



Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 05:27 AM EDT

PDB ID : 11DE / pdb_000011de
EMDB ID : EMD-75632
Title : Human Slo1-Charybdotoxin complex under divalent chelated condition - gating ring masked map
Authors : Chowdhury, S.; Pal, K.; Kallure, G.S.
Deposited on : 2026-02-18
Resolution : 3.00 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:

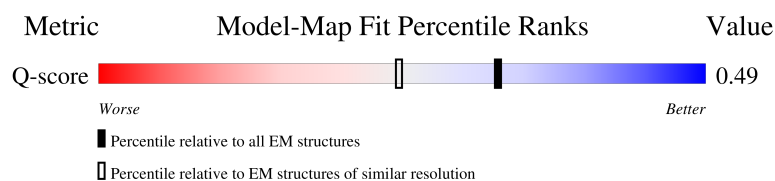
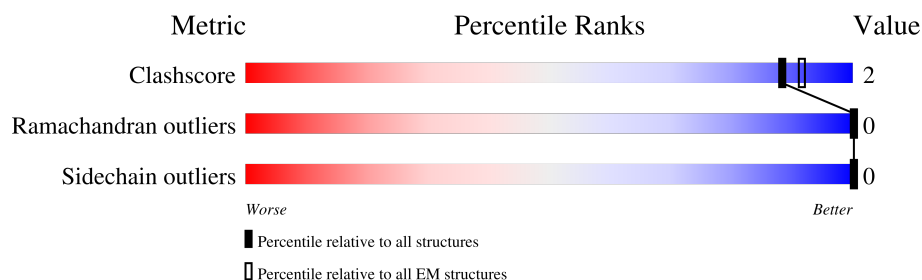
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1065	
1	B	1065	
1	C	1065	
1	D	1065	

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Mol	Chain	Length	Quality of chain
2	Y	37	

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
4	LBN	A	1104	X	-	-	-
4	LBN	A	1105	X	-	-	-
4	LBN	A	1119	X	-	-	-
4	LBN	A	1120	X	-	-	-
4	LBN	B	1102	X	-	-	-
4	LBN	B	1103	X	-	-	-
4	LBN	B	1106	X	-	-	-
4	LBN	B	1107	X	-	-	-
4	LBN	B	1120	X	-	-	-
4	LBN	B	1121	X	-	-	-
4	LBN	C	1101	X	-	-	-
4	LBN	C	1102	X	-	-	-
4	LBN	C	1103	X	-	-	-
4	LBN	C	1116	X	-	-	-
4	LBN	C	1117	X	-	-	-
4	LBN	D	1101	X	-	-	-
4	LBN	D	1103	X	-	-	-
4	LBN	D	1104	X	-	-	-
4	LBN	D	1116	X	-	-	-
4	LBN	D	1117	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11546 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 Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	263	Total	C	N	O	S	0	0
			2140	1442	329	358	11		
1	B	263	Total	C	N	O	S	0	0
			2140	1442	329	358	11		
1	C	263	Total	C	N	O	S	0	0
			2140	1442	329	358	11		
1	D	263	Total	C	N	O	S	0	0
			2140	1442	329	358	11		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1057	SER	-	expression tag	UNP Q12791
A	1058	ASN	-	expression tag	UNP Q12791
A	1059	SER	-	expression tag	UNP Q12791
A	1060	LEU	-	expression tag	UNP Q12791
A	1061	GLU	-	expression tag	UNP Q12791
A	1062	VAL	-	expression tag	UNP Q12791
A	1063	LEU	-	expression tag	UNP Q12791
A	1064	PHE	-	expression tag	UNP Q12791
A	1065	GLN	-	expression tag	UNP Q12791
B	1057	SER	-	expression tag	UNP Q12791
B	1058	ASN	-	expression tag	UNP Q12791
B	1059	SER	-	expression tag	UNP Q12791
B	1060	LEU	-	expression tag	UNP Q12791
B	1061	GLU	-	expression tag	UNP Q12791
B	1062	VAL	-	expression tag	UNP Q12791
B	1063	LEU	-	expression tag	UNP Q12791
B	1064	PHE	-	expression tag	UNP Q12791
B	1065	GLN	-	expression tag	UNP Q12791
C	1057	SER	-	expression tag	UNP Q12791
C	1058	ASN	-	expression tag	UNP Q12791
C	1059	SER	-	expression tag	UNP Q12791
C	1060	LEU	-	expression tag	UNP Q12791

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1061	GLU	-	expression tag	UNP Q12791
C	1062	VAL	-	expression tag	UNP Q12791
C	1063	LEU	-	expression tag	UNP Q12791
C	1064	PHE	-	expression tag	UNP Q12791
C	1065	GLN	-	expression tag	UNP Q12791
D	1057	SER	-	expression tag	UNP Q12791
D	1058	ASN	-	expression tag	UNP Q12791
D	1059	SER	-	expression tag	UNP Q12791
D	1060	LEU	-	expression tag	UNP Q12791
D	1061	GLU	-	expression tag	UNP Q12791
D	1062	VAL	-	expression tag	UNP Q12791
D	1063	LEU	-	expression tag	UNP Q12791
D	1064	PHE	-	expression tag	UNP Q12791
D	1065	GLN	-	expression tag	UNP Q12791

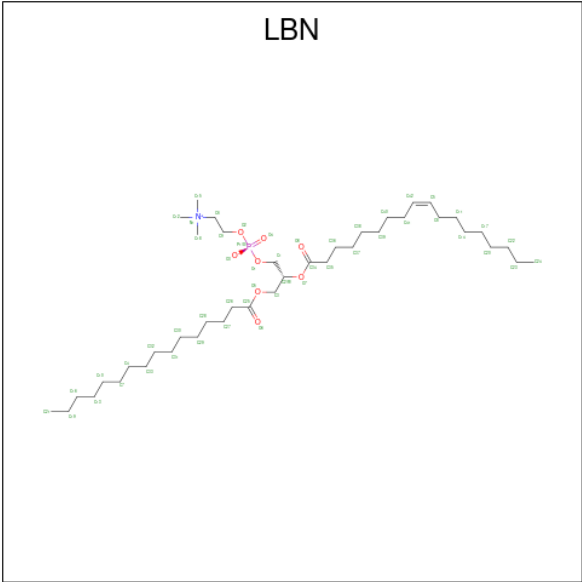
- Molecule 2 is a protein called Potassium channel toxin alpha-KTx 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	37	Total	C	N	O	S	0	0
			295	176	57	55	7		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	K	0
			2	2	
3	B	1	Total	K	0
			1	1	

- Molecule 4 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	O			0
			14	12	2			
4	A	1	Total	C	O	P		
			38	29	8	1		
4	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
4	A	1	Total	C	O			0
			15	13	2			
4	A	1	Total	C	O			0
			19	17	2			
4	A	1	Total	C	O			0
			13	11	2			
4	A	1	Total	C	O	P		
			29	20	8	1		
4	A	1	Total	C	O	P		
			36	27	8	1		
4	B	1	Total	C	O	P		
			22	14	7	1		
4	B	1	Total	C	O	P		
			22	14	7	1		
4	B	1	Total	C	O			0
			14	12	2			
4	B	1	Total	C	O			0
			14	12	2			
4	B	1	Total	C	O	P		
			39	30	8	1		
4	B	1	Total	C	N	O	P	0
			46	36	1	8	1	

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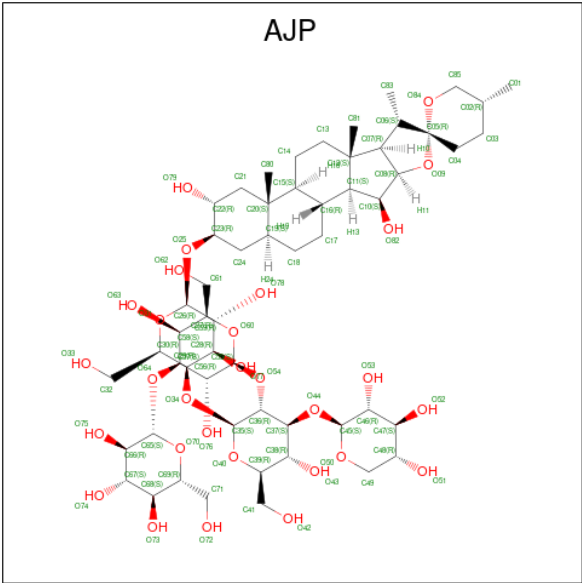
Mol	Chain	Residues	Atoms				AltConf	
4	B	1	Total 15	C 13	O 2		0	
4	B	1	Total 19	C 17	O 2		0	
4	B	1	Total 13	C 11	O 2		0	
4	B	1	Total 29	C 20	O 8	P 1	0	
4	B	1	Total 36	C 27	O 8	P 1	0	
4	C	1	Total 22	C 14	O 7	P 1	0	
4	C	1	Total 39	C 30	O 8	P 1	0	
4	C	1	Total 47	C 37	N 1	O 8	P 1	0
4	C	1	Total 15	C 13	O 2		0	
4	C	1	Total 19	C 17	O 2		0	
4	C	1	Total 13	C 11	O 2		0	
4	C	1	Total 29	C 20	O 8	P 1	0	
4	C	1	Total 36	C 27	O 8	P 1	0	
4	D	1	Total 22	C 14	O 7	P 1	0	
4	D	1	Total 14	C 12	O 2		0	
4	D	1	Total 39	C 30	O 8	P 1	0	
4	D	1	Total 47	C 37	N 1	O 8	P 1	0
4	D	1	Total 15	C 13	O 2		0	
4	D	1	Total 19	C 17	O 2		0	
4	D	1	Total 13	C 11	O 2		0	
4	D	1	Total 29	C 20	O 8	P 1	0	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
4	D	1	36	27	8	1	0

- Molecule 5 is Digitonin (CCD ID: AJP) (formula: C₅₆H₉₂O₂₉).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	A	1	54	39	15	0
5	A	1	54	39	15	0
5	A	1	32	27	5	0
5	A	1	43	33	10	0
5	A	1	32	27	5	0
5	A	1	65	45	20	0
5	A	1	43	33	10	0
5	A	1	43	33	10	0
5	A	1	54	39	15	0
5	A	1	54	39	15	0

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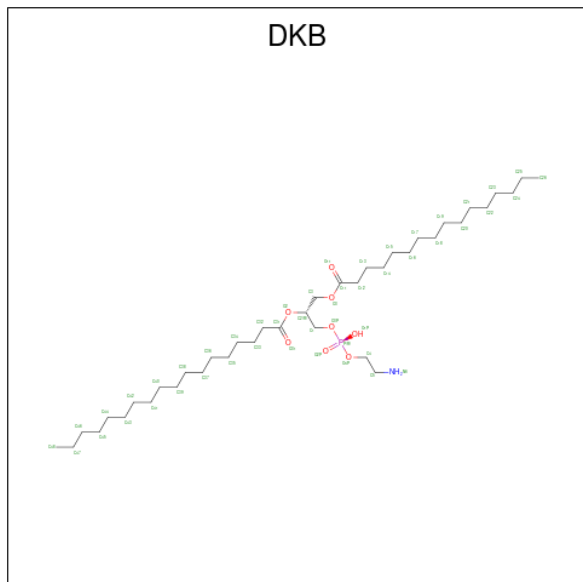
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			54	39	15	
5	B	1	Total	C	O	0
			54	39	15	
5	B	1	Total	C	O	0
			32	27	5	
5	B	1	Total	C	O	0
			43	33	10	
5	B	1	Total	C	O	0
			32	27	5	
5	B	1	Total	C	O	0
			65	45	20	
5	B	1	Total	C	O	0
			43	33	10	
5	B	1	Total	C	O	0
			43	33	10	
5	B	1	Total	C	O	0
			54	39	15	
5	C	1	Total	C	O	0
			54	39	15	
5	C	1	Total	C	O	0
			54	39	15	
5	C	1	Total	C	O	0
			32	27	5	
5	C	1	Total	C	O	0
			43	33	10	
5	C	1	Total	C	O	0
			32	27	5	
5	C	1	Total	C	O	0
			65	45	20	
5	C	1	Total	C	O	0
			43	33	10	
5	C	1	Total	C	O	0
			43	33	10	
5	C	1	Total	C	O	0
			54	39	15	
5	D	1	Total	C	O	0
			54	39	15	
5	D	1	Total	C	O	0
			54	39	15	
5	D	1	Total	C	O	0
			32	27	5	

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Mol	Chain	Residues	Atoms			AltConf
5	D	1	Total	C	O	0
			43	33	10	
5	D	1	Total	C	O	0
			32	27	5	
5	D	1	Total	C	O	0
			65	45	20	
5	D	1	Total	C	O	0
			43	33	10	
5	D	1	Total	C	O	0
			43	33	10	

- Molecule 6 is [(2R)-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] octadecanoate (CCD ID: DKB) (formula: $C_{39}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	C	0
			18	18	
6	B	1	Total	C	0
			18	18	
6	C	1	Total	C	0
			18	18	
6	D	1	Total	C	0
			18	18	

- Molecule 7 is water.

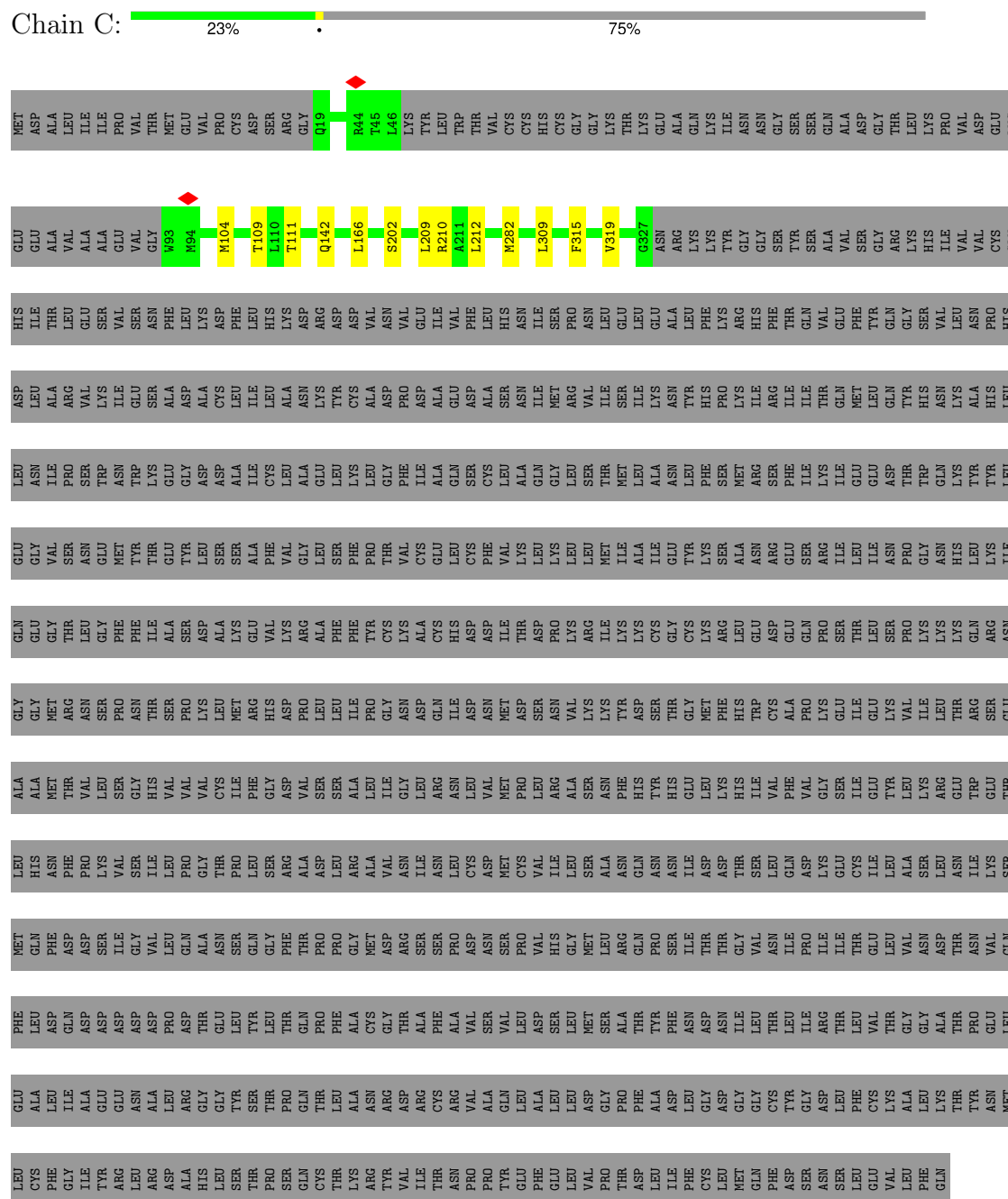
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total 1	O 1	0
7	B	1	Total 1	O 1	0
7	C	1	Total 1	O 1	0
7	D	1	Total 1	O 1	0

VAL	PRO	THR	ASP	LEU	ILE	PHE	CYS	LEU	MET	GLN	PHE	ASP	SER	ASN	SER	LEU	GLU	VAL	LEU	PHE	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

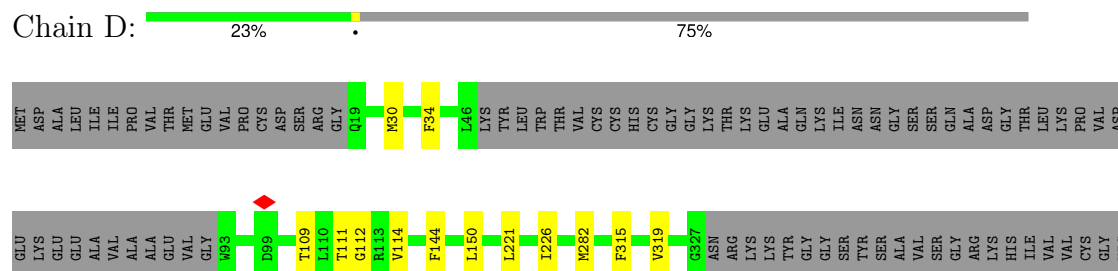
- Chain B: 23% 1% 75%

SER
LEU
GLU
VAL
LEU
PHE
GLN

- 



- Molecule 1: Calcium-activated potassium channel subunit alpha-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	283043	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 ($e^-/\text{\AA}^2$)	72	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.204	Depositor
Minimum map value	-0.747	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	276.47998, 276.47998, 276.47998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9215999, 0.9215999, 0.9215999	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: K, LBN, AJP, PCA, DKB

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	0.17	0/2202	0.37	0/2999
1	B	0.16	0/2202	0.37	0/2999
1	C	0.16	0/2202	0.33	0/2999
1	D	0.17	0/2202	0.36	0/2999
2	Y	0.16	0/292	0.42	0/389
All	All	0.17	0/9100	0.36	0/12385

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	2140	0	2155	15	0
1	B	2140	0	2155	12	0
1	C	2140	0	2155	8	0
1	D	2140	0	2155	7	0
2	Y	295	0	282	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	209	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	269	0	0	0	0
4	C	220	0	0	0	0
4	D	234	0	0	0	0
5	A	474	0	0	0	0
5	B	420	0	0	0	0
5	C	420	0	0	0	0
5	D	366	0	0	0	0
6	A	18	0	0	0	0
6	B	18	0	0	0	0
6	C	18	0	0	0	0
6	D	18	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	11546	0	8902	39	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 2.

All (39) 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:B:292:ASP:HA	2:Y:29:MET:HE1	1.78	0.66
1:A:185:VAL:HG12	1:A:210:ARG:HH21	1.68	0.58
1:A:234:LYS:HD2	1:A:325:LEU:HD21	1.88	0.56
1:C:315:PHE:O	1:C:319:VAL:HG23	2.10	0.52
1:A:109:THR:HG22	1:A:111:THR:H	1.76	0.51
1:B:221:LEU:HD22	1:B:226:ILE:HD12	1.93	0.51
1:B:109:THR:HG22	1:B:111:THR:H	1.77	0.49
1:D:111:THR:HA	1:D:114:VAL:HG12	1.94	0.49
1:B:143:ASN:HB3	1:B:146:LYS:HG2	1.95	0.49
1:A:315:PHE:O	1:A:319:VAL:HG23	2.13	0.48
1:D:315:PHE:O	1:D:319:VAL:HG23	2.14	0.48
1:B:315:PHE:O	1:B:319:VAL:HG23	2.14	0.48
1:C:104:MET:HE1	1:C:166:LEU:HD21	1.97	0.46
1:B:309:LEU:HG	1:C:282:MET:HE2	1.97	0.46
1:D:30:MET:HE3	1:D:34:PHE:HE2	1.81	0.46
1:C:309:LEU:HG	1:D:282:MET:HE2	1.97	0.45
1:A:115:LEU:HB3	1:A:163:TYR:HE1	1.80	0.45
1:B:37:LEU:HD12	1:B:178:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:THR:HG23	1:D:112:GLY:H	1.81	0.45
1:A:182:ASN:HD22	1:A:213:ARG:NH1	2.15	0.44
1:A:116:VAL:HG21	1:A:223:PHE:HE2	1.82	0.44
1:A:100:TRP:O	1:A:104:MET:HG2	2.18	0.44
1:B:294:TYR:CE2	1:B:296:LYS:HB3	2.53	0.44
1:A:157:ASN:OD1	1:A:193:VAL:HG21	2.18	0.43
1:A:41:LEU:HD12	1:A:41:LEU:HA	1.89	0.43
1:B:142:GLN:HG2	1:B:202:SER:HB2	2.01	0.43
1:A:309:LEU:HG	1:B:282:MET:HE2	2.02	0.42
1:D:144:PHE:HB3	1:D:150:LEU:HD22	2.02	0.42
1:A:270:GLN:HB2	1:A:296:LYS:HE2	2.01	0.42
1:C:142:GLN:CD	1:C:202:SER:HB3	2.44	0.42
1:C:209:LEU:O	1:C:212:LEU:HB2	2.20	0.41
1:A:122:LEU:HD22	1:A:156:PHE:CE1	2.56	0.41
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.91	0.41
1:B:21:MET:HA	1:B:21:MET:HE2	2.02	0.41
1:B:195:VAL:O	1:B:199:LEU:HD23	2.22	0.40
1:C:109:THR:HG22	1:C:111:THR:H	1.86	0.40
1:D:221:LEU:HD22	1:D:226:ILE:HD12	2.03	0.40
1:C:210:ARG:HD3	1:C:210:ARG:HA	1.90	0.40
1:A:227:LEU:HD22	1:A:232:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/1065 (24%)	255 (98%)	4 (2%)	0	100	100
1	B	259/1065 (24%)	252 (97%)	7 (3%)	0	100	100
1	C	259/1065 (24%)	253 (98%)	6 (2%)	0	100	100
1	D	259/1065 (24%)	254 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	1071/4297 (25%)	1048 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/937 (25%)	231 (100%)	0	100	100
1	B	231/937 (25%)	231 (100%)	0	100	100
1	C	231/937 (25%)	231 (100%)	0	100	100
1	D	231/937 (25%)	231 (100%)	0	100	100
2	Y	35/35 (100%)	35 (100%)	0	100	100
All	All	959/3783 (25%)	959 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	258	ASN
1	A	268	ASN
1	B	258	ASN
1	C	216	GLN
1	C	222	GLN
1	C	267	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	PCA	Y	1	2	7,8,9	0.67	0	9,10,12	1.27	1 (11%)

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	PCA	Y	1	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	Y	1	PCA	CB-CA-N	2.21	109.33	103.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 79 ligands modelled in this entry, 3 are monoatomic - leaving 76 for Mogul analysis.

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	$\# Z > 2$
5	AJP	D	1112	-	49,49,95	0.15	0	75,80,149	0.35	0
5	AJP	C	1110	-	49,49,95	0.15	0	75,80,149	0.34	0
4	LBN	C	1101	-	21,21,51	0.83	1 (4%)	23,25,59	1.04	2 (8%)
5	AJP	C	1109	-	73,73,95	0.15	0	111,116,149	0.45	0
4	LBN	D	1104	-	46,46,51	0.52	0	52,54,59	0.52	0
4	LBN	A	1117	-	18,18,51	0.26	0	18,18,59	0.38	0
4	LBN	D	1103	-	38,38,51	0.67	1 (2%)	41,43,59	0.81	2 (4%)
5	AJP	D	1106	-	61,61,95	0.16	0	93,98,149	0.49	1 (1%)
4	LBN	B	1103	-	21,21,51	0.83	1 (4%)	23,25,59	1.04	2 (8%)
4	LBN	A	1120	-	35,35,51	0.72	1 (2%)	38,40,59	0.85	2 (5%)
5	AJP	B	1112	-	37,37,95	0.22	0	58,62,149	0.52	1 (1%)
4	LBN	B	1102	-	21,21,51	0.83	1 (4%)	23,25,59	1.05	2 (8%)
5	AJP	B	1113	-	73,73,95	0.17	0	111,116,149	0.46	0
4	LBN	B	1121	-	35,35,51	0.71	1 (2%)	38,40,59	0.87	2 (5%)
5	AJP	B	1116	-	61,61,95	0.14	0	93,98,149	0.36	0
4	LBN	B	1120	-	28,28,51	0.80	1 (3%)	31,33,59	0.93	2 (6%)
5	AJP	C	1104	-	61,61,95	0.17	0	93,98,149	0.51	1 (1%)
4	LBN	C	1114	-	18,18,51	0.27	0	18,18,59	0.39	0
4	LBN	B	1105	-	13,13,51	0.35	0	13,13,59	0.42	0
4	LBN	A	1119	-	28,28,51	0.79	1 (3%)	31,33,59	0.94	2 (6%)
4	LBN	B	1107	-	45,45,51	0.53	0	51,53,59	0.53	0
4	LBN	D	1114	-	18,18,51	0.27	0	18,18,59	0.39	0
4	LBN	D	1116	-	28,28,51	0.80	1 (3%)	31,33,59	0.93	2 (6%)
4	LBN	B	1106	-	38,38,51	0.69	1 (2%)	41,43,59	0.81	2 (4%)
4	LBN	D	1117	-	35,35,51	0.71	1 (2%)	38,40,59	0.86	2 (5%)
4	LBN	C	1115	-	12,12,51	0.89	1 (8%)	12,12,59	0.85	1 (8%)
5	AJP	A	1106	-	61,61,95	0.19	0	93,98,149	0.57	1 (1%)
5	AJP	C	1108	-	37,37,95	0.21	0	58,62,149	0.51	1 (1%)
5	AJP	A	1108	-	37,37,95	0.21	0	58,62,149	0.50	1 (1%)
5	AJP	D	1107	-	37,37,95	0.20	0	58,62,149	0.50	1 (1%)
4	LBN	A	1116	-	14,14,51	1.23	2 (14%)	14,14,59	1.42	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	AJP	B	1111	-	49,49,95	0.15	0	75,80,149	0.34	0
4	LBN	C	1113	-	14,14,51	1.23	2 (14%)	14,14,59	1.42	2 (14%)
4	LBN	B	1118	-	18,18,51	0.27	0	18,18,59	0.38	0
4	LBN	B	1119	-	12,12,51	0.89	1 (8%)	12,12,59	0.85	1 (8%)
5	AJP	A	1109	-	49,49,95	0.15	0	75,80,149	0.35	0
5	AJP	B	1114	-	49,49,95	0.15	0	75,80,149	0.36	0
5	AJP	C	1105	-	61,61,95	0.16	0	93,98,149	0.51	0
5	AJP	C	1106	-	37,37,95	0.22	0	58,62,149	0.54	1 (1%)
4	LBN	D	1101	-	21,21,51	0.84	1 (4%)	23,25,59	1.05	2 (8%)
5	AJP	D	1111	-	49,49,95	0.12	0	75,80,149	0.35	0
6	DKB	B	1122	-	17,17,48	0.19	0	16,16,53	0.26	0
6	DKB	D	1118	-	17,17,48	0.21	0	16,16,53	0.22	0
5	AJP	B	1108	-	61,61,95	0.16	0	93,98,149	0.50	1 (1%)
4	LBN	C	1103	-	46,46,51	0.52	0	52,54,59	0.45	0
5	AJP	C	1112	-	61,61,95	0.15	0	93,98,149	0.37	0
5	AJP	B	1115	-	49,49,95	0.16	0	75,80,149	0.38	0
4	LBN	C	1102	-	38,38,51	0.68	1 (2%)	41,43,59	0.81	2 (4%)
5	AJP	A	1110	-	37,37,95	0.22	0	58,62,149	0.51	1 (1%)
5	AJP	A	1112	-	49,49,95	0.17	0	75,80,149	0.47	0
5	AJP	B	1109	-	61,61,95	0.16	0	93,98,149	0.48	0
4	LBN	D	1102	-	13,13,51	1.29	2 (15%)	13,13,59	1.47	2 (15%)
5	AJP	B	1110	-	37,37,95	0.21	0	58,62,149	0.47	1 (1%)
5	AJP	D	1110	-	73,73,95	0.15	0	111,116,149	0.45	0
5	AJP	D	1109	-	37,37,95	0.22	0	58,62,149	0.51	1 (1%)
5	AJP	D	1108	-	49,49,95	0.14	0	75,80,149	0.35	0
4	LBN	C	1117	-	35,35,51	0.70	1 (2%)	38,40,59	0.86	2 (5%)
5	AJP	A	1107	-	61,61,95	0.15	0	93,98,149	0.44	0
4	LBN	B	1117	-	14,14,51	1.24	2 (14%)	14,14,59	1.43	2 (14%)
4	LBN	C	1116	-	28,28,51	0.80	1 (3%)	31,33,59	0.95	2 (6%)
5	AJP	A	1114	-	61,61,95	0.14	0	93,98,149	0.36	0
4	LBN	D	1113	-	14,14,51	1.24	2 (14%)	14,14,59	1.42	2 (14%)
4	LBN	A	1104	-	37,37,51	0.69	1 (2%)	40,42,59	0.84	2 (5%)
5	AJP	C	1111	-	49,49,95	0.16	0	75,80,149	0.35	0
5	AJP	C	1107	-	49,49,95	0.14	0	75,80,149	0.37	0
6	DKB	A	1121	-	17,17,48	0.21	0	16,16,53	0.23	0
5	AJP	A	1111	-	73,73,95	0.15	0	111,116,149	0.45	0
4	LBN	B	1104	-	13,13,51	1.30	2 (15%)	13,13,59	1.49	2 (15%)
6	DKB	C	1118	-	17,17,48	0.20	0	16,16,53	0.24	0
4	LBN	A	1103	-	13,13,51	0.34	0	13,13,59	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LBN	A	1105	-	44,44,51	0.53	0	50,52,59	0.50	0
4	LBN	D	1115	-	12,12,51	0.89	1 (8%)	12,12,59	0.85	1 (8%)
5	AJP	A	1115	-	61,61,95	0.13	0	93,98,149	0.35	0
4	LBN	A	1118	-	12,12,51	0.89	1 (8%)	12,12,59	0.85	1 (8%)
5	AJP	A	1113	-	49,49,95	0.16	0	75,80,149	0.51	1 (1%)
5	AJP	D	1105	-	61,61,95	0.16	0	93,98,149	0.49	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
5	AJP	D	1112	-	-	3/6/121/220	0/7/7/11
5	AJP	C	1110	-	-	2/6/121/220	0/7/7/11
4	LBN	C	1101	-	1/1/3/7	5/21/21/55	-
5	AJP	C	1109	-	-	3/18/173/220	0/9/9/11
4	LBN	D	1104	-	1/1/5/7	18/50/50/55	-
4	LBN	D	1103	-	1/1/4/7	10/40/40/55	-
4	LBN	A	1117	-	-	2/16/16/55	-
5	AJP	D	1106	-	-	0/12/147/220	0/8/8/11
4	LBN	B	1103	-	1/1/3/7	8/21/21/55	-
4	LBN	A	1120	-	1/1/4/7	3/37/37/55	-
5	AJP	B	1112	-	-	-	0/6/6/11
4	LBN	B	1102	-	1/1/3/7	4/21/21/55	-
5	AJP	B	1113	-	-	5/18/173/220	0/9/9/11
4	LBN	B	1121	-	1/1/4/7	6/37/37/55	-
5	AJP	B	1116	-	-	3/12/147/220	0/8/8/11
4	LBN	B	1120	-	1/1/4/7	3/30/30/55	-
5	AJP	C	1104	-	-	2/12/147/220	1/8/8/11
4	LBN	C	1114	-	-	2/16/16/55	-
4	LBN	A	1119	-	1/1/4/7	9/30/30/55	-
4	LBN	B	1105	-	-	2/11/11/55	-
4	LBN	B	1107	-	1/1/5/7	13/49/49/55	-
4	LBN	D	1114	-	-	3/16/16/55	-
4	LBN	D	1116	-	1/1/4/7	5/30/30/55	-
4	LBN	B	1106	-	1/1/4/7	9/40/40/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LBN	D	1117	-	1/1/4/7	4/37/37/55	-
4	LBN	C	1115	-	-	3/10/10/55	-
5	AJP	A	1106	-	-	5/12/147/220	1/8/8/11
5	AJP	C	1108	-	-	-	0/6/6/11
5	AJP	A	1108	-	-	-	0/6/6/11
5	AJP	D	1107	-	-	-	0/6/6/11
4	LBN	A	1116	-	-	0/12/12/55	-
5	AJP	B	1111	-	-	0/6/121/220	0/7/7/11
4	LBN	C	1113	-	-	2/12/12/55	-
4	LBN	B	1118	-	-	2/16/16/55	-
4	LBN	B	1119	-	-	3/10/10/55	-
5	AJP	A	1109	-	-	0/6/121/220	0/7/7/11
5	AJP	B	1114	-	-	1/6/121/220	0/7/7/11
5	AJP	C	1105	-	-	0/12/147/220	0/8/8/11
5	AJP	D	1111	-	-	2/6/121/220	0/7/7/11
4	LBN	D	1101	-	1/1/3/7	3/21/21/55	-
6	DKB	B	1122	-	-	6/15/15/52	-
5	AJP	C	1106	-	-	-	0/6/6/11
6	DKB	D	1118	-	-	3/15/15/52	-
5	AJP	B	1108	-	-	5/12/147/220	1/8/8/11
4	LBN	C	1103	-	1/1/5/7	6/50/50/55	-
5	AJP	C	1112	-	-	2/12/147/220	0/8/8/11
5	AJP	B	1115	-	-	1/6/121/220	0/7/7/11
4	LBN	C	1102	-	1/1/4/7	13/40/40/55	-
5	AJP	B	1109	-	-	1/12/147/220	0/8/8/11
5	AJP	A	1112	-	-	0/6/121/220	0/7/7/11
5	AJP	A	1110	-	-	-	0/6/6/11
4	LBN	D	1102	-	-	2/11/11/55	-
5	AJP	D	1110	-	-	3/18/173/220	0/9/9/11
5	AJP	B	1110	-	-	-	0/6/6/11
5	AJP	D	1109	-	-	-	0/6/6/11
5	AJP	D	1108	-	-	0/6/121/220	0/7/7/11
4	LBN	C	1117	-	1/1/4/7	7/37/37/55	-
5	AJP	A	1107	-	-	1/12/147/220	0/8/8/11
4	LBN	C	1116	-	1/1/4/7	3/30/30/55	-
4	LBN	B	1117	-	-	2/12/12/55	-
5	AJP	A	1114	-	-	2/12/147/220	0/8/8/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LBN	D	1113	-	-	2/12/12/55	-
4	LBN	A	1104	-	1/1/4/7	9/39/39/55	-
5	AJP	C	1111	-	-	1/6/121/220	0/7/7/11
5	AJP	C	1107	-	-	1/6/121/220	0/7/7/11
6	DKB	A	1121	-	-	0/15/15/52	-
5	AJP	A	1111	-	-	6/18/173/220	0/9/9/11
4	LBN	B	1104	-	-	3/11/11/55	-
6	DKB	C	1118	-	-	5/15/15/52	-
4	LBN	A	1105	-	1/1/5/7	15/48/48/55	-
4	LBN	A	1103	-	-	2/11/11/55	-
4	LBN	D	1115	-	-	3/10/10/55	-
5	AJP	A	1115	-	-	4/12/147/220	0/8/8/11
4	LBN	A	1118	-	-	3/10/10/55	-
5	AJP	A	1113	-	-	1/6/121/220	0/7/7/11
5	AJP	D	1105	-	-	3/12/147/220	1/8/8/11

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1104	LBN	O8-C34	3.50	1.33	1.22
4	D	1113	LBN	O8-C34	3.48	1.33	1.22
4	C	1113	LBN	O8-C34	3.46	1.33	1.22
4	D	1102	LBN	O8-C34	3.46	1.33	1.22
4	A	1116	LBN	O8-C34	3.46	1.33	1.22
4	B	1117	LBN	O8-C34	3.46	1.33	1.22
4	B	1120	LBN	P1-O2	3.06	1.66	1.54
4	A	1119	LBN	P1-O2	3.06	1.66	1.54
4	D	1101	LBN	P1-O2	3.06	1.66	1.54
4	B	1103	LBN	P1-O2	3.05	1.66	1.54
4	D	1116	LBN	P1-O2	3.04	1.66	1.54
4	A	1120	LBN	P1-O2	3.04	1.66	1.54
4	B	1102	LBN	P1-O2	3.04	1.66	1.54
4	C	1116	LBN	P1-O2	3.04	1.66	1.54
4	C	1102	LBN	P1-O2	3.04	1.66	1.54
4	C	1101	LBN	P1-O2	3.03	1.66	1.54
4	A	1104	LBN	P1-O2	3.02	1.66	1.54
4	B	1121	LBN	P1-O2	3.01	1.66	1.54
4	D	1117	LBN	P1-O2	3.01	1.66	1.54
4	B	1106	LBN	P1-O2	3.01	1.66	1.54
4	D	1103	LBN	P1-O2	3.00	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1113	LBN	O7-C34	-3.00	1.20	1.30
4	B	1117	LBN	O7-C34	-2.99	1.20	1.30
4	B	1104	LBN	O7-C34	-2.99	1.20	1.30
4	C	1117	LBN	P1-O2	2.98	1.65	1.54
4	A	1116	LBN	O7-C34	-2.97	1.21	1.30
4	C	1113	LBN	O7-C34	-2.97	1.21	1.30
4	D	1102	LBN	O7-C34	-2.96	1.21	1.30
4	B	1119	LBN	C4-C33	-2.91	1.33	1.51
4	D	1115	LBN	C4-C33	-2.90	1.33	1.51
4	C	1115	LBN	C4-C33	-2.90	1.33	1.51
4	A	1118	LBN	C4-C33	-2.89	1.33	1.51

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1117	LBN	O8-C34-C35	-3.83	110.94	123.09
4	B	1104	LBN	O8-C34-C35	-3.83	110.94	123.09
4	D	1113	LBN	O8-C34-C35	-3.80	111.03	123.09
4	C	1113	LBN	O8-C34-C35	-3.80	111.05	123.09
4	A	1116	LBN	O8-C34-C35	-3.79	111.07	123.09
4	D	1102	LBN	O8-C34-C35	-3.78	111.09	123.09
4	B	1104	LBN	O7-C34-C35	3.65	125.54	114.00
4	B	1117	LBN	O7-C34-C35	3.64	125.49	114.00
4	D	1102	LBN	O7-C34-C35	3.63	125.47	114.00
4	A	1116	LBN	O7-C34-C35	3.63	125.47	114.00
4	D	1113	LBN	O7-C34-C35	3.63	125.46	114.00
4	C	1113	LBN	O7-C34-C35	3.62	125.45	114.00
4	C	1117	LBN	O2-P1-O1	-3.56	97.40	106.67
4	D	1117	LBN	O2-P1-O1	-3.52	97.50	106.67
4	B	1120	LBN	O2-P1-O1	-3.51	97.52	106.67
4	B	1102	LBN	O2-P1-O1	-3.45	97.67	106.67
4	C	1116	LBN	O2-P1-O1	-3.45	97.69	106.67
4	D	1103	LBN	O2-P1-O1	-3.44	97.70	106.67
4	D	1101	LBN	O2-P1-O1	-3.43	97.72	106.67
4	A	1120	LBN	O2-P1-O1	-3.42	97.74	106.67
4	C	1101	LBN	O2-P1-O1	-3.42	97.74	106.67
4	B	1121	LBN	O2-P1-O1	-3.42	97.75	106.67
4	A	1104	LBN	O2-P1-O1	-3.41	97.77	106.67
4	D	1116	LBN	O2-P1-O1	-3.41	97.78	106.67
4	B	1103	LBN	O2-P1-O1	-3.41	97.79	106.67
4	A	1119	LBN	O2-P1-O1	-3.39	97.83	106.67
4	C	1102	LBN	O2-P1-O1	-3.34	97.96	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1106	LBN	O2-P1-O1	-3.29	98.09	106.67
5	D	1107	AJP	C19-C24-C23	-2.93	110.92	114.40
5	C	1106	AJP	C19-C24-C23	-2.87	110.99	114.40
5	A	1108	AJP	C19-C24-C23	-2.86	110.99	114.40
5	C	1108	AJP	C19-C24-C23	-2.86	111.00	114.40
5	B	1112	AJP	C19-C24-C23	-2.85	111.02	114.40
5	A	1110	AJP	C19-C24-C23	-2.69	111.20	114.40
4	C	1117	LBN	O3-P1-O4	2.69	121.30	110.83
5	D	1109	AJP	C19-C24-C23	-2.67	111.22	114.40
4	D	1103	LBN	O3-P1-O4	2.67	121.25	110.83
4	C	1101	LBN	O3-P1-O4	2.67	121.23	110.83
4	B	1121	LBN	O3-P1-O4	2.67	121.22	110.83
4	A	1104	LBN	O3-P1-O4	2.66	121.21	110.83
4	A	1119	LBN	O3-P1-O4	2.66	121.20	110.83
4	D	1117	LBN	O3-P1-O4	2.66	121.20	110.83
4	B	1103	LBN	O3-P1-O4	2.66	121.18	110.83
4	C	1102	LBN	O3-P1-O4	2.65	121.16	110.83
4	A	1120	LBN	O3-P1-O4	2.64	121.14	110.83
4	C	1116	LBN	O3-P1-O4	2.64	121.12	110.83
4	B	1102	LBN	O3-P1-O4	2.64	121.11	110.83
4	B	1106	LBN	O3-P1-O4	2.64	121.11	110.83
4	D	1101	LBN	O3-P1-O4	2.63	121.08	110.83
4	B	1120	LBN	O3-P1-O4	2.61	120.99	110.83
4	D	1116	LBN	O3-P1-O4	2.60	120.97	110.83
5	B	1110	AJP	C19-C24-C23	-2.52	111.40	114.40
5	B	1108	AJP	C20-C21-C22	2.29	117.93	114.17
5	D	1105	AJP	C20-C21-C22	2.21	117.80	114.17
5	A	1106	AJP	C20-C21-C22	2.14	117.69	114.17
5	A	1113	AJP	C26-O31-C30	2.13	117.89	113.72
4	C	1115	LBN	C7-C4-C33	2.13	127.78	113.36
4	A	1118	LBN	C7-C4-C33	2.12	127.70	113.36
4	D	1115	LBN	C7-C4-C33	2.12	127.70	113.36
4	B	1119	LBN	C7-C4-C33	2.12	127.69	113.36
5	C	1104	AJP	C20-C21-C22	2.06	117.55	114.17
5	D	1106	AJP	O40-C35-C36	2.02	114.51	110.37

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1104	LBN	C2
4	A	1105	LBN	C2
4	A	1119	LBN	C2

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Mol	Chain	Res	Type	Atom
4	A	1120	LBN	C2
4	B	1102	LBN	C2
4	B	1103	LBN	C2
4	B	1106	LBN	C2
4	B	1107	LBN	C2
4	B	1120	LBN	C2
4	B	1121	LBN	C2
4	C	1101	LBN	C2
4	C	1102	LBN	C2
4	C	1103	LBN	C2
4	C	1116	LBN	C2
4	C	1117	LBN	C2
4	D	1101	LBN	C2
4	D	1103	LBN	C2
4	D	1104	LBN	C2
4	D	1116	LBN	C2
4	D	1117	LBN	C2

All (260) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1104	LBN	C1-O1-P1-O2
4	A	1104	LBN	C1-O1-P1-O3
4	A	1105	LBN	O1-C1-C2-O7
4	A	1105	LBN	C1-O1-P1-O2
4	A	1105	LBN	C1-O1-P1-O4
4	A	1105	LBN	C9-O2-P1-O3
4	A	1105	LBN	O8-C34-O7-C2
4	A	1119	LBN	C1-O1-P1-O3
4	A	1120	LBN	C1-O1-P1-O2
4	A	1120	LBN	C1-O1-P1-O3
4	A	1120	LBN	C1-O1-P1-O4
4	B	1103	LBN	O1-C1-C2-C3
4	B	1103	LBN	C1-O1-P1-O2
4	B	1106	LBN	C1-O1-P1-O2
4	B	1106	LBN	C1-O1-P1-O3
4	B	1106	LBN	C1-O1-P1-O4
4	B	1107	LBN	C1-O1-P1-O2
4	B	1107	LBN	C1-O1-P1-O3
4	B	1107	LBN	C1-O1-P1-O4
4	B	1107	LBN	O8-C34-O7-C2
4	B	1121	LBN	C1-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
4	B	1121	LBN	C1-O1-P1-O3
4	C	1101	LBN	C1-O1-P1-O2
4	C	1101	LBN	C1-O1-P1-O3
4	C	1101	LBN	C1-O1-P1-O4
4	C	1102	LBN	C1-O1-P1-O2
4	C	1102	LBN	C1-O1-P1-O3
4	C	1103	LBN	N1-C6-C9-O2
4	C	1117	LBN	C1-O1-P1-O2
4	C	1117	LBN	C1-O1-P1-O3
4	C	1117	LBN	C1-O1-P1-O4
4	D	1101	LBN	C1-O1-P1-O2
4	D	1101	LBN	C1-O1-P1-O3
4	D	1103	LBN	C1-O1-P1-O2
4	D	1103	LBN	C1-O1-P1-O3
4	D	1104	LBN	C1-O1-P1-O4
4	D	1104	LBN	C9-O2-P1-O1
4	D	1104	LBN	C9-O2-P1-O3
4	D	1104	LBN	C9-O2-P1-O4
4	D	1104	LBN	C35-C34-O7-C2
4	D	1116	LBN	C1-O1-P1-O2
4	D	1116	LBN	C1-O1-P1-O3
4	D	1116	LBN	C1-O1-P1-O4
4	D	1117	LBN	C1-O1-P1-O2
4	D	1117	LBN	C1-O1-P1-O3
4	D	1117	LBN	C1-O1-P1-O4
5	D	1110	AJP	O60-C55-O54-C36
5	C	1104	AJP	C36-C35-O34-C29
5	B	1114	AJP	O31-C26-O25-C23
5	B	1108	AJP	O31-C26-O25-C23
5	B	1108	AJP	O40-C35-O34-C29
5	D	1105	AJP	O40-C35-O34-C29
5	D	1110	AJP	C56-C55-O54-C36
5	D	1105	AJP	O31-C26-O25-C23
4	D	1104	LBN	O8-C34-O7-C2
4	A	1119	LBN	C26-C25-O5-C3
4	A	1105	LBN	C35-C34-O7-C2
4	B	1107	LBN	C35-C34-O7-C2
4	A	1119	LBN	O6-C25-O5-C3
5	A	1106	AJP	O31-C26-O25-C23
4	B	1103	LBN	O1-C1-C2-O7
5	B	1113	AJP	O60-C59-C61-O62
5	C	1110	AJP	O31-C26-O25-C23

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Mol	Chain	Res	Type	Atoms
4	D	1104	LBN	C25-C26-C27-C28
5	C	1109	AJP	C56-C55-O54-C36
5	A	1106	AJP	O31-C30-C32-O33
5	C	1110	AJP	C27-C26-O25-C23
5	B	1113	AJP	C56-C55-O54-C36
5	D	1105	AJP	C36-C35-O34-C29
5	C	1109	AJP	O60-C55-O54-C36
5	C	1111	AJP	O31-C30-C32-O33
5	B	1115	AJP	O31-C30-C32-O33
5	D	1112	AJP	O31-C30-C32-O33
4	A	1119	LBN	C35-C34-O7-C2
4	C	1102	LBN	C25-C26-C27-C28
4	C	1102	LBN	C11-C14-C17-C20
5	B	1113	AJP	O60-C55-O54-C36
4	A	1104	LBN	C37-C38-C39-C40
4	B	1106	LBN	C37-C38-C39-C40
6	C	1118	DKB	C34-C35-C36-C37
4	B	1106	LBN	C26-C27-C28-C29
4	D	1116	LBN	C35-C34-O7-C2
4	A	1119	LBN	O8-C34-O7-C2
5	C	1107	AJP	O31-C30-C32-O33
4	B	1121	LBN	C35-C34-O7-C2
4	C	1103	LBN	C35-C34-O7-C2
4	A	1104	LBN	C11-C14-C17-C20
4	A	1118	LBN	C31-C32-C33-C4
4	B	1119	LBN	C31-C32-C33-C4
5	B	1116	AJP	O40-C39-C41-O42
4	B	1121	LBN	O8-C34-O7-C2
5	A	1115	AJP	O31-C30-C32-O33
5	B	1109	AJP	O31-C30-C32-O33
5	C	1104	AJP	O40-C39-C41-O42
5	B	1108	AJP	O40-C39-C41-O42
4	D	1115	LBN	C31-C32-C33-C4
5	A	1111	AJP	O31-C30-C32-O33
5	B	1113	AJP	O31-C30-C32-O33
4	A	1104	LBN	C36-C37-C38-C39
4	C	1115	LBN	C31-C32-C33-C4
4	C	1103	LBN	C28-C29-C30-C31
5	A	1107	AJP	O31-C30-C32-O33
5	C	1109	AJP	O31-C30-C32-O33
5	A	1115	AJP	O40-C39-C41-O42
4	D	1116	LBN	O8-C34-O7-C2

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Mol	Chain	Res	Type	Atoms
5	D	1110	AJP	O60-C59-C61-O62
4	D	1104	LBN	C26-C27-C28-C29
4	A	1104	LBN	C38-C39-C40-C41
5	A	1114	AJP	C30-C29-O34-C35
5	A	1114	AJP	C28-C29-O34-C35
4	A	1104	LBN	C1-O1-P1-O4
4	D	1103	LBN	C1-O1-P1-O4
5	A	1113	AJP	O31-C30-C32-O33
4	B	1102	LBN	C26-C25-O5-C3
4	C	1102	LBN	C38-C39-C40-C41
4	C	1102	LBN	C14-C11-C8-C5
5	A	1111	AJP	C56-C55-O54-C36
4	A	1105	LBN	C26-C27-C28-C29
4	B	1121	LBN	C38-C39-C40-C41
5	C	1112	AJP	O40-C35-O34-C29
4	C	1103	LBN	O8-C34-O7-C2
5	B	1108	AJP	C27-C26-O25-C23
4	C	1102	LBN	C1-C2-C3-O5
4	B	1107	LBN	O1-C1-C2-O7
5	C	1112	AJP	C36-C35-O34-C29
5	B	1108	AJP	C36-C35-O34-C29
4	D	1103	LBN	C11-C14-C17-C20
6	B	1122	DKB	C40-C41-C42-C43
4	C	1103	LBN	C11-C14-C17-C20
4	D	1117	LBN	C25-C26-C27-C28
4	B	1102	LBN	O6-C25-O5-C3
4	D	1103	LBN	C26-C25-O5-C3
4	A	1105	LBN	O1-C1-C2-C3
4	A	1119	LBN	O1-C1-C2-C3
5	B	1113	AJP	C58-C59-C61-O62
4	D	1104	LBN	C38-C39-C40-C41
4	A	1119	LBN	C1-O1-P1-O2
4	B	1120	LBN	C1-O1-P1-O3
4	C	1101	LBN	O7-C2-C3-O5
6	B	1122	DKB	C41-C42-C43-C44
4	D	1104	LBN	C1-C2-C3-O5
4	D	1103	LBN	O6-C25-O5-C3
4	A	1105	LBN	C6-C9-O2-P1
6	D	1118	DKB	C42-C43-C44-C45
4	B	1107	LBN	N1-C6-C9-O2
5	A	1111	AJP	O60-C55-O54-C36
6	D	1118	DKB	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
4	B	1107	LBN	O1-C1-C2-C3
4	C	1116	LBN	C35-C34-O7-C2
4	C	1116	LBN	O8-C34-O7-C2
4	A	1119	LBN	O1-C1-C2-O7
5	A	1115	AJP	O40-C35-O34-C29
5	A	1115	AJP	C36-C35-O34-C29
4	B	1106	LBN	C11-C14-C17-C20
4	A	1105	LBN	C1-O1-P1-O3
4	A	1105	LBN	C9-O2-P1-O1
4	A	1105	LBN	C9-O2-P1-O4
6	C	1118	DKB	C38-C39-C40-C41
4	A	1105	LBN	C2-C1-O1-P1
4	B	1102	LBN	C1-O1-P1-O4
4	B	1121	LBN	C1-O1-P1-O4
4	C	1102	LBN	C1-O1-P1-O4
4	D	1103	LBN	C38-C39-C40-C41
5	B	1116	AJP	O40-C35-O34-C29
4	B	1106	LBN	C40-C41-C42-C5
4	B	1120	LBN	C30-C31-C32-C33
4	C	1102	LBN	O6-C25-O5-C3
5	D	1112	AJP	O31-C26-O25-C23
4	C	1102	LBN	C26-C25-O5-C3
4	C	1117	LBN	O8-C34-O7-C2
4	C	1117	LBN	C35-C34-O7-C2
5	A	1106	AJP	C28-C29-O34-C35
5	B	1116	AJP	C36-C35-O34-C29
5	A	1106	AJP	C30-C29-O34-C35
6	D	1118	DKB	C40-C41-C42-C43
4	C	1101	LBN	C2-C1-O1-P1
4	B	1104	LBN	C38-C39-C40-C41
5	D	1112	AJP	C27-C26-O25-C23
4	D	1115	LBN	O6-C25-C26-C27
4	A	1119	LBN	C3-C2-O7-C34
5	D	1111	AJP	O31-C26-O25-C23
4	D	1115	LBN	O5-C25-C26-C27
4	A	1103	LBN	O8-C34-C35-C36
4	A	1118	LBN	O6-C25-C26-C27
4	B	1105	LBN	O8-C34-C35-C36
4	D	1104	LBN	O1-C1-C2-O7
5	A	1111	AJP	O40-C35-O34-C29
4	C	1114	LBN	O8-C34-C35-C36
4	B	1119	LBN	O6-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
4	A	1117	LBN	O8-C34-C35-C36
6	B	1122	DKB	C38-C39-C40-C41
5	A	1111	AJP	C58-C59-C61-O62
4	B	1118	LBN	O8-C34-C35-C36
4	D	1103	LBN	O8-C34-O7-C2
4	A	1103	LBN	O7-C34-C35-C36
5	A	1111	AJP	C36-C35-O34-C29
4	B	1103	LBN	C26-C25-O5-C3
4	A	1118	LBN	O5-C25-C26-C27
4	D	1102	LBN	O7-C34-C35-C36
4	D	1103	LBN	C20-C22-C23-C24
4	B	1120	LBN	C35-C36-C37-C38
4	B	1106	LBN	C20-C22-C23-C24
4	C	1114	LBN	O7-C34-C35-C36
4	B	1103	LBN	O6-C25-O5-C3
4	C	1102	LBN	C20-C22-C23-C24
4	B	1118	LBN	O7-C34-C35-C36
4	B	1119	LBN	O5-C25-C26-C27
4	B	1105	LBN	O7-C34-C35-C36
4	B	1106	LBN	C36-C37-C38-C39
4	D	1104	LBN	O6-C25-O5-C3
4	C	1113	LBN	O7-C34-C35-C36
6	C	1118	DKB	C33-C34-C35-C36
5	D	1111	AJP	C27-C26-O25-C23
4	C	1103	LBN	C37-C38-C39-C40
4	D	1104	LBN	C11-C14-C17-C20
4	A	1117	LBN	O7-C34-C35-C36
4	B	1104	LBN	O7-C34-C35-C36
4	D	1102	LBN	O8-C34-C35-C36
4	D	1104	LBN	C26-C25-O5-C3
4	B	1103	LBN	C1-O1-P1-O3
4	B	1103	LBN	C1-O1-P1-O4
4	C	1116	LBN	C1-O1-P1-O3
4	B	1117	LBN	O7-C34-C35-C36
4	D	1114	LBN	C14-C17-C20-C22
6	B	1122	DKB	C37-C38-C39-C40
4	A	1104	LBN	C20-C22-C23-C24
4	C	1102	LBN	C40-C41-C42-C5
4	C	1113	LBN	O8-C34-C35-C36
4	D	1113	LBN	O7-C34-C35-C36
6	B	1122	DKB	C36-C37-C38-C39
4	D	1113	LBN	O8-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
4	D	1103	LBN	C35-C34-O7-C2
4	D	1114	LBN	O8-C34-C35-C36
4	C	1117	LBN	O5-C25-C26-C27
4	B	1104	LBN	O8-C34-C35-C36
4	C	1115	LBN	O6-C25-C26-C27
5	A	1106	AJP	C29-C30-C32-O33
4	B	1117	LBN	O8-C34-C35-C36
4	B	1107	LBN	C2-C1-O1-P1
4	A	1105	LBN	C37-C38-C39-C40
4	B	1102	LBN	O1-C1-C2-O7
4	D	1104	LBN	C9-C6-N1-C18
4	B	1107	LBN	C37-C38-C39-C40
4	D	1104	LBN	O5-C25-C26-C27
6	B	1122	DKB	C43-C44-C45-C46
4	B	1107	LBN	C9-C6-N1-C15
4	D	1104	LBN	C9-C6-N1-C12
4	B	1103	LBN	O7-C2-C3-O5
4	C	1115	LBN	O5-C25-C26-C27
4	D	1114	LBN	O7-C34-C35-C36
4	B	1107	LBN	C9-C6-N1-C12
4	D	1104	LBN	C9-C6-N1-C15
4	C	1117	LBN	O6-C25-C26-C27
4	B	1107	LBN	C34-C35-C36-C37
4	A	1105	LBN	C8-C11-C14-C17
4	C	1102	LBN	O7-C2-C3-O5
4	A	1104	LBN	O7-C34-C35-C36
4	D	1101	LBN	O7-C2-C3-O5
6	C	1118	DKB	C39-C40-C41-C42
6	C	1118	DKB	C36-C37-C38-C39

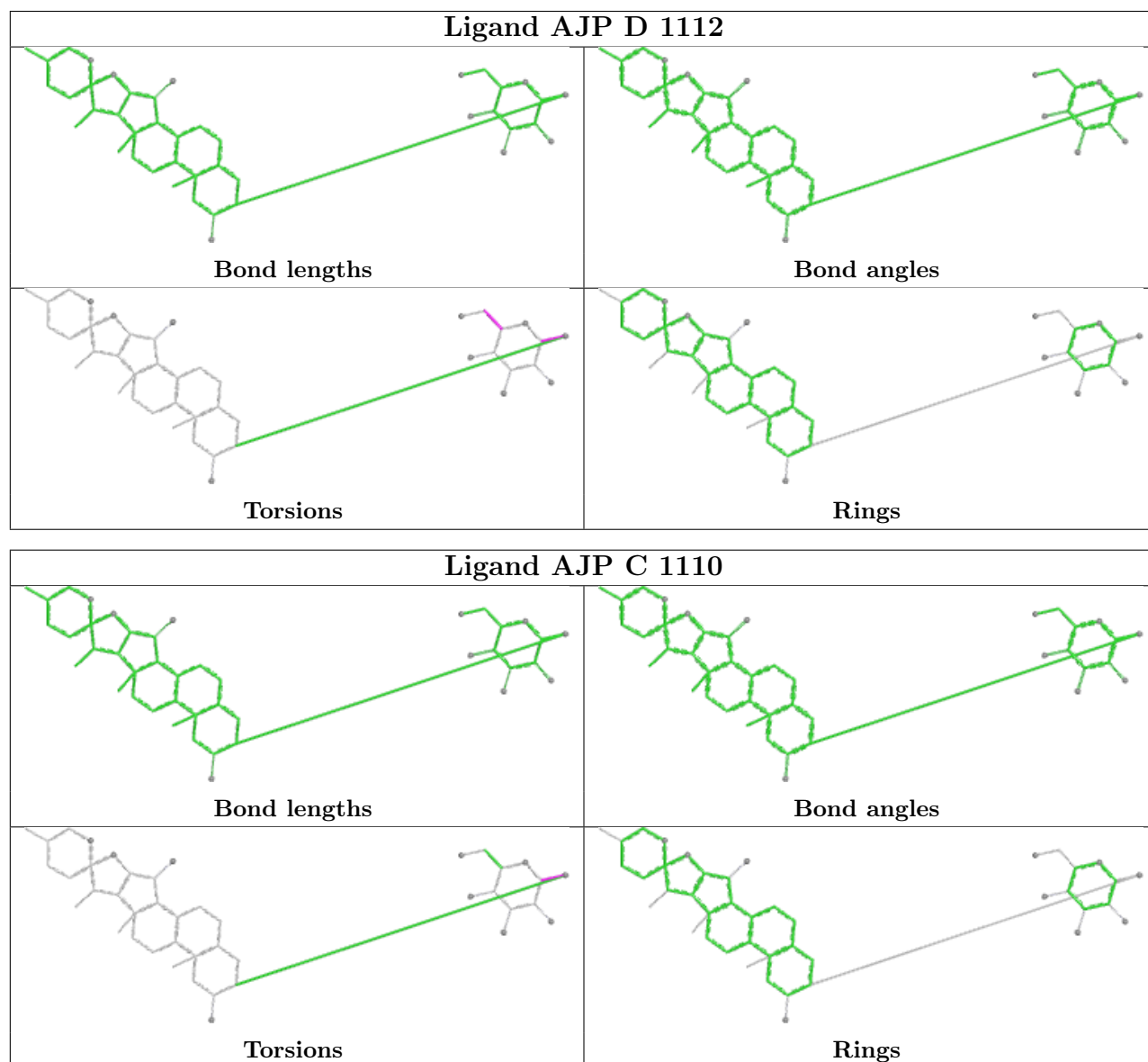
All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1104	AJP	C19-C20-C21-C22-C23-C24
5	A	1106	AJP	C19-C20-C21-C22-C23-C24
5	B	1108	AJP	C19-C20-C21-C22-C23-C24
5	D	1105	AJP	C19-C20-C21-C22-C23-C24

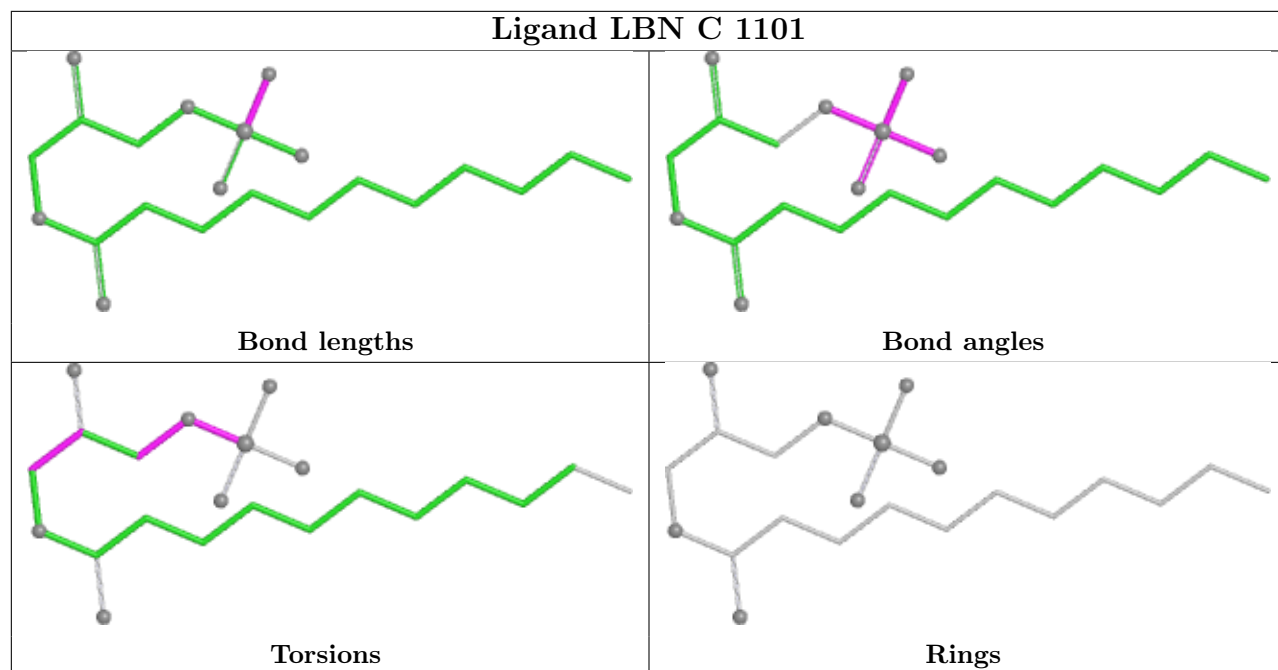
No monomer is involved in short contacts.

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

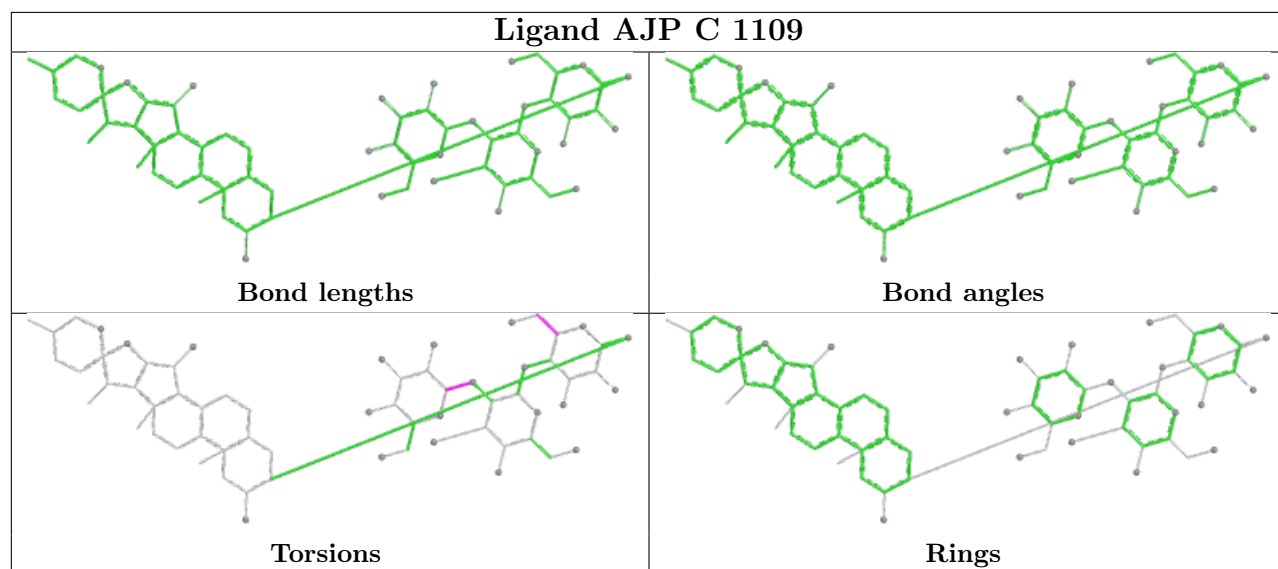
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

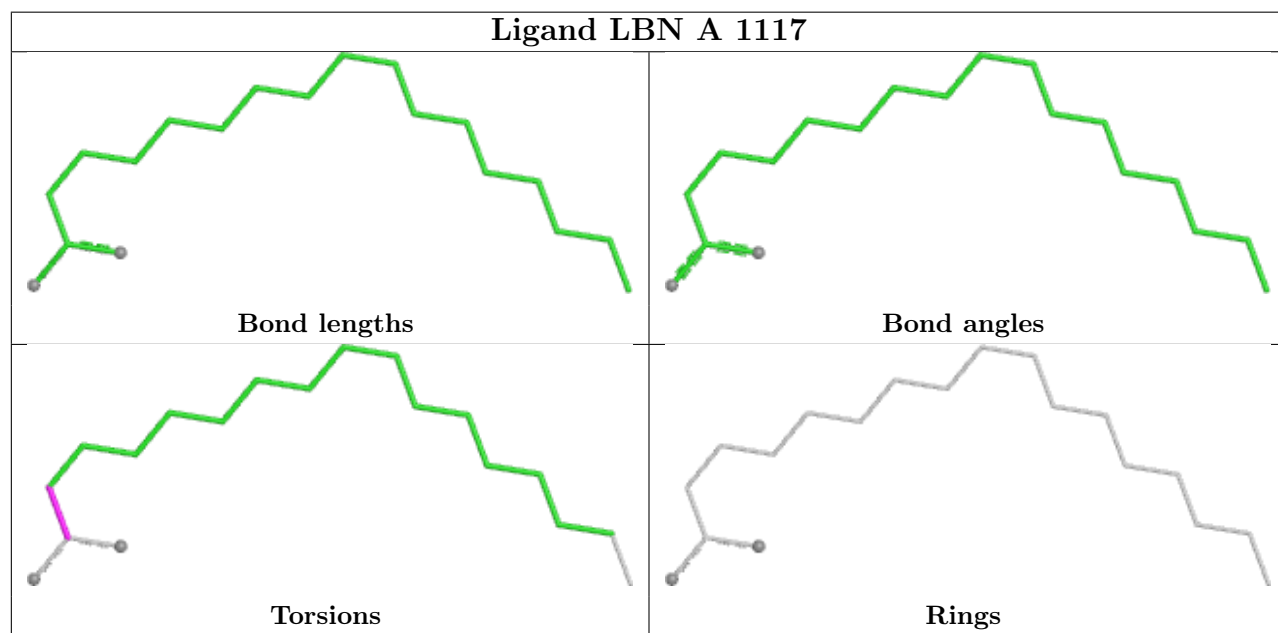
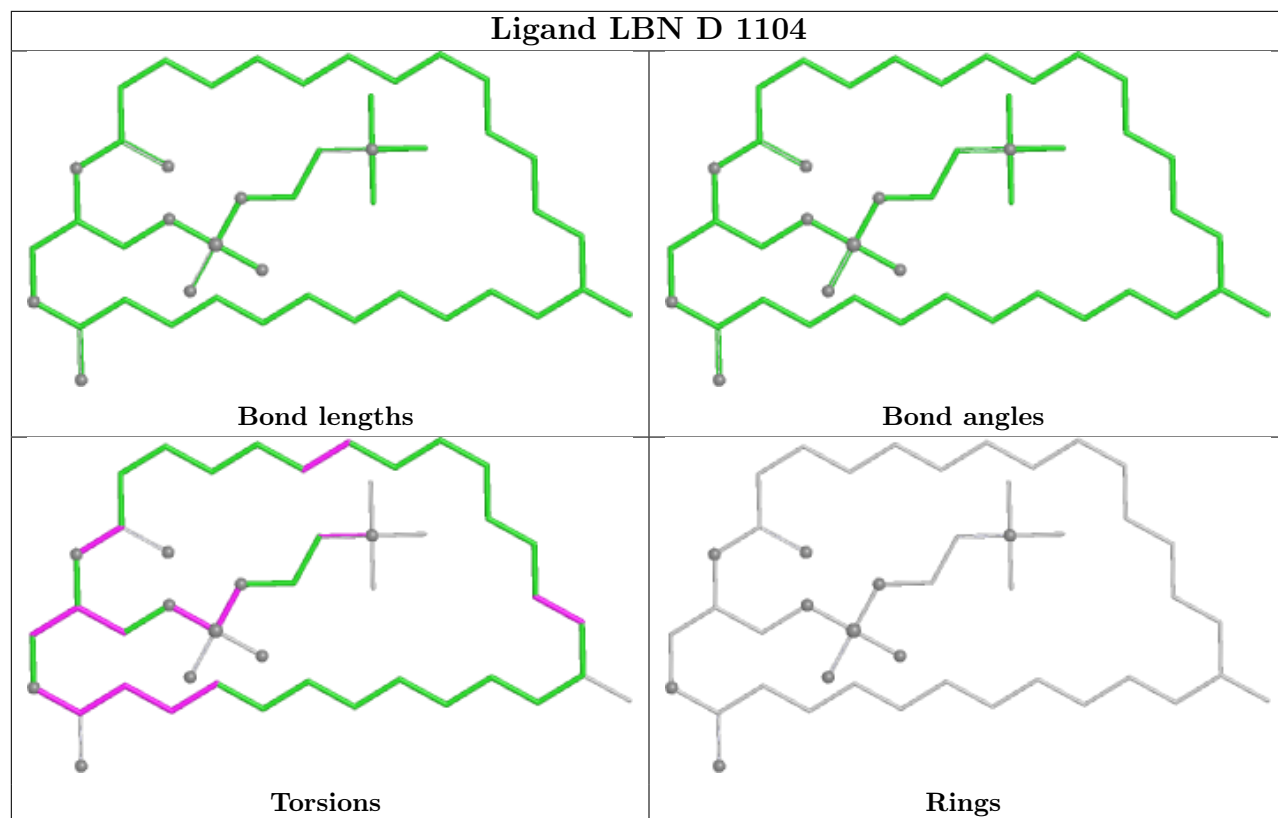


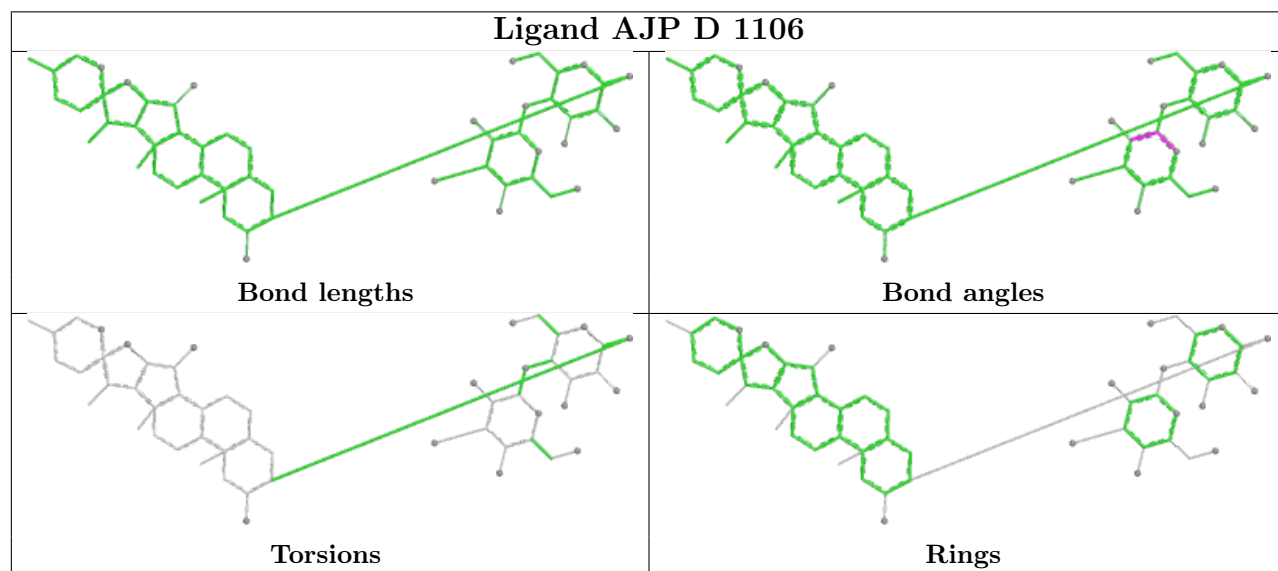
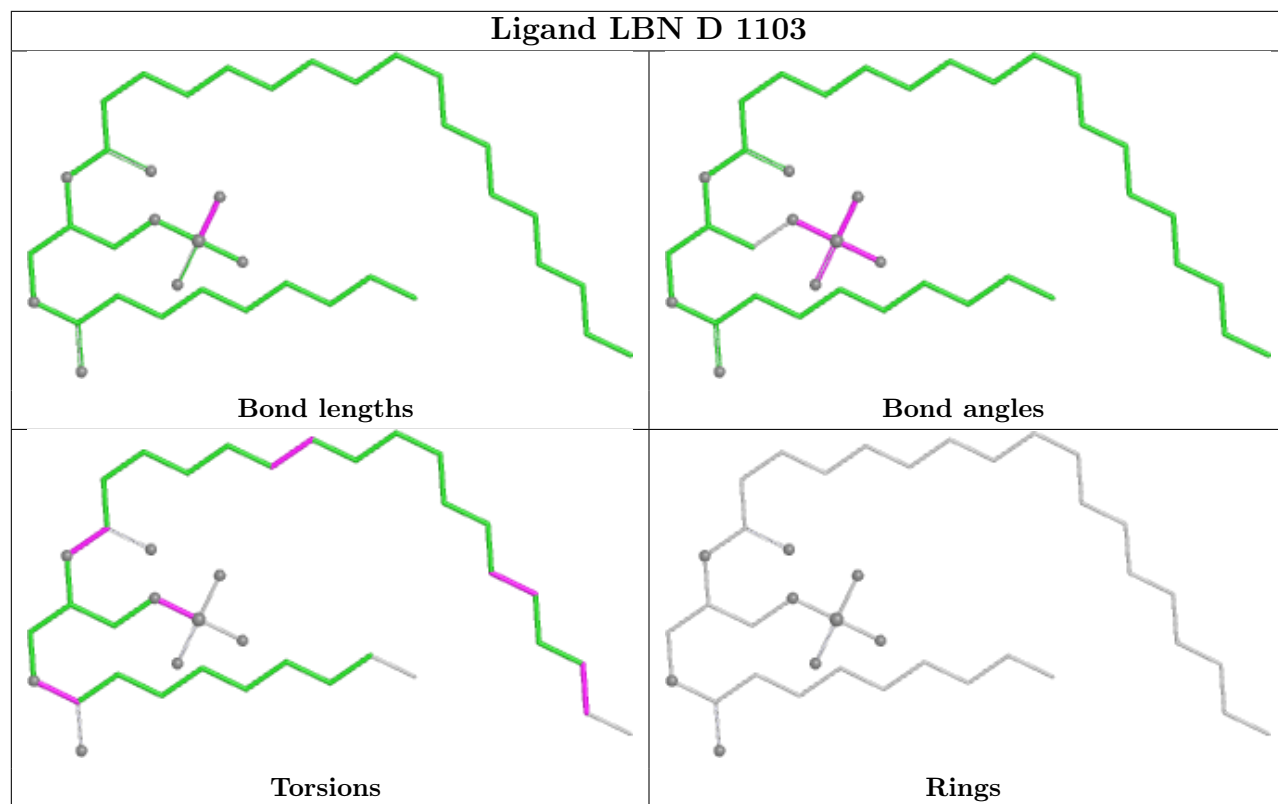
Ligand LBN C 1101

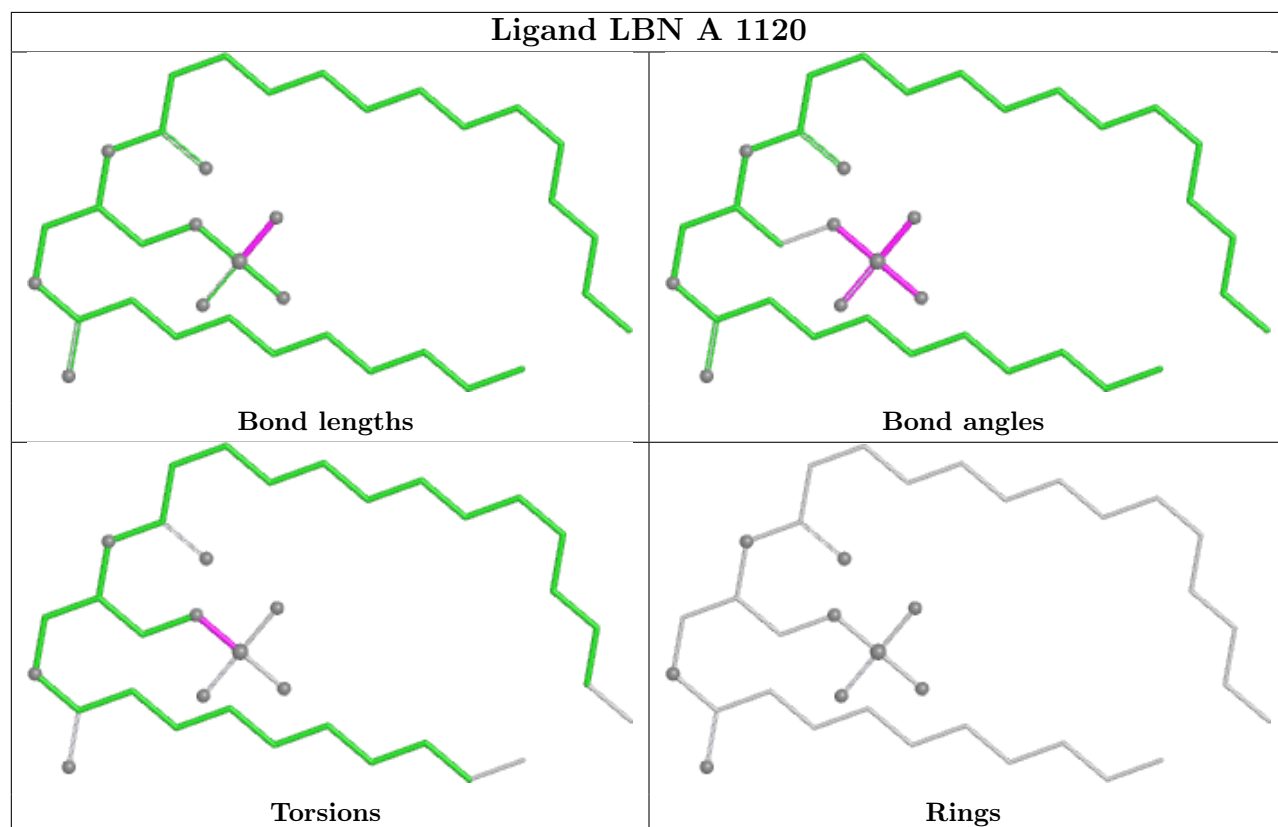
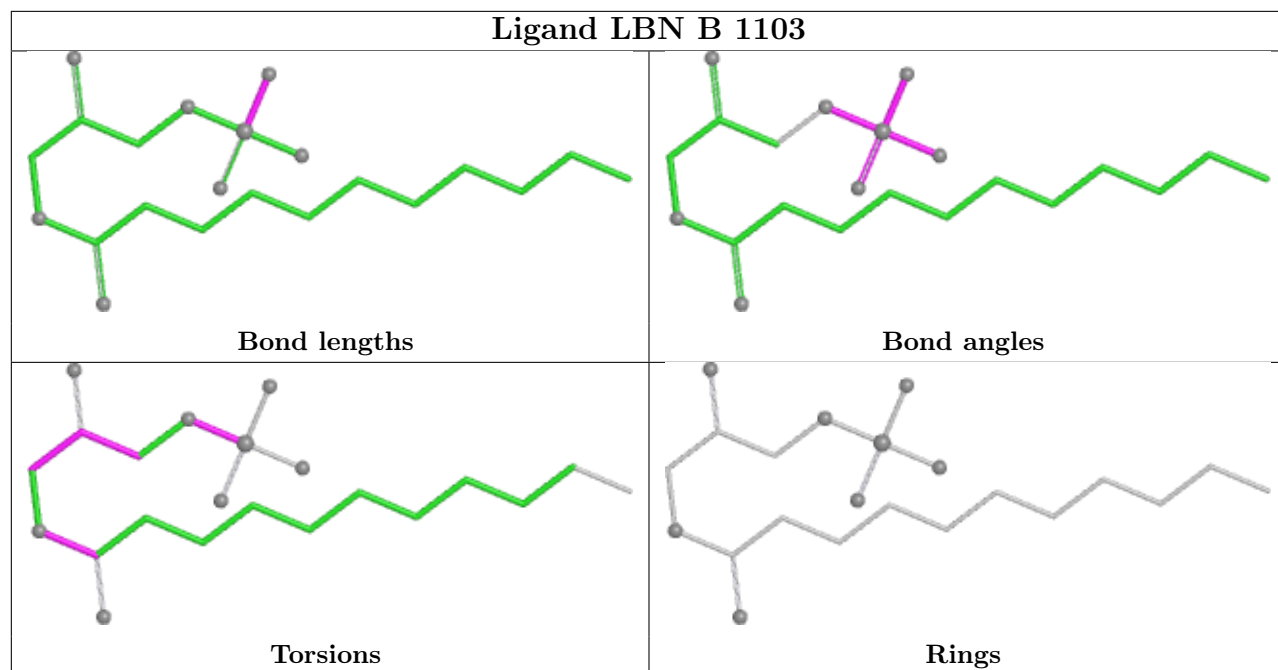


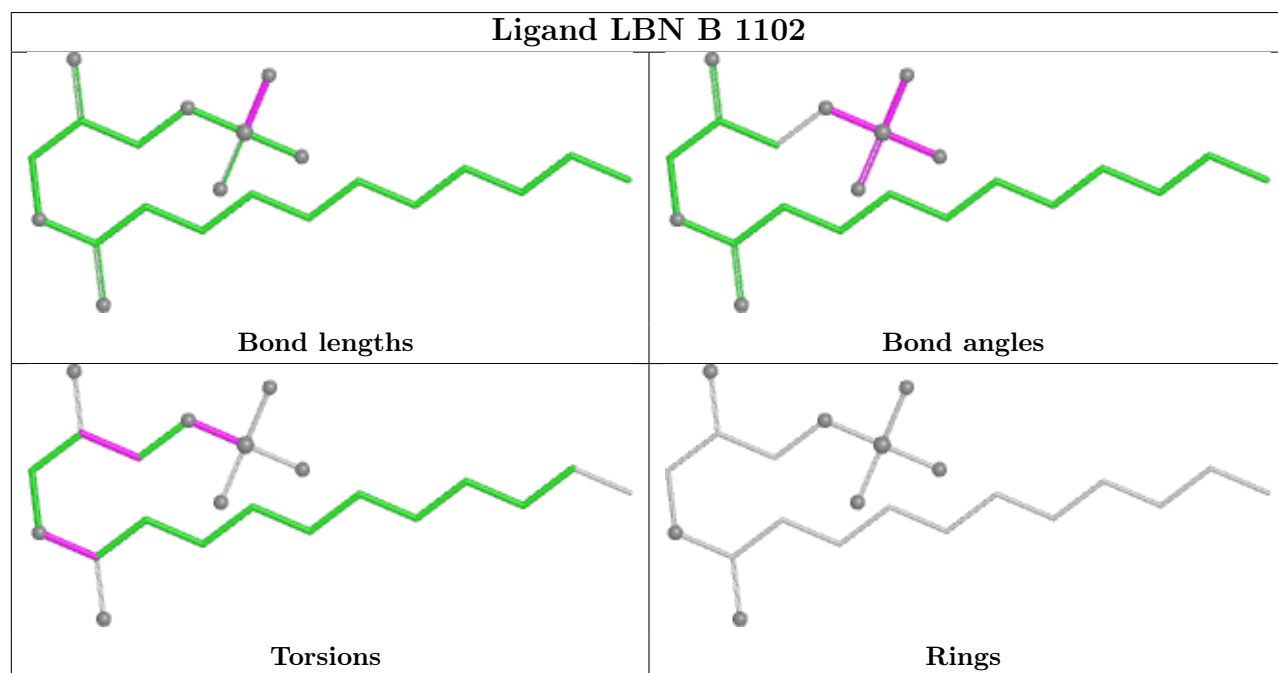
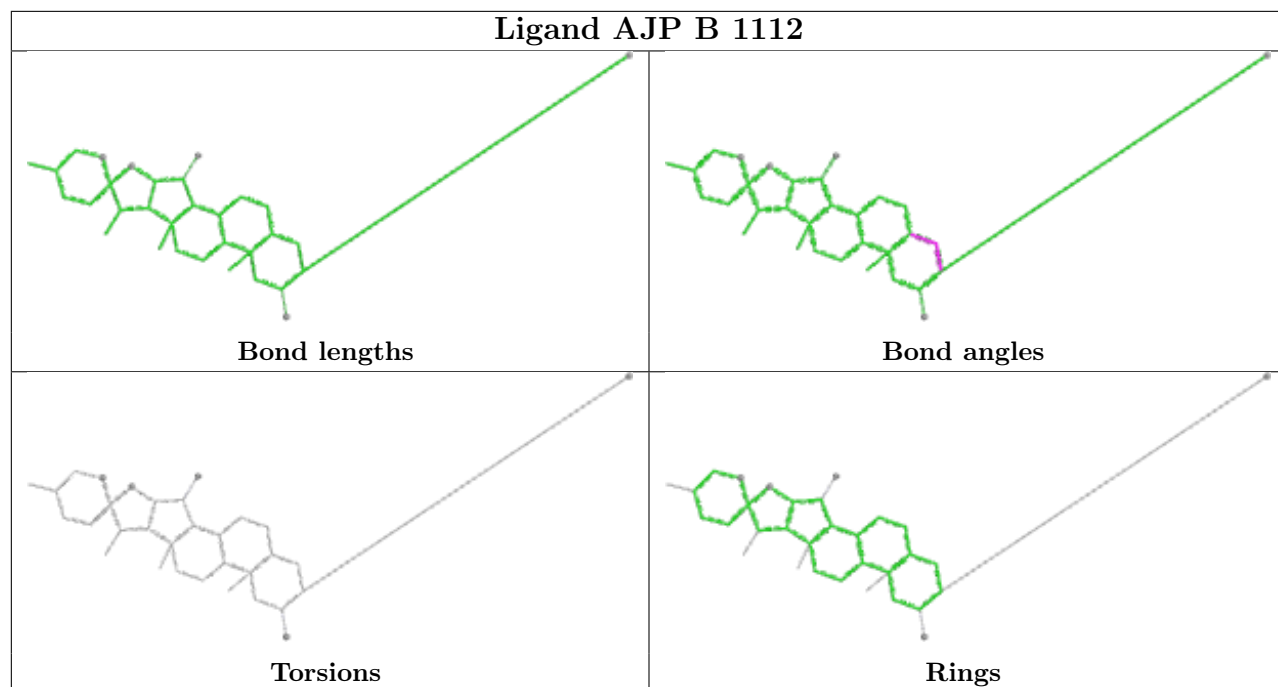
Ligand AJP C 1109

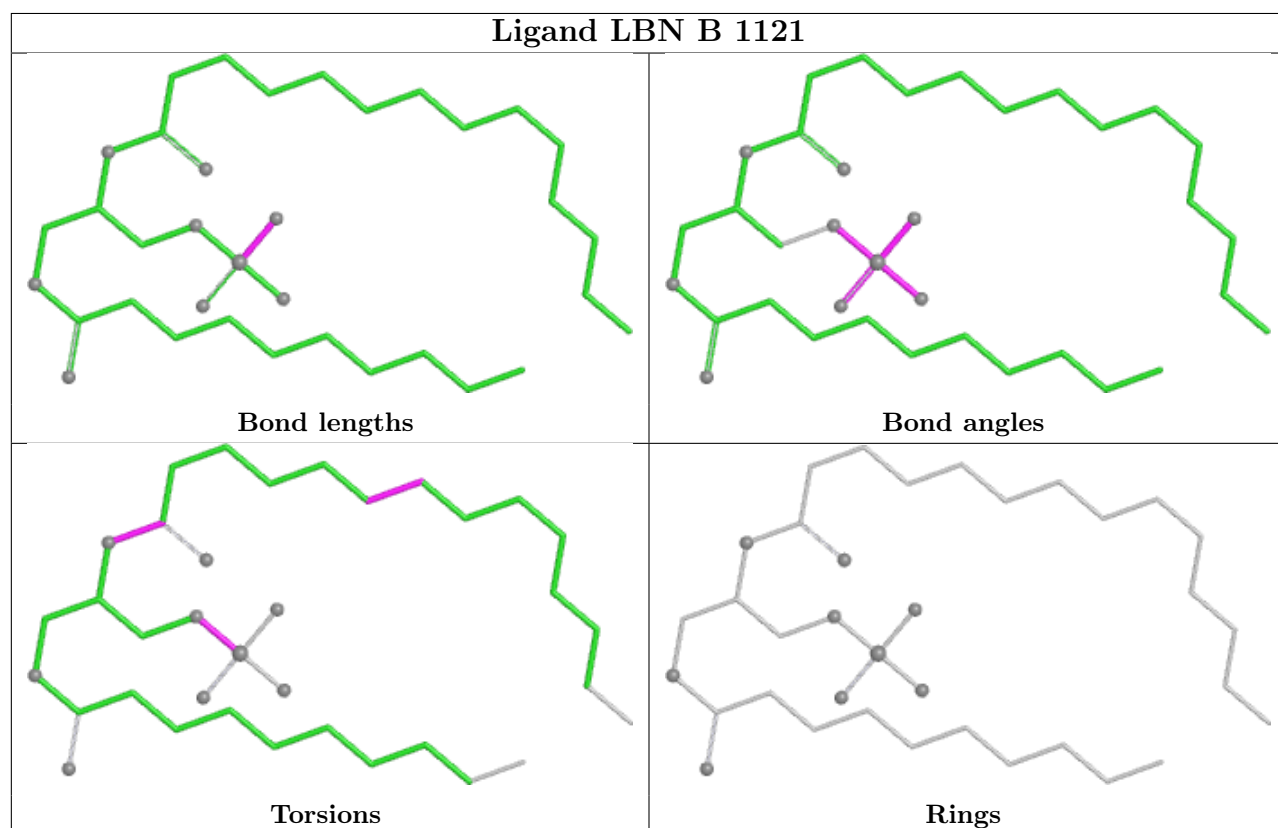
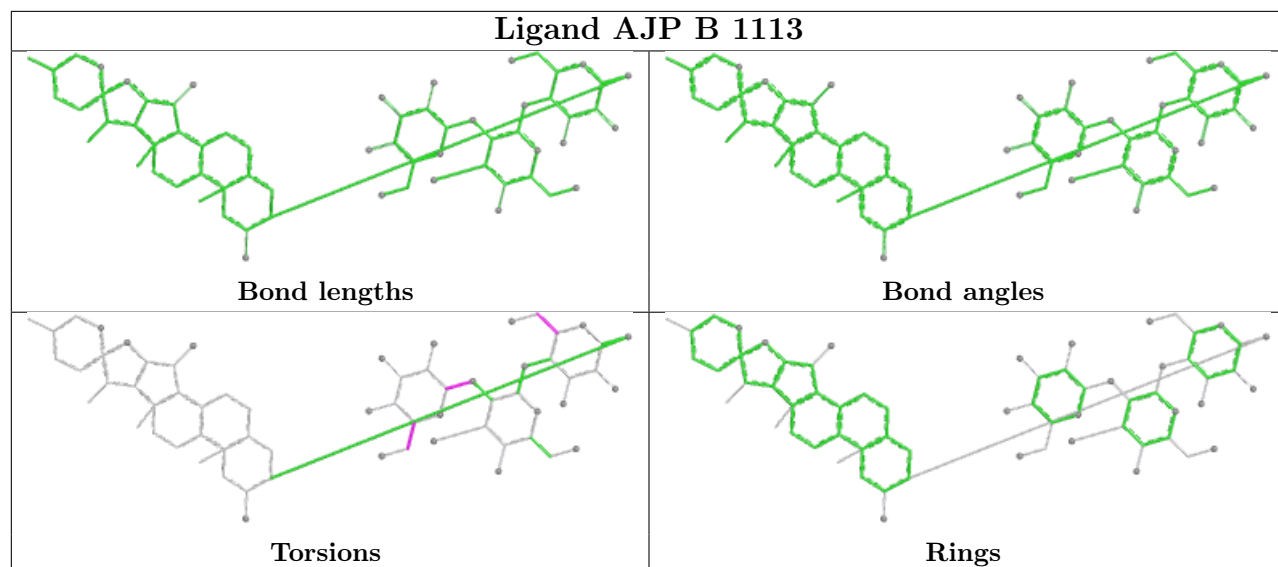


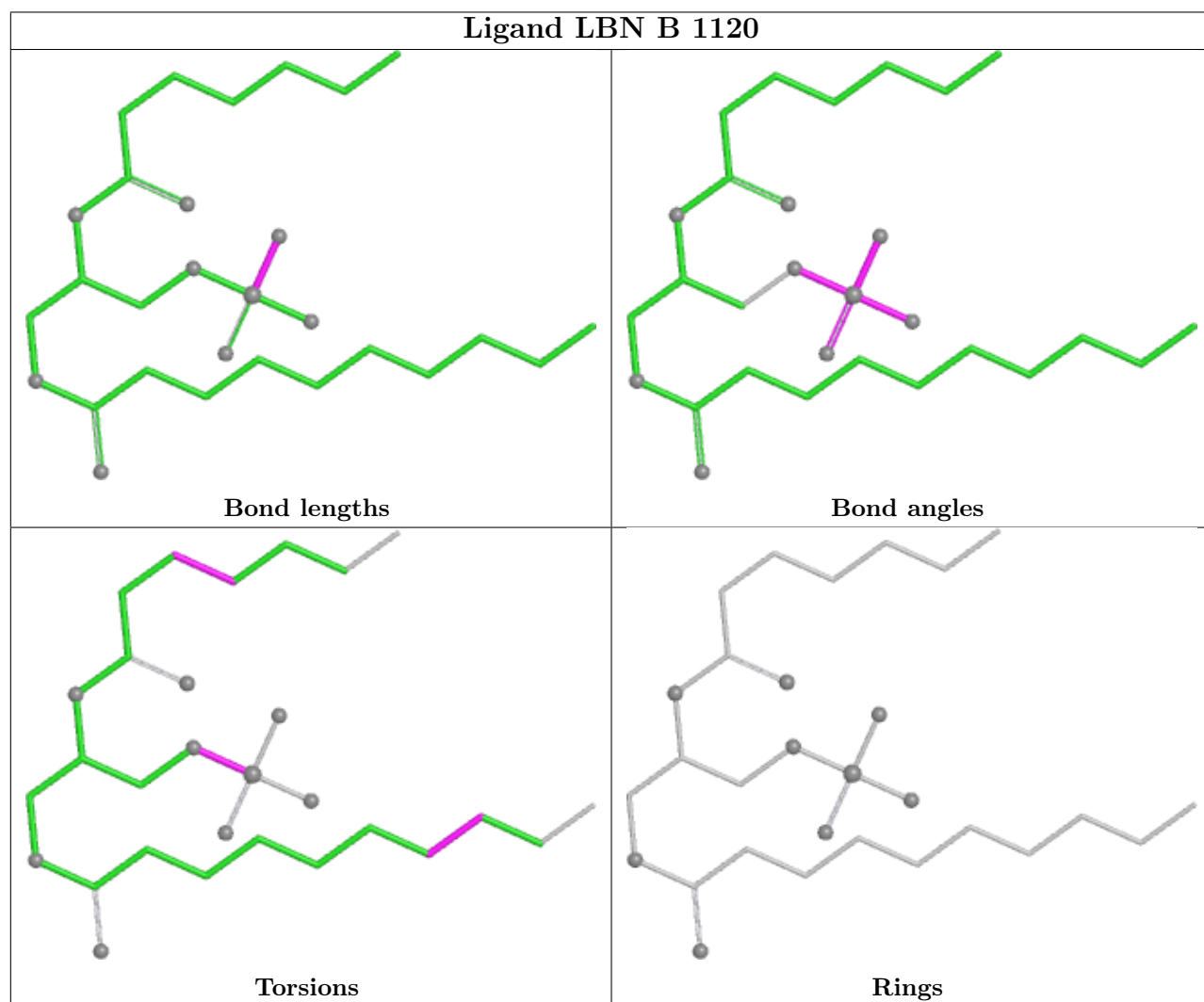
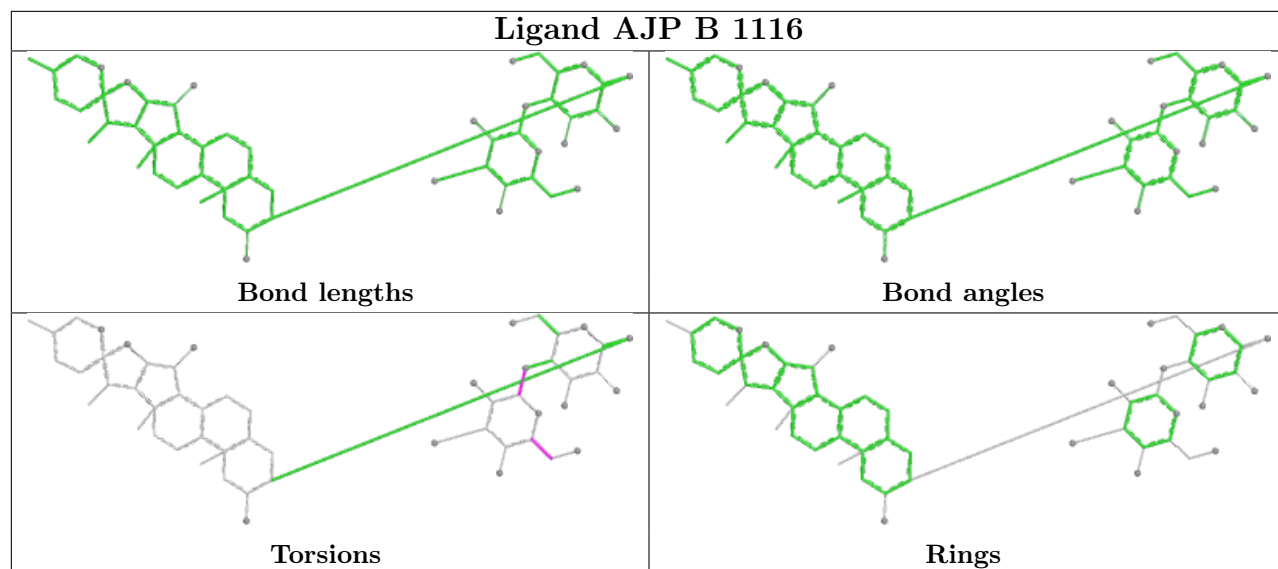


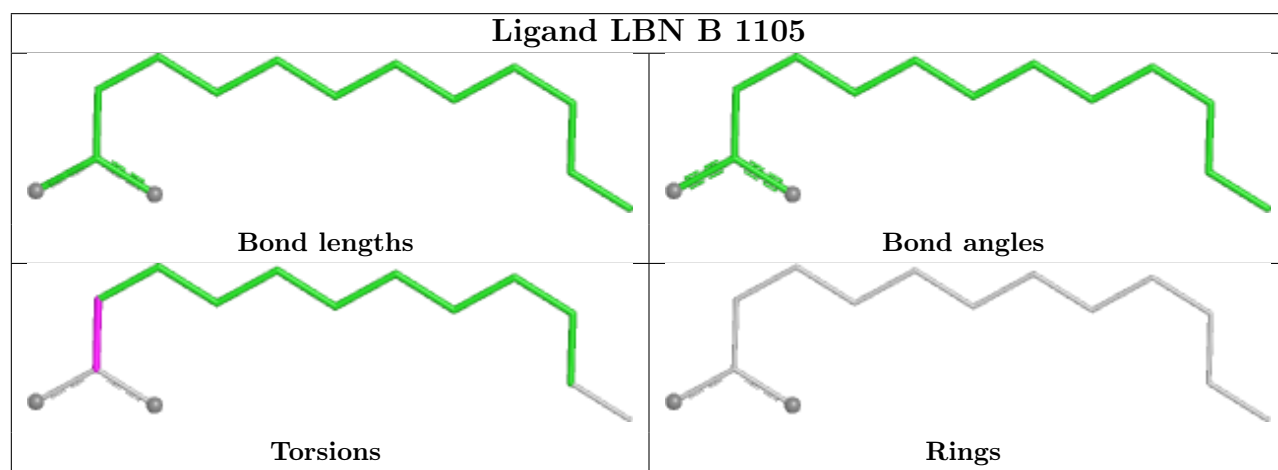
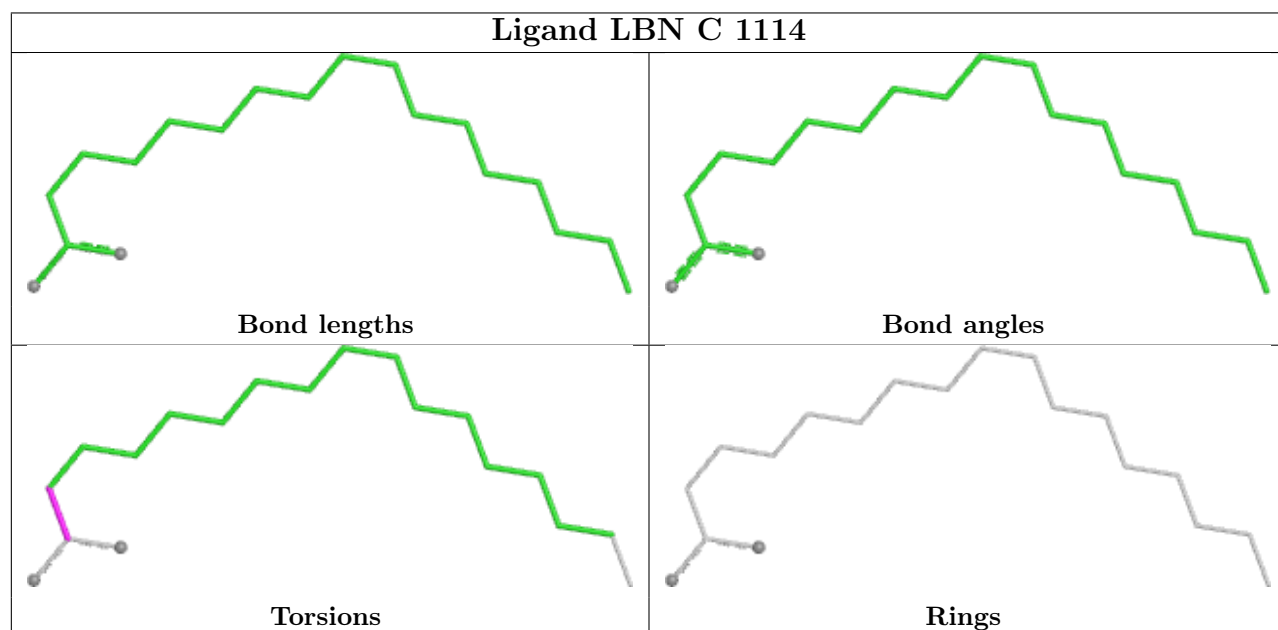
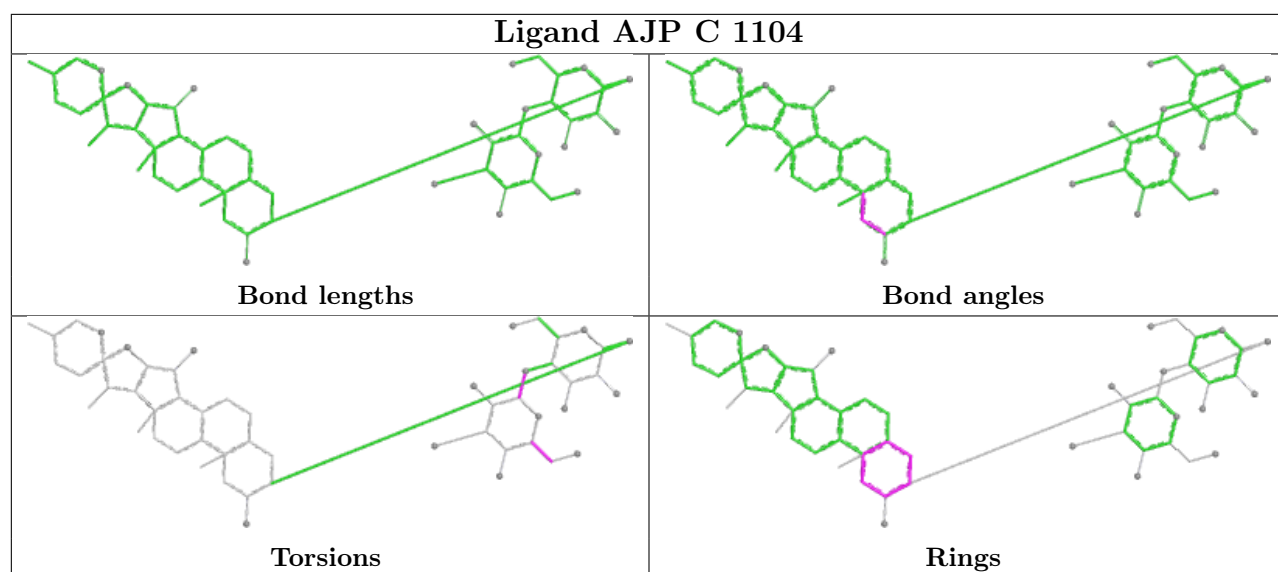


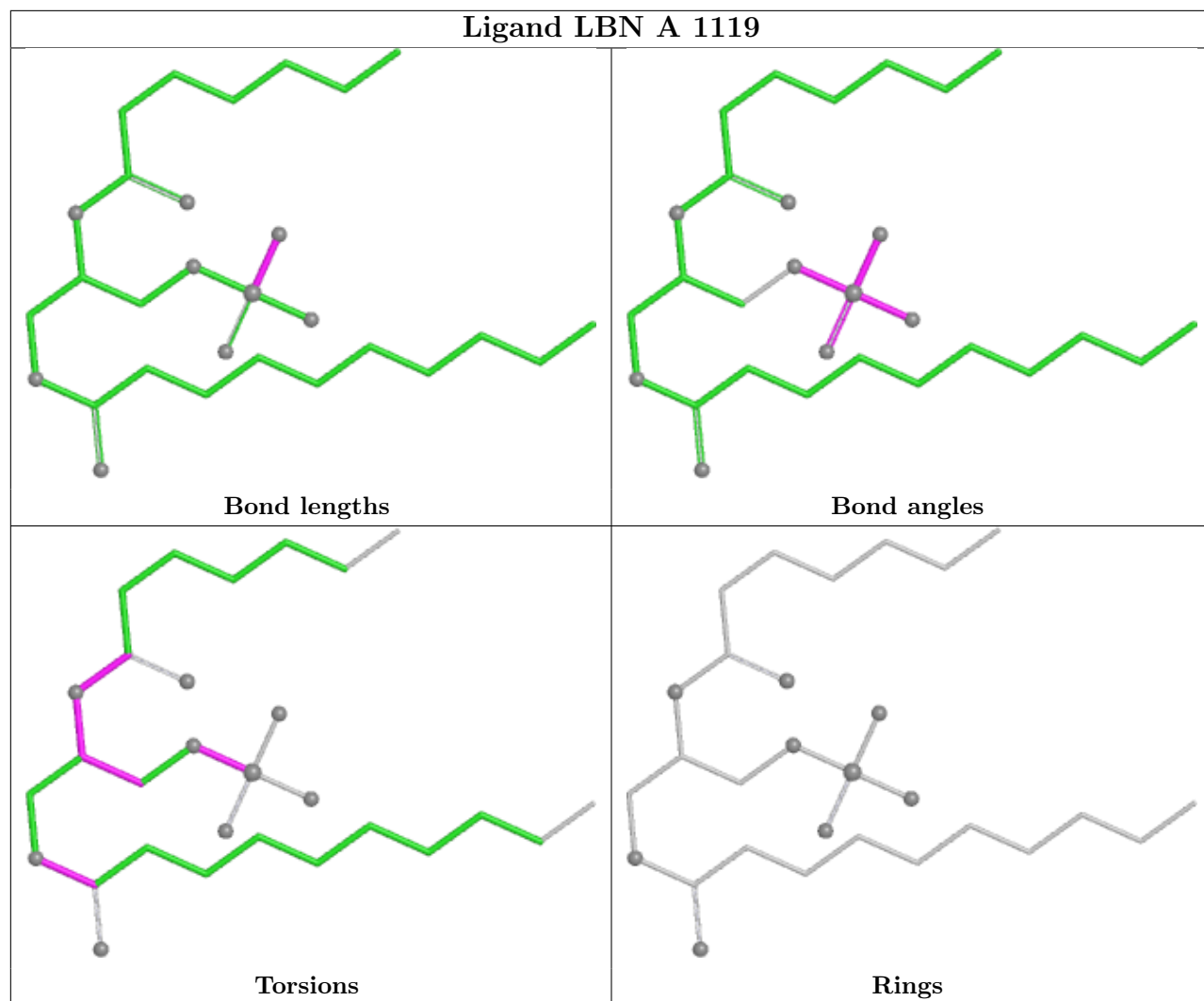


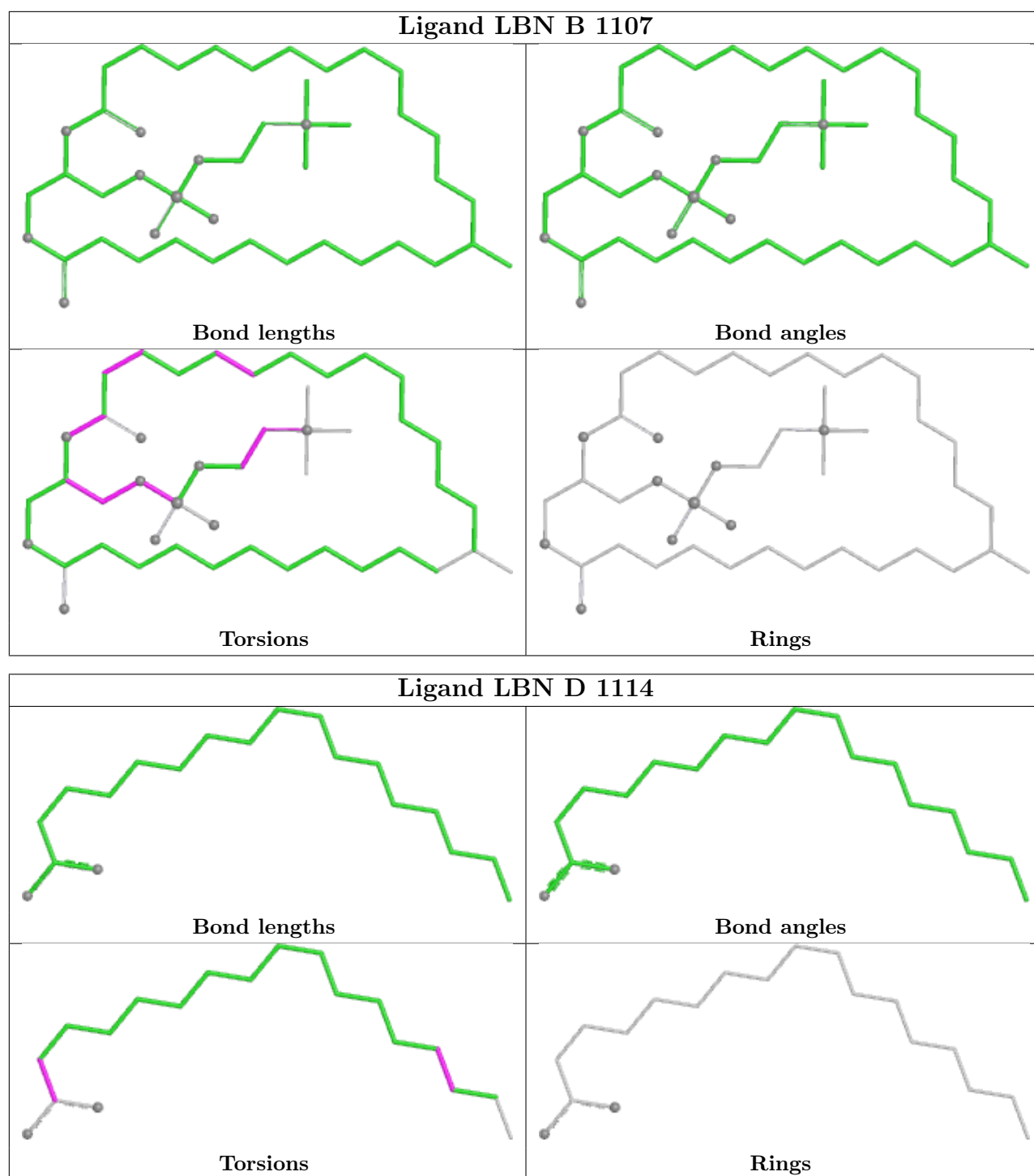


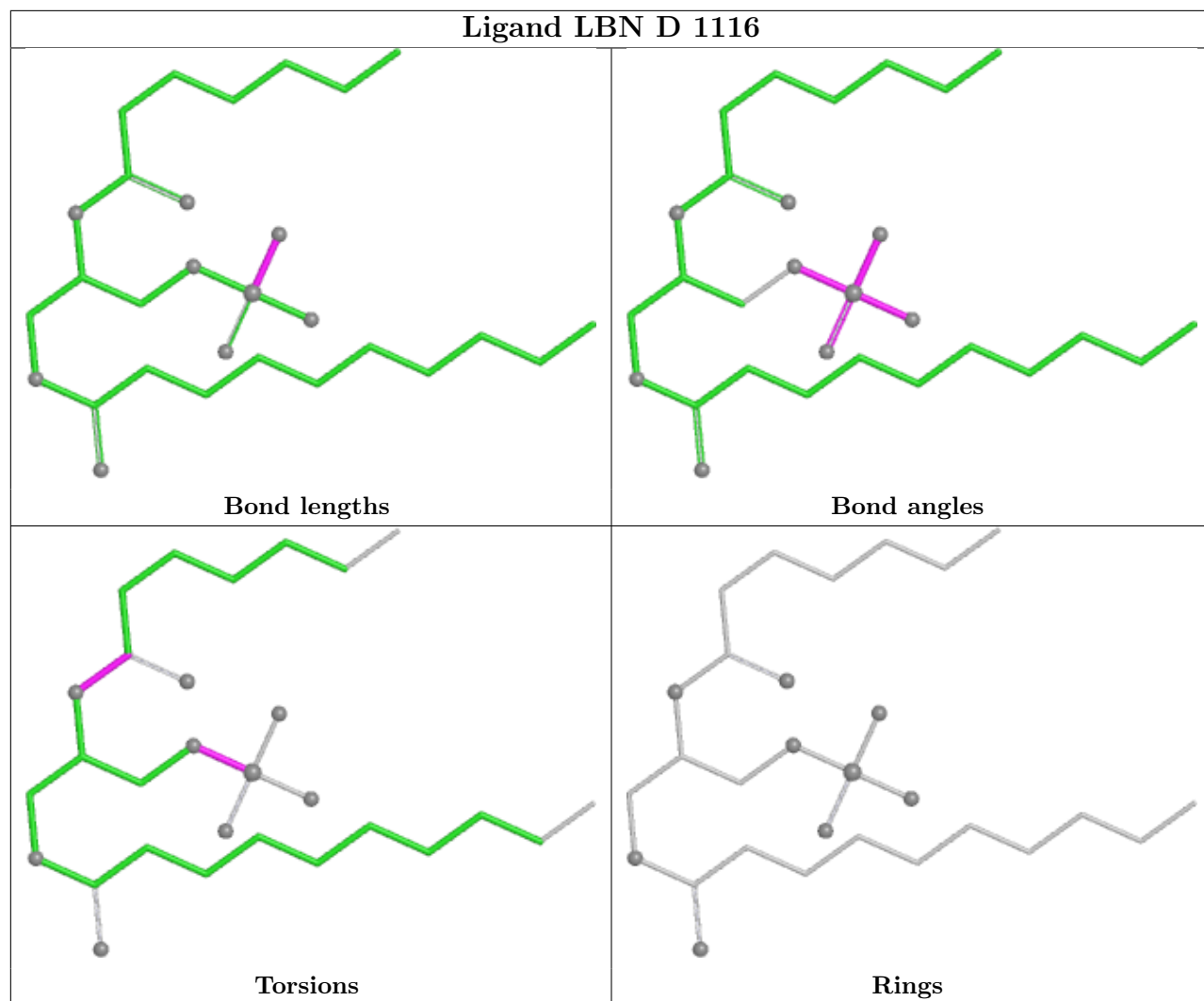


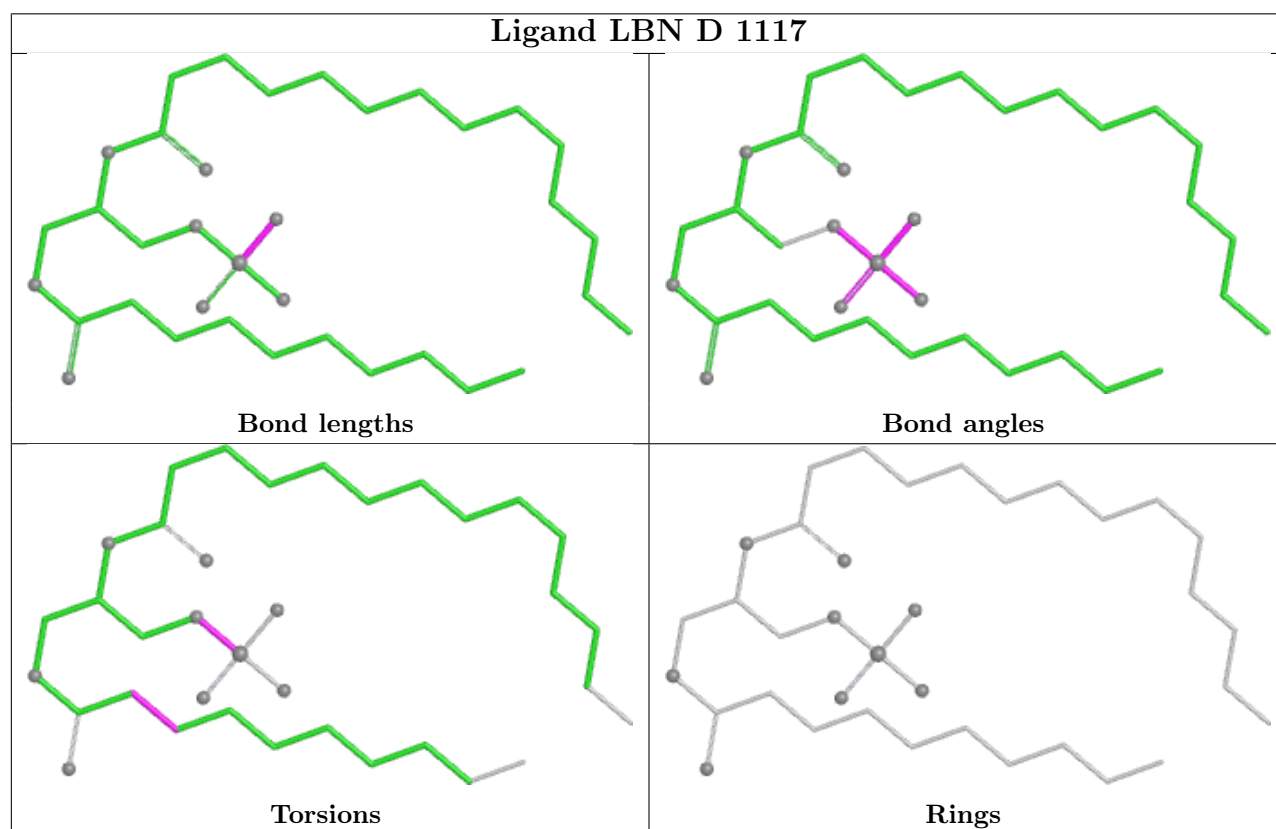
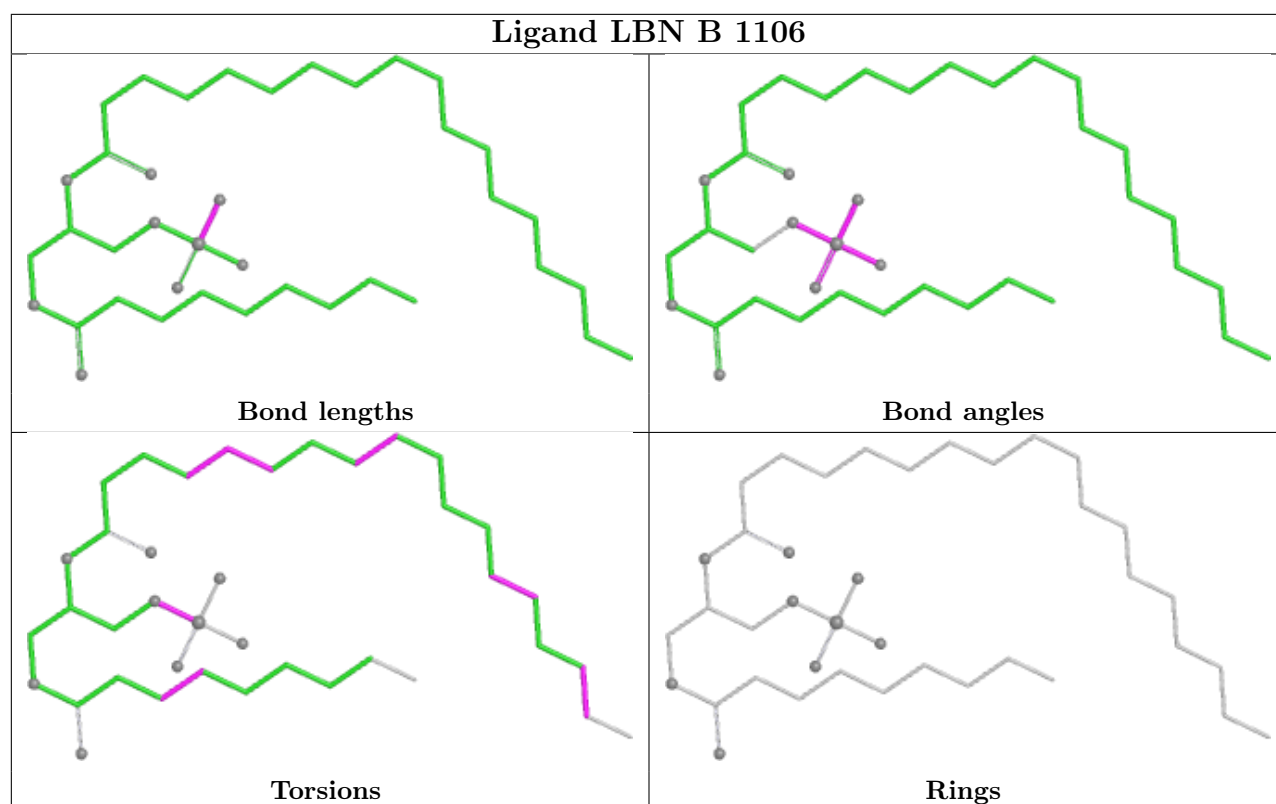


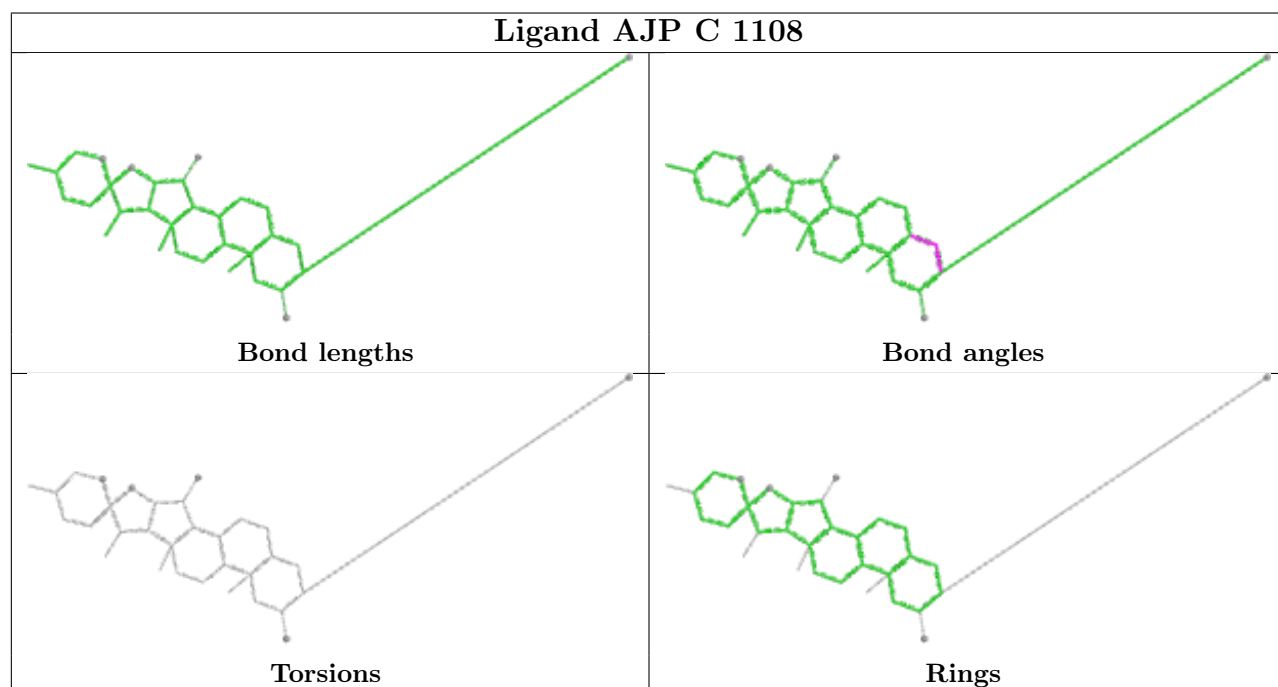
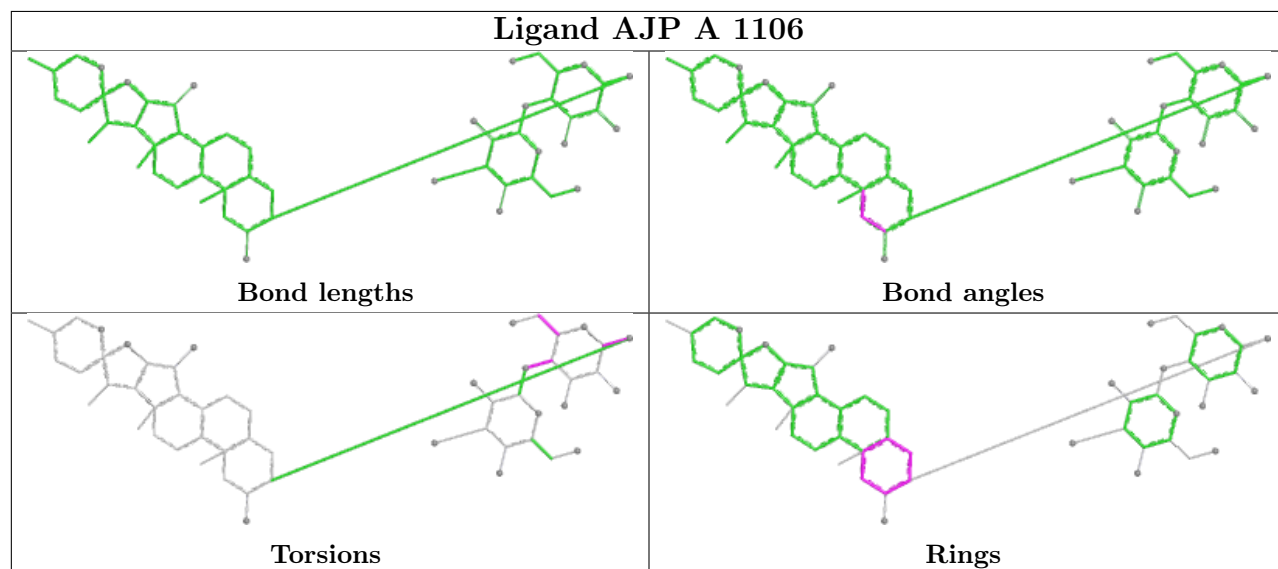
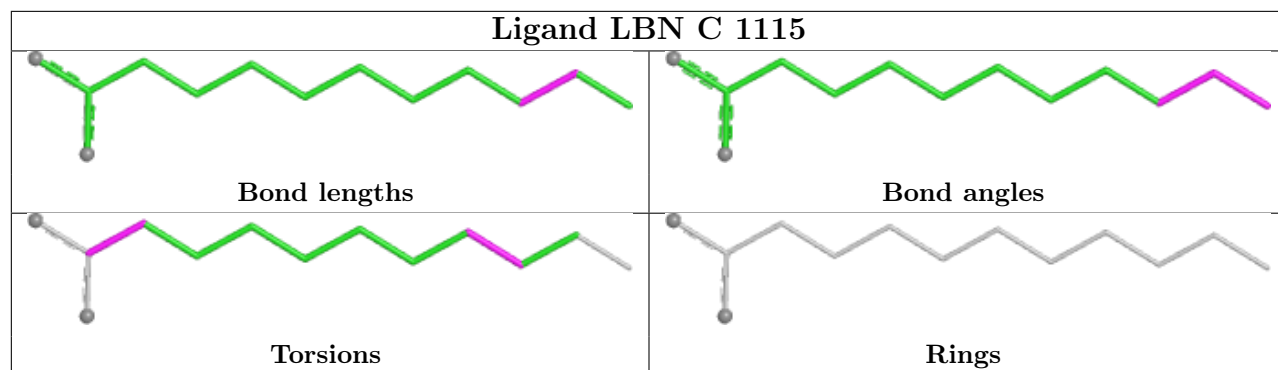


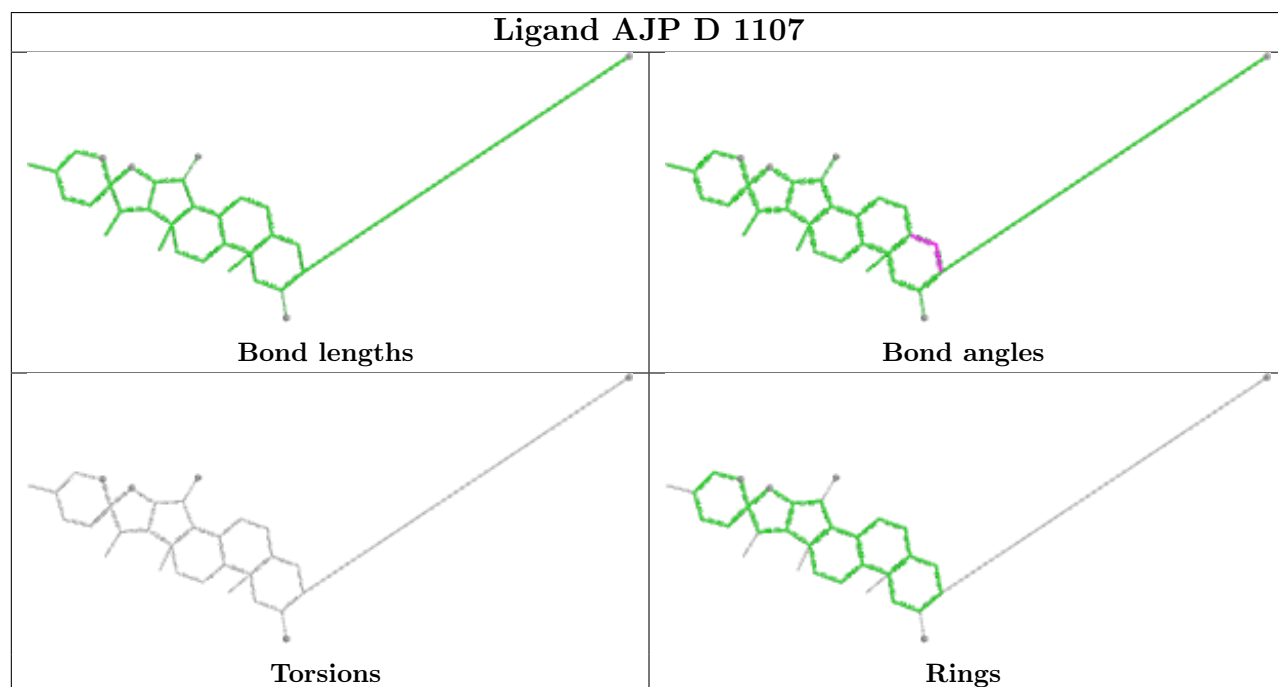
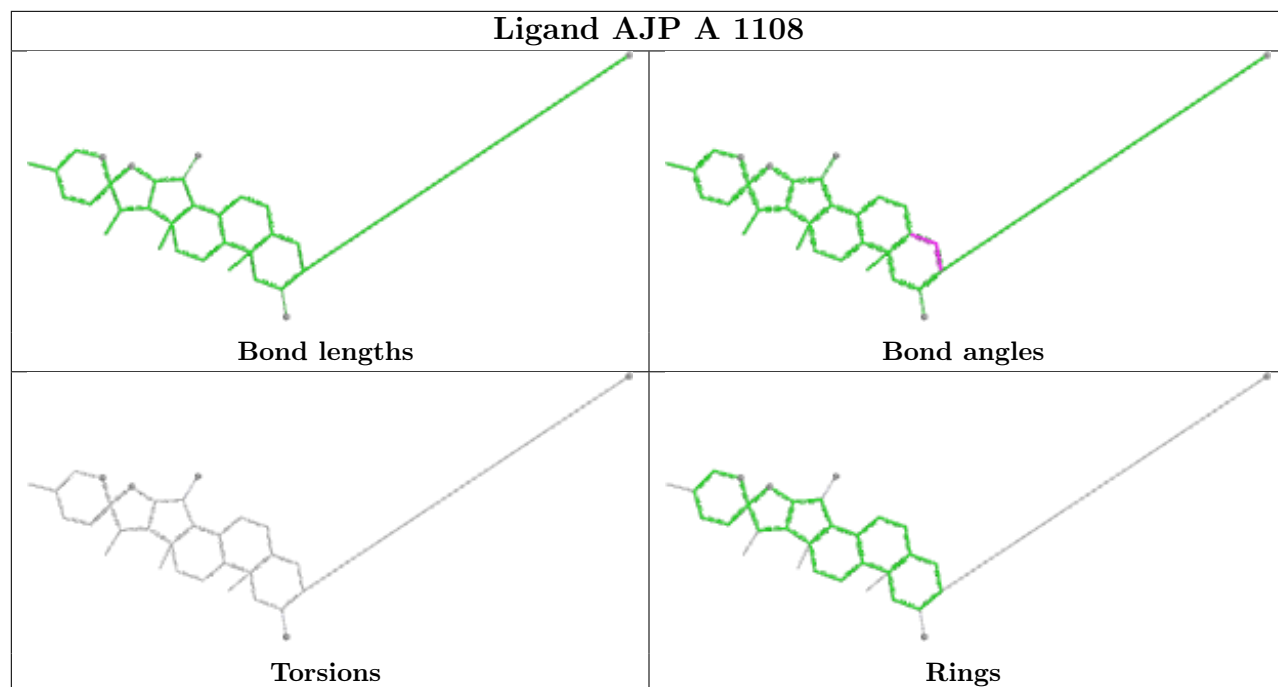


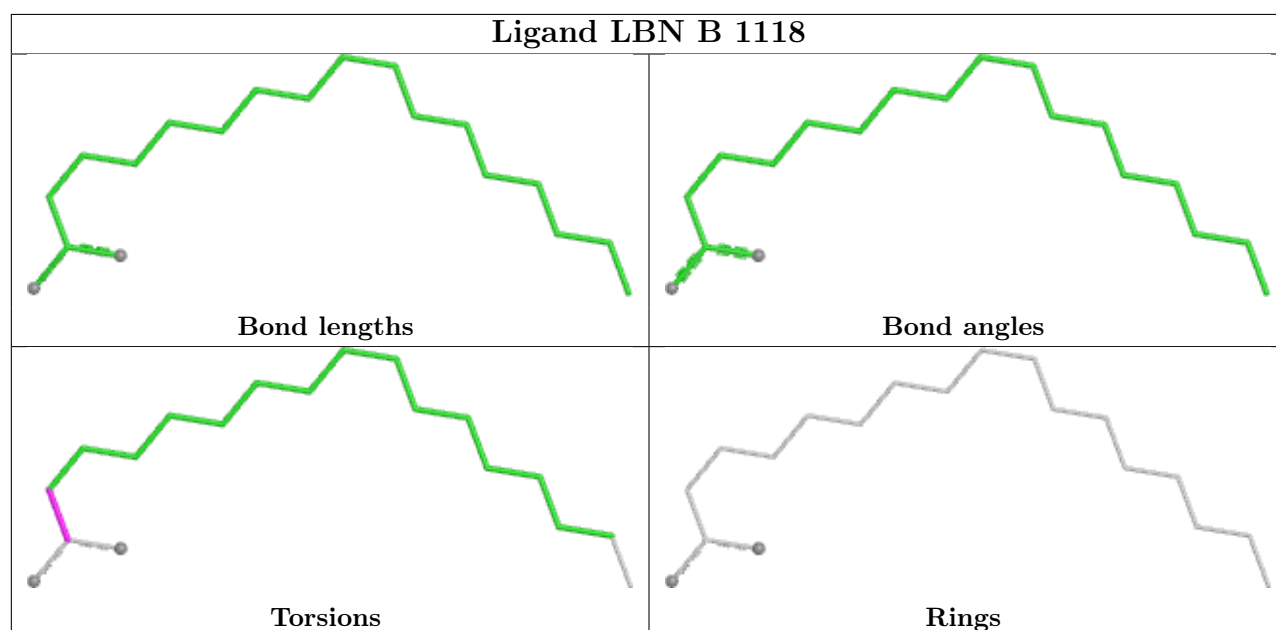
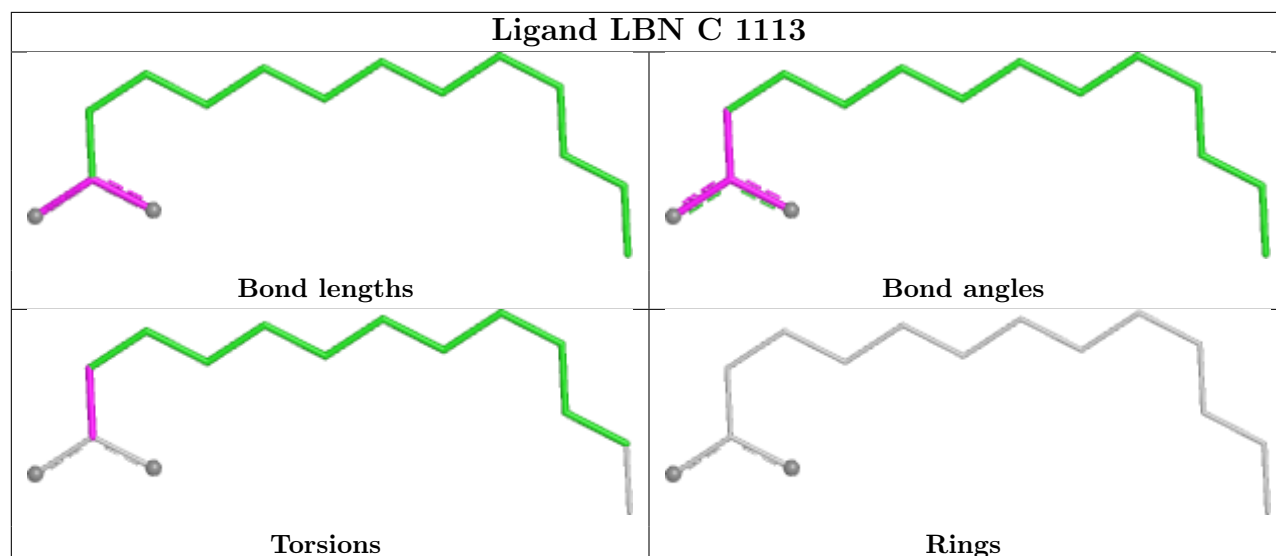
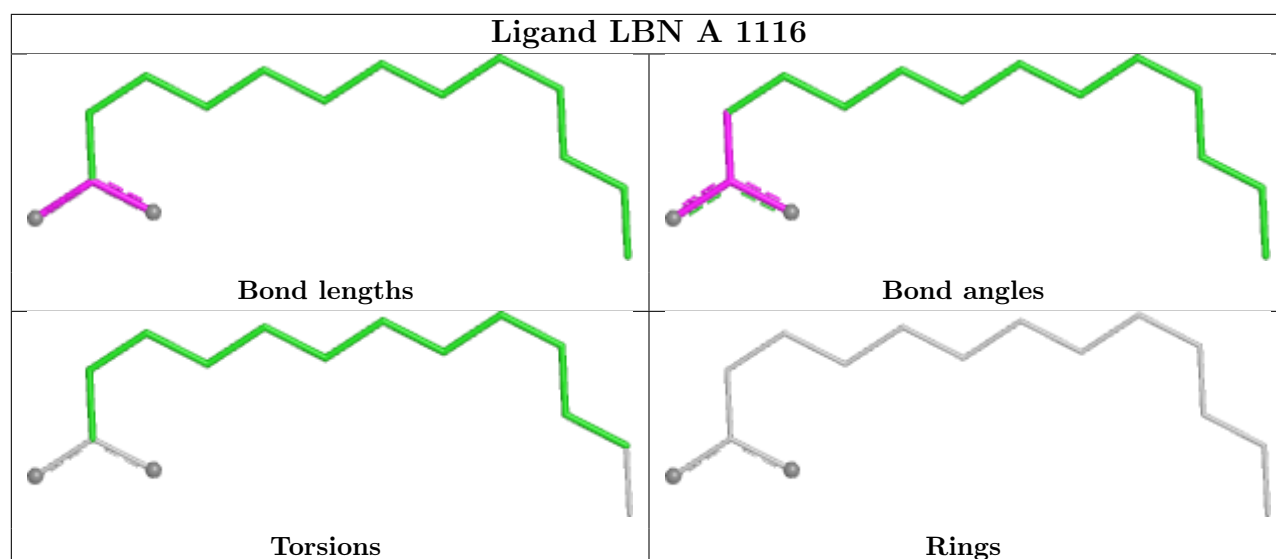


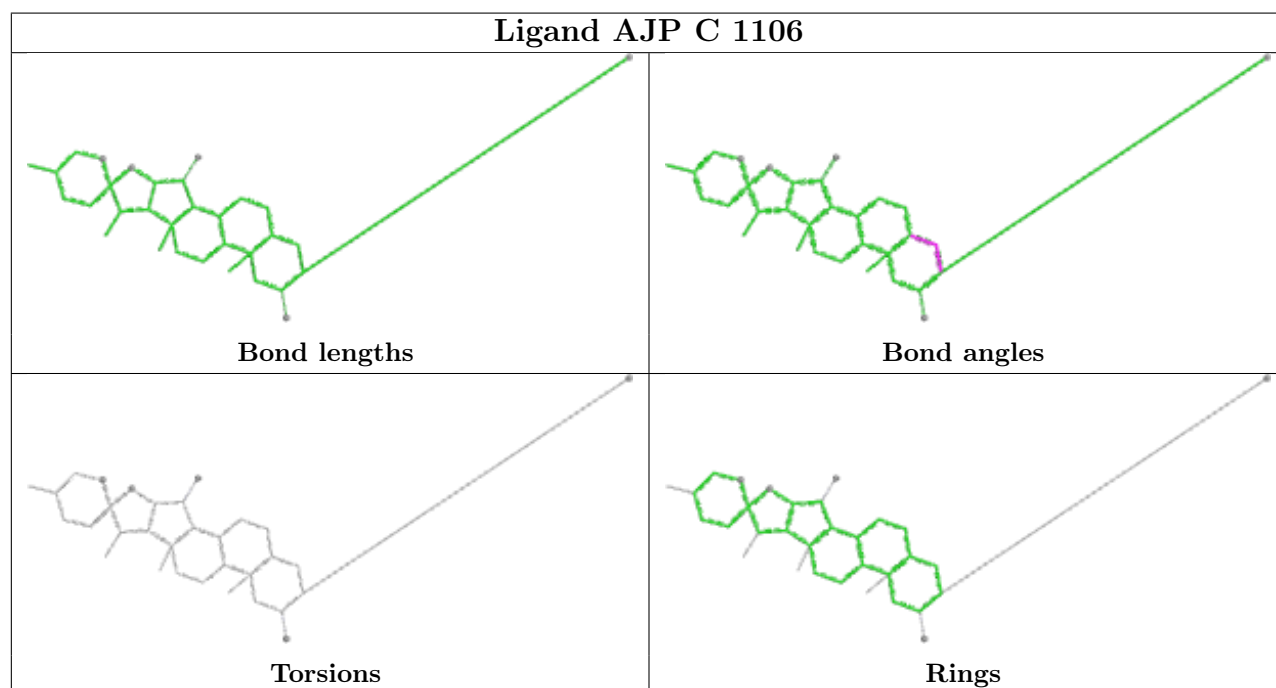
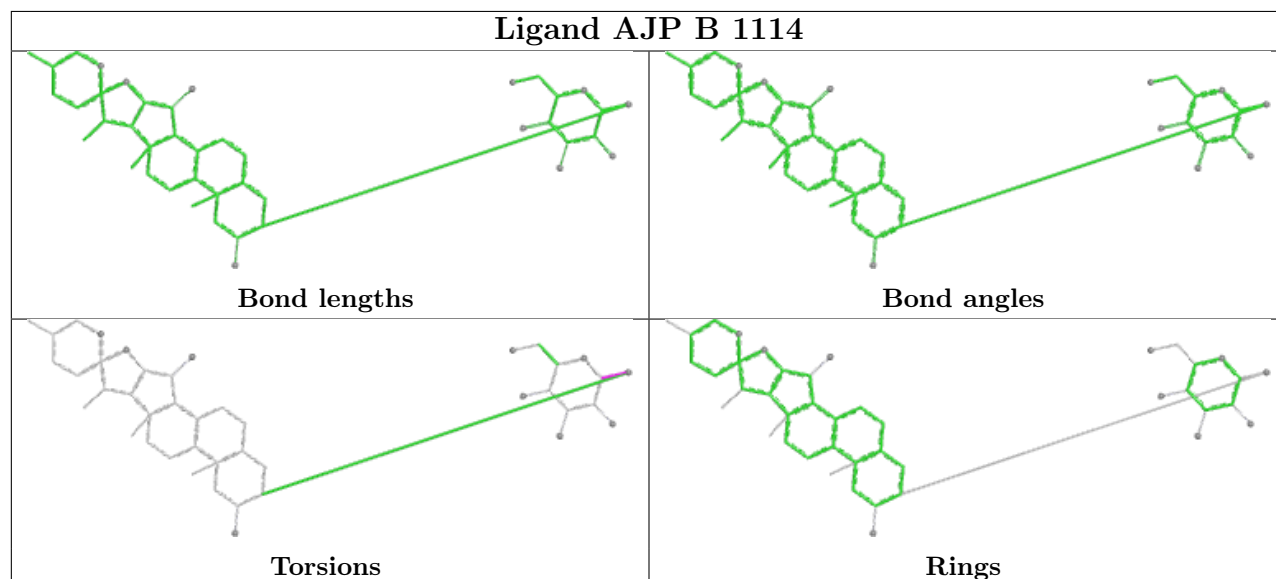
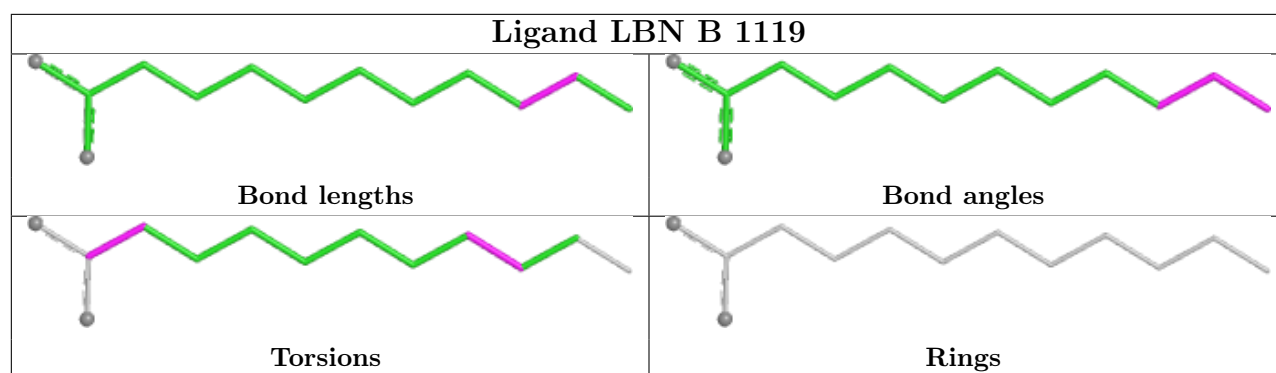


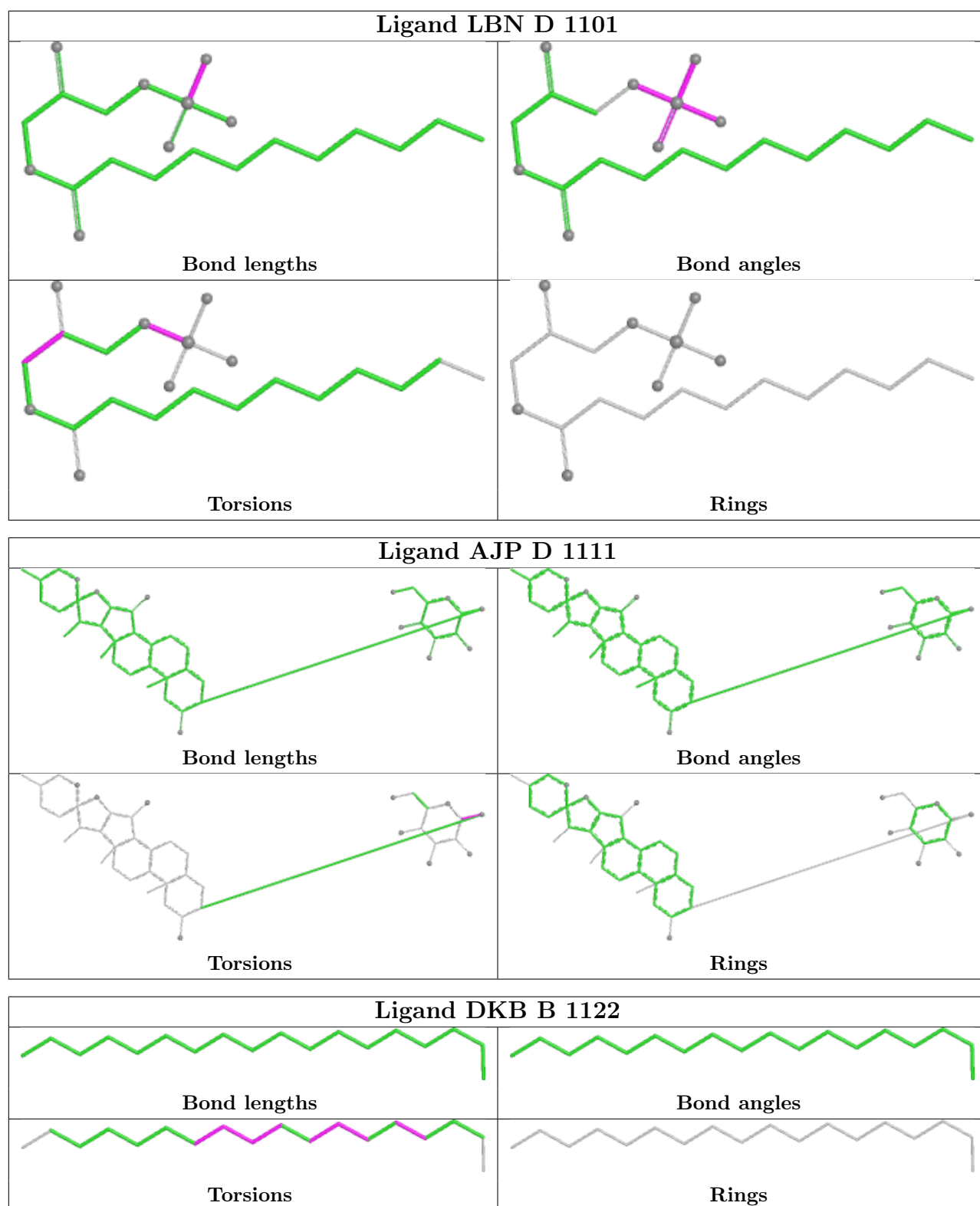


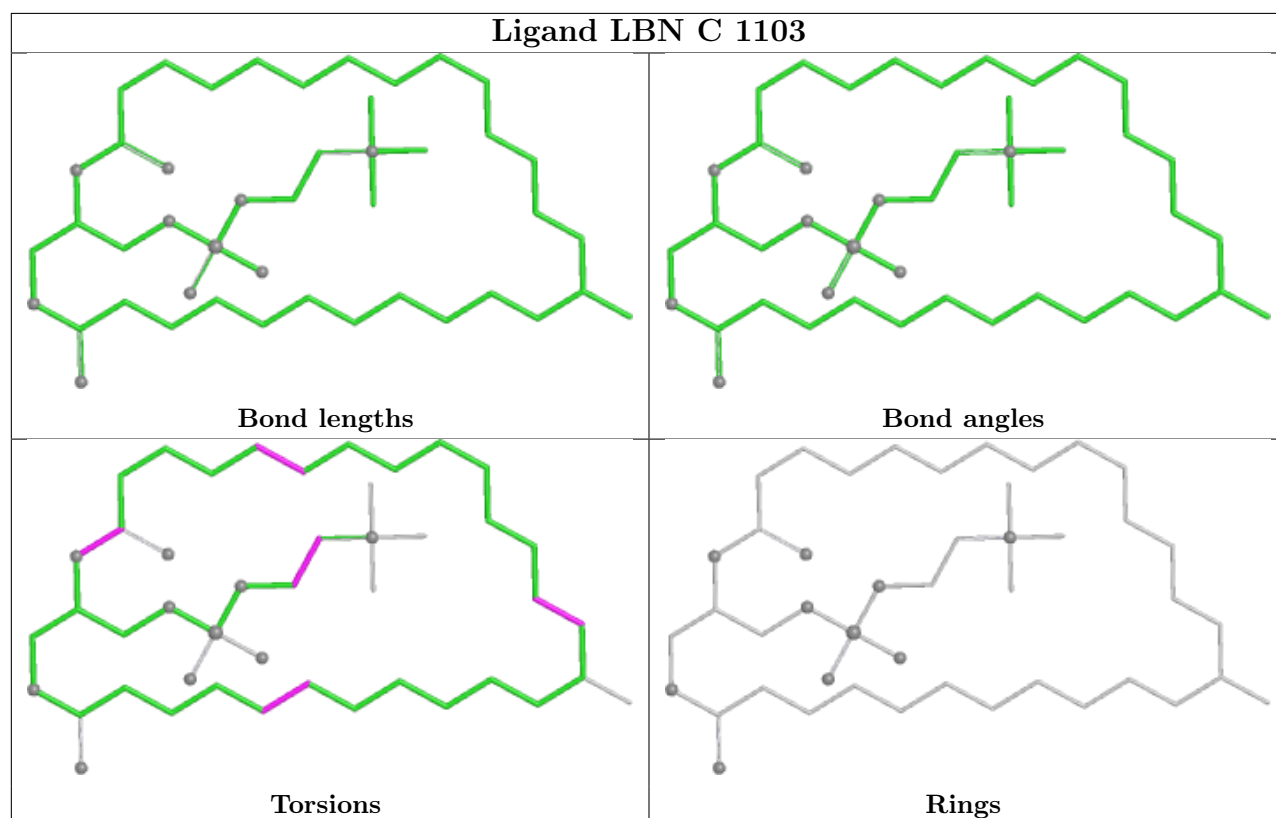
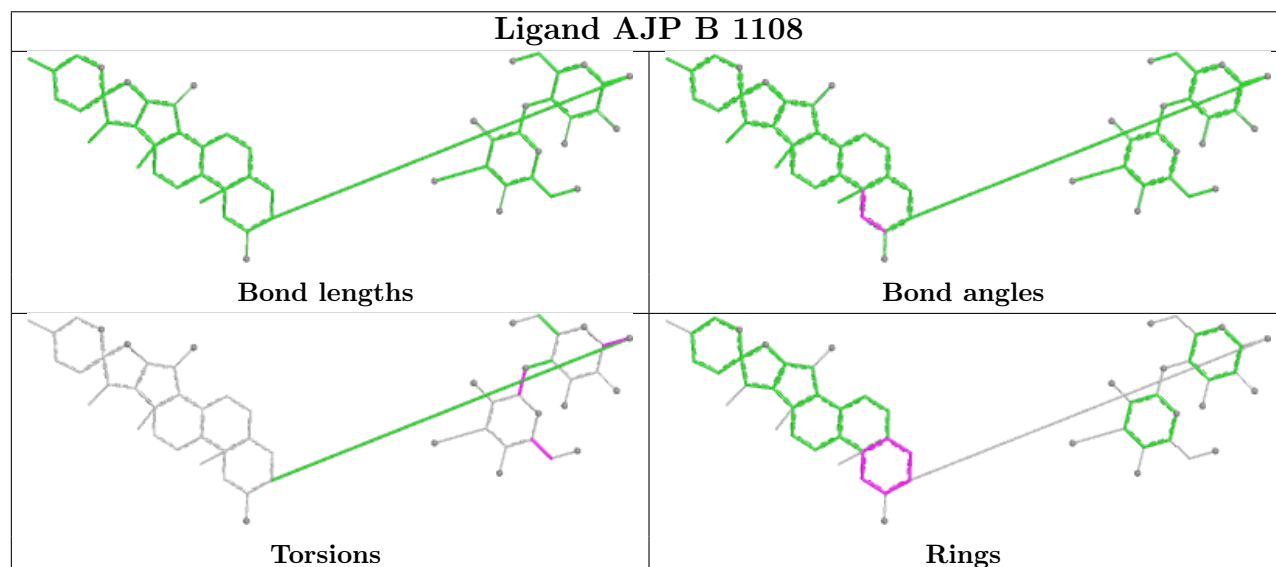
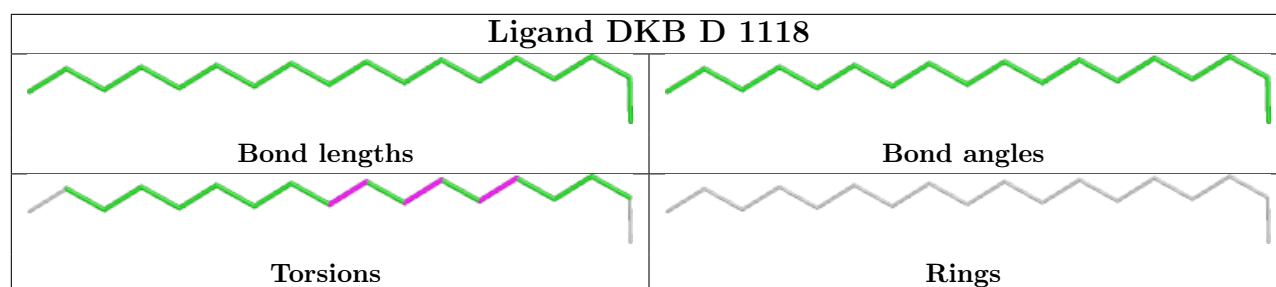


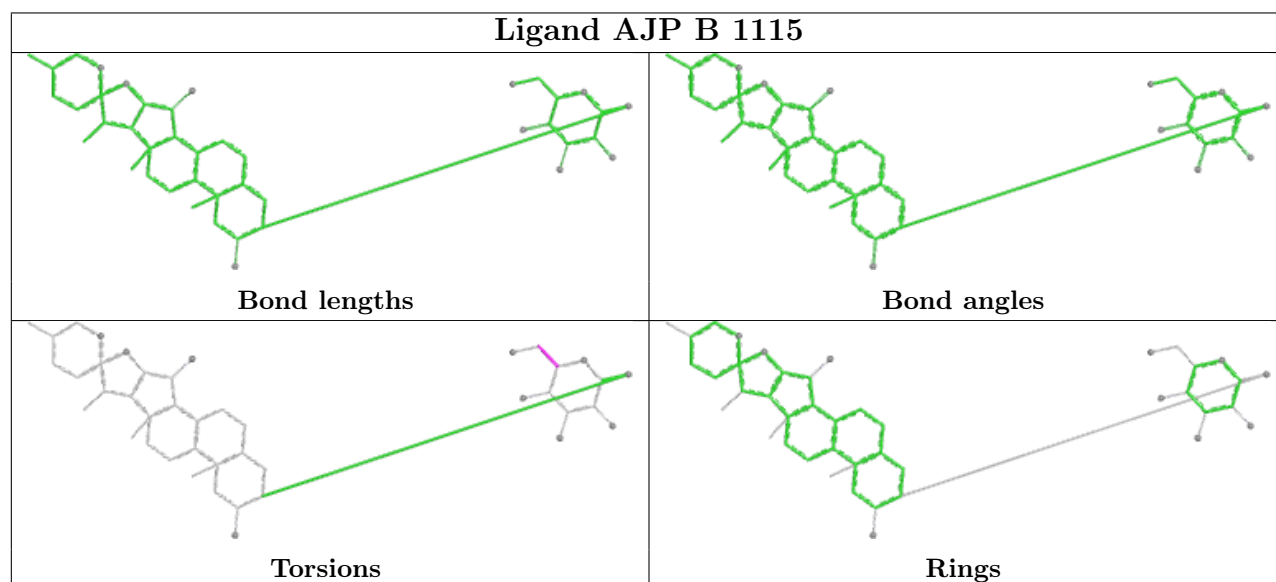
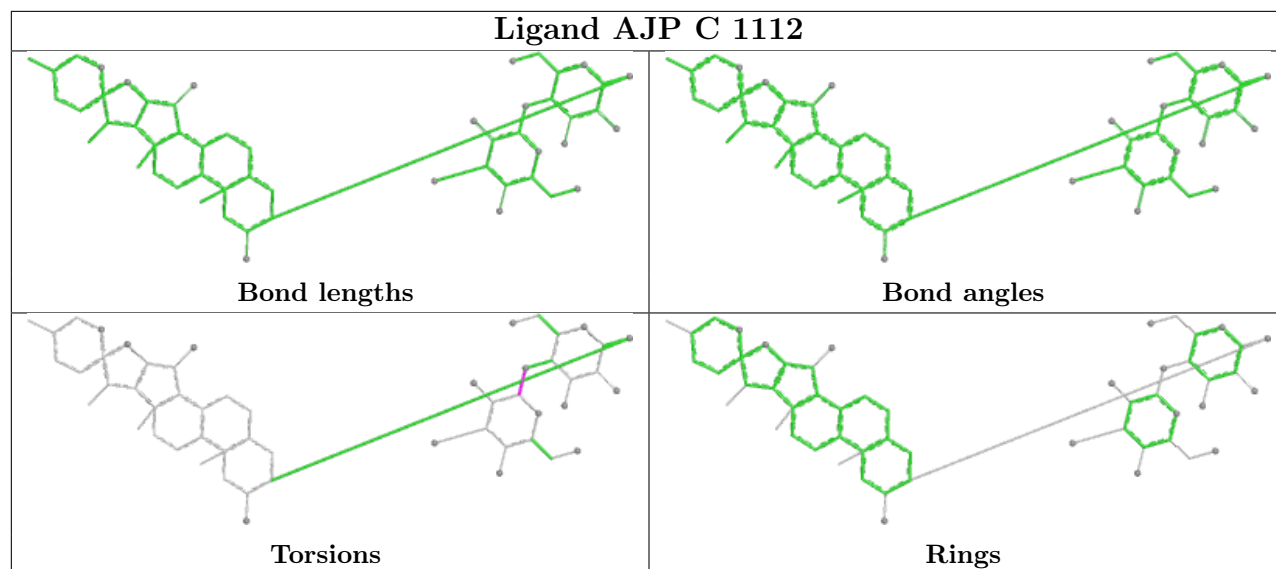


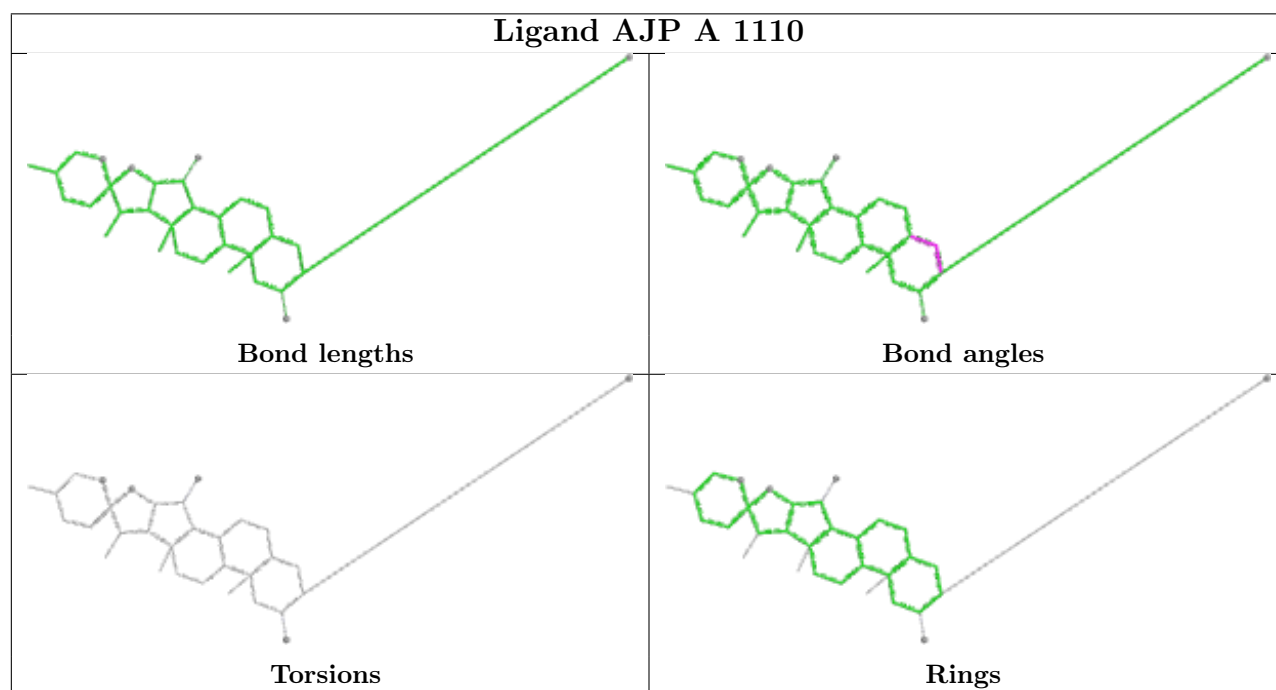
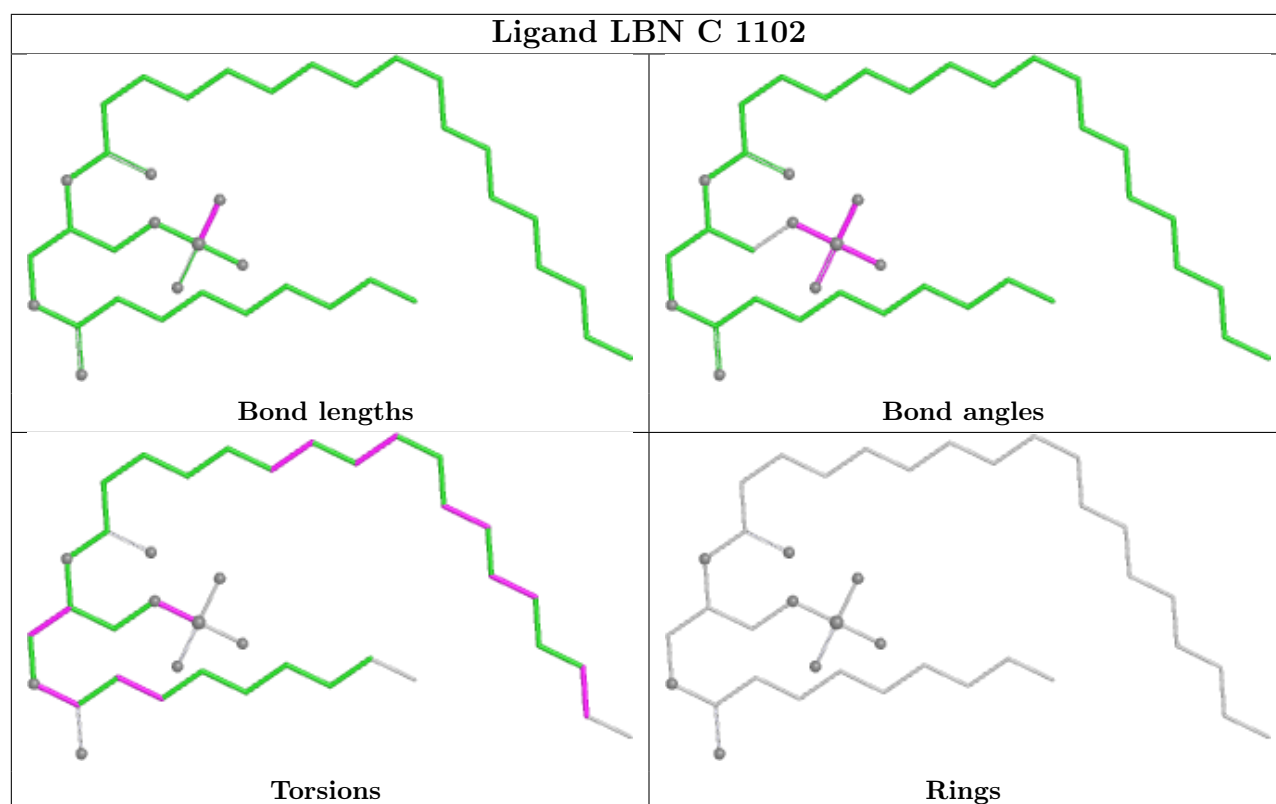


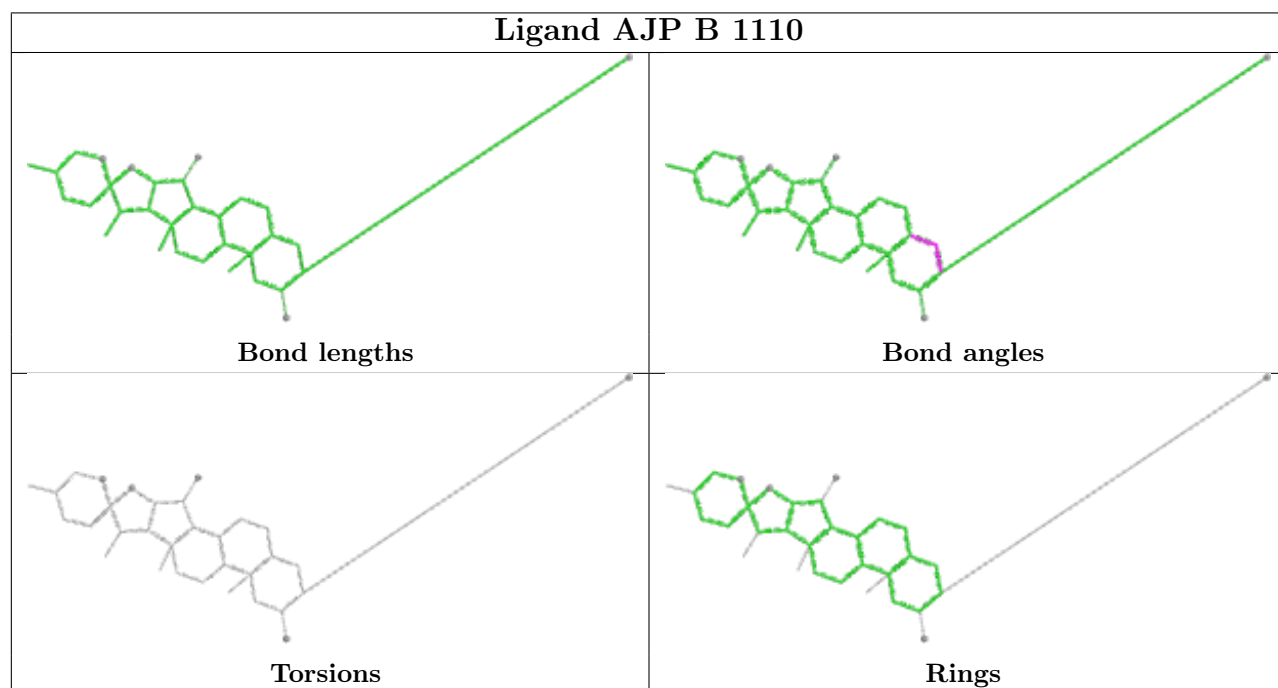
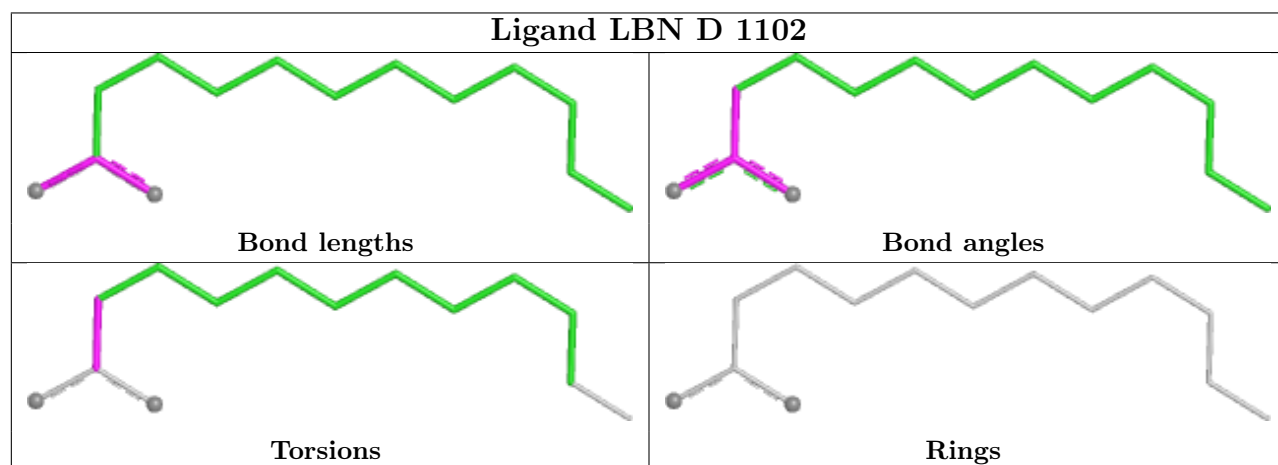
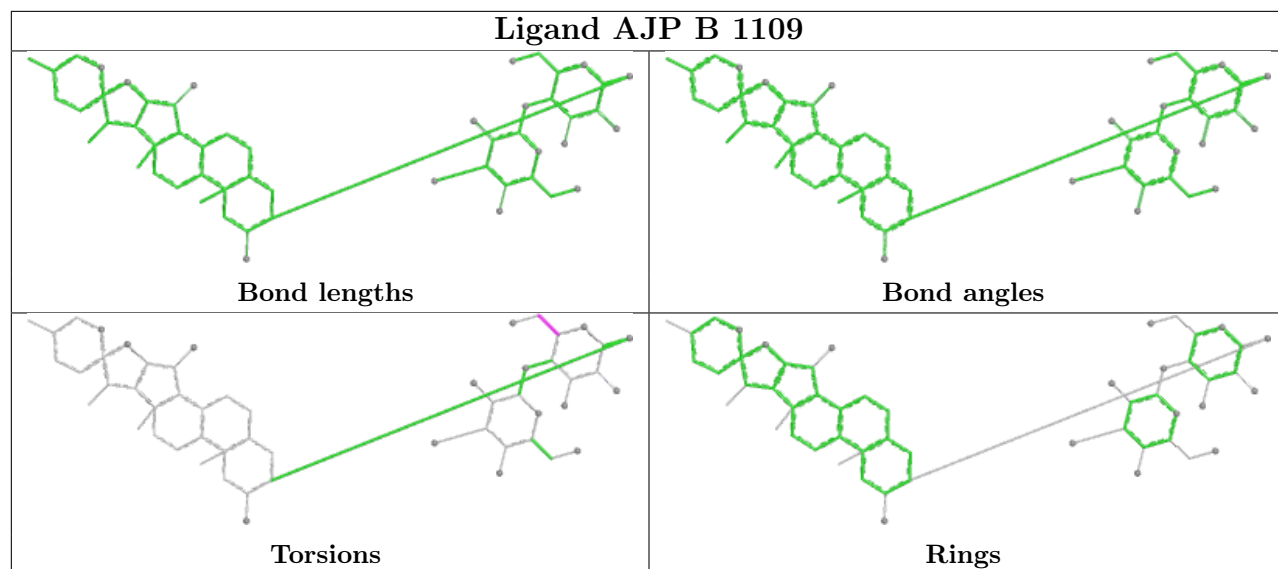


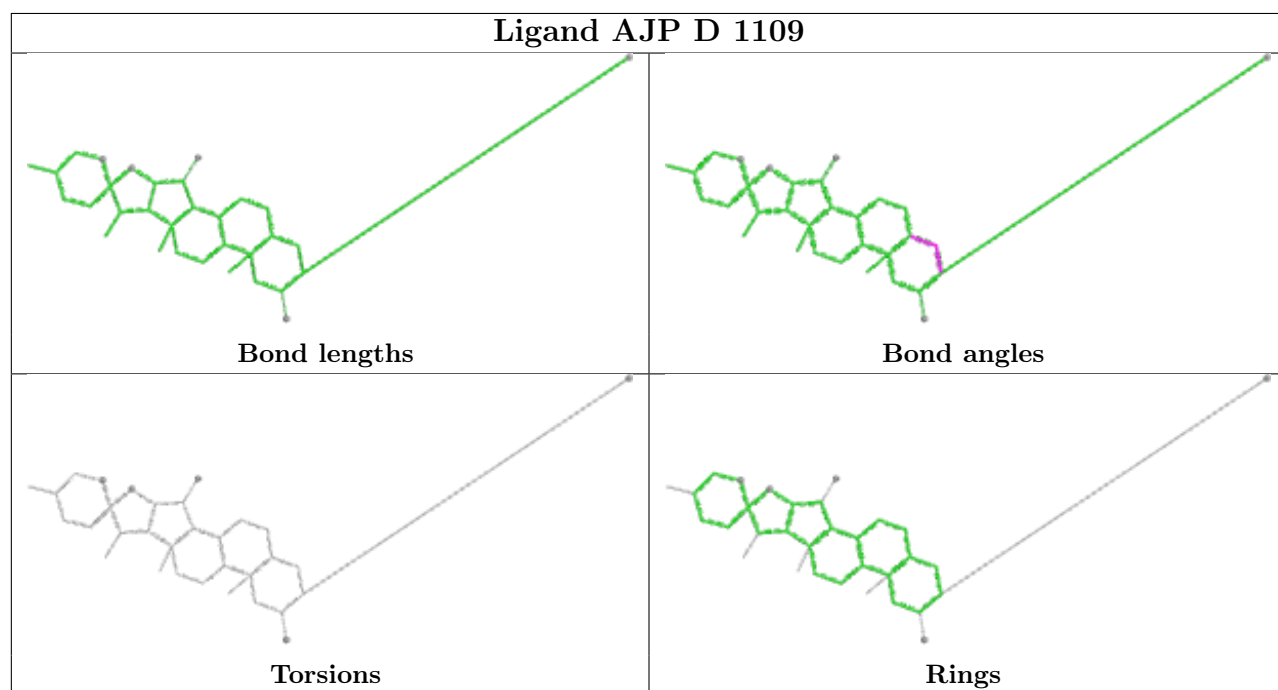
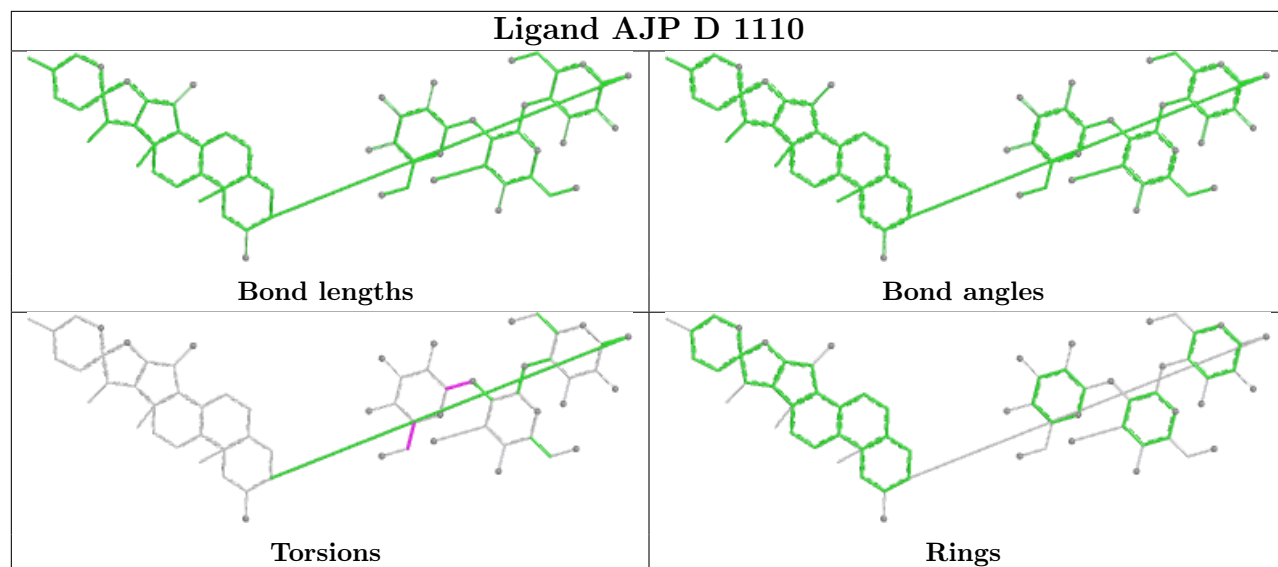


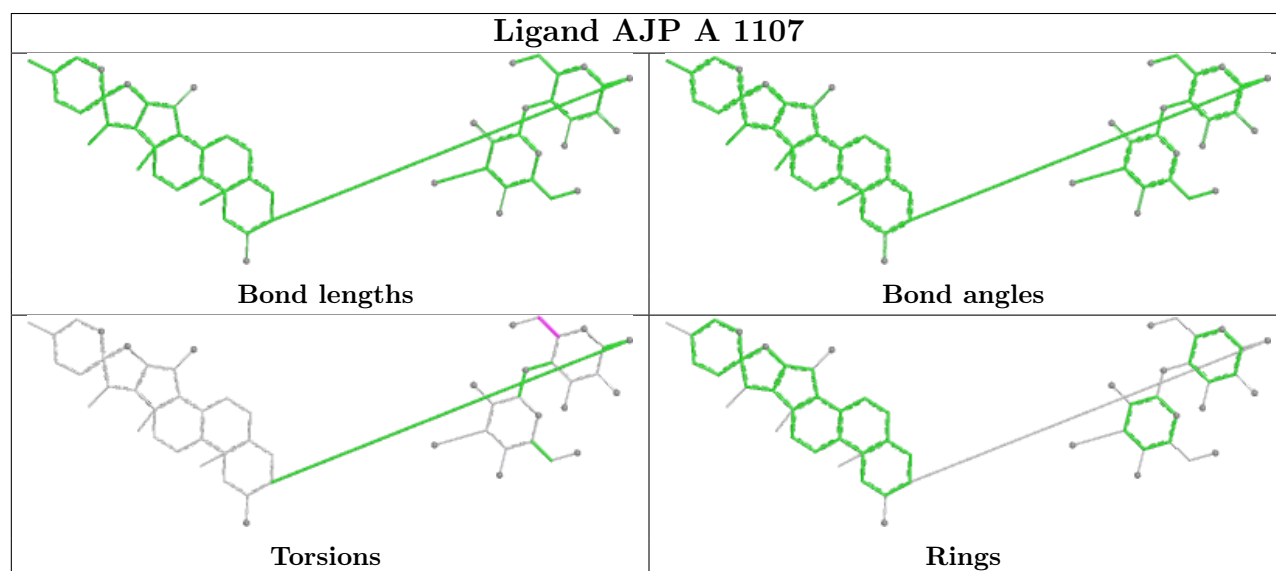
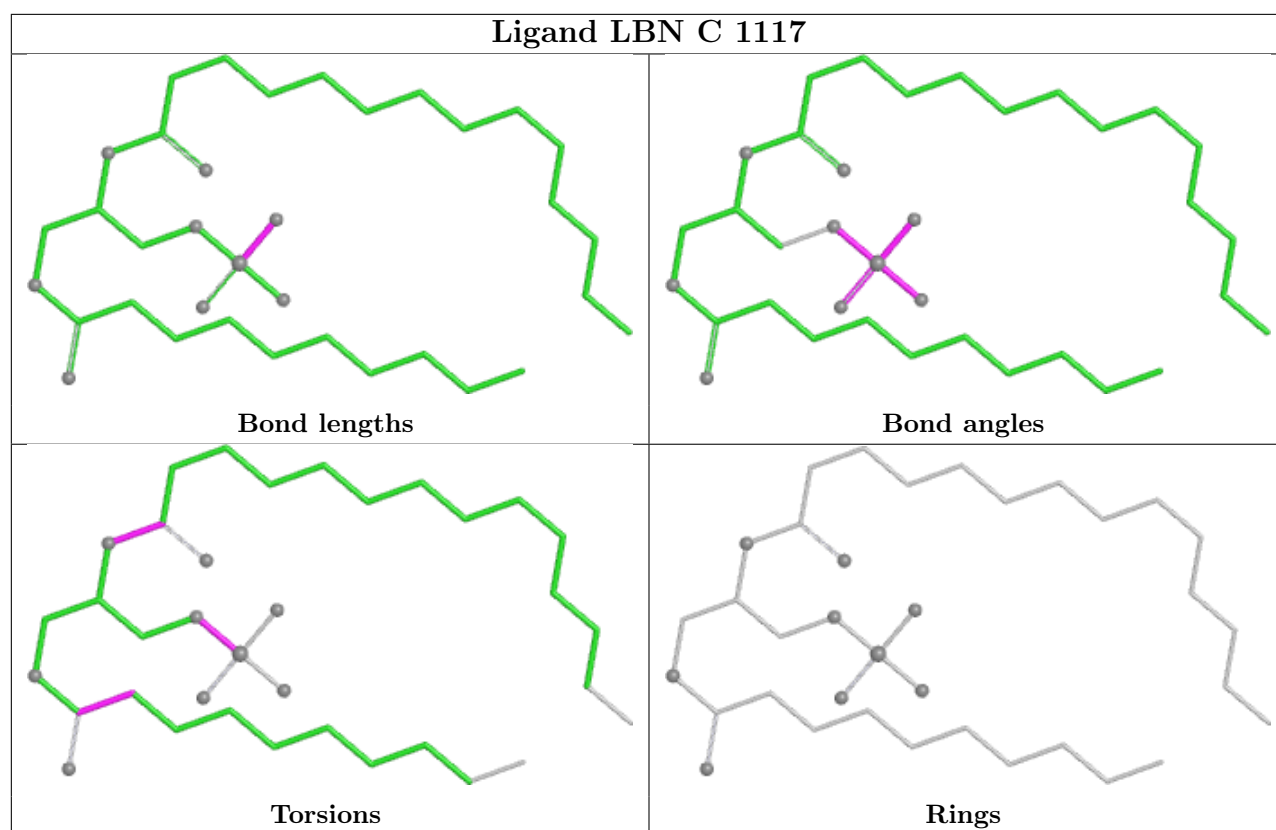


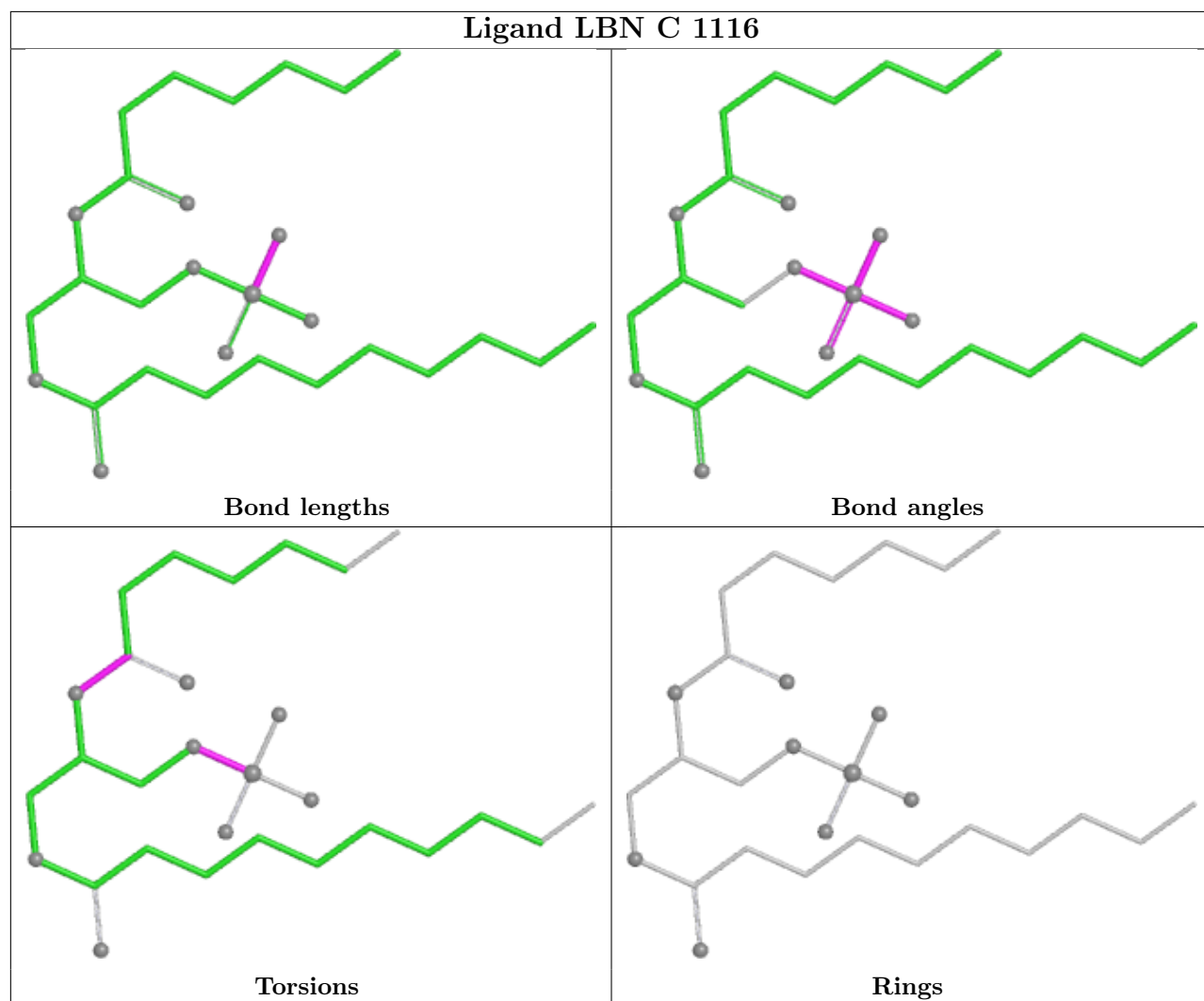
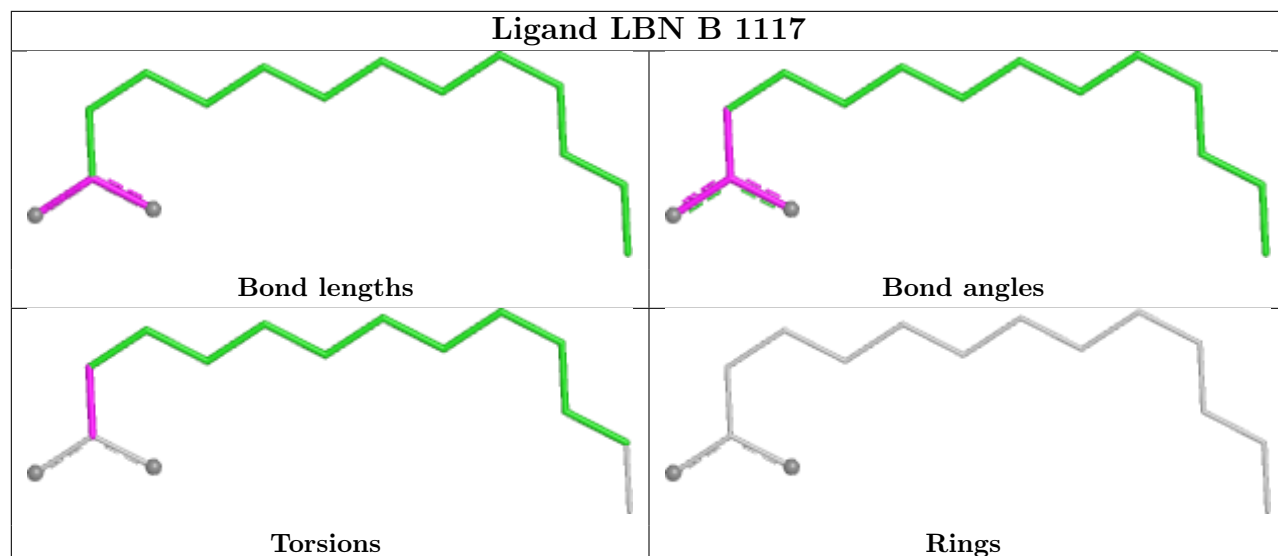


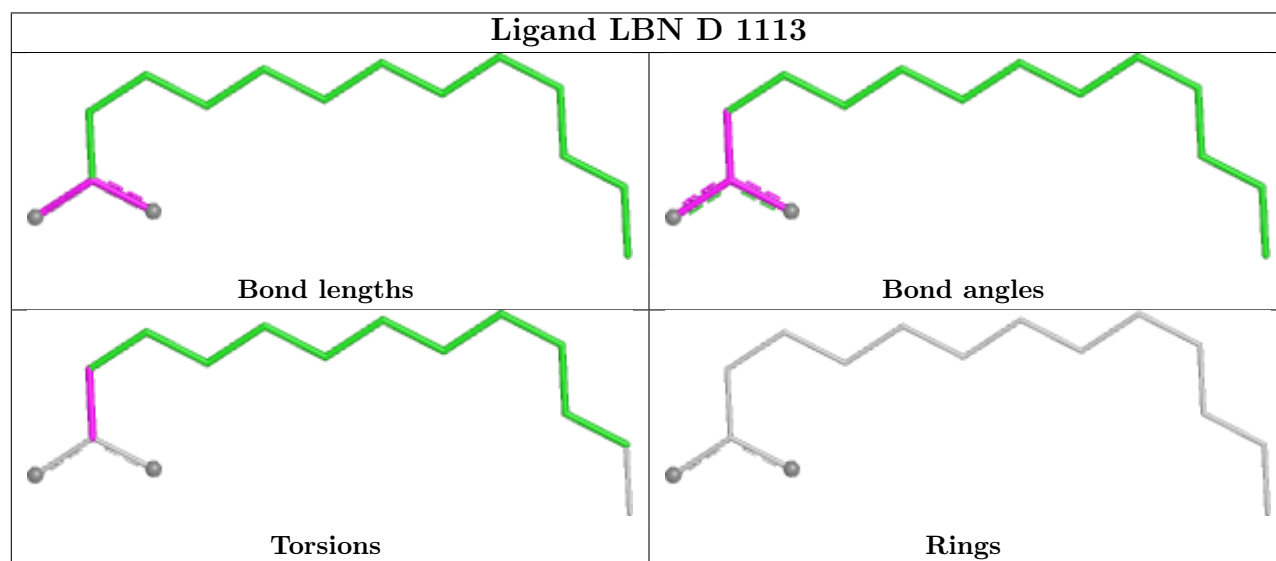
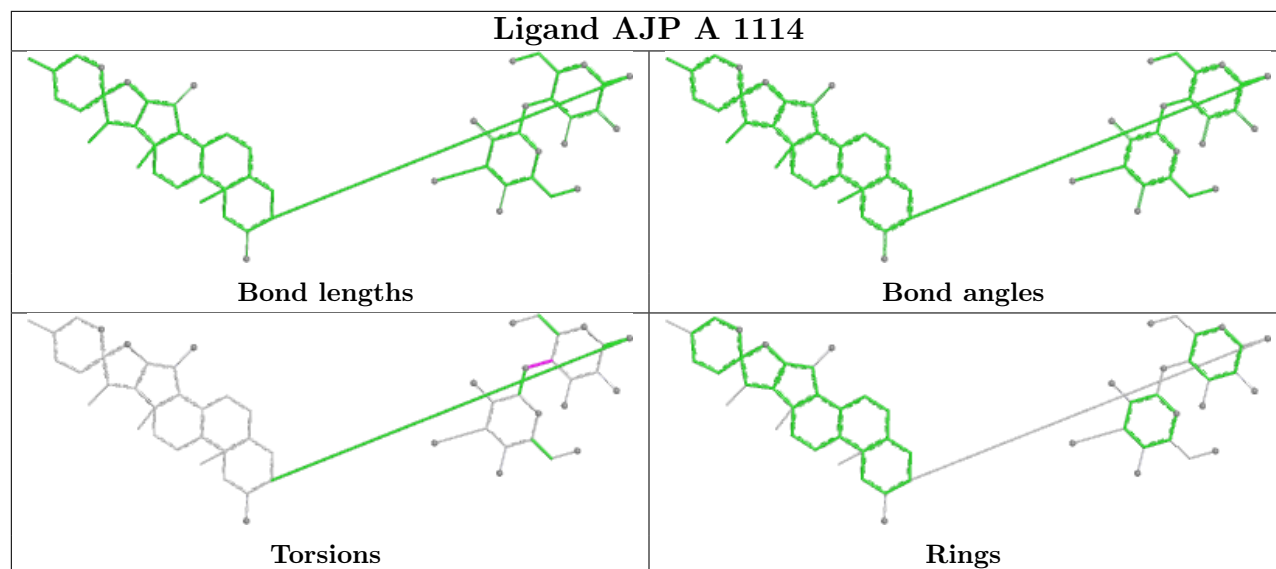


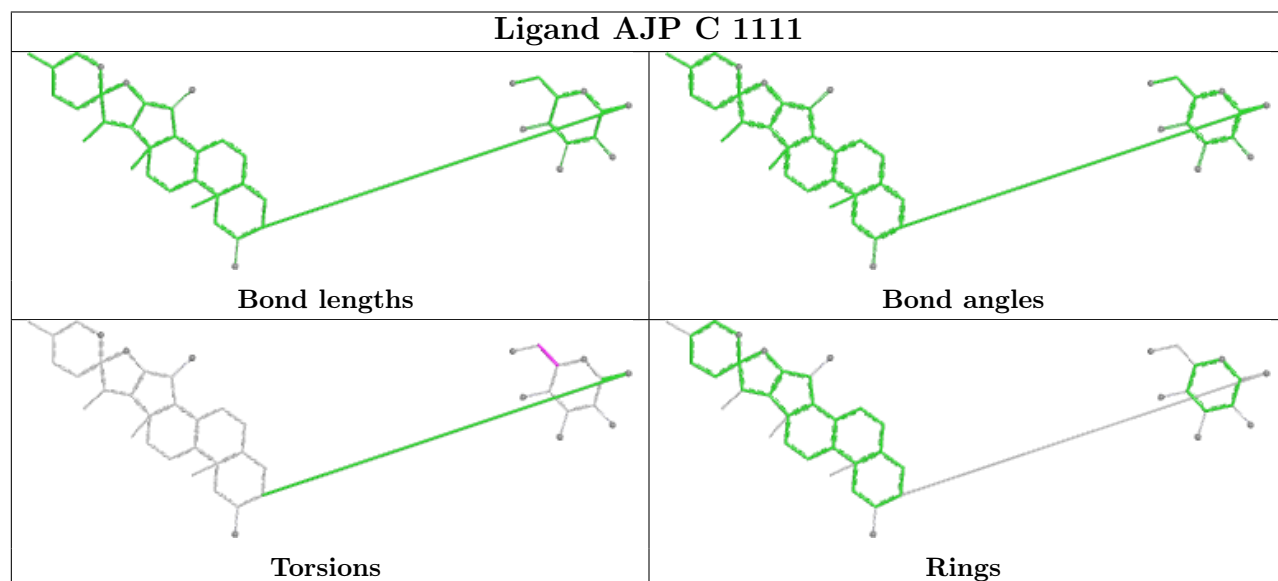
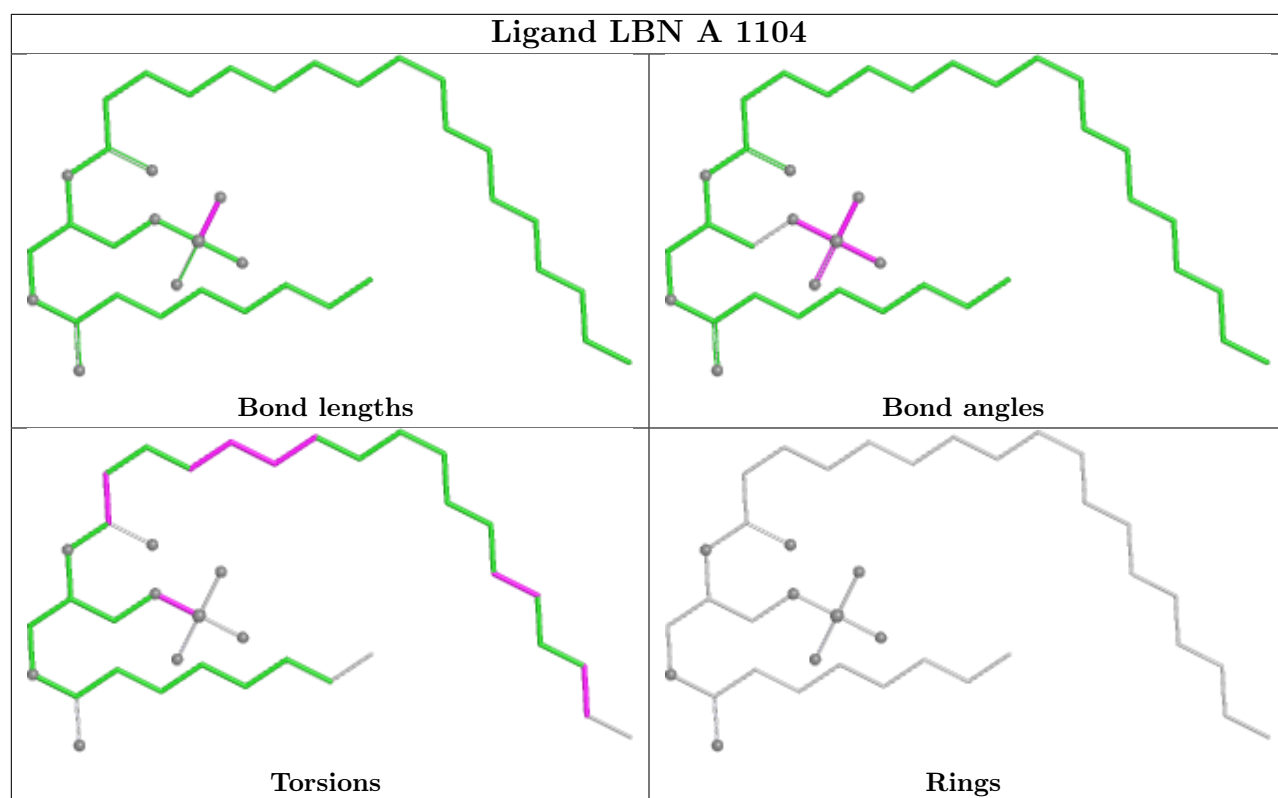


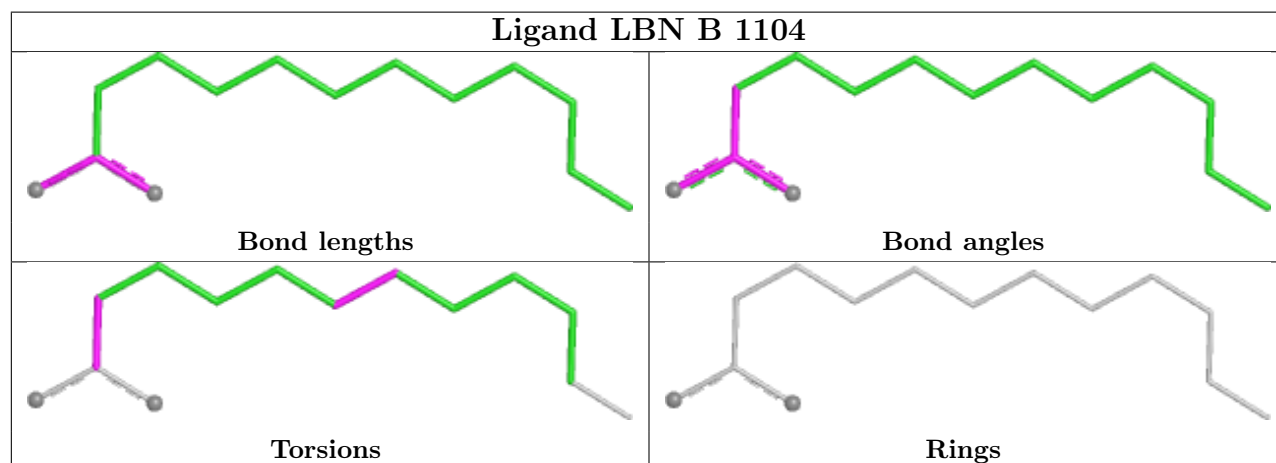
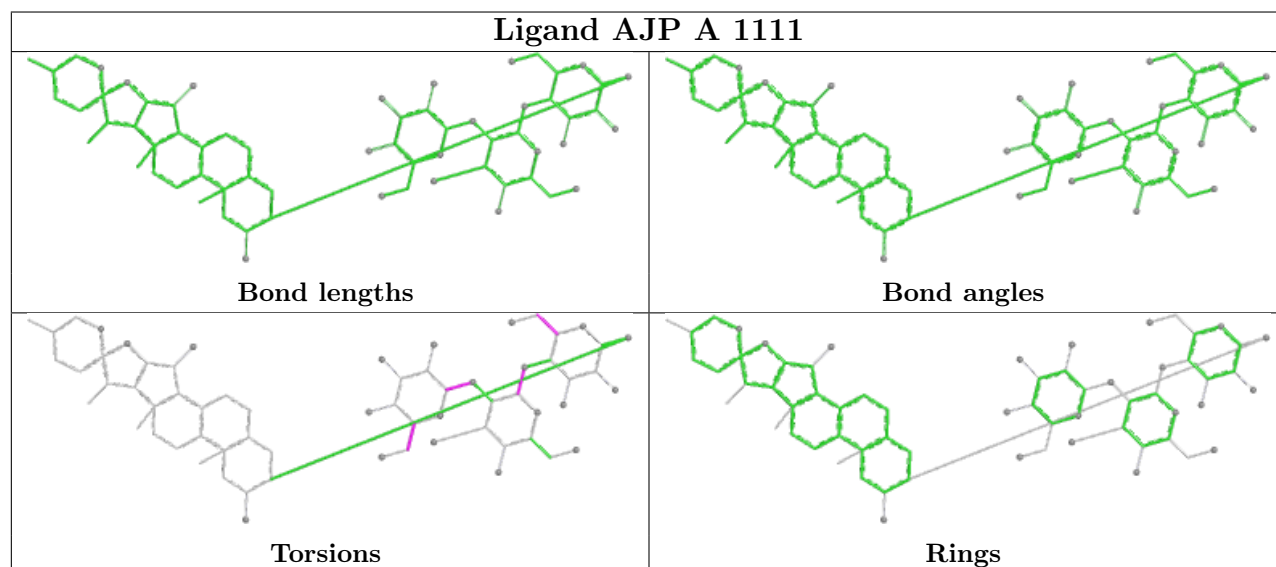
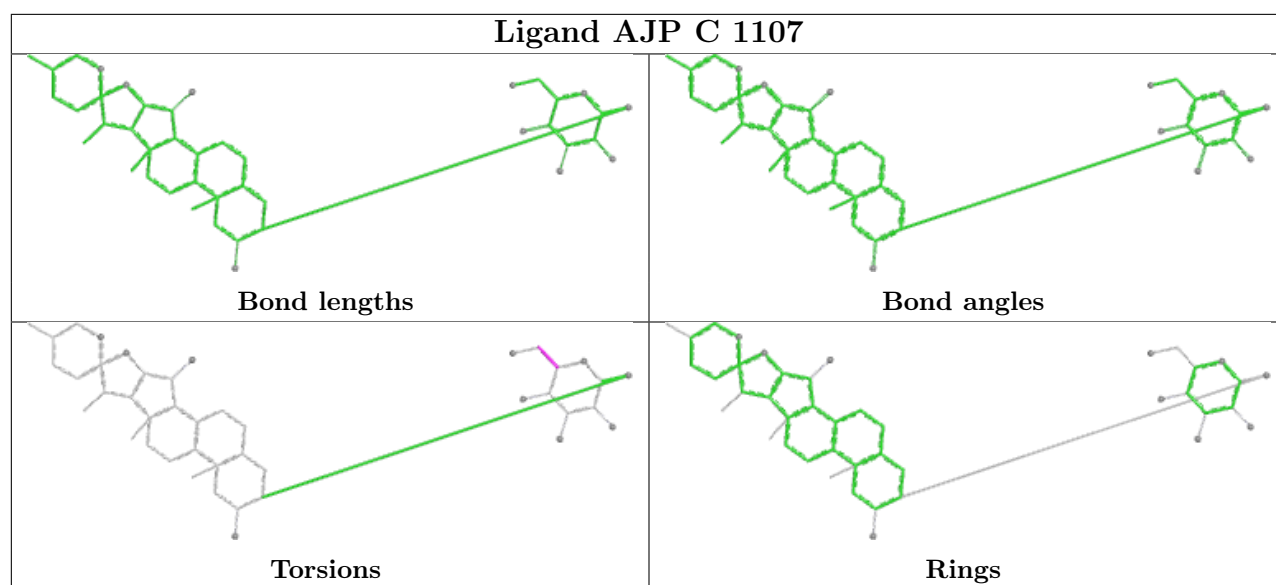


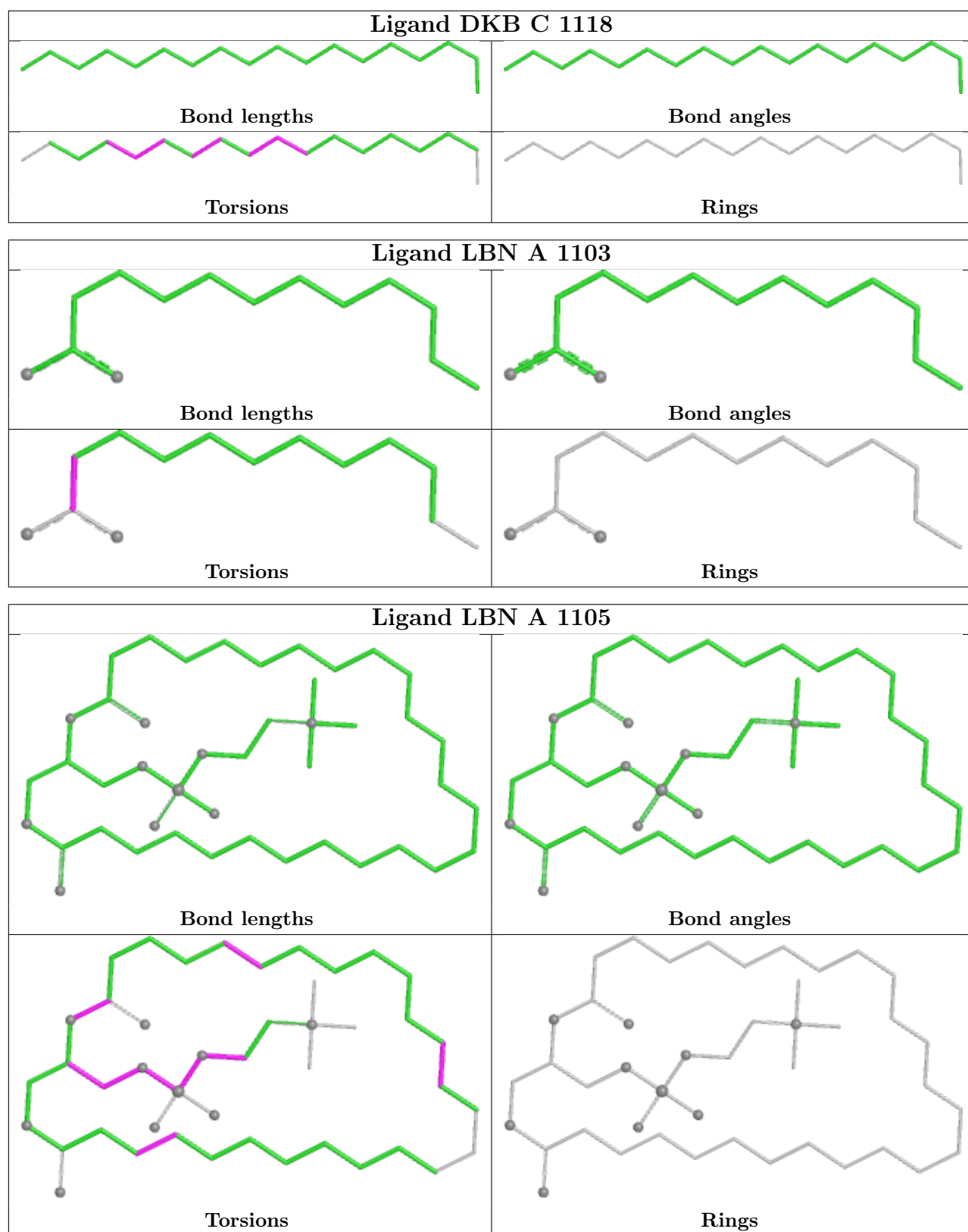


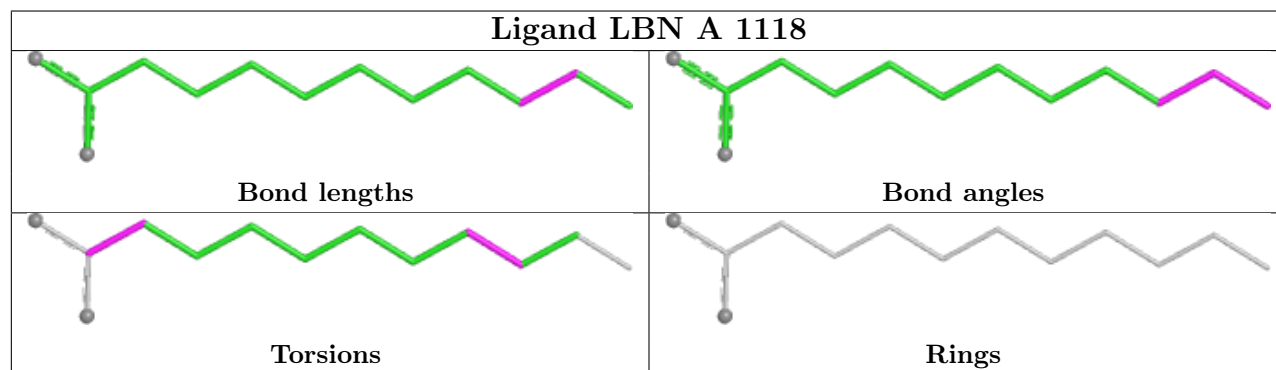
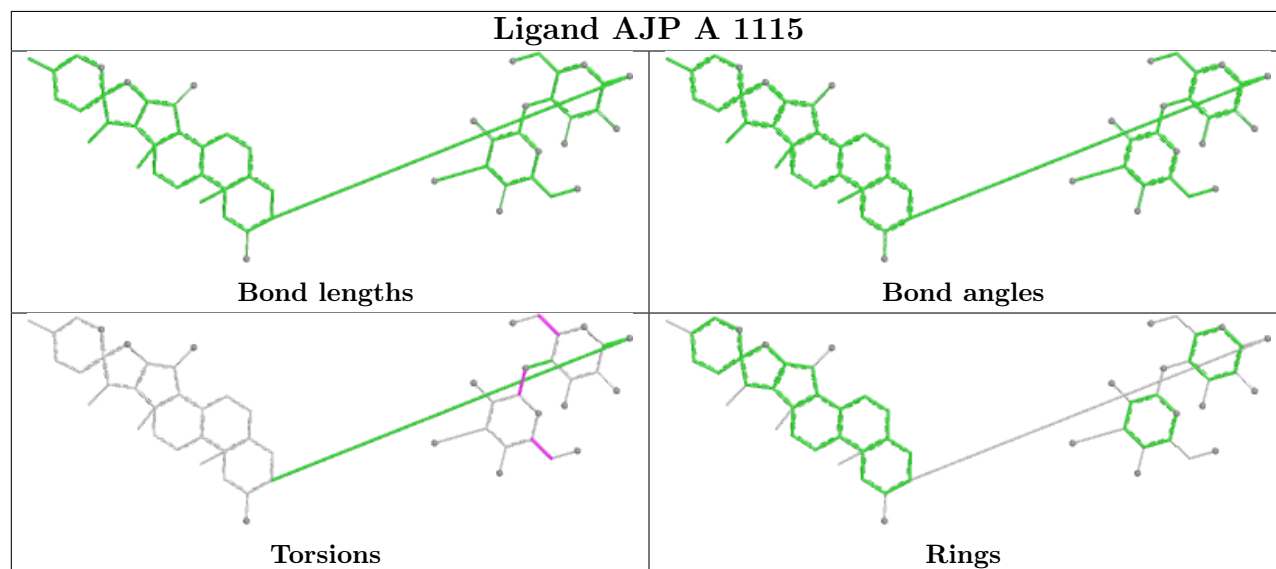
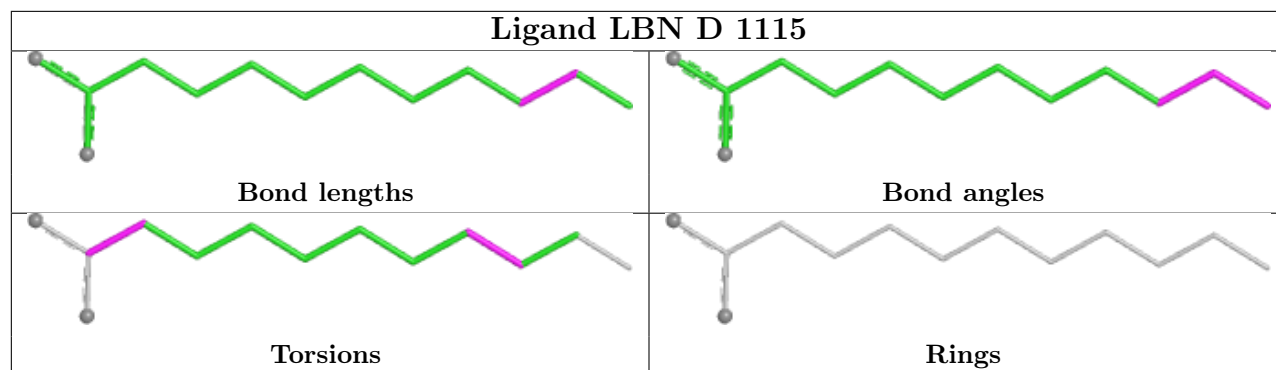


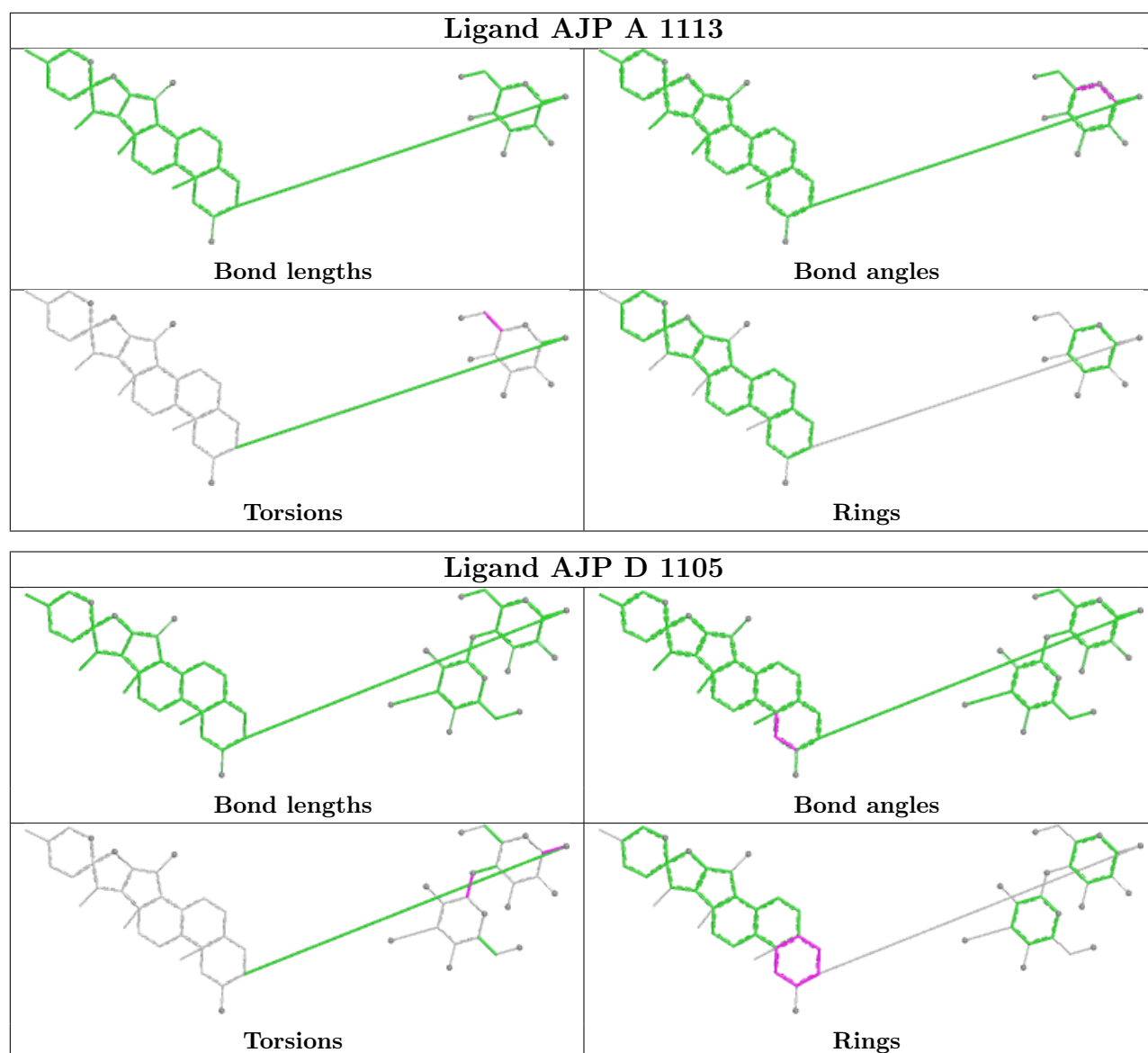












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

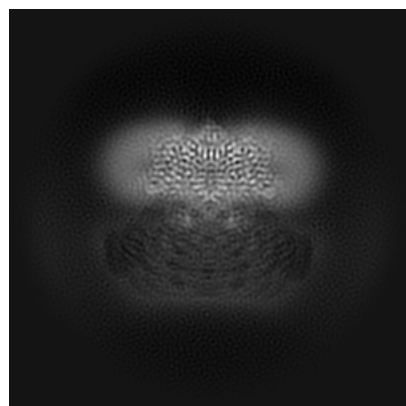
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75632. These allow visual inspection of the internal detail of the map and identification of artifacts.

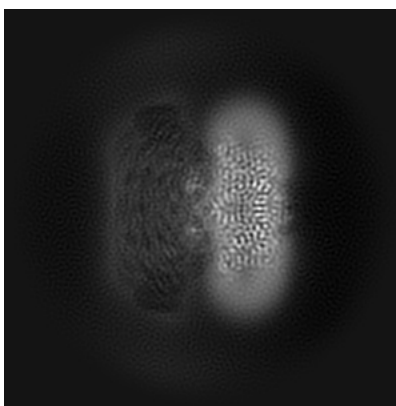
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

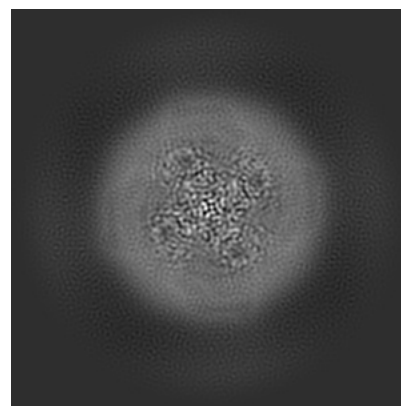
6.1.1 Primary map



X

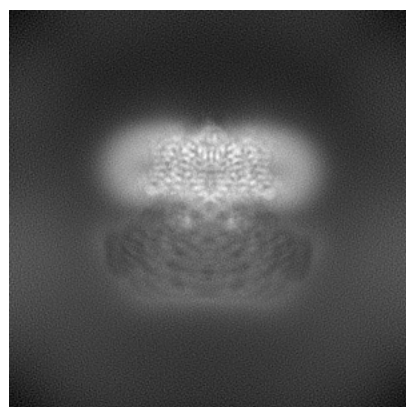


Y

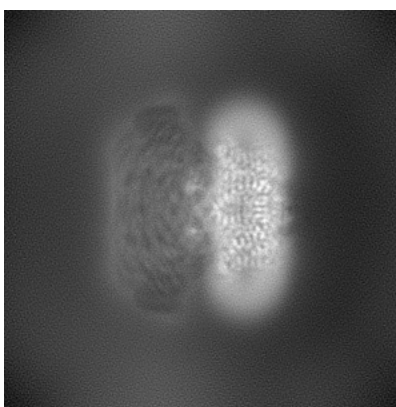


Z

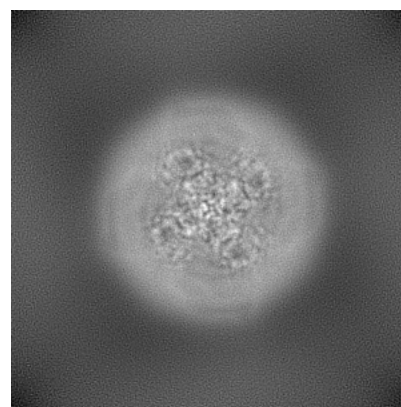
6.1.2 Raw map



X



Y

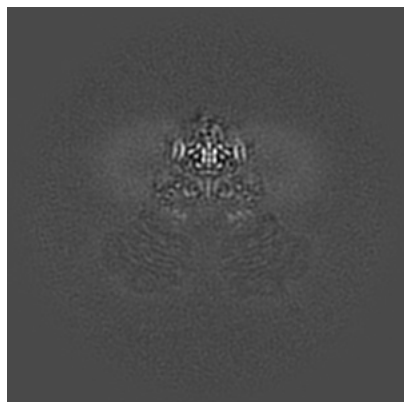


Z

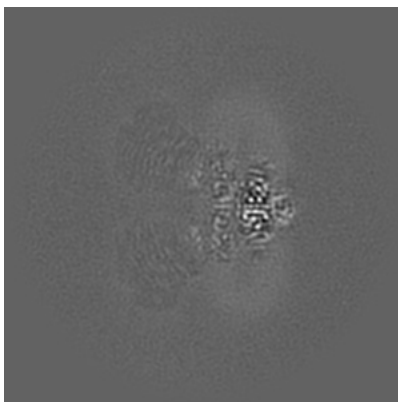
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

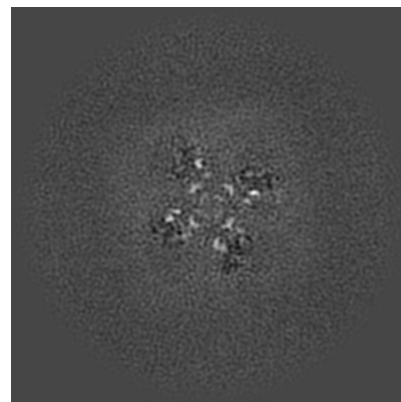
6.2.1 Primary map



X Index: 150

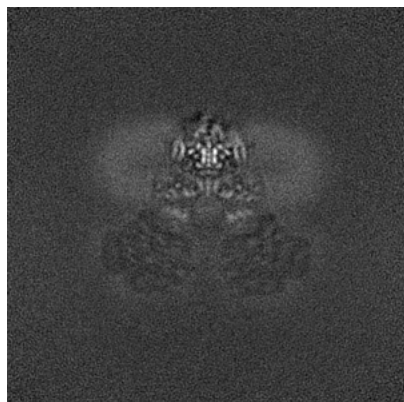


Y Index: 150

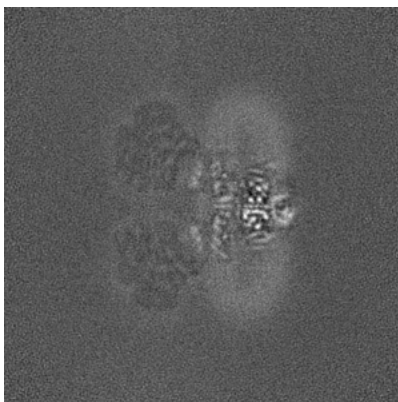


Z Index: 150

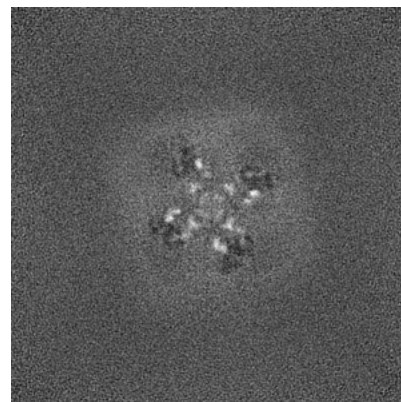
6.2.2 Raw map



X Index: 150



Y Index: 150

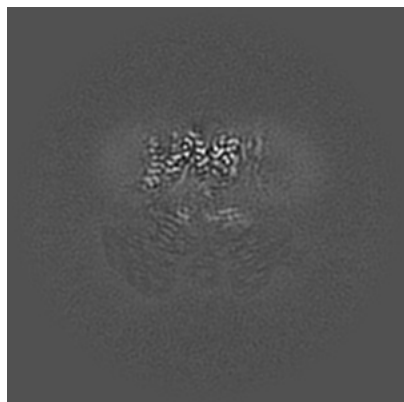


Z Index: 150

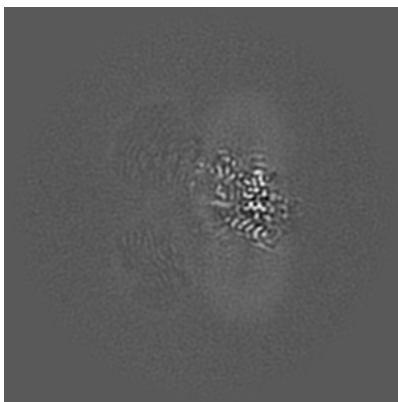
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

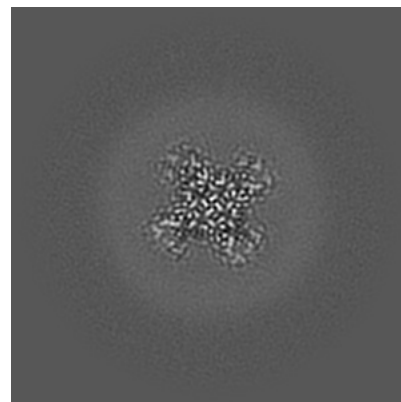
6.3.1 Primary map



X Index: 167

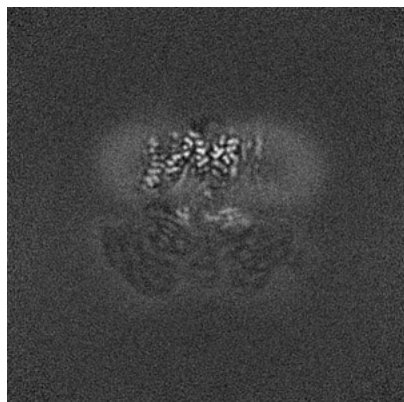


Y Index: 156

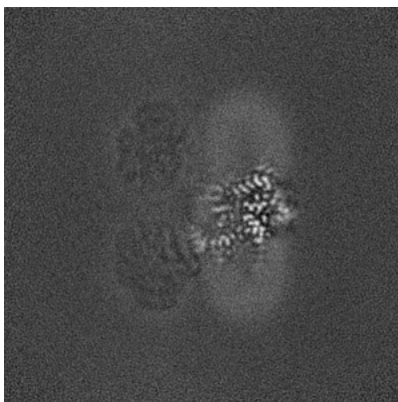


Z Index: 191

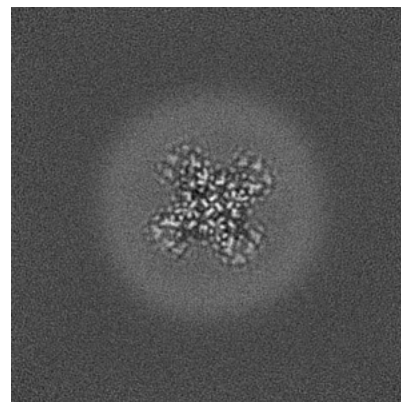
6.3.2 Raw map



X Index: 167



Y Index: 146

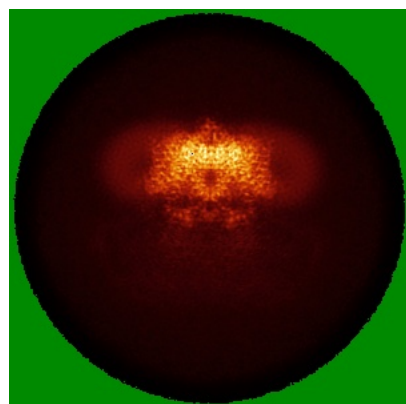


Z Index: 191

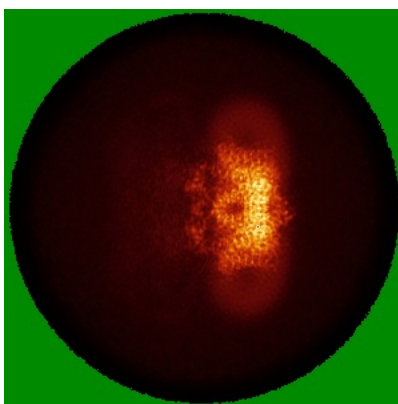
The images above show the largest variance slices of the map in three orthogonal directions.

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

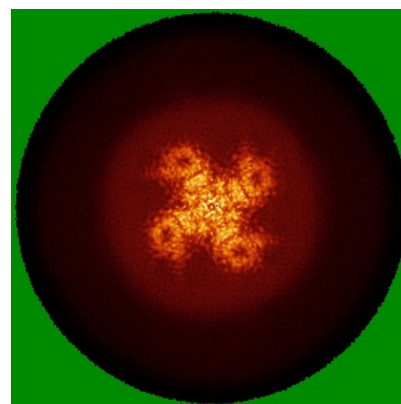
6.4.1 Primary map



X

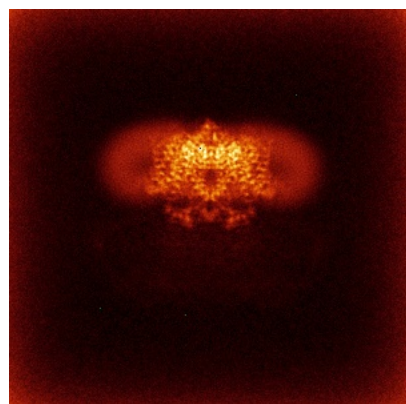


Y

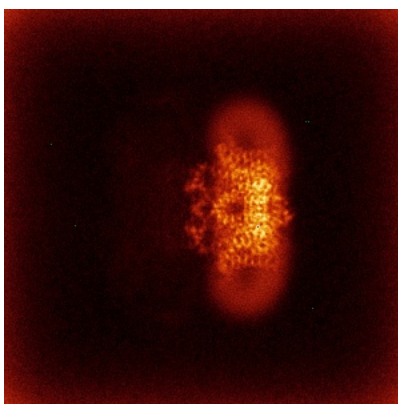


Z

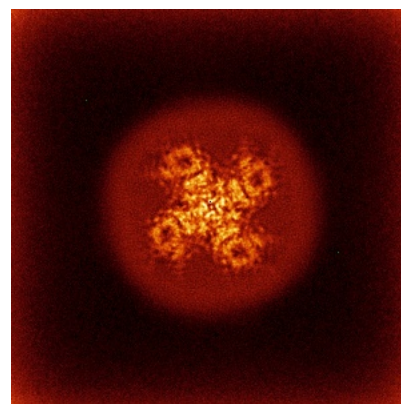
6.4.2 Raw map



X



Y

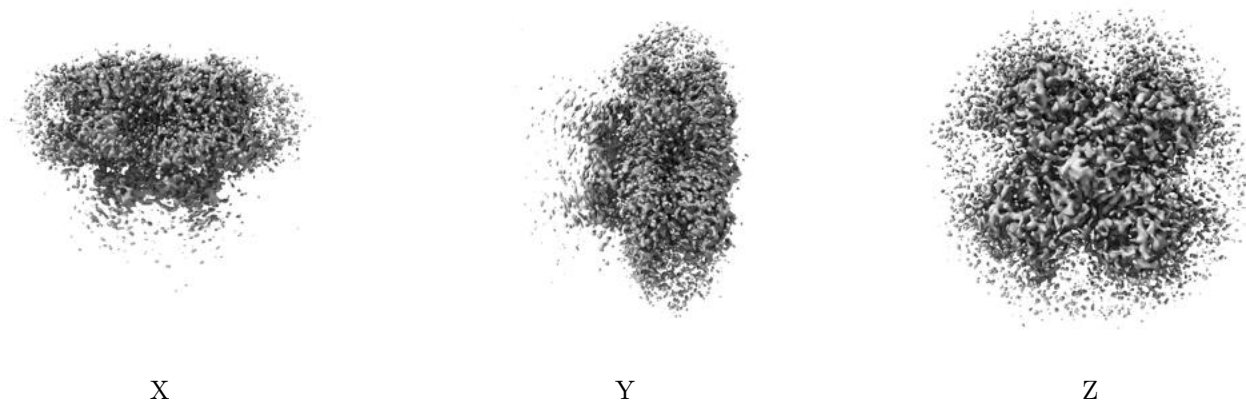


Z

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

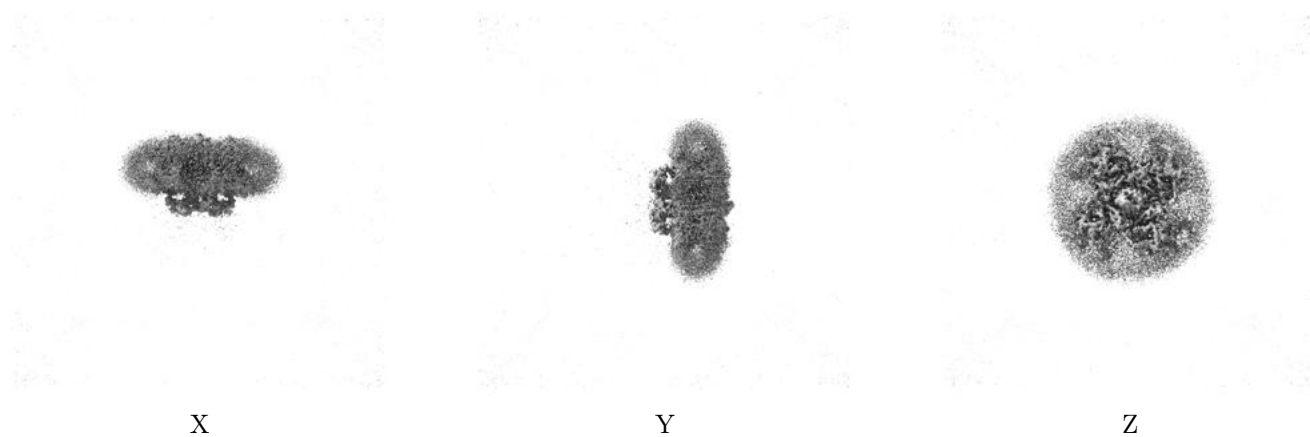
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

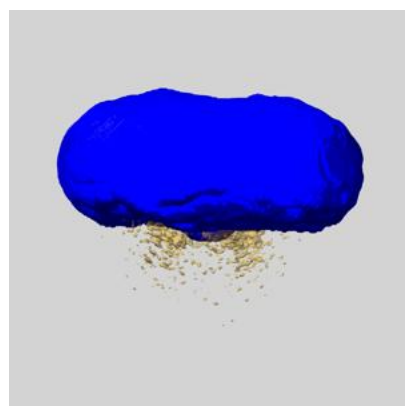
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

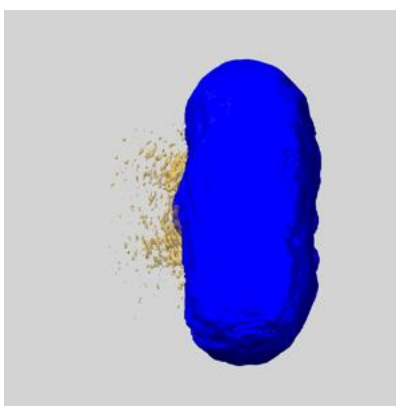
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

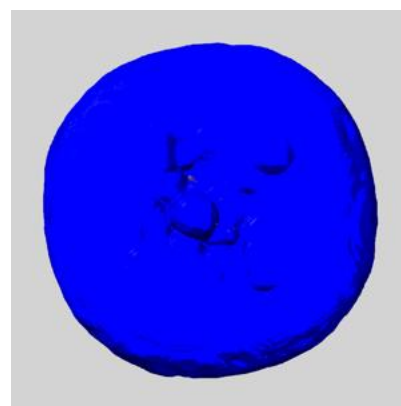
6.6.1 emd_75632_msk_1.map [i](#)



X



Y

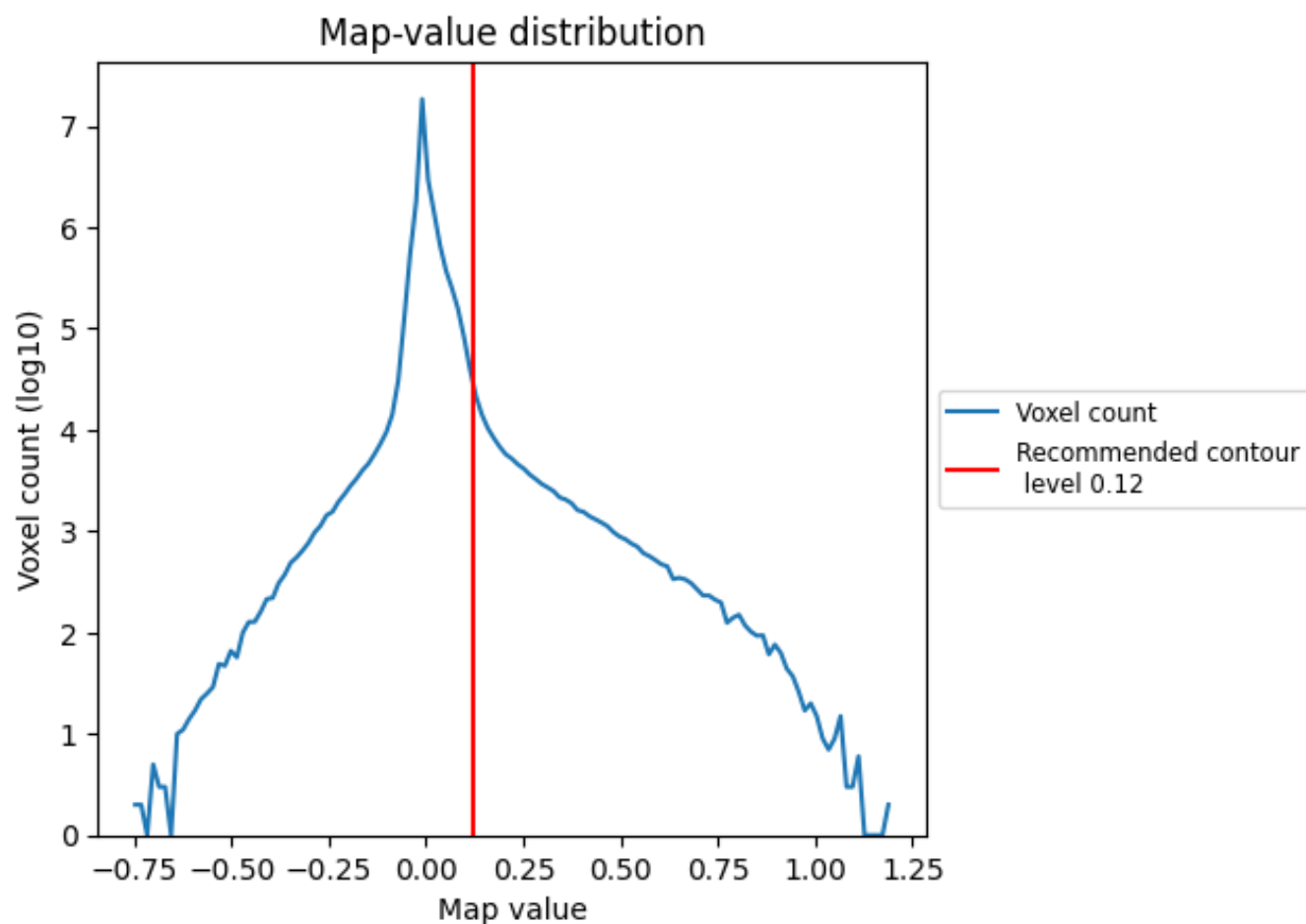


Z

7 Map analysis [i](#)

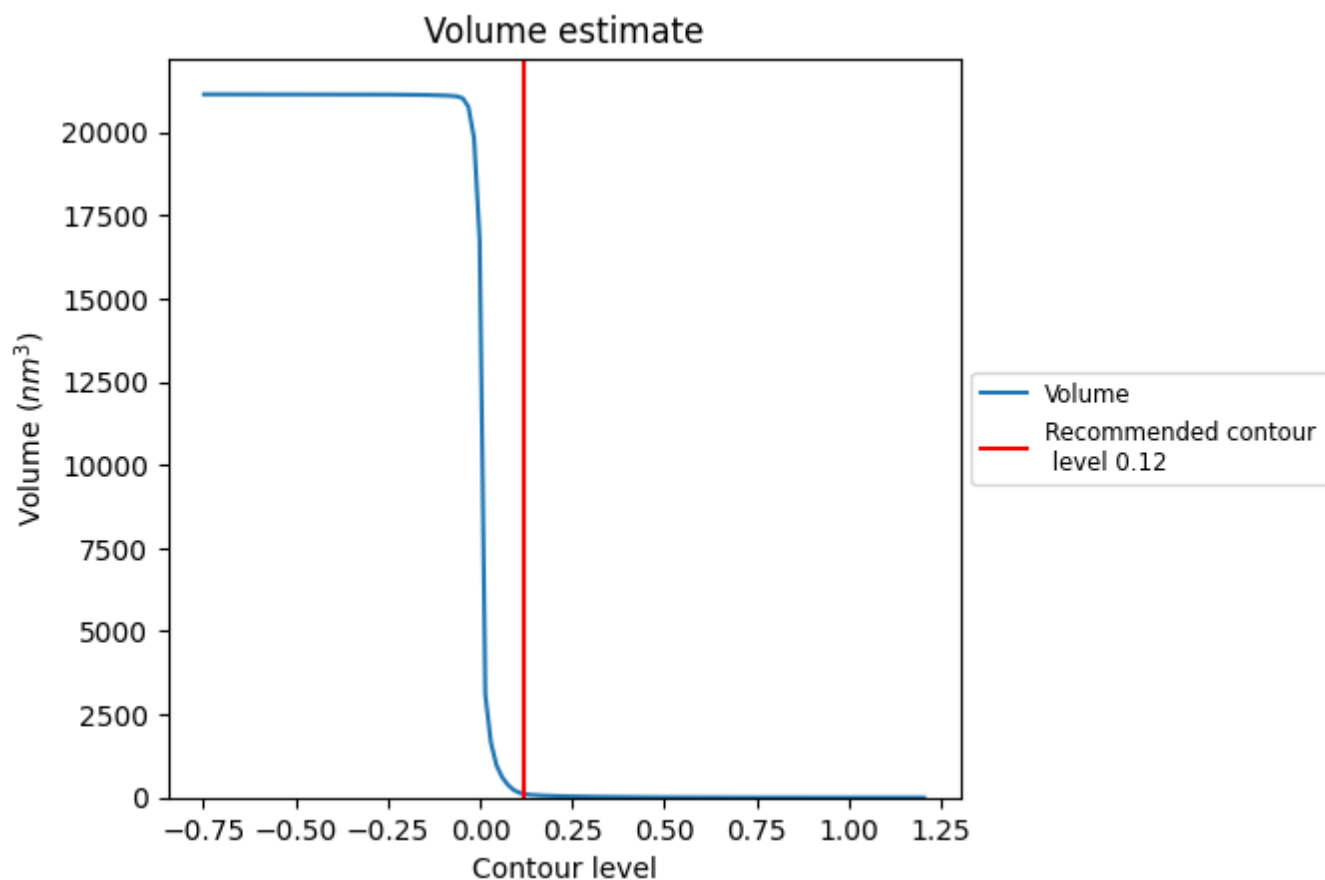
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

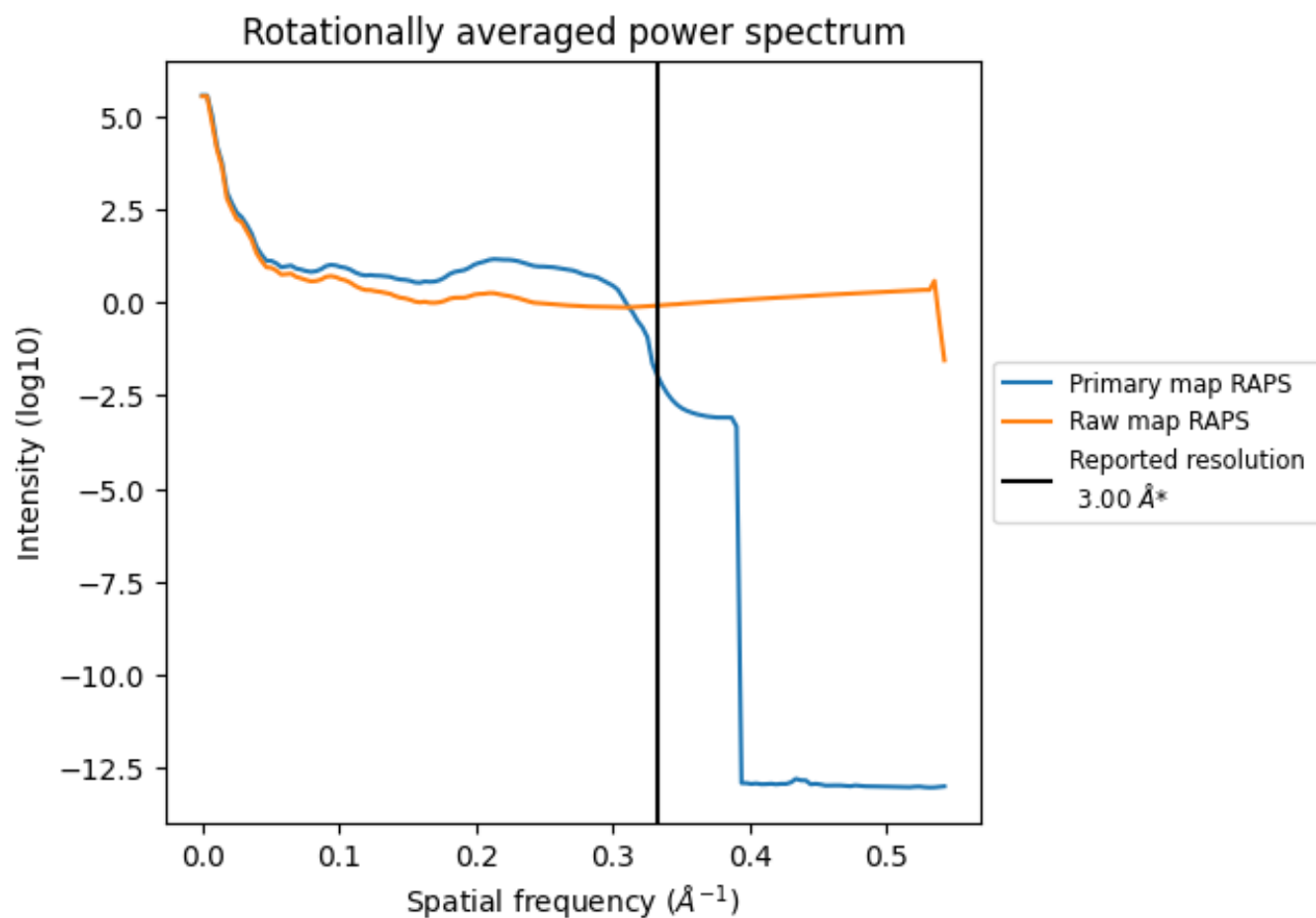
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 110 nm^3 ; this corresponds to an approximate mass of 99 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

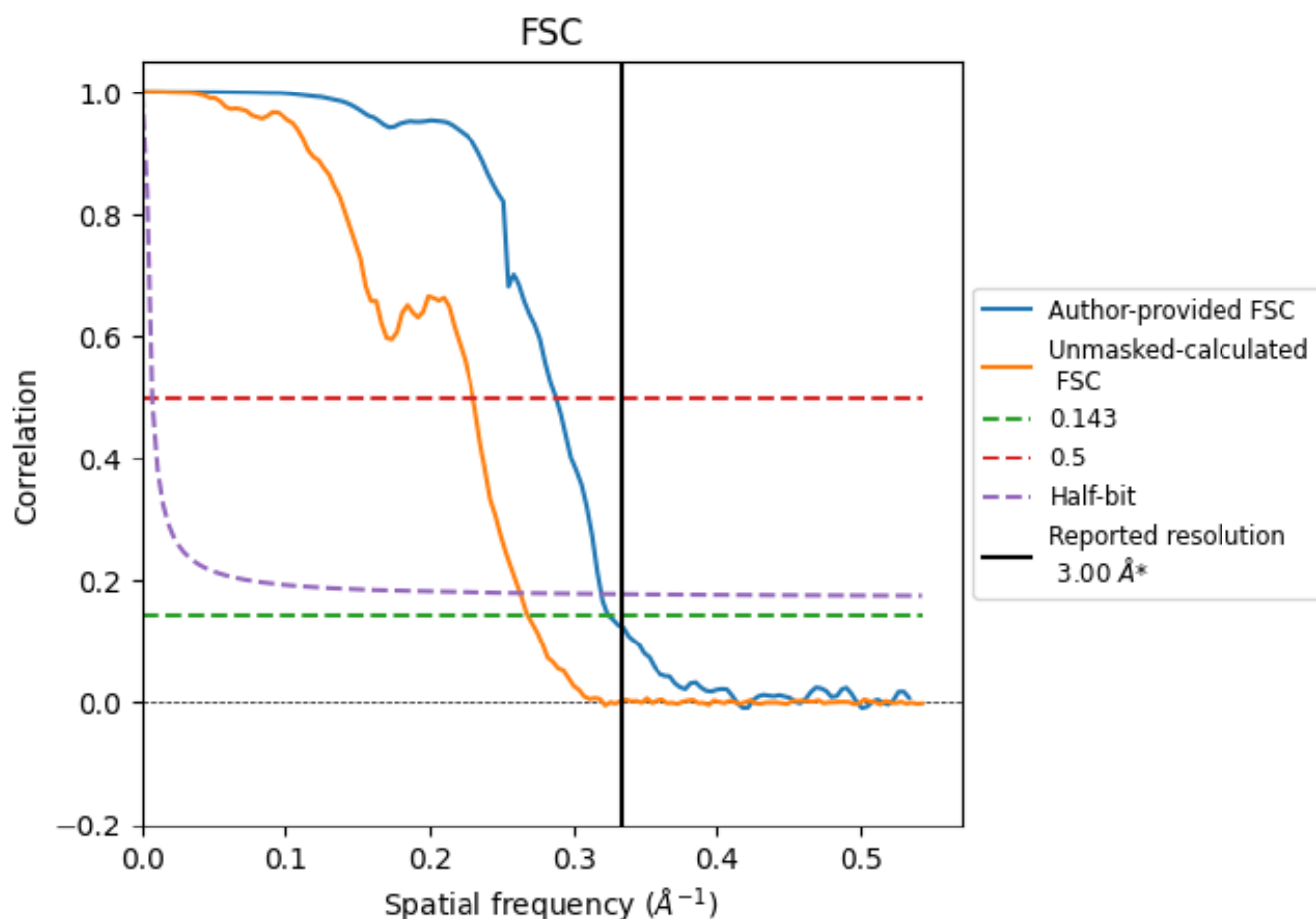


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

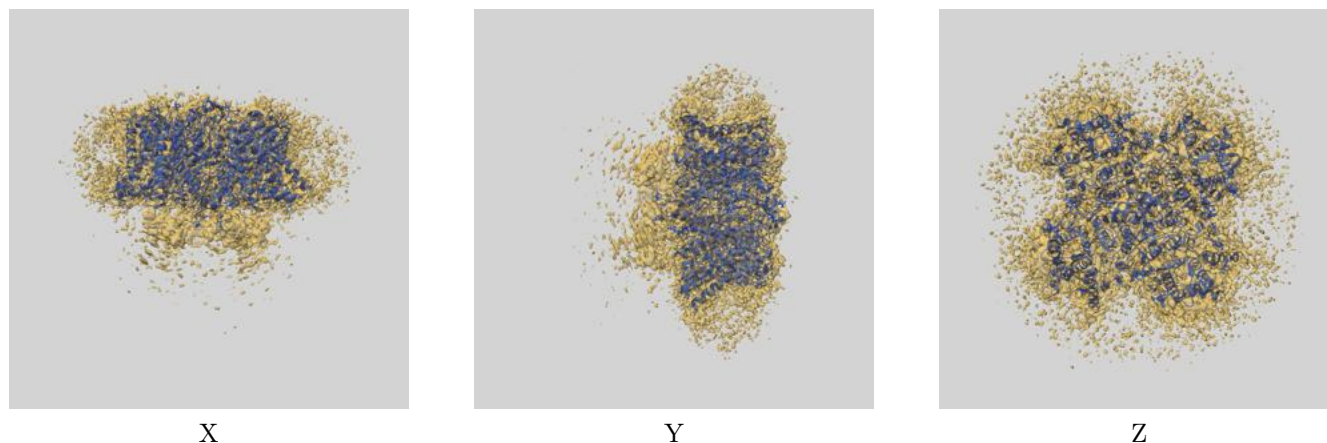
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.08	3.47	3.13
Unmasked-calculated*	3.73	4.35	3.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.73 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

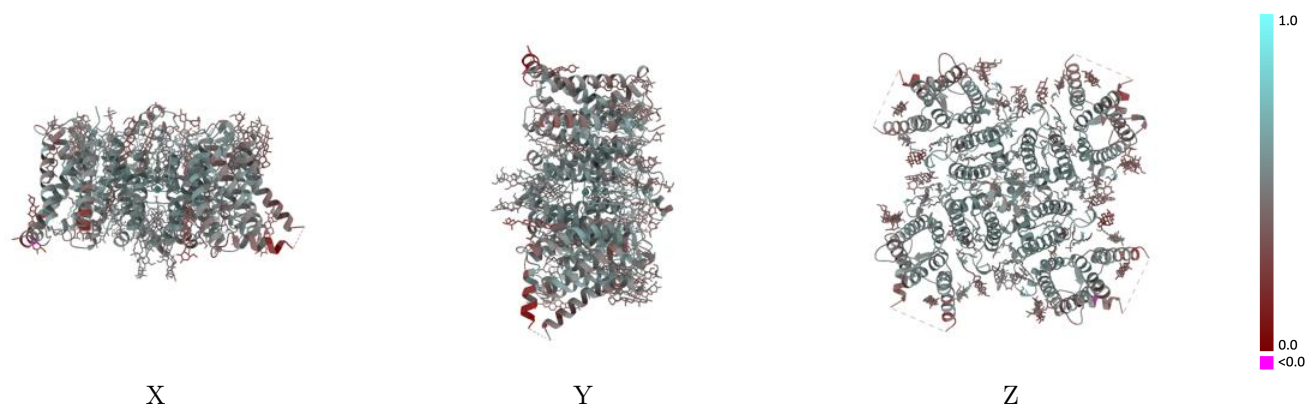
This section contains information regarding the fit between EMDB map EMD-75632 and PDB model 11DE. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



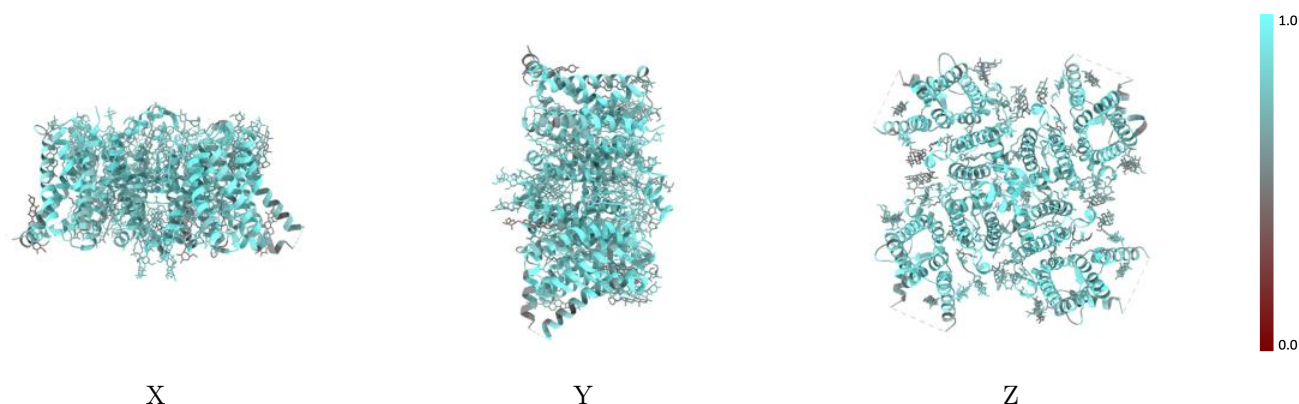
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



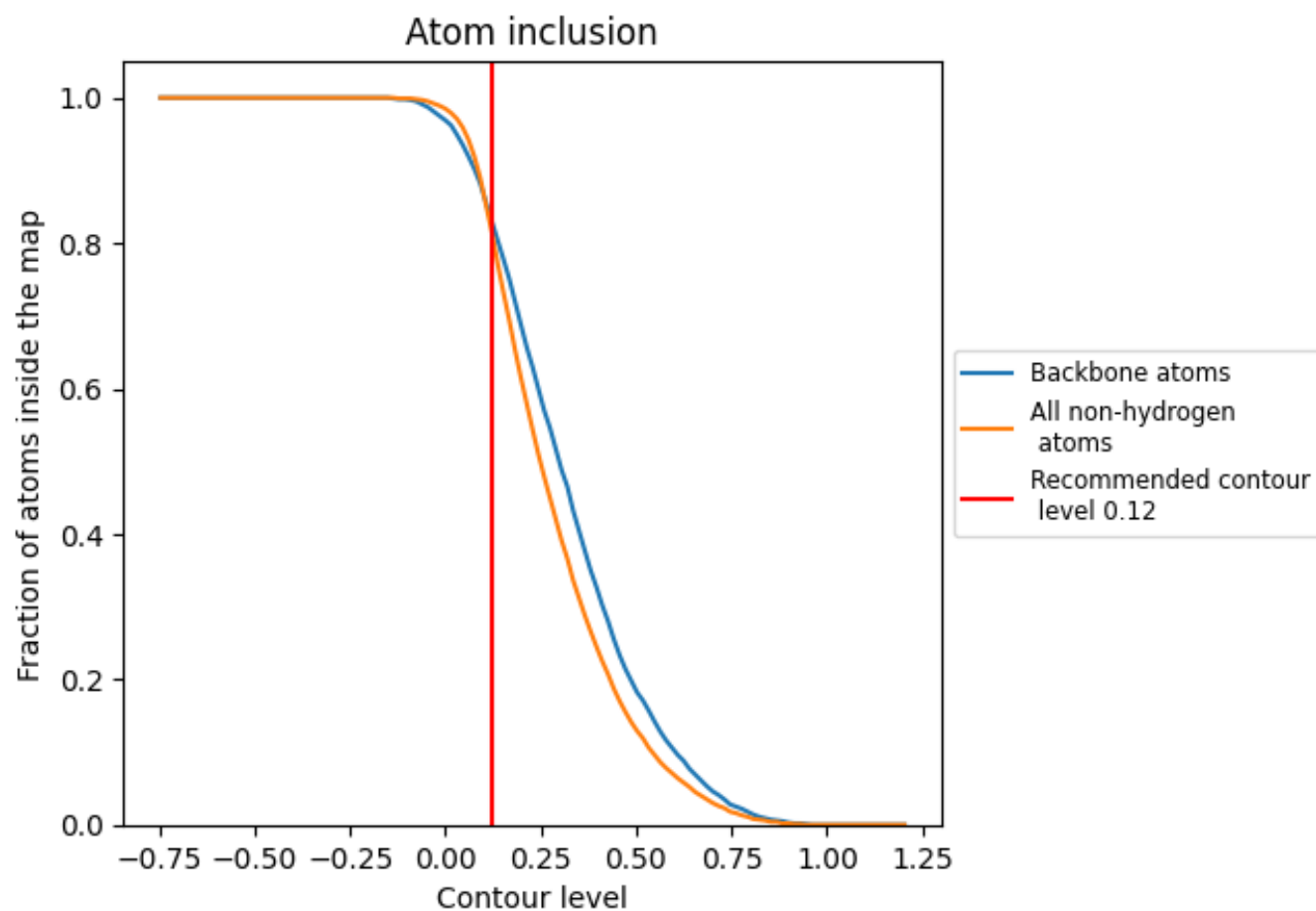
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8200	0.4900
A	0.8160	0.4830
B	0.8120	0.4840
C	0.8290	0.4990
D	0.8210	0.4920
Y	0.9020	0.4930

