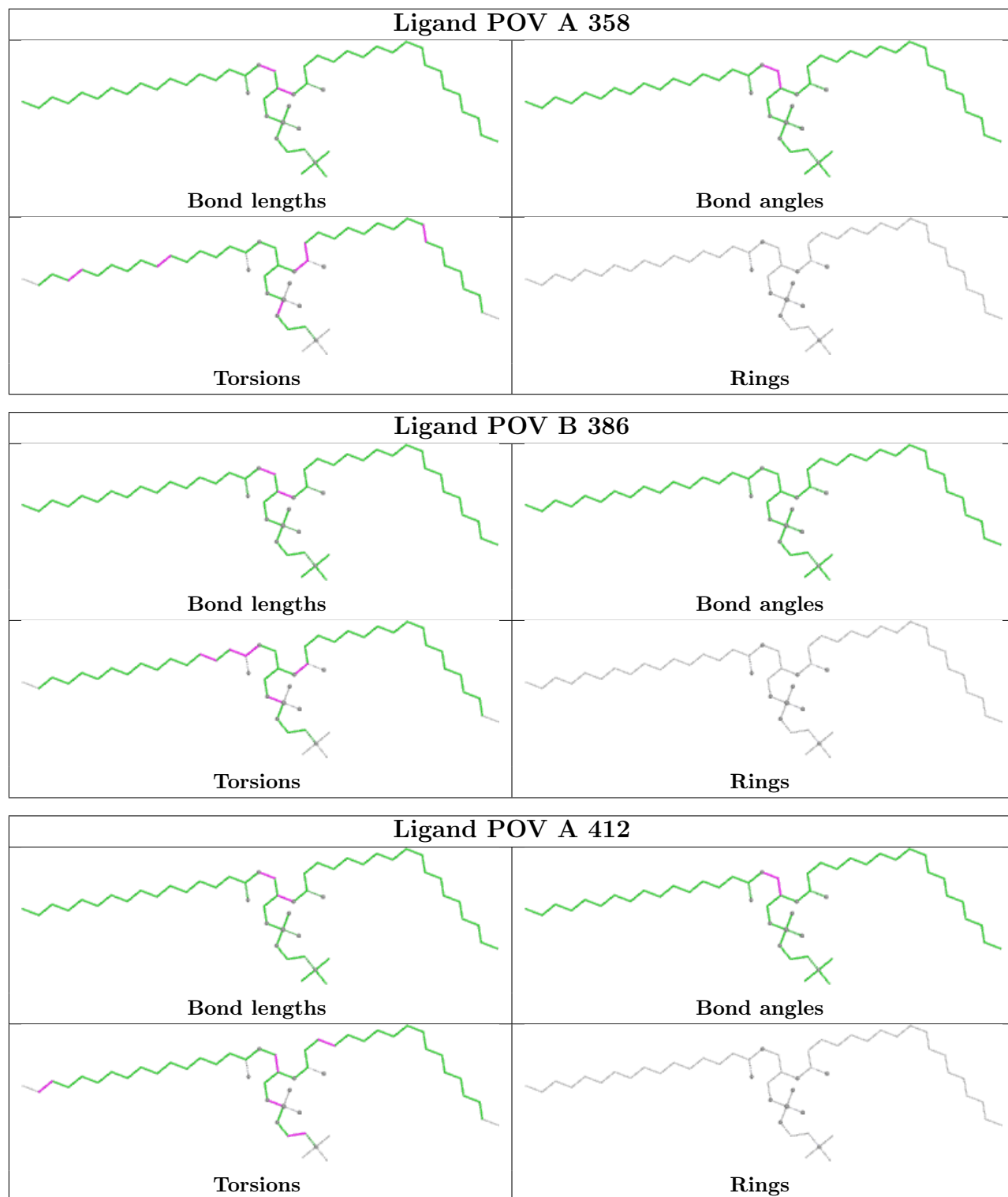


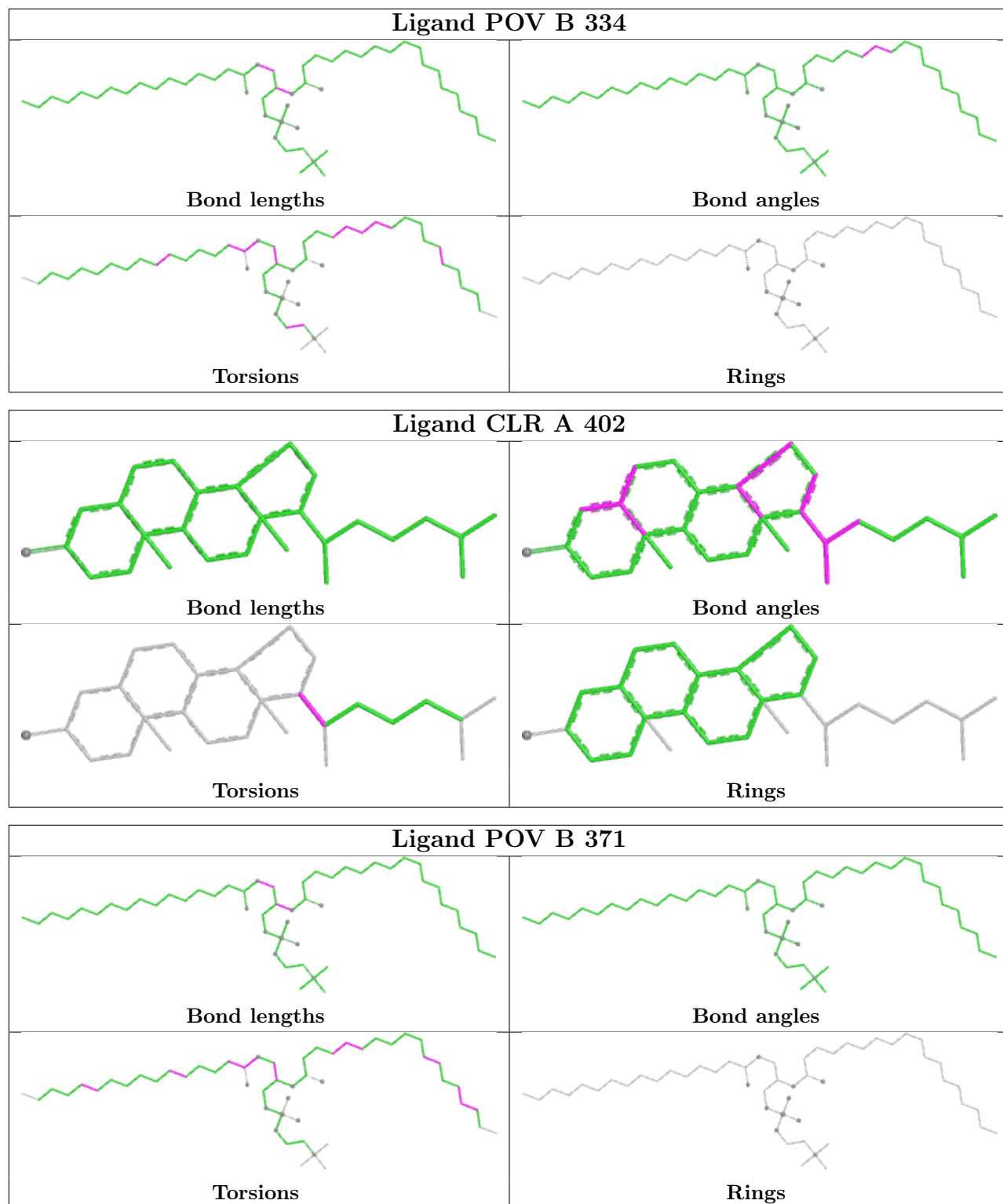


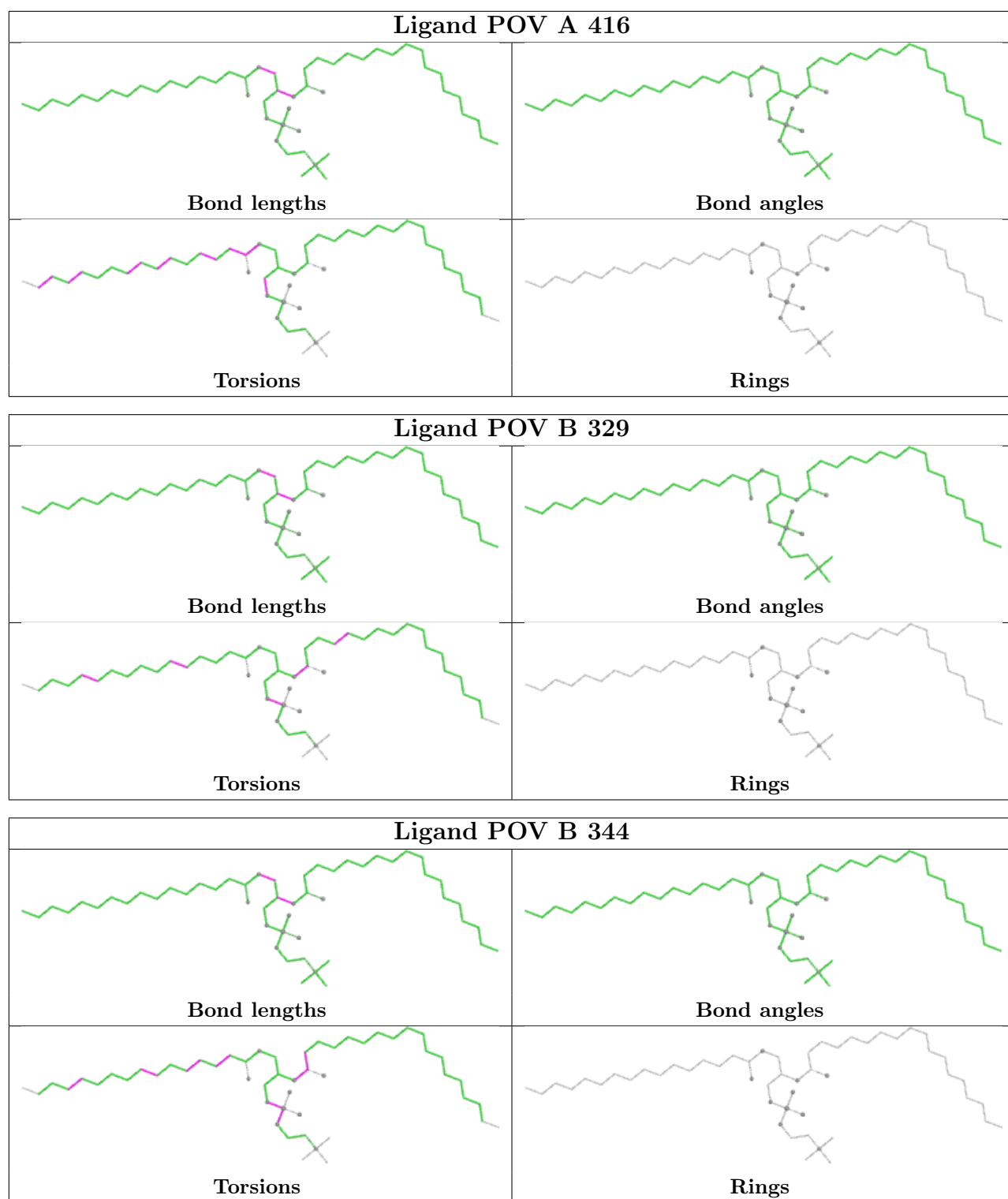


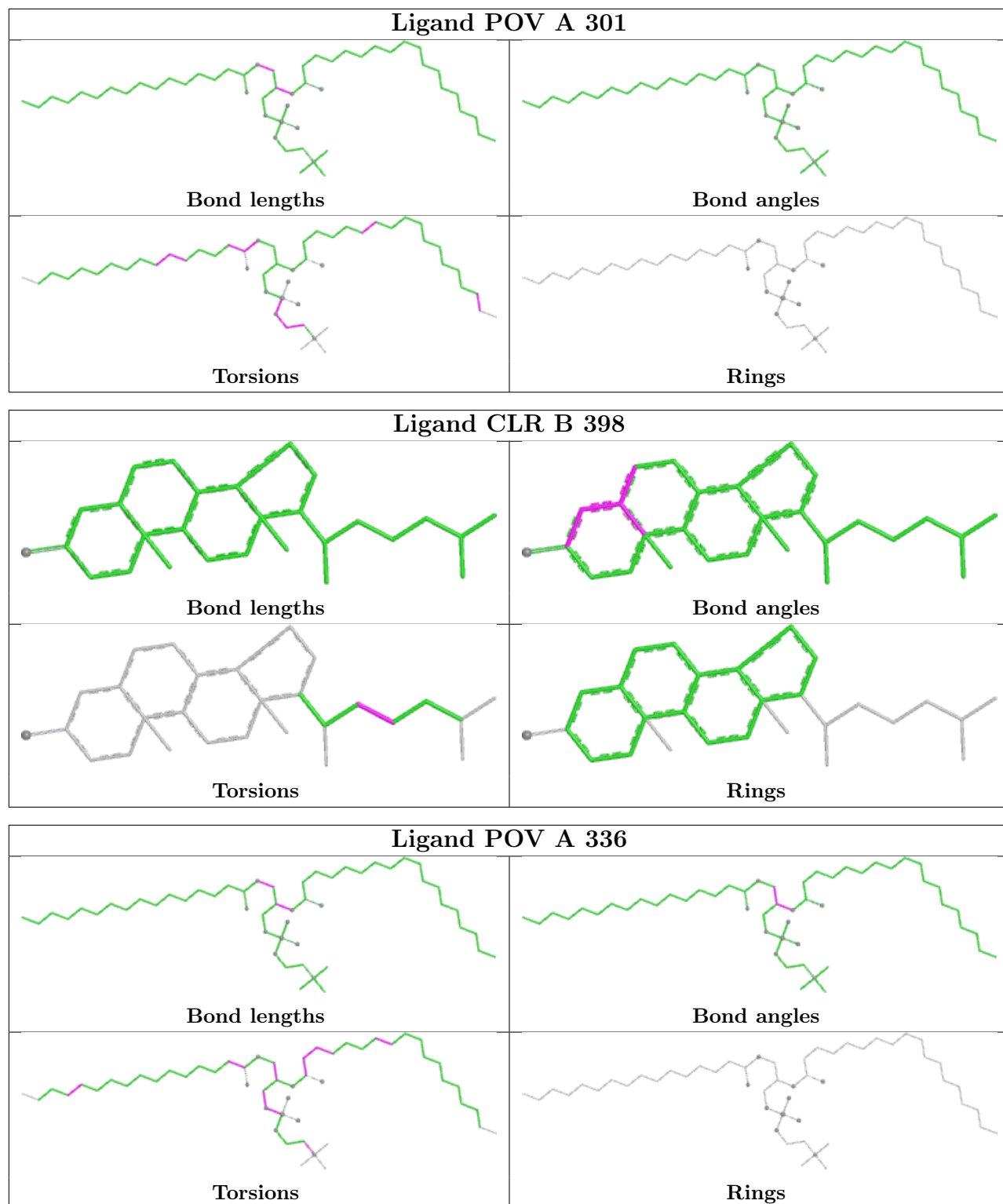


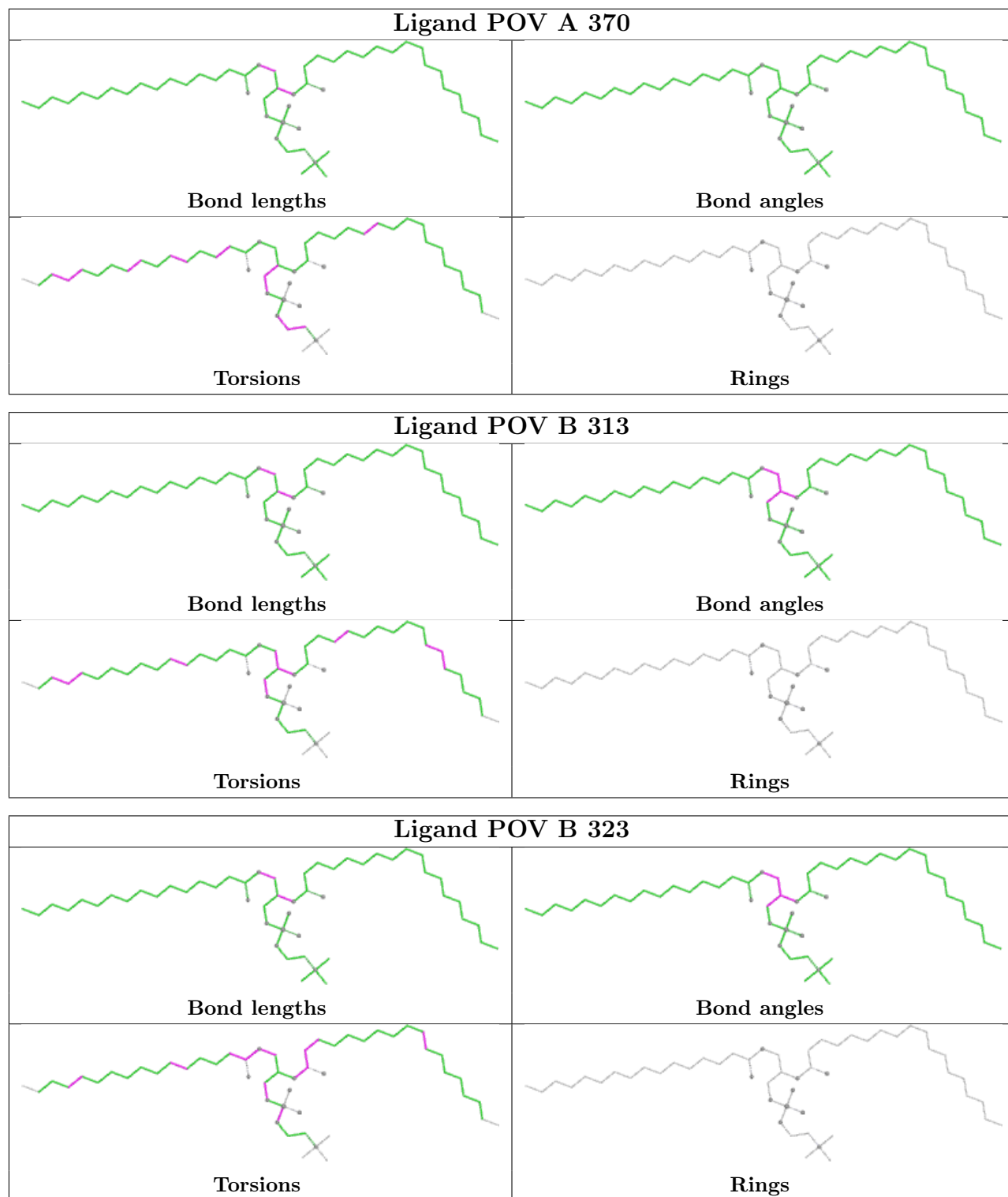


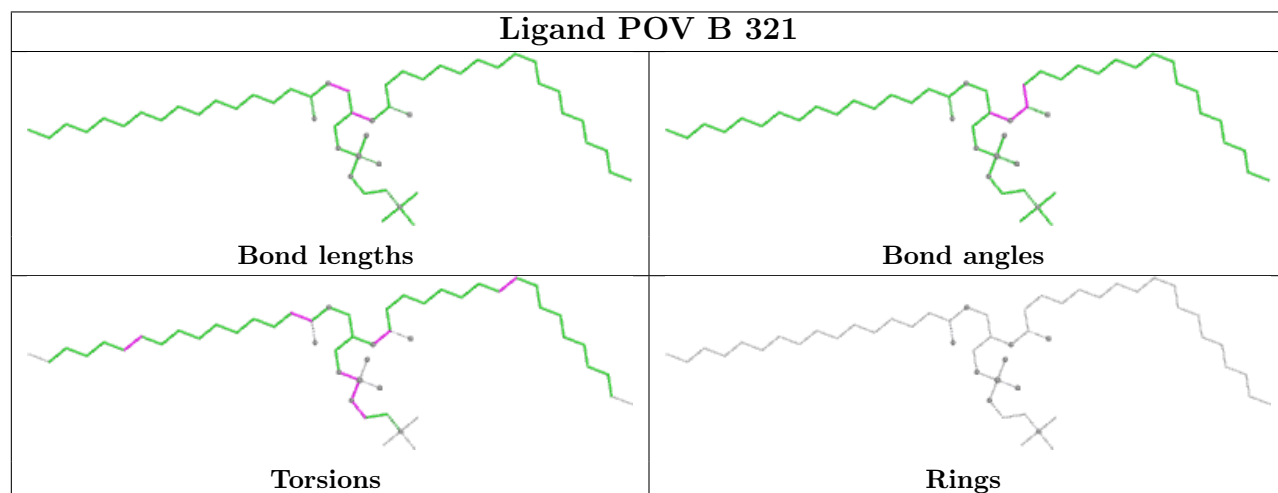
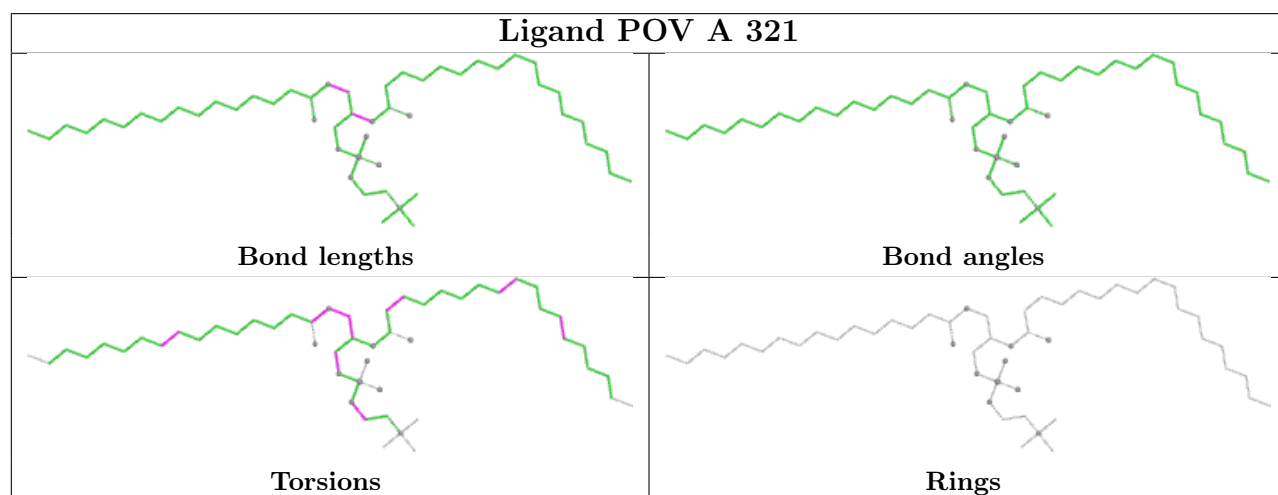
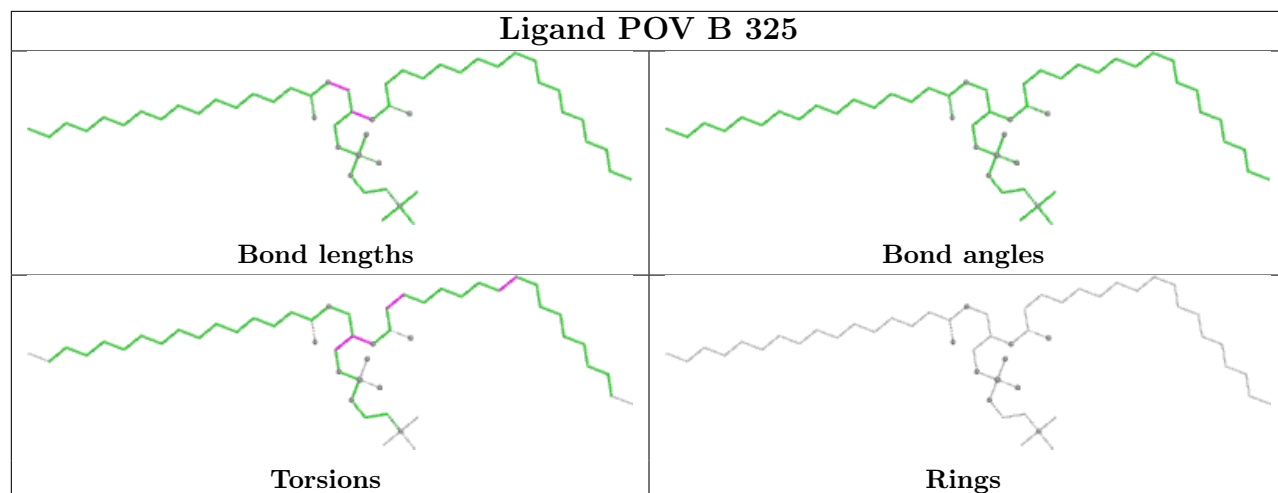


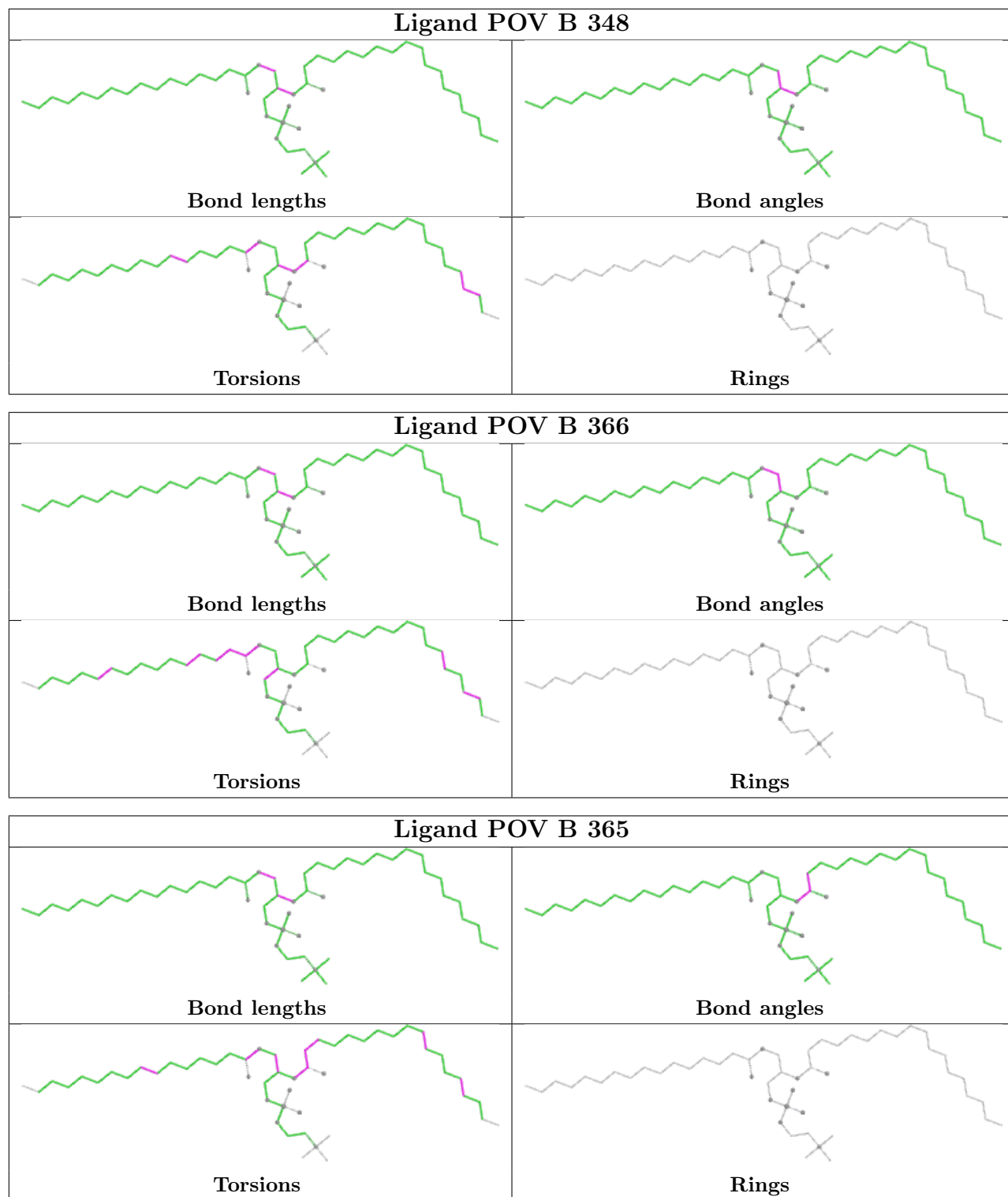


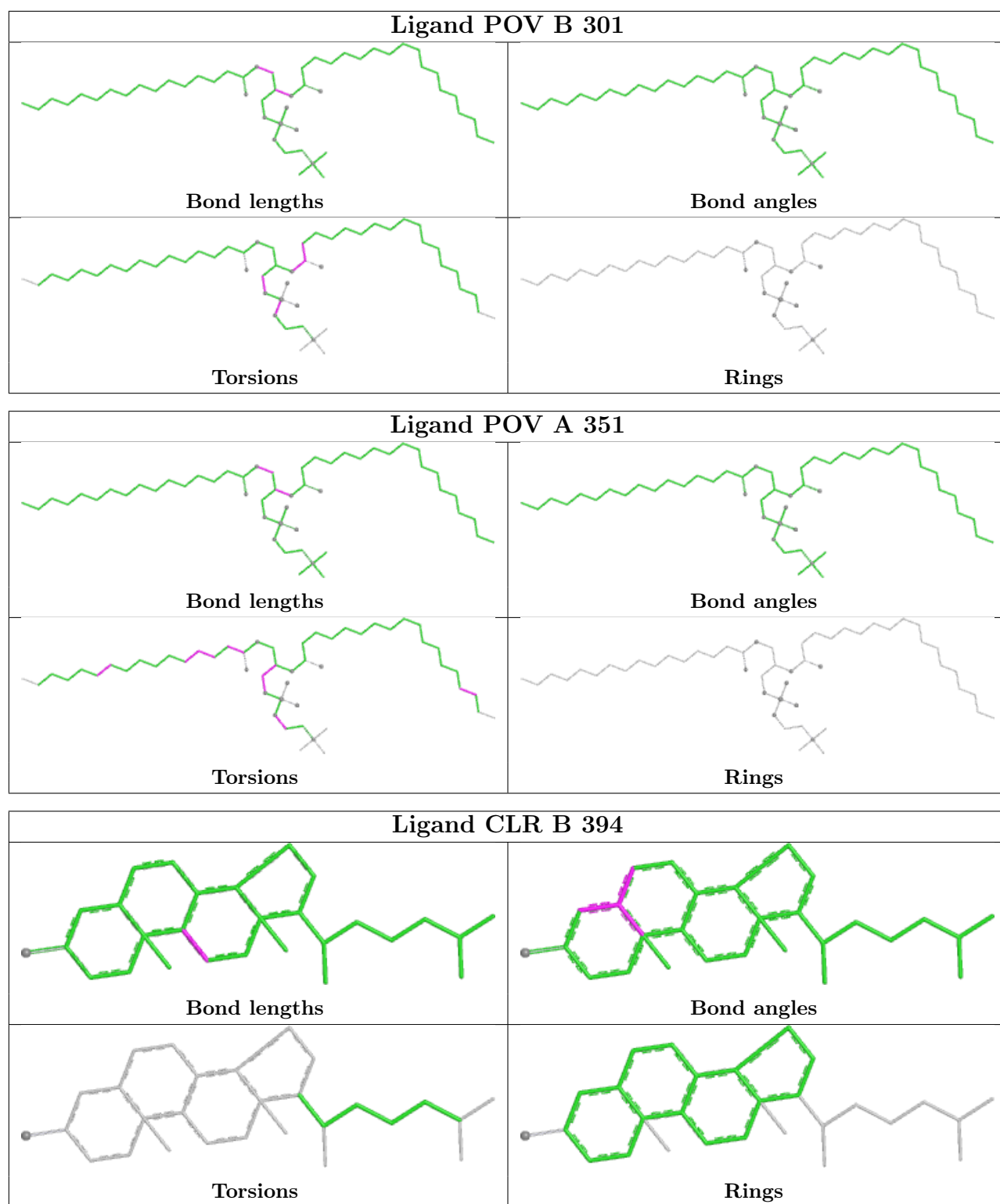


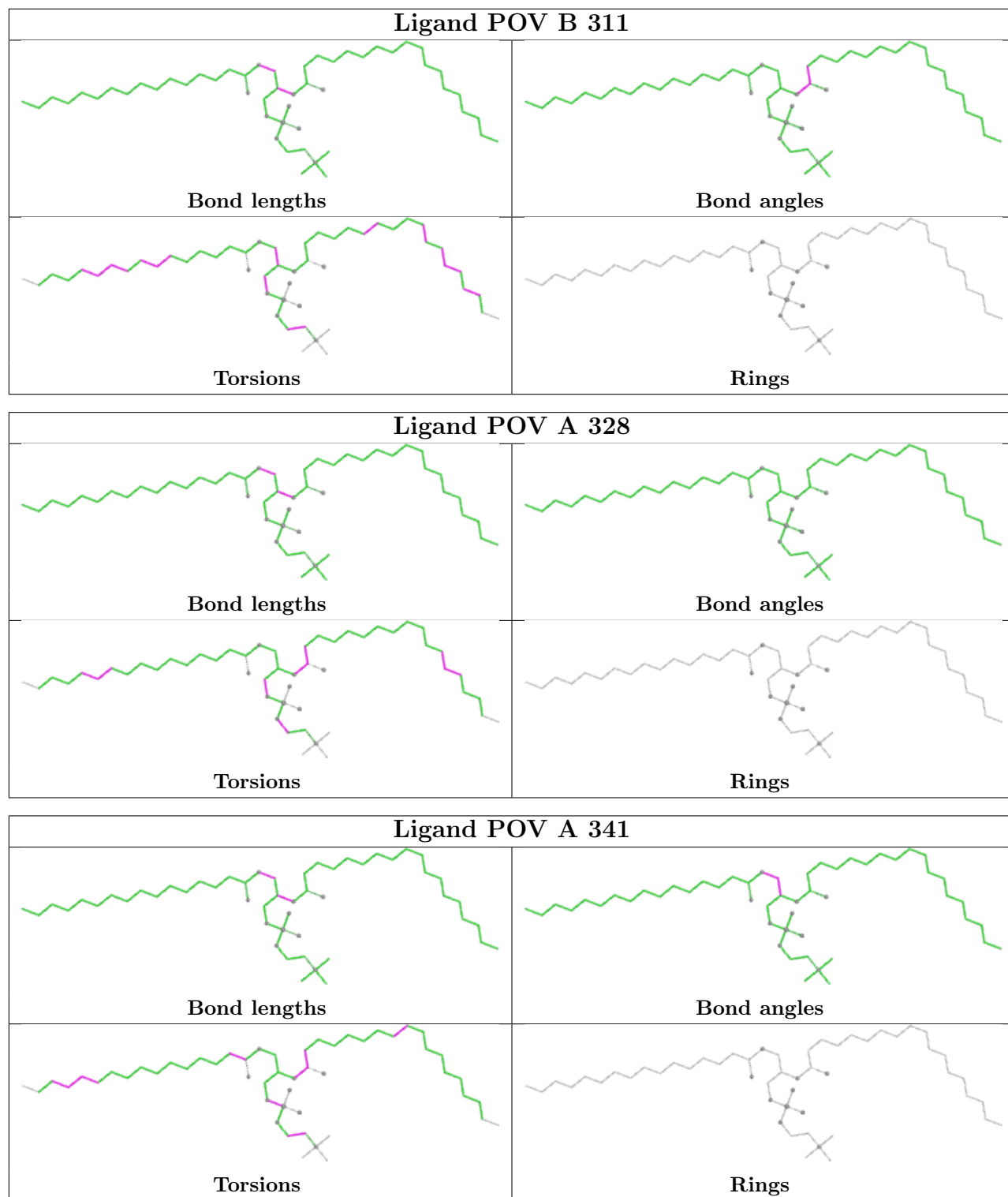


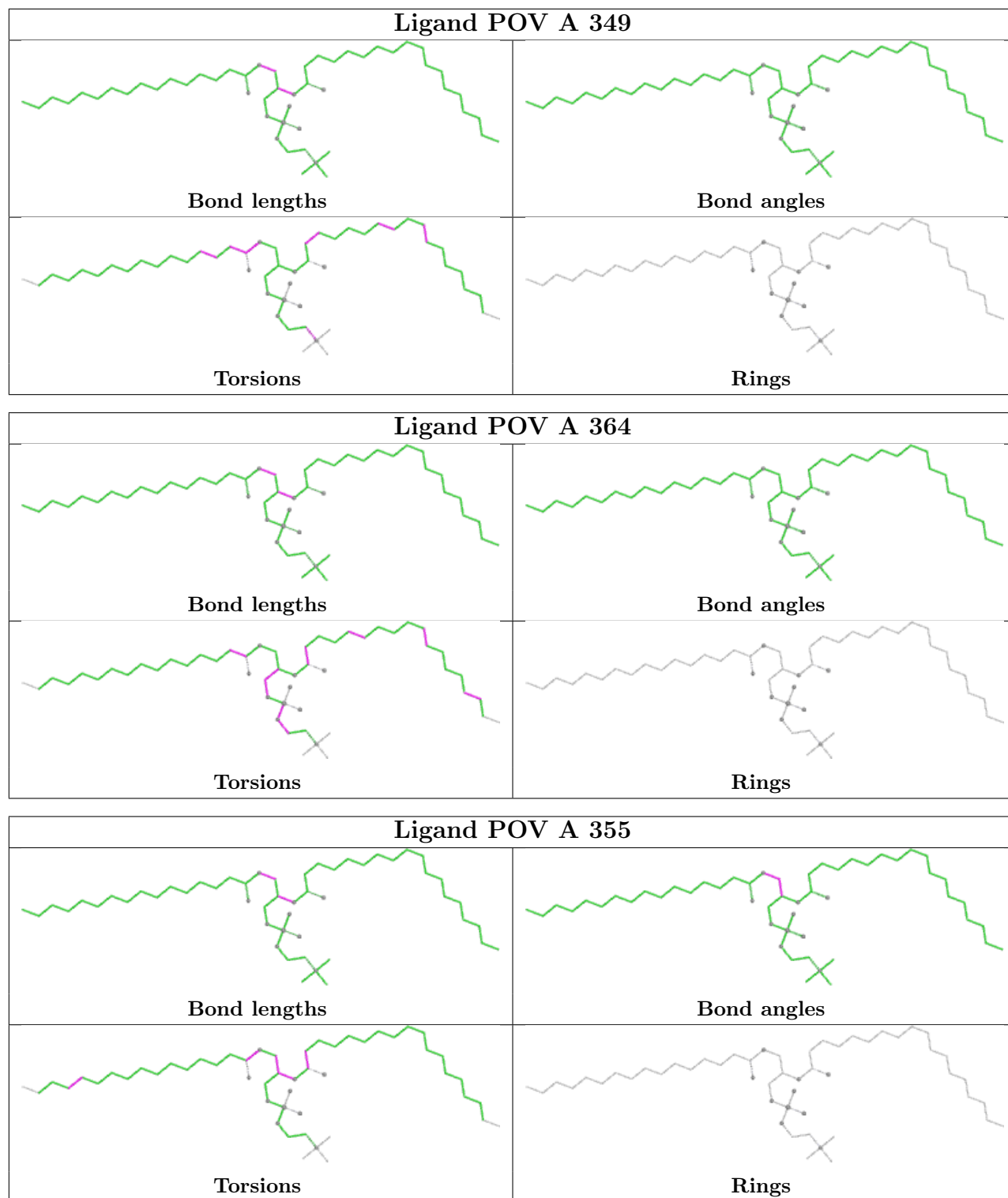


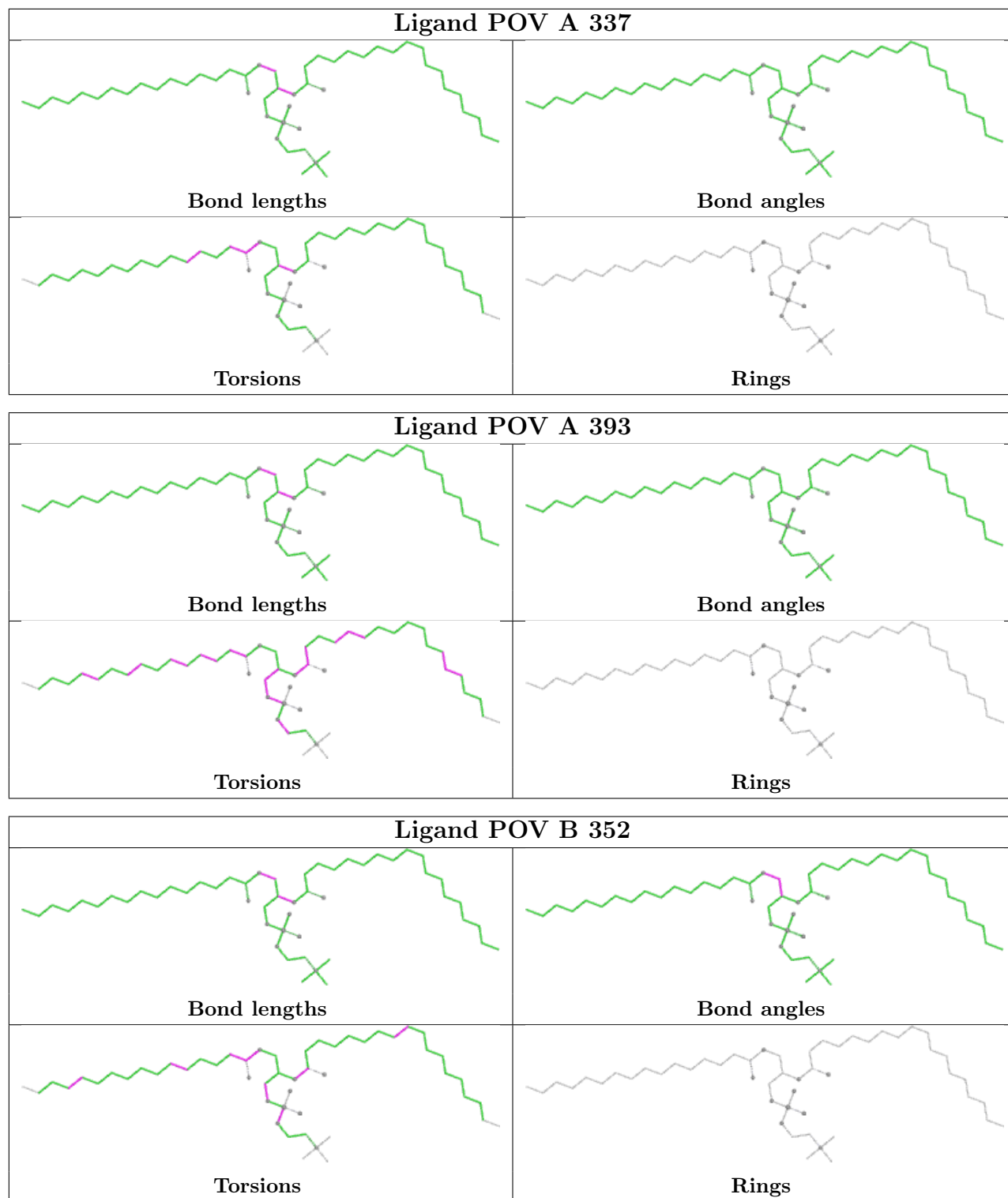


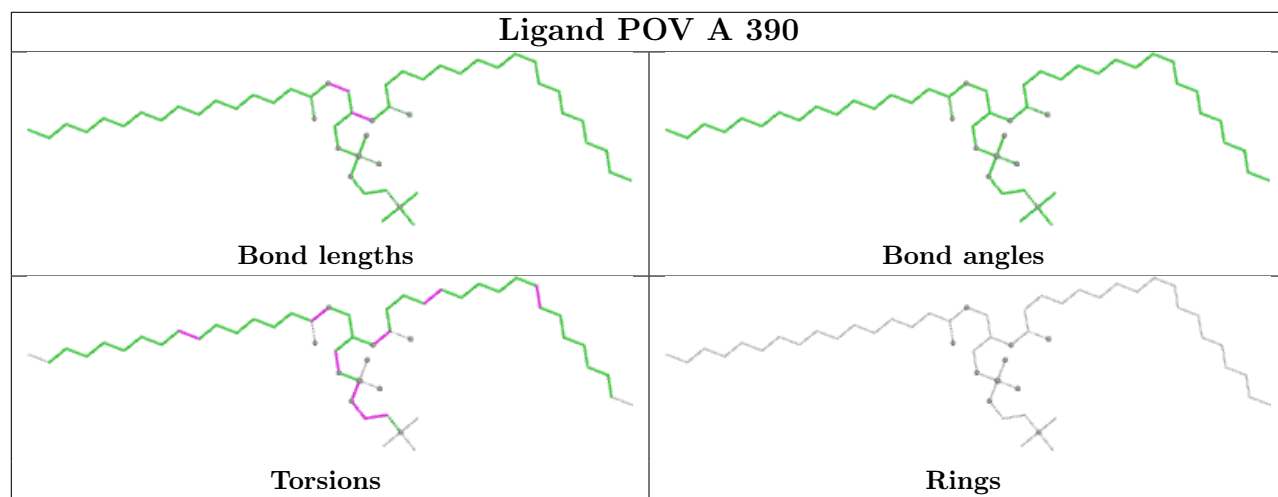
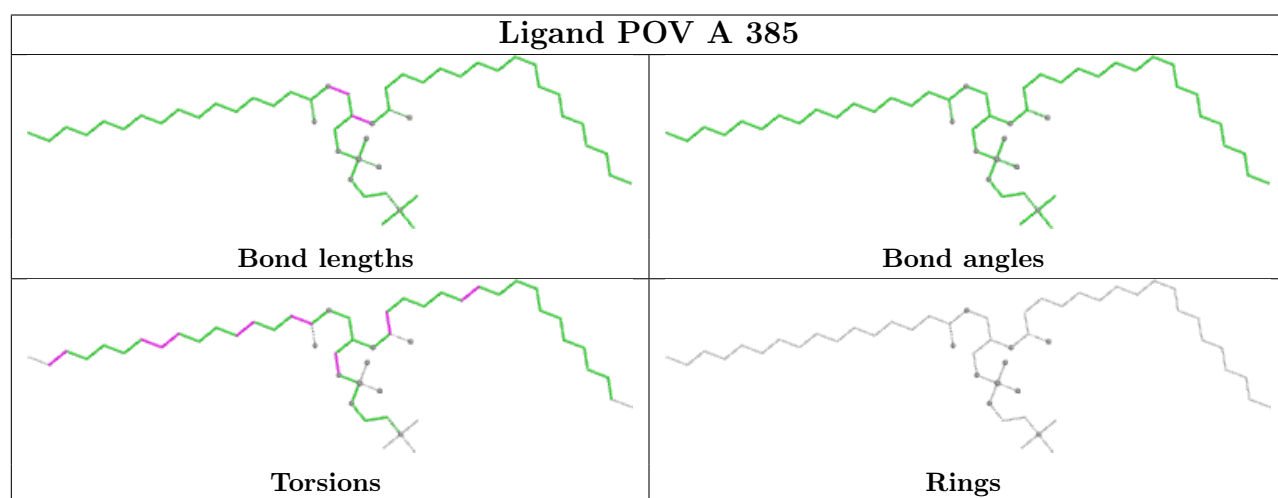
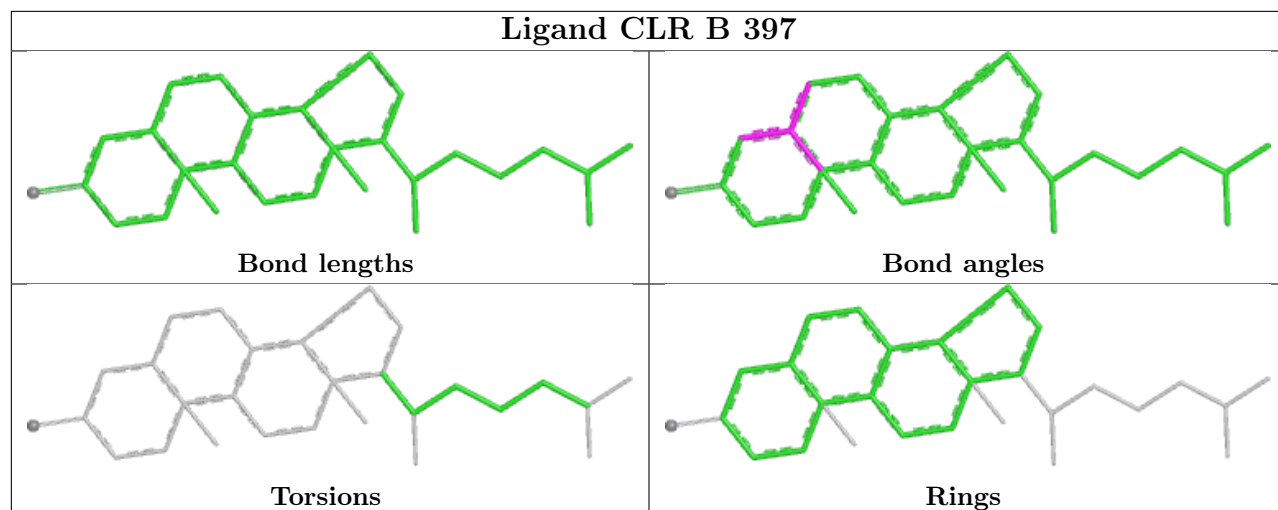


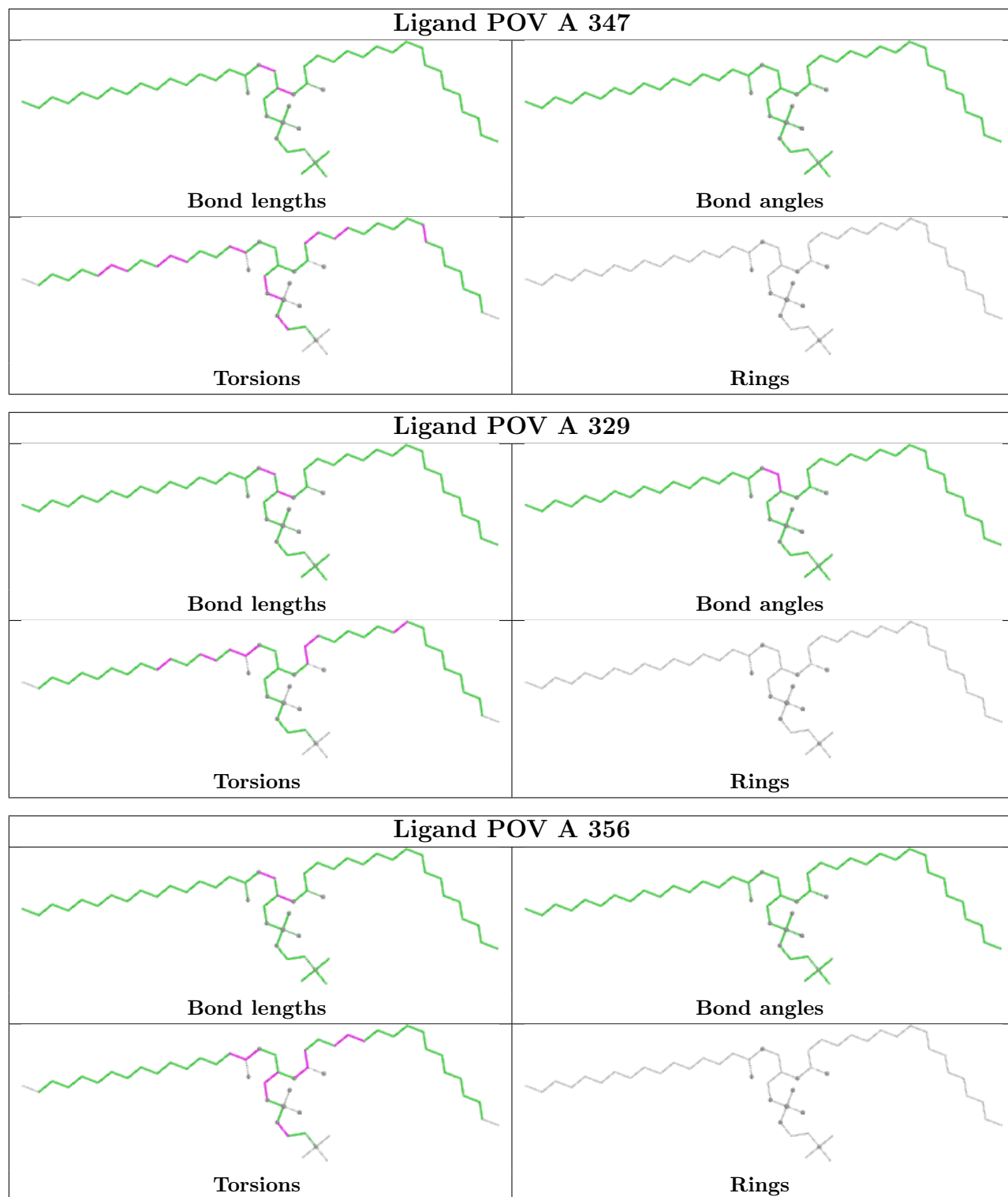


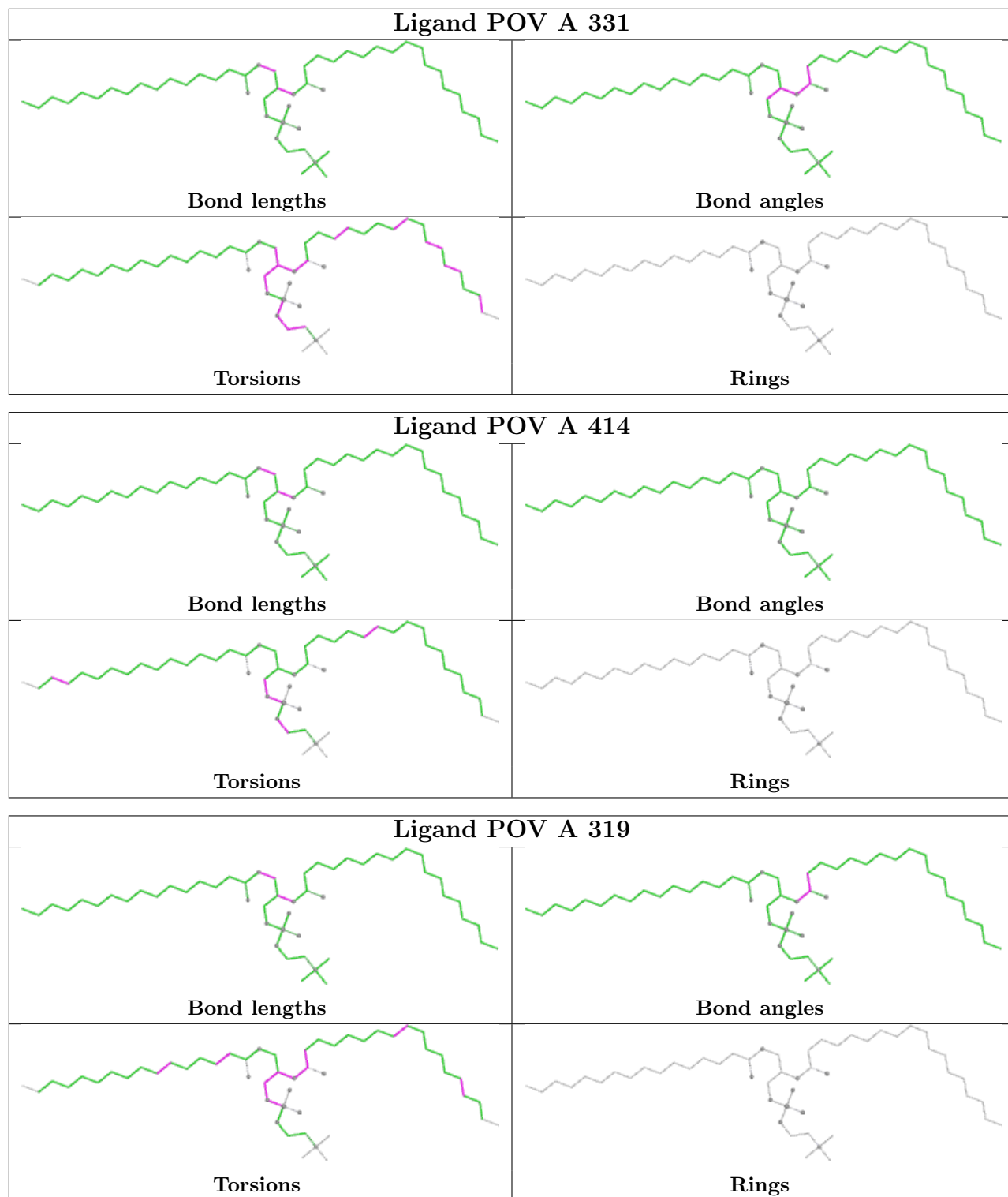


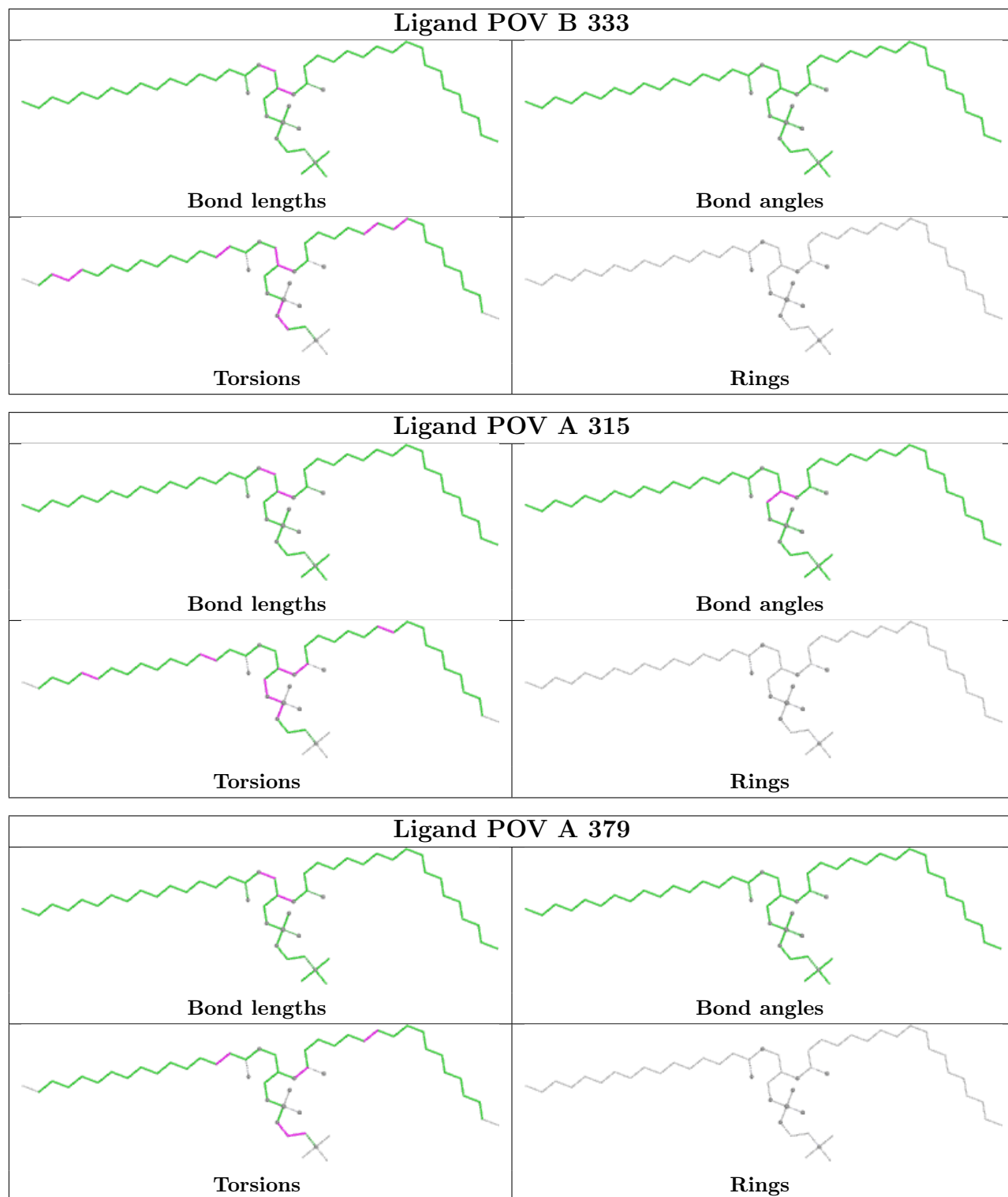


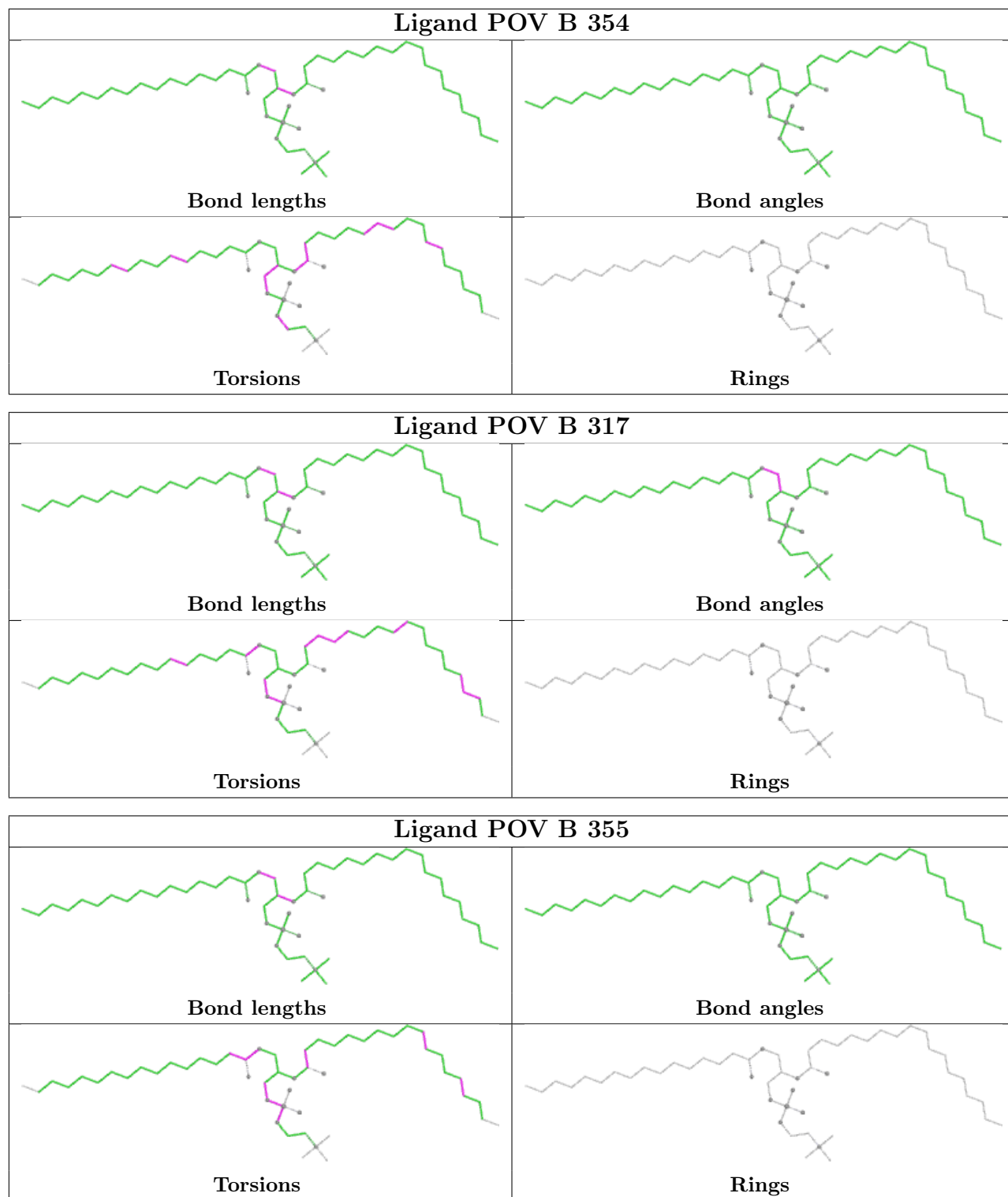


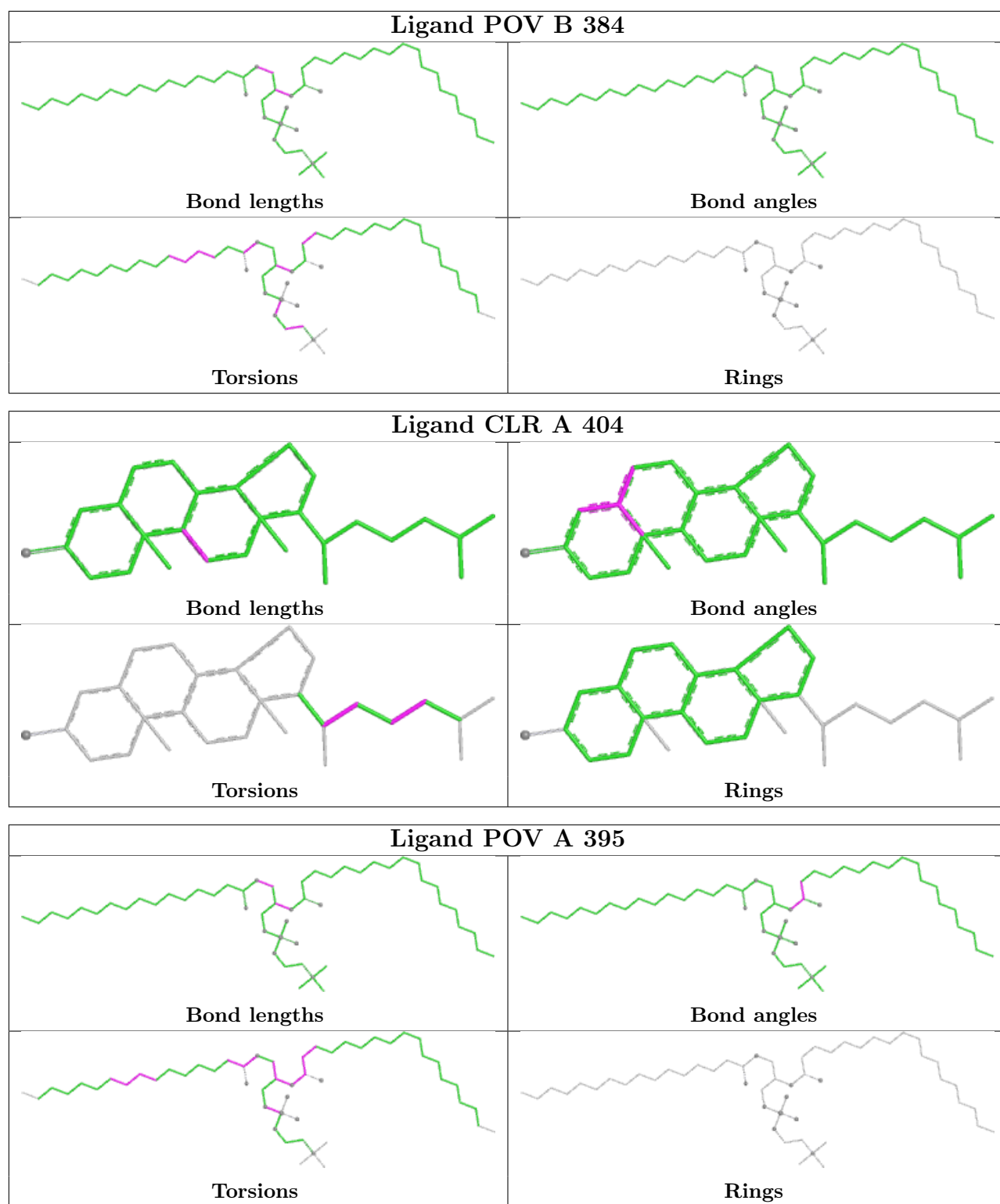


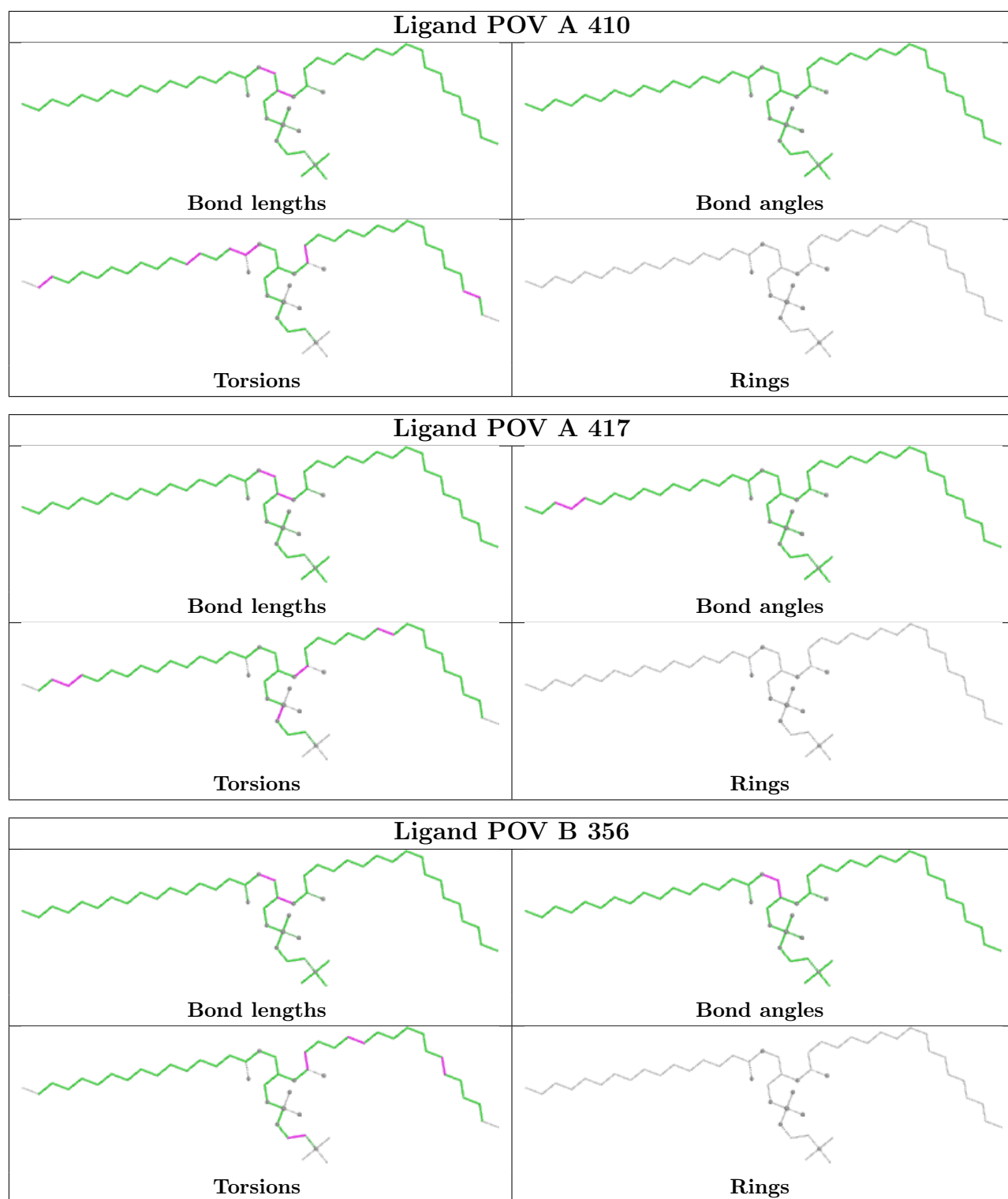


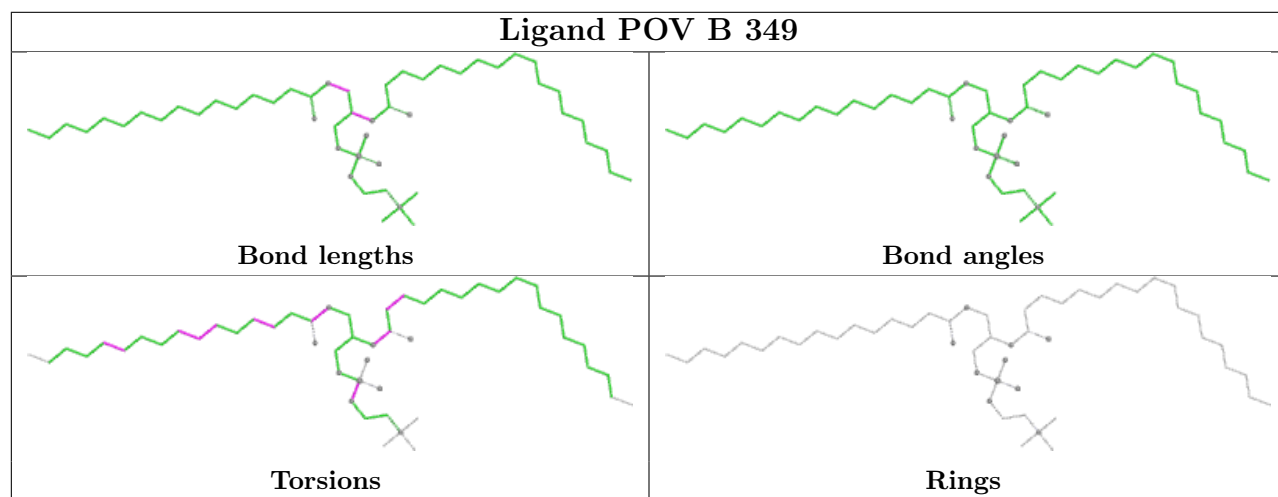
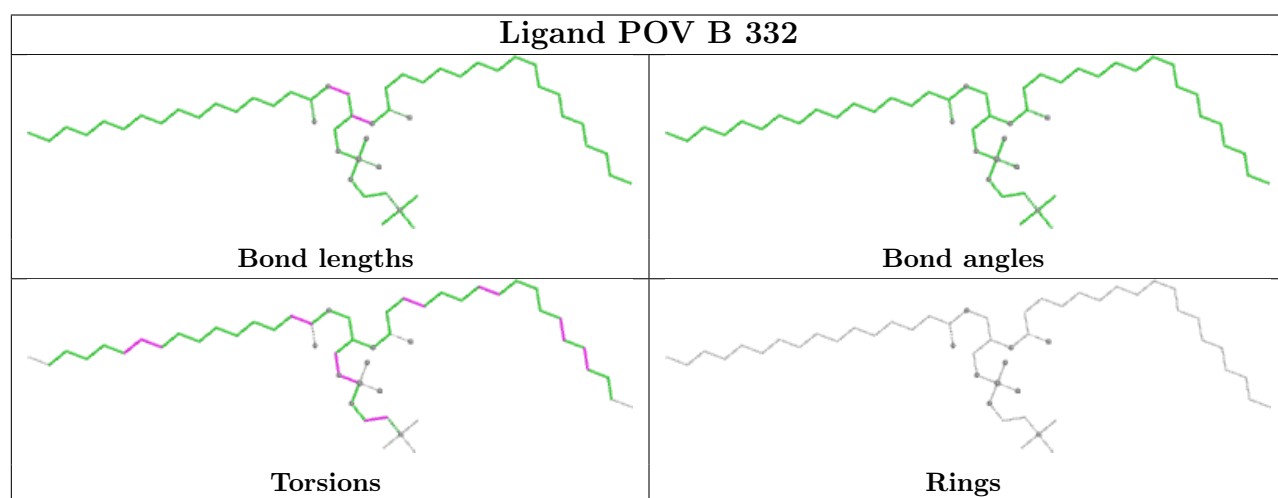
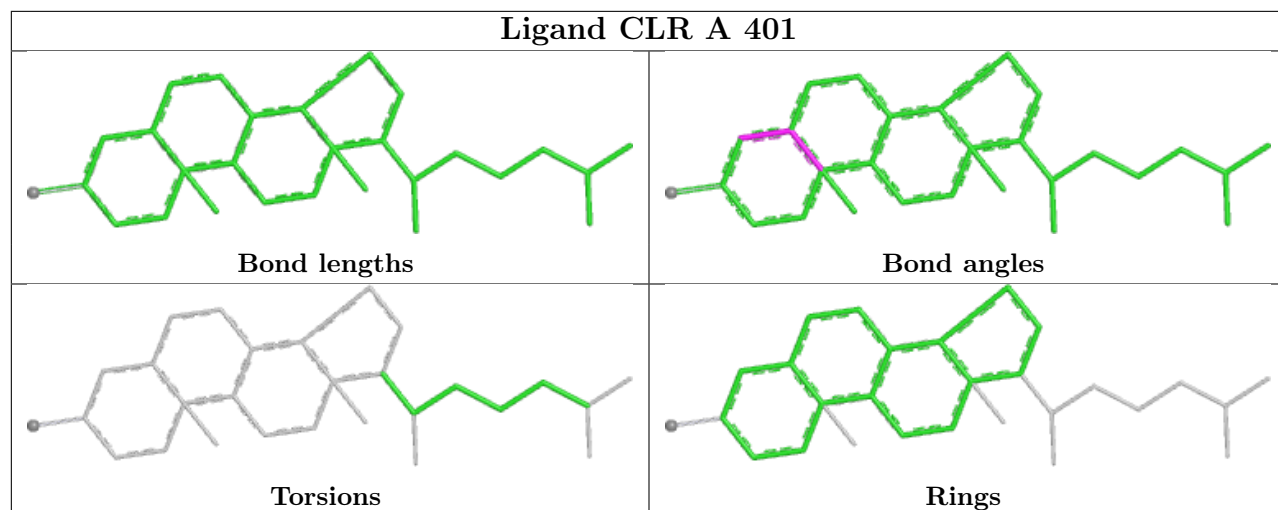


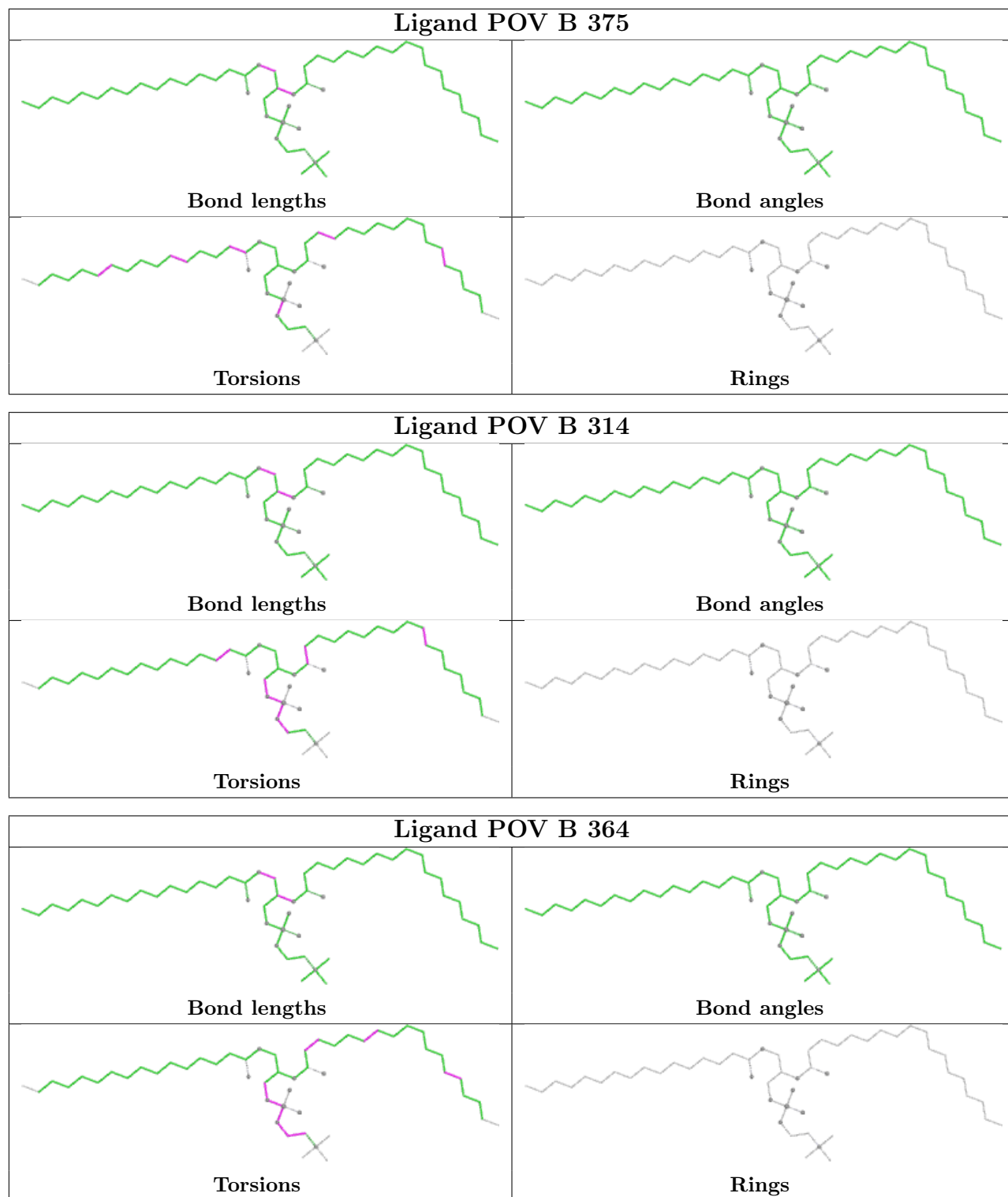


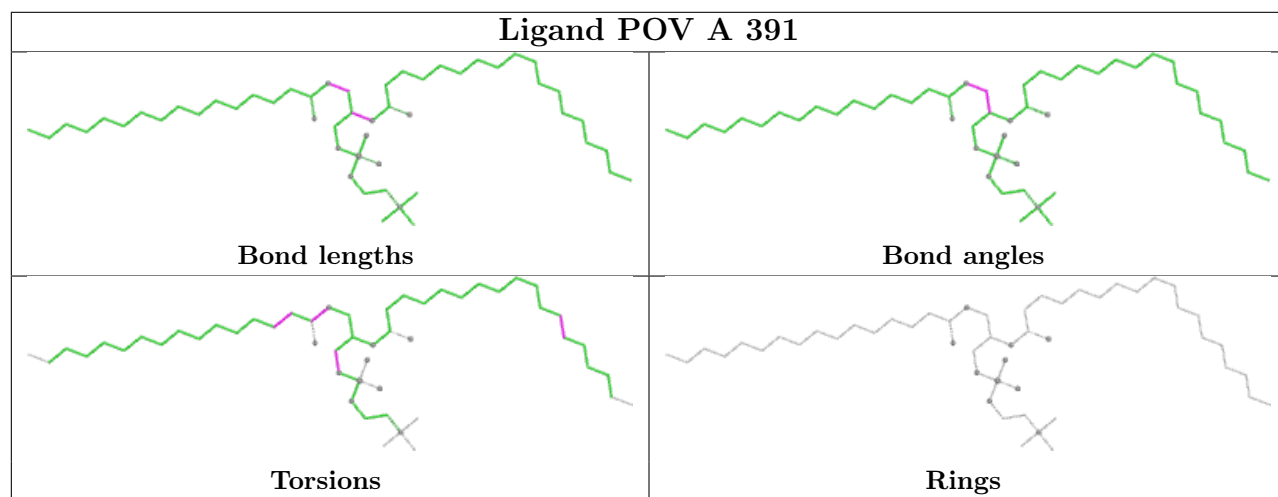
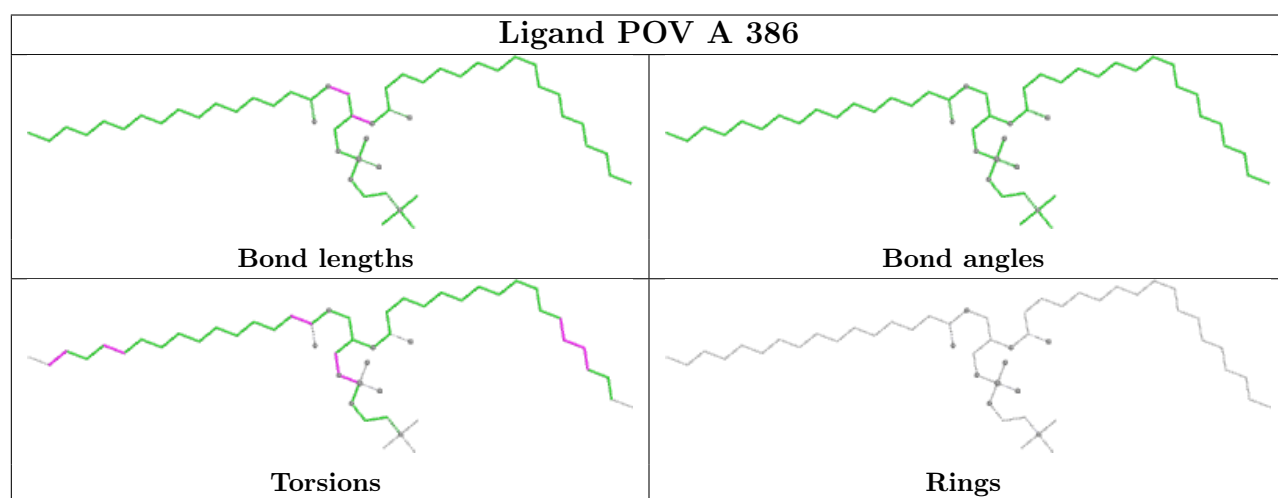
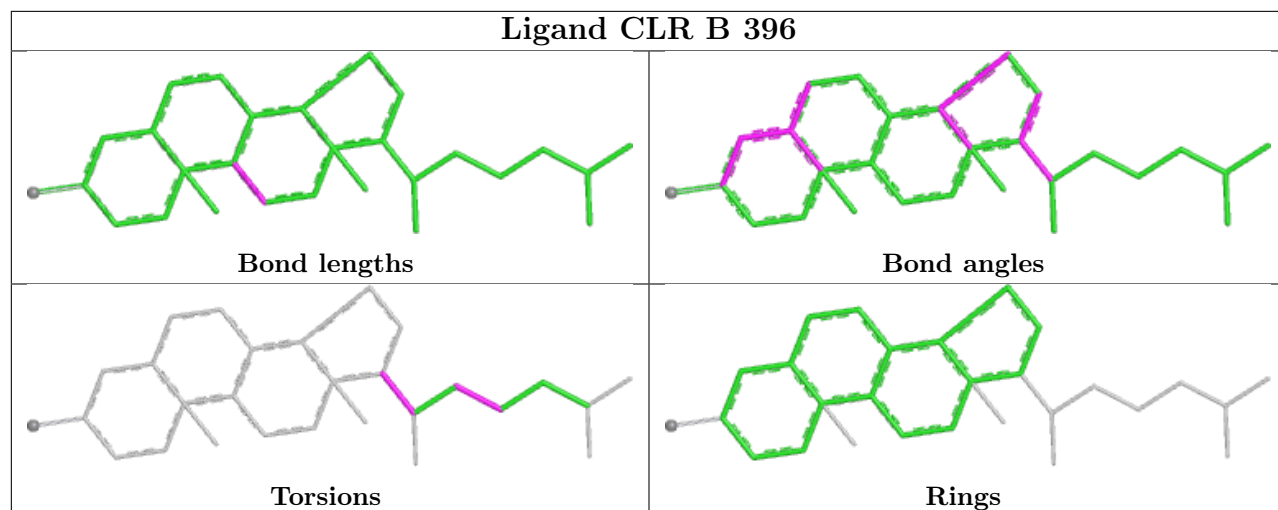


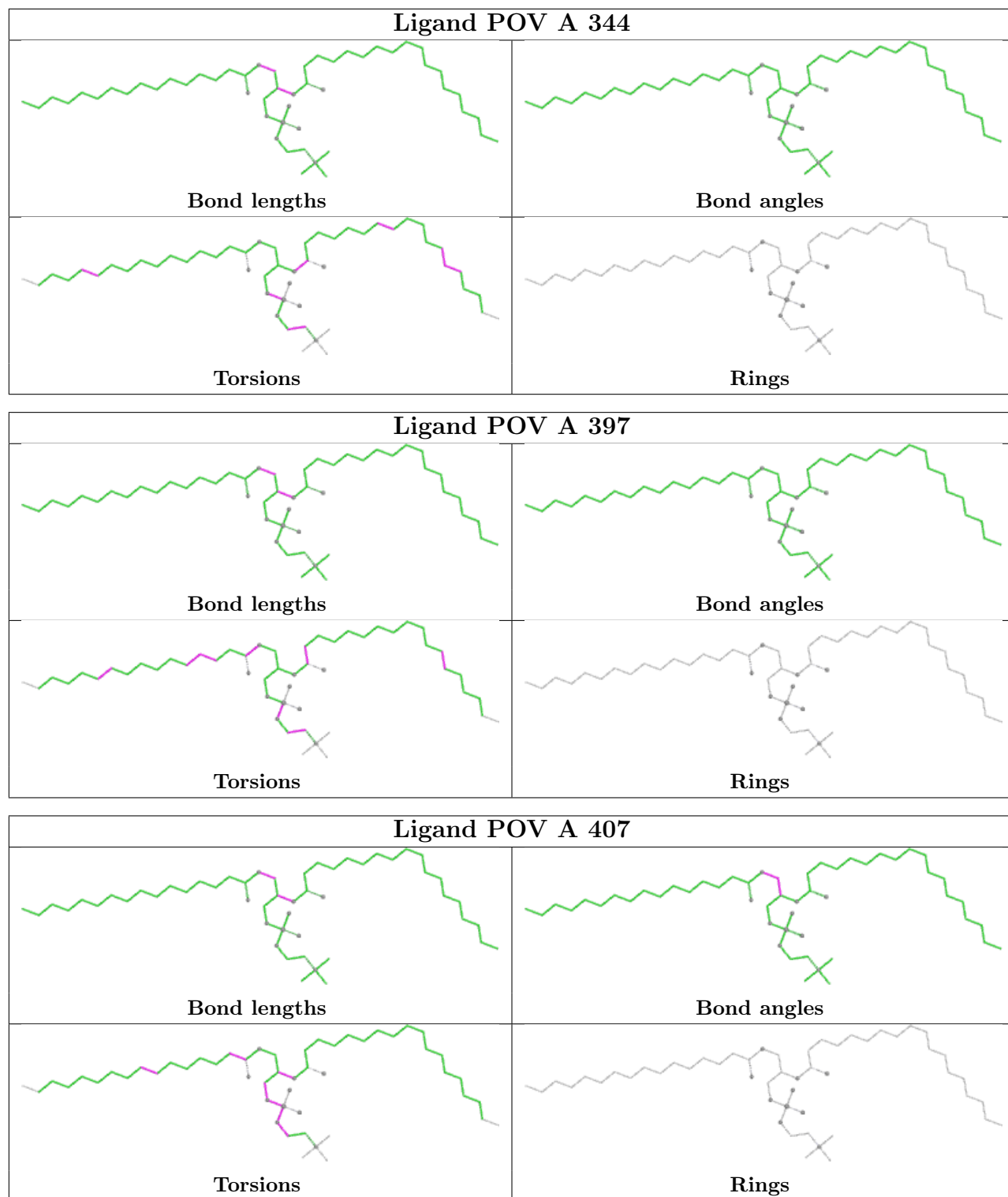




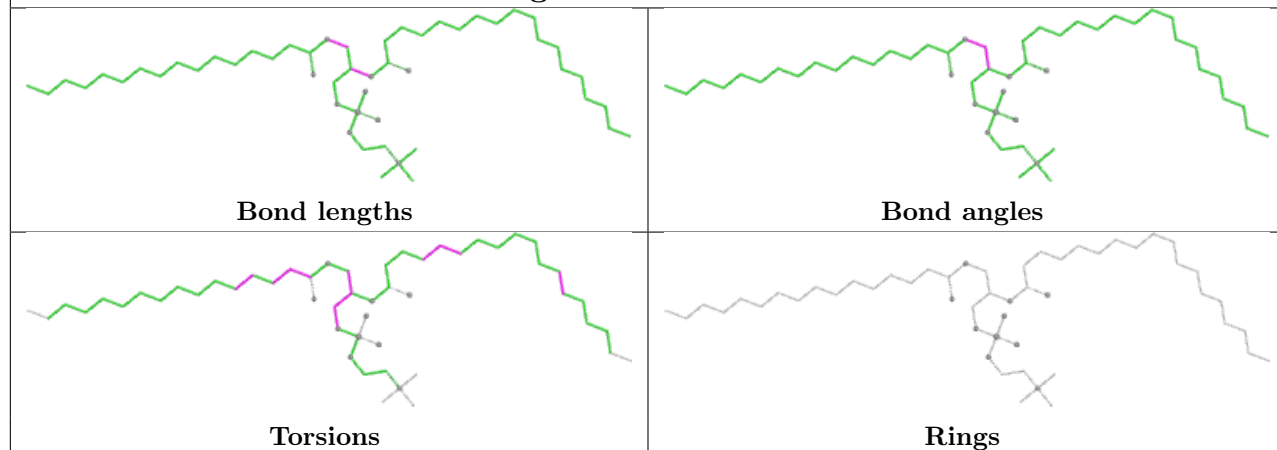




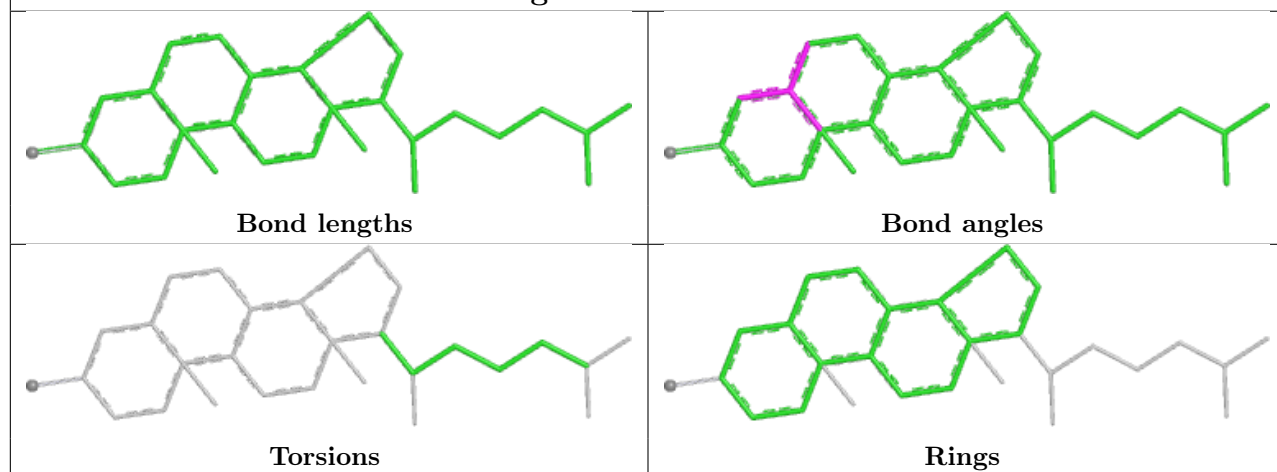




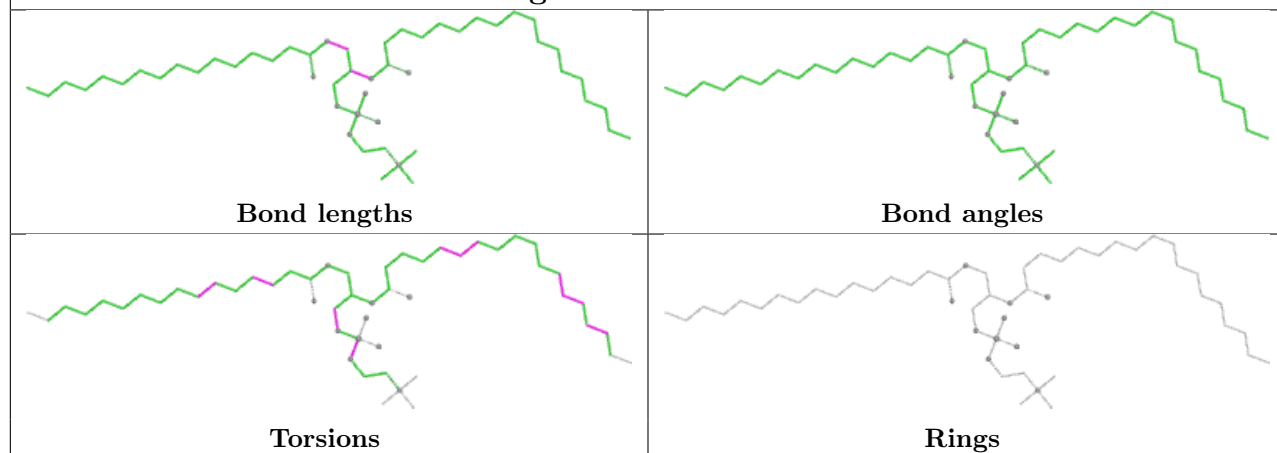
Ligand POV B 304

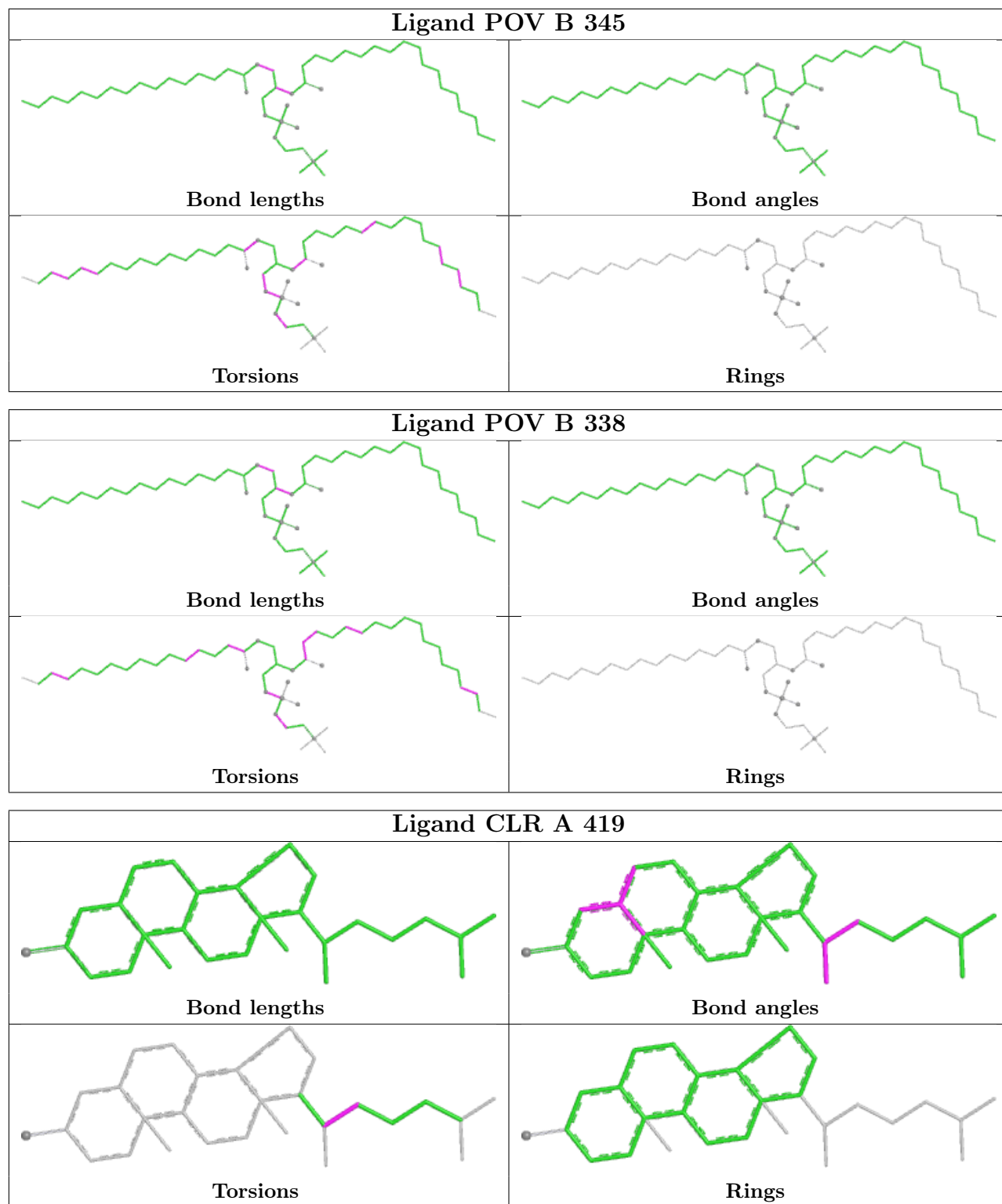


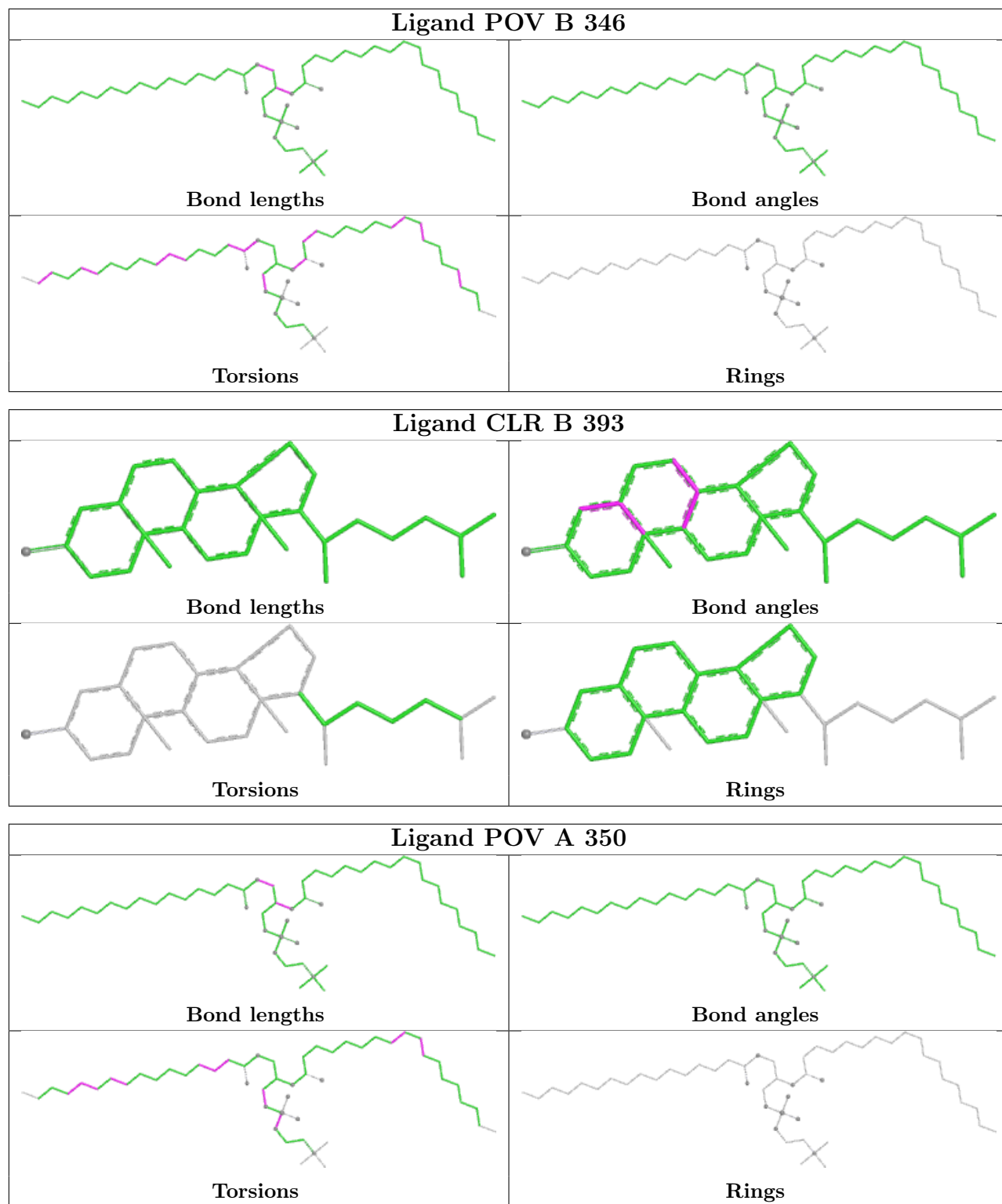
Ligand CLR A 403

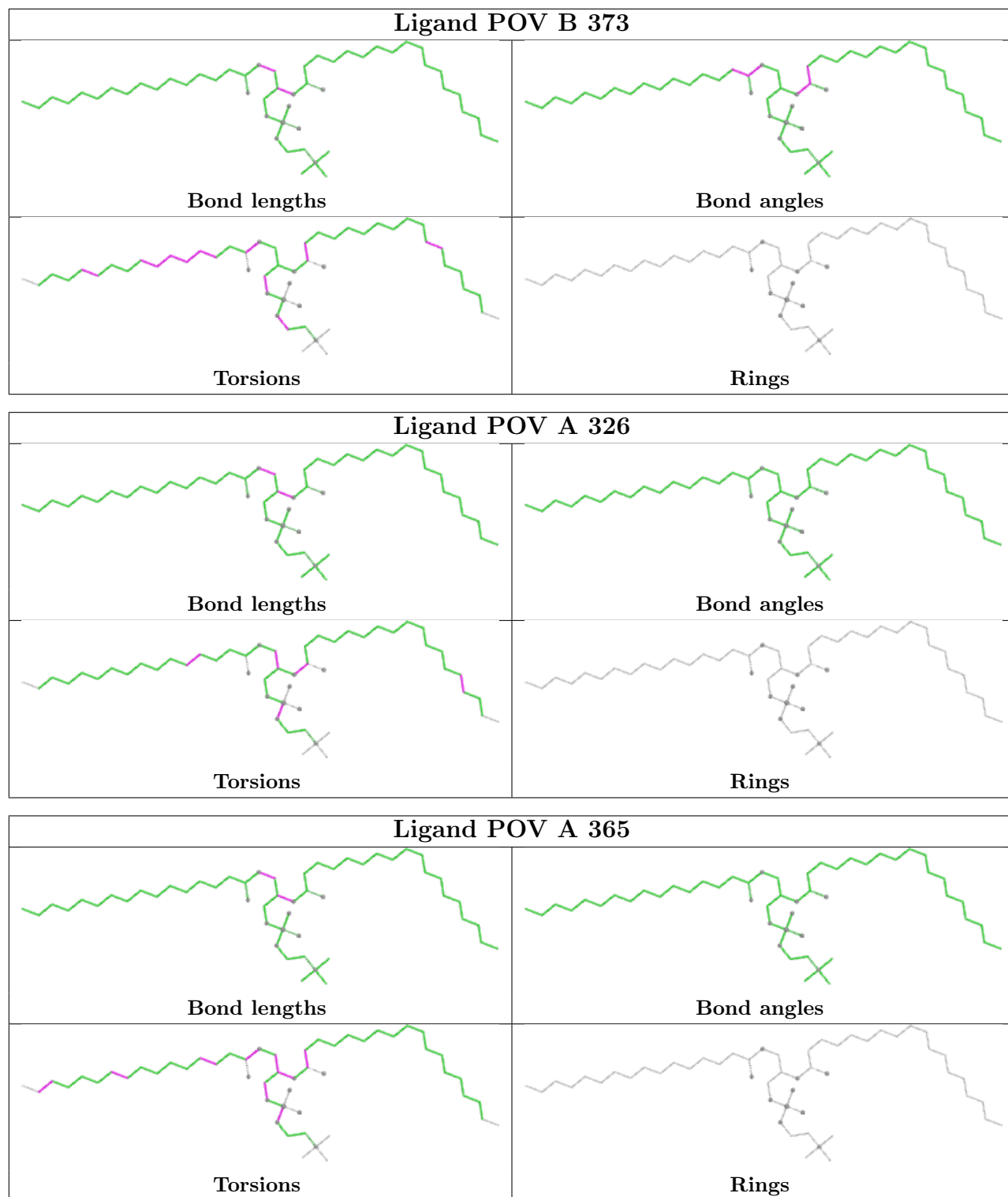


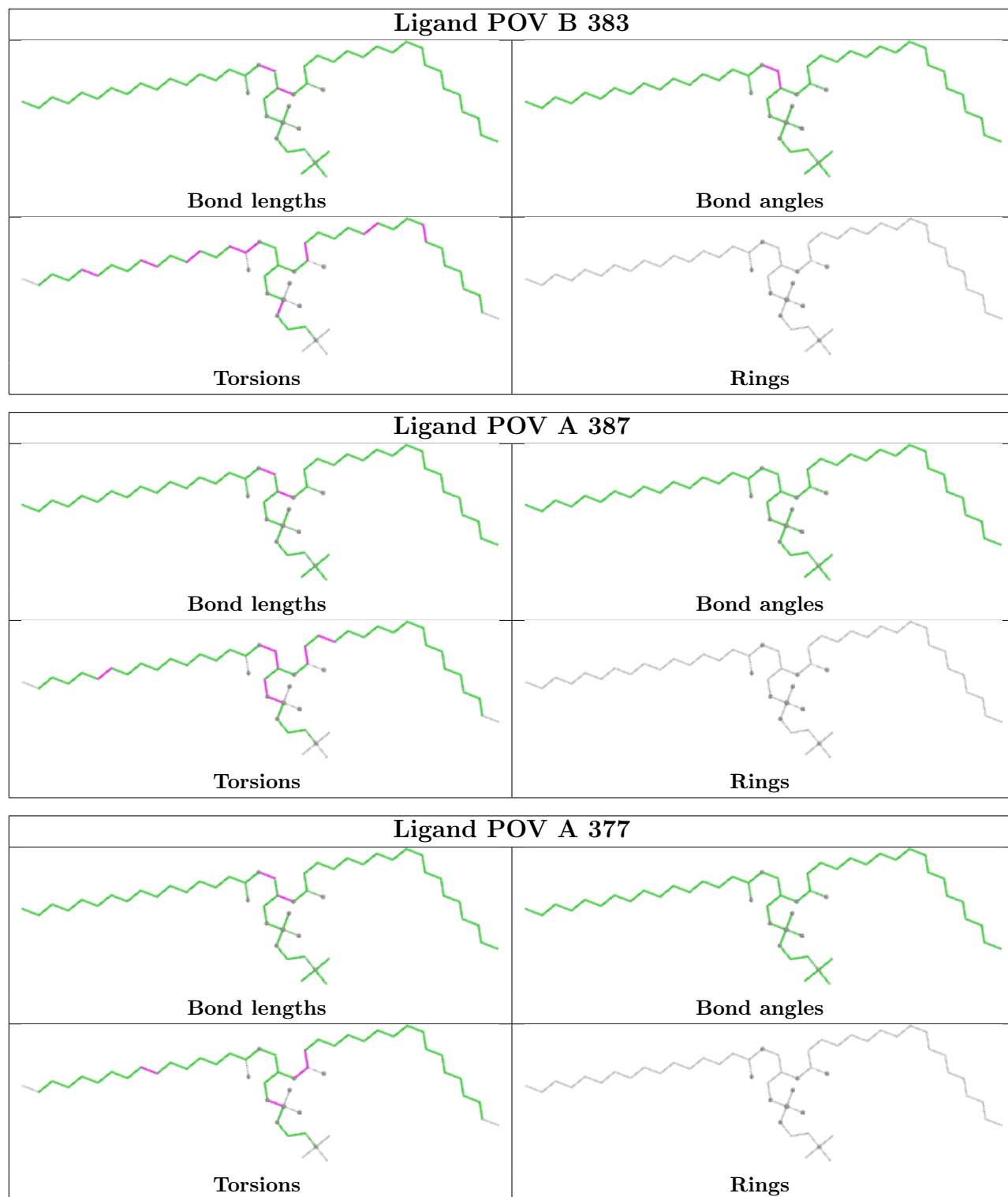
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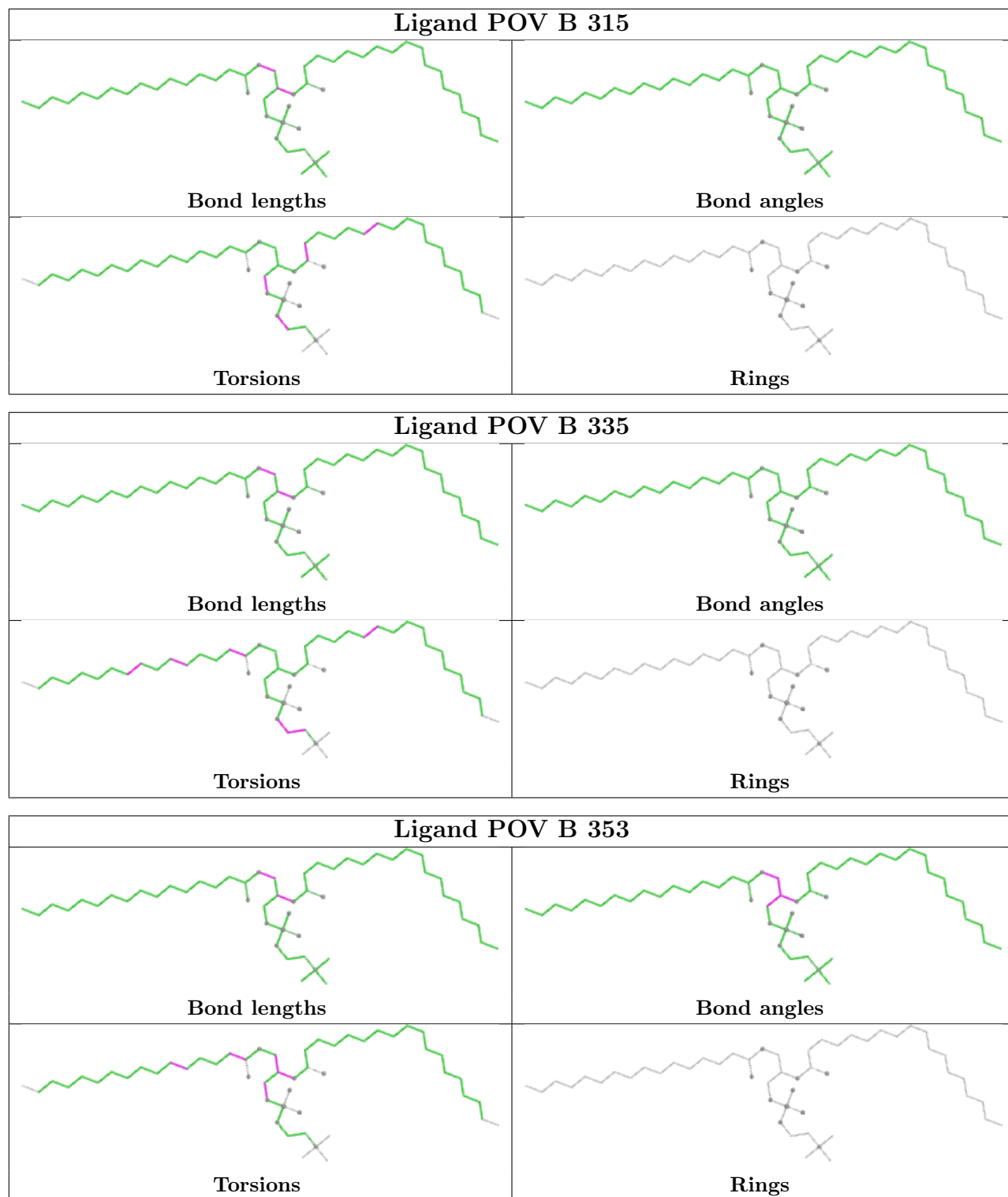


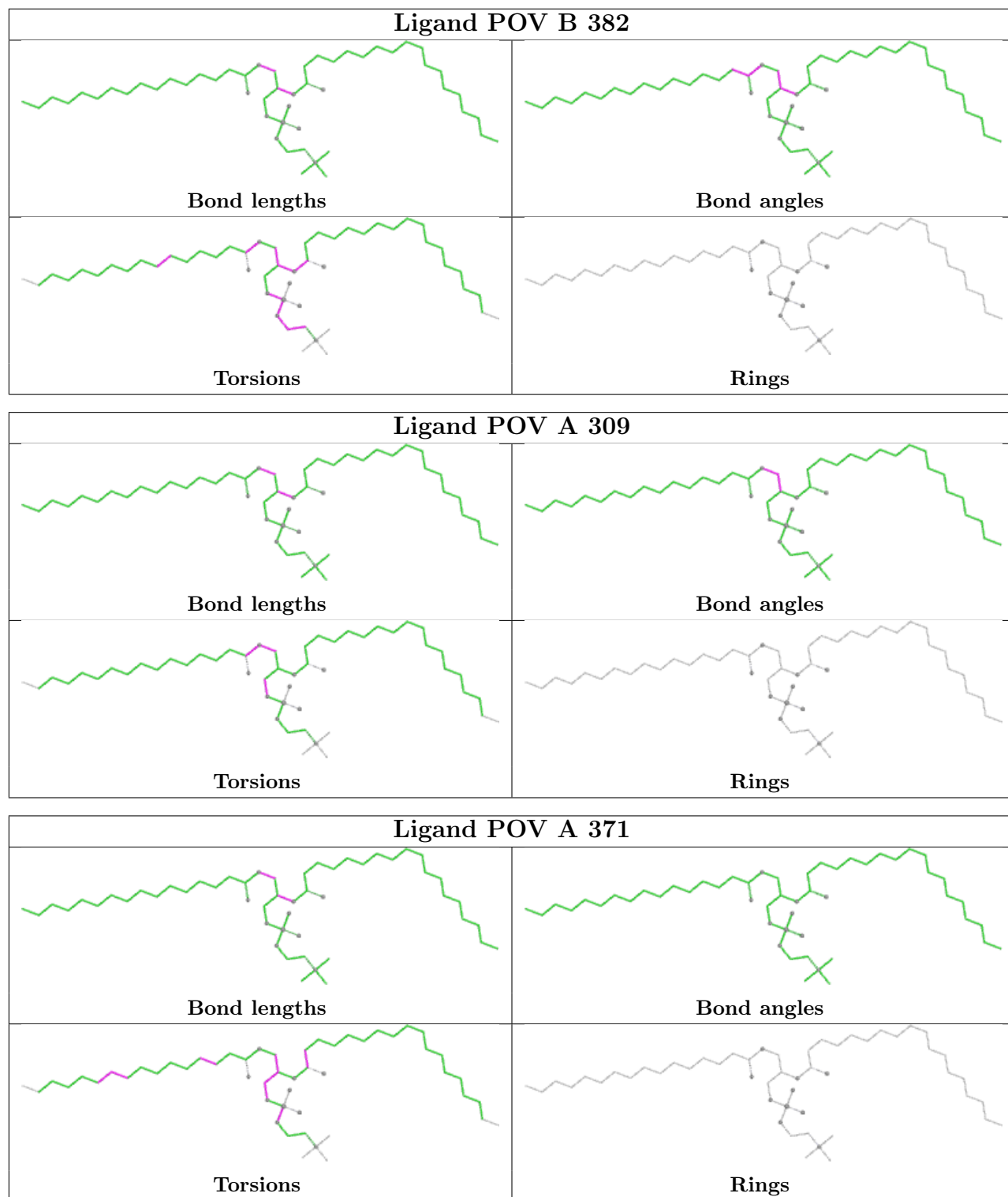


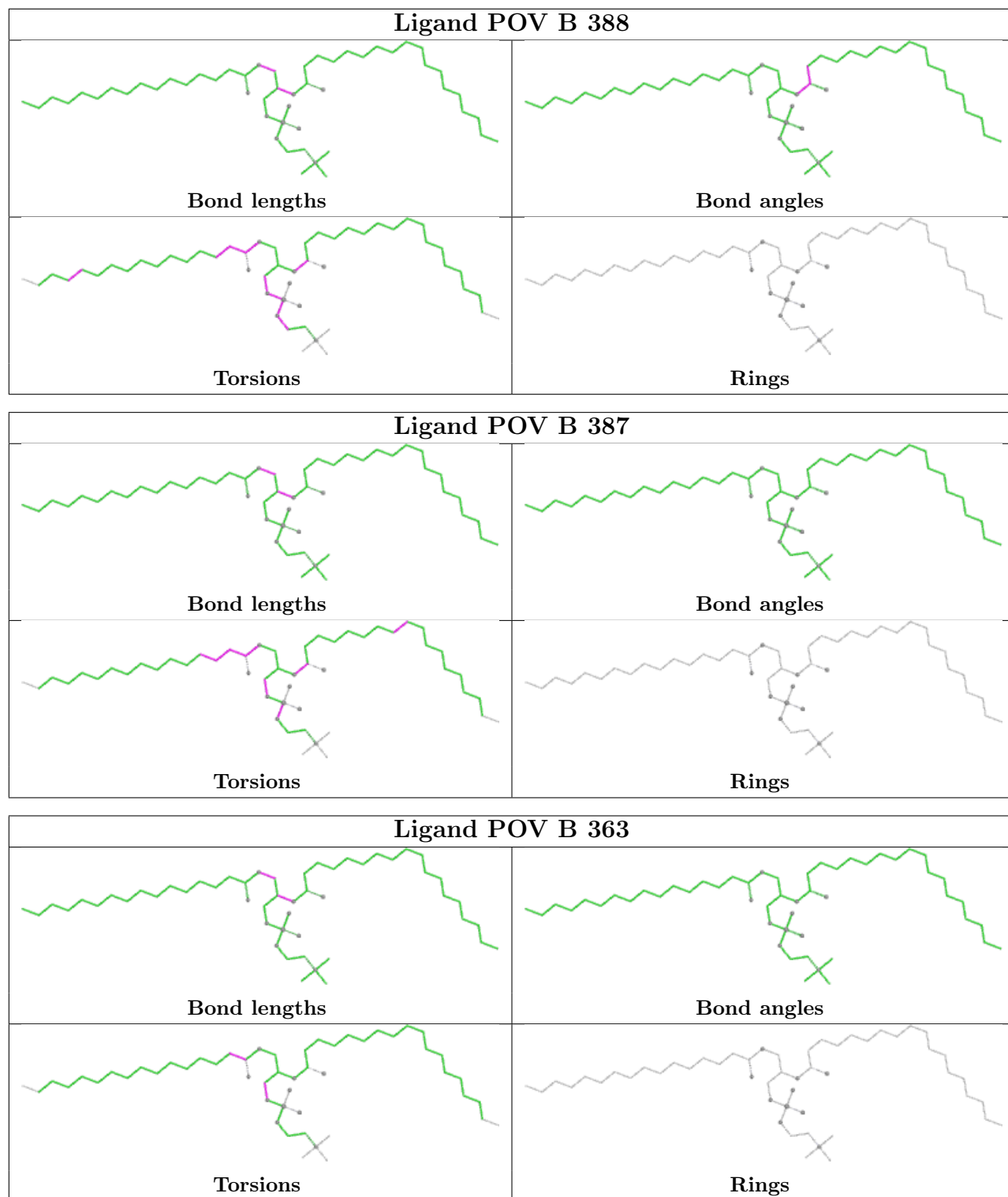


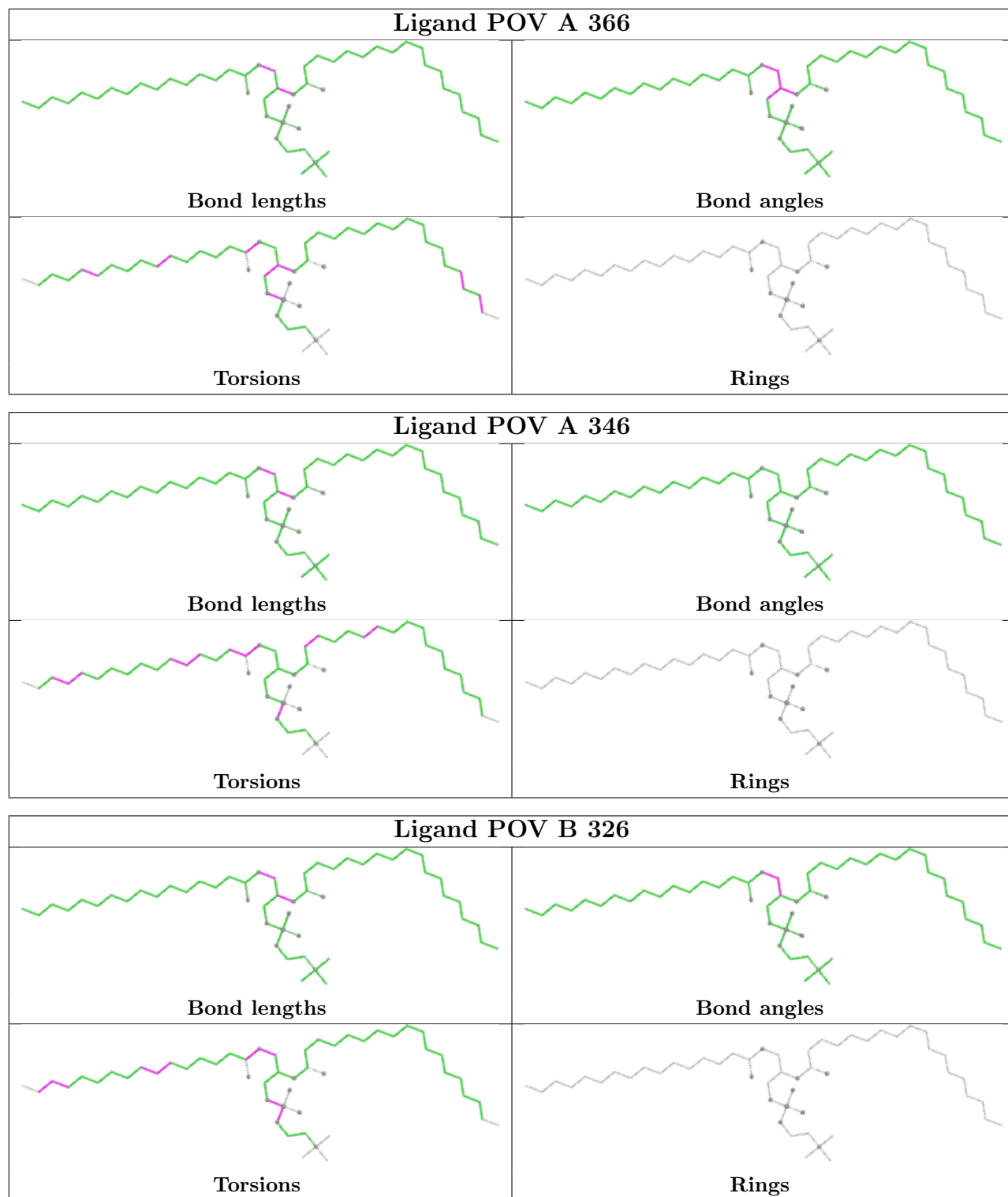


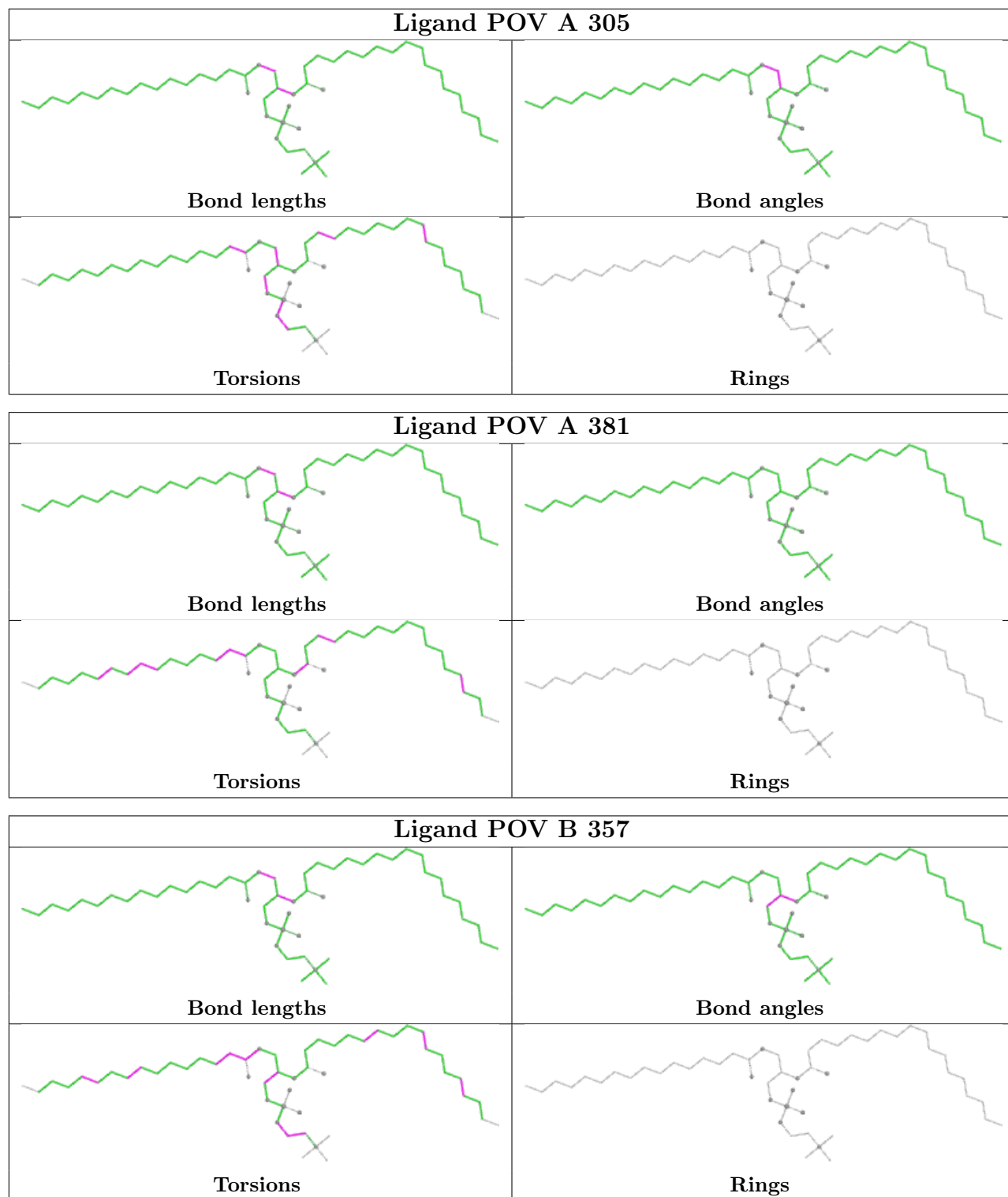




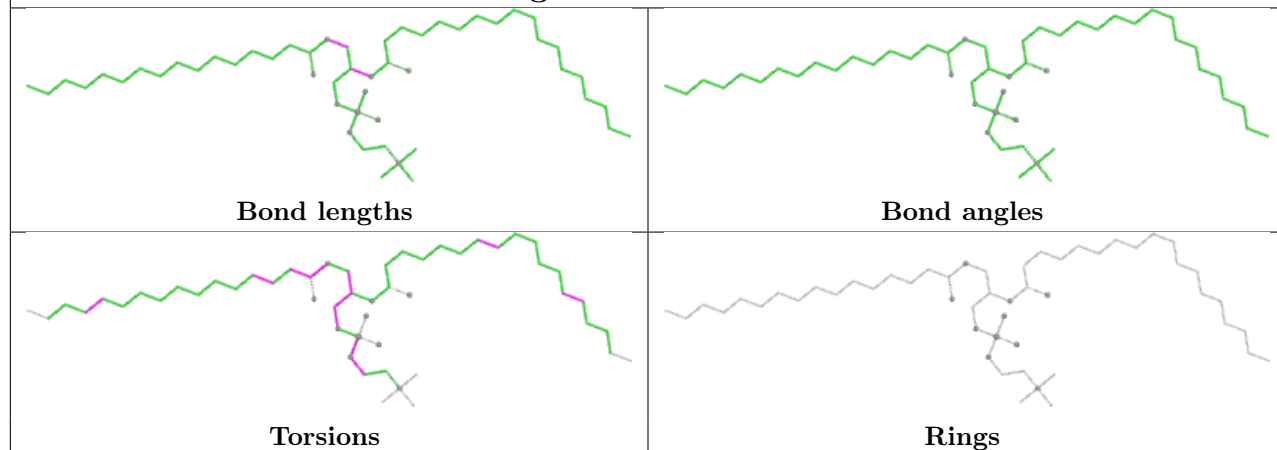




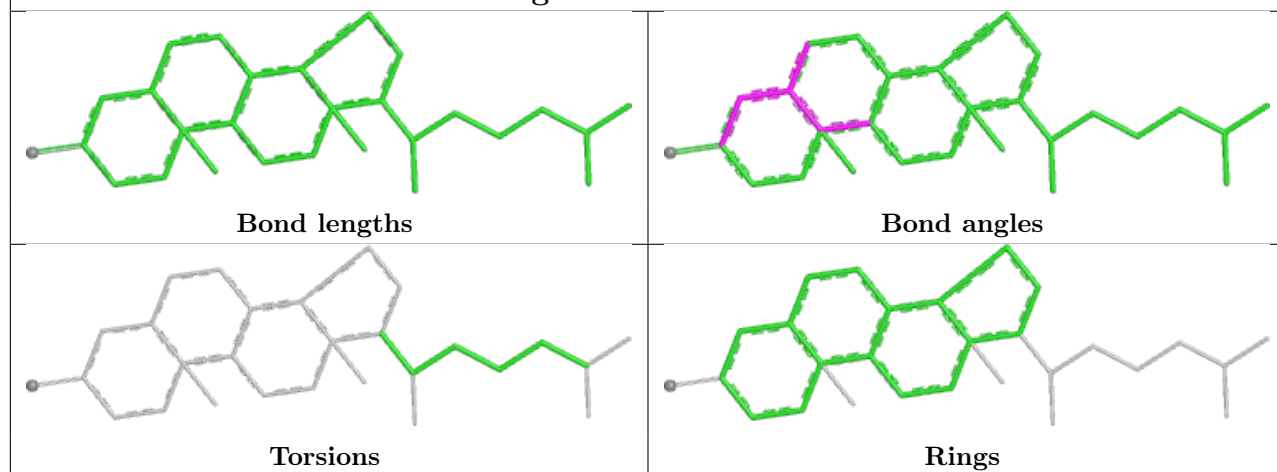




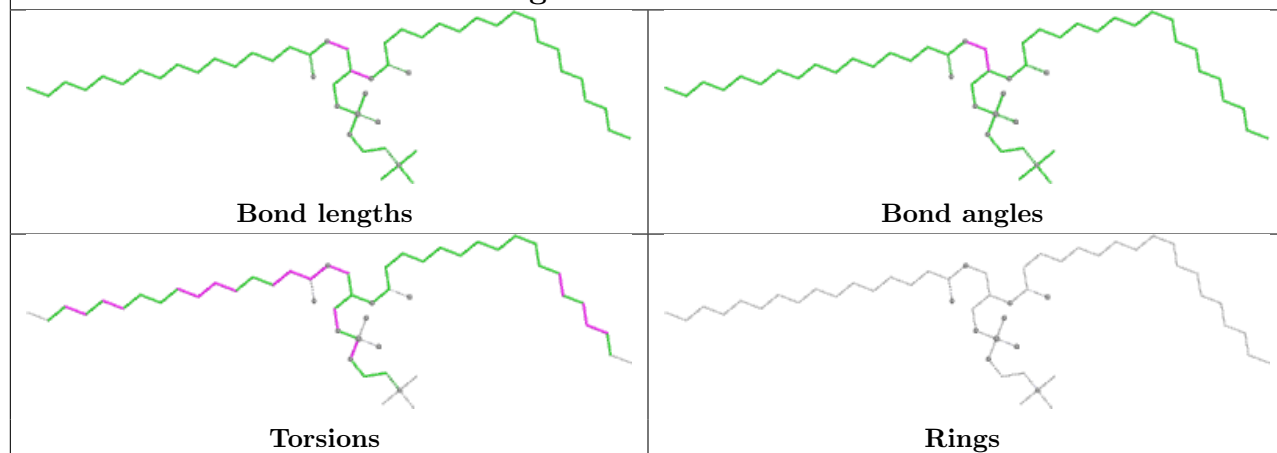
Ligand POV B 381

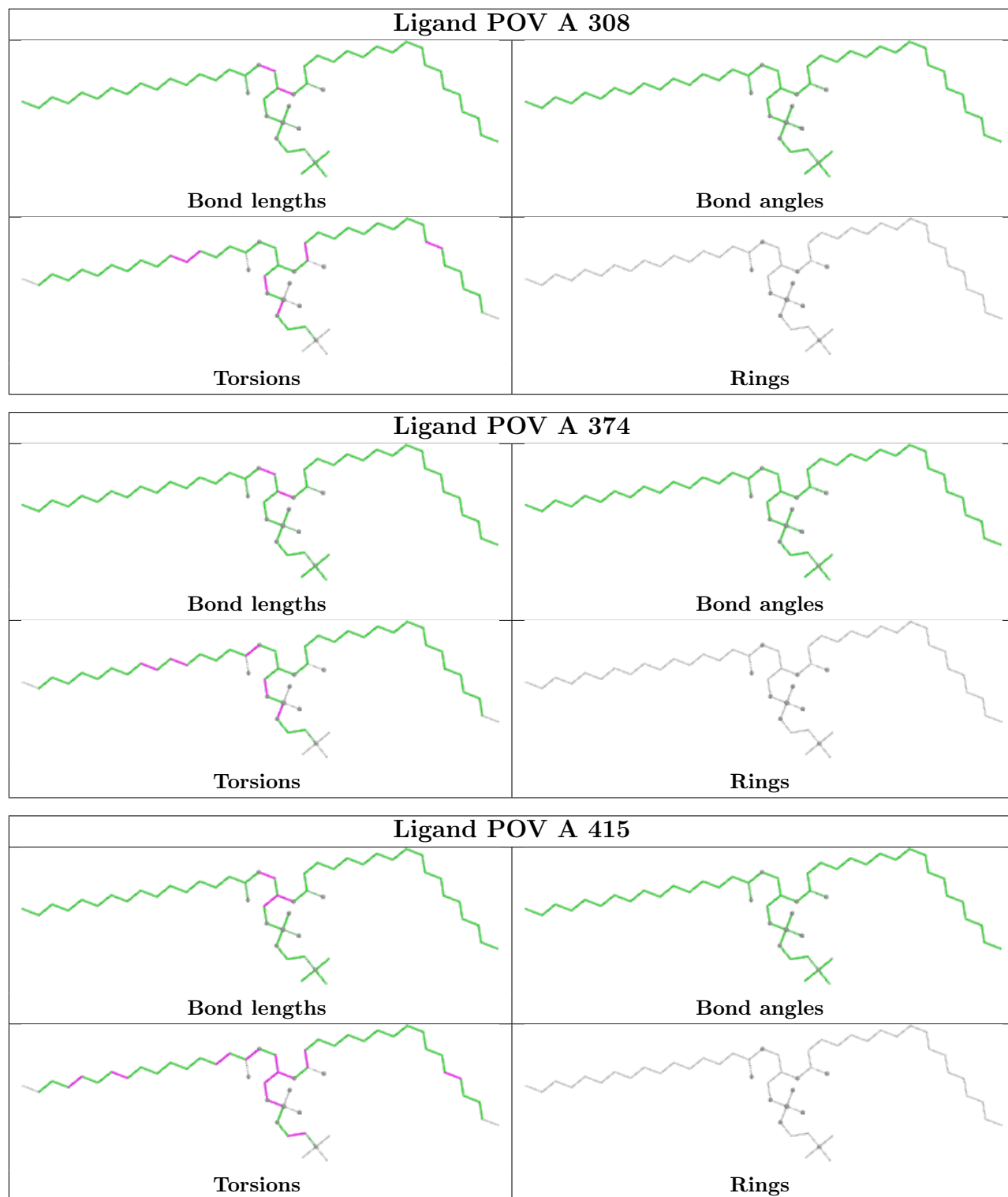


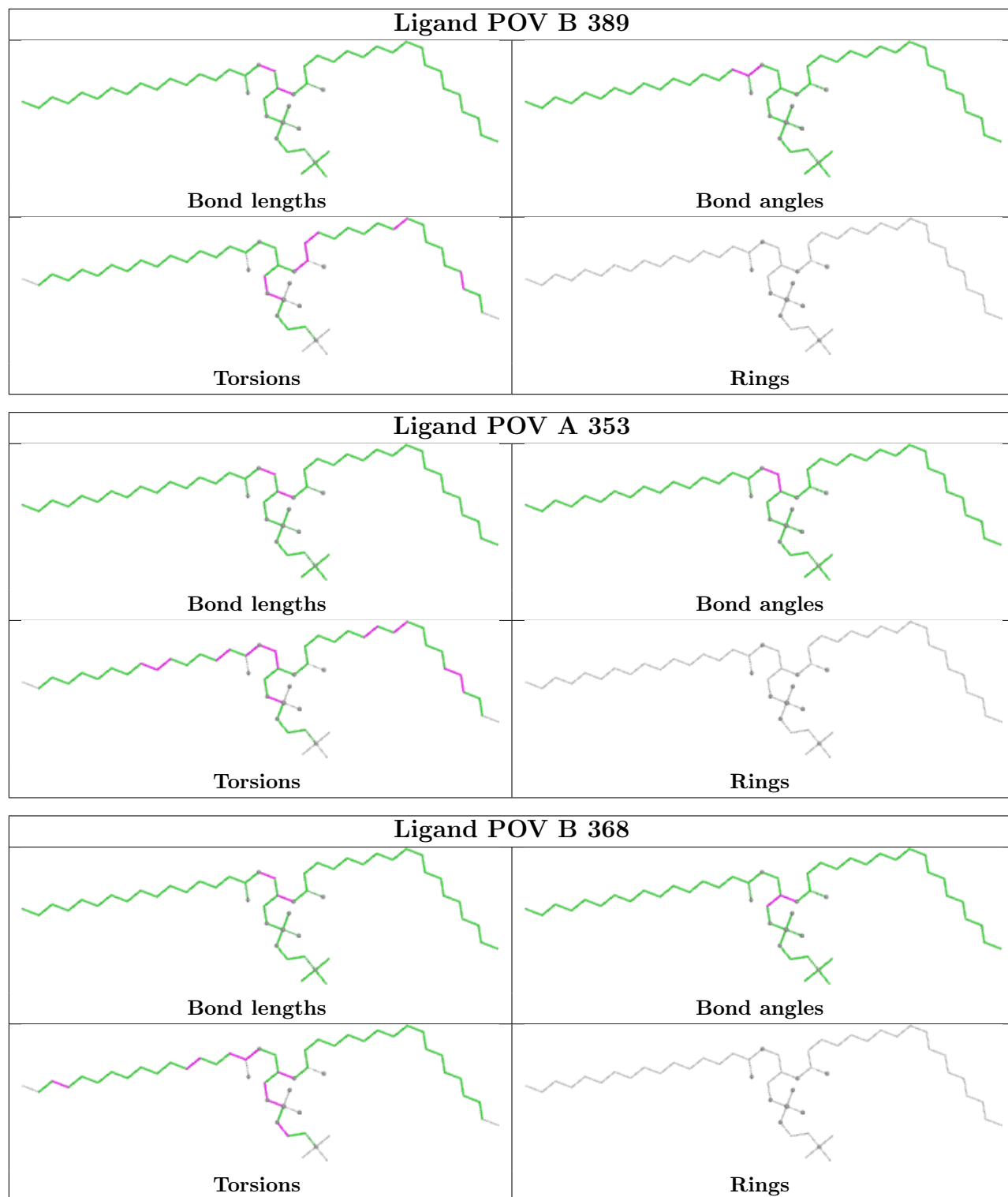
Ligand CLR B 395

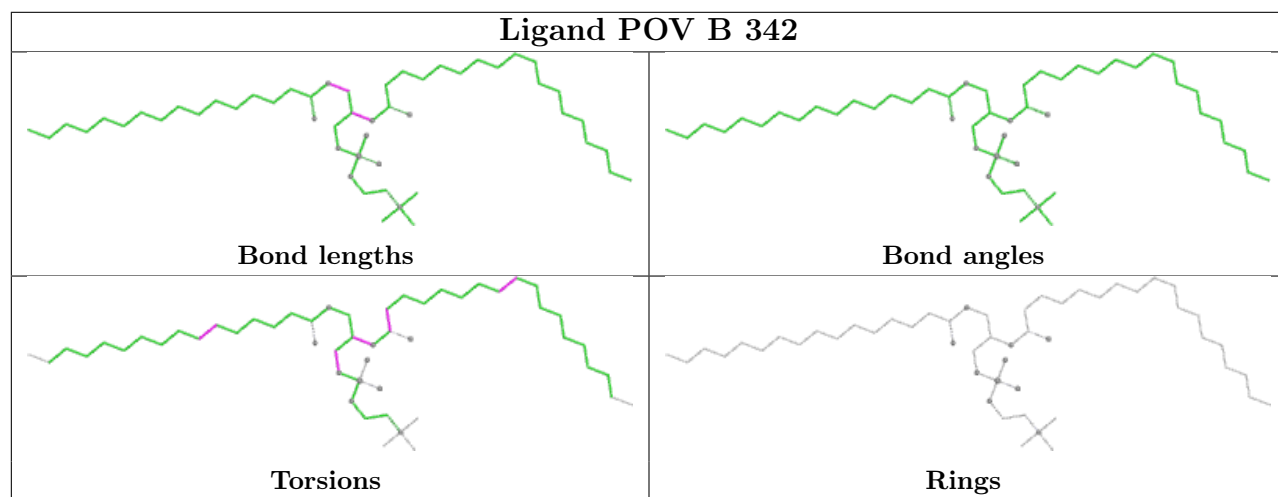
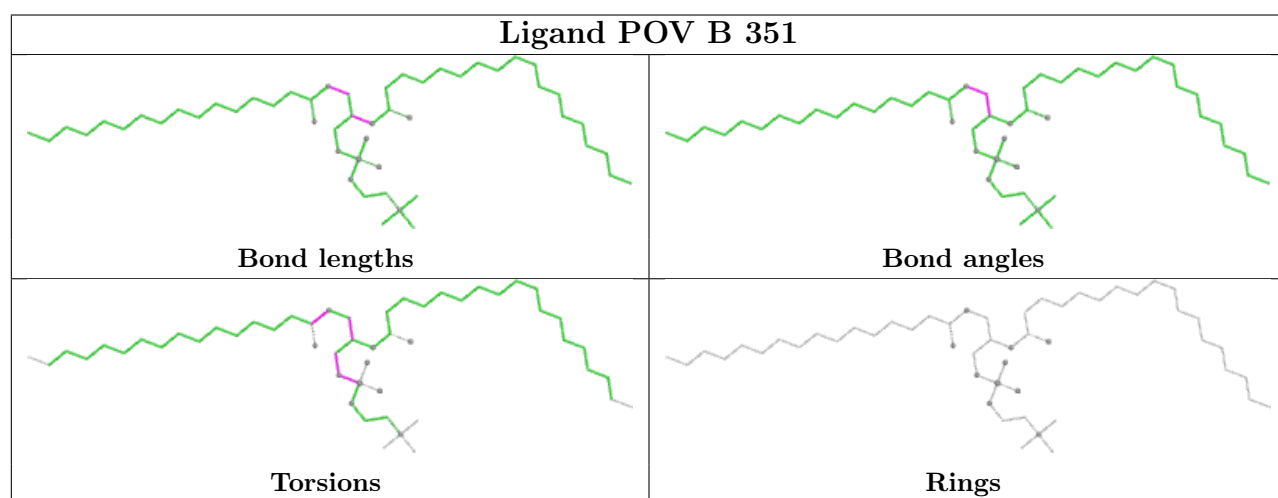
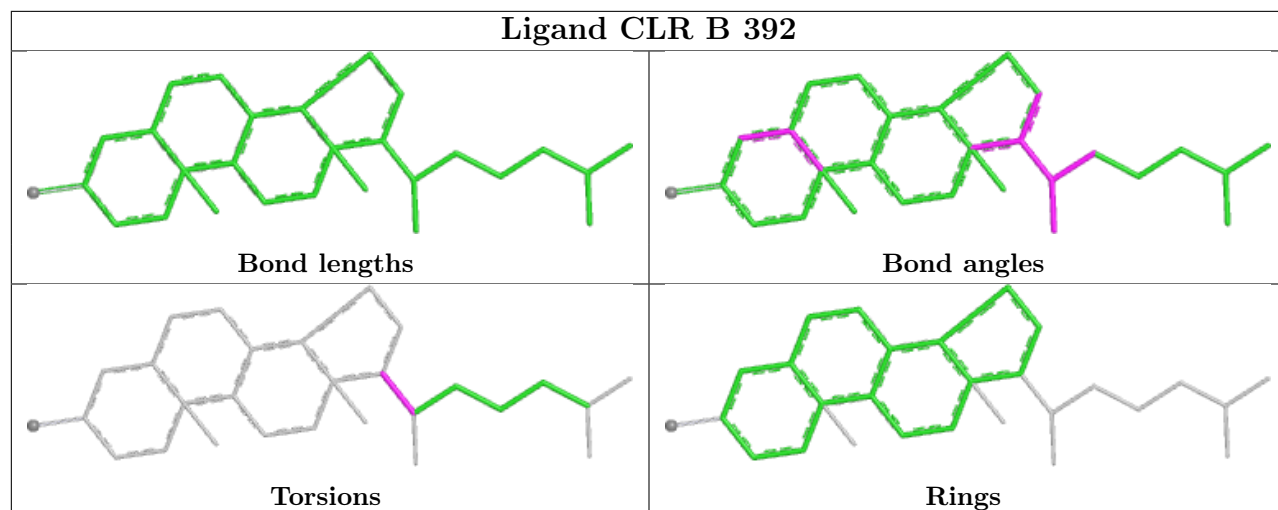


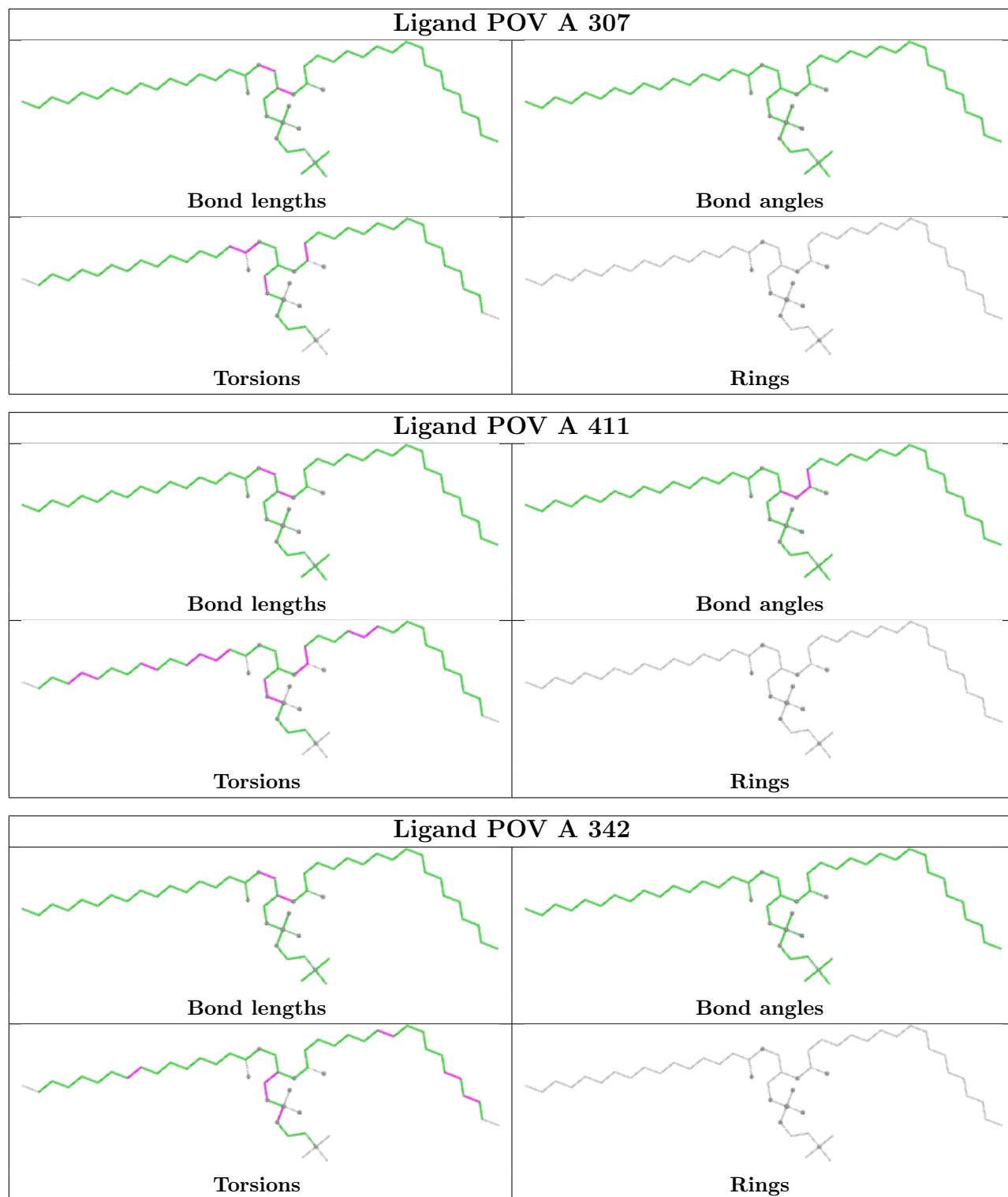
Ligand POV A 311

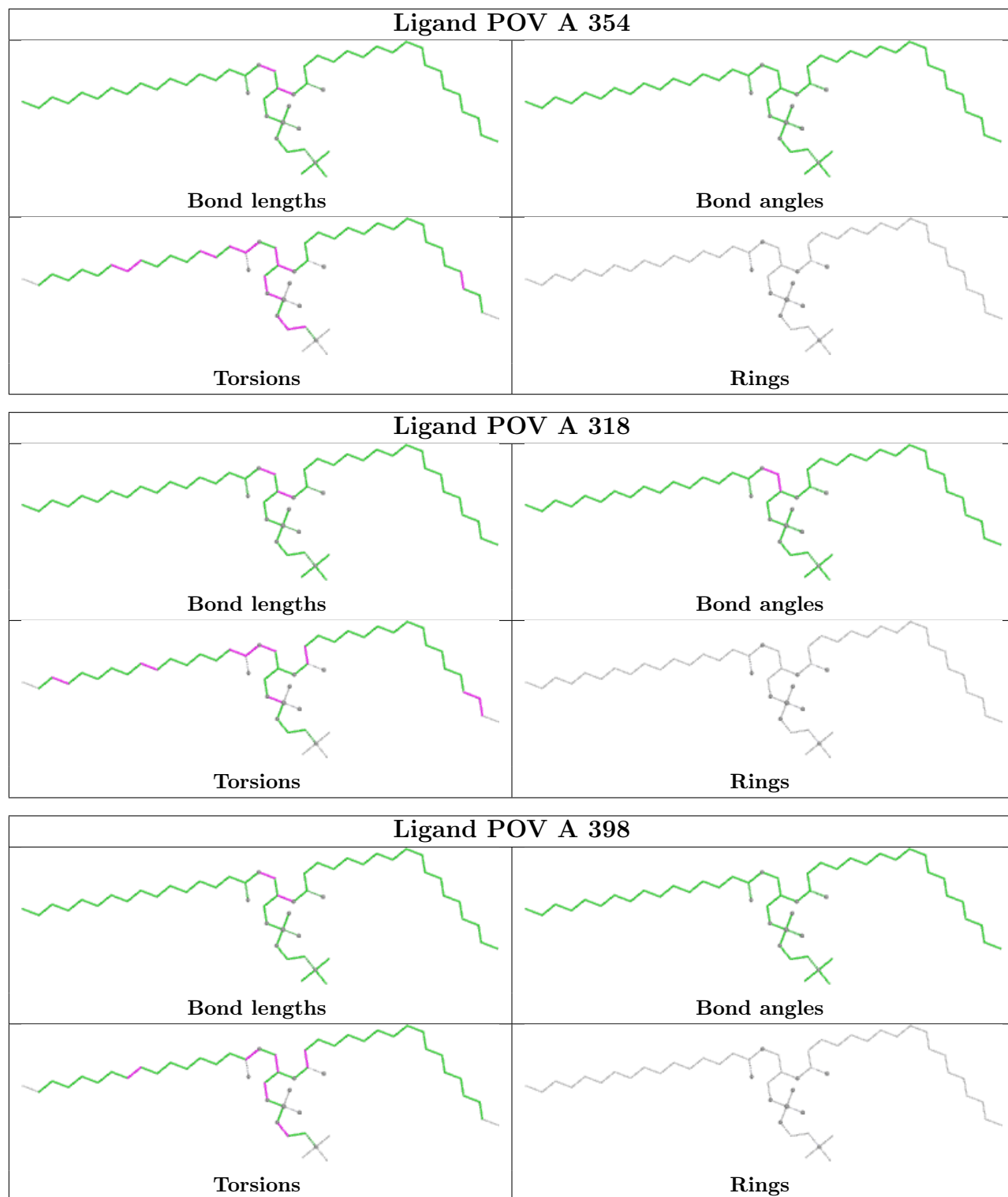


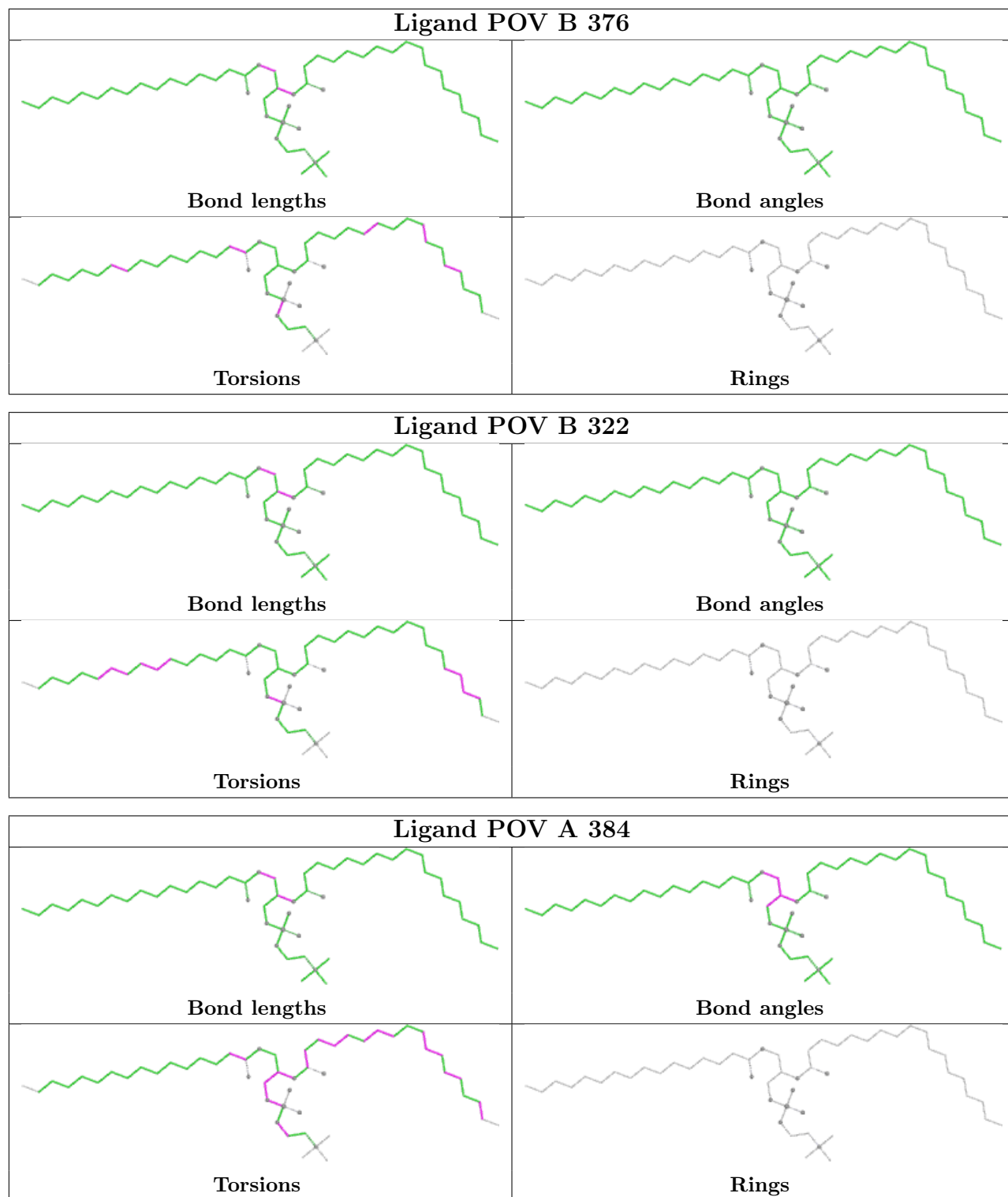


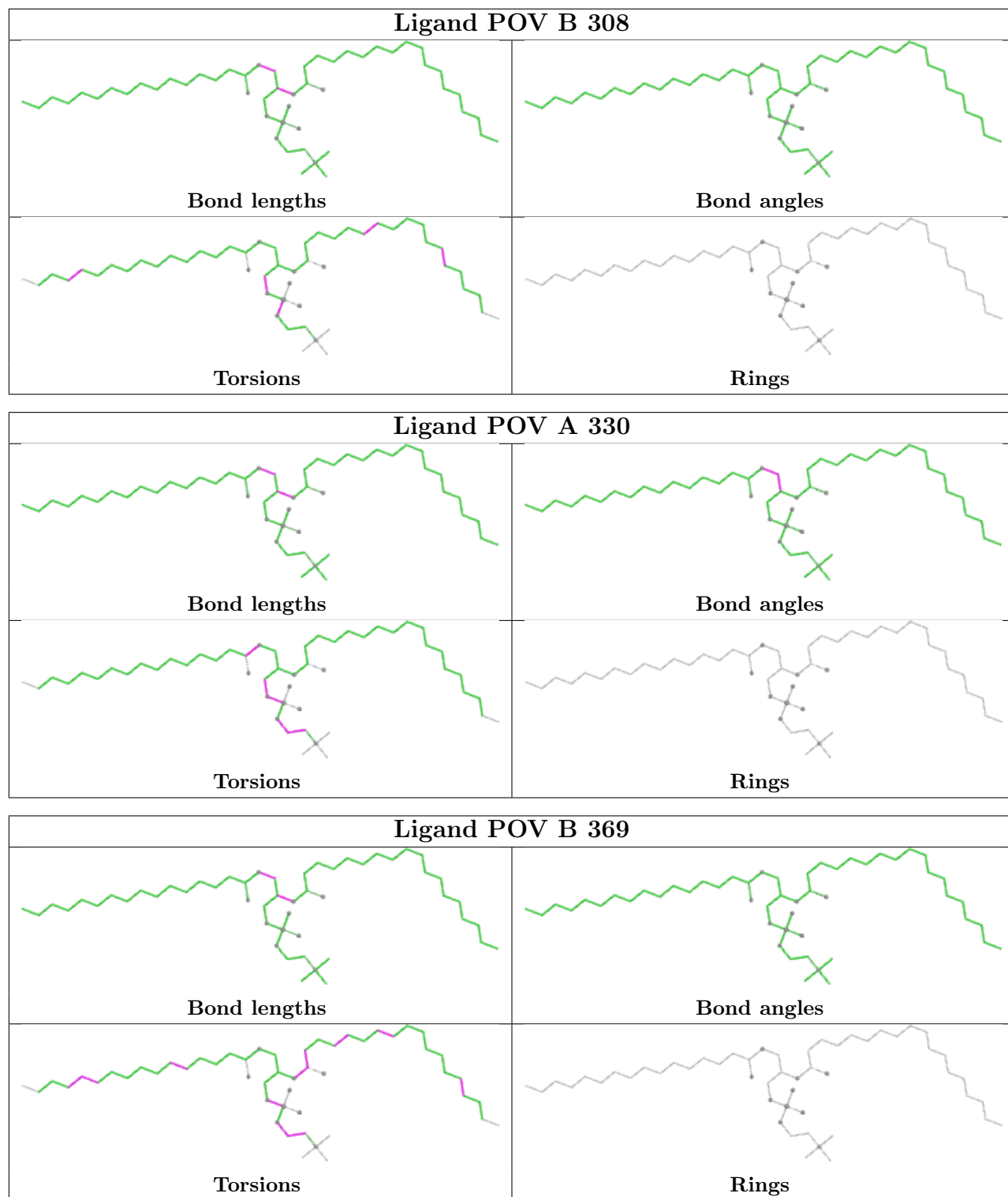


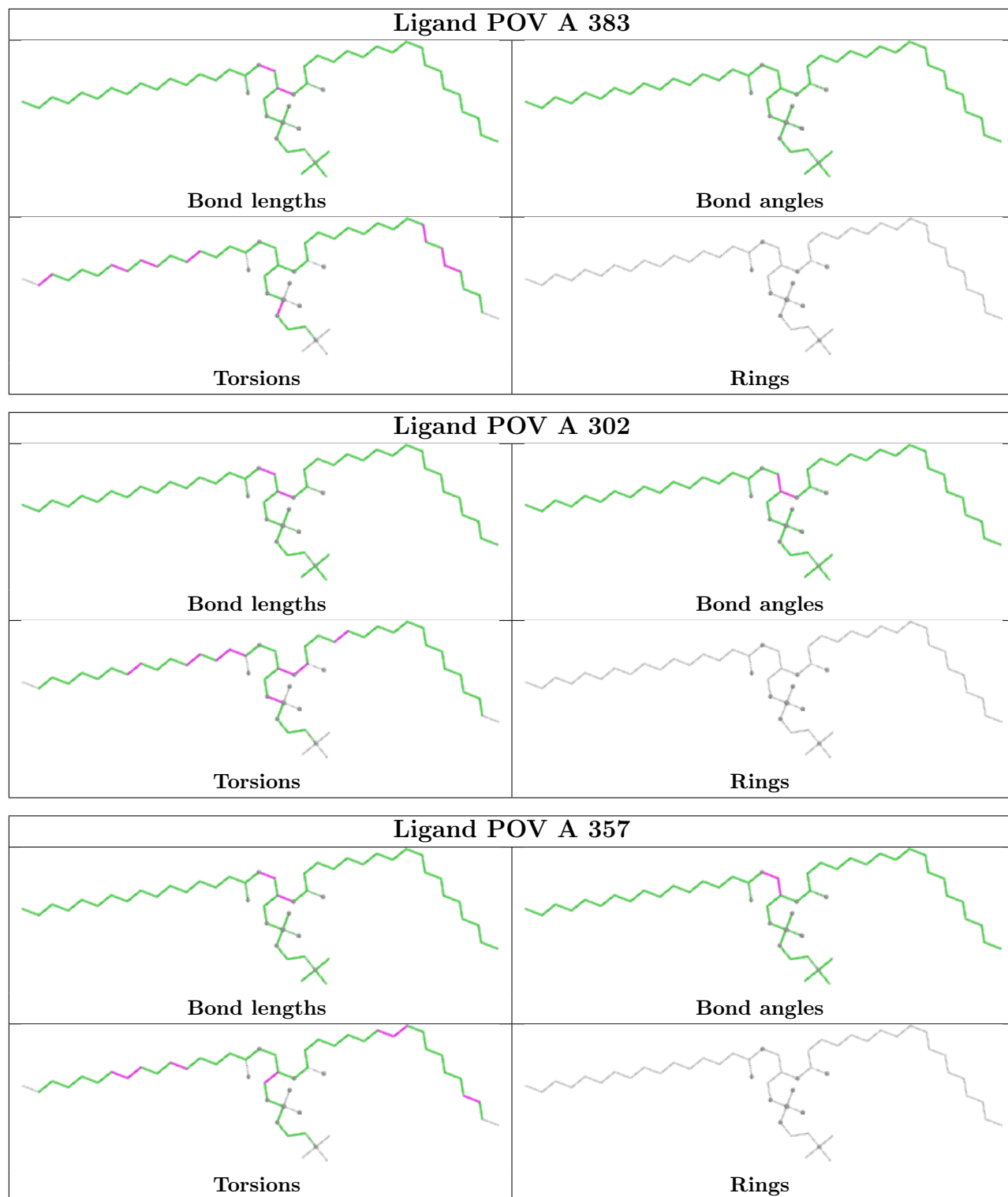


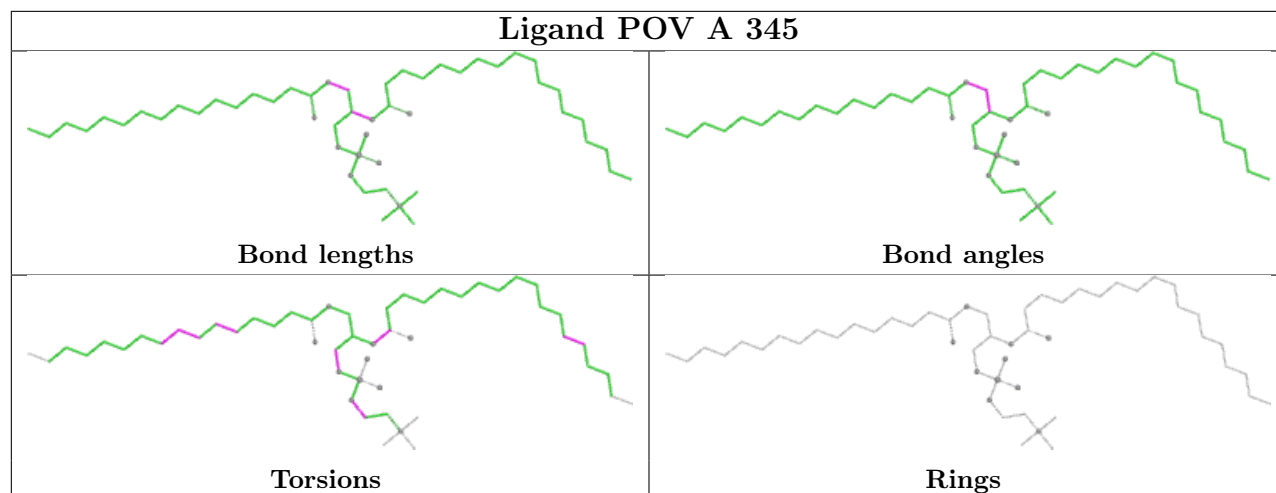












4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.