



Full wwPDB EM Validation Report ⓘ

May 3, 2026 – 12:33 AM JST

PDB ID : 9L0U / pdb_00009l0u
EMDB ID : EMD-62723
Title : Cryo-EM structure of human lipid phosphate phosphatase 1 complexed with PO4.MAG
Authors : Yang, M.; Qian, H.W.
Deposited on : 2024-12-13
Resolution : 2.28 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

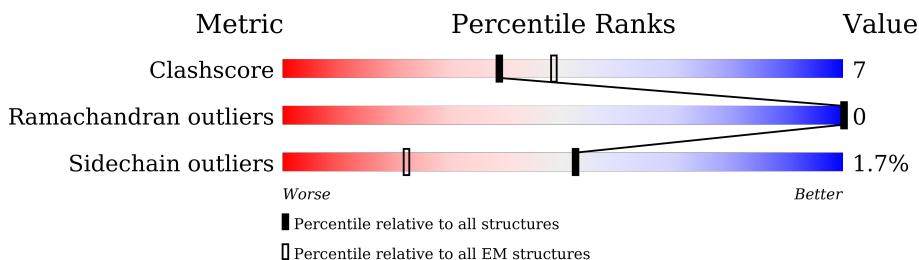
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.28 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	284	73% 15% 11%
1	B	284	72% 17% 11%
1	C	284	72% 16% 11%
1	D	284	71% 18% 11%

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
7	PO4	B	307	-	-	X	-
7	PO4	C	307	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PO4	D	307	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9064 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

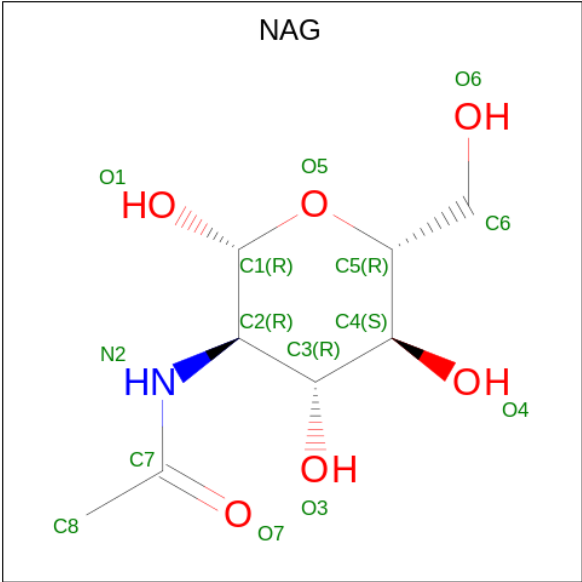
- Molecule 1 is a protein called Phospholipid phosphatase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	252	Total 2003	C 1312	N 329	O 352	S 10	0	0
1	B	252	Total 2003	C 1312	N 329	O 352	S 10	0	0
1	C	252	Total 2003	C 1312	N 329	O 352	S 10	0	0
1	D	252	Total 2003	C 1312	N 329	O 352	S 10	0	0

There are 4 discrepancies between the modelled and reference sequences:

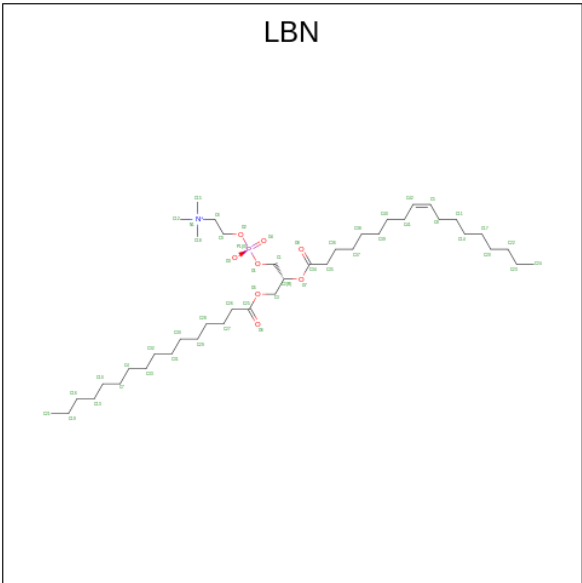
Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ALA	HIS	engineered mutation	UNP O14494
B	223	ALA	HIS	engineered mutation	UNP O14494
C	223	ALA	HIS	engineered mutation	UNP O14494
D	223	ALA	HIS	engineered mutation	UNP O14494

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



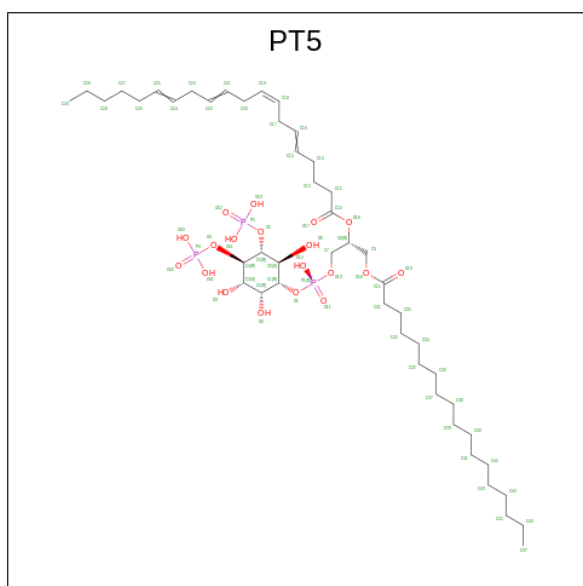
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	14	8	1	5	0
2	B	1	14	8	1	5	0
2	C	1	14	8	1	5	0
2	D	1	14	8	1	5	0

- Molecule 3 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



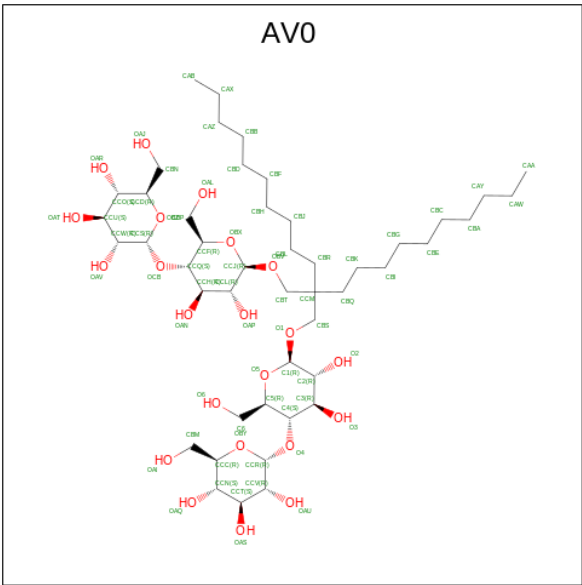
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			45	36	8	1	
3	B	1	Total	C	O	P	0
			45	36	8	1	
3	C	1	Total	C	O	P	0
			45	36	8	1	
3	D	1	Total	C	O	P	0
			45	36	8	1	

- Molecule 4 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: C₄₇H₈₅O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



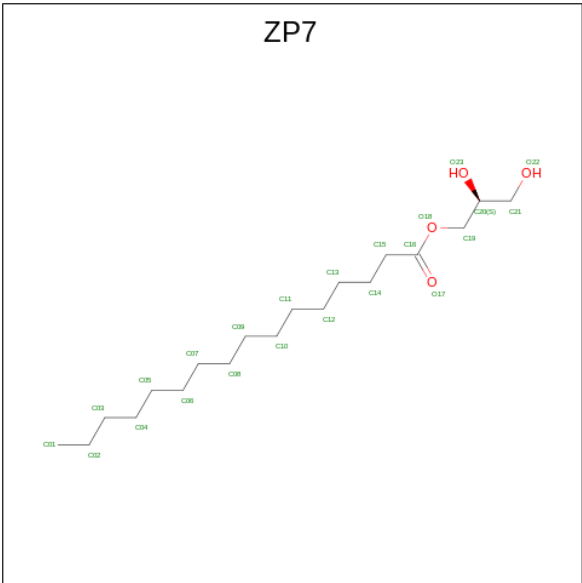
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			62	40	19	3	
4	B	1	Total	C	O	P	0
			62	40	19	3	
4	C	1	Total	C	O	P	0
			62	40	19	3	
4	D	1	Total	C	O	P	0
			62	40	19	3	

- Molecule 5 is Lauryl Maltose Neopentyl Glycol (CCD ID: AV0) (formula: C₄₇H₈₈O₂₂).



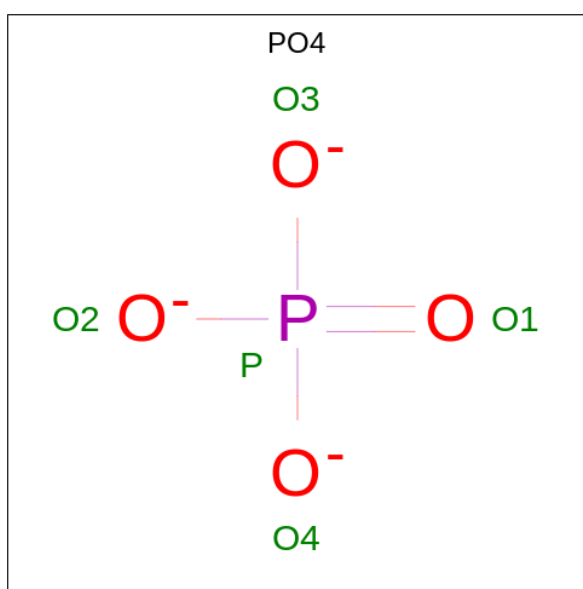
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			58	41	17	
5	B	1	Total	C	O	0
			58	41	17	
5	C	1	Total	C	O	0
			58	41	17	
5	D	1	Total	C	O	0
			58	41	17	

- Molecule 6 is (2S)-2,3-dihydroxypropyl hexadecanoate (CCD ID: ZP7) (formula: C₁₉H₃₈O₄) (labeled as "Ligand of Interest" by depositor).



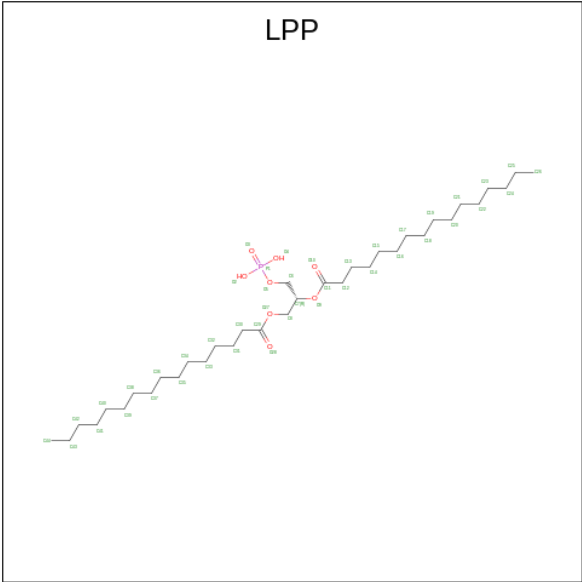
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			23	19	4	
6	B	1	Total	C	O	0
			23	19	4	
6	C	1	Total	C	O	0
			23	19	4	
6	D	1	Total	C	O	0
			23	19	4	

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	O	P	0
			5	4	1	
7	B	1	Total	O	P	0
			5	4	1	
7	C	1	Total	O	P	0
			5	4	1	
7	D	1	Total	O	P	0
			5	4	1	

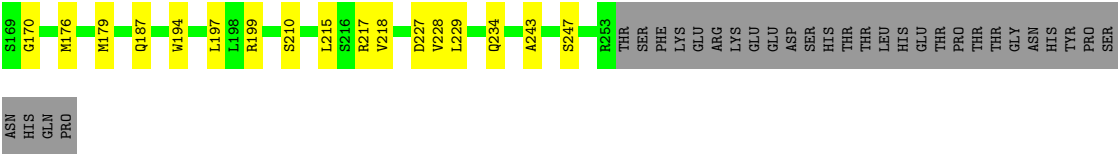
- Molecule 8 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O	P	0
			44	35	8	1	
8	B	1	Total	C	O	P	0
			44	35	8	1	
8	C	1	Total	C	O	P	0
			44	35	8	1	
8	D	1	Total	C	O	P	0
			44	35	8	1	

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	12	Total	O	0
			12	12	
9	B	12	Total	O	0
			12	12	
9	C	12	Total	O	0
			12	12	
9	D	12	Total	O	0
			12	12	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	512703	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZP7, NAG, LPP, AV0, LBN, PO4, PT5

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/2054	0.54	0/2789
1	B	0.24	0/2054	0.49	0/2789
1	C	0.24	0/2054	0.49	0/2789
1	D	0.24	0/2054	0.49	0/2789
All	All	0.25	0/8216	0.50	0/11156

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2003	0	2015	28	0
1	B	2003	0	2015	31	0
1	C	2003	0	2015	31	0
1	D	2003	0	2015	33	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	45	0	0	0	0
3	C	45	0	0	0	0
3	D	45	0	0	0	0
4	A	62	0	65	5	0
4	B	62	0	65	4	0
4	C	62	0	65	3	0
4	D	62	0	65	4	0
5	A	58	0	0	0	0
5	B	58	0	0	0	0
5	C	58	0	0	0	0
5	D	58	0	0	0	0
6	A	23	0	0	1	0
6	B	23	0	0	1	0
6	C	23	0	0	1	0
6	D	23	0	0	1	0
7	A	5	0	0	1	0
7	B	5	0	0	2	0
7	C	5	0	0	2	0
7	D	5	0	0	2	0
8	A	44	0	67	3	0
8	B	44	0	67	3	0
8	C	44	0	67	4	0
8	D	44	0	67	3	0
9	A	12	0	0	0	0
9	B	12	0	0	0	0
9	C	12	0	0	0	0
9	D	12	0	0	0	0
All	All	9064	0	8640	128	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 7.

All (128) 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:D:104:THR:HG21	1:D:247:SER:HB3	1.75	0.69
1:C:104:THR:HG21	1:C:247:SER:HB3	1.75	0.69
1:B:104:THR:HG21	1:B:247:SER:HB3	1.75	0.68
1:A:104:THR:HG21	1:A:247:SER:HB3	1.75	0.67
1:D:52:ASP:OD1	1:D:217:ARG:NH1	2.18	0.64
1:D:127:ARG:NH1	1:D:162:GLU:O	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:NH1	1:B:162:GLU:O	2.30	0.61
1:C:52:ASP:OD1	1:C:217:ARG:NH1	2.19	0.61
1:C:53:THR:HG22	1:C:54:ILE:HG13	1.83	0.60
1:B:53:THR:HG22	1:B:54:ILE:HG13	1.83	0.60
1:A:116:THR:HG22	1:A:120:LYS:HD2	1.83	0.60
1:A:187:GLN:HA	1:A:199:ARG:HD2	1.85	0.59
1:C:116:THR:HG22	1:C:120:LYS:HD2	1.84	0.58
1:D:116:THR:HG22	1:D:120:LYS:HD2	1.84	0.58
1:C:127:ARG:NH1	1:C:162:GLU:O	2.31	0.58
1:B:116:THR:HG22	1:B:120:LYS:HD2	1.84	0.58
1:B:137:ASP:OD1	1:B:139:SER:OG	2.23	0.56
1:B:187:GLN:HA	1:B:199:ARG:HD2	1.86	0.56
1:C:187:GLN:HA	1:C:199:ARG:HD2	1.87	0.56
1:D:187:GLN:HA	1:D:199:ARG:HD2	1.87	0.56
1:C:137:ASP:OD1	1:C:139:SER:OG	2.24	0.55
1:C:243:ALA:O	1:C:247:SER:OG	2.23	0.55
1:B:243:ALA:O	1:B:247:SER:OG	2.24	0.55
1:D:137:ASP:OD1	1:D:139:SER:OG	2.25	0.54
1:D:243:ALA:O	1:D:247:SER:OG	2.24	0.54
1:B:127:ARG:HD3	1:B:129:HIS:CE1	2.44	0.53
1:A:125:ARG:NH1	1:A:227:ASP:OD1	2.41	0.53
1:D:127:ARG:HD3	1:D:129:HIS:CE1	2.44	0.52
1:A:88:SER:HB2	4:A:303:PT5:H16	1.92	0.52
1:A:243:ALA:O	1:A:247:SER:OG	2.27	0.51
1:A:218:VAL:HG23	1:A:228:VAL:HG21	1.92	0.51
1:D:116:THR:HG21	1:D:170:GLY:HA2	1.93	0.51
1:B:127:ARG:NH2	7:B:307:PO4:O3	2.45	0.50
1:A:116:THR:HG21	1:A:170:GLY:HA2	1.94	0.50
1:C:127:ARG:NH2	7:C:307:PO4:O3	2.44	0.50
1:D:127:ARG:NH2	7:D:307:PO4:O3	2.45	0.50
1:C:116:THR:HG21	1:C:170:GLY:HA2	1.93	0.49
1:C:137:ASP:OD2	1:C:140:LYS:NZ	2.41	0.49
1:A:13:ASP:HB3	4:A:303:PT5:H62	1.94	0.49
1:C:127:ARG:HD3	1:C:129:HIS:CE1	2.47	0.49
1:B:13:ASP:HB3	4:B:304:PT5:H62	1.94	0.49
1:B:116:THR:HG21	1:B:170:GLY:HA2	1.93	0.49
1:C:13:ASP:HB3	4:C:304:PT5:H62	1.94	0.49
1:D:13:ASP:HB3	4:D:304:PT5:H62	1.94	0.49
1:B:42:ASP:OD1	1:B:44:SER:OG	2.30	0.49
1:A:218:VAL:HG11	8:A:307:LPP:H302	1.94	0.49
8:B:301:LPP:H261	8:B:301:LPP:H411	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ASP:OD1	1:D:44:SER:OG	2.32	0.48
1:A:27:LEU:HA	1:A:31:HIS:HB2	1.96	0.48
1:A:120:LYS:HB3	1:A:165:LEU:HD22	1.95	0.48
1:B:10:VAL:HG11	4:B:304:PT5:H27	1.96	0.48
1:C:10:VAL:HG11	4:C:304:PT5:H27	1.96	0.48
1:A:167:PHE:HA	1:A:168:TYR:HA	1.64	0.47
1:C:125:ARG:NH1	1:C:227:ASP:OD1	2.48	0.47
1:D:120:LYS:HB3	1:D:165:LEU:HD22	1.96	0.47
1:D:10:VAL:HG11	4:D:304:PT5:H27	1.95	0.47
1:D:125:ARG:NH1	1:D:227:ASP:OD1	2.48	0.47
8:C:301:LPP:H411	8:C:301:LPP:H261	1.96	0.47
1:A:10:VAL:HG11	4:A:303:PT5:H27	1.96	0.47
1:A:42:ASP:OD1	1:A:44:SER:OG	2.31	0.47
1:B:52:ASP:OD1	1:B:217:ARG:NH1	2.28	0.47
1:B:120:LYS:HB3	1:B:165:LEU:HD22	1.97	0.47
8:D:301:LPP:H411	8:D:301:LPP:H261	1.97	0.46
1:C:28:THR:HG23	1:C:117:ASP:OD2	2.15	0.46
1:C:120:LYS:HB3	1:C:165:LEU:HD22	1.97	0.46
8:A:307:LPP:H411	8:A:307:LPP:H261	1.96	0.46
1:B:28:THR:HG23	1:B:117:ASP:OD2	2.15	0.46
1:A:215:LEU:HD13	1:D:119:ALA:HA	1.98	0.46
1:A:28:THR:HG23	1:A:117:ASP:OD2	2.16	0.46
1:D:28:THR:HG23	1:D:117:ASP:OD2	2.16	0.46
1:A:75:GLU:OE1	1:A:97:THR:HB	2.16	0.45
1:C:40:CYS:O	1:C:46:LYS:NZ	2.49	0.45
1:D:40:CYS:O	1:D:46:LYS:NZ	2.49	0.45
1:D:167:PHE:HA	1:D:168:TYR:HA	1.63	0.45
1:C:218:VAL:HG11	8:C:301:LPP:H302	1.99	0.45
1:A:176:MET:HE2	1:A:210:SER:OG	2.16	0.45
6:A:305:ZP7:O22	7:A:306:PO4:O1	2.34	0.45
1:B:63:ILE:HG23	1:B:179:MET:HE3	1.99	0.44
1:C:229:LEU:HD11	8:C:301:LPP:H241	2.00	0.44
6:C:306:ZP7:O22	7:C:307:PO4:O1	2.35	0.44
6:D:306:ZP7:O22	7:D:307:PO4:O1	2.35	0.44
1:D:229:LEU:HD11	8:D:301:LPP:H241	2.00	0.44
1:B:125:ARG:NH1	1:B:227:ASP:OD1	2.48	0.44
1:D:218:VAL:HG11	8:D:301:LPP:H302	2.00	0.44
1:D:63:ILE:HG23	1:D:179:MET:HE3	1.99	0.44
1:A:6:ARG:HA	1:A:9:TYR:HD2	1.82	0.44
1:B:229:LEU:HD11	8:B:301:LPP:H241	2.00	0.44
6:B:306:ZP7:O22	7:B:307:PO4:O1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:HG11	8:B:301:LPP:H302	1.99	0.44
1:C:63:ILE:HG23	1:C:179:MET:HE3	1.99	0.44
1:D:53:THR:HG22	1:D:54:ILE:HG13	2.00	0.44
1:A:103:GLY:HA2	4:A:303:PT5:H69	2.00	0.43
1:B:167:PHE:HA	1:B:168:TYR:HA	1.63	0.43
1:B:218:VAL:HG23	1:B:228:VAL:HG21	2.01	0.43
1:A:53:THR:HG22	1:A:54:ILE:HG13	2.01	0.42
1:B:123:ILE:HD13	1:B:123:ILE:HA	1.85	0.42
1:B:194:TRP:CD1	1:B:194:TRP:H	2.38	0.42
1:D:6:ARG:HA	1:D:9:TYR:HD2	1.84	0.42
1:C:6:ARG:HA	1:C:9:TYR:HD2	1.85	0.42
1:D:137:ASP:OD2	1:D:140:LYS:NZ	2.40	0.42
1:D:194:TRP:CD1	1:D:194:TRP:H	2.37	0.42
1:D:100:LYS:HG2	4:D:304:PT5:H54	2.01	0.42
1:A:119:ALA:HA	1:B:215:LEU:HD13	2.00	0.42
1:D:123:ILE:HD13	1:D:123:ILE:HA	1.85	0.42
1:D:176:MET:HE2	1:D:210:SER:OG	2.20	0.42
1:D:218:VAL:HG23	1:D:228:VAL:HG21	2.02	0.42
1:C:123:ILE:HD13	1:C:123:ILE:HA	1.85	0.42
1:D:197:LEU:HD23	1:D:197:LEU:HA	1.85	0.42
1:C:218:VAL:HG23	1:C:228:VAL:HG21	2.02	0.41
1:C:176:MET:HE2	1:C:210:SER:OG	2.20	0.41
1:A:194:TRP:CD1	1:A:194:TRP:H	2.37	0.41
1:B:100:LYS:HG2	4:B:304:PT5:H54	2.03	0.41
1:B:6:ARG:HA	1:B:9:TYR:HD2	1.84	0.41
1:C:167:PHE:HA	1:C:168:TYR:HA	1.63	0.41
1:B:40:CYS:O	1:B:46:LYS:NZ	2.51	0.41
1:C:100:LYS:HG2	4:C:304:PT5:H54	2.03	0.41
8:C:301:LPP:H402	8:C:301:LPP:H372	1.96	0.41
1:A:63:ILE:HG23	1:A:179:MET:HE3	2.02	0.41
1:A:176:MET:HG2	1:A:232:LEU:O	2.20	0.41
1:C:119:ALA:HA	1:D:215:LEU:HD13	2.02	0.41
1:C:194:TRP:H	1:C:194:TRP:CD1	2.37	0.41
1:A:96:ALA:HA	4:A:303:PT5:H22	2.03	0.41
1:A:229:LEU:HD11	8:A:307:LPP:H241	2.03	0.41
1:B:119:ALA:HA	1:C:215:LEU:HD13	2.02	0.41
1:C:197:LEU:HD23	1:C:197:LEU:HA	1.85	0.40
1:B:103:GLY:HA2	4:B:304:PT5:H69	2.04	0.40
1:D:103:GLY:HA2	4:D:304:PT5:H69	2.03	0.40
1:B:176:MET:HG2	1:B:232:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	250/284 (88%)	244 (98%)	6 (2%)	0	100	100
1	B	250/284 (88%)	245 (98%)	5 (2%)	0	100	100
1	C	250/284 (88%)	245 (98%)	5 (2%)	0	100	100
1	D	250/284 (88%)	245 (98%)	5 (2%)	0	100	100
All	All	1000/1136 (88%)	979 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/247 (87%)	212 (98%)	4 (2%)	50	66
1	B	216/247 (87%)	212 (98%)	4 (2%)	50	66
1	C	216/247 (87%)	212 (98%)	4 (2%)	50	66
1	D	216/247 (87%)	213 (99%)	3 (1%)	59	74
All	All	864/988 (87%)	849 (98%)	15 (2%)	52	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	31	HIS

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Mol	Chain	Res	Type
1	A	113	GLN
1	A	234	GLN
1	B	15	LEU
1	B	53	THR
1	B	142	ASN
1	B	234	GLN
1	C	15	LEU
1	C	53	THR
1	C	142	ASN
1	C	234	GLN
1	D	15	LEU
1	D	142	ASN
1	D	234	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	85	HIS
1	C	85	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PO4	A	306	-	4,4,4	1.12	0	6,6,6	0.46	0
3	LBN	B	303	-	44,44,51	1.26	6 (13%)	48,49,59	1.18	3 (6%)
3	LBN	A	302	-	44,44,51	1.27	6 (13%)	48,49,59	1.19	3 (6%)
4	PT5	C	304	-	62,62,69	0.86	2 (3%)	76,80,87	0.97	3 (3%)
7	PO4	C	307	-	4,4,4	1.13	0	6,6,6	0.39	0
3	LBN	D	303	-	44,44,51	1.27	6 (13%)	48,49,59	1.19	3 (6%)
6	ZP7	B	306	-	22,22,22	0.84	2 (9%)	23,23,23	0.77	1 (4%)
8	LPP	A	307	-	43,43,43	0.91	3 (6%)	47,48,48	1.09	2 (4%)
4	PT5	D	304	-	62,62,69	0.86	2 (3%)	76,80,87	0.97	2 (2%)
5	AV0	C	305	-	60,60,72	0.51	0	78,80,98	1.22	5 (6%)
7	PO4	B	307	-	4,4,4	1.12	0	6,6,6	0.39	0
8	LPP	B	301	-	43,43,43	0.91	3 (6%)	47,48,48	1.09	2 (4%)
8	LPP	C	301	-	43,43,43	0.91	3 (6%)	47,48,48	1.09	2 (4%)
2	NAG	C	302	1	14,14,15	0.49	0	17,19,21	1.17	2 (11%)
2	NAG	A	301	1	14,14,15	0.92	1 (7%)	17,19,21	1.01	2 (11%)
5	AV0	D	305	-	60,60,72	0.51	0	78,80,98	1.22	5 (6%)
6	ZP7	C	306	-	22,22,22	0.83	2 (9%)	23,23,23	0.77	1 (4%)
6	ZP7	D	306	-	22,22,22	0.84	2 (9%)	23,23,23	0.77	1 (4%)
8	LPP	D	301	-	43,43,43	0.91	3 (6%)	47,48,48	1.09	2 (4%)
2	NAG	B	302	1	14,14,15	0.49	0	17,19,21	1.16	2 (11%)
5	AV0	A	304	-	60,60,72	0.50	0	78,80,98	1.22	6 (7%)
3	LBN	C	303	-	44,44,51	1.27	6 (13%)	48,49,59	1.19	3 (6%)
2	NAG	D	302	1	14,14,15	0.50	0	17,19,21	1.16	2 (11%)
7	PO4	D	307	-	4,4,4	1.14	0	6,6,6	0.39	0
4	PT5	A	303	-	62,62,69	0.86	2 (3%)	76,80,87	0.98	2 (2%)
6	ZP7	A	305	-	22,22,22	0.83	2 (9%)	23,23,23	0.78	1 (4%)
5	AV0	B	305	-	60,60,72	0.51	0	78,80,98	1.22	6 (7%)
4	PT5	B	304	-	62,62,69	0.86	2 (3%)	76,80,87	0.97	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LBN	B	303	-	-	20/46/46/55	-
3	LBN	A	302	-	-	21/46/46/55	-
4	PT5	C	304	-	-	17/59/83/90	0/1/1/1
3	LBN	D	303	-	-	20/46/46/55	-
6	ZP7	B	306	-	-	6/22/22/22	-
8	LPP	A	307	-	-	13/45/45/45	-
4	PT5	D	304	-	-	17/59/83/90	0/1/1/1
5	AV0	C	305	-	-	27/44/104/130	0/3/3/4
8	LPP	B	301	-	-	14/45/45/45	-
8	LPP	C	301	-	-	14/45/45/45	-
2	NAG	C	302	1	-	1/6/23/26	0/1/1/1
2	NAG	A	301	1	-	2/6/23/26	0/1/1/1
5	AV0	D	305	-	-	27/44/104/130	0/3/3/4
6	ZP7	C	306	-	-	7/22/22/22	-
6	ZP7	D	306	-	-	6/22/22/22	-
8	LPP	D	301	-	-	14/45/45/45	-
2	NAG	B	302	1	-	1/6/23/26	0/1/1/1
5	AV0	A	304	-	-	28/44/104/130	0/3/3/4
3	LBN	C	303	-	-	20/46/46/55	-
2	NAG	D	302	1	-	1/6/23/26	0/1/1/1
4	PT5	A	303	-	-	17/59/83/90	0/1/1/1
6	ZP7	A	305	-	-	10/22/22/22	-
5	AV0	B	305	-	-	27/44/104/130	0/3/3/4
4	PT5	B	304	-	-	17/59/83/90	0/1/1/1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	304	PT5	O18-C11	4.12	1.45	1.33
4	A	303	PT5	O18-C11	4.12	1.45	1.33
4	C	304	PT5	O18-C11	4.11	1.45	1.33
4	B	304	PT5	O18-C11	4.11	1.45	1.33
4	B	304	PT5	O16-C10	3.94	1.45	1.34
4	C	304	PT5	O16-C10	3.93	1.45	1.34
4	D	304	PT5	O16-C10	3.93	1.45	1.34
4	A	303	PT5	O16-C10	3.92	1.45	1.34
3	C	303	LBN	C42-C5	3.69	1.53	1.31
3	B	303	LBN	C42-C5	3.69	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	LBN	C42-C5	3.69	1.53	1.31
3	D	303	LBN	C42-C5	3.68	1.53	1.31
3	D	303	LBN	C33-C4	-3.52	1.31	1.51
3	A	302	LBN	C33-C4	-3.52	1.31	1.51
3	B	303	LBN	C33-C4	-3.51	1.31	1.51
3	C	303	LBN	C33-C4	-3.51	1.31	1.51
3	B	303	LBN	C41-C42	-3.22	1.31	1.50
3	C	303	LBN	C41-C42	-3.22	1.31	1.50
3	D	303	LBN	C41-C42	-3.22	1.32	1.50
3	A	302	LBN	C41-C42	-3.21	1.32	1.50
2	A	301	NAG	O5-C1	-3.10	1.38	1.43
8	C	301	LPP	O9-C7	-2.76	1.39	1.46
8	B	301	LPP	O9-C7	-2.75	1.39	1.46
8	D	301	LPP	O9-C7	-2.75	1.39	1.46
8	A	307	LPP	O9-C7	-2.74	1.39	1.46
3	D	303	LBN	O7-C2	-2.60	1.40	1.46
3	B	303	LBN	O7-C2	-2.59	1.40	1.46
8	C	301	LPP	O27-C29	2.59	1.40	1.33
3	A	302	LBN	O7-C2	-2.57	1.40	1.46
8	B	301	LPP	O27-C29	2.57	1.40	1.33
8	A	307	LPP	O27-C29	2.57	1.40	1.33
3	C	303	LBN	O7-C2	-2.57	1.40	1.46
8	D	301	LPP	O27-C29	2.57	1.40	1.33
3	D	303	LBN	O5-C25	2.40	1.40	1.33
3	C	303	LBN	O5-C25	2.39	1.40	1.33
6	A	305	ZP7	O18-C19	-2.38	1.39	1.45
6	B	306	ZP7	O18-C19	-2.38	1.39	1.45
6	D	306	ZP7	O18-C19	-2.37	1.39	1.45
3	B	303	LBN	O5-C25	2.37	1.40	1.33
6	C	306	ZP7	O18-C19	-2.37	1.39	1.45
3	A	302	LBN	O5-C25	2.36	1.40	1.33
6	B	306	ZP7	O18-C16	2.29	1.40	1.33
6	D	306	ZP7	O18-C16	2.27	1.40	1.33
6	C	306	ZP7	O18-C16	2.25	1.39	1.33
6	A	305	ZP7	O18-C16	2.25	1.39	1.33
3	A	302	LBN	O5-C3	-2.21	1.40	1.45
3	C	303	LBN	O5-C3	-2.18	1.40	1.45
3	D	303	LBN	O5-C3	-2.17	1.40	1.45
3	B	303	LBN	O5-C3	-2.17	1.40	1.45
8	B	301	LPP	O9-C11	2.09	1.40	1.34
8	C	301	LPP	O9-C11	2.08	1.40	1.34
8	D	301	LPP	O9-C11	2.06	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	307	LPP	O9-C11	2.05	1.40	1.34

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	305	AV0	O1-C1-C2	5.22	116.46	108.30
5	A	304	AV0	O1-C1-C2	5.21	116.44	108.30
5	B	305	AV0	O1-C1-C2	5.20	116.42	108.30
5	D	305	AV0	O1-C1-C2	5.20	116.42	108.30
3	D	303	LBN	O7-C34-C35	4.17	120.49	111.50
3	C	303	LBN	O7-C34-C35	4.17	120.49	111.50
3	A	302	LBN	O7-C34-C35	4.16	120.48	111.50
3	B	303	LBN	O7-C34-C35	4.06	120.26	111.50
8	B	301	LPP	O9-C11-C12	3.79	119.67	111.50
8	C	301	LPP	O9-C11-C12	3.79	119.66	111.50
8	D	301	LPP	O9-C11-C12	3.78	119.66	111.50
8	A	307	LPP	O9-C11-C12	3.78	119.65	111.50
4	C	304	PT5	O16-C10-C12	3.77	119.64	111.50
5	D	305	AV0	CCR-OBY-CCC	3.76	121.07	113.69
5	A	304	AV0	CCR-OBY-CCC	3.75	121.06	113.69
5	C	305	AV0	CCR-OBY-CCC	3.74	121.03	113.69
4	B	304	PT5	O16-C10-C12	3.74	119.56	111.50
5	B	305	AV0	CCR-OBY-CCC	3.73	121.01	113.69
4	A	303	PT5	O16-C10-C12	3.73	119.54	111.50
4	D	304	PT5	O16-C10-C12	3.71	119.50	111.50
5	A	304	AV0	CBS-O1-C1	3.69	122.95	113.36
5	D	305	AV0	CBS-O1-C1	3.66	122.87	113.36
5	B	305	AV0	CBS-O1-C1	3.65	122.84	113.36
5	C	305	AV0	CBS-O1-C1	3.64	122.82	113.36
5	C	305	AV0	O2-C2-C3	-3.39	102.52	110.35
5	D	305	AV0	O2-C2-C3	-3.38	102.54	110.35
5	B	305	AV0	O2-C2-C3	-3.36	102.58	110.35
5	A	304	AV0	O2-C2-C3	-3.35	102.60	110.35
2	B	302	NAG	C1-O5-C5	3.13	116.43	112.19
2	C	302	NAG	C1-O5-C5	3.13	116.43	112.19
2	D	302	NAG	C1-O5-C5	3.11	116.41	112.19
2	A	301	NAG	C3-C4-C5	3.08	115.73	110.24
2	C	302	NAG	C3-C4-C5	2.86	115.35	110.24
2	D	302	NAG	C3-C4-C5	2.85	115.33	110.24
2	B	302	NAG	C3-C4-C5	2.82	115.26	110.24
4	D	304	PT5	O18-C11-C31	2.69	120.36	111.91
4	A	303	PT5	O18-C11-C31	2.66	120.25	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	304	PT5	O18-C11-C31	2.60	120.08	111.91
4	B	304	PT5	O18-C11-C31	2.60	120.06	111.91
6	C	306	ZP7	O18-C16-C15	2.49	119.73	111.91
6	B	306	ZP7	O18-C16-C15	2.48	119.69	111.91
6	D	306	ZP7	O18-C16-C15	2.48	119.69	111.91
6	A	305	ZP7	O18-C16-C15	2.46	119.62	111.91
3	C	303	LBN	O5-C25-C26	2.45	119.58	111.91
3	D	303	LBN	O5-C25-C26	2.43	119.54	111.91
3	A	302	LBN	O5-C25-C26	2.42	119.51	111.91
3	B	303	LBN	O5-C25-C26	2.42	119.50	111.91
8	B	301	LPP	O27-C29-C30	2.28	119.07	111.91
8	A	307	LPP	O27-C29-C30	2.28	119.06	111.91
8	C	301	LPP	O27-C29-C30	2.28	119.06	111.91
8	D	301	LPP	O27-C29-C30	2.27	119.04	111.91
5	C	305	AV0	CBT-OBV-CCJ	2.11	118.86	113.36
5	B	305	AV0	CBT-OBV-CCJ	2.10	118.83	113.36
2	A	301	NAG	C4-C3-C2	2.09	114.08	111.02
5	D	305	AV0	CBT-OBV-CCJ	2.07	118.74	113.36
5	A	304	AV0	CBT-OBV-CCJ	2.06	118.71	113.36
5	A	304	AV0	C2-C3-C4	2.01	114.28	109.68
4	C	304	PT5	C12-C13-C14	-2.01	109.64	113.23
5	B	305	AV0	C2-C3-C4	2.01	114.27	109.68
3	A	302	LBN	C8-C5-C42	-2.01	109.33	124.73
3	B	303	LBN	C8-C5-C42	-2.01	109.33	124.73
3	C	303	LBN	C8-C5-C42	-2.00	109.37	124.73
3	D	303	LBN	C8-C5-C42	-2.00	109.37	124.73

There are no chirality outliers.

All (347) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	PT5	C7-O13-P1-O11
4	A	303	PT5	C7-O13-P1-O1
4	A	303	PT5	C1-O1-P1-O12
4	B	304	PT5	C7-O13-P1-O11
4	B	304	PT5	C7-O13-P1-O1
4	B	304	PT5	C1-O1-P1-O12
4	B	304	PT5	O17-C10-O16-C8
4	C	304	PT5	C7-O13-P1-O11
4	C	304	PT5	C7-O13-P1-O1
4	C	304	PT5	C1-O1-P1-O12
4	D	304	PT5	C7-O13-P1-O11

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Mol	Chain	Res	Type	Atoms
4	D	304	PT5	C7-O13-P1-O1
4	D	304	PT5	C1-O1-P1-O12
4	D	304	PT5	O17-C10-O16-C8
5	A	304	AV0	C2-C1-O1-CBS
5	A	304	AV0	O5-C1-O1-CBS
5	A	304	AV0	CBK-CBQ-CCM-CBR
5	A	304	AV0	CBK-CBQ-CCM-CBS
5	A	304	AV0	CBK-CBQ-CCM-CBT
5	A	304	AV0	CBL-CBR-CCM-CBQ
5	A	304	AV0	CBL-CBR-CCM-CBS
5	B	305	AV0	C2-C1-O1-CBS
5	B	305	AV0	O5-C1-O1-CBS
5	B	305	AV0	CBK-CBQ-CCM-CBR
5	B	305	AV0	CBK-CBQ-CCM-CBS
5	B	305	AV0	CBK-CBQ-CCM-CBT
5	B	305	AV0	CBL-CBR-CCM-CBQ
5	B	305	AV0	CBL-CBR-CCM-CBS
5	B	305	AV0	OBX-CCJ-OBV-CBT
5	C	305	AV0	C2-C1-O1-CBS
5	C	305	AV0	O5-C1-O1-CBS
5	C	305	AV0	CBK-CBQ-CCM-CBR
5	C	305	AV0	CBK-CBQ-CCM-CBS
5	C	305	AV0	CBK-CBQ-CCM-CBT
5	C	305	AV0	CBL-CBR-CCM-CBQ
5	C	305	AV0	CBL-CBR-CCM-CBS
5	C	305	AV0	OBX-CCJ-OBV-CBT
5	D	305	AV0	C2-C1-O1-CBS
5	D	305	AV0	O5-C1-O1-CBS
5	D	305	AV0	CBK-CBQ-CCM-CBR
5	D	305	AV0	CBK-CBQ-CCM-CBS
5	D	305	AV0	CBK-CBQ-CCM-CBT
5	D	305	AV0	CBL-CBR-CCM-CBQ
5	D	305	AV0	CBL-CBR-CCM-CBS
5	D	305	AV0	OBX-CCJ-OBV-CBT
8	A	307	LPP	C6-O5-P1-O2
8	B	301	LPP	C6-O5-P1-O2
8	C	301	LPP	C6-O5-P1-O2
8	D	301	LPP	C6-O5-P1-O2
5	A	304	AV0	OBY-CCR-O4-C4
5	B	305	AV0	OBY-CCR-O4-C4
5	C	305	AV0	OBY-CCR-O4-C4
5	D	305	AV0	OBY-CCR-O4-C4

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Mol	Chain	Res	Type	Atoms
4	A	303	PT5	O17-C10-O16-C8
4	C	304	PT5	O17-C10-O16-C8
4	B	304	PT5	C12-C10-O16-C8
4	C	304	PT5	C12-C10-O16-C8
4	D	304	PT5	C12-C10-O16-C8
5	B	305	AV0	OAI-CBM-CCC-OBY
5	C	305	AV0	OAI-CBM-CCC-OBY
5	A	304	AV0	OAI-CBM-CCC-OBY
5	D	305	AV0	OAI-CBM-CCC-OBY
4	A	303	PT5	C12-C10-O16-C8
2	A	301	NAG	C4-C5-C6-O6
5	A	304	AV0	OBX-CCJ-OBV-CBT
5	B	305	AV0	OAI-CBM-CCC-CCN
5	C	305	AV0	OAI-CBM-CCC-CCN
5	D	305	AV0	OAI-CBM-CCC-CCN
3	A	302	LBN	C26-C25-O5-C3
3	B	303	LBN	C26-C25-O5-C3
3	C	303	LBN	C26-C25-O5-C3
3	D	303	LBN	C26-C25-O5-C3
5	A	304	AV0	CCL-CCJ-OBV-CBT
5	B	305	AV0	CCL-CCJ-OBV-CBT
5	C	305	AV0	CCL-CCJ-OBV-CBT
5	D	305	AV0	CCL-CCJ-OBV-CBT
2	A	301	NAG	O5-C5-C6-O6
6	B	306	ZP7	C08-C09-C10-C11
6	D	306	ZP7	C08-C09-C10-C11
5	A	304	AV0	C4-C5-C6-O6
5	A	304	AV0	OAL-CBP-CCF-CCQ
5	B	305	AV0	OAL-CBP-CCF-CCQ
5	C	305	AV0	OAL-CBP-CCF-CCQ
5	D	305	AV0	OAL-CBP-CCF-CCQ
5	A	304	AV0	CBJ-CBL-CBR-CCM
5	B	305	AV0	CBJ-CBL-CBR-CCM
5	C	305	AV0	CBJ-CBL-CBR-CCM
5	D	305	AV0	CBJ-CBL-CBR-CCM
6	C	306	ZP7	C08-C09-C10-C11
6	A	305	ZP7	C08-C09-C10-C11
5	A	304	AV0	OAI-CBM-CCC-CCN
3	B	303	LBN	O6-C25-O5-C3
3	C	303	LBN	O6-C25-O5-C3
3	D	303	LBN	O6-C25-O5-C3
3	A	302	LBN	O6-C25-O5-C3

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Mol	Chain	Res	Type	Atoms
3	A	302	LBN	C41-C42-C5-C8
3	B	303	LBN	C41-C42-C5-C8
3	C	303	LBN	C41-C42-C5-C8
3	D	303	LBN	C41-C42-C5-C8
5	A	304	AV0	O5-C5-C6-O6
5	B	305	AV0	C4-C5-C6-O6
5	D	305	AV0	C4-C5-C6-O6
4	B	304	PT5	C40-C41-C42-C43
4	C	304	PT5	C40-C41-C42-C43
4	A	303	PT5	C40-C41-C42-C43
4	D	304	PT5	C40-C41-C42-C43
6	D	306	ZP7	C10-C11-C12-C13
5	C	305	AV0	C4-C5-C6-O6
6	B	306	ZP7	C10-C11-C12-C13
6	C	306	ZP7	C10-C11-C12-C13
8	A	307	LPP	C34-C35-C36-C37
4	A	303	PT5	C38-C39-C40-C41
5	A	304	AV0	CBI-CBK-CBQ-CCM
4	B	304	PT5	C38-C39-C40-C41
4	C	304	PT5	C38-C39-C40-C41
4	D	304	PT5	C38-C39-C40-C41
6	A	305	ZP7	C10-C11-C12-C13
5	A	304	AV0	OAL-CBP-CCF-OBX
5	B	305	AV0	OAL-CBP-CCF-OBX
5	D	305	AV0	OAL-CBP-CCF-OBX
8	C	301	LPP	C34-C35-C36-C37
8	D	301	LPP	C34-C35-C36-C37
5	C	305	AV0	OAL-CBP-CCF-OBX
8	B	301	LPP	C34-C35-C36-C37
8	D	301	LPP	C39-C40-C41-C42
3	B	303	LBN	C39-C40-C41-C42
3	C	303	LBN	C38-C39-C40-C41
3	D	303	LBN	C38-C39-C40-C41
5	A	304	AV0	CBE-CBG-CBI-CBK
5	B	305	AV0	CBE-CBG-CBI-CBK
5	C	305	AV0	CBE-CBG-CBI-CBK
5	D	305	AV0	CBE-CBG-CBI-CBK
8	A	307	LPP	C39-C40-C41-C42
8	B	301	LPP	C39-C40-C41-C42
8	C	301	LPP	C39-C40-C41-C42
8	C	301	LPP	C40-C41-C42-C43
3	A	302	LBN	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
3	B	303	LBN	C38-C39-C40-C41
8	B	301	LPP	C40-C41-C42-C43
8	D	301	LPP	C40-C41-C42-C43
8	A	307	LPP	C40-C41-C42-C43
5	A	304	AV0	CBG-CBI-CBK-CBQ
5	C	305	AV0	CBI-CBK-CBQ-CCM
5	D	305	AV0	CBI-CBK-CBQ-CCM
5	D	305	AV0	O5-C5-C6-O6
5	B	305	AV0	O5-C5-C6-O6
3	A	302	LBN	C39-C40-C41-C42
3	C	303	LBN	C39-C40-C41-C42
3	D	303	LBN	C39-C40-C41-C42
5	C	305	AV0	O5-C5-C6-O6
5	B	305	AV0	CBI-CBK-CBQ-CCM
5	B	305	AV0	CBG-CBI-CBK-CBQ
5	D	305	AV0	CBG-CBI-CBK-CBQ
8	B	301	LPP	C36-C37-C38-C39
5	C	305	AV0	CBG-CBI-CBK-CBQ
8	D	301	LPP	C36-C37-C38-C39
8	C	301	LPP	C36-C37-C38-C39
6	B	306	ZP7	C01-C02-C03-C04
6	C	306	ZP7	C01-C02-C03-C04
6	D	306	ZP7	C01-C02-C03-C04
5	A	304	AV0	CAZ-CBB-CBD-CBF
3	A	302	LBN	C33-C4-C7-C10
3	A	302	LBN	C27-C28-C29-C30
5	B	305	AV0	CAZ-CBB-CBD-CBF
5	C	305	AV0	CAZ-CBB-CBD-CBF
5	D	305	AV0	CAZ-CBB-CBD-CBF
4	B	304	PT5	C34-C35-C36-C37
4	C	304	PT5	C34-C35-C36-C37
4	D	304	PT5	C34-C35-C36-C37
3	A	302	LBN	C35-C34-O7-C2
3	B	303	LBN	C35-C34-O7-C2
3	C	303	LBN	C35-C34-O7-C2
3	D	303	LBN	C35-C34-O7-C2
3	B	303	LBN	C27-C28-C29-C30
3	C	303	LBN	C27-C28-C29-C30
3	D	303	LBN	C27-C28-C29-C30
3	A	302	LBN	O8-C34-O7-C2
3	B	303	LBN	O8-C34-O7-C2
3	C	303	LBN	O8-C34-O7-C2

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Mol	Chain	Res	Type	Atoms
8	A	307	LPP	C36-C37-C38-C39
4	A	303	PT5	C34-C35-C36-C37
4	A	303	PT5	C33-C34-C35-C36
4	C	304	PT5	C33-C34-C35-C36
4	B	304	PT5	C33-C34-C35-C36
3	D	303	LBN	O8-C34-O7-C2
4	D	304	PT5	C33-C34-C35-C36
5	B	305	AV0	CBA-CBC-CBE-CBG
5	D	305	AV0	CBA-CBC-CBE-CBG
5	A	304	AV0	CBA-CBC-CBE-CBG
5	C	305	AV0	CBA-CBC-CBE-CBG
3	D	303	LBN	C33-C4-C7-C10
3	B	303	LBN	C33-C4-C7-C10
3	C	303	LBN	C33-C4-C7-C10
2	B	302	NAG	O5-C5-C6-O6
2	D	302	NAG	O5-C5-C6-O6
4	A	303	PT5	C7-C8-O16-C10
4	B	304	PT5	C7-C8-O16-C10
4	C	304	PT5	C7-C8-O16-C10
4	D	304	PT5	C7-C8-O16-C10
2	C	302	NAG	O5-C5-C6-O6
3	B	303	LBN	C14-C17-C20-C22
3	C	303	LBN	C14-C17-C20-C22
3	D	303	LBN	C14-C17-C20-C22
6	A	305	ZP7	C01-C02-C03-C04
6	A	305	ZP7	C15-C16-O18-C19
4	A	303	PT5	C1-O1-P1-O13
4	B	304	PT5	C1-O1-P1-O13
4	C	304	PT5	C1-O1-P1-O13
3	A	302	LBN	C14-C17-C20-C22
3	A	302	LBN	C1-C2-C3-O5
3	B	303	LBN	C1-C2-C3-O5
3	C	303	LBN	C1-C2-C3-O5
3	D	303	LBN	C1-C2-C3-O5
4	B	304	PT5	C1-O1-P1-O11
4	C	304	PT5	C1-O1-P1-O11
4	D	304	PT5	C1-O1-P1-O11
3	A	302	LBN	C31-C32-C33-C4
4	A	303	PT5	C15-C16-C17-C18
4	B	304	PT5	C15-C16-C17-C18
4	C	304	PT5	C15-C16-C17-C18
4	D	304	PT5	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
3	A	302	LBN	C8-C11-C14-C17
3	D	303	LBN	C8-C11-C14-C17
3	B	303	LBN	C8-C11-C14-C17
3	C	303	LBN	C8-C11-C14-C17
6	A	305	ZP7	C04-C05-C06-C07
3	A	302	LBN	C28-C29-C30-C31
3	D	303	LBN	C28-C29-C30-C31
3	C	303	LBN	C28-C29-C30-C31
4	D	304	PT5	C1-O1-P1-O13
3	B	303	LBN	C28-C29-C30-C31
8	A	307	LPP	C6-O5-P1-O4
8	B	301	LPP	C6-O5-P1-O4
8	C	301	LPP	C6-O5-P1-O4
8	D	301	LPP	C6-O5-P1-O4
6	A	305	ZP7	C03-C04-C05-C06
6	A	305	ZP7	O17-C16-O18-C19
6	B	306	ZP7	C11-C12-C13-C14
3	B	303	LBN	O7-C2-C3-O5
3	D	303	LBN	O7-C2-C3-O5
6	C	306	ZP7	C11-C12-C13-C14
6	D	306	ZP7	C11-C12-C13-C14
5	A	304	AV0	O1-CBS-CCM-CBR
5	B	305	AV0	O1-CBS-CCM-CBQ
5	B	305	AV0	O1-CBS-CCM-CBR
5	C	305	AV0	O1-CBS-CCM-CBR
5	D	305	AV0	O1-CBS-CCM-CBQ
5	D	305	AV0	O1-CBS-CCM-CBR
3	B	303	LBN	C14-C11-C8-C5
8	A	307	LPP	C35-C36-C37-C38
6	A	305	ZP7	C12-C13-C14-C15
8	C	301	LPP	C35-C36-C37-C38
4	A	303	PT5	C10-C12-C13-C14
8	D	301	LPP	C35-C36-C37-C38
8	B	301	LPP	C35-C36-C37-C38
3	C	303	LBN	C30-C31-C32-C33
5	B	305	AV0	O1-CBS-CCM-CBT
5	D	305	AV0	O1-CBS-CCM-CBT
3	D	303	LBN	C30-C31-C32-C33
6	D	306	ZP7	C15-C16-O18-C19
5	A	304	AV0	O1-CBS-CCM-CBT
5	C	305	AV0	O1-CBS-CCM-CBT
3	A	302	LBN	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
3	B	303	LBN	C30-C31-C32-C33
6	C	306	ZP7	C15-C16-O18-C19
6	A	305	ZP7	C11-C12-C13-C14
3	A	302	LBN	O7-C2-C3-O5
3	C	303	LBN	O7-C2-C3-O5
6	B	306	ZP7	C15-C16-O18-C19
3	A	302	LBN	C14-C11-C8-C5
3	C	303	LBN	C14-C11-C8-C5
3	D	303	LBN	C14-C11-C8-C5
3	A	302	LBN	C40-C41-C42-C5
3	B	303	LBN	C40-C41-C42-C5
3	C	303	LBN	C40-C41-C42-C5
3	D	303	LBN	C40-C41-C42-C5
6	D	306	ZP7	O17-C16-O18-C19
8	A	307	LPP	C6-O5-P1-O3
8	B	301	LPP	C6-O5-P1-O3
8	C	301	LPP	C6-O5-P1-O3
8	D	301	LPP	C6-O5-P1-O3
6	B	306	ZP7	O17-C16-O18-C19
6	C	306	ZP7	O17-C16-O18-C19
3	C	303	LBN	O1-C1-C2-O7
3	D	303	LBN	O1-C1-C2-O7
3	C	303	LBN	C42-C5-C8-C11
8	A	307	LPP	C6-C7-C8-O27
8	B	301	LPP	C6-C7-C8-O27
8	C	301	LPP	C6-C7-C8-O27
8	D	301	LPP	C6-C7-C8-O27
3	A	302	LBN	C42-C5-C8-C11
3	B	303	LBN	C42-C5-C8-C11
3	D	303	LBN	C42-C5-C8-C11
4	C	304	PT5	C39-C40-C41-C42
4	A	303	PT5	C1-O1-P1-O11
4	A	303	PT5	C39-C40-C41-C42
4	B	304	PT5	C39-C40-C41-C42
4	D	304	PT5	C39-C40-C41-C42
3	A	302	LBN	O1-C1-C2-O7
3	B	303	LBN	O1-C1-C2-O7
8	B	301	LPP	C32-C33-C34-C35
8	D	301	LPP	C32-C33-C34-C35
4	D	304	PT5	C10-C12-C13-C14
5	A	304	AV0	CBB-CBD-CBF-CBH
8	C	301	LPP	C32-C33-C34-C35

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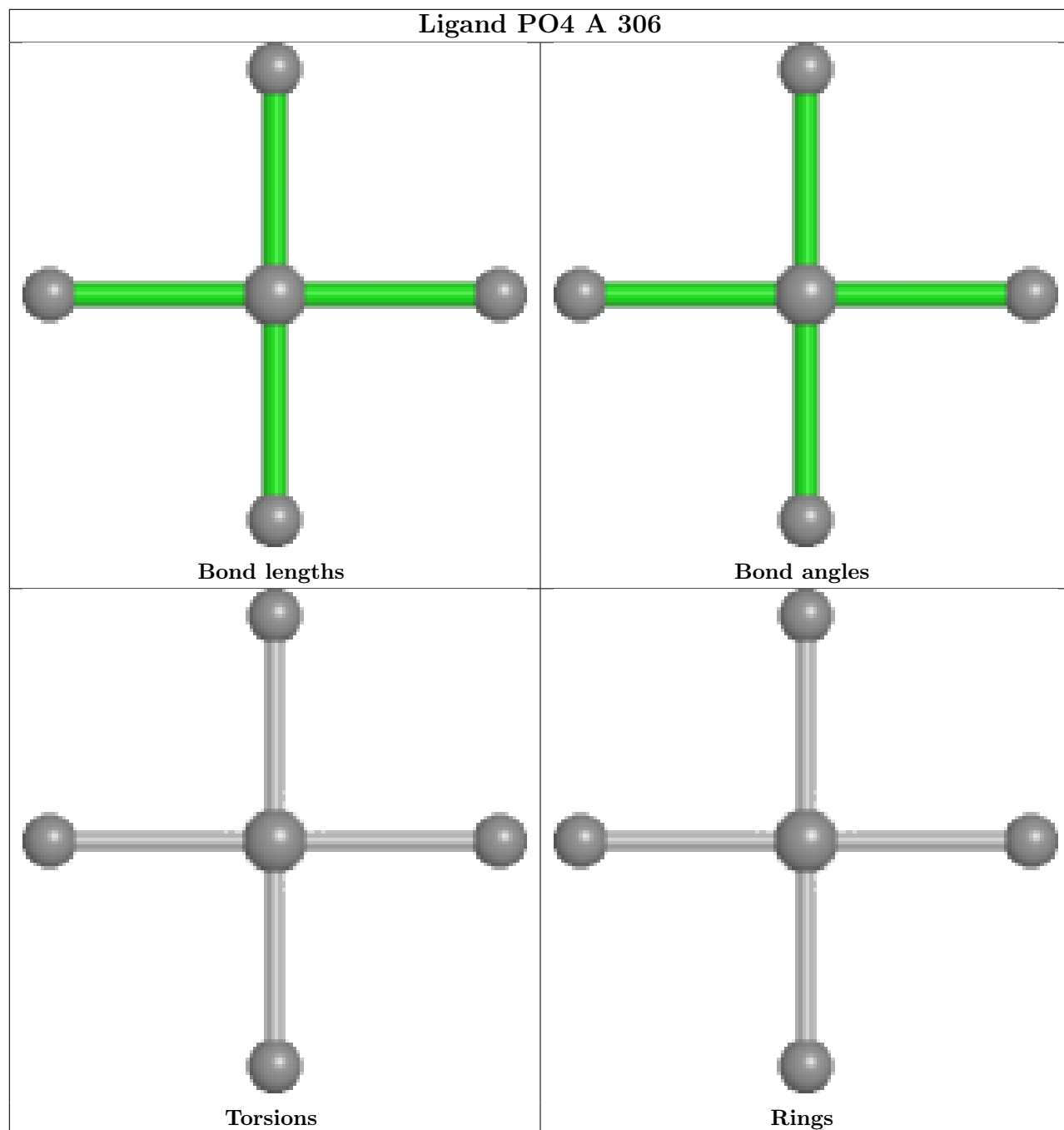
Mol	Chain	Res	Type	Atoms
5	C	305	AV0	CBB-CBD-CBF-CBH
5	A	304	AV0	CBF-CBH-CBJ-CBL
5	B	305	AV0	CBB-CBD-CBF-CBH
5	D	305	AV0	CBB-CBD-CBF-CBH
6	A	305	ZP7	C14-C15-C16-O18
4	B	304	PT5	O16-C10-C12-C13
4	C	304	PT5	O16-C10-C12-C13
4	D	304	PT5	O16-C10-C12-C13
8	B	301	LPP	O9-C11-C12-C13
8	A	307	LPP	C19-C20-C21-C22
4	A	303	PT5	O16-C10-C12-C13
8	A	307	LPP	C21-C22-C23-C24
8	D	301	LPP	C19-C20-C21-C22
8	A	307	LPP	O9-C11-C12-C13
8	C	301	LPP	O9-C11-C12-C13
8	D	301	LPP	O9-C11-C12-C13
8	B	301	LPP	C19-C20-C21-C22
8	C	301	LPP	C19-C20-C21-C22
5	B	305	AV0	CBF-CBH-CBJ-CBL
5	C	305	AV0	CBF-CBH-CBJ-CBL
5	D	305	AV0	CBF-CBH-CBJ-CBL
5	A	304	AV0	CBC-CBE-CBG-CBI
5	A	304	AV0	O1-CBS-CCM-CBQ
5	C	305	AV0	O1-CBS-CCM-CBQ
4	D	304	PT5	O17-C10-C12-C13
4	C	304	PT5	C10-C12-C13-C14
4	B	304	PT5	O17-C10-C12-C13
4	A	303	PT5	O17-C10-C12-C13
8	C	301	LPP	O10-C11-C12-C13
8	D	301	LPP	O10-C11-C12-C13
8	C	301	LPP	C21-C22-C23-C24
4	C	304	PT5	O17-C10-C12-C13
8	A	307	LPP	O10-C11-C12-C13
8	D	301	LPP	C21-C22-C23-C24
8	B	301	LPP	O10-C11-C12-C13
8	B	301	LPP	C21-C22-C23-C24
4	B	304	PT5	C10-C12-C13-C14
3	C	303	LBN	O7-C34-C35-C36
3	A	302	LBN	O7-C34-C35-C36
3	D	303	LBN	O7-C34-C35-C36
3	B	303	LBN	O7-C34-C35-C36
6	C	306	ZP7	C14-C15-C16-O18

There are no ring outliers.

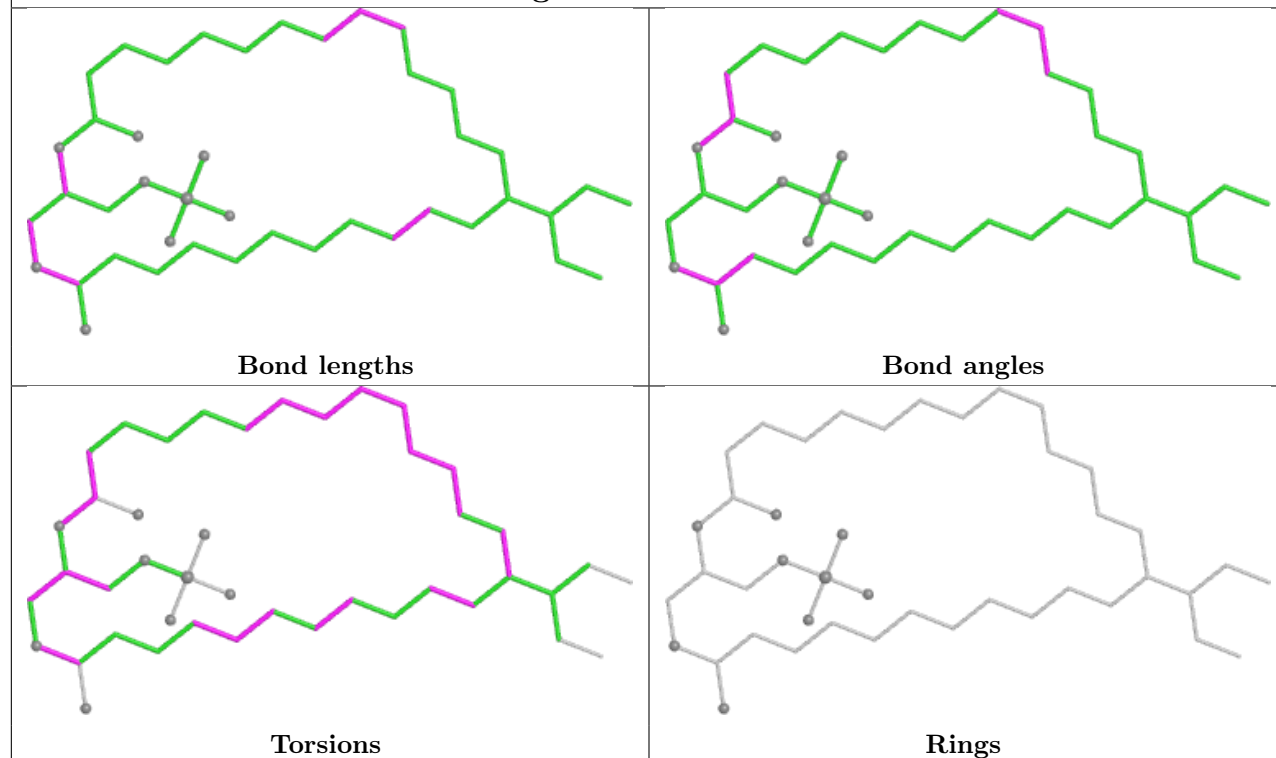
16 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	306	PO4	1	0
4	C	304	PT5	3	0
7	C	307	PO4	2	0
6	B	306	ZP7	1	0
8	A	307	LPP	3	0
4	D	304	PT5	4	0
7	B	307	PO4	2	0
8	B	301	LPP	3	0
8	C	301	LPP	4	0
6	C	306	ZP7	1	0
6	D	306	ZP7	1	0
8	D	301	LPP	3	0
7	D	307	PO4	2	0
4	A	303	PT5	5	0
6	A	305	ZP7	1	0
4	B	304	PT5	4	0

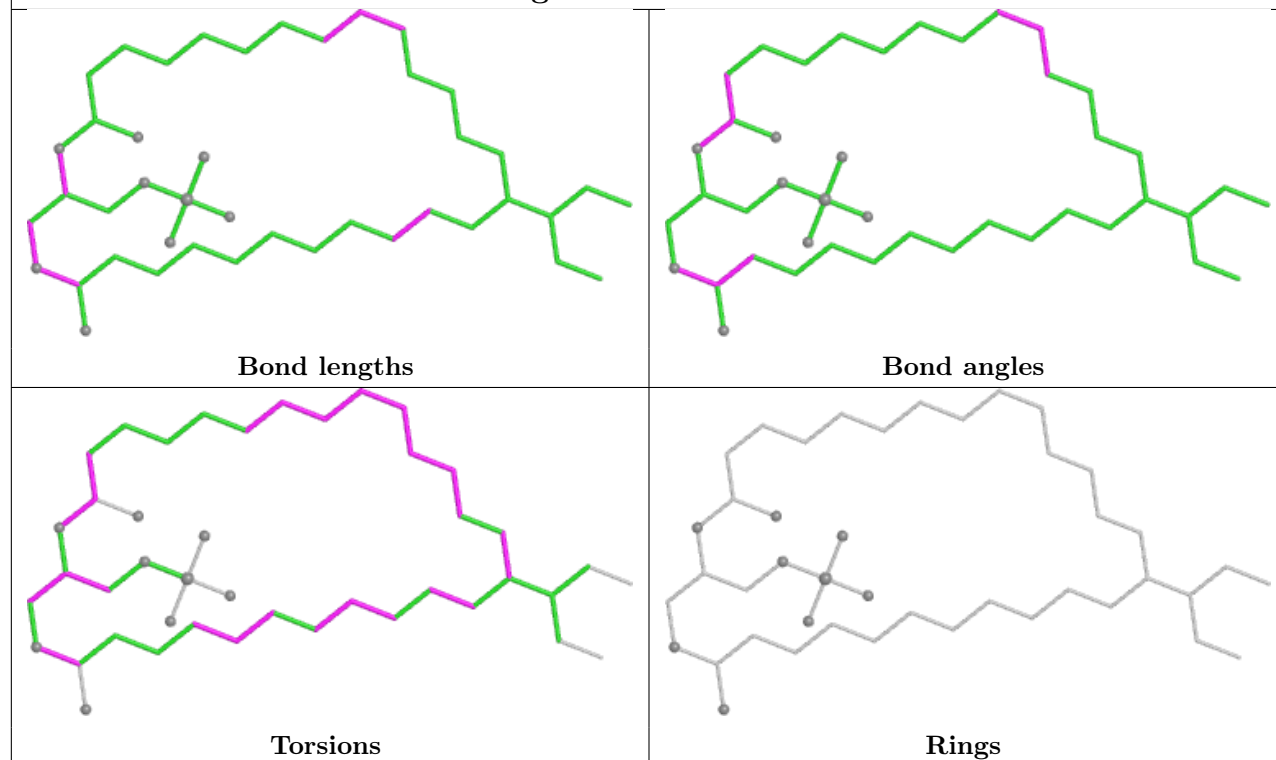
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

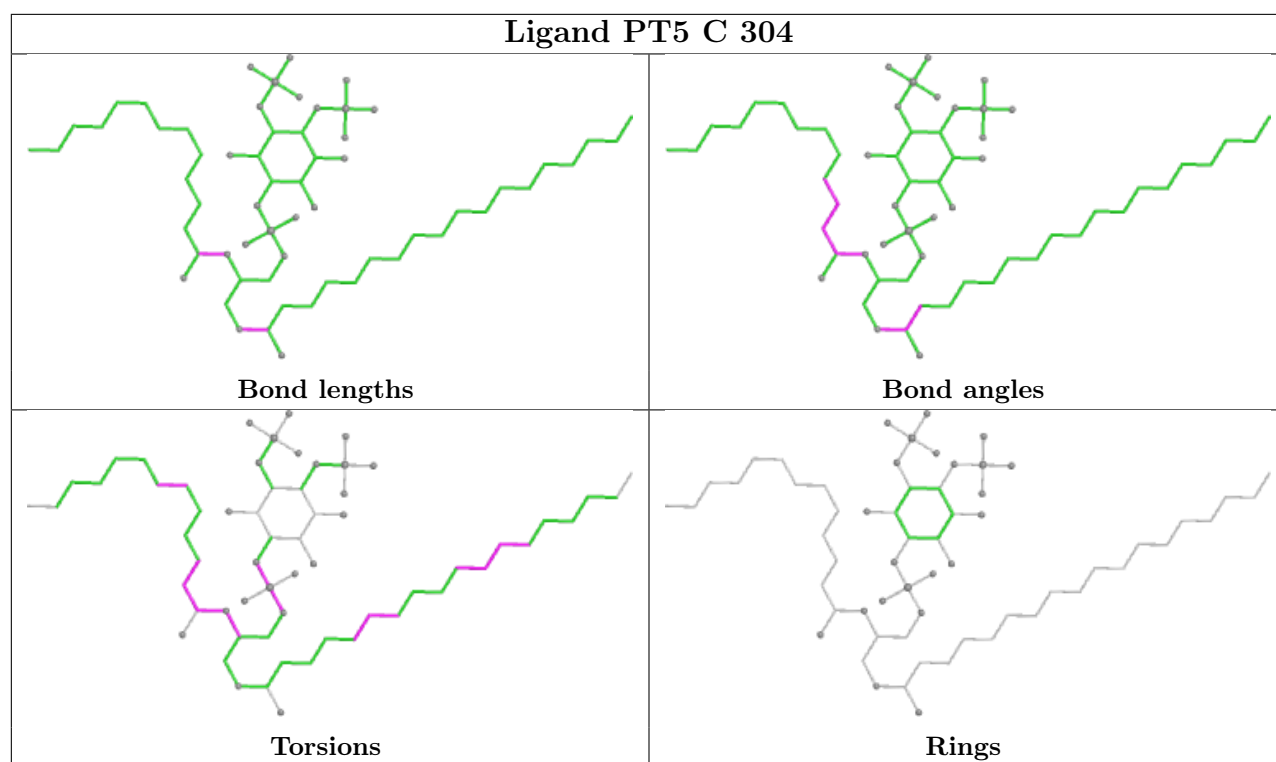


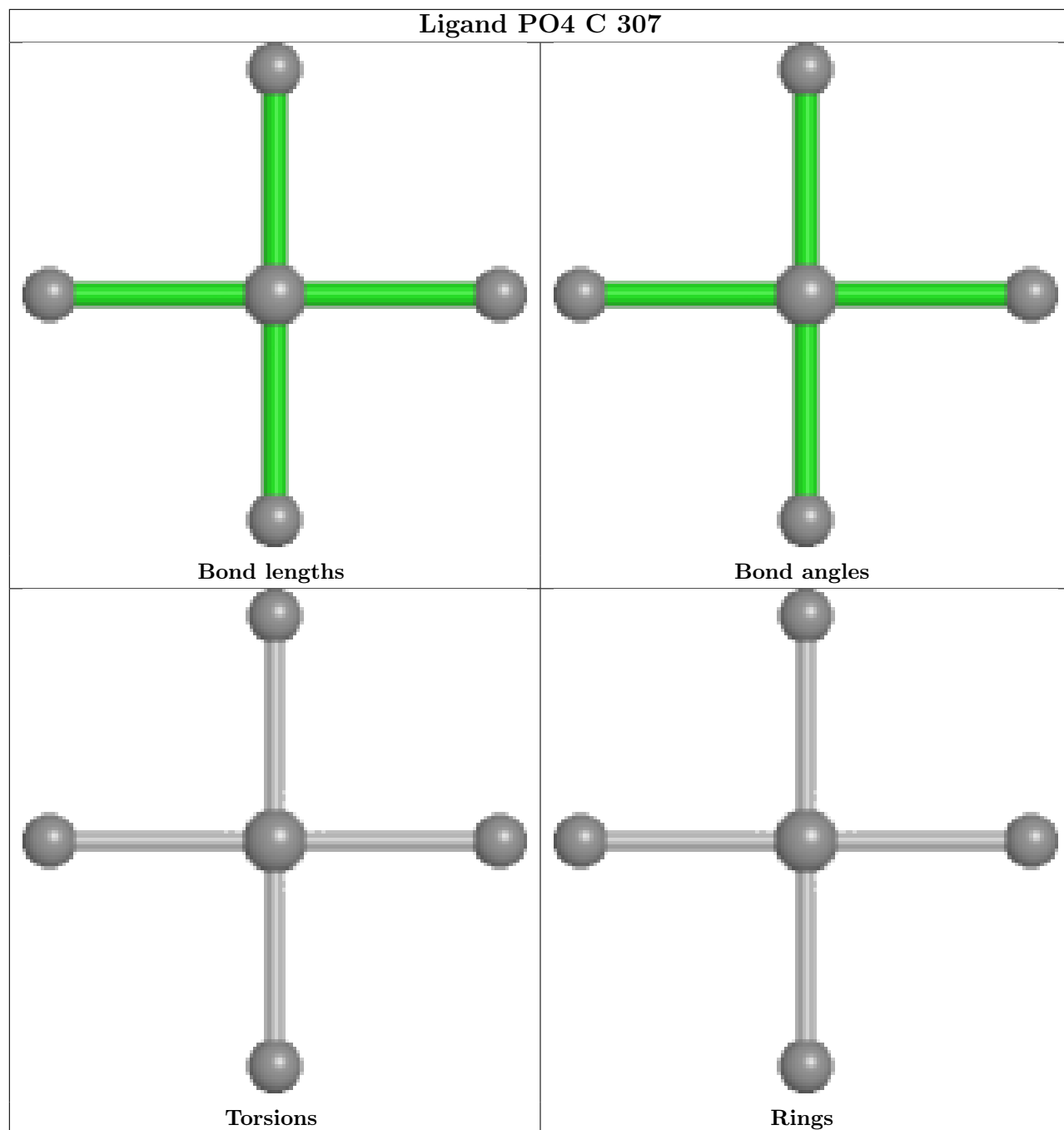
Ligand LBN B 303

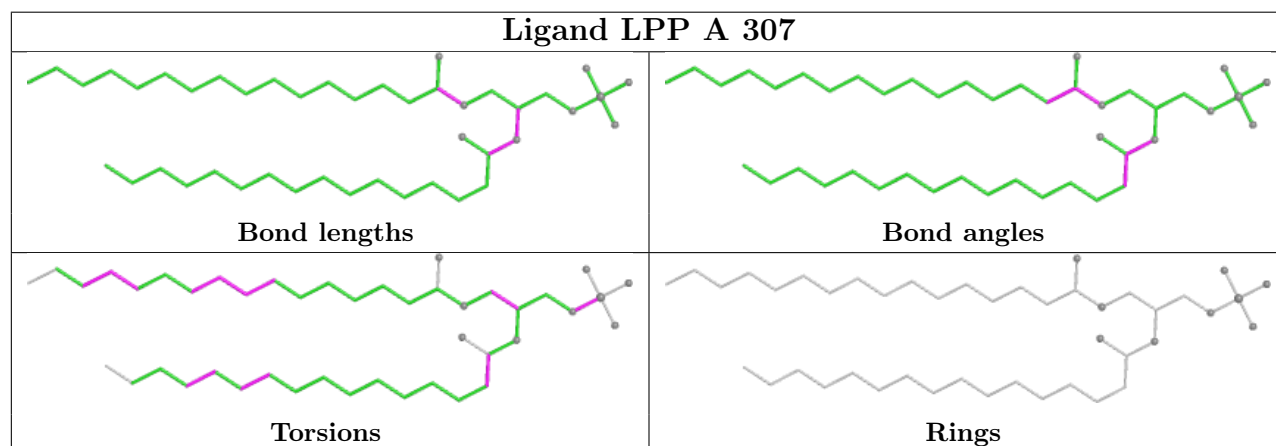
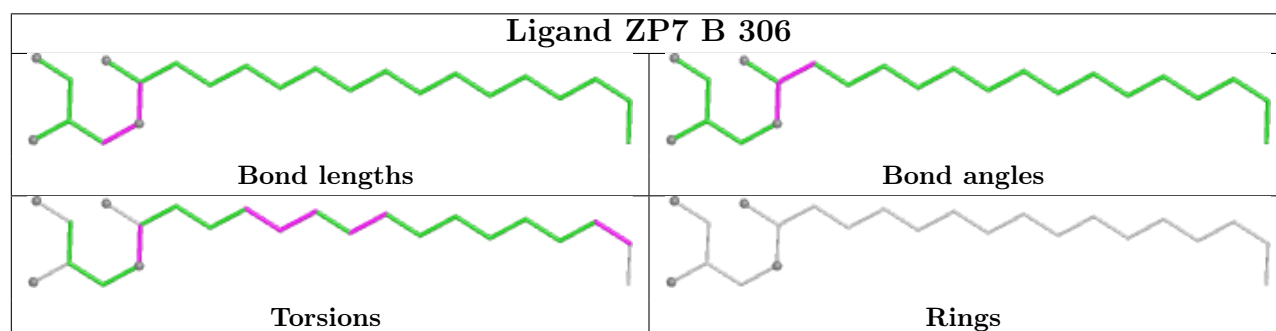
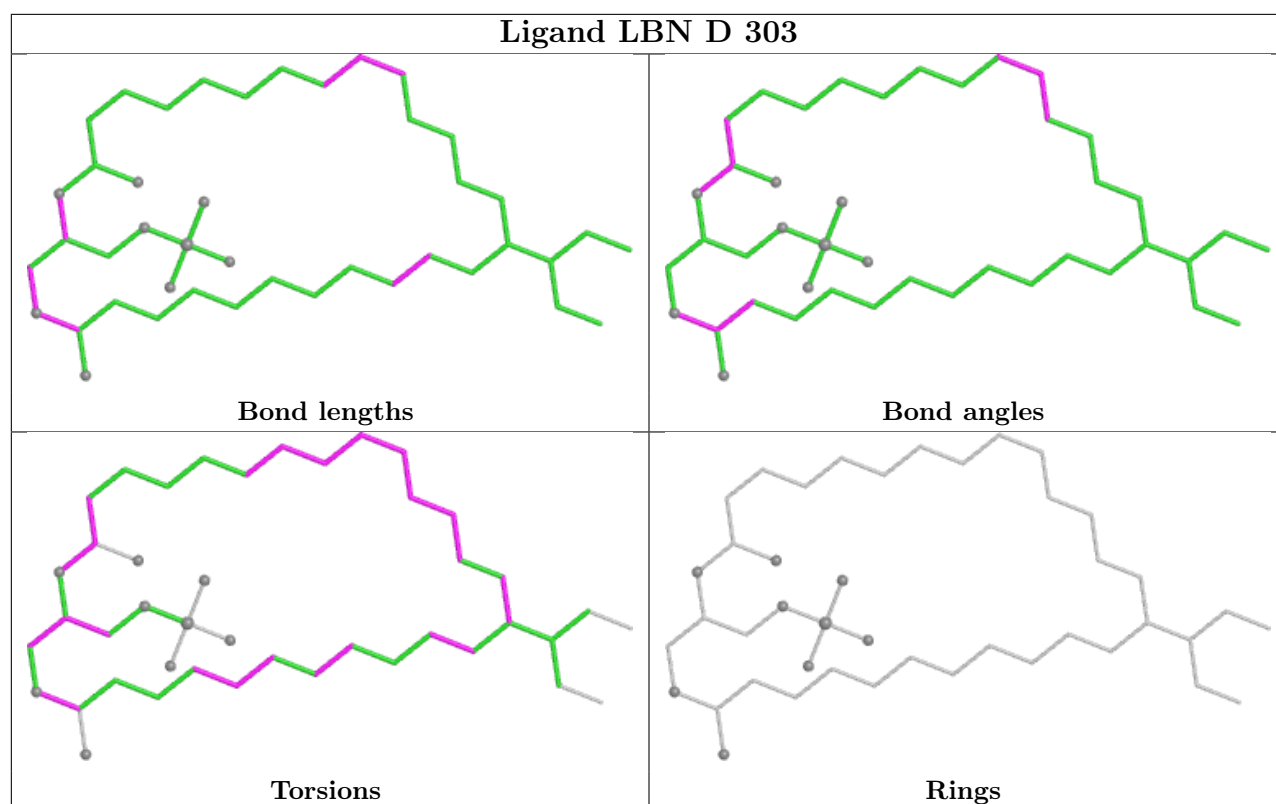


Ligand LBN A 302

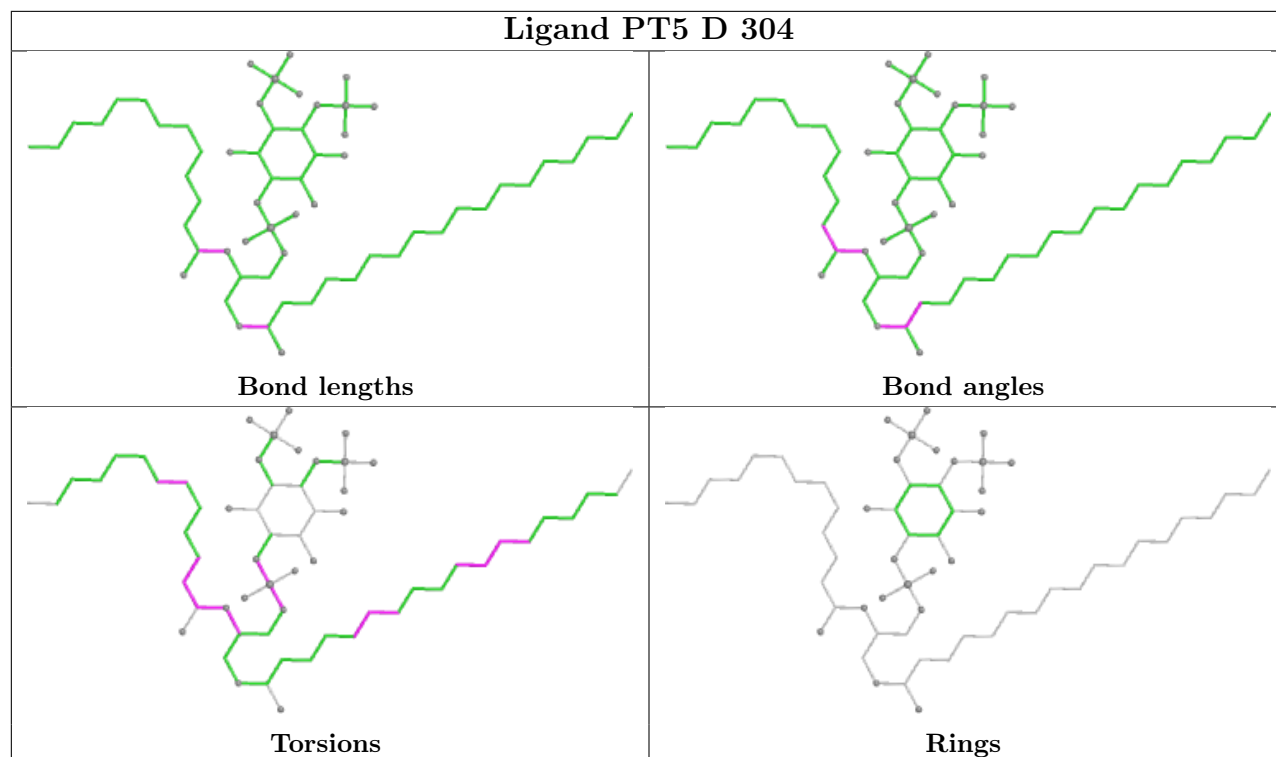




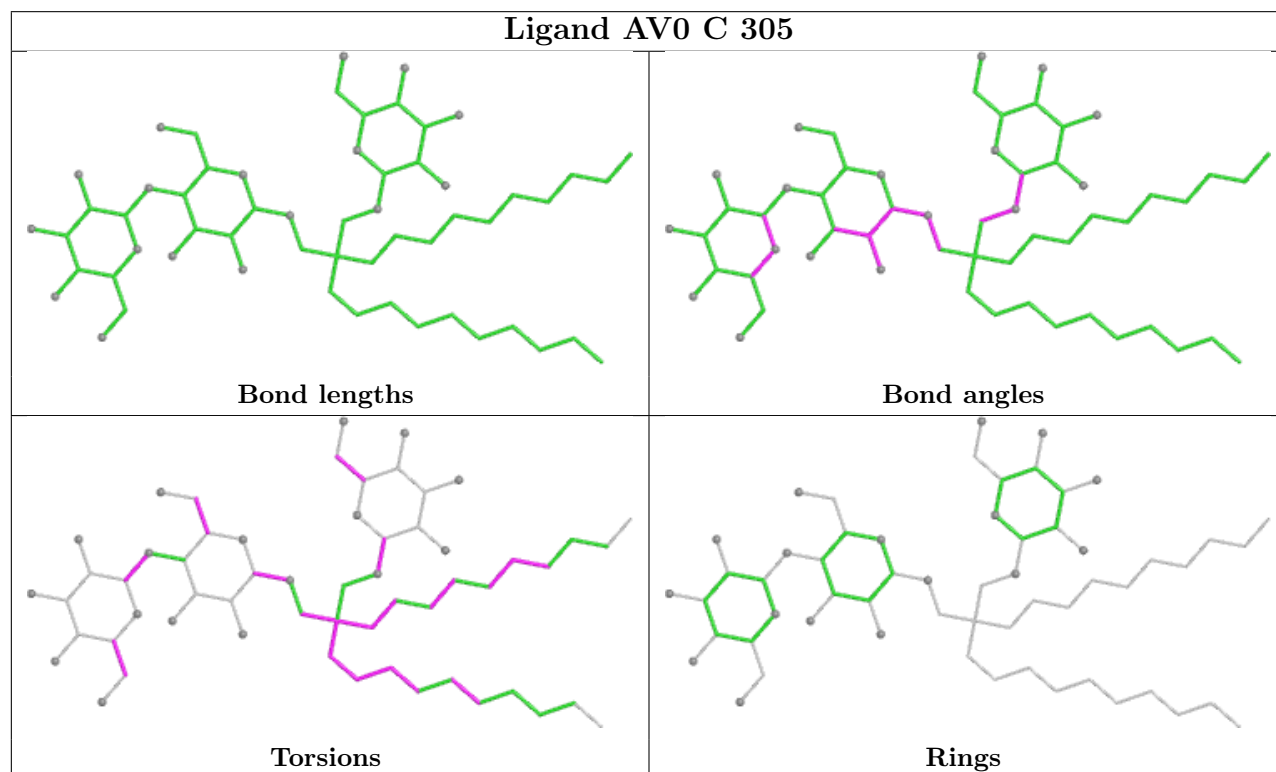


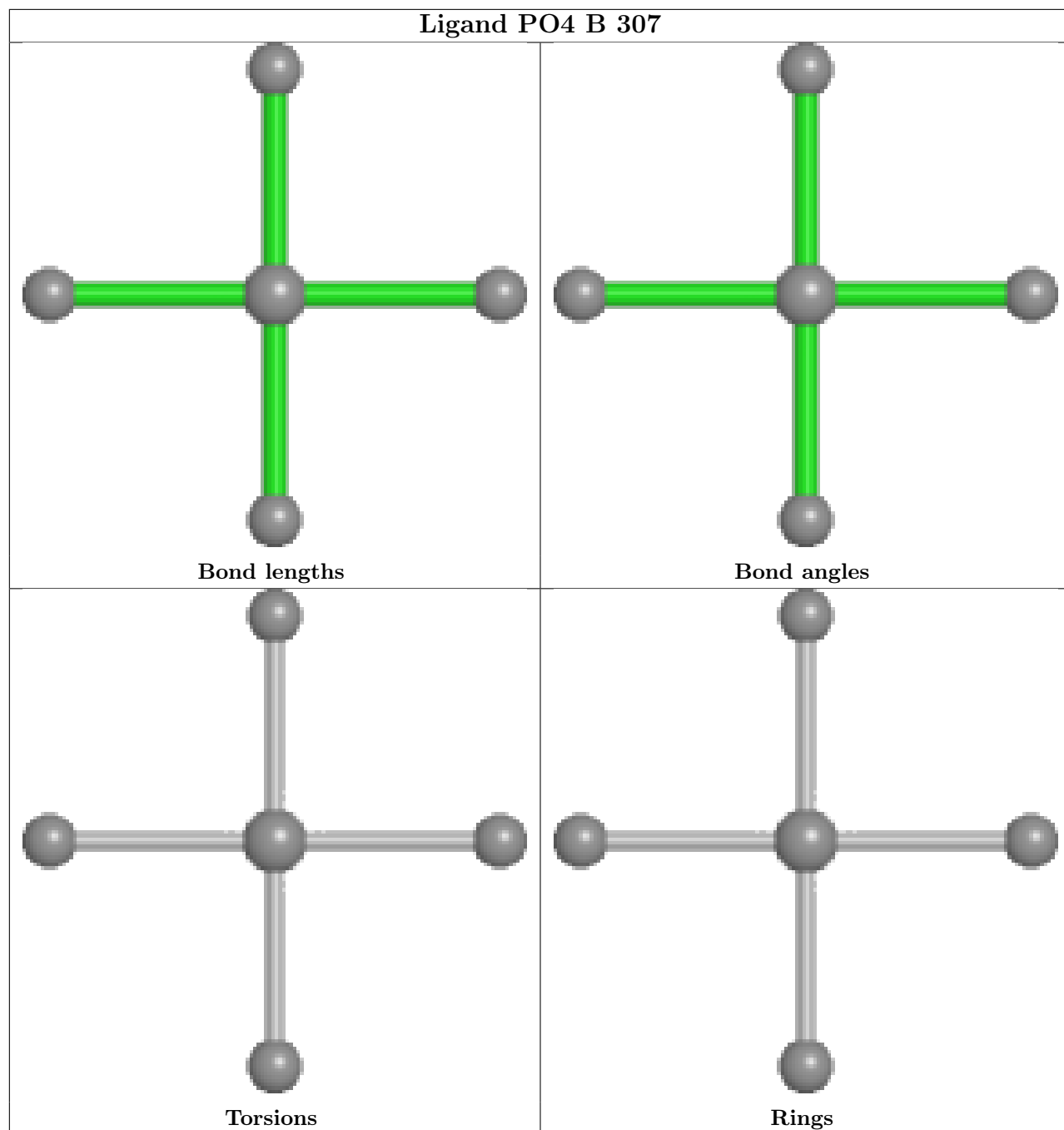


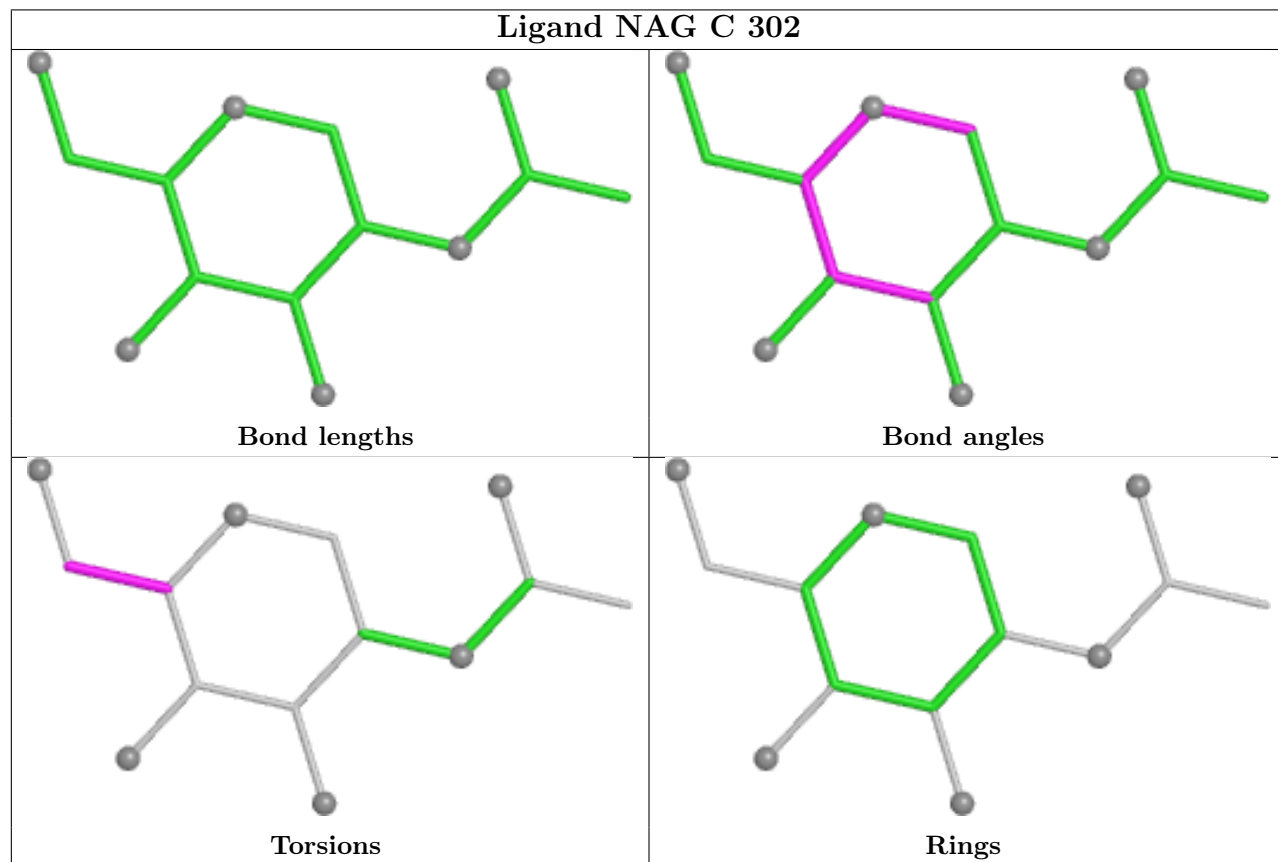
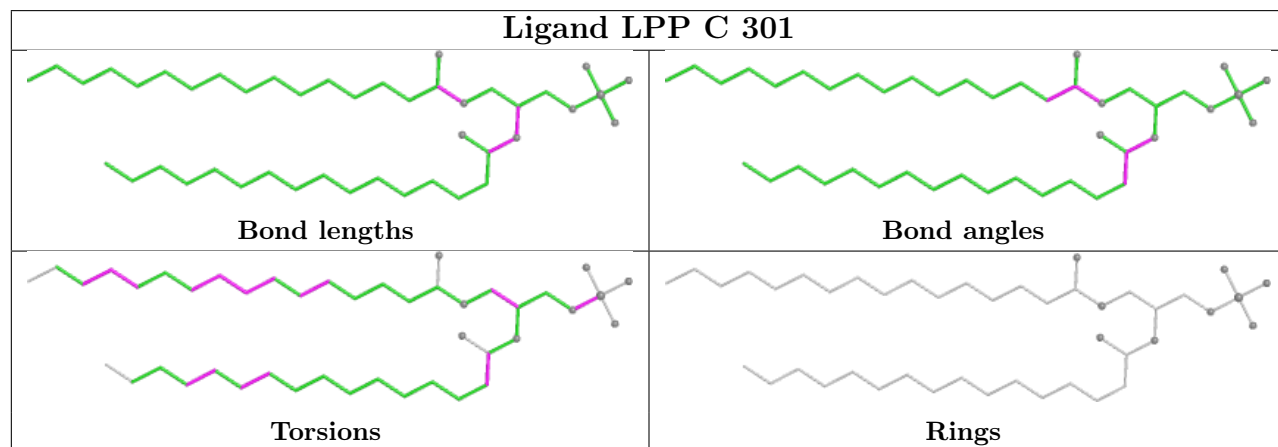
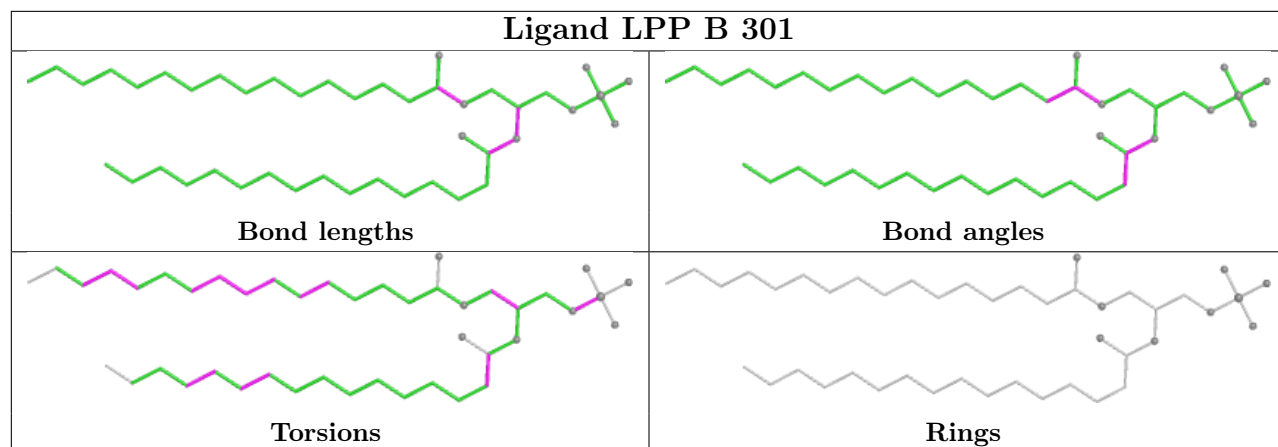
Ligand PT5 D 304

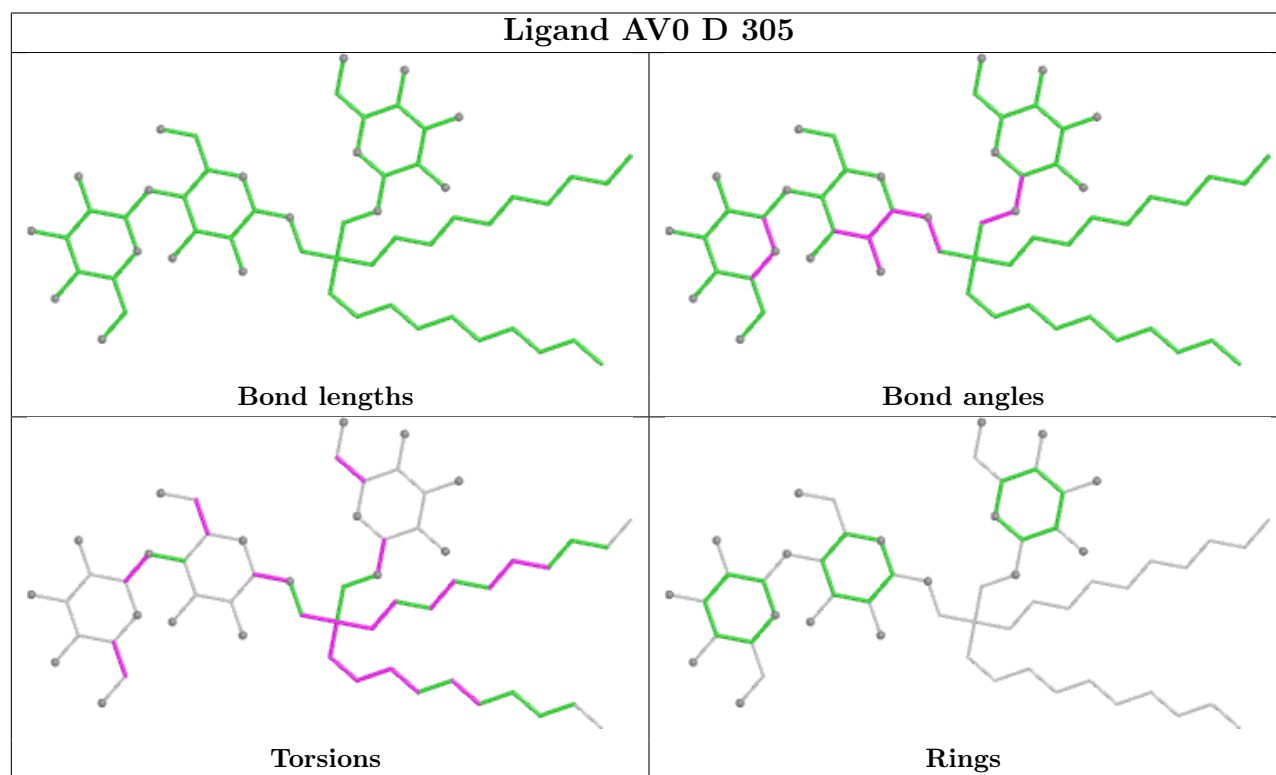
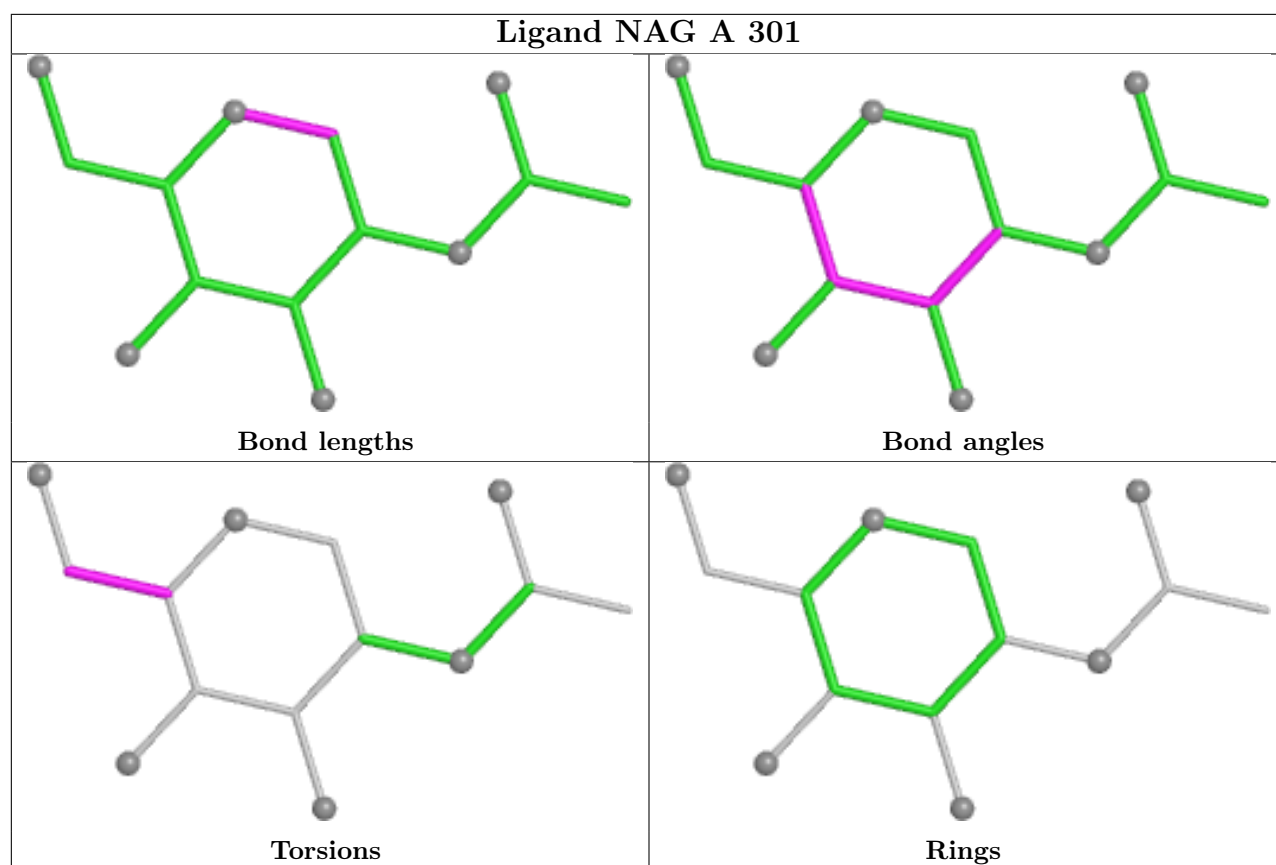


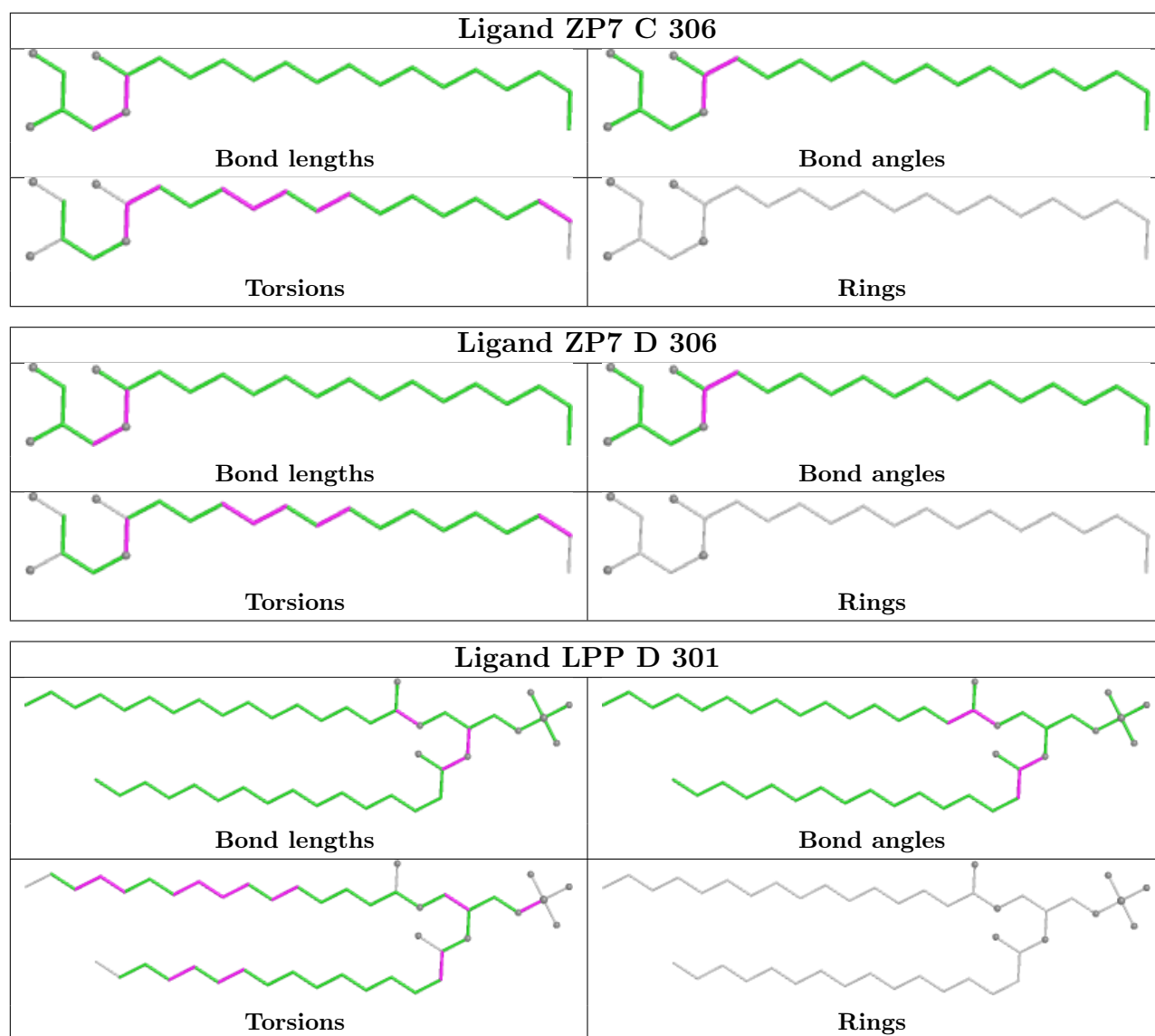
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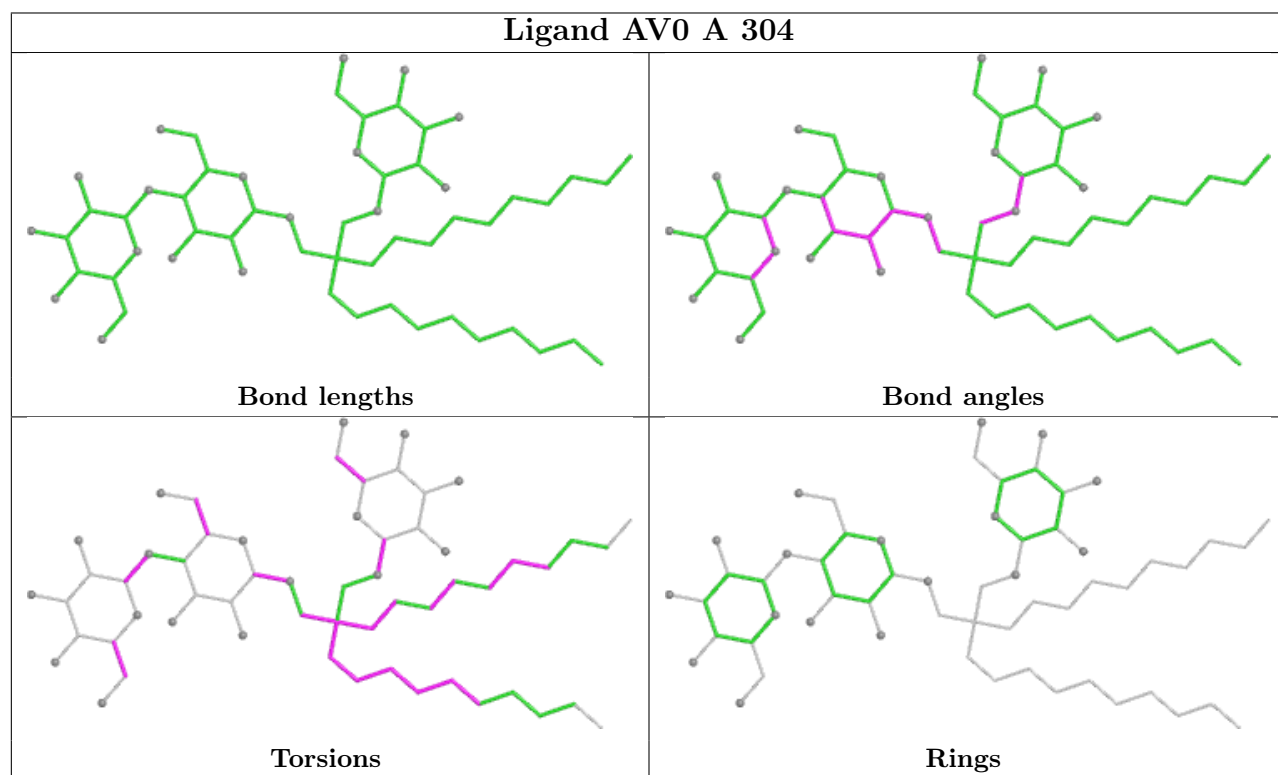
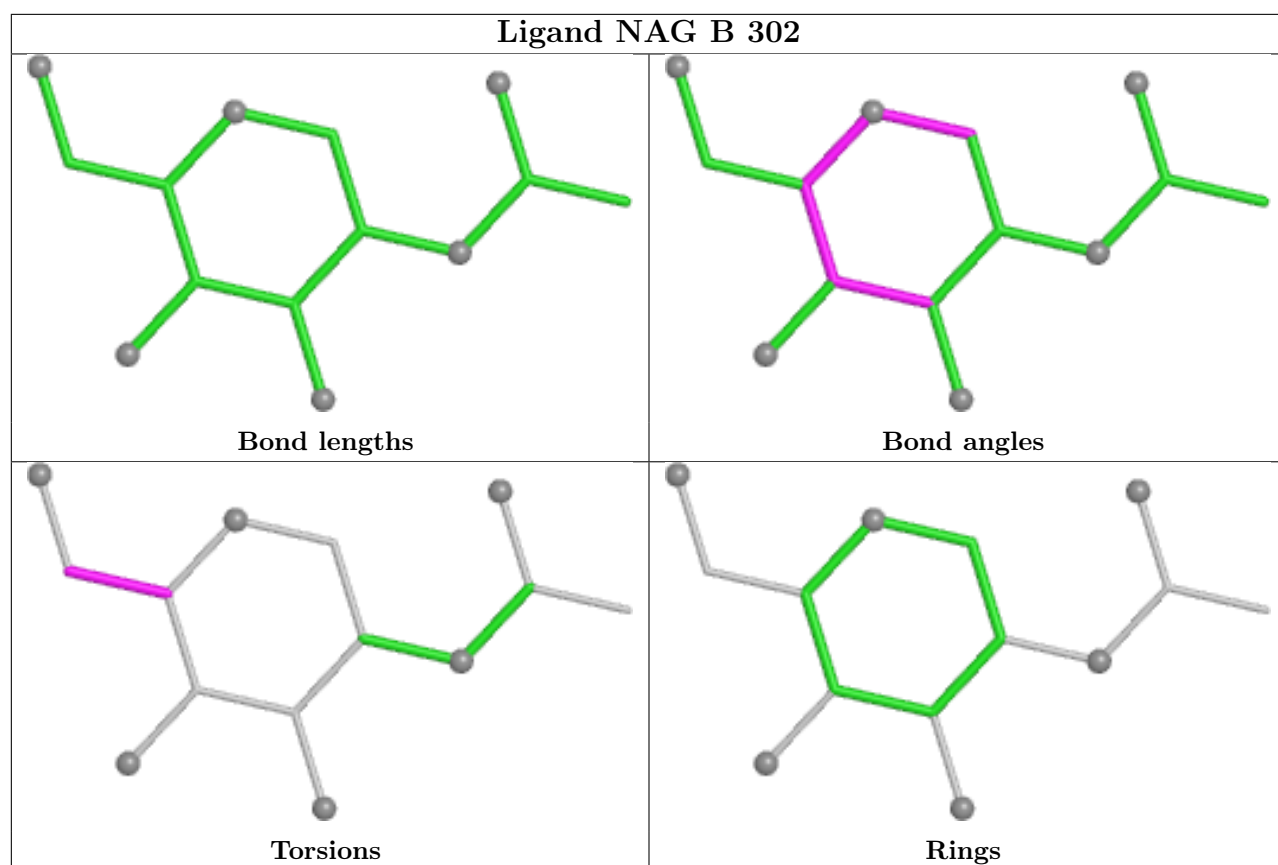


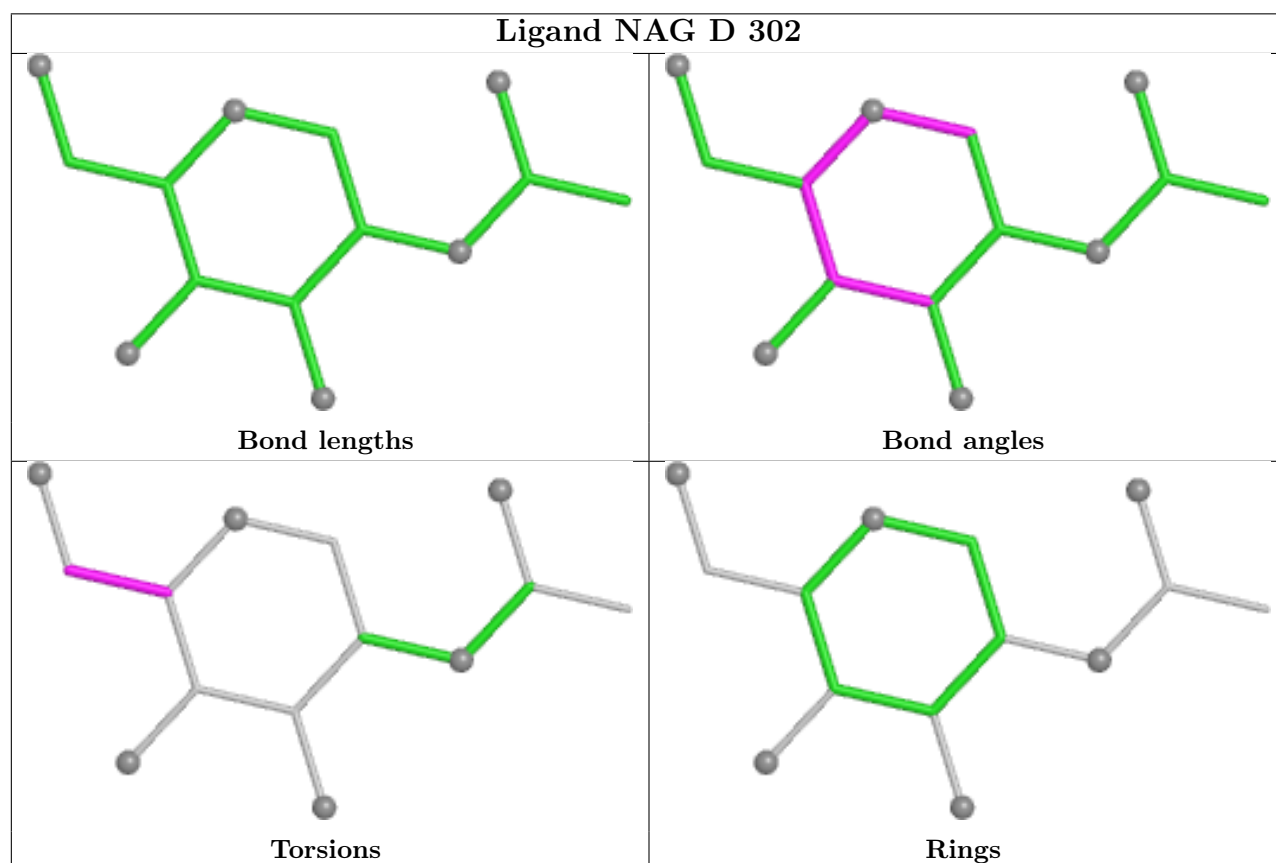
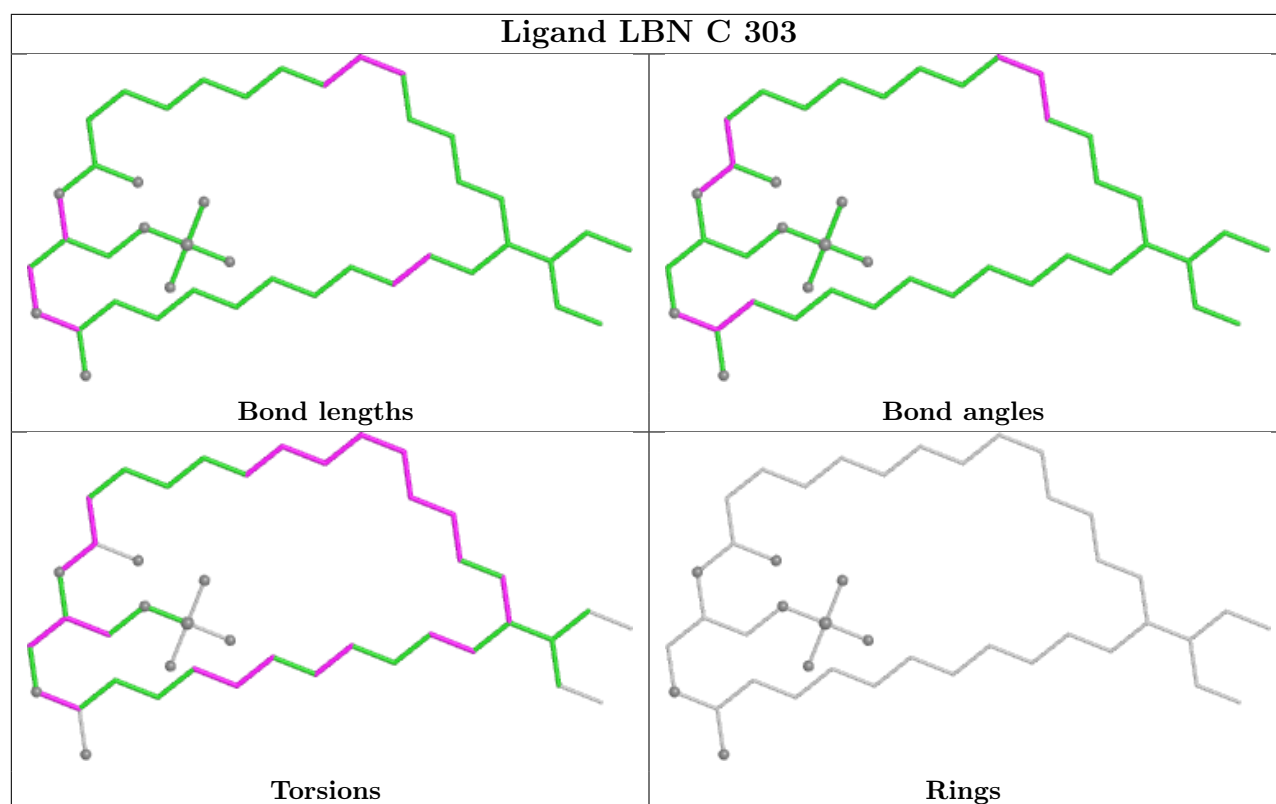


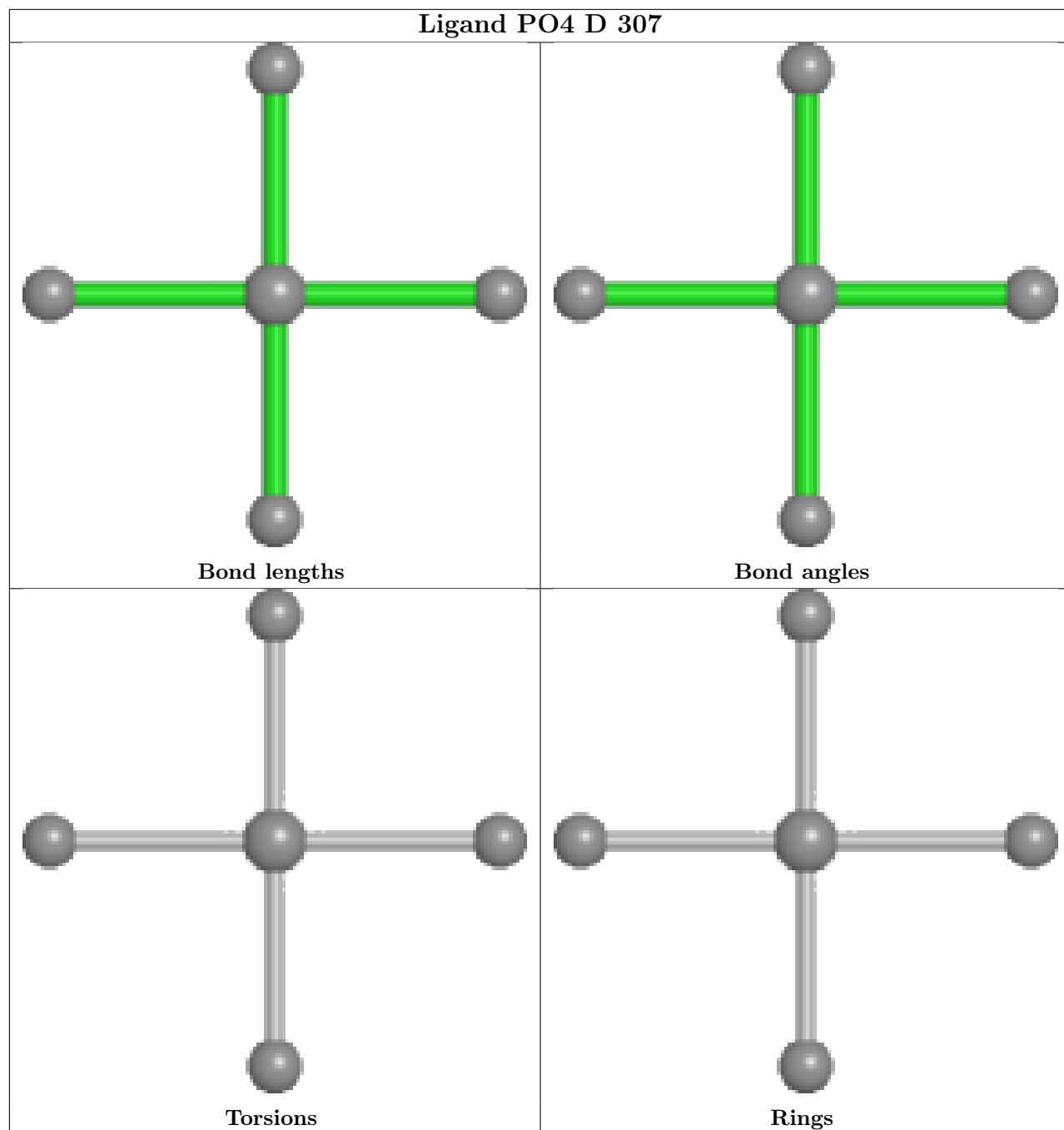


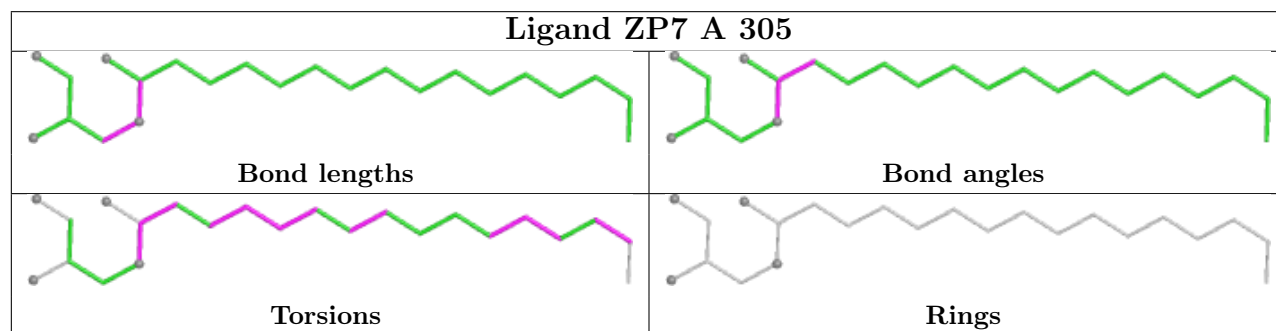
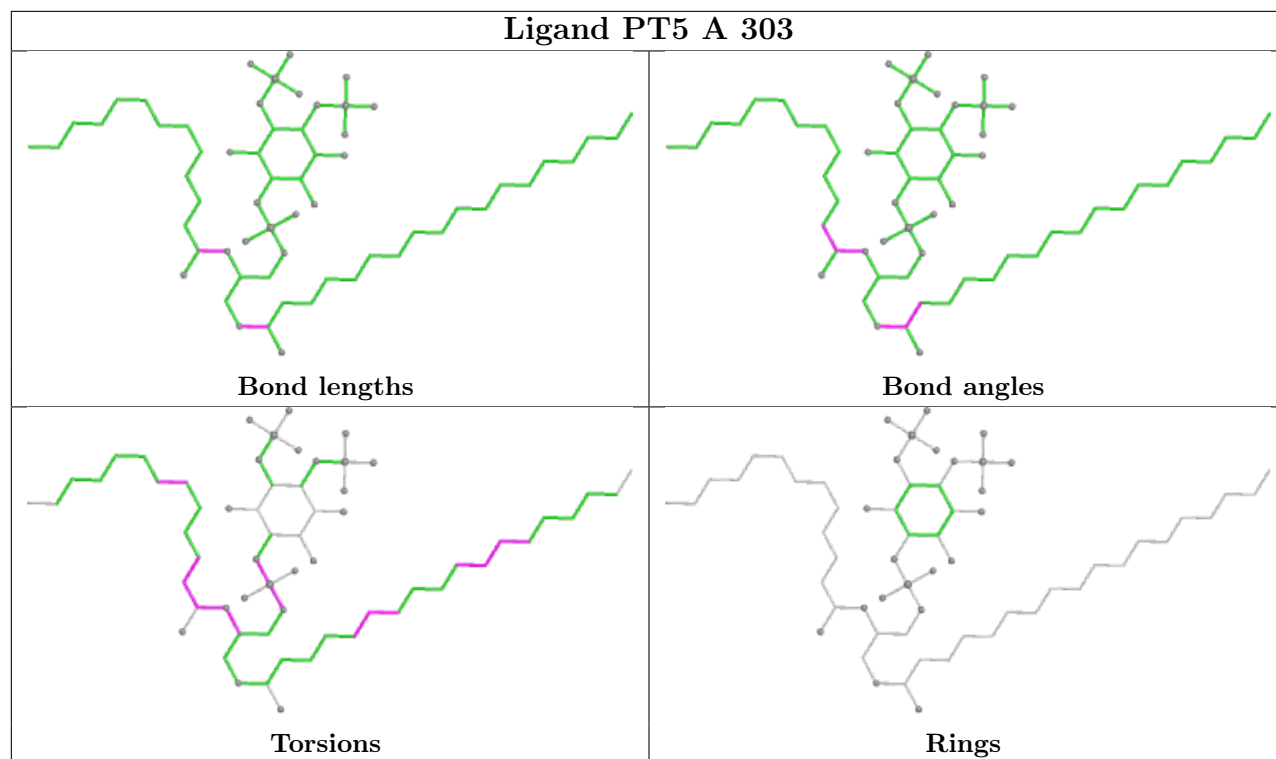


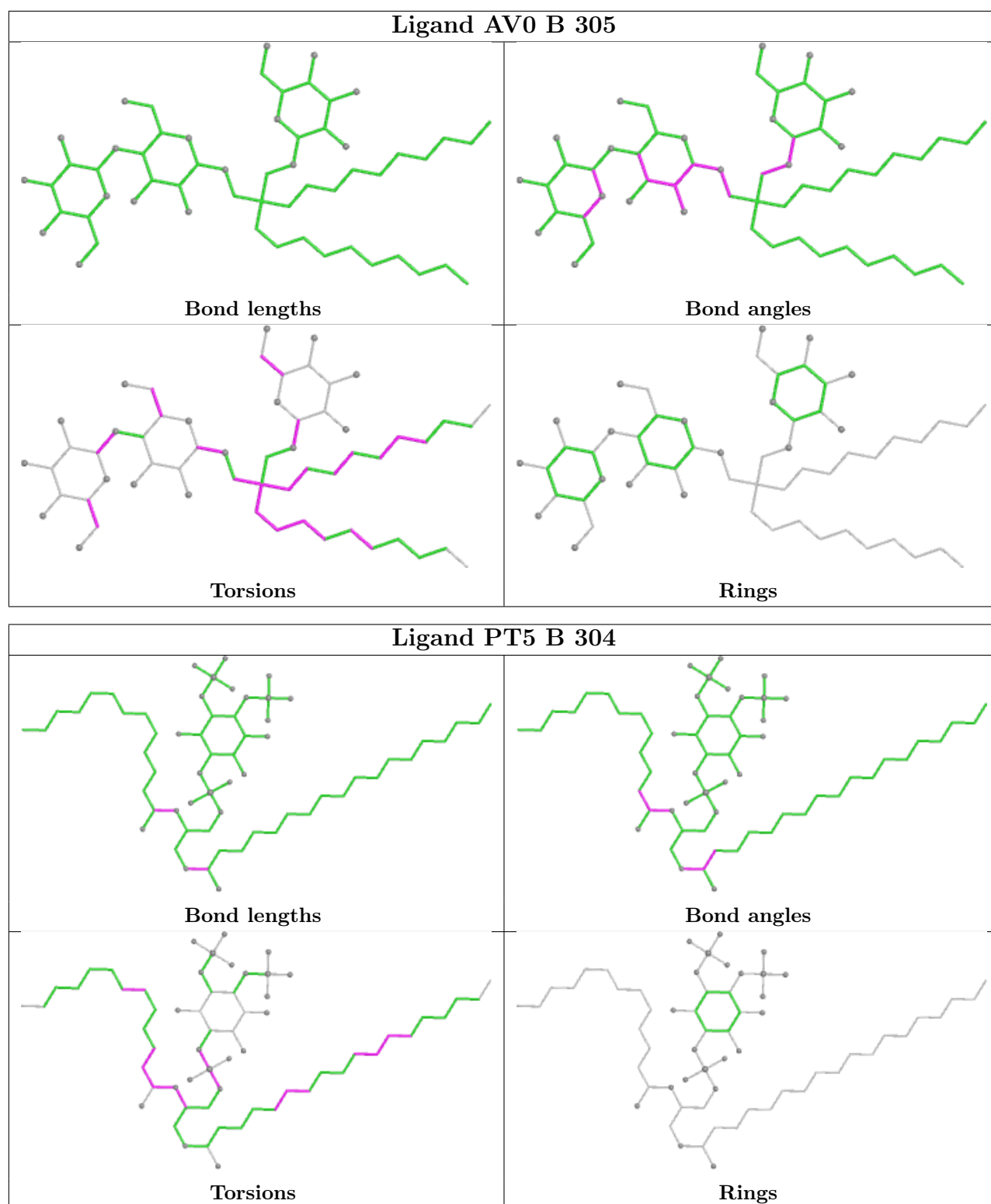












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.