



Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 06:04 AM EDT

PDB ID : 11CZ / pdb_000011cz
EMDB ID : EMD-75627
Title : Human Slo1-paxilline complex under divalent chelated condition - full model
Authors : Chowdhury, S.; Pal, K.; Kallure, G.S.
Deposited on : 2026-02-18
Resolution : 2.60 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

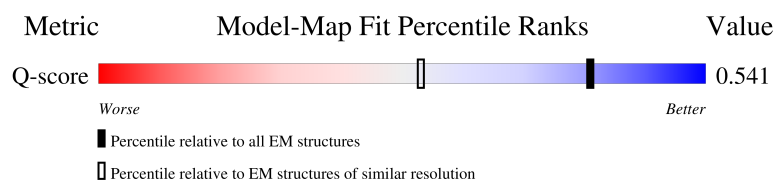
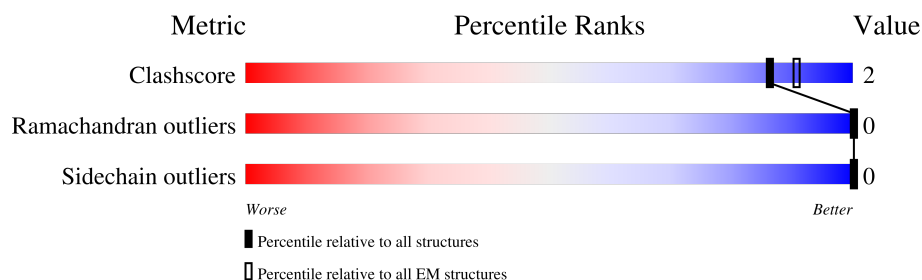
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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	

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
3	LBN	A	1107	X	-	-	-
3	LBN	A	1108	X	-	-	-
3	LBN	A	1109	X	-	-	-
3	LBN	A	1110	X	-	-	-
3	LBN	A	1111	X	-	-	-
3	LBN	A	1114	X	-	-	-
3	LBN	A	1115	X	-	-	-
3	LBN	A	1116	X	-	-	-
3	LBN	B	1102	X	-	-	-
3	LBN	B	1103	X	-	-	-
3	LBN	B	1104	X	-	-	-
3	LBN	B	1105	X	-	-	-
3	LBN	B	1108	X	-	-	-
3	LBN	B	1109	X	-	-	-
3	LBN	B	1110	X	-	-	-
3	LBN	C	1102	X	-	-	-
3	LBN	C	1103	X	-	-	-
3	LBN	C	1104	X	-	-	-
3	LBN	C	1107	X	-	-	-
3	LBN	C	1108	X	-	-	-
3	LBN	C	1109	X	-	-	-
3	LBN	D	1102	X	-	-	-
3	LBN	D	1103	X	-	-	-
3	LBN	D	1104	X	-	-	-
3	LBN	D	1105	X	-	-	-
3	LBN	D	1108	X	-	-	-
3	LBN	D	1109	X	-	-	-
3	LBN	D	1110	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31279 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	895	Total	C	N	O	S	0	0
			7143	4639	1165	1293	46		
1	B	895	Total	C	N	O	S	0	0
			7143	4639	1165	1293	46		
1	C	895	Total	C	N	O	S	0	0
			7143	4639	1165	1293	46		
1	D	895	Total	C	N	O	S	0	0
			7143	4639	1165	1293	46		

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

Continued on next page...

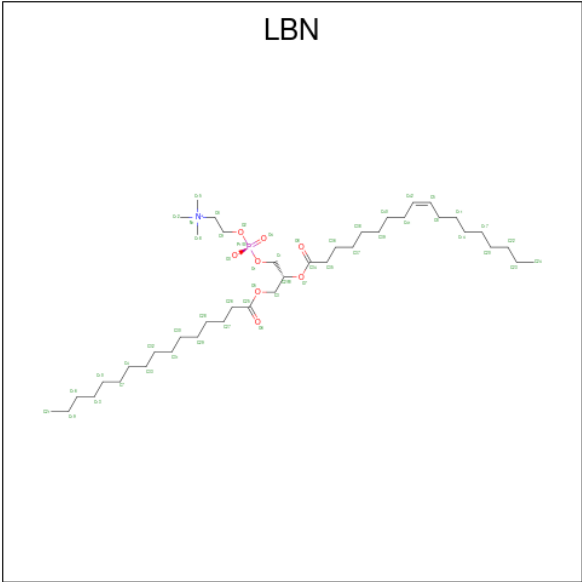
Continued from previous page...

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

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

- Molecule 3 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



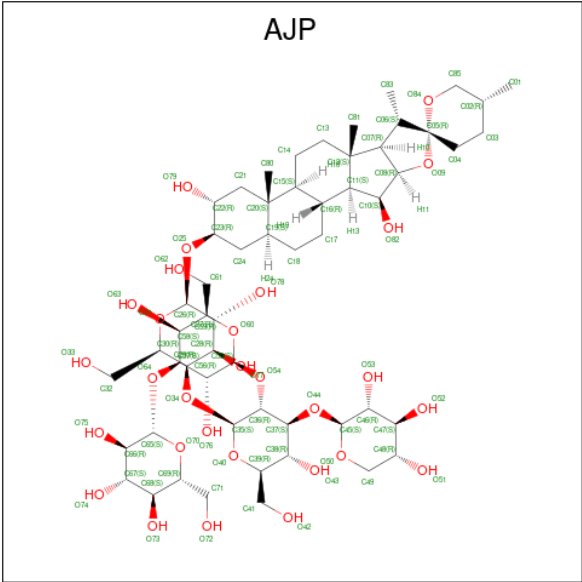
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			22	14	7	1	
3	A	1	Total	C	O	P	0
			22	14	7	1	
3	A	1	Total	C	O	P	0
			22	14	7	1	
3	A	1	Total	C	O	P	0
			34	25	8	1	
3	A	1	Total	C	O	P	0
			36	27	8	1	
3	A	1	Total	C	O	P	0
			31	22	8	1	
3	A	1	Total	C	O	P	0
			20	12	7	1	
3	A	1	Total	C	O	P	0
			29	20	8	1	
3	B	1	Total	C	O	P	0
			22	14	7	1	
3	B	1	Total	C	O	P	0
			22	14	7	1	
3	B	1	Total	C	O	P	0
			34	25	8	1	
3	B	1	Total	C	O	P	0
			35	26	8	1	
3	B	1	Total	C	O	P	0
			29	20	8	1	
3	B	1	Total	C	O	P	0
			31	22	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	O	P	0
			20	12	7	1	
3	C	1	Total	C	O	P	0
			22	14	7	1	
3	C	1	Total	C	O	P	0
			34	25	8	1	
3	C	1	Total	C	O	P	0
			35	26	8	1	
3	C	1	Total	C	O	P	0
			29	20	8	1	
3	C	1	Total	C	O	P	0
			31	22	8	1	
3	C	1	Total	C	O	P	0
			20	12	7	1	
3	D	1	Total	C	O	P	0
			22	14	7	1	
3	D	1	Total	C	O	P	0
			22	14	7	1	
3	D	1	Total	C	O	P	0
			34	25	8	1	
3	D	1	Total	C	O	P	0
			36	27	8	1	
3	D	1	Total	C	O	P	0
			29	20	8	1	
3	D	1	Total	C	O	P	0
			31	22	8	1	
3	D	1	Total	C	O	P	0
			20	12	7	1	

- Molecule 4 is Digitonin (CCD ID: AJP) (formula: $C_{56}H_{92}O_{29}$).



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

Continued on next page...

Continued from previous page...

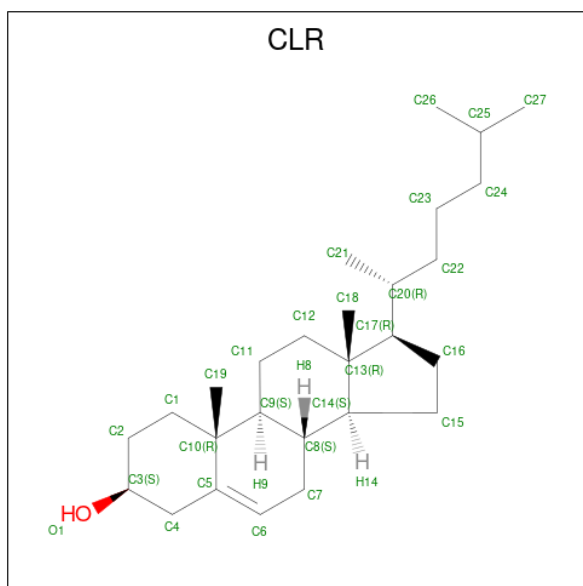
Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	C	O	0
			65	45	20	
4	B	1	Total	C	O	0
			43	33	10	
4	B	1	Total	C	O	0
			43	33	10	
4	B	1	Total	C	O	0
			43	33	10	
4	C	1	Total	C	O	0
			54	39	15	
4	C	1	Total	C	O	0
			43	33	10	
4	C	1	Total	C	O	0
			43	33	10	
4	C	1	Total	C	O	0
			43	33	10	
4	C	1	Total	C	O	0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

Continued on next page...

Continued from previous page...

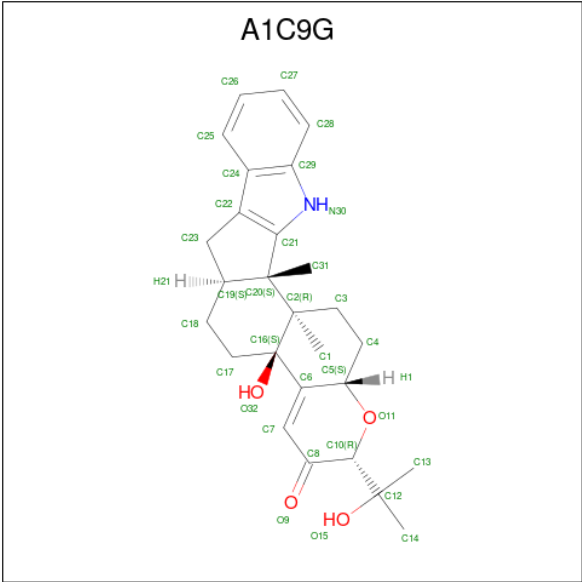
Mol	Chain	Residues	Atoms			AltConf
4	D	1	Total	C	O	0
			43	33	10	

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	C	1	Total	C	O	0
			28	27	1	
5	D	1	Total	C	O	0
			28	27	1	

- Molecule 6 is Paxilline (CCD ID: A1C9G) (formula: $C_{27}H_{33}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			32	27	1	4	
6	B	1	Total	C	N	O	0
			32	27	1	4	
6	C	1	Total	C	N	O	0
			32	27	1	4	
6	D	1	Total	C	N	O	0
			32	27	1	4	

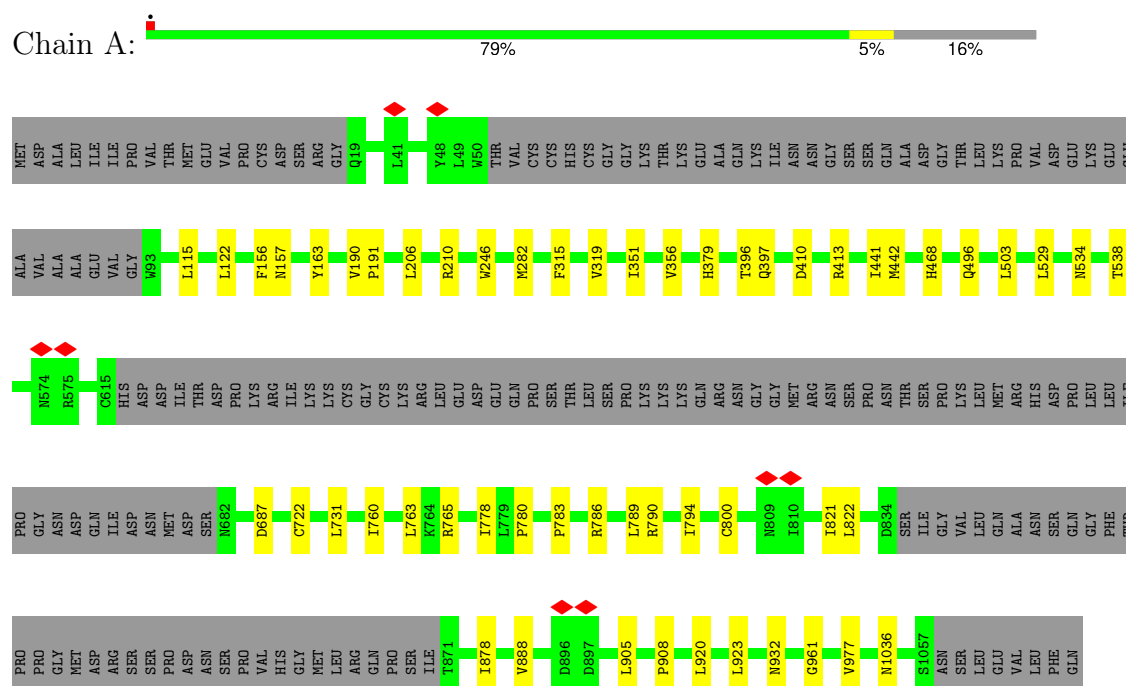
- Molecule 7 is water.

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

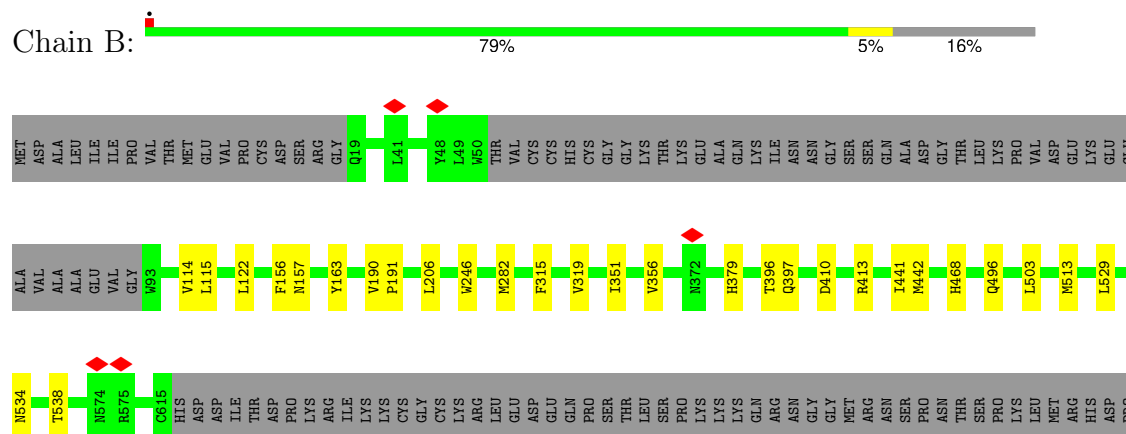
3 Residue-property plots [i](#)

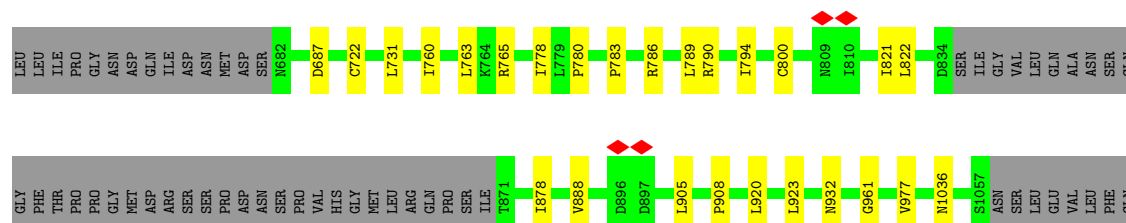
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

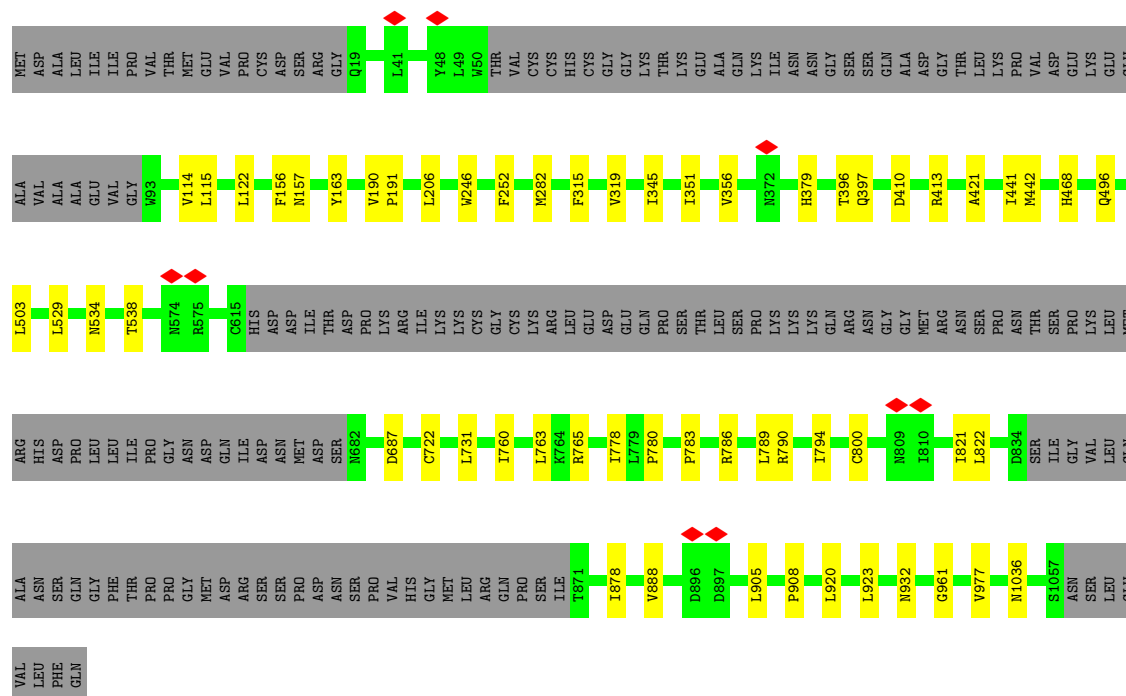
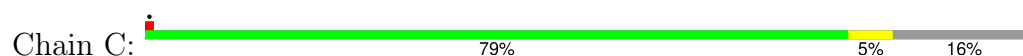


- Molecule 1: Calcium-activated potassium channel subunit alpha-1

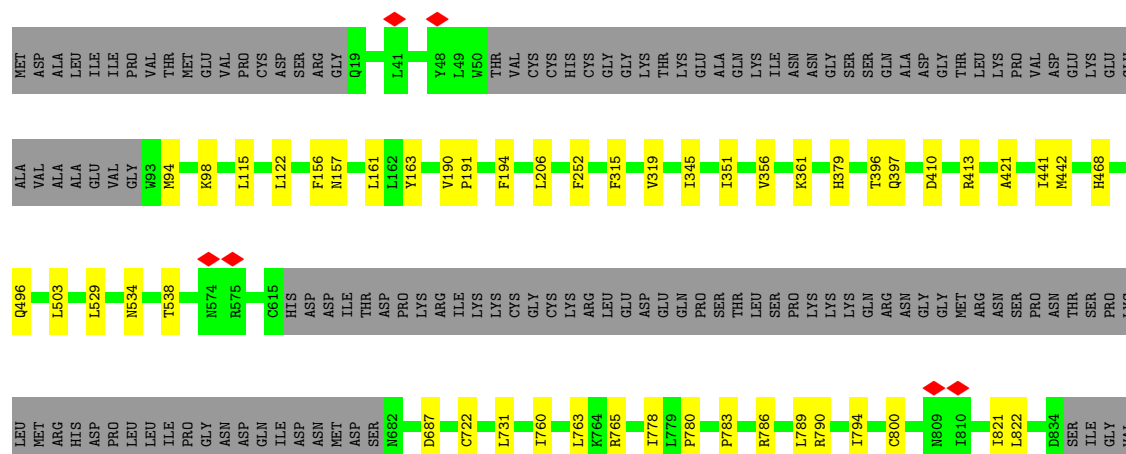
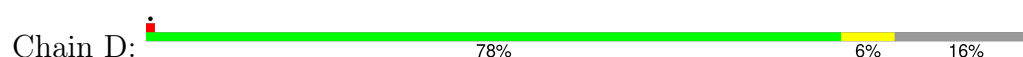


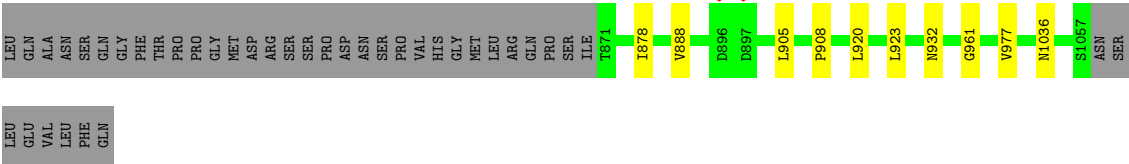


• Molecule 1: Calcium-activated potassium channel subunit alpha-1



• 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	359852	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	0.410	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	291.19998, 291.19998, 291.19998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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, A1C9G, CLR, AJP

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	0.18	0/7310	0.31	0/9923
1	B	0.18	0/7310	0.31	0/9923
1	C	0.18	0/7310	0.31	0/9923
1	D	0.18	0/7310	0.31	0/9923
All	All	0.18	0/29240	0.31	0/39692

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	7143	0	7129	32	0
1	B	7143	0	7129	33	0
1	C	7143	0	7129	34	0
1	D	7143	0	7129	36	0
2	A	6	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	216	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	193	0	0	0	0
3	C	171	0	0	0	0
3	D	194	0	0	0	0
4	A	420	0	0	0	0
4	B	420	0	0	1	0
4	C	420	0	0	1	0
4	D	420	0	0	0	0
5	A	28	0	46	1	0
5	B	28	0	46	1	0
5	C	28	0	46	2	0
5	D	28	0	46	2	0
6	A	32	0	0	0	0
6	B	32	0	0	0	0
6	C	32	0	0	0	0
6	D	32	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	31279	0	28700	127	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 (127) 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:722:CYS:HB3	1:D:783:PRO:HB3	1.64	0.80
1:C:722:CYS:HB3	1:C:783:PRO:HB3	1.64	0.79
1:B:722:CYS:HB3	1:B:783:PRO:HB3	1.64	0.78
1:A:722:CYS:HB3	1:A:783:PRO:HB3	1.64	0.78
1:D:351:ILE:HD12	1:D:379:HIS:HB2	1.76	0.68
1:A:351:ILE:HD12	1:A:379:HIS:HB2	1.76	0.68
1:C:351:ILE:HD12	1:C:379:HIS:HB2	1.76	0.67
1:A:800:CYS:HB3	1:A:878:ILE:HG22	1.78	0.66
1:B:351:ILE:HD12	1:B:379:HIS:HB2	1.77	0.66
1:D:800:CYS:HB3	1:D:878:ILE:HG22	1.78	0.65
1:C:800:CYS:HB3	1:C:878:ILE:HG22	1.78	0.65
1:B:800:CYS:HB3	1:B:878:ILE:HG22	1.78	0.64
1:A:503:LEU:HD22	1:A:977:VAL:HG11	1.82	0.61
1:C:503:LEU:HD22	1:C:977:VAL:HG11	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:LEU:HD22	1:D:977:VAL:HG11	1.82	0.61
1:B:503:LEU:HD22	1:B:977:VAL:HG11	1.82	0.61
1:A:396:THR:HG23	1:A:397:GLN:HG3	1.86	0.58
1:B:396:THR:HG23	1:B:397:GLN:HG3	1.86	0.58
1:D:396:THR:HG23	1:D:397:GLN:HG3	1.86	0.57
1:C:396:THR:HG23	1:C:397:GLN:HG3	1.86	0.56
1:C:206:LEU:HD11	5:C:1106:CLR:H121	1.91	0.53
1:B:115:LEU:HB3	1:B:163:TYR:HE1	1.77	0.49
1:D:496:GLN:HB3	1:D:503:LEU:HD23	1.95	0.48
1:C:115:LEU:HB3	1:C:163:TYR:HE1	1.77	0.48
1:C:496:GLN:HB3	1:C:503:LEU:HD23	1.95	0.48
1:A:496:GLN:HB3	1:A:503:LEU:HD23	1.95	0.48
1:C:410:ASP:HA	1:C:413:ARG:HG3	1.96	0.48
1:D:315:PHE:O	1:D:319:VAL:HG23	2.14	0.48
1:A:315:PHE:O	1:A:319:VAL:HG23	2.14	0.48
1:C:315:PHE:O	1:C:319:VAL:HG23	2.14	0.48
1:D:115:LEU:HB3	1:D:163:TYR:HE1	1.78	0.48
1:D:410:ASP:HA	1:D:413:ARG:HG3	1.96	0.48
1:A:731:LEU:HD21	1:A:765:ARG:HE	1.79	0.48
1:B:496:GLN:HB3	1:B:503:LEU:HD23	1.96	0.48
1:A:410:ASP:HA	1:A:413:ARG:HG3	1.96	0.47
1:C:441:ILE:HG21	1:D:822:LEU:HD11	1.96	0.47
1:C:731:LEU:HD21	1:C:765:ARG:HE	1.80	0.47
1:A:157:ASN:HD21	1:A:190:VAL:HA	1.80	0.47
1:D:157:ASN:HD21	1:D:190:VAL:HA	1.80	0.47
1:A:351:ILE:HG23	1:A:356:VAL:HG21	1.97	0.47
1:B:731:LEU:HD21	1:B:765:ARG:HE	1.80	0.47
1:D:731:LEU:HD21	1:D:765:ARG:HE	1.80	0.47
1:B:441:ILE:HG21	1:C:822:LEU:HD11	1.96	0.47
1:D:351:ILE:HG23	1:D:356:VAL:HG21	1.97	0.46
1:A:441:ILE:HG21	1:B:822:LEU:HD11	1.97	0.46
1:B:157:ASN:HD21	1:B:190:VAL:HA	1.81	0.46
1:B:315:PHE:O	1:B:319:VAL:HG23	2.14	0.46
1:A:115:LEU:HB3	1:A:163:TYR:HE1	1.81	0.46
1:C:351:ILE:HG23	1:C:356:VAL:HG21	1.97	0.46
1:A:822:LEU:HD11	1:D:441:ILE:HG21	1.96	0.46
1:B:441:ILE:HD13	1:B:468:HIS:HB2	1.98	0.46
1:D:786:ARG:O	1:D:790:ARG:HG3	2.16	0.45
1:B:410:ASP:HA	1:B:413:ARG:HG3	1.96	0.45
1:B:786:ARG:O	1:B:790:ARG:HG3	2.16	0.45
1:A:210:ARG:HD3	1:A:210:ARG:HA	1.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:763:LEU:HD13	1:D:778:ILE:HG23	1.99	0.45
1:B:351:ILE:HG23	1:B:356:VAL:HG21	1.98	0.45
1:C:786:ARG:O	1:C:790:ARG:HG3	2.16	0.45
1:A:786:ARG:O	1:A:790:ARG:HG3	2.16	0.45
1:C:114:VAL:HG12	4:C:1116:AJP:O82	2.17	0.45
1:A:920:LEU:O	1:A:923:LEU:HB3	2.17	0.45
1:D:920:LEU:O	1:D:923:LEU:HB3	2.17	0.45
1:C:763:LEU:HD13	1:C:778:ILE:HG23	1.99	0.44
1:C:920:LEU:O	1:C:923:LEU:HB3	2.17	0.44
1:A:763:LEU:HD13	1:A:778:ILE:HG23	1.99	0.44
1:A:442:MET:HE3	1:B:821:ILE:HD12	2.00	0.44
1:B:888:VAL:HG22	1:B:908:PRO:HB2	2.00	0.44
1:B:920:LEU:O	1:B:923:LEU:HB3	2.17	0.44
1:C:687:ASP:HA	1:C:961:GLY:HA2	1.99	0.44
1:B:114:VAL:HG12	4:B:1117:AJP:O82	2.18	0.44
1:D:206:LEU:HD11	5:D:1107:CLR:H121	2.00	0.43
1:A:206:LEU:HD11	5:A:1113:CLR:H121	2.00	0.43
1:B:122:LEU:HD22	1:B:156:PHE:CE1	2.54	0.43
1:A:534:ASN:ND2	1:A:1036:ASN:HB3	2.34	0.43
1:A:821:ILE:HD12	1:D:442:MET:HE3	2.00	0.43
1:B:442:MET:HE3	1:C:821:ILE:HD12	2.00	0.43
1:A:122:LEU:HD22	1:A:156:PHE:CE1	2.54	0.43
1:C:534:ASN:ND2	1:C:1036:ASN:HB3	2.34	0.43
1:D:122:LEU:HD22	1:D:156:PHE:CE1	2.54	0.43
1:D:888:VAL:HG22	1:D:908:PRO:HB2	2.00	0.43
1:B:529:LEU:HD21	1:B:905:LEU:HD21	2.01	0.43
1:C:888:VAL:HG22	1:C:908:PRO:HB2	2.00	0.43
1:D:534:ASN:ND2	1:D:1036:ASN:HB3	2.34	0.43
1:B:763:LEU:HD13	1:B:778:ILE:HG23	1.99	0.43
1:D:529:LEU:HD21	1:D:905:LEU:HD21	2.01	0.43
1:B:760:ILE:HB	1:B:780:PRO:HB3	2.00	0.43
1:B:789:LEU:HD22	1:B:794:ILE:HD12	2.01	0.43
1:C:760:ILE:HB	1:C:780:PRO:HB3	2.00	0.43
1:D:538:THR:HG21	1:D:932:ASN:HB2	2.01	0.43
1:C:442:MET:HE3	1:D:821:ILE:HD12	2.00	0.42
1:A:529:LEU:HD21	1:A:905:LEU:HD21	2.01	0.42
1:A:888:VAL:HG22	1:A:908:PRO:HB2	2.00	0.42
1:C:122:LEU:HD22	1:C:156:PHE:CE1	2.53	0.42
1:A:538:THR:HG21	1:A:932:ASN:HB2	2.01	0.42
1:A:789:LEU:HD22	1:A:794:ILE:HD12	2.01	0.42
1:D:687:ASP:HA	1:D:961:GLY:HA2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:THR:HG21	1:C:932:ASN:HB2	2.01	0.42
1:C:157:ASN:HD21	1:C:190:VAL:HA	1.84	0.42
1:C:529:LEU:HD21	1:C:905:LEU:HD21	2.02	0.42
1:C:789:LEU:HD22	1:C:794:ILE:HD12	2.01	0.42
1:D:98:LYS:HE2	1:D:98:LYS:HB3	1.87	0.42
1:B:534:ASN:ND2	1:B:1036:ASN:HB3	2.34	0.42
1:A:190:VAL:HB	1:A:191:PRO:HD3	2.01	0.41
1:A:687:ASP:HA	1:A:961:GLY:HA2	2.02	0.41
1:C:190:VAL:HB	1:C:191:PRO:HD3	2.02	0.41
1:C:252:PHE:HE1	5:C:1106:CLR:H182	1.86	0.41
1:D:94:MET:HE3	1:D:94:MET:HB3	1.97	0.41
1:D:190:VAL:HB	1:D:191:PRO:HD3	2.01	0.41
1:B:687:ASP:HA	1:B:961:GLY:HA2	2.02	0.41
1:C:441:ILE:HD13	1:C:468:HIS:HB2	2.03	0.41
1:D:789:LEU:HD22	1:D:794:ILE:HD12	2.01	0.41
1:A:246:TRP:CE3	1:A:282:MET:HE1	2.56	0.41
1:B:206:LEU:HD11	5:B:1107:CLR:H121	2.03	0.41
1:B:246:TRP:CE3	1:B:282:MET:HE1	2.56	0.41
1:B:538:THR:HG21	1:B:932:ASN:HB2	2.01	0.41
1:D:161:LEU:HD22	1:D:194:PHE:HZ	1.85	0.41
1:D:361:LYS:HE3	1:D:361:LYS:HB2	1.86	0.41
1:A:760:ILE:HB	1:A:780:PRO:HB3	2.01	0.41
1:B:190:VAL:HB	1:B:191:PRO:HD3	2.01	0.41
1:C:345:ILE:HD12	1:C:421:ALA:HB3	2.03	0.41
1:D:441:ILE:HD13	1:D:468:HIS:HB2	2.03	0.41
1:D:760:ILE:HB	1:D:780:PRO:HB3	2.02	0.41
1:D:345:ILE:HD12	1:D:421:ALA:HB3	2.03	0.41
1:D:252:PHE:HE1	5:D:1107:CLR:H182	1.85	0.40
1:A:441:ILE:HD13	1:A:468:HIS:HB2	2.03	0.40
1:C:246:TRP:CE3	1:C:282:MET:HE1	2.56	0.40
1:B:513:MET:HE3	1:B:513:MET:HB3	1.93	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	887/1065 (83%)	872 (98%)	15 (2%)	0	100	100
1	B	887/1065 (83%)	871 (98%)	16 (2%)	0	100	100
1	C	887/1065 (83%)	872 (98%)	15 (2%)	0	100	100
1	D	887/1065 (83%)	871 (98%)	16 (2%)	0	100	100
All	All	3548/4260 (83%)	3486 (98%)	62 (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	787/937 (84%)	787 (100%)	0	100	100
1	B	787/937 (84%)	787 (100%)	0	100	100
1	C	787/937 (84%)	787 (100%)	0	100	100
1	D	787/937 (84%)	787 (100%)	0	100	100
All	All	3148/3748 (84%)	3148 (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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	258	ASN
1	A	270	GLN
1	A	816	GLN
1	B	157	ASN
1	B	258	ASN
1	B	270	GLN
1	B	409	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	258	ASN
1	C	270	GLN
1	C	816	GLN
1	D	157	ASN
1	D	258	ASN
1	D	270	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](#)

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](#)

Of 81 ligands modelled in this entry, 9 are monoatomic - leaving 72 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	$\# Z > 2$
3	LBN	C	1107	-	28,28,51	0.81	1 (3%)	31,33,59	0.93	2 (6%)
3	LBN	A	1111	-	35,35,51	0.71	1 (2%)	38,40,59	0.93	3 (7%)
5	CLR	C	1106	-	31,31,31	0.41	0	48,48,48	0.74	1 (2%)
4	AJP	D	1118	-	49,49,95	0.14	0	75,80,149	0.35	0
4	AJP	B	1112	-	49,49,95	0.17	0	75,80,149	0.51	1 (1%)
3	LBN	D	1102	-	21,21,51	0.84	1 (4%)	23,25,59	1.05	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LBN	D	1105	-	35,35,51	0.71	1 (2%)	38,40,59	0.96	3 (7%)
4	AJP	C	1112	-	49,49,95	0.20	0	75,80,149	0.57	0
5	CLR	B	1107	-	31,31,31	0.41	0	48,48,48	0.70	1 (2%)
4	AJP	A	1117	-	49,49,95	0.15	0	75,80,149	0.36	0
3	LBN	D	1103	-	21,21,51	0.84	1 (4%)	23,25,59	1.06	2 (8%)
3	LBN	B	1109	-	30,30,51	0.76	1 (3%)	33,35,59	0.91	2 (6%)
3	LBN	D	1108	-	28,28,51	0.80	1 (3%)	31,33,59	0.93	2 (6%)
3	LBN	D	1110	-	19,19,51	0.88	1 (5%)	21,23,59	1.09	2 (9%)
3	LBN	A	1114	-	30,30,51	0.76	1 (3%)	33,35,59	0.90	2 (6%)
3	LBN	C	1102	-	21,21,51	0.84	1 (4%)	23,25,59	1.06	2 (8%)
4	AJP	A	1122	-	49,49,95	0.15	0	75,80,149	0.36	0
6	A1C9G	C	1118	-	35,37,37	0.34	0	44,63,63	0.73	1 (2%)
4	AJP	B	1115	-	73,73,95	0.15	0	111,116,149	0.44	0
6	A1C9G	B	1119	-	35,37,37	0.34	0	44,63,63	0.73	1 (2%)
4	AJP	D	1106	-	61,61,95	0.19	0	93,98,149	0.45	0
6	A1C9G	A	1125	-	35,37,37	0.35	0	44,63,63	0.73	1 (2%)
4	AJP	D	1115	-	73,73,95	0.14	0	111,116,149	0.44	0
4	AJP	D	1112	-	49,49,95	0.19	0	75,80,149	0.51	0
3	LBN	C	1108	-	30,30,51	0.76	1 (3%)	33,35,59	0.91	2 (6%)
4	AJP	A	1123	-	49,49,95	0.17	0	75,80,149	0.46	0
5	CLR	D	1107	-	31,31,31	0.40	0	48,48,48	0.70	1 (2%)
4	AJP	C	1115	-	49,49,95	0.14	0	75,80,149	0.36	0
3	LBN	D	1104	-	33,33,51	0.74	1 (3%)	36,38,59	0.87	2 (5%)
4	AJP	C	1110	-	49,49,95	0.15	0	75,80,149	0.54	1 (1%)
3	LBN	C	1103	-	33,33,51	0.74	1 (3%)	36,38,59	0.86	2 (5%)
4	AJP	B	1117	-	49,49,95	0.17	0	75,80,149	0.47	0
3	LBN	C	1109	-	19,19,51	0.88	1 (5%)	21,23,59	1.09	2 (9%)
4	AJP	A	1119	-	49,49,95	0.16	0	75,80,149	0.36	0
3	LBN	D	1109	-	30,30,51	0.76	1 (3%)	33,35,59	0.91	2 (6%)
3	LBN	B	1108	-	28,28,51	0.80	1 (3%)	31,33,59	0.93	2 (6%)
4	AJP	B	1116	-	49,49,95	0.15	0	75,80,149	0.35	0
4	AJP	C	1105	-	61,61,95	0.17	0	93,98,149	0.57	1 (1%)
4	AJP	C	1113	-	49,49,95	0.16	0	75,80,149	0.38	0
4	AJP	D	1117	-	49,49,95	0.18	0	75,80,149	0.53	1 (1%)
3	LBN	A	1110	-	33,33,51	0.74	1 (3%)	36,38,59	0.86	2 (5%)
4	AJP	A	1118	-	49,49,95	0.16	0	75,80,149	0.39	0
4	AJP	D	1114	-	49,49,95	0.16	0	75,80,149	0.37	0
3	LBN	B	1103	-	21,21,51	0.84	1 (4%)	23,25,59	1.05	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	A1C9G	D	1119	-	35,37,37	0.34	0	44,63,63	0.73	1 (2%)
4	AJP	C	1117	-	49,49,95	0.14	0	75,80,149	0.39	0
4	AJP	B	1106	-	61,61,95	0.18	0	93,98,149	0.50	0
3	LBN	B	1110	-	19,19,51	0.88	1 (5%)	21,23,59	1.09	2 (9%)
3	LBN	A	1109	-	21,21,51	0.83	1 (4%)	23,25,59	1.06	2 (8%)
3	LBN	A	1116	-	28,28,51	0.80	1 (3%)	31,33,59	0.92	2 (6%)
3	LBN	C	1104	-	34,34,51	0.71	1 (2%)	37,39,59	0.95	3 (8%)
4	AJP	A	1121	-	73,73,95	0.15	0	111,116,149	0.44	0
4	AJP	B	1113	-	49,49,95	0.14	0	75,80,149	0.55	0
4	AJP	C	1116	-	49,49,95	0.18	0	75,80,149	0.46	0
3	LBN	A	1108	-	21,21,51	0.84	1 (4%)	23,25,59	1.07	2 (8%)
4	AJP	A	1112	-	61,61,95	0.16	0	93,98,149	0.49	1 (1%)
4	AJP	A	1124	-	49,49,95	0.13	0	75,80,149	0.36	0
3	LBN	A	1115	-	19,19,51	0.88	1 (5%)	21,23,59	1.09	2 (9%)
4	AJP	C	1111	-	49,49,95	0.23	0	75,80,149	0.65	3 (4%)
4	AJP	D	1113	-	49,49,95	0.15	0	75,80,149	0.34	0
5	CLR	A	1113	-	31,31,31	0.41	0	48,48,48	0.73	1 (2%)
3	LBN	B	1104	-	33,33,51	0.74	1 (3%)	36,38,59	0.87	2 (5%)
4	AJP	C	1114	-	73,73,95	0.15	0	111,116,149	0.45	0
4	AJP	B	1111	-	49,49,95	0.15	0	75,80,149	0.37	0
3	LBN	B	1105	-	34,34,51	0.71	1 (2%)	37,39,59	0.93	3 (8%)
3	LBN	A	1107	-	21,21,51	0.84	1 (4%)	23,25,59	1.06	2 (8%)
4	AJP	D	1111	-	49,49,95	0.15	0	75,80,149	0.36	0
4	AJP	B	1118	-	49,49,95	0.13	0	75,80,149	0.34	0
3	LBN	B	1102	-	21,21,51	0.83	1 (4%)	23,25,59	1.06	2 (8%)
4	AJP	B	1114	-	49,49,95	0.16	0	75,80,149	0.38	0
4	AJP	D	1116	-	49,49,95	0.16	0	75,80,149	0.47	0
4	AJP	A	1120	-	49,49,95	0.16	0	75,80,149	0.37	0

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	C	1107	-	1/1/4/7	5/30/30/55	-
3	LBN	A	1111	-	1/1/4/7	8/37/37/55	-
5	CLR	C	1106	-	-	2/10/68/68	0/4/4/4
4	AJP	D	1118	-	-	3/6/121/220	0/7/7/11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AJP	B	1112	-	-	1/6/121/220	1/7/7/11
3	LBN	D	1102	-	1/1/3/7	6/21/21/55	-
3	LBN	D	1105	-	1/1/4/7	8/37/37/55	-
4	AJP	C	1112	-	-	1/6/121/220	0/7/7/11
5	CLR	B	1107	-	-	2/10/68/68	0/4/4/4
4	AJP	A	1117	-	-	0/6/121/220	0/7/7/11
3	LBN	D	1103	-	1/1/3/7	3/21/21/55	-
3	LBN	B	1109	-	1/1/4/7	6/32/32/55	-
3	LBN	D	1108	-	1/1/4/7	5/30/30/55	-
3	LBN	D	1110	-	1/1/3/7	5/19/19/55	-
3	LBN	A	1114	-	1/1/4/7	6/32/32/55	-
3	LBN	C	1102	-	1/1/3/7	3/21/21/55	-
4	AJP	A	1122	-	-	1/6/121/220	0/7/7/11
6	A1C9G	C	1118	-	-	0/6/74/74	0/6/6/6
4	AJP	B	1115	-	-	4/18/173/220	0/9/9/11
6	A1C9G	B	1119	-	-	0/6/74/74	0/6/6/6
4	AJP	D	1106	-	-	6/12/147/220	0/8/8/11
6	A1C9G	A	1125	-	-	0/6/74/74	0/6/6/6
4	AJP	D	1115	-	-	4/18/173/220	0/9/9/11
4	AJP	D	1112	-	-	2/6/121/220	0/7/7/11
3	LBN	C	1108	-	1/1/4/7	7/32/32/55	-
4	AJP	A	1123	-	-	0/6/121/220	0/7/7/11
5	CLR	D	1107	-	-	4/10/68/68	0/4/4/4
4	AJP	C	1115	-	-	2/6/121/220	0/7/7/11
3	LBN	D	1104	-	1/1/4/7	7/35/35/55	-
4	AJP	C	1110	-	-	0/6/121/220	0/7/7/11
3	LBN	C	1103	-	1/1/4/7	9/35/35/55	-
4	AJP	B	1117	-	-	2/6/121/220	0/7/7/11
3	LBN	C	1109	-	1/1/3/7	5/19/19/55	-
4	AJP	A	1119	-	-	0/6/121/220	0/7/7/11
3	LBN	D	1109	-	1/1/4/7	6/32/32/55	-
3	LBN	B	1108	-	1/1/4/7	5/30/30/55	-
4	AJP	B	1116	-	-	2/6/121/220	0/7/7/11
4	AJP	C	1105	-	-	6/12/147/220	1/8/8/11
4	AJP	C	1113	-	-	0/6/121/220	0/7/7/11
4	AJP	D	1117	-	-	3/6/121/220	1/7/7/11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LBN	A	1110	-	1/1/4/7	7/35/35/55	-
4	AJP	A	1118	-	-	1/6/121/220	0/7/7/11
4	AJP	D	1114	-	-	0/6/121/220	0/7/7/11
3	LBN	B	1103	-	1/1/3/7	6/21/21/55	-
6	A1C9G	D	1119	-	-	0/6/74/74	0/6/6/6
4	AJP	C	1117	-	-	2/6/121/220	0/7/7/11
4	AJP	B	1106	-	-	5/12/147/220	0/8/8/11
3	LBN	B	1110	-	1/1/3/7	5/19/19/55	-
3	LBN	A	1109	-	1/1/3/7	3/21/21/55	-
3	LBN	A	1116	-	1/1/4/7	5/30/30/55	-
3	LBN	C	1104	-	1/1/4/7	10/36/36/55	-
4	AJP	A	1121	-	-	4/18/173/220	0/9/9/11
4	AJP	B	1113	-	-	2/6/121/220	0/7/7/11
4	AJP	C	1116	-	-	1/6/121/220	0/7/7/11
3	LBN	A	1108	-	1/1/3/7	5/21/21/55	-
4	AJP	A	1112	-	-	4/12/147/220	1/8/8/11
4	AJP	A	1124	-	-	2/6/121/220	0/7/7/11
3	LBN	A	1115	-	1/1/3/7	5/19/19/55	-
4	AJP	C	1111	-	-	1/6/121/220	0/7/7/11
4	AJP	D	1113	-	-	2/6/121/220	0/7/7/11
5	CLR	A	1113	-	-	2/10/68/68	0/4/4/4
3	LBN	B	1104	-	1/1/4/7	8/35/35/55	-
4	AJP	C	1114	-	-	6/18/173/220	0/9/9/11
4	AJP	B	1111	-	-	0/6/121/220	0/7/7/11
3	LBN	B	1105	-	1/1/4/7	9/36/36/55	-
3	LBN	A	1107	-	1/1/3/7	6/21/21/55	-
4	AJP	D	1111	-	-	0/6/121/220	0/7/7/11
4	AJP	B	1118	-	-	0/6/121/220	0/7/7/11
3	LBN	B	1102	-	1/1/3/7	3/21/21/55	-
4	AJP	B	1114	-	-	0/6/121/220	0/7/7/11
4	AJP	D	1116	-	-	1/6/121/220	0/7/7/11
4	AJP	A	1120	-	-	0/6/121/220	0/7/7/11

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1110	LBN	P1-O2	3.07	1.66	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1110	LBN	P1-O2	3.07	1.66	1.54
3	B	1110	LBN	P1-O2	3.06	1.66	1.54
3	C	1103	LBN	P1-O2	3.06	1.66	1.54
3	C	1109	LBN	P1-O2	3.06	1.66	1.54
3	B	1108	LBN	P1-O2	3.05	1.66	1.54
3	C	1107	LBN	P1-O2	3.05	1.66	1.54
3	A	1108	LBN	P1-O2	3.05	1.66	1.54
3	B	1104	LBN	P1-O2	3.05	1.66	1.54
3	B	1109	LBN	P1-O2	3.05	1.66	1.54
3	C	1102	LBN	P1-O2	3.05	1.66	1.54
3	C	1108	LBN	P1-O2	3.05	1.66	1.54
3	D	1108	LBN	P1-O2	3.04	1.66	1.54
3	A	1111	LBN	P1-O2	3.04	1.66	1.54
3	D	1103	LBN	P1-O2	3.04	1.66	1.54
3	D	1104	LBN	P1-O2	3.04	1.66	1.54
3	A	1109	LBN	P1-O2	3.04	1.66	1.54
3	A	1115	LBN	P1-O2	3.04	1.66	1.54
3	A	1107	LBN	P1-O2	3.04	1.66	1.54
3	D	1105	LBN	P1-O2	3.04	1.66	1.54
3	B	1102	LBN	P1-O2	3.03	1.66	1.54
3	A	1114	LBN	P1-O2	3.03	1.66	1.54
3	D	1109	LBN	P1-O2	3.03	1.66	1.54
3	D	1102	LBN	P1-O2	3.03	1.66	1.54
3	B	1103	LBN	P1-O2	3.03	1.66	1.54
3	A	1116	LBN	P1-O2	3.02	1.66	1.54
3	C	1104	LBN	P1-O2	3.02	1.66	1.54
3	B	1105	LBN	P1-O2	3.02	1.66	1.54

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1108	LBN	O2-P1-O1	-3.50	97.53	106.67
3	A	1111	LBN	O2-P1-O1	-3.48	97.58	106.67
3	B	1109	LBN	O2-P1-O1	-3.48	97.60	106.67
3	D	1105	LBN	O2-P1-O1	-3.48	97.60	106.67
3	B	1104	LBN	O2-P1-O1	-3.47	97.62	106.67
3	D	1104	LBN	O2-P1-O1	-3.47	97.62	106.67
3	C	1104	LBN	O2-P1-O1	-3.47	97.63	106.67
3	B	1105	LBN	O2-P1-O1	-3.46	97.65	106.67
3	D	1109	LBN	O2-P1-O1	-3.46	97.65	106.67
3	C	1108	LBN	O2-P1-O1	-3.46	97.65	106.67
3	D	1103	LBN	O2-P1-O1	-3.46	97.66	106.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1102	LBN	O2-P1-O1	-3.46	97.66	106.67
3	B	1102	LBN	O2-P1-O1	-3.46	97.66	106.67
3	A	1109	LBN	O2-P1-O1	-3.46	97.66	106.67
3	A	1114	LBN	O2-P1-O1	-3.44	97.69	106.67
3	C	1103	LBN	O2-P1-O1	-3.44	97.69	106.67
3	A	1110	LBN	O2-P1-O1	-3.44	97.71	106.67
3	B	1103	LBN	O2-P1-O1	-3.43	97.73	106.67
3	B	1110	LBN	O2-P1-O1	-3.43	97.73	106.67
3	A	1115	LBN	O2-P1-O1	-3.42	97.74	106.67
3	D	1110	LBN	O2-P1-O1	-3.42	97.75	106.67
3	A	1107	LBN	O2-P1-O1	-3.42	97.76	106.67
3	D	1102	LBN	O2-P1-O1	-3.41	97.77	106.67
3	B	1108	LBN	O2-P1-O1	-3.41	97.77	106.67
3	C	1107	LBN	O2-P1-O1	-3.41	97.77	106.67
3	C	1109	LBN	O2-P1-O1	-3.41	97.78	106.67
3	D	1108	LBN	O2-P1-O1	-3.40	97.81	106.67
3	A	1116	LBN	O2-P1-O1	-3.38	97.84	106.67
5	C	1106	CLR	C17-C13-C14	2.72	103.22	100.10
3	C	1107	LBN	O3-P1-O4	2.68	121.28	110.83
3	B	1108	LBN	O3-P1-O4	2.67	121.26	110.83
3	D	1108	LBN	O3-P1-O4	2.67	121.25	110.83
3	A	1116	LBN	O3-P1-O4	2.67	121.23	110.83
3	B	1109	LBN	O3-P1-O4	2.65	121.17	110.83
3	D	1103	LBN	O3-P1-O4	2.65	121.16	110.83
3	A	1108	LBN	O3-P1-O4	2.65	121.15	110.83
3	A	1109	LBN	O3-P1-O4	2.64	121.13	110.83
3	A	1114	LBN	O3-P1-O4	2.64	121.13	110.83
3	C	1108	LBN	O3-P1-O4	2.64	121.13	110.83
3	B	1102	LBN	O3-P1-O4	2.64	121.12	110.83
3	D	1109	LBN	O3-P1-O4	2.64	121.12	110.83
3	D	1102	LBN	O3-P1-O4	2.64	121.12	110.83
3	C	1102	LBN	O3-P1-O4	2.64	121.11	110.83
3	B	1103	LBN	O3-P1-O4	2.64	121.10	110.83
3	B	1104	LBN	O3-P1-O4	2.63	121.09	110.83
3	A	1115	LBN	O3-P1-O4	2.63	121.09	110.83
3	B	1110	LBN	O3-P1-O4	2.63	121.08	110.83
3	D	1110	LBN	O3-P1-O4	2.63	121.08	110.83
3	A	1107	LBN	O3-P1-O4	2.63	121.08	110.83
3	C	1109	LBN	O3-P1-O4	2.63	121.07	110.83
3	A	1110	LBN	O3-P1-O4	2.63	121.06	110.83
3	D	1104	LBN	O3-P1-O4	2.61	121.01	110.83
3	C	1103	LBN	O3-P1-O4	2.60	120.97	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1113	CLR	C17-C13-C14	2.60	103.08	100.10
4	C	1111	AJP	C26-O25-C23	2.58	119.58	115.27
3	B	1105	LBN	O3-P1-O4	2.57	120.86	110.83
3	D	1105	LBN	O3-P1-O4	2.57	120.85	110.83
3	A	1111	LBN	O3-P1-O4	2.57	120.85	110.83
3	C	1104	LBN	O3-P1-O4	2.55	120.78	110.83
4	C	1111	AJP	O79-C22-C21	-2.54	104.07	109.97
3	D	1105	LBN	C2-O7-C34	2.46	123.68	117.80
5	B	1107	CLR	C17-C13-C14	2.46	102.92	100.10
5	D	1107	CLR	C17-C13-C14	2.43	102.89	100.10
3	C	1104	LBN	C2-O7-C34	2.30	123.30	117.80
4	D	1117	AJP	C20-C21-C22	2.24	117.86	114.17
4	B	1112	AJP	C20-C21-C22	2.23	117.83	114.17
4	A	1112	AJP	C20-C21-C22	2.16	117.72	114.17
6	B	1119	A1C9G	O32-C16-C2	2.13	112.51	107.72
4	C	1111	AJP	C21-C22-C23	2.12	113.30	110.46
6	D	1119	A1C9G	O32-C16-C2	2.12	112.48	107.72
4	C	1105	AJP	C20-C21-C22	2.11	117.64	114.17
3	A	1111	LBN	C2-O7-C34	2.11	122.86	117.80
6	C	1118	A1C9G	O32-C16-C2	2.10	112.44	107.72
6	A	1125	A1C9G	O32-C16-C2	2.10	112.43	107.72
4	C	1110	AJP	C26-O31-C30	2.06	117.74	113.72
3	B	1105	LBN	C2-O7-C34	2.01	122.61	117.80

All (28) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1107	LBN	C2
3	A	1108	LBN	C2
3	A	1109	LBN	C2
3	A	1110	LBN	C2
3	A	1111	LBN	C2
3	A	1114	LBN	C2
3	A	1115	LBN	C2
3	A	1116	LBN	C2
3	B	1102	LBN	C2
3	B	1103	LBN	C2
3	B	1104	LBN	C2
3	B	1105	LBN	C2
3	B	1108	LBN	C2
3	B	1109	LBN	C2
3	B	1110	LBN	C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	C	1102	LBN	C2
3	C	1103	LBN	C2
3	C	1104	LBN	C2
3	C	1107	LBN	C2
3	C	1108	LBN	C2
3	C	1109	LBN	C2
3	D	1102	LBN	C2
3	D	1103	LBN	C2
3	D	1104	LBN	C2
3	D	1105	LBN	C2
3	D	1108	LBN	C2
3	D	1109	LBN	C2
3	D	1110	LBN	C2

All (244) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1107	LBN	C1-O1-P1-O2
3	A	1107	LBN	C1-O1-P1-O3
3	A	1107	LBN	C1-O1-P1-O4
3	A	1110	LBN	C1-O1-P1-O2
3	A	1110	LBN	C1-O1-P1-O3
3	A	1110	LBN	C1-O1-P1-O4
3	A	1114	LBN	C1-O1-P1-O2
3	A	1114	LBN	C1-O1-P1-O3
3	A	1115	LBN	C1-O1-P1-O2
3	A	1115	LBN	C1-O1-P1-O3
3	A	1116	LBN	C1-O1-P1-O2
3	A	1116	LBN	C1-O1-P1-O3
3	A	1116	LBN	C1-O1-P1-O4
3	B	1103	LBN	C1-O1-P1-O2
3	B	1103	LBN	C1-O1-P1-O3
3	B	1104	LBN	C1-O1-P1-O2
3	B	1104	LBN	C1-O1-P1-O3
3	B	1108	LBN	C1-O1-P1-O2
3	B	1108	LBN	C1-O1-P1-O3
3	B	1108	LBN	C1-O1-P1-O4
3	B	1109	LBN	C1-O1-P1-O2
3	B	1109	LBN	C1-O1-P1-O3
3	B	1110	LBN	C1-O1-P1-O2
3	B	1110	LBN	C1-O1-P1-O3
3	C	1103	LBN	C1-O1-P1-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1103	LBN	C1-O1-P1-O3
3	C	1103	LBN	C1-O1-P1-O4
3	C	1104	LBN	C1-O1-P1-O2
3	C	1107	LBN	C1-O1-P1-O2
3	C	1107	LBN	C1-O1-P1-O3
3	C	1107	LBN	C1-O1-P1-O4
3	C	1108	LBN	C1-O1-P1-O2
3	C	1108	LBN	C1-O1-P1-O3
3	C	1109	LBN	C1-O1-P1-O2
3	C	1109	LBN	C1-O1-P1-O3
3	D	1102	LBN	C1-O1-P1-O2
3	D	1102	LBN	C1-O1-P1-O3
3	D	1102	LBN	C1-O1-P1-O4
3	D	1104	LBN	C1-O1-P1-O2
3	D	1104	LBN	C1-O1-P1-O3
3	D	1108	LBN	C1-O1-P1-O2
3	D	1108	LBN	C1-O1-P1-O3
3	D	1108	LBN	C1-O1-P1-O4
3	D	1109	LBN	C1-O1-P1-O2
3	D	1109	LBN	C1-O1-P1-O3
3	D	1110	LBN	C1-O1-P1-O2
3	D	1110	LBN	C1-O1-P1-O3
4	B	1112	AJP	O31-C26-O25-C23
4	B	1117	AJP	C24-C23-O25-C26
4	C	1111	AJP	C22-C23-O25-C26
4	C	1112	AJP	C22-C23-O25-C26
4	C	1116	AJP	C24-C23-O25-C26
4	C	1117	AJP	C27-C26-O25-C23
4	B	1106	AJP	O40-C35-O34-C29
4	B	1106	AJP	C36-C35-O34-C29
4	A	1112	AJP	O31-C26-O25-C23
4	A	1112	AJP	O40-C35-O34-C29
4	A	1118	AJP	O31-C26-O25-C23
4	A	1121	AJP	O60-C55-O54-C36
4	A	1122	AJP	O31-C26-O25-C23
4	B	1115	AJP	O60-C55-O54-C36
4	C	1114	AJP	O60-C55-O54-C36
4	D	1115	AJP	O60-C55-O54-C36
4	D	1118	AJP	O31-C26-O25-C23
4	C	1115	AJP	O31-C26-O25-C23
4	C	1105	AJP	O31-C26-O25-C23
4	A	1112	AJP	C27-C26-O25-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1121	AJP	C56-C55-O54-C36
4	B	1115	AJP	C56-C55-O54-C36
4	D	1115	AJP	C56-C55-O54-C36
4	C	1114	AJP	C56-C55-O54-C36
4	C	1105	AJP	C27-C26-O25-C23
4	B	1116	AJP	O31-C26-O25-C23
4	B	1116	AJP	C27-C26-O25-C23
3	C	1104	LBN	C35-C34-O7-C2
3	D	1105	LBN	C35-C34-O7-C2
4	A	1124	AJP	O31-C26-O25-C23
4	A	1124	AJP	C27-C26-O25-C23
3	D	1105	LBN	O8-C34-O7-C2
3	A	1108	LBN	O1-C1-C2-C3
4	B	1113	AJP	O31-C30-C32-O33
4	C	1114	AJP	C58-C59-C61-O62
3	A	1107	LBN	O1-C1-C2-O7
3	B	1103	LBN	O1-C1-C2-O7
3	D	1102	LBN	O1-C1-C2-O7
3	A	1111	LBN	C35-C34-O7-C2
4	D	1116	AJP	O31-C26-O25-C23
3	C	1104	LBN	O8-C34-O7-C2
3	A	1110	LBN	C25-C26-C27-C28
3	A	1108	LBN	O1-C1-C2-O7
3	A	1109	LBN	O1-C1-C2-O7
3	A	1115	LBN	O1-C1-C2-O7
3	B	1102	LBN	O1-C1-C2-O7
3	B	1110	LBN	O1-C1-C2-O7
3	C	1102	LBN	O1-C1-C2-O7
3	C	1109	LBN	O1-C1-C2-O7
3	D	1103	LBN	O1-C1-C2-O7
3	D	1110	LBN	O1-C1-C2-O7
3	A	1111	LBN	O8-C34-O7-C2
3	B	1105	LBN	C35-C34-O7-C2
3	B	1105	LBN	O8-C34-O7-C2
3	A	1107	LBN	O1-C1-C2-C3
3	A	1109	LBN	O1-C1-C2-C3
3	A	1115	LBN	O1-C1-C2-C3
3	B	1102	LBN	O1-C1-C2-C3
3	B	1103	LBN	O1-C1-C2-C3
3	B	1110	LBN	O1-C1-C2-C3
3	C	1102	LBN	O1-C1-C2-C3
3	C	1109	LBN	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	1102	LBN	O1-C1-C2-C3
3	D	1103	LBN	O1-C1-C2-C3
3	D	1110	LBN	O1-C1-C2-C3
5	C	1106	CLR	C20-C22-C23-C24
5	D	1107	CLR	C20-C22-C23-C24
5	A	1113	CLR	C20-C22-C23-C24
5	B	1107	CLR	C20-C22-C23-C24
4	C	1114	AJP	O60-C59-C61-O62
4	C	1105	AJP	O31-C30-C32-O33
4	D	1118	AJP	O31-C30-C32-O33
3	A	1111	LBN	C36-C37-C38-C39
4	A	1112	AJP	O31-C30-C32-O33
3	B	1105	LBN	C35-C36-C37-C38
4	C	1105	AJP	C30-C29-O34-C35
3	B	1105	LBN	C34-C35-C36-C37
4	D	1117	AJP	O31-C30-C32-O33
3	C	1104	LBN	C35-C36-C37-C38
4	C	1117	AJP	O31-C30-C32-O33
4	B	1106	AJP	O31-C30-C32-O33
3	B	1105	LBN	C36-C37-C38-C39
3	D	1104	LBN	C35-C34-O7-C2
4	C	1105	AJP	C28-C29-O34-C35
5	D	1107	CLR	C22-C23-C24-C25
4	C	1114	AJP	O31-C30-C32-O33
5	B	1107	CLR	C22-C23-C24-C25
4	D	1106	AJP	O31-C26-O25-C23
4	A	1121	AJP	O31-C30-C32-O33
4	B	1115	AJP	O31-C30-C32-O33
4	D	1115	AJP	O31-C30-C32-O33
3	B	1104	LBN	C35-C34-O7-C2
5	A	1113	CLR	C22-C23-C24-C25
3	D	1105	LBN	C36-C37-C38-C39
5	C	1106	CLR	C22-C23-C24-C25
4	C	1114	AJP	O40-C39-C41-O42
3	C	1104	LBN	C38-C39-C40-C41
4	D	1106	AJP	O40-C39-C41-O42
4	C	1105	AJP	O40-C39-C41-O42
3	A	1114	LBN	O1-C1-C2-C3
3	B	1109	LBN	O1-C1-C2-C3
3	C	1108	LBN	O1-C1-C2-C3
3	D	1109	LBN	O1-C1-C2-C3
3	C	1103	LBN	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	1106	AJP	C27-C26-O25-C23
4	D	1106	AJP	O31-C30-C32-O33
4	C	1115	AJP	O31-C30-C32-O33
3	A	1114	LBN	C1-O1-P1-O4
3	B	1103	LBN	C1-O1-P1-O4
3	B	1104	LBN	C1-O1-P1-O4
3	B	1109	LBN	C1-O1-P1-O4
3	C	1108	LBN	C1-O1-P1-O4
3	D	1104	LBN	C1-O1-P1-O4
3	D	1109	LBN	C1-O1-P1-O4
3	A	1108	LBN	C27-C28-C29-C30
3	A	1107	LBN	C27-C28-C29-C30
3	B	1103	LBN	C27-C28-C29-C30
3	D	1102	LBN	C27-C28-C29-C30
4	D	1118	AJP	C27-C26-O25-C23
3	A	1116	LBN	O1-C1-C2-O7
3	B	1108	LBN	O1-C1-C2-O7
3	C	1107	LBN	O1-C1-C2-O7
3	D	1108	LBN	O1-C1-C2-O7
3	D	1105	LBN	C35-C36-C37-C38
3	D	1104	LBN	O8-C34-O7-C2
4	D	1106	AJP	O40-C35-O34-C29
3	D	1105	LBN	C38-C39-C40-C41
3	B	1104	LBN	O8-C34-O7-C2
3	D	1109	LBN	O1-C1-C2-O7
3	C	1104	LBN	C36-C37-C38-C39
3	C	1103	LBN	O7-C2-C3-O5
3	A	1109	LBN	C1-O1-P1-O3
3	B	1102	LBN	C1-O1-P1-O3
3	C	1102	LBN	C1-O1-P1-O3
3	D	1103	LBN	C1-O1-P1-O3
3	D	1105	LBN	C1-O1-P1-O2
4	D	1106	AJP	C36-C35-O34-C29
3	B	1109	LBN	O1-C1-C2-O7
3	A	1110	LBN	O7-C2-C3-O5
3	B	1109	LBN	C25-C26-C27-C28
3	A	1114	LBN	O1-C1-C2-O7
3	C	1108	LBN	O1-C1-C2-O7
3	A	1111	LBN	C40-C41-C42-C5
3	D	1109	LBN	C25-C26-C27-C28
4	D	1117	AJP	O31-C26-O25-C23
4	B	1106	AJP	O31-C26-O25-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1111	LBN	C37-C38-C39-C40
3	C	1108	LBN	C25-C26-C27-C28
3	A	1115	LBN	C1-O1-P1-O4
3	B	1110	LBN	C1-O1-P1-O4
3	C	1109	LBN	C1-O1-P1-O4
3	D	1110	LBN	C1-O1-P1-O4
4	D	1113	AJP	O31-C26-O25-C23
3	A	1111	LBN	C3-C2-O7-C34
3	B	1105	LBN	C3-C2-O7-C34
3	D	1105	LBN	C3-C2-O7-C34
4	D	1117	AJP	C27-C26-O25-C23
3	A	1116	LBN	O1-C1-C2-C3
3	B	1108	LBN	O1-C1-C2-C3
3	C	1107	LBN	O1-C1-C2-C3
3	D	1108	LBN	O1-C1-C2-C3
3	B	1105	LBN	O7-C2-C3-O5
4	A	1121	AJP	C58-C59-C61-O62
4	D	1113	AJP	C27-C26-O25-C23
4	B	1106	AJP	C27-C26-O25-C23
4	B	1115	AJP	C58-C59-C61-O62
3	A	1114	LBN	C25-C26-C27-C28
3	C	1104	LBN	C3-C2-O7-C34
3	A	1111	LBN	O7-C2-C3-O5
3	C	1103	LBN	O8-C34-O7-C2
3	A	1110	LBN	C1-C2-C3-O5
3	B	1104	LBN	C36-C37-C38-C39
5	D	1107	CLR	C23-C24-C25-C26
3	A	1108	LBN	C1-O1-P1-O3
3	A	1108	LBN	C1-O1-P1-O4
3	C	1104	LBN	C1-O1-P1-O3
3	C	1104	LBN	C1-O1-P1-O4
3	D	1104	LBN	C36-C37-C38-C39
3	C	1108	LBN	C36-C37-C38-C39
3	D	1105	LBN	C26-C27-C28-C29
3	C	1103	LBN	C1-C2-C3-O5
3	D	1104	LBN	C25-C26-C27-C28
3	C	1104	LBN	C26-C27-C28-C29
3	C	1103	LBN	C36-C37-C38-C39
4	D	1112	AJP	C29-C30-C32-O33
3	C	1103	LBN	C35-C34-O7-C2
3	A	1111	LBN	C26-C27-C28-C29
3	B	1104	LBN	O7-C2-C3-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1105	LBN	C40-C41-C42-C5
3	A	1110	LBN	C36-C37-C38-C39
3	B	1105	LBN	C26-C27-C28-C29
3	B	1104	LBN	C25-C26-C27-C28
5	D	1107	CLR	C23-C24-C25-C27
4	B	1117	AJP	O31-C26-O25-C23
4	D	1115	AJP	C58-C59-C61-O62
4	B	1113	AJP	C29-C30-C32-O33
4	D	1112	AJP	O31-C30-C32-O33

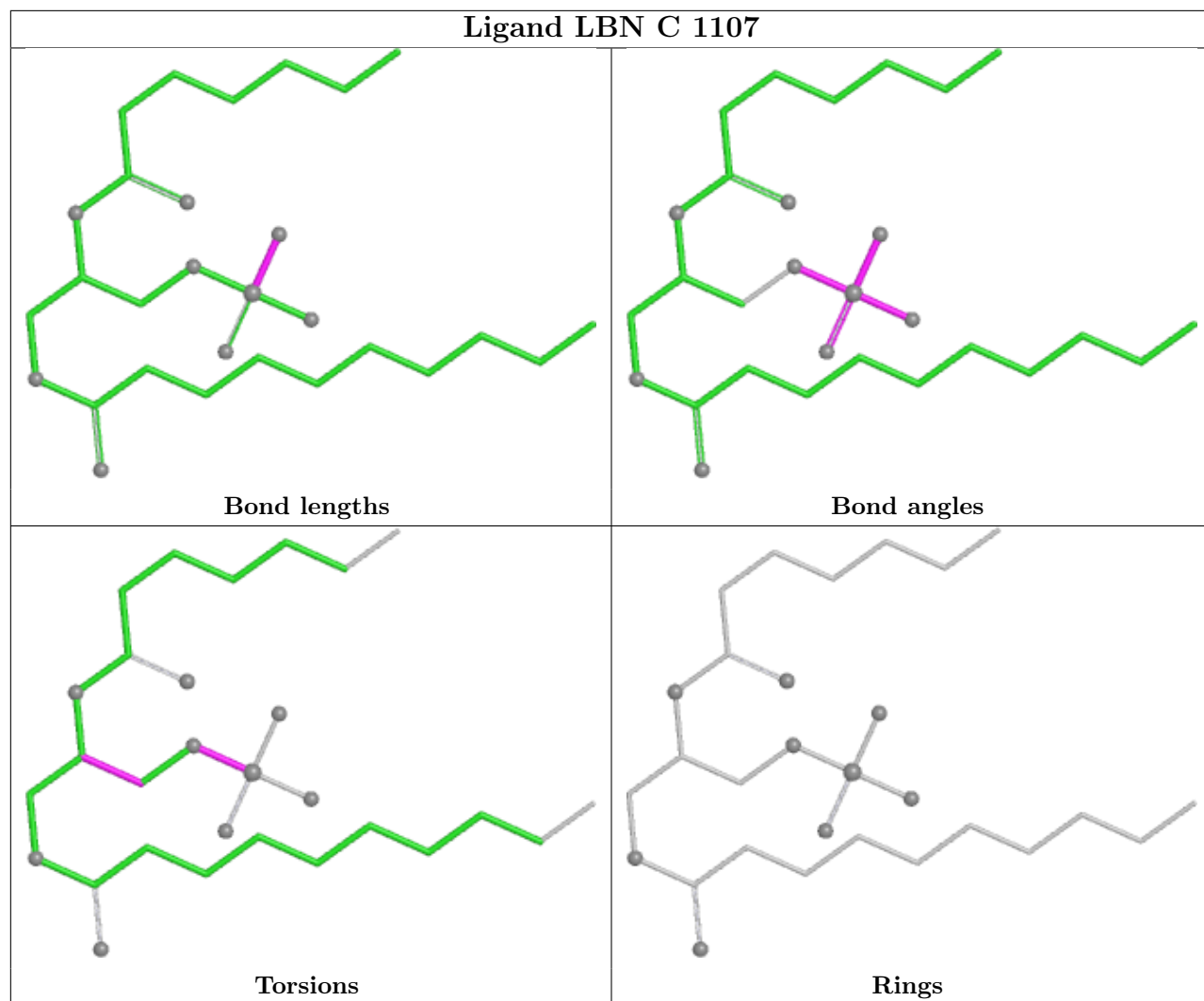
All (4) ring outliers are listed below:

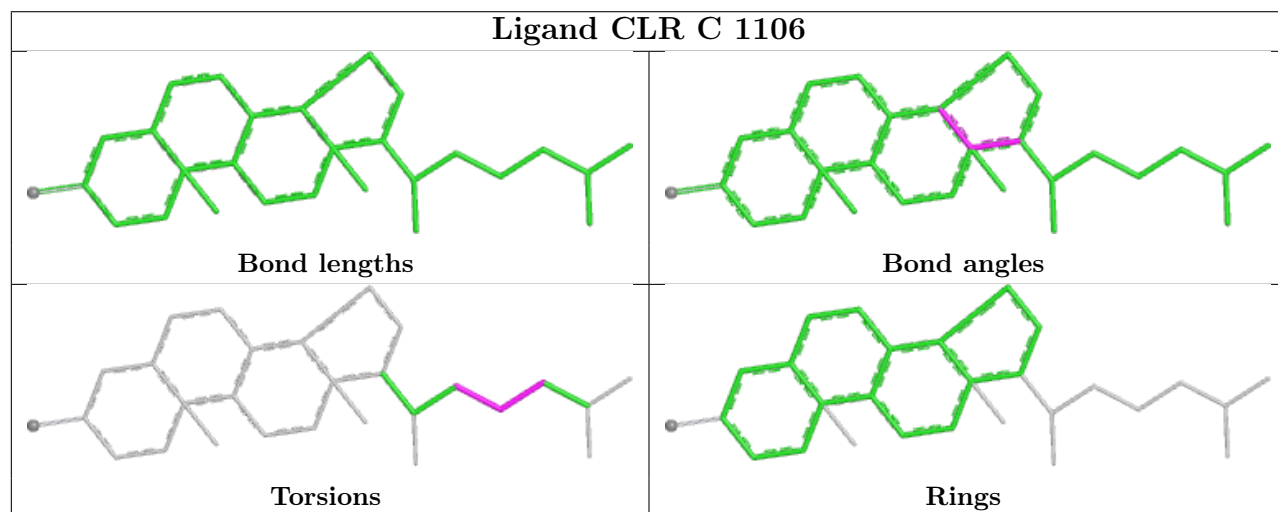
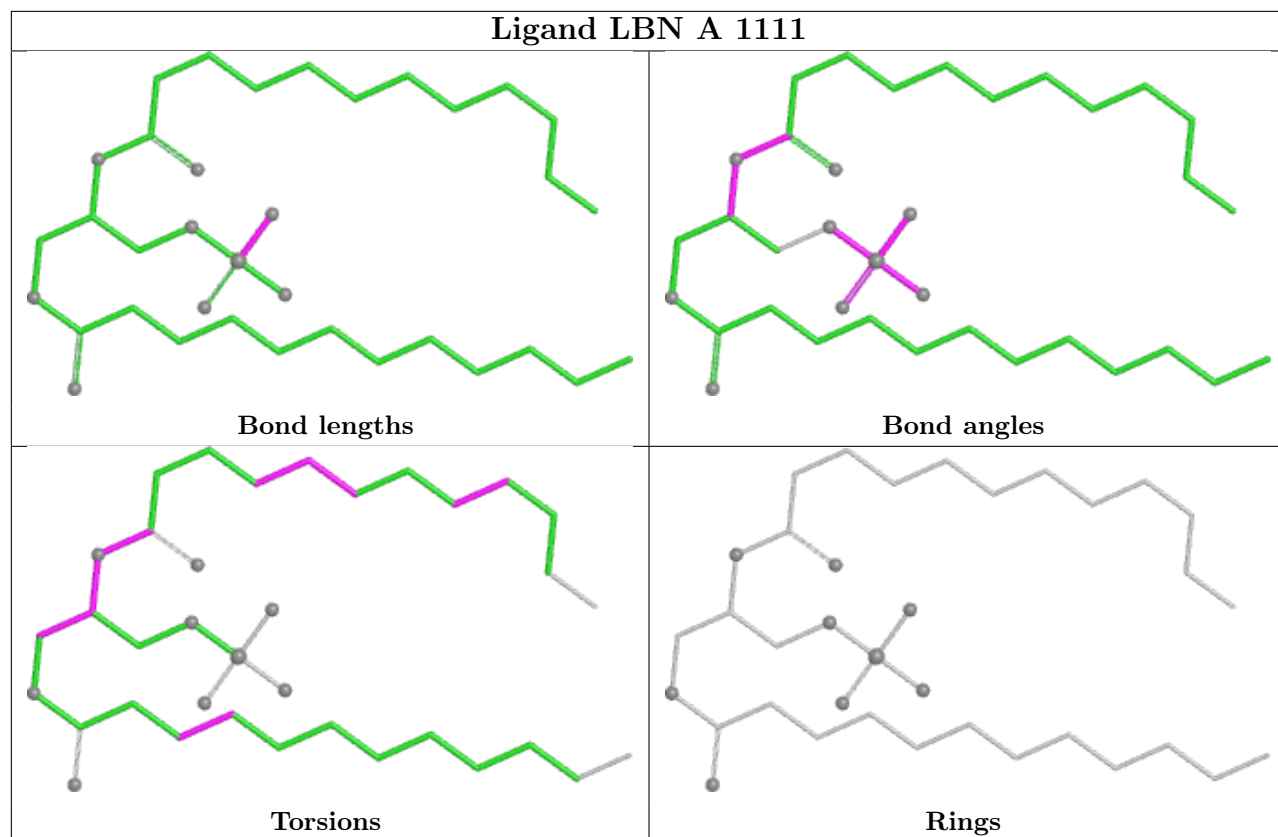
Mol	Chain	Res	Type	Atoms
4	C	1105	AJP	C19-C20-C21-C22-C23-C24
4	A	1112	AJP	C19-C20-C21-C22-C23-C24
4	D	1117	AJP	C19-C20-C21-C22-C23-C24
4	B	1112	AJP	C19-C20-C21-C22-C23-C24

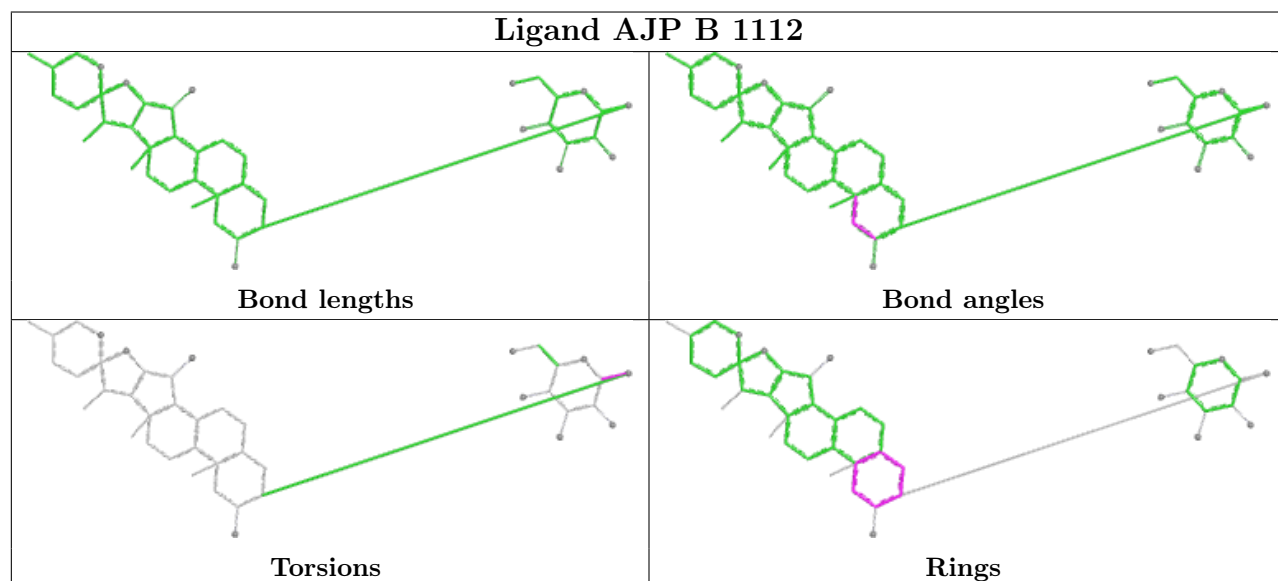
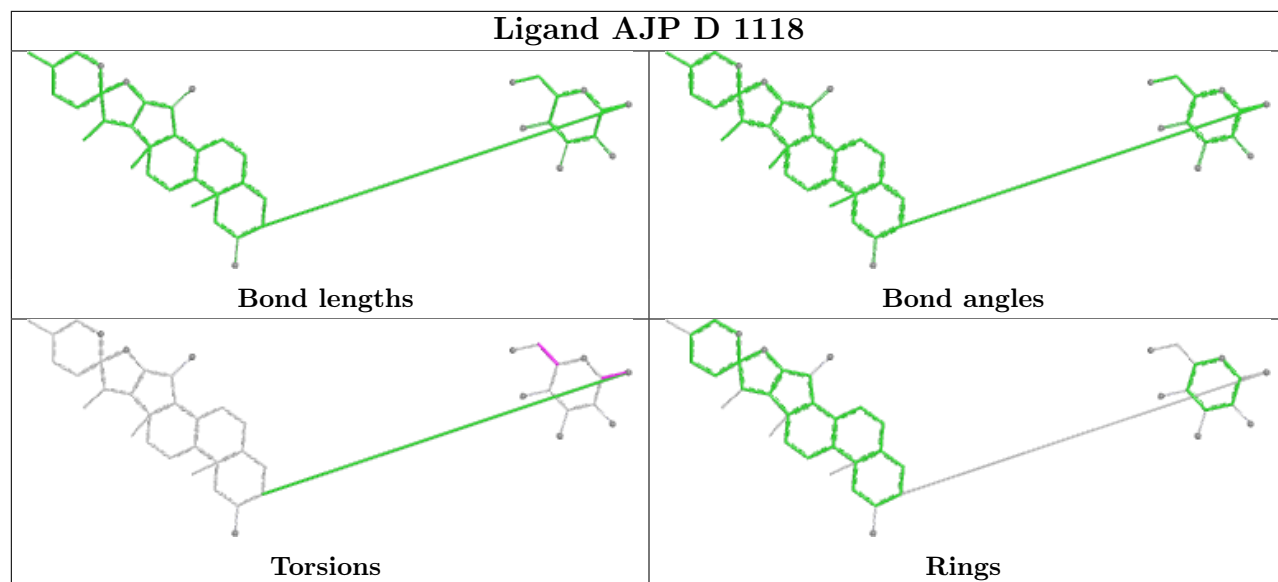
6 monomers are involved in 8 short contacts:

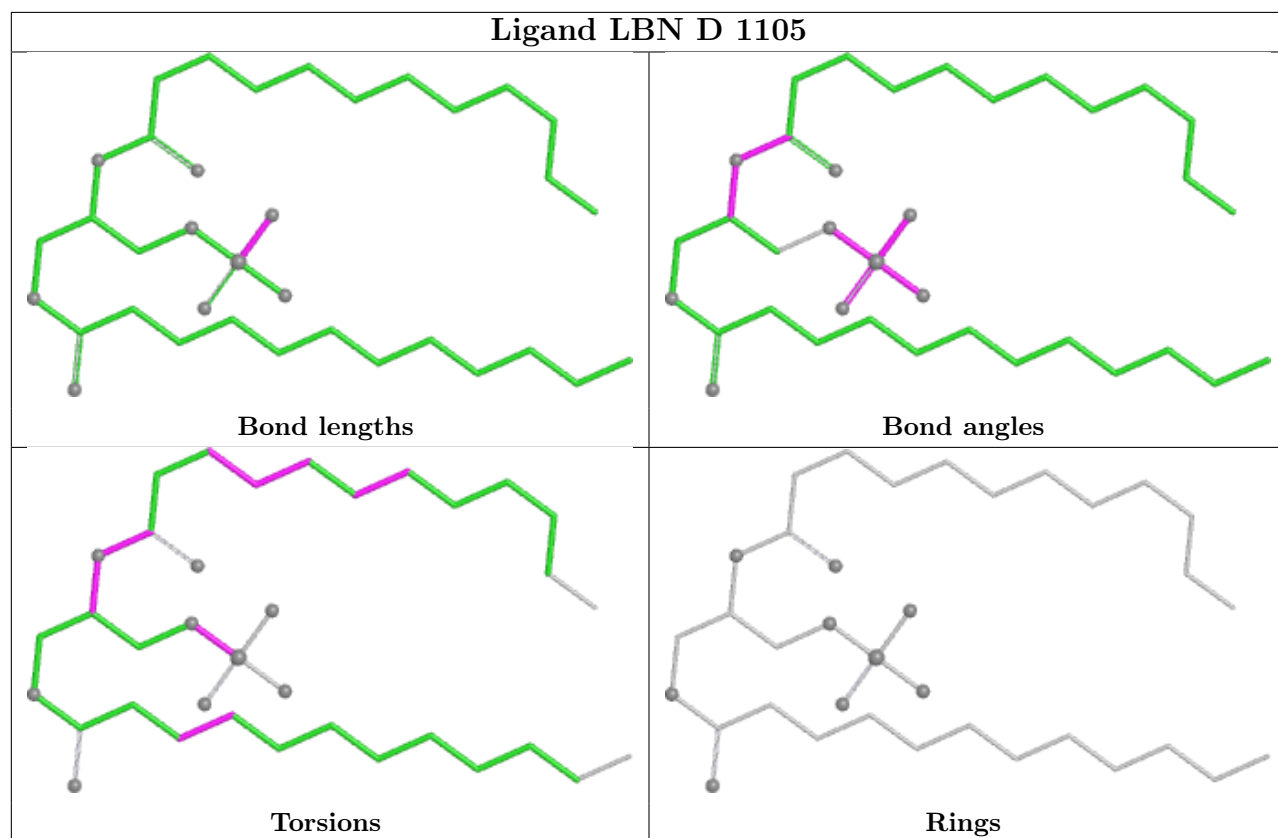
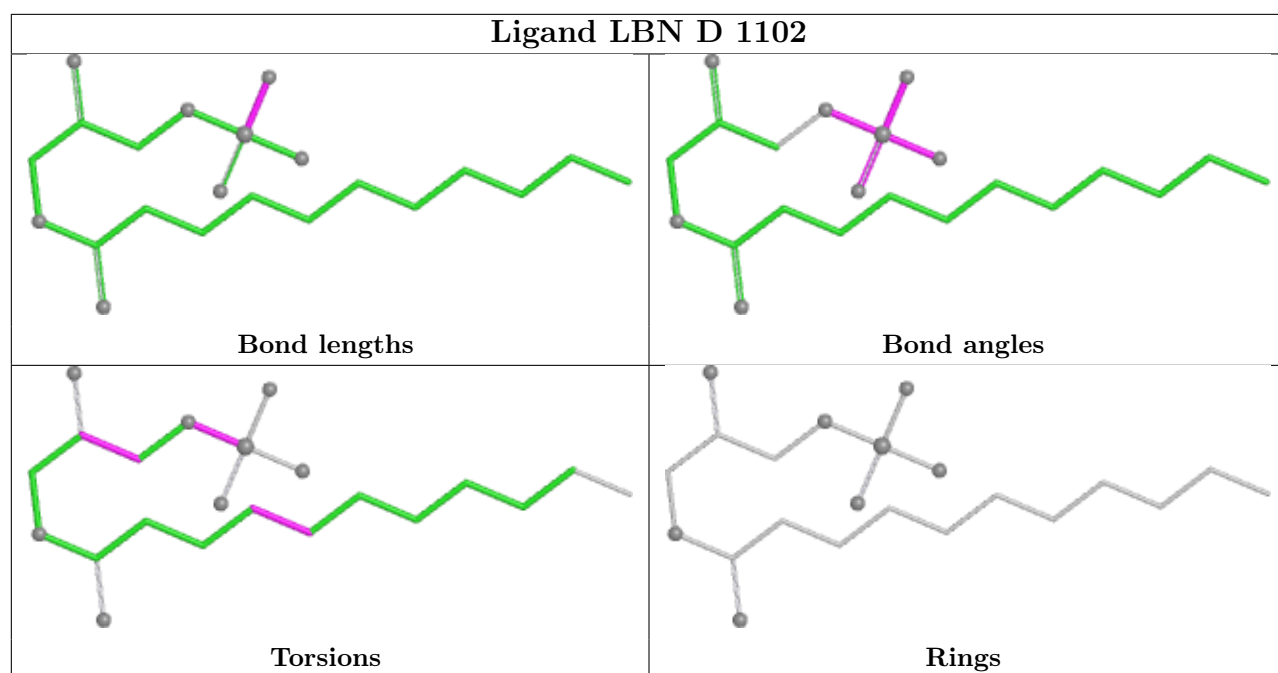
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1106	CLR	2	0
5	B	1107	CLR	1	0
5	D	1107	CLR	2	0
4	B	1117	AJP	1	0
4	C	1116	AJP	1	0
5	A	1113	CLR	1	0

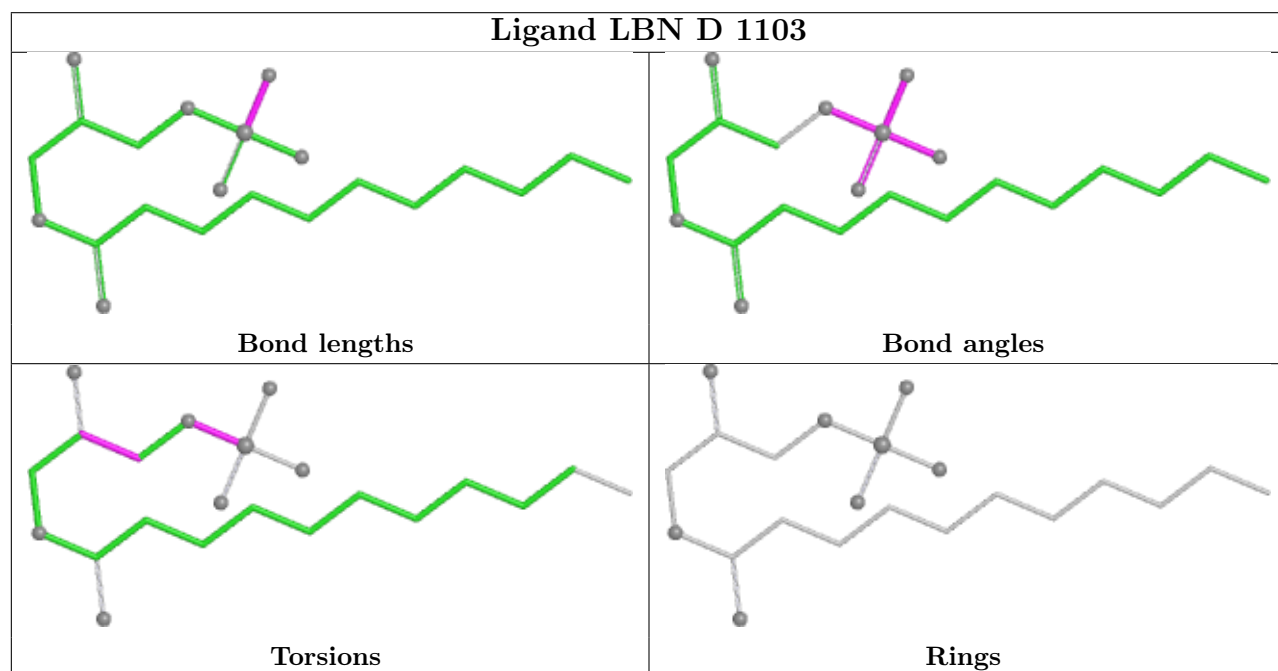
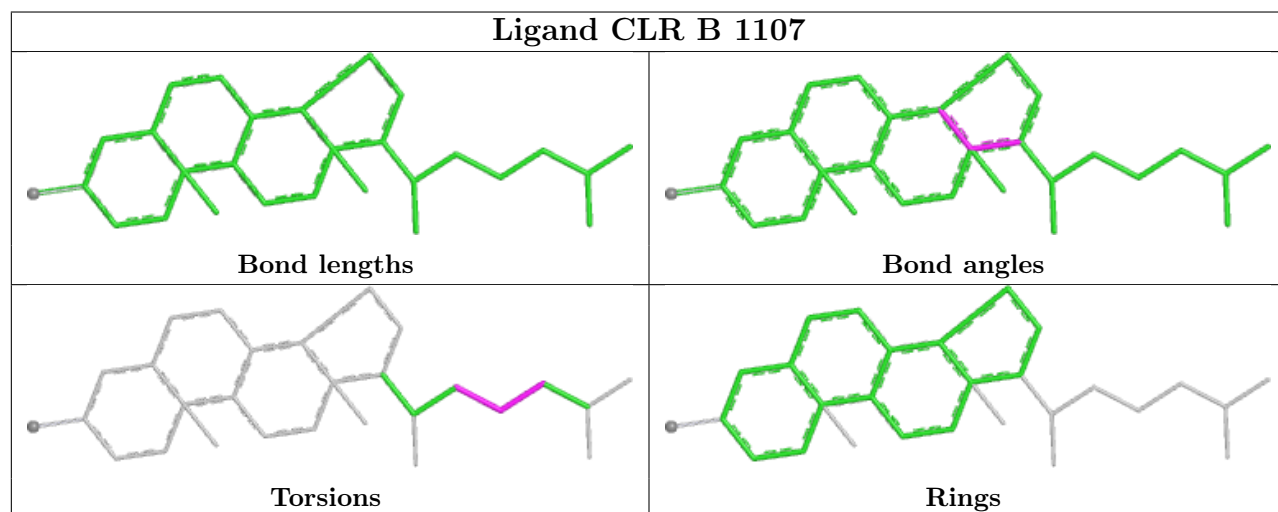
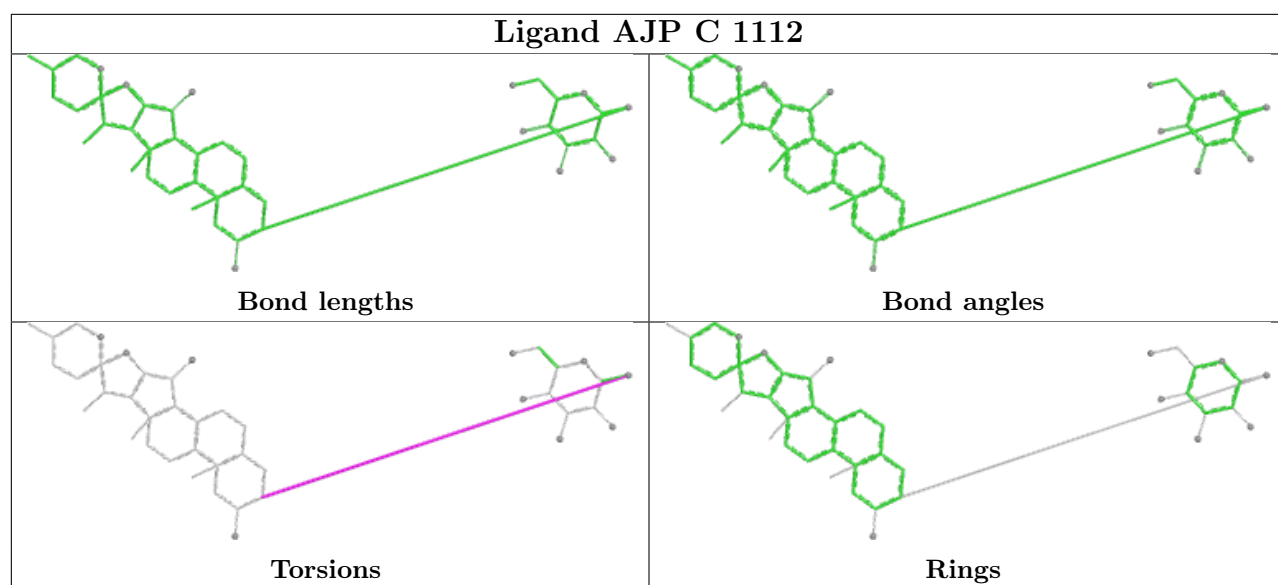
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

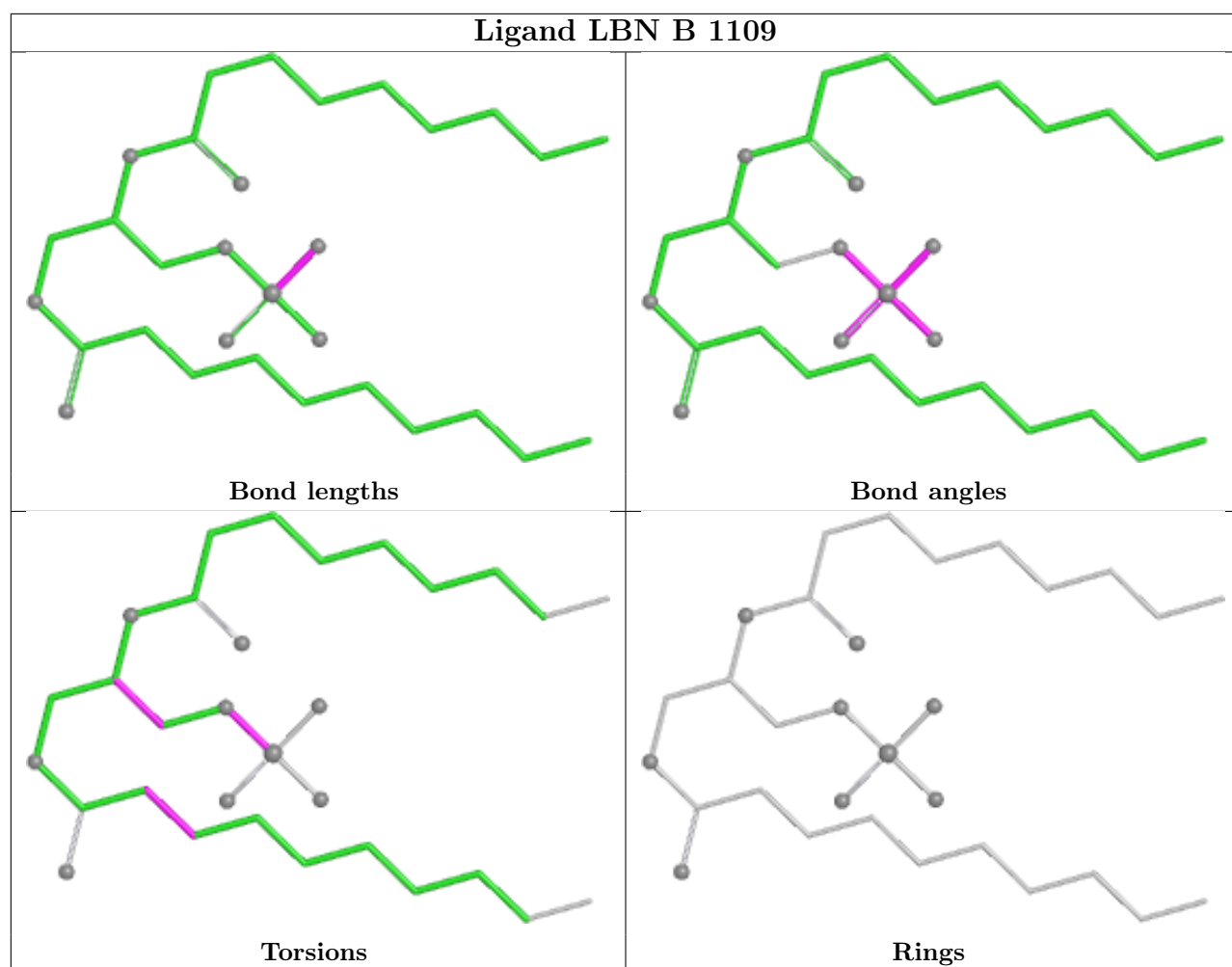


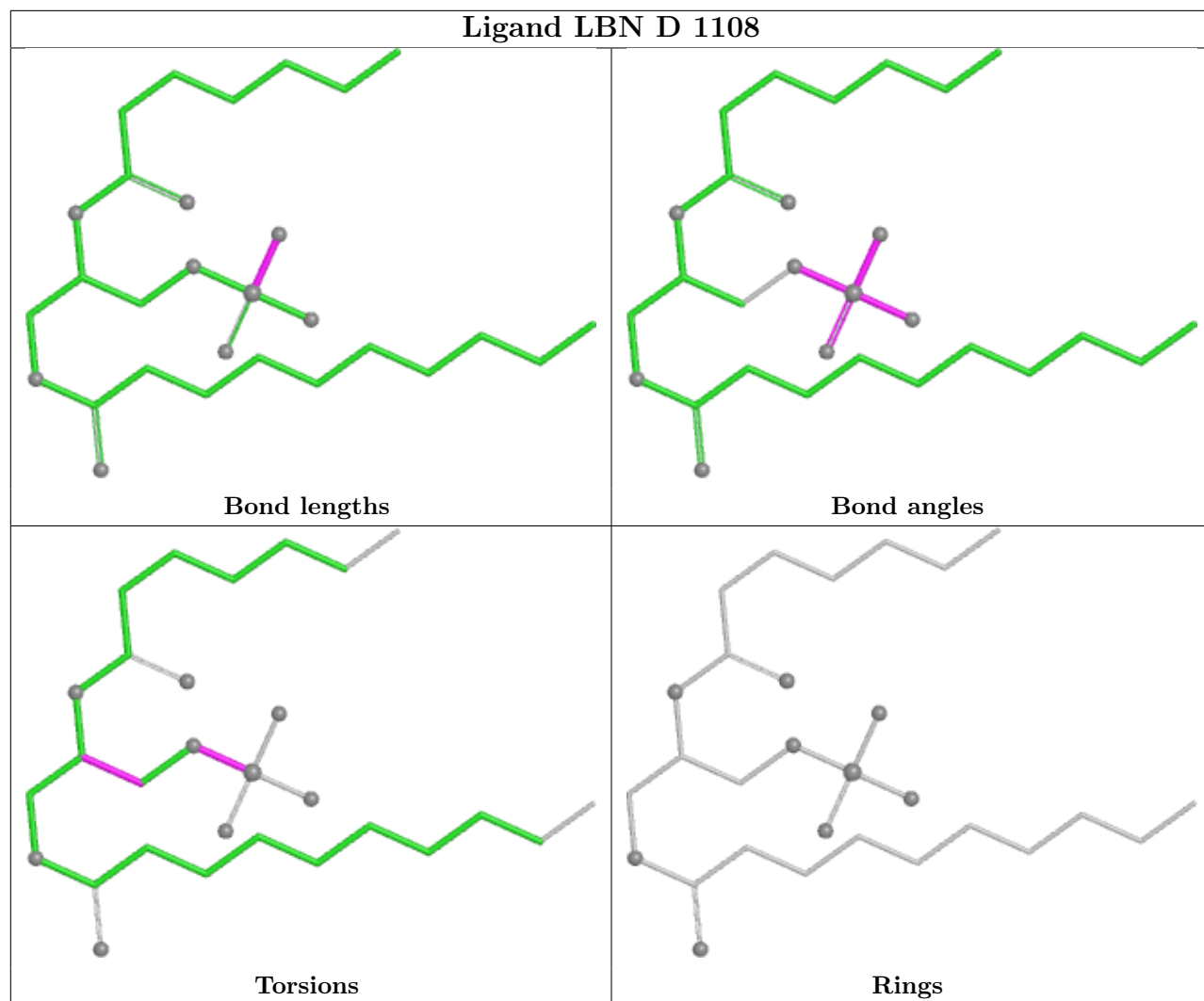


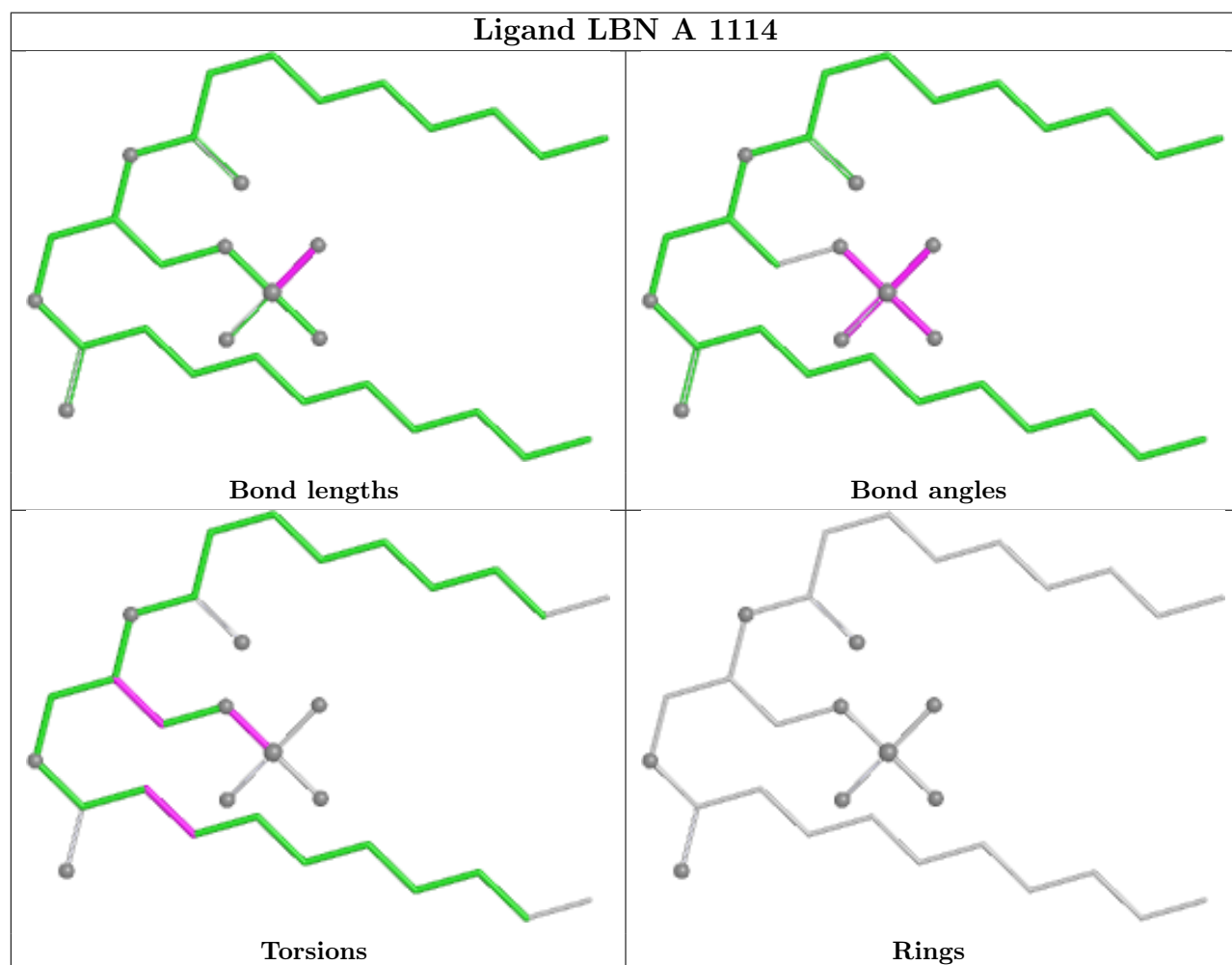
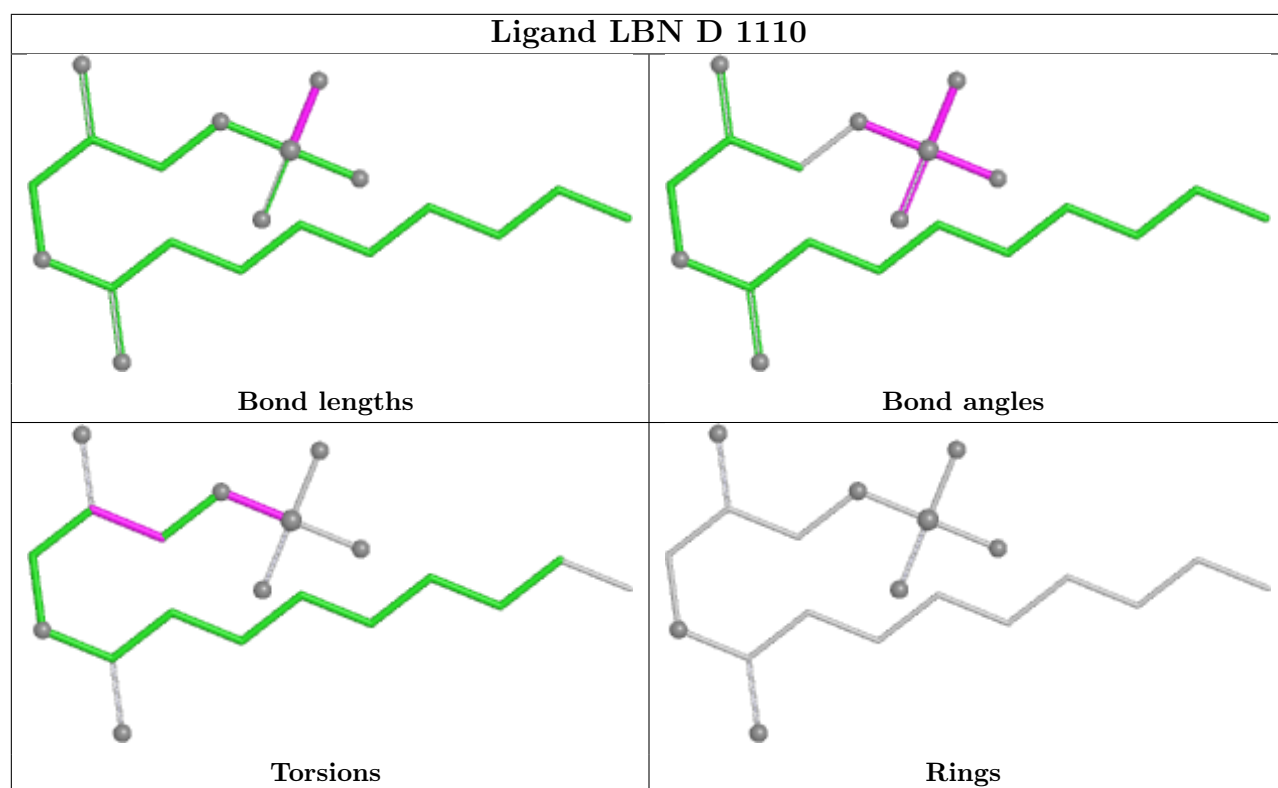


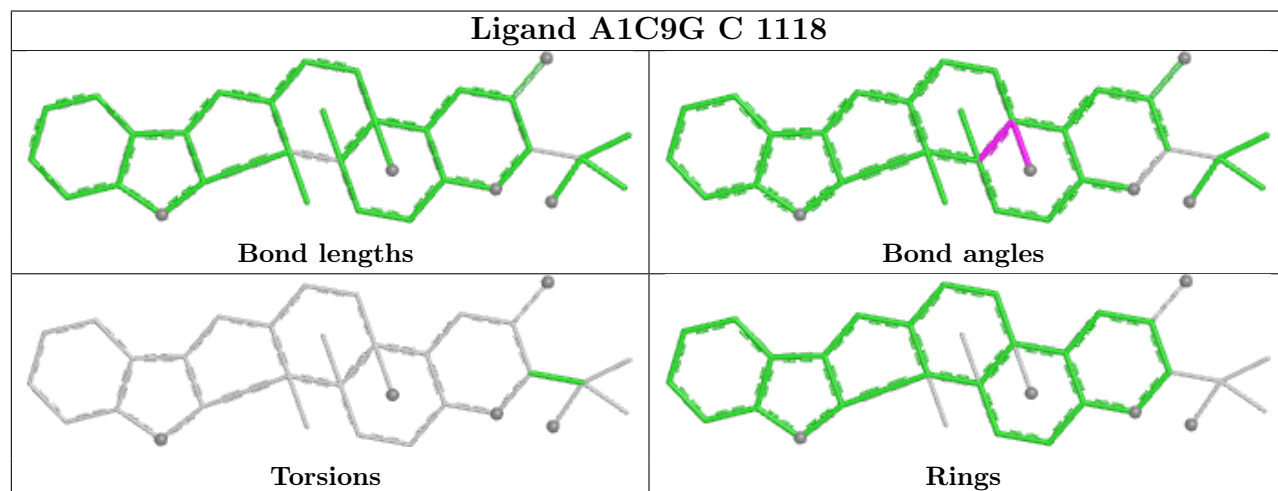
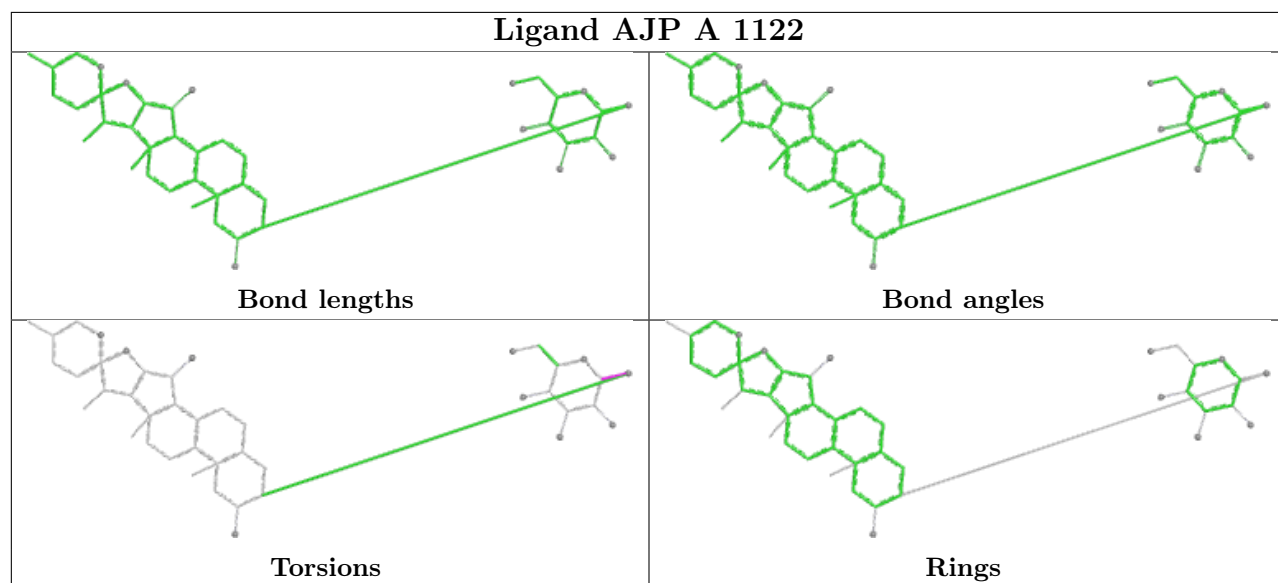
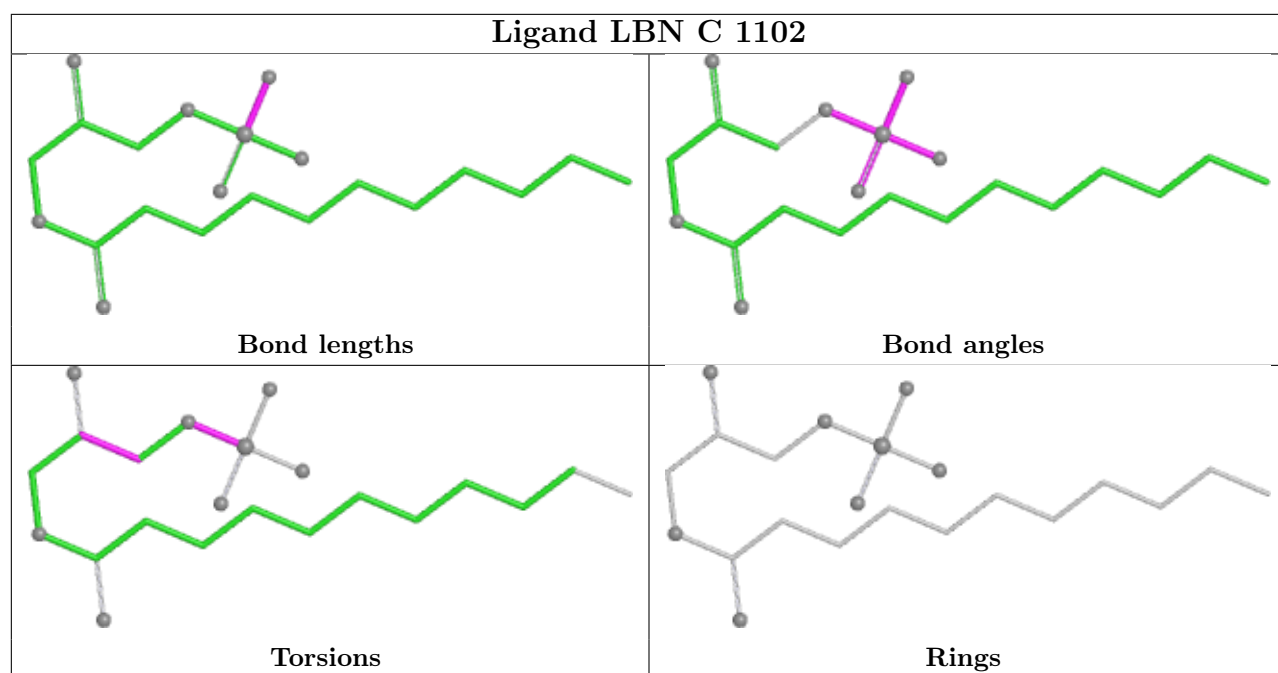


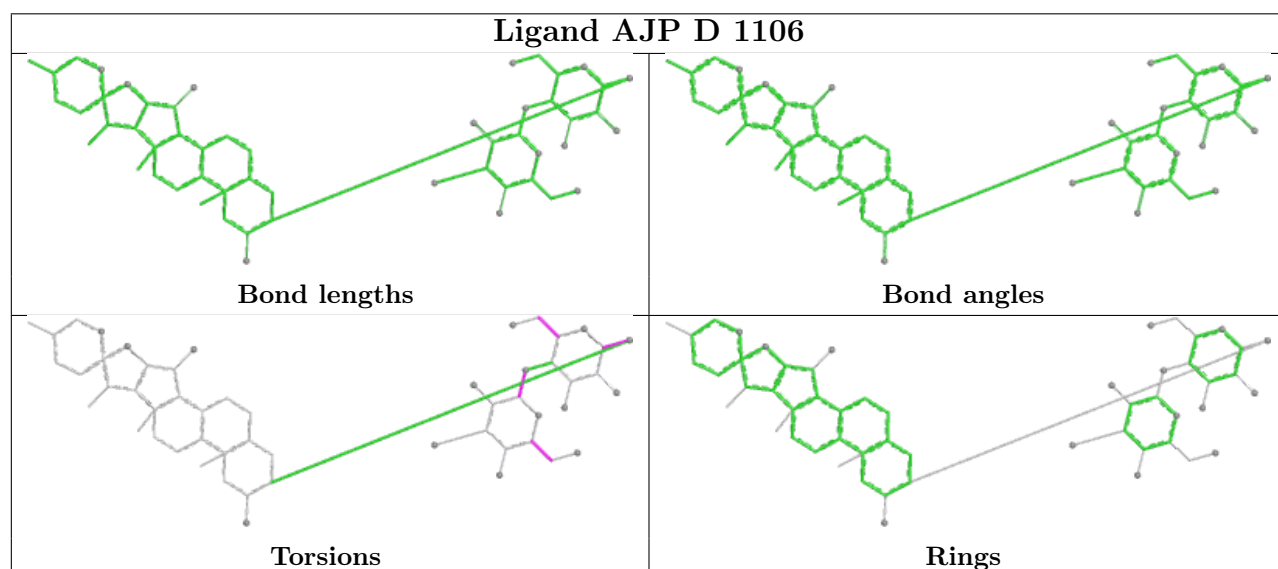
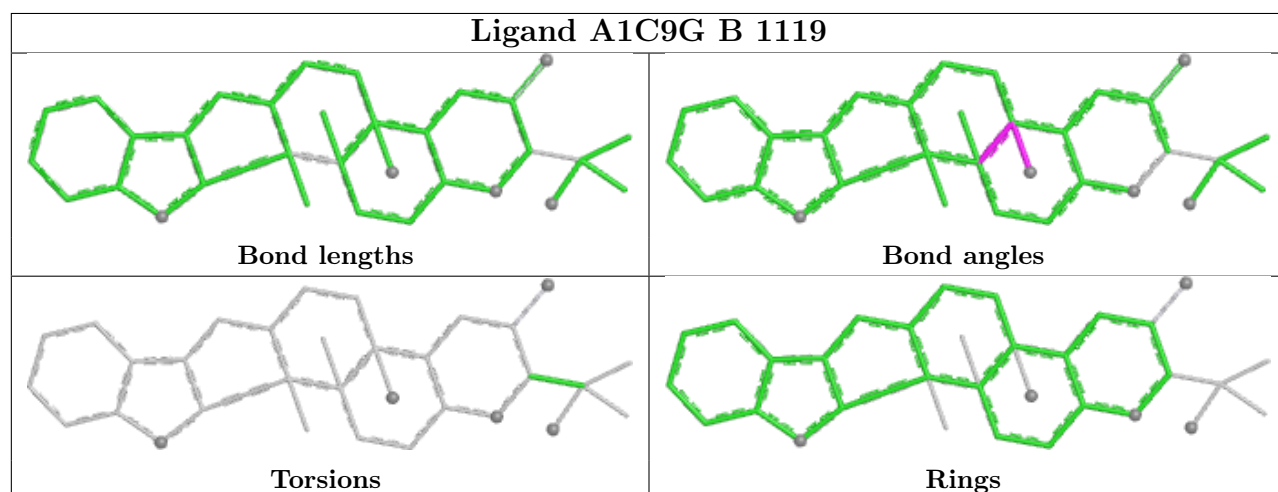
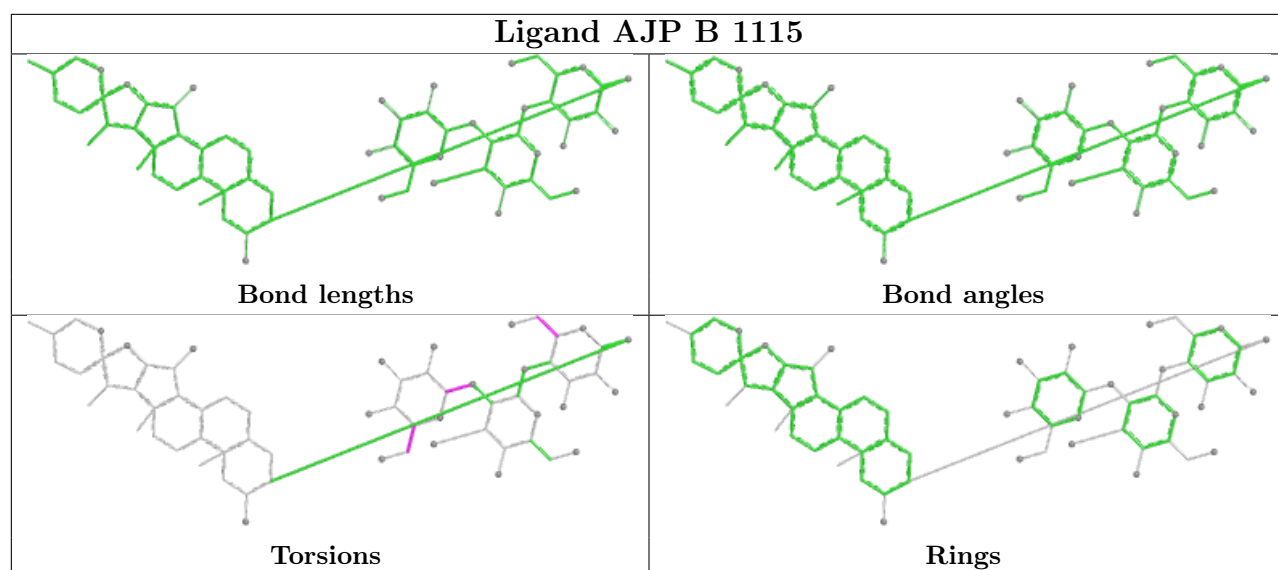


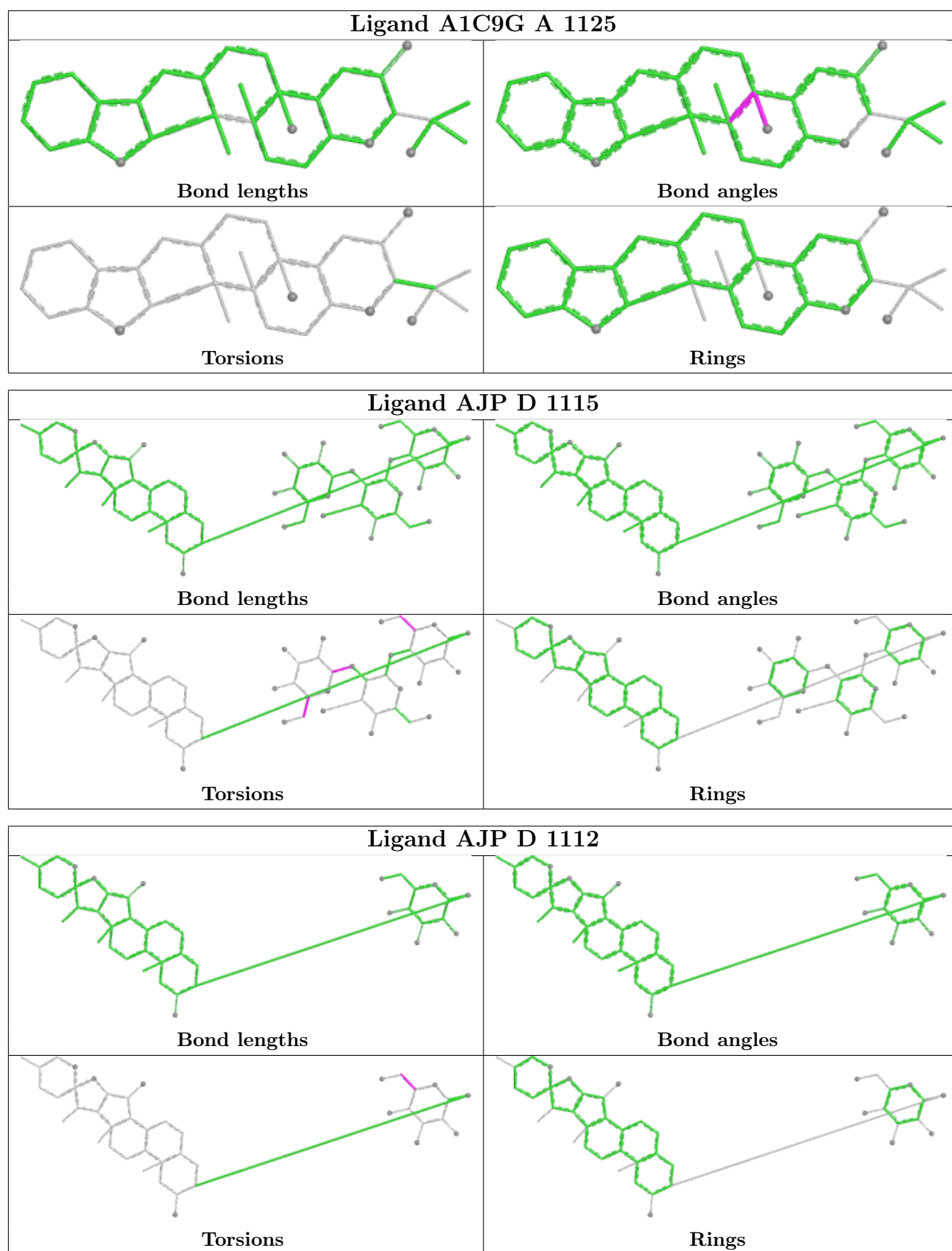


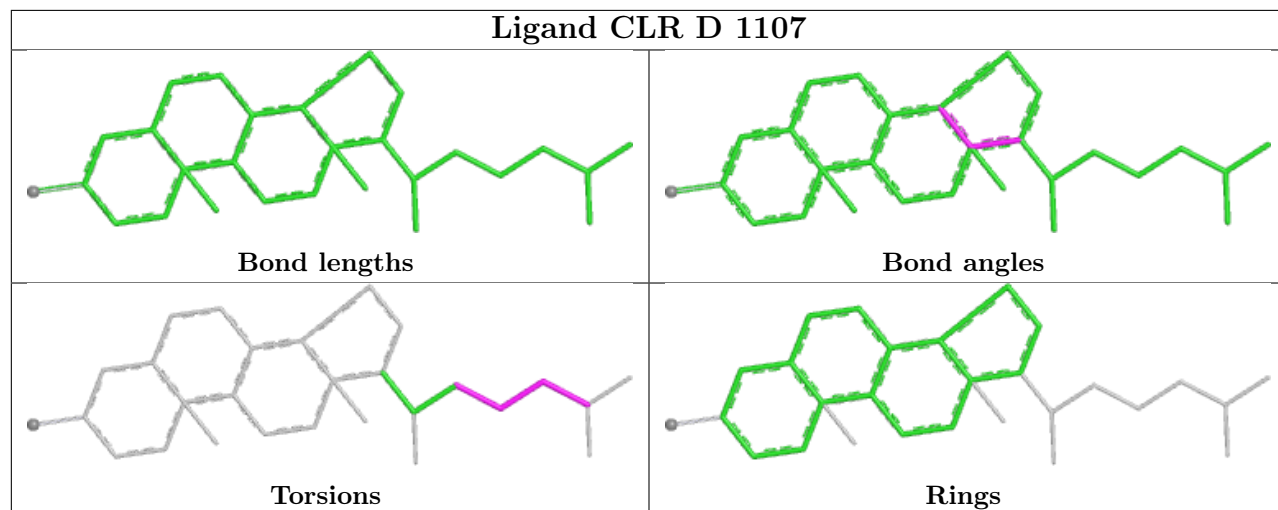
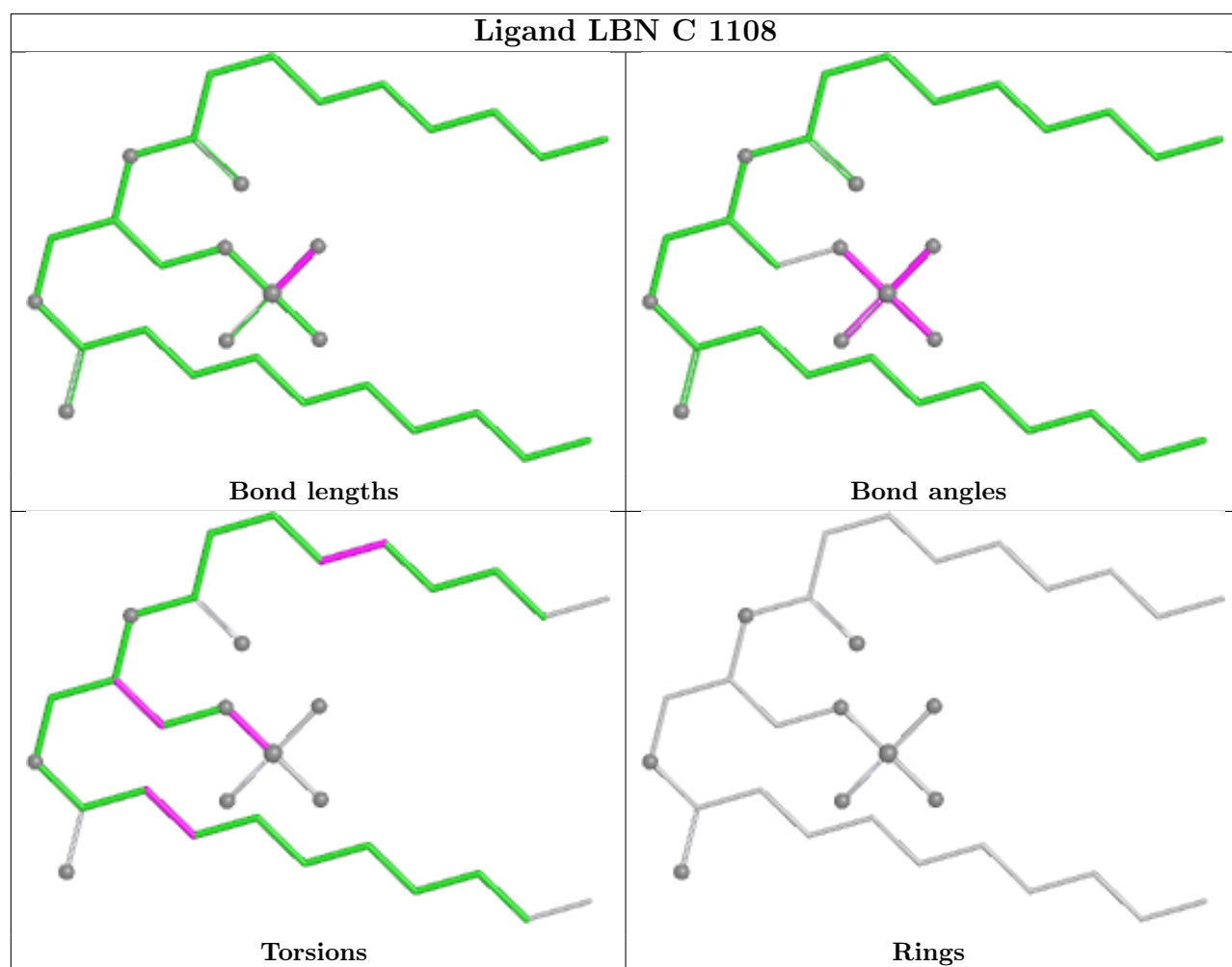


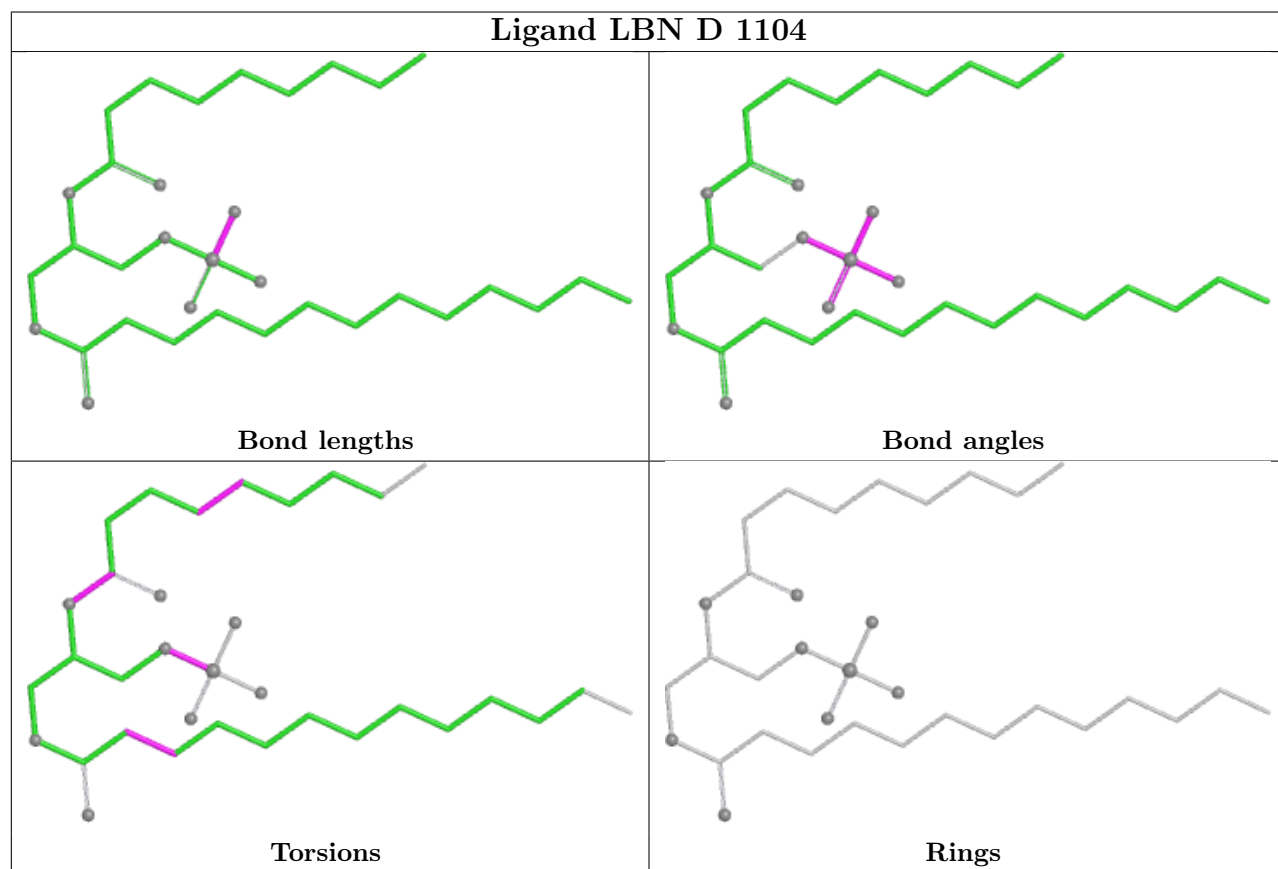
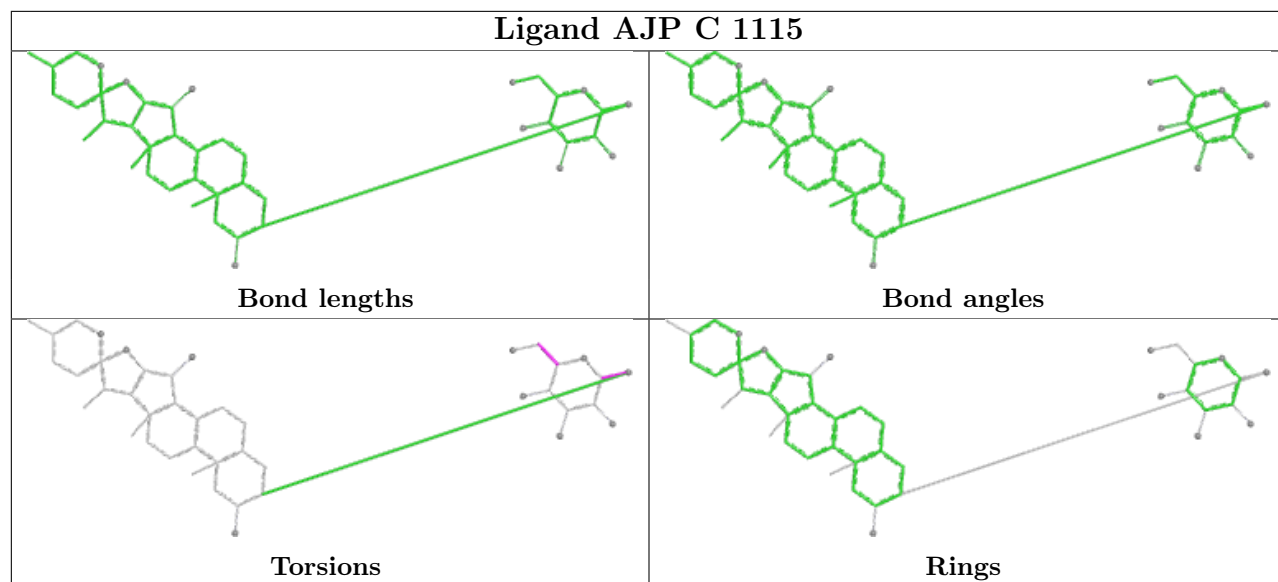


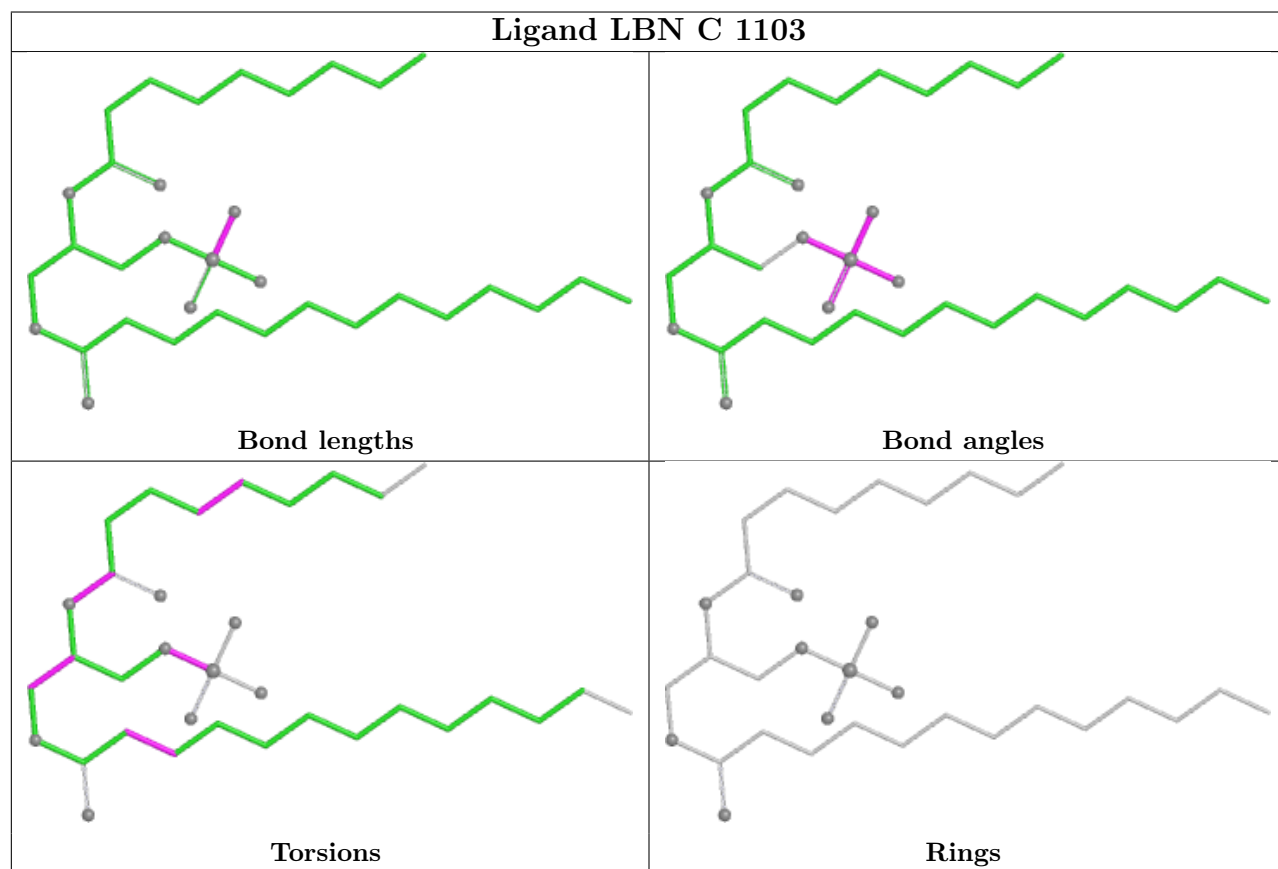
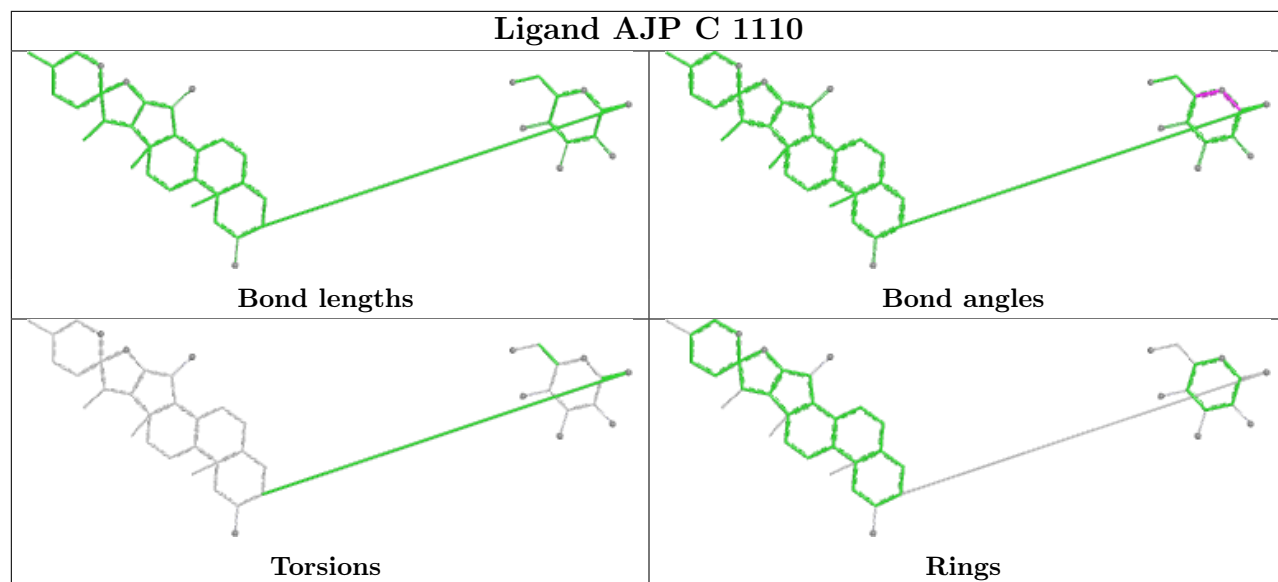


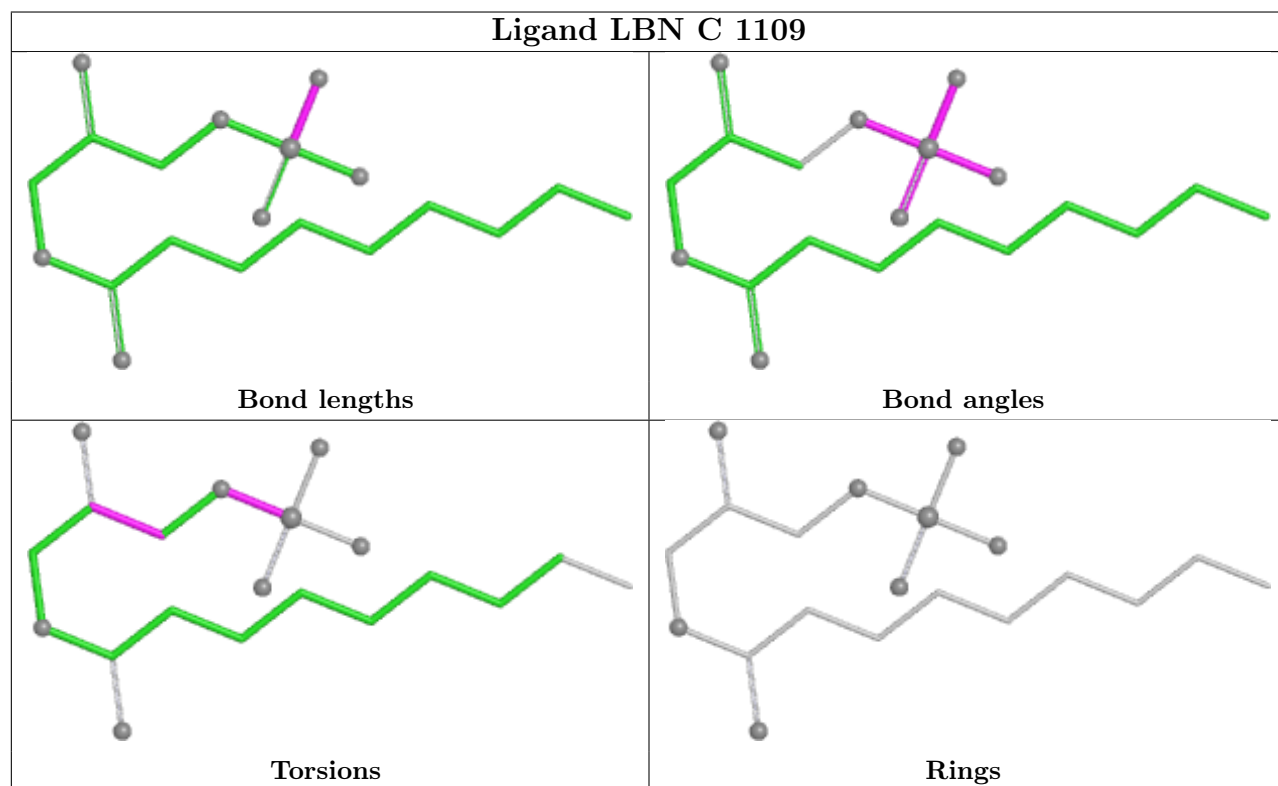
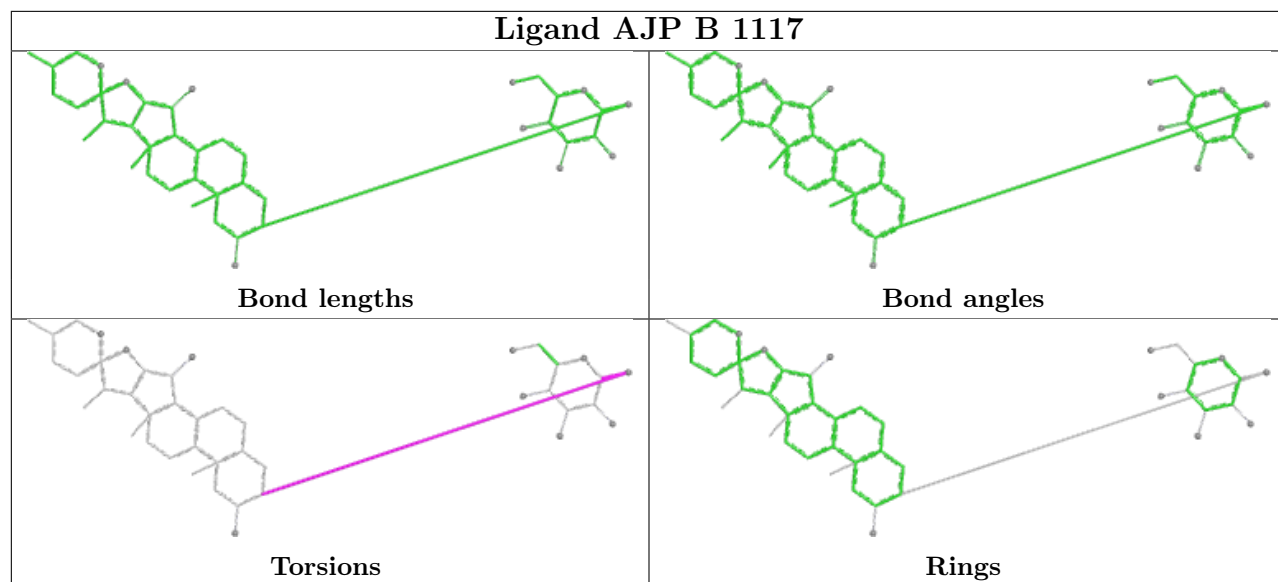


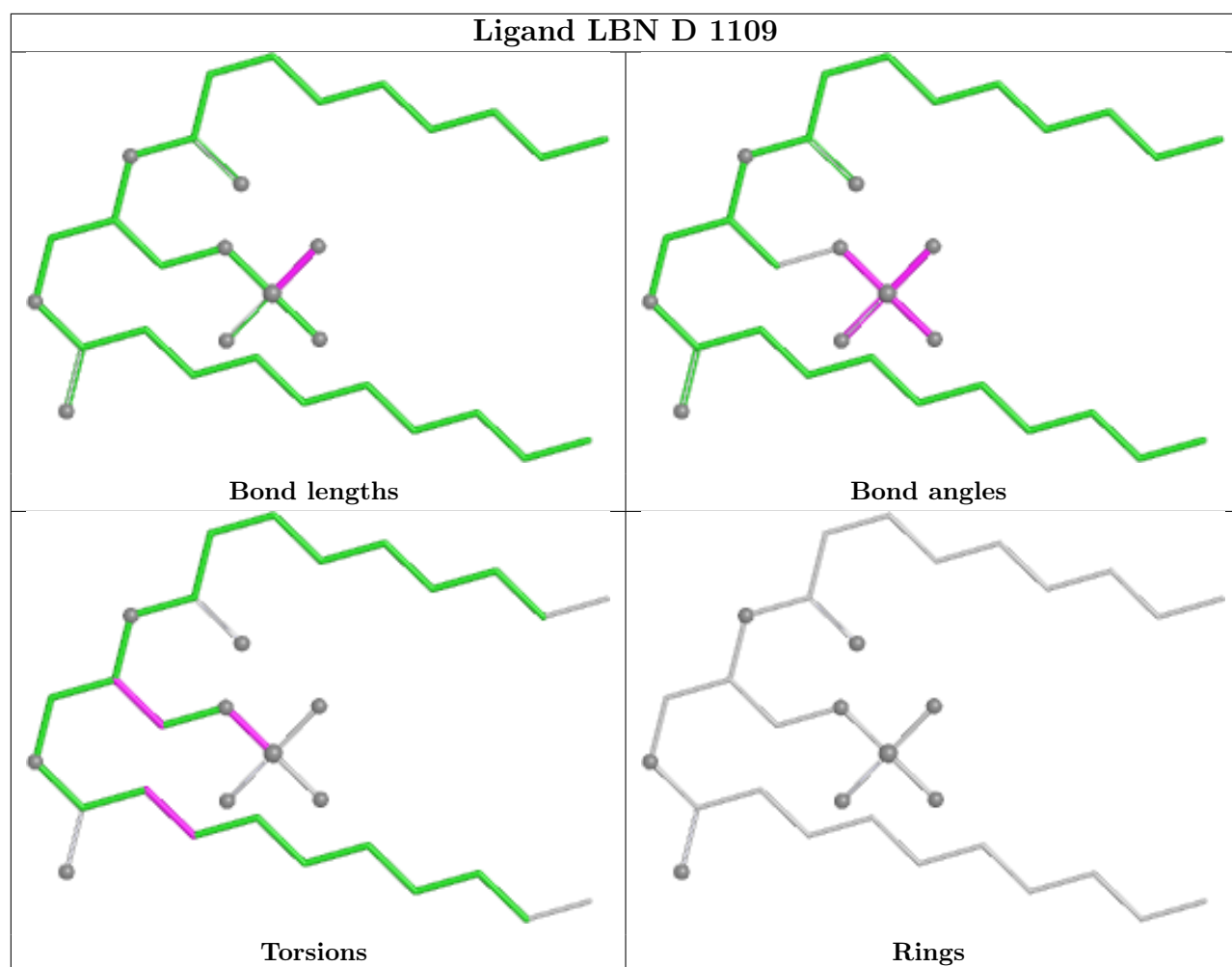




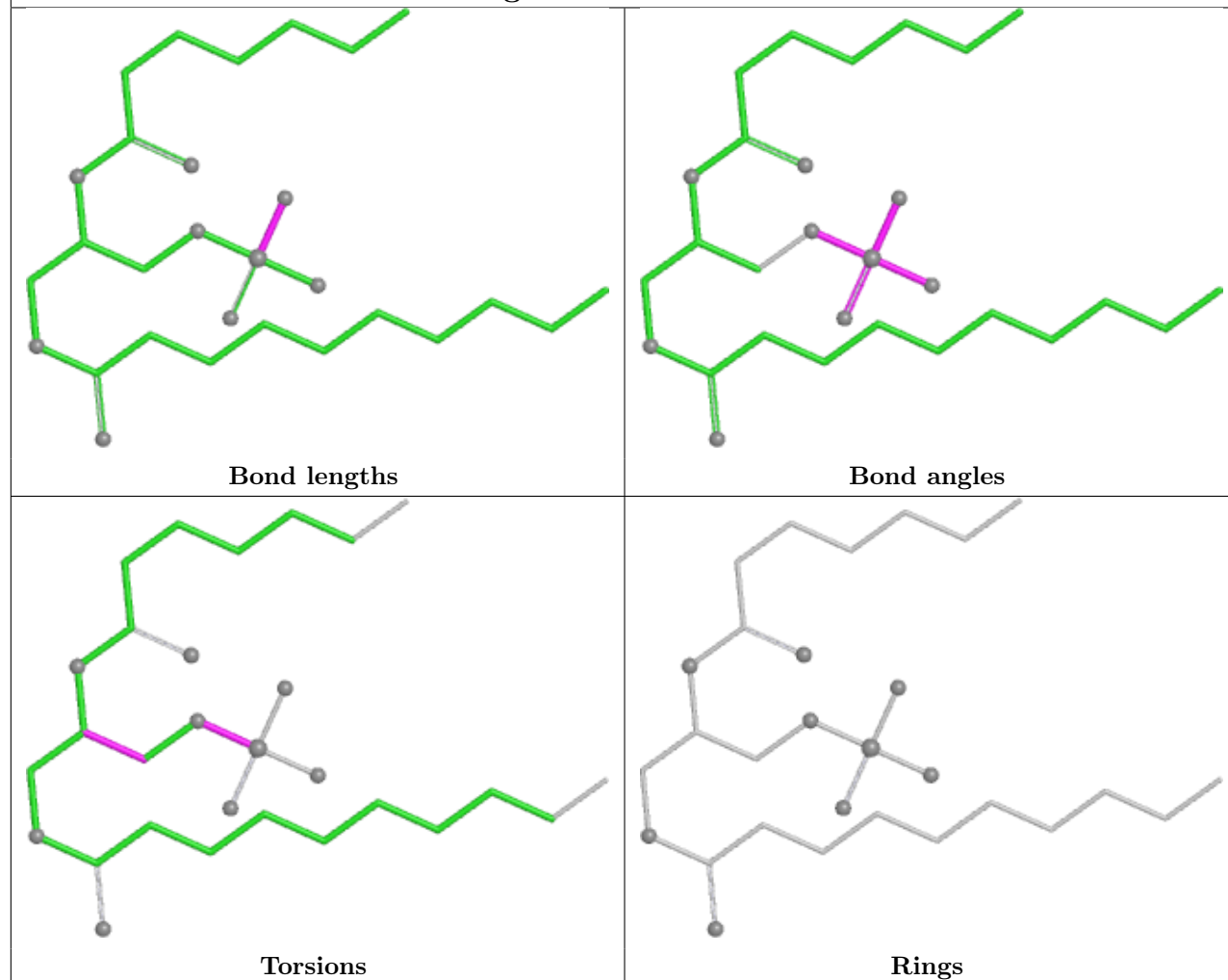




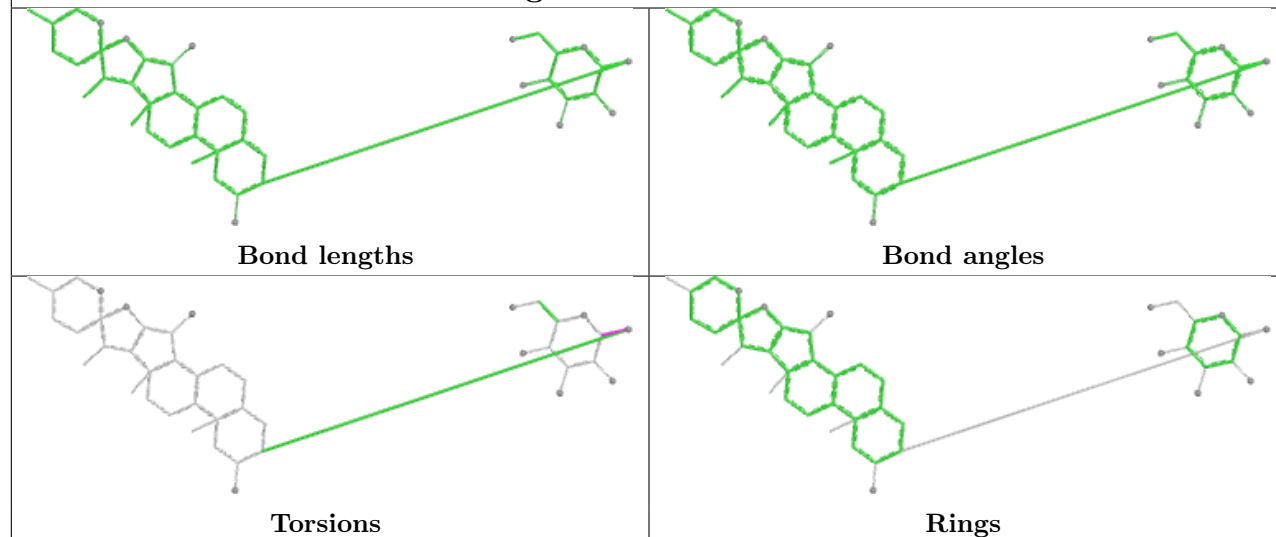


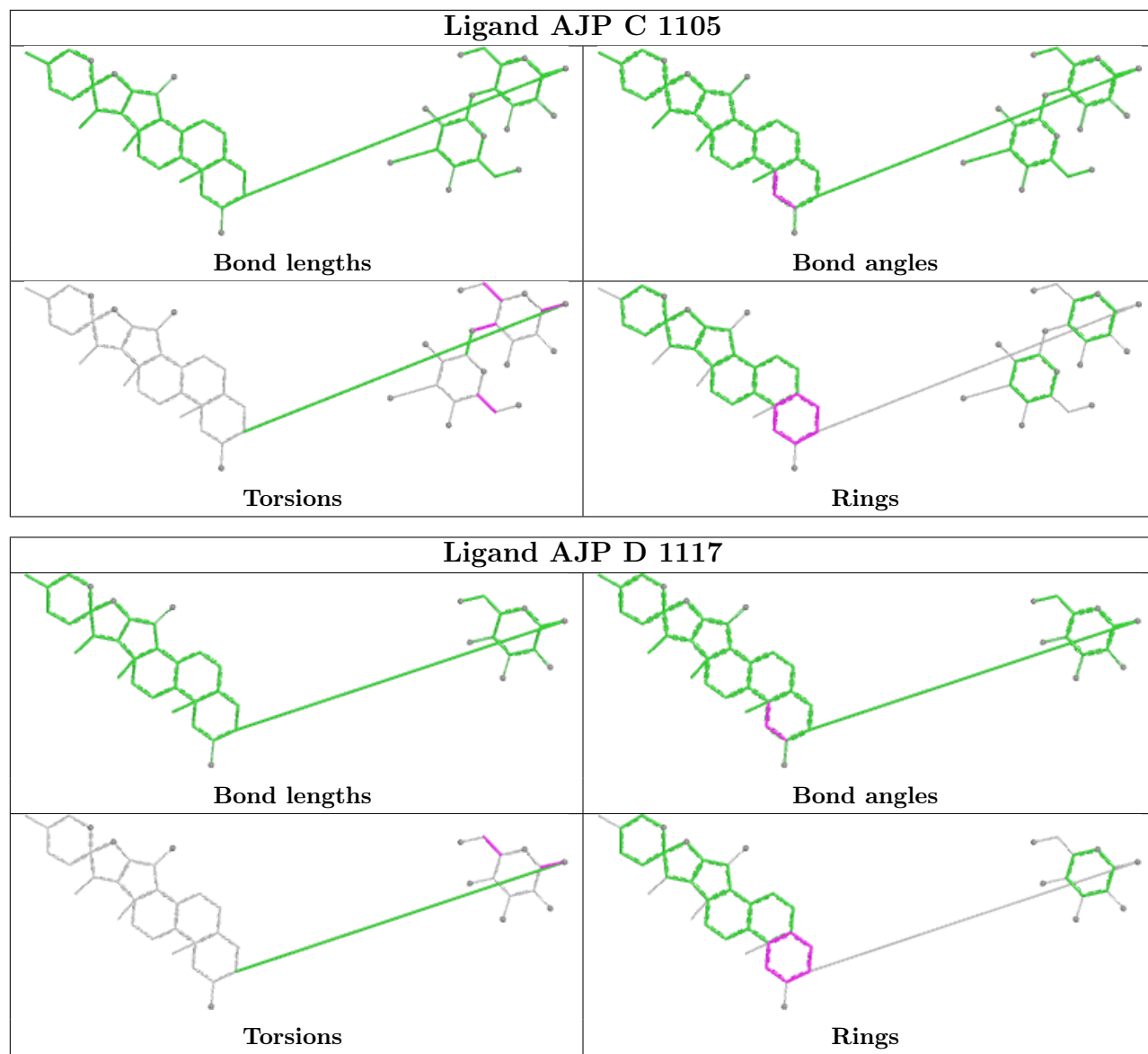


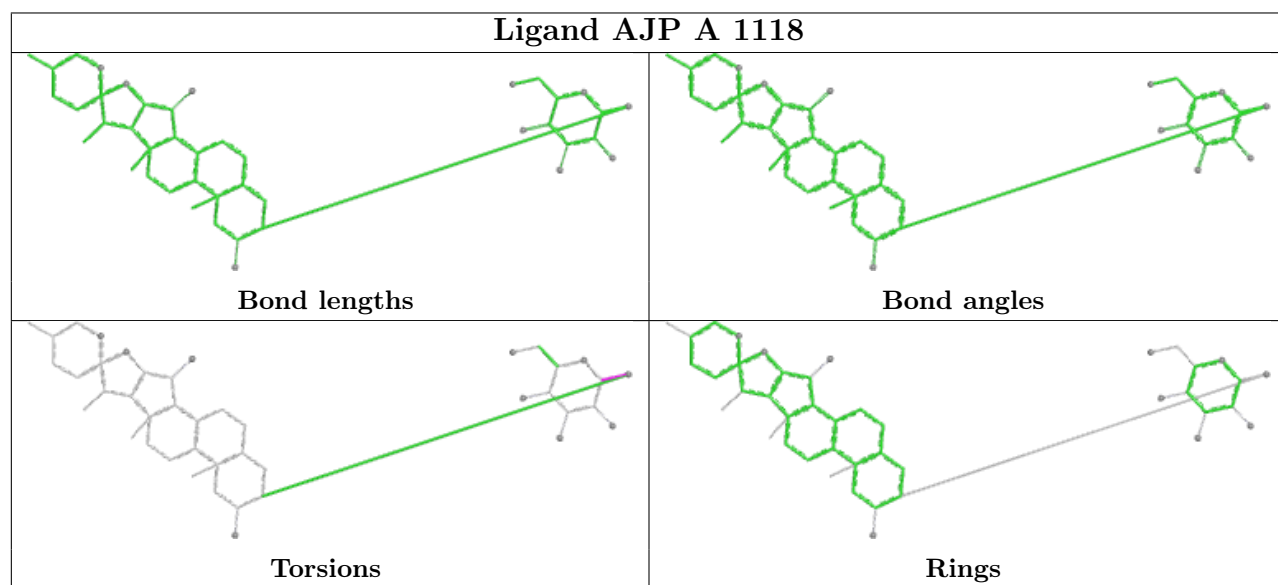
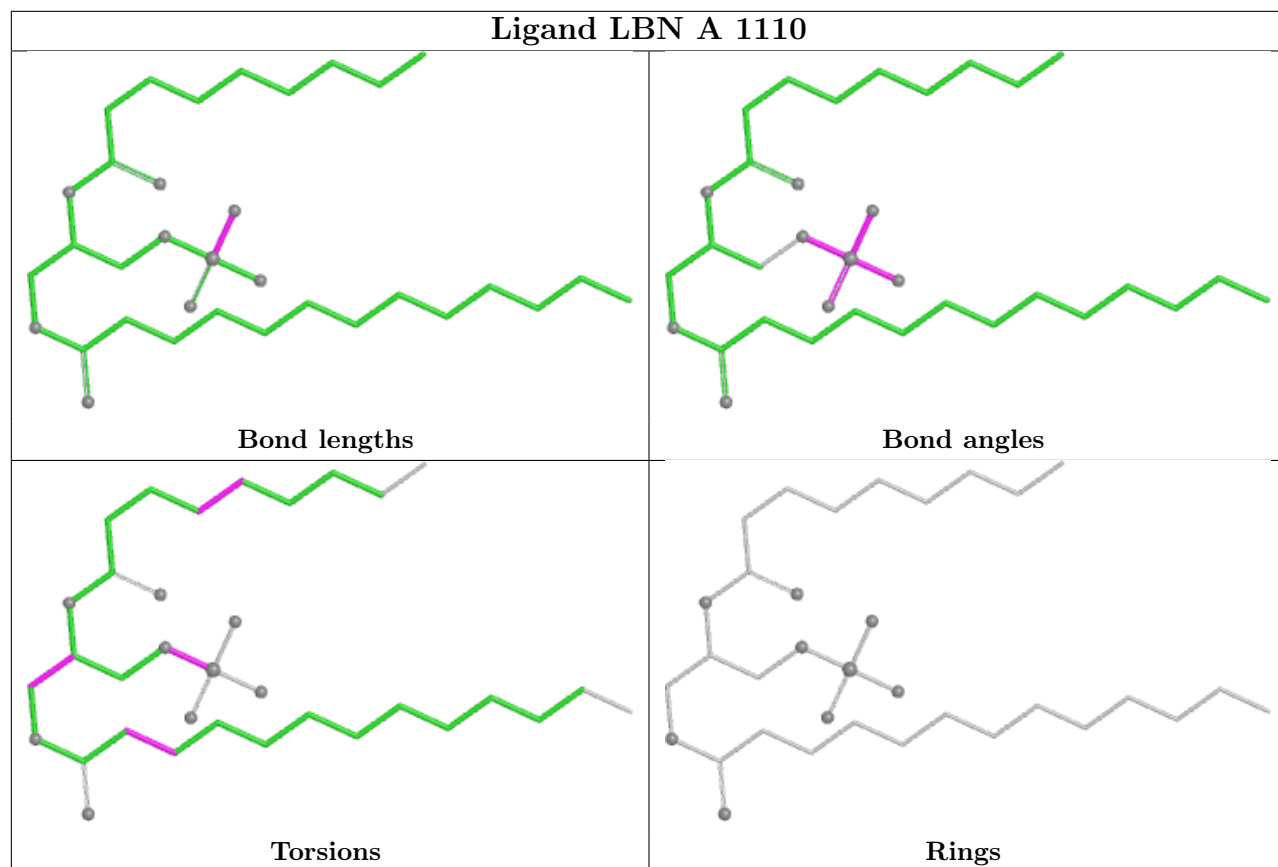
Ligand LBN B 1108

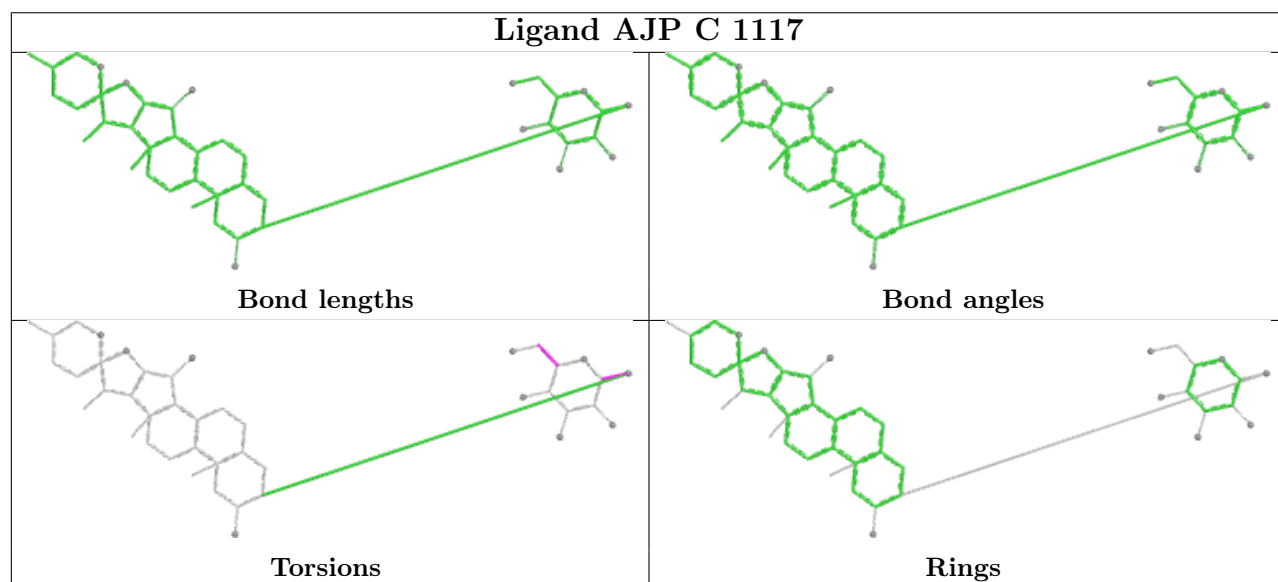
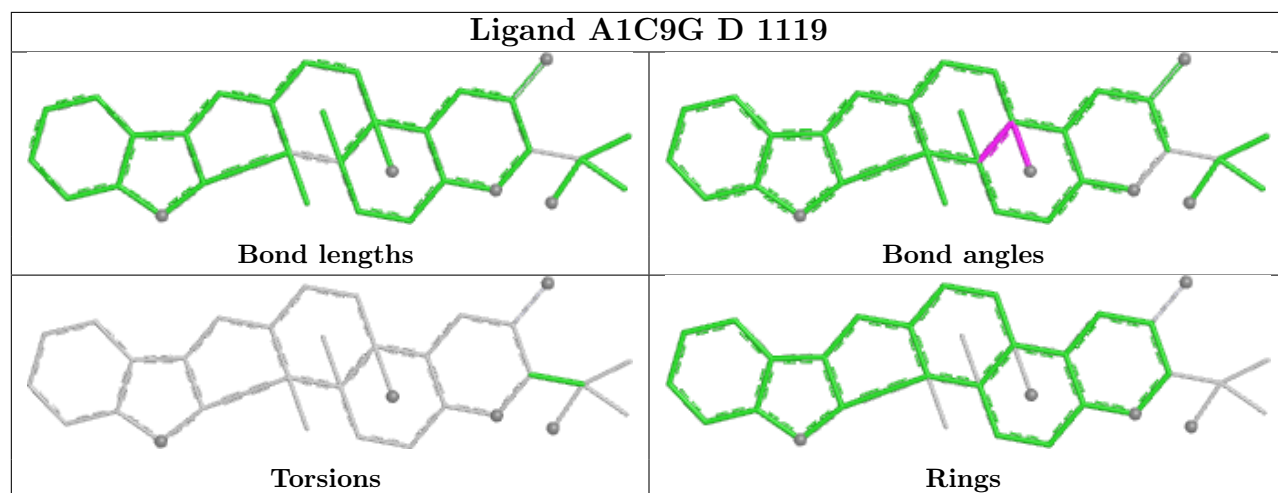
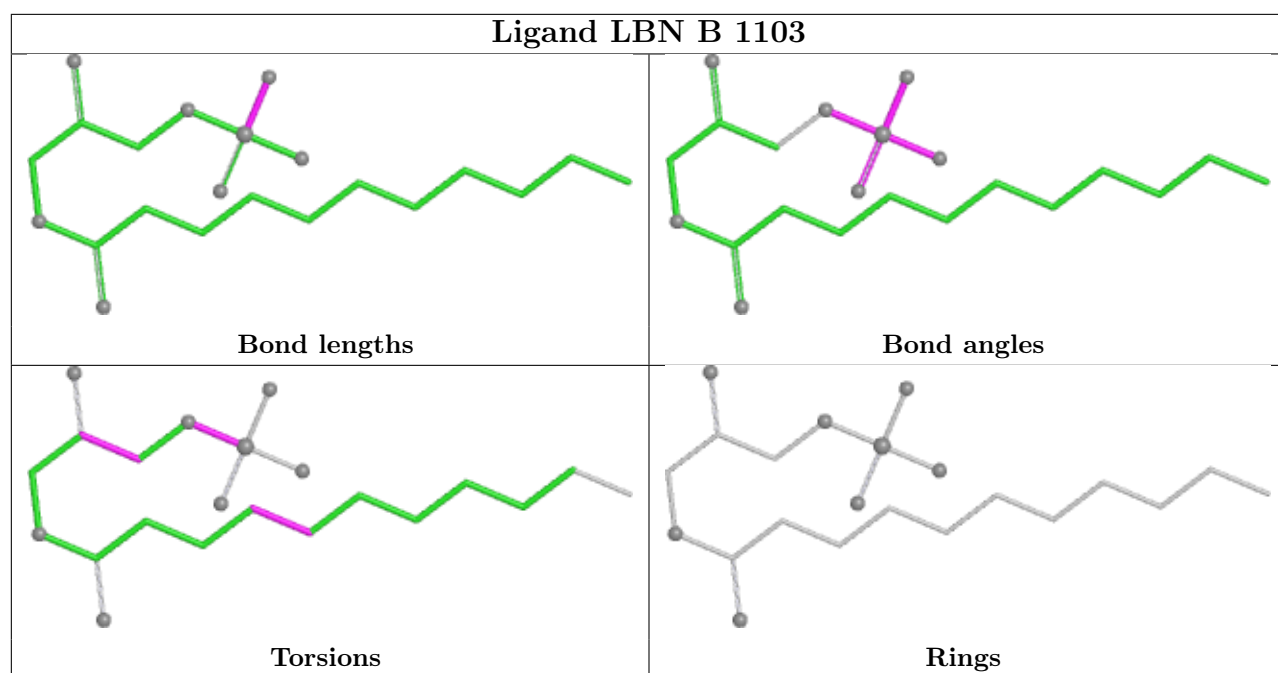


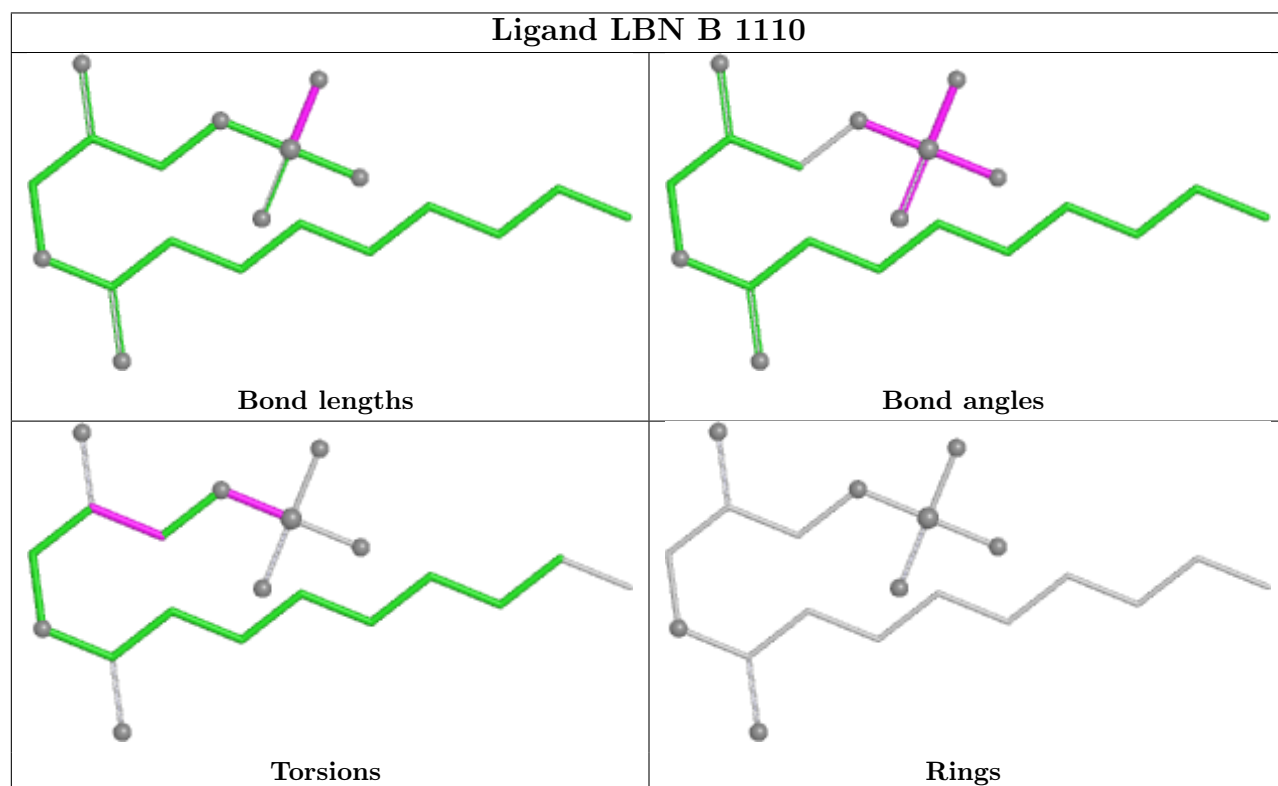
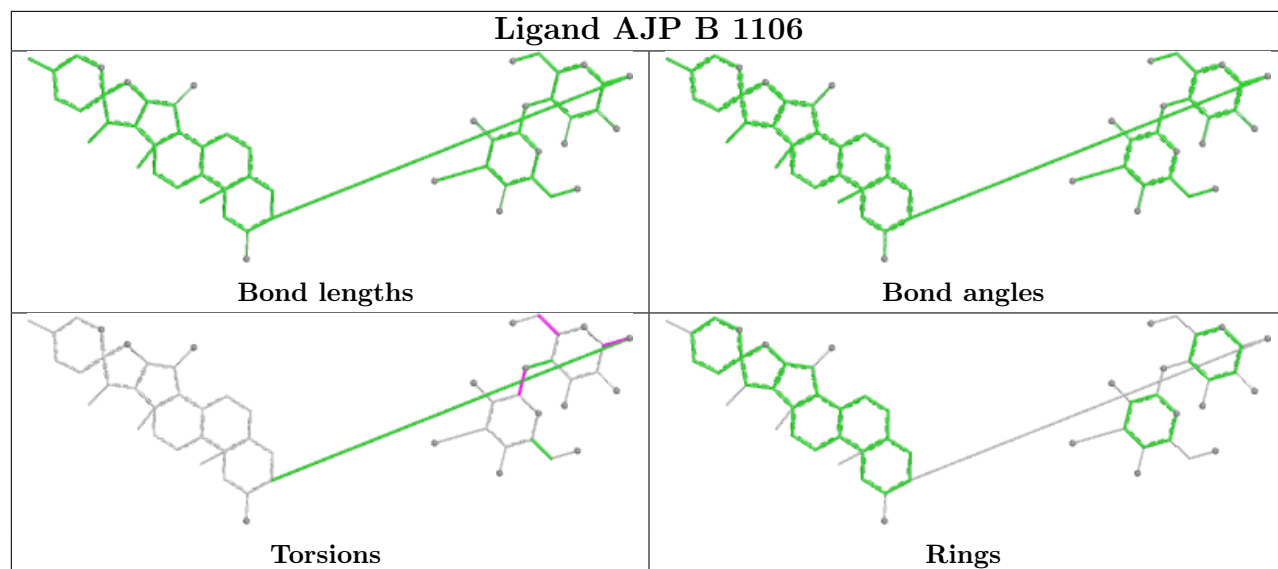
Ligand AJP B 1116



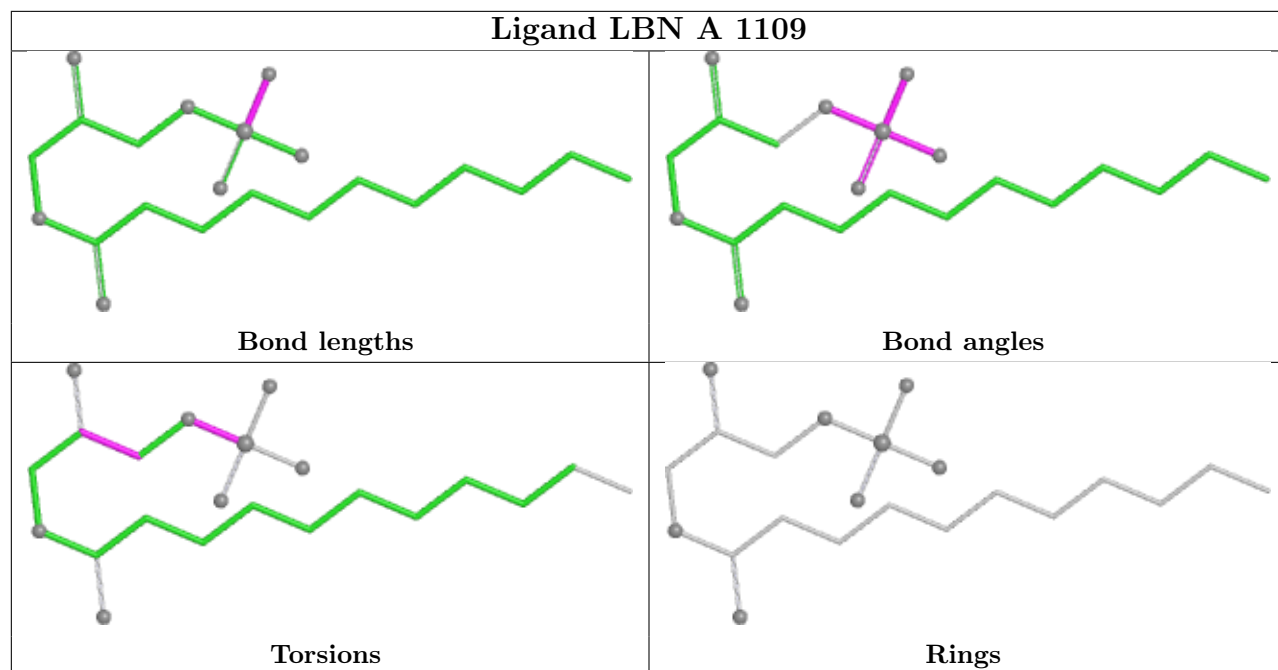




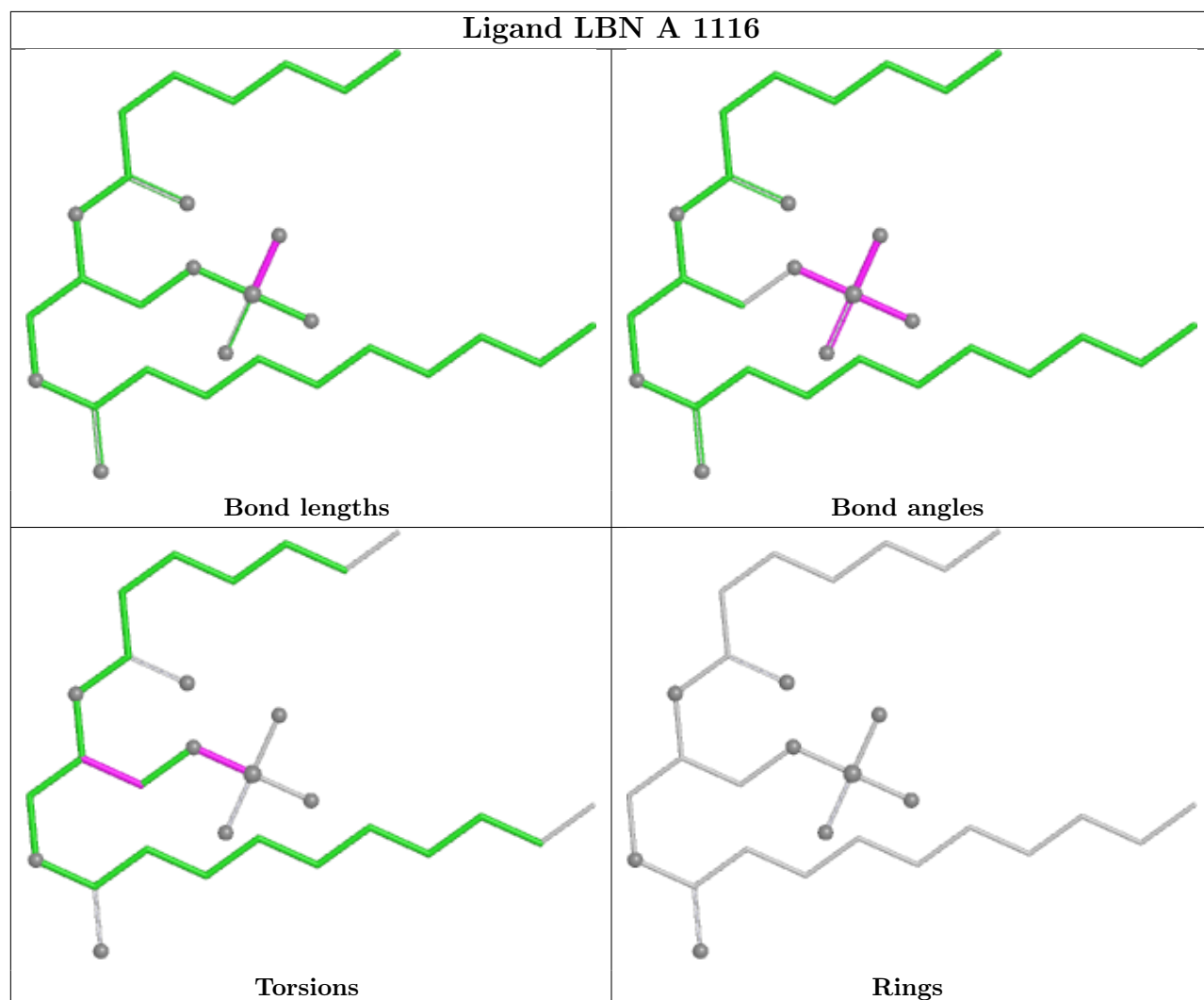


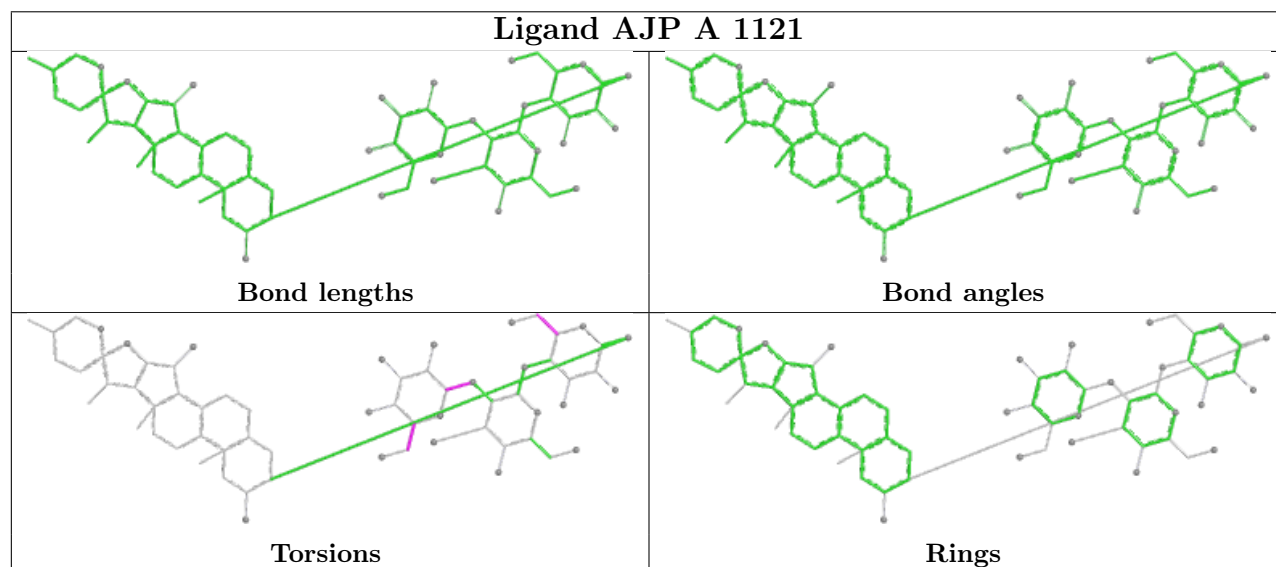
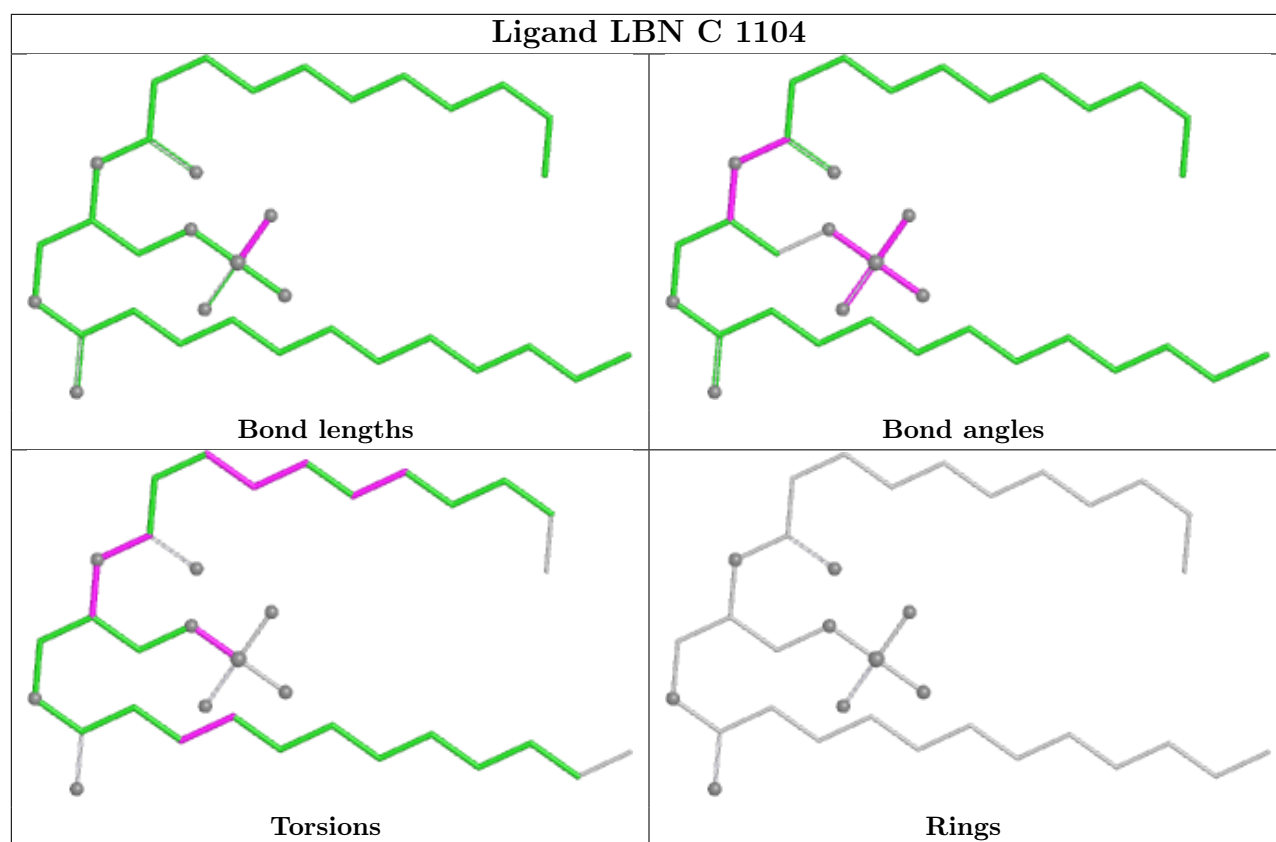


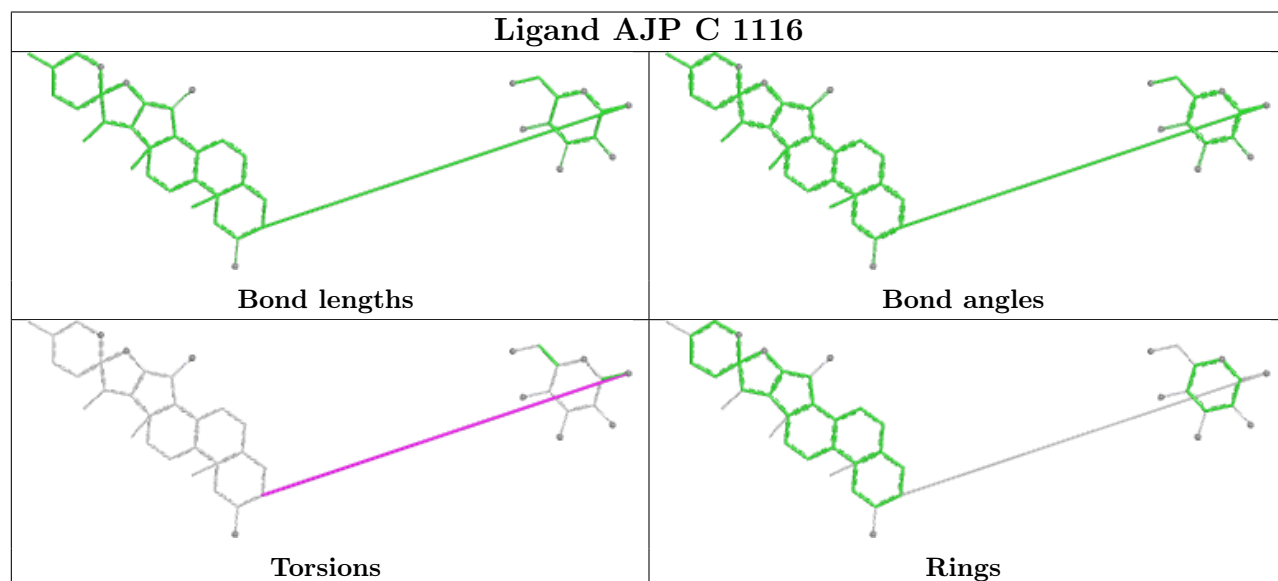
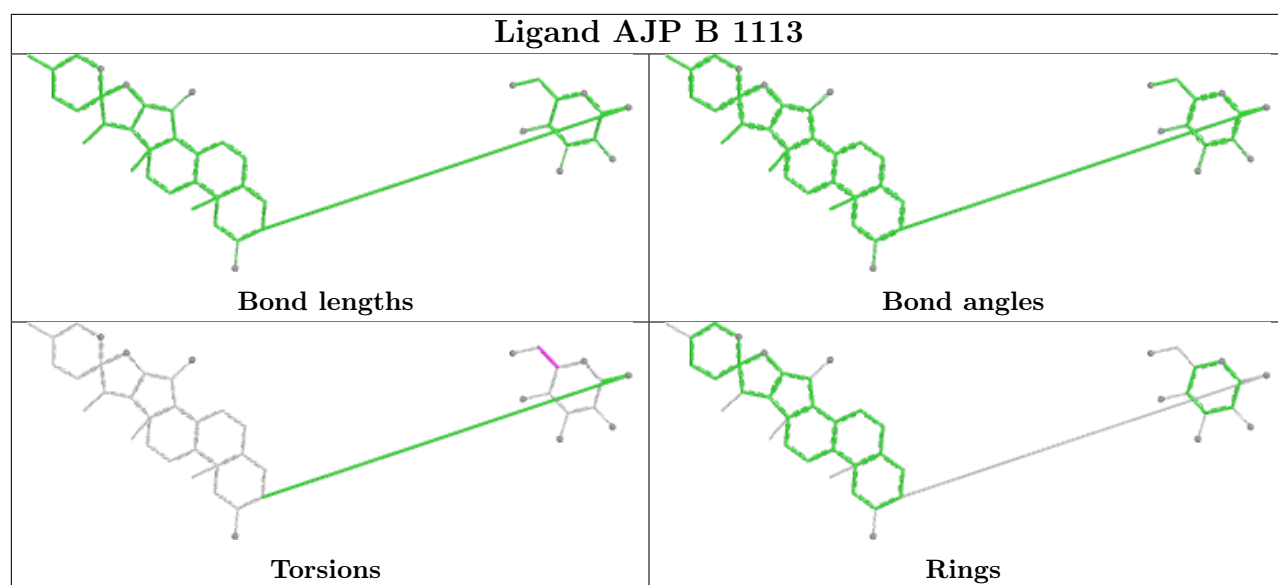
Ligand LBN A 1109

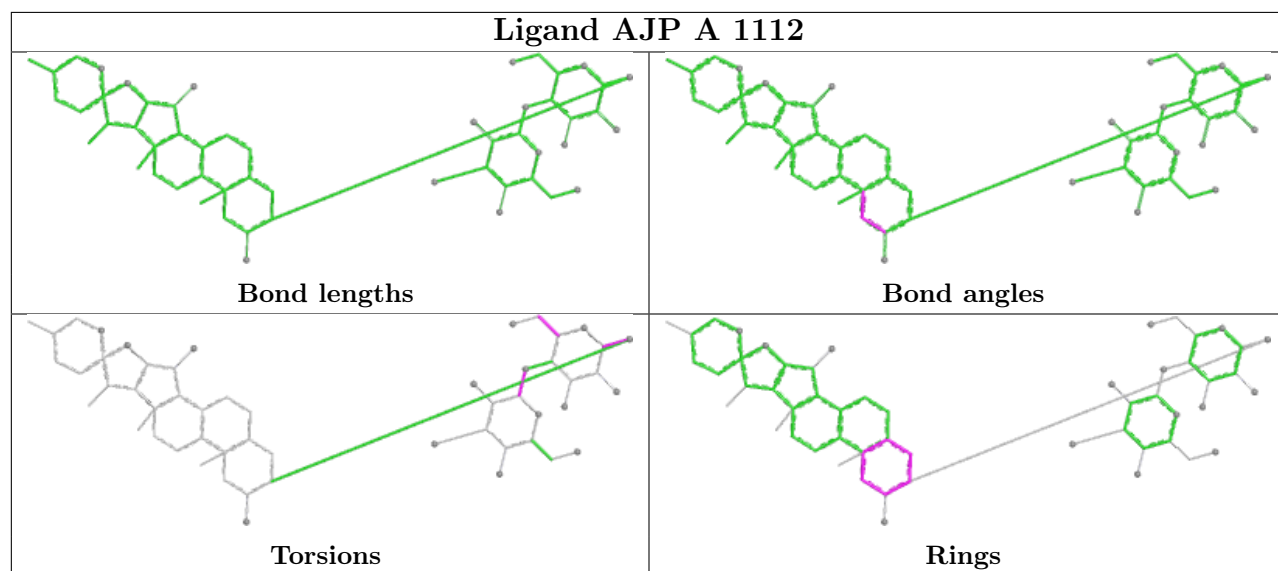
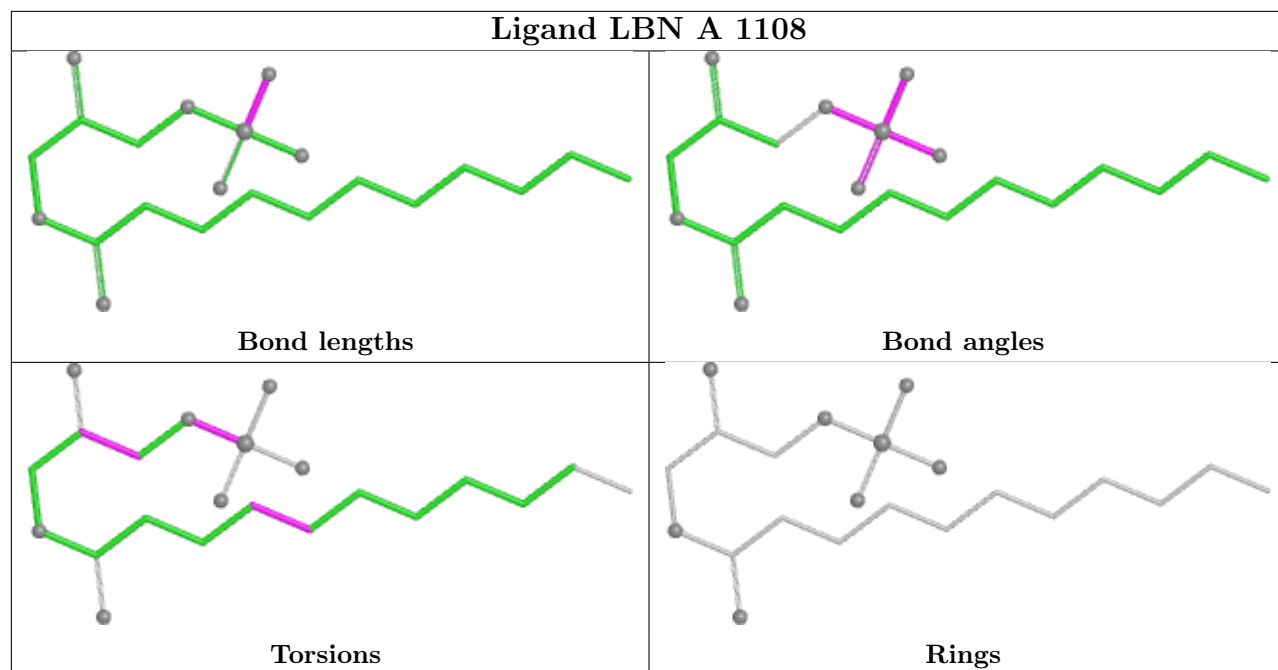


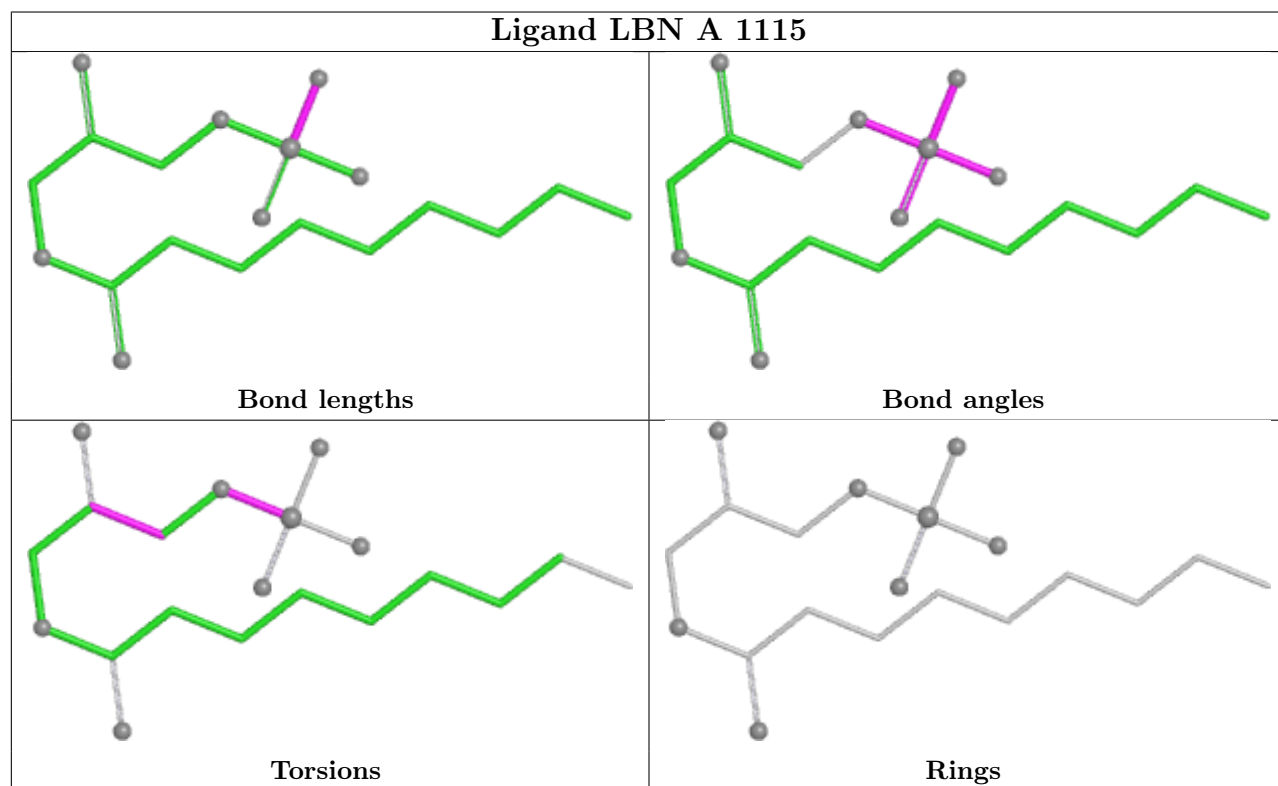
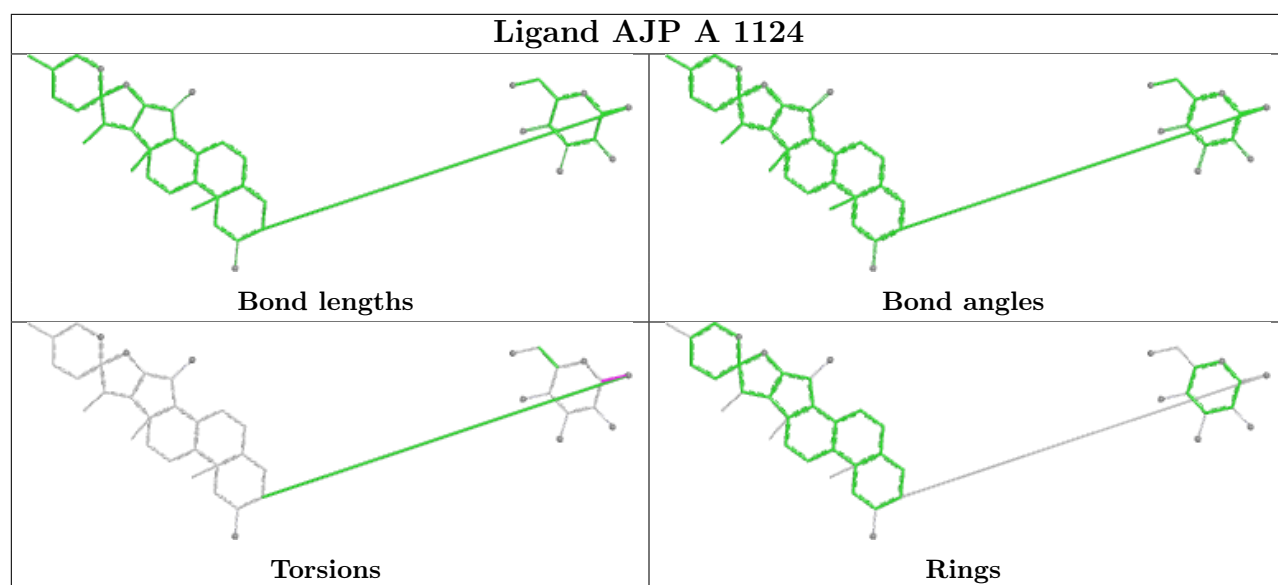
Ligand LBN A 1116

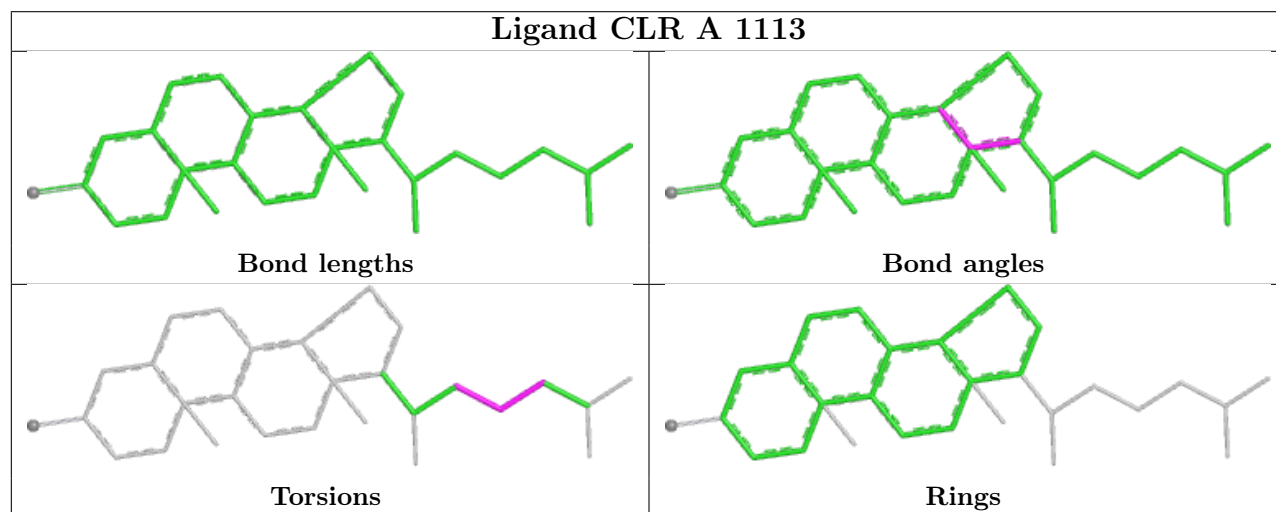
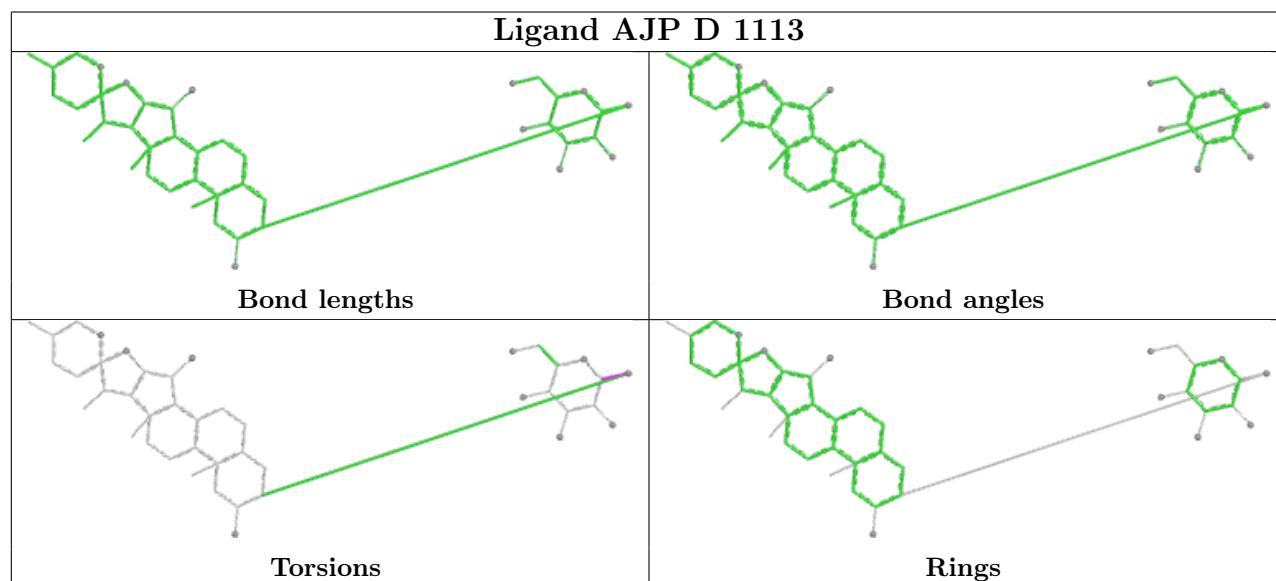
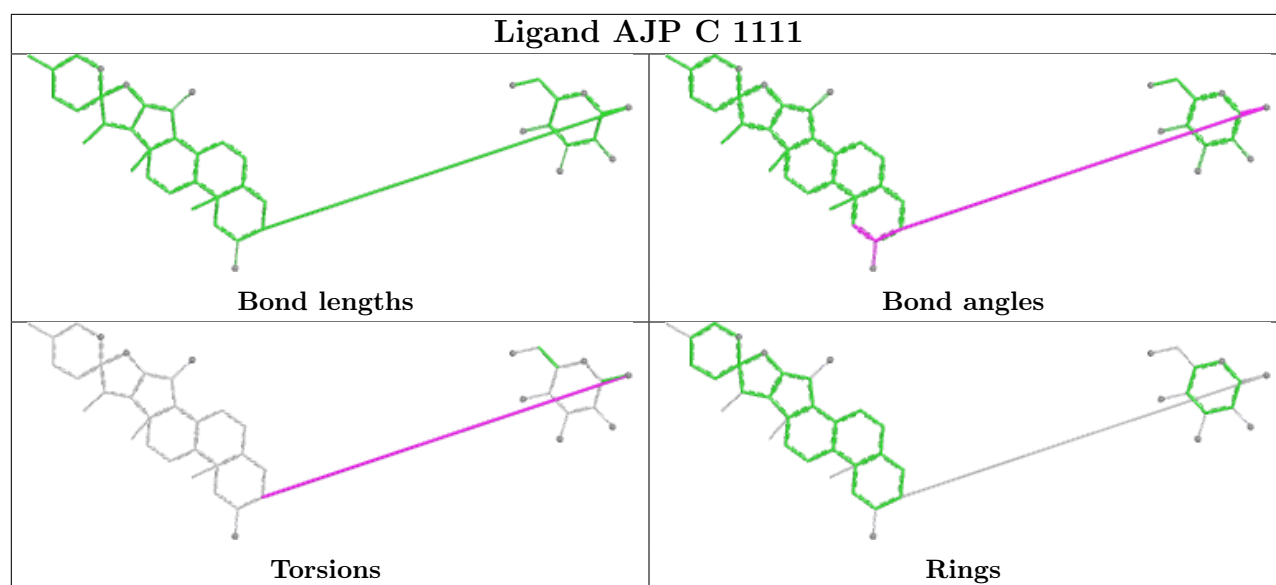


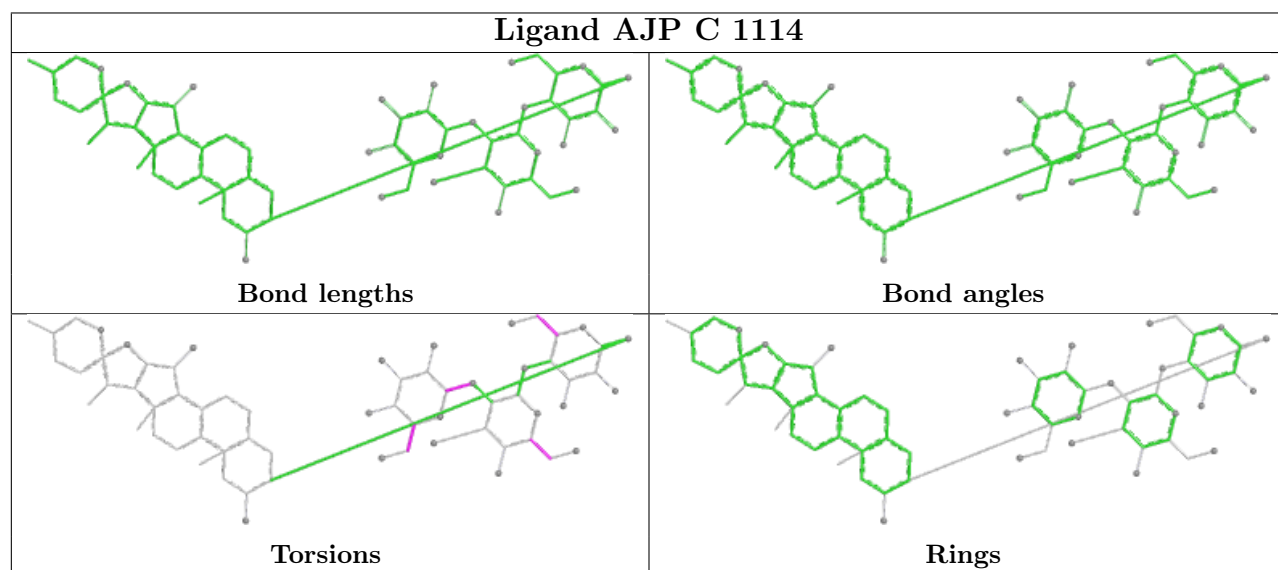
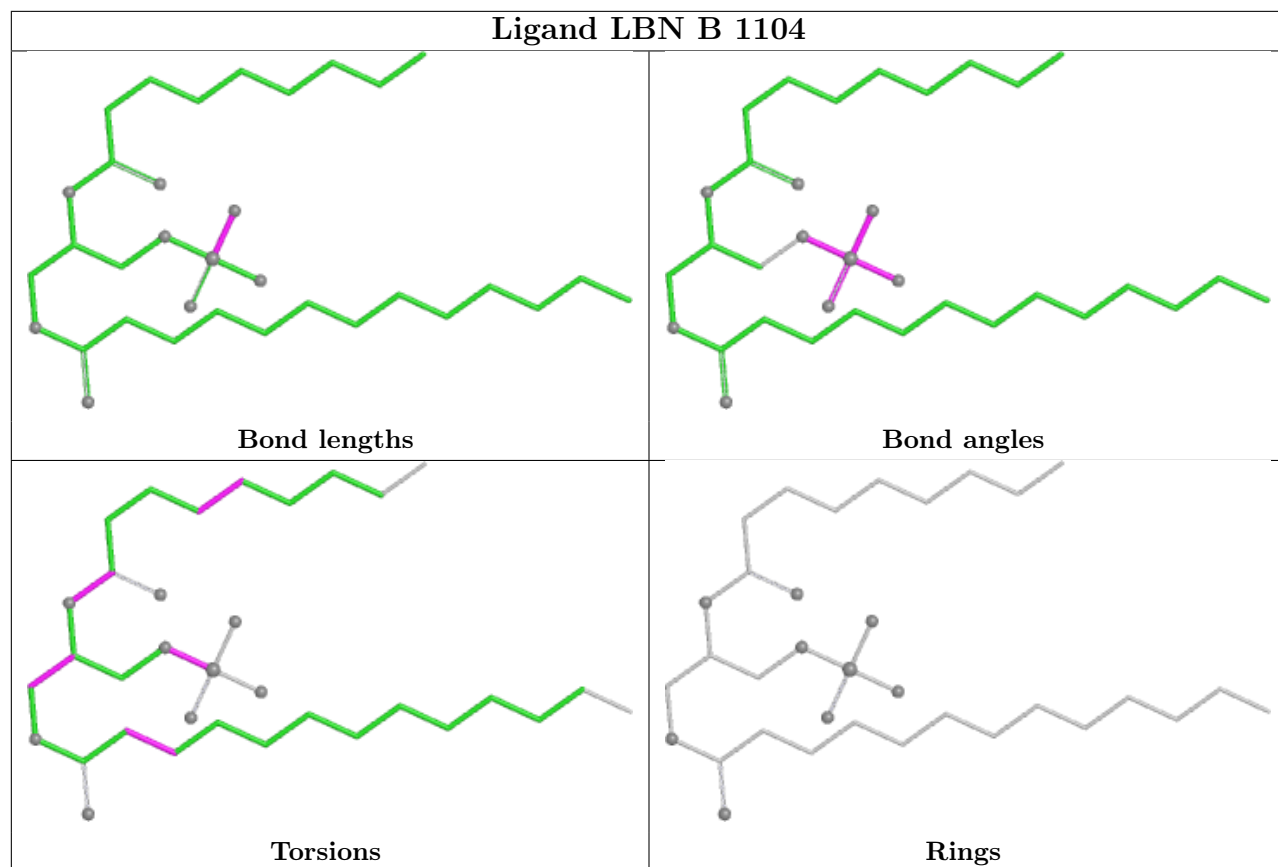


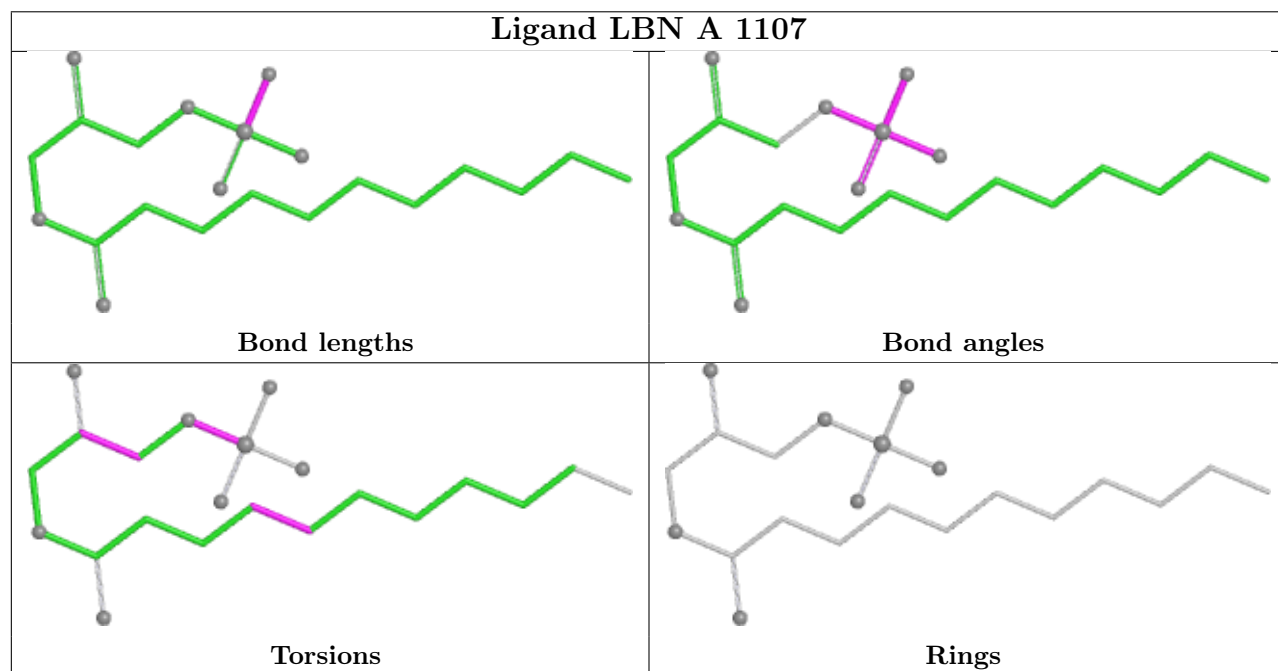
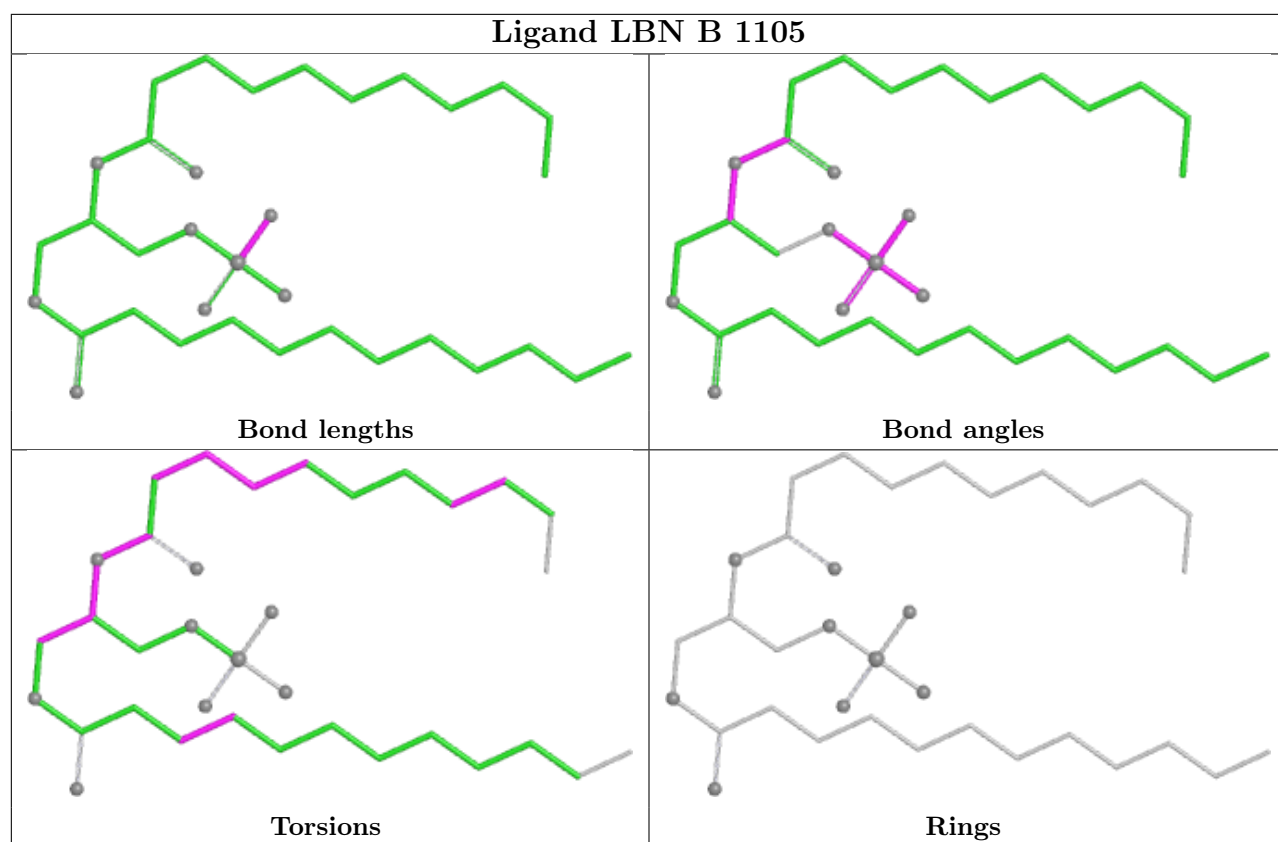


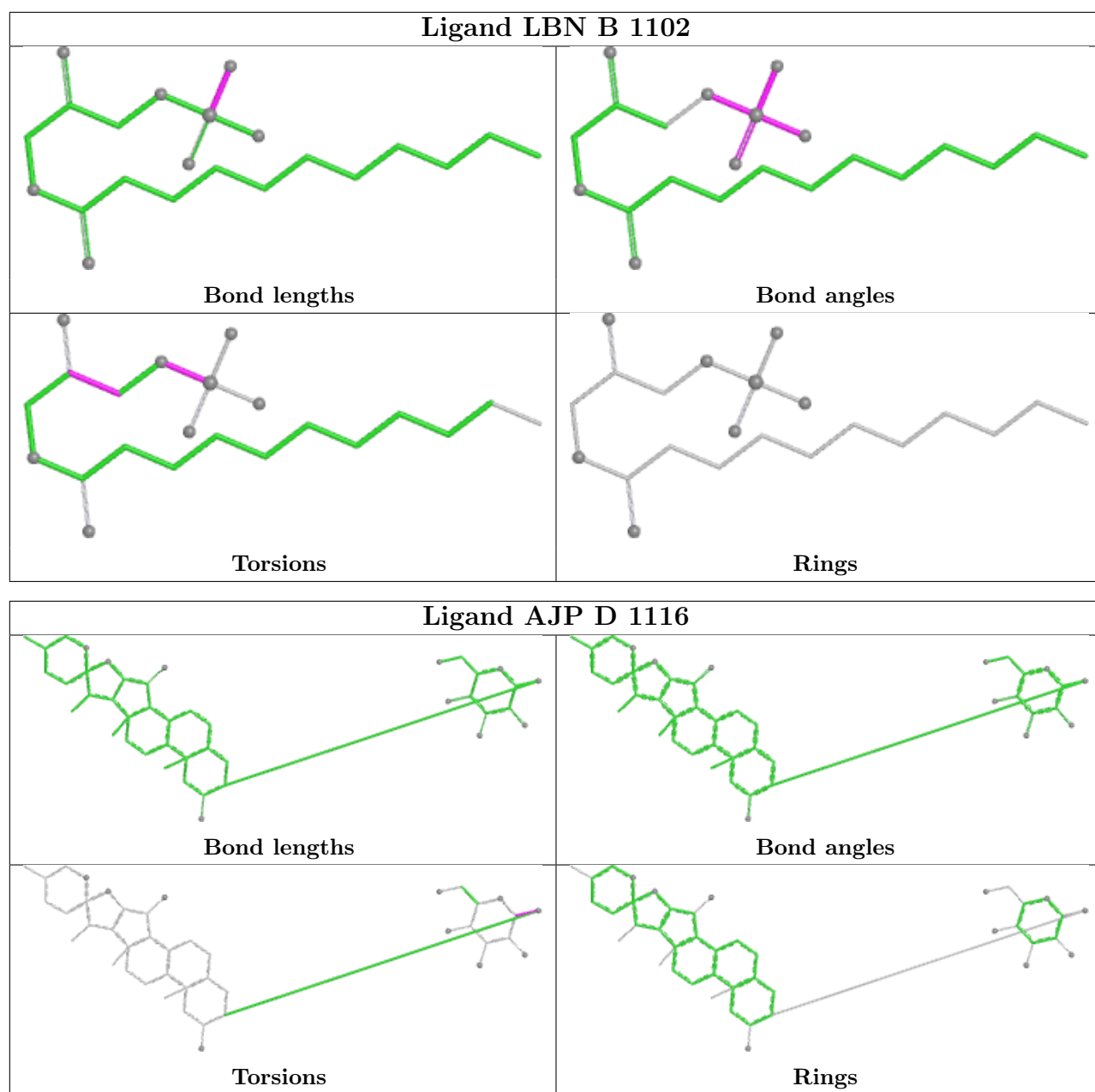












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

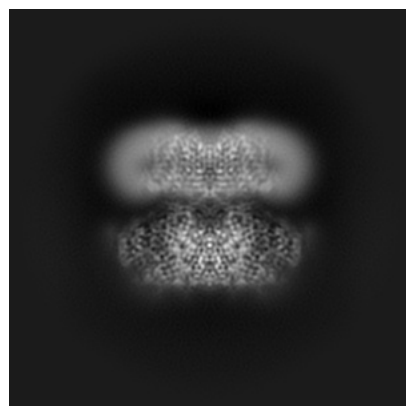
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75627. These allow visual inspection of the internal detail of the map and identification of artifacts.

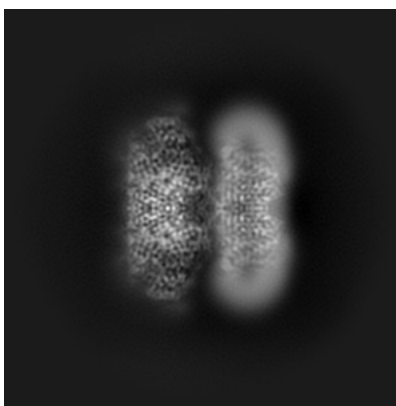
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

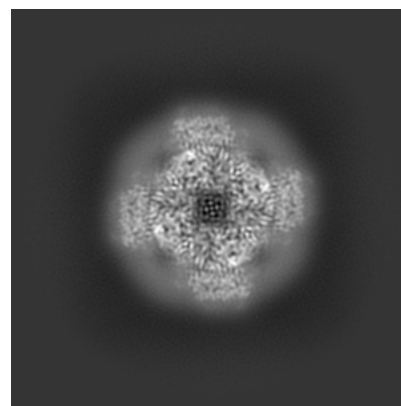
6.1.1 Primary map



X

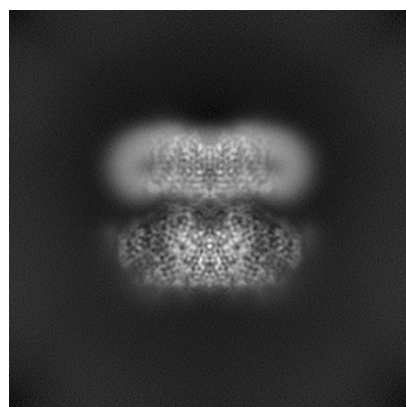


Y

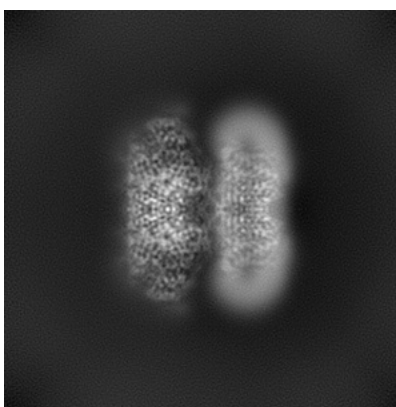


Z

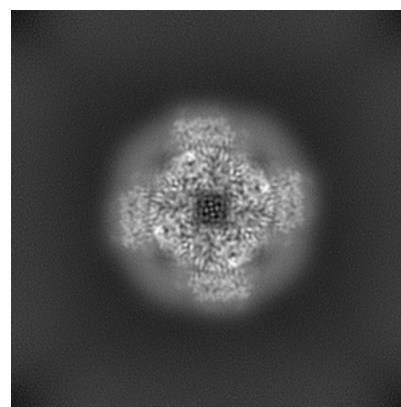
6.1.2 Raw map



X



Y

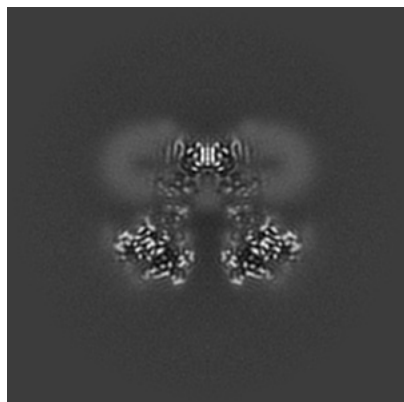


Z

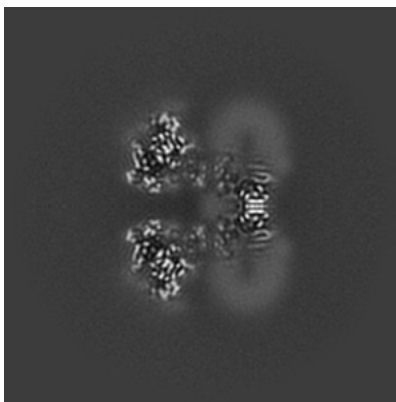
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

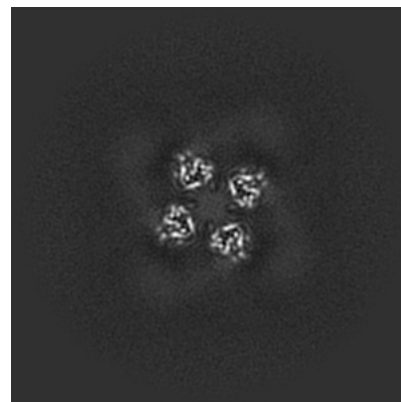
6.2.1 Primary map



X Index: 140

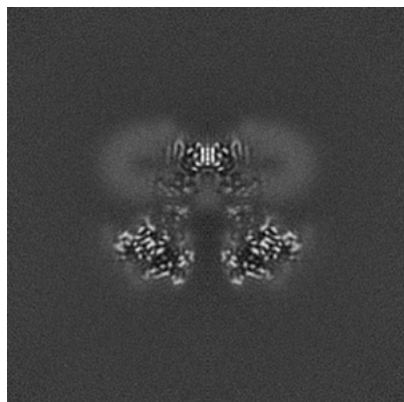


Y Index: 140

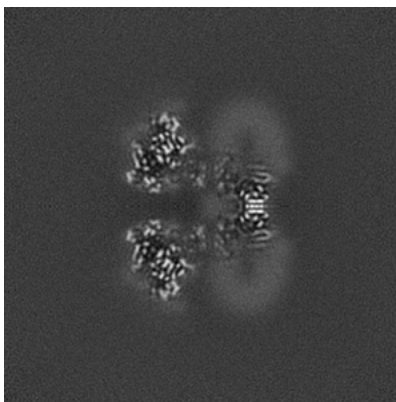


Z Index: 140

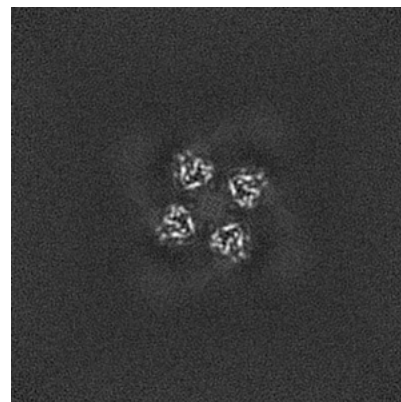
6.2.2 Raw map



X Index: 140



Y Index: 140

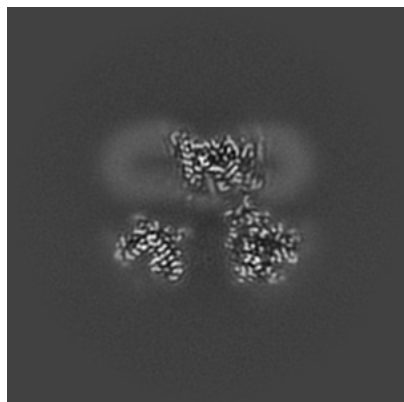


Z Index: 140

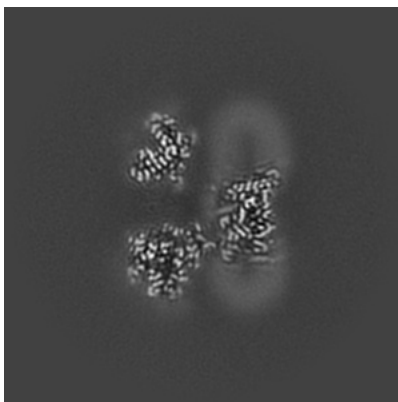
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

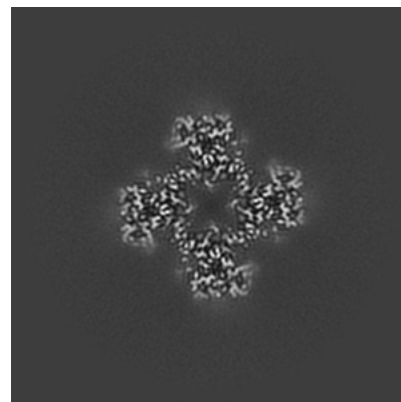
6.3.1 Primary map



X Index: 133

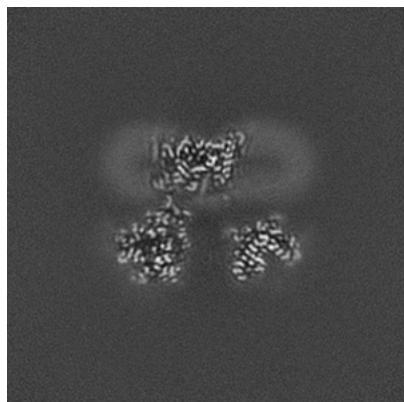


Y Index: 133

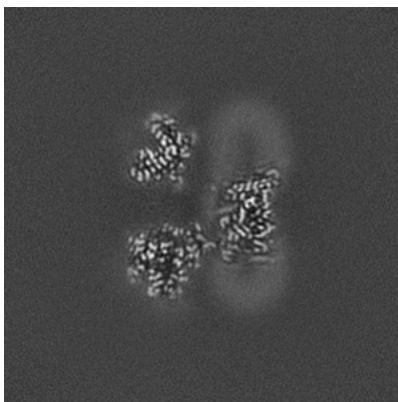


Z Index: 109

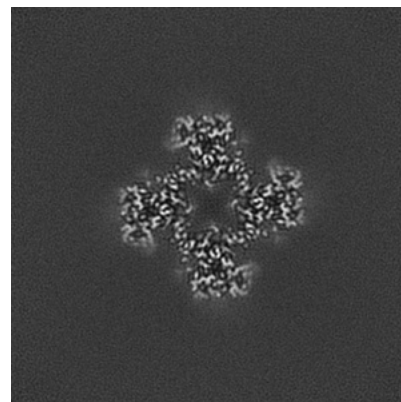
6.3.2 Raw map



X Index: 147



Y Index: 133

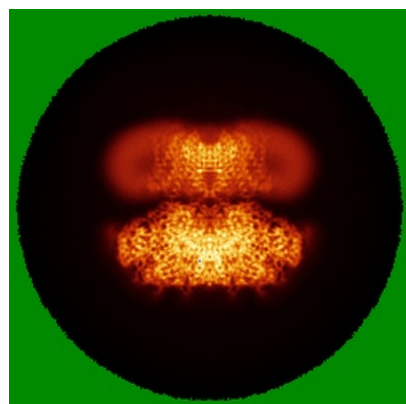


Z Index: 109

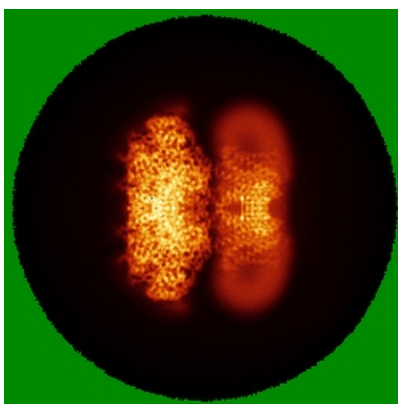
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

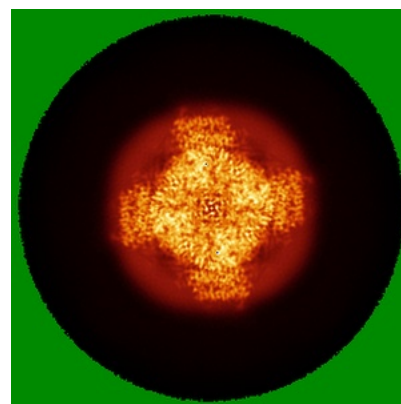
6.4.1 Primary map



X

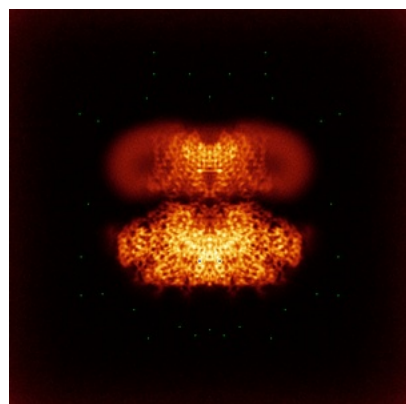


Y

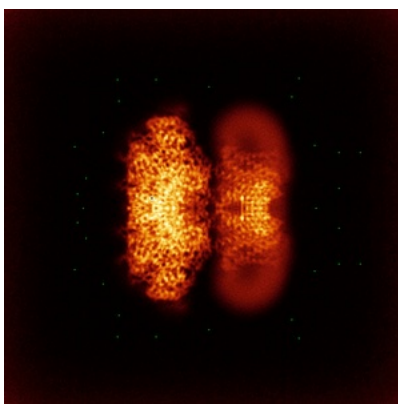


Z

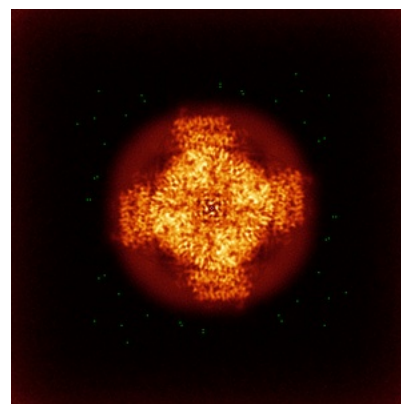
6.4.2 Raw map



X



Y

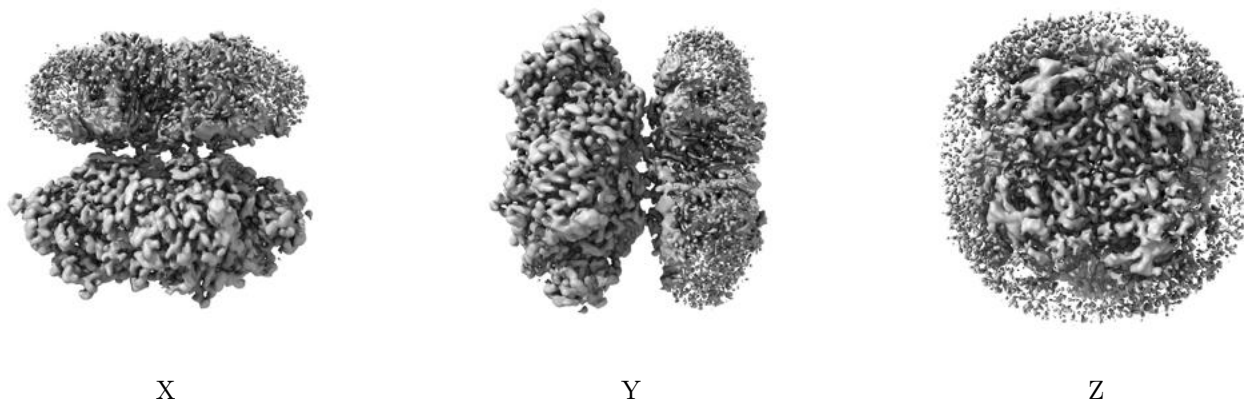


Z

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.

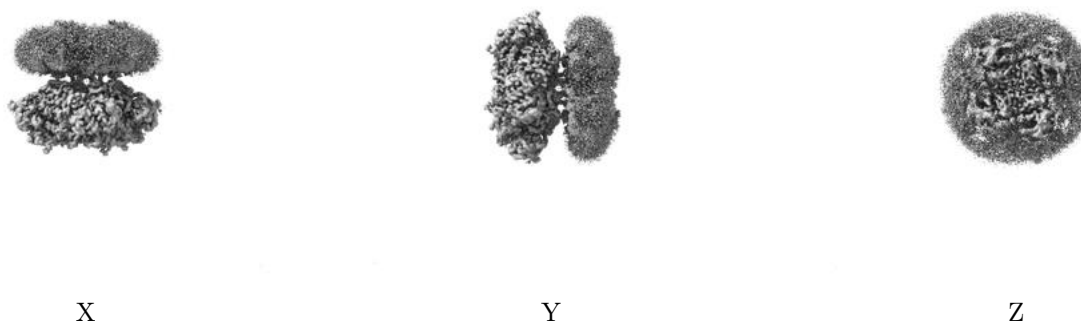
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

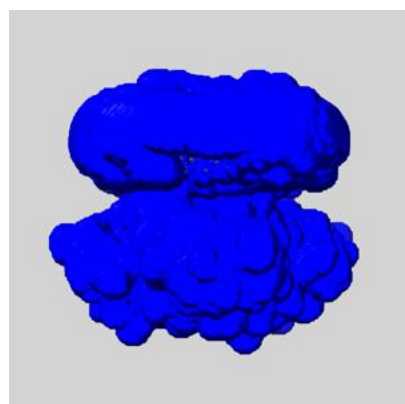
6.6 Mask visualisation [i](#)

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

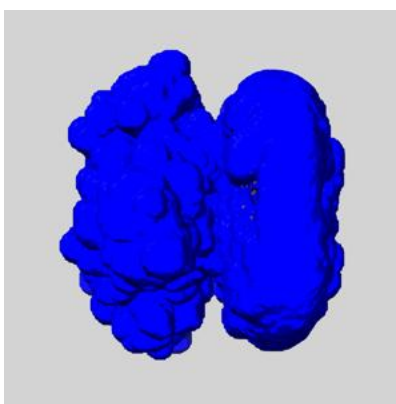
A mask typically either:

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

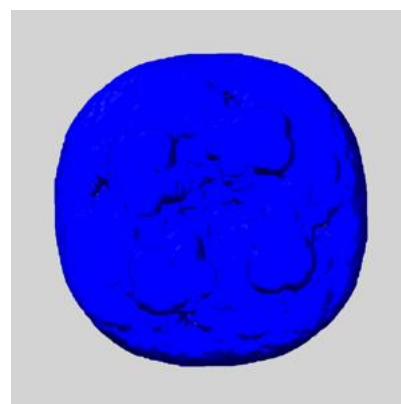
6.6.1 emd_75627_msk_1.map [i](#)



X



Y

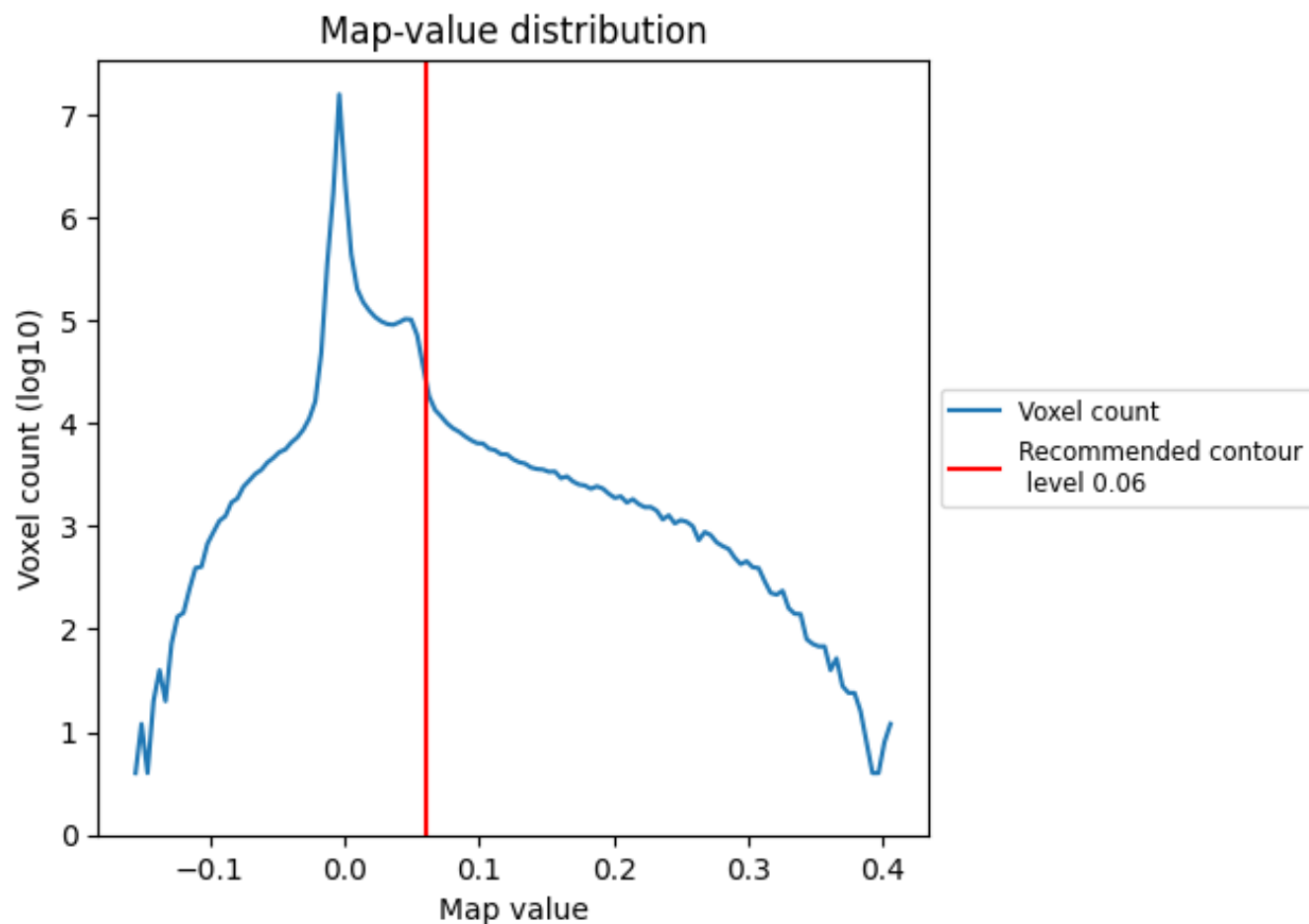


Z

7 Map analysis [i](#)

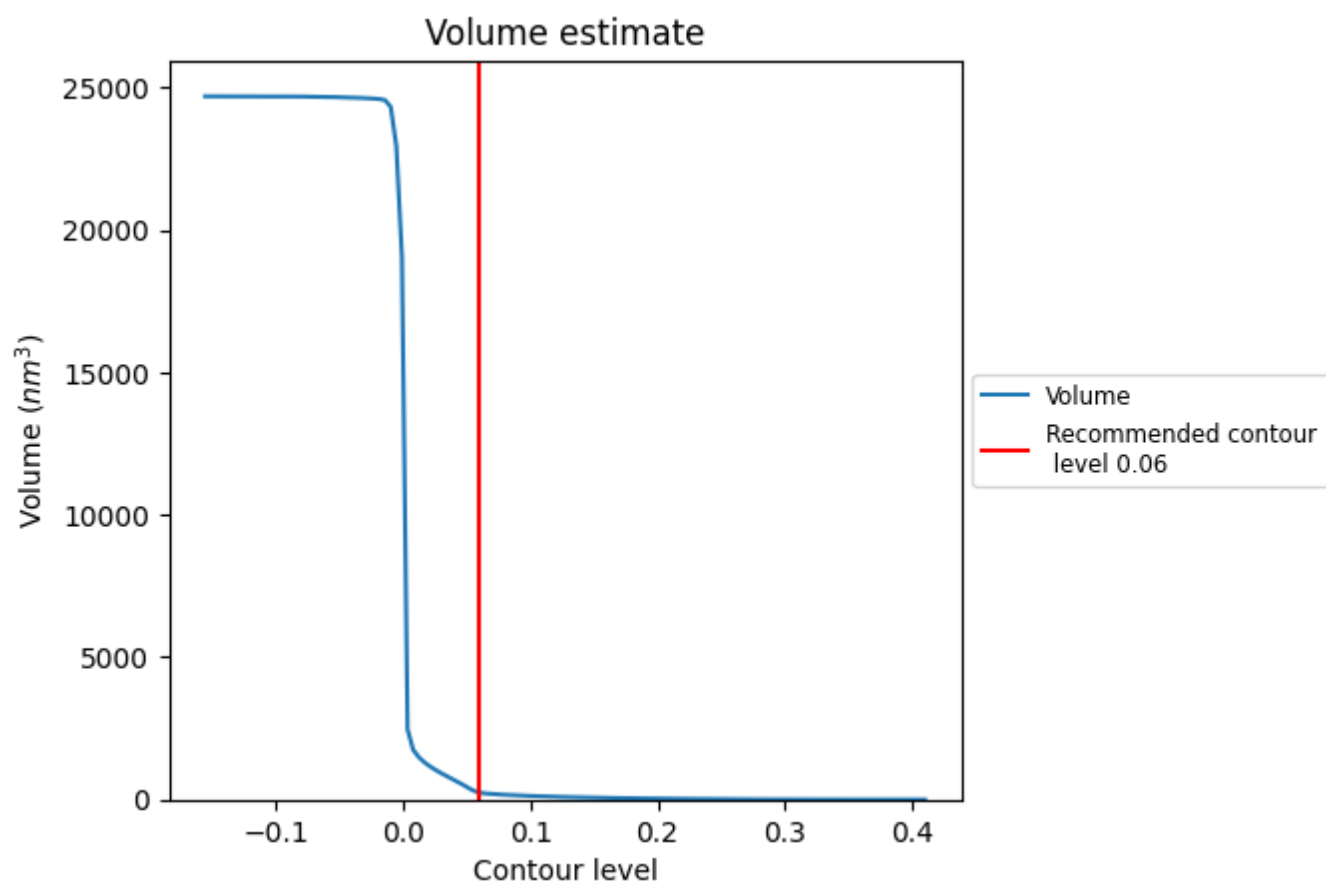
This section contains the results of statistical analysis of the map.

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.

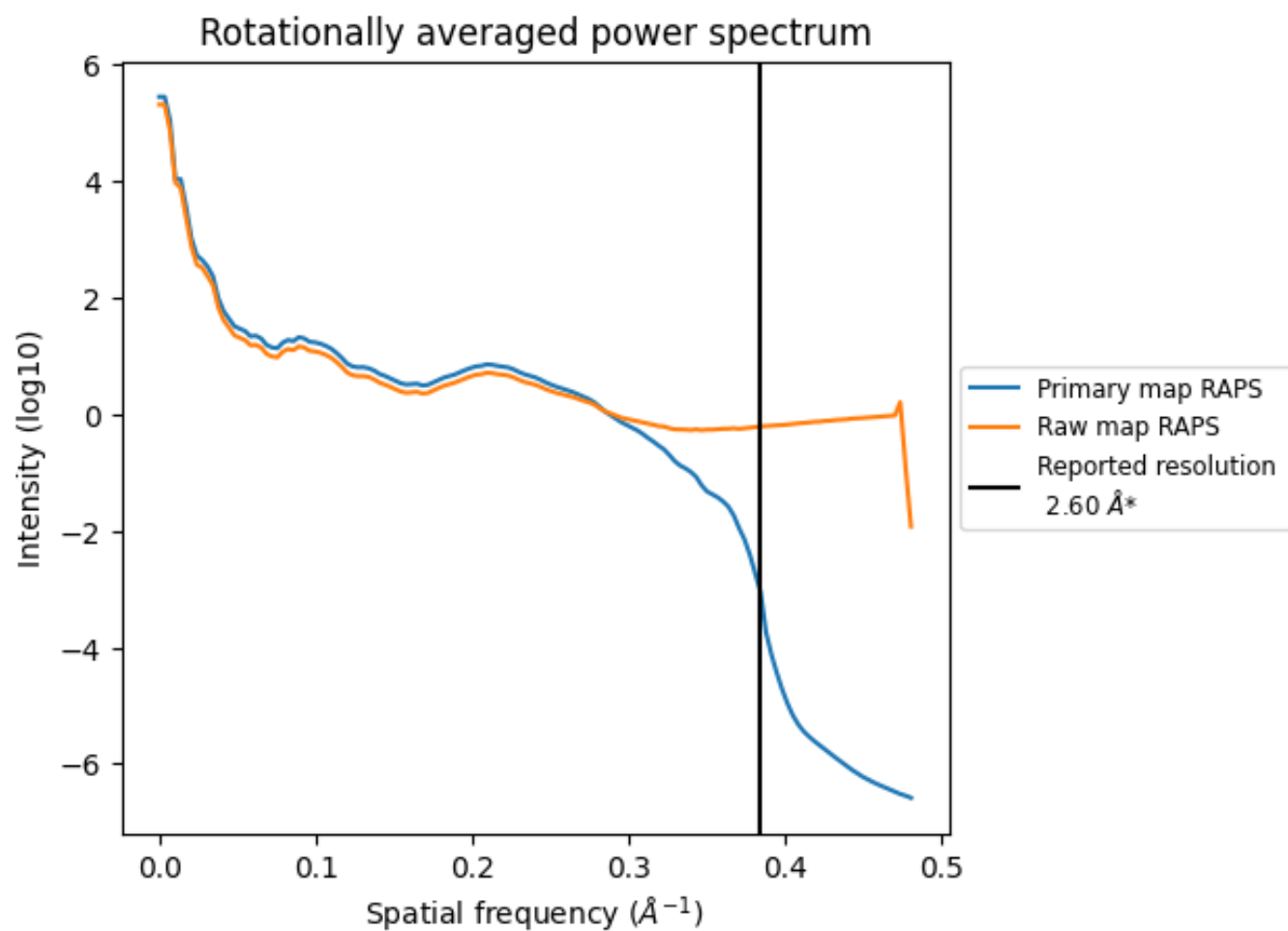
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm³; this corresponds to an approximate mass of 226 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 ⓘ

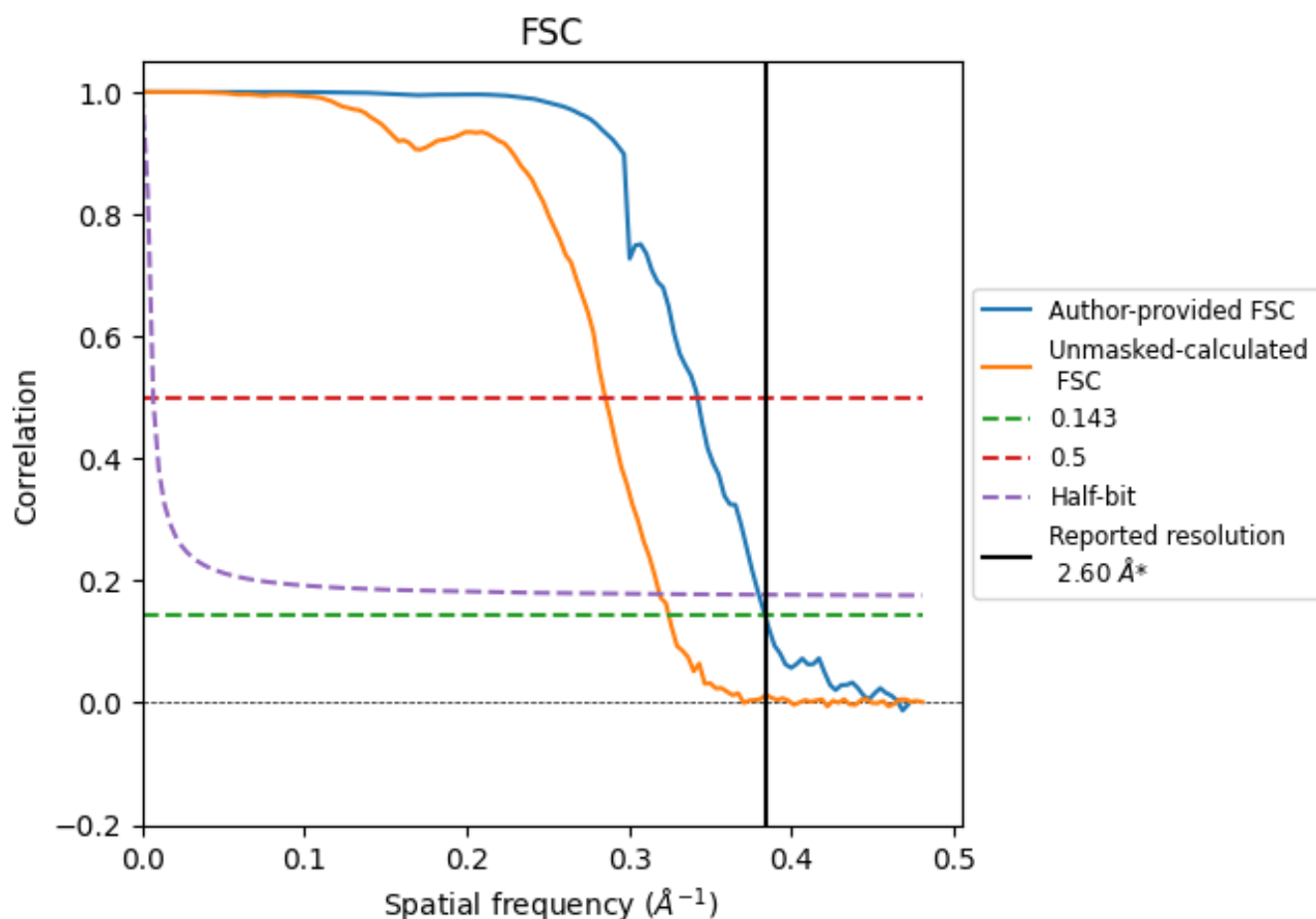


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

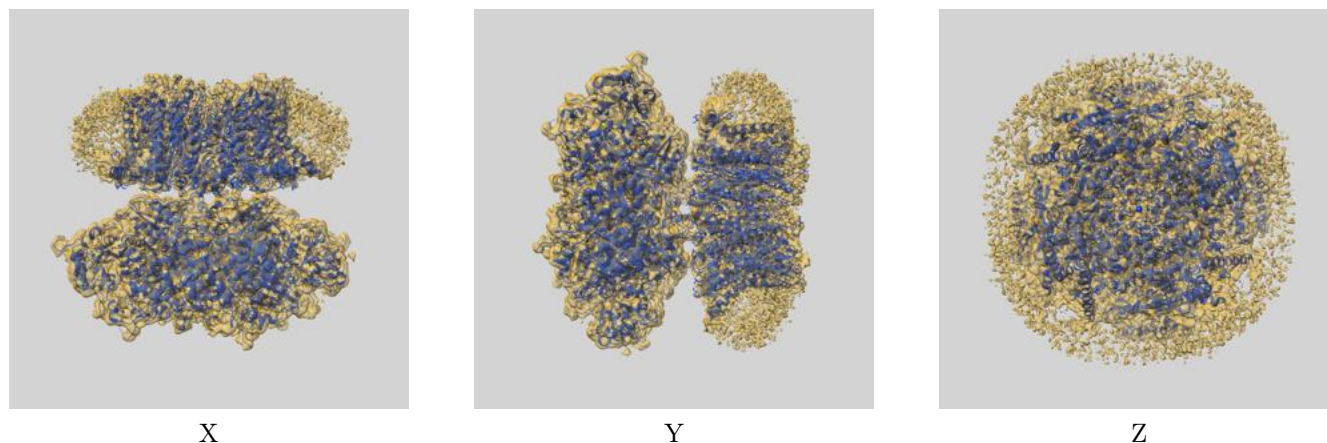
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	2.92	2.63
Unmasked-calculated*	3.08	3.50	3.14

*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 3.08 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

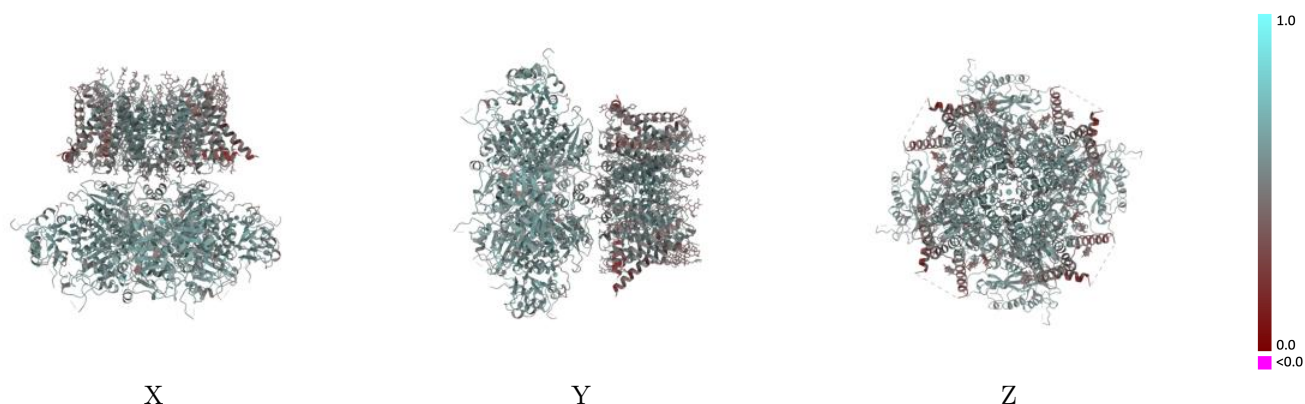
This section contains information regarding the fit between EMDB map EMD-75627 and PDB model 11CZ. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



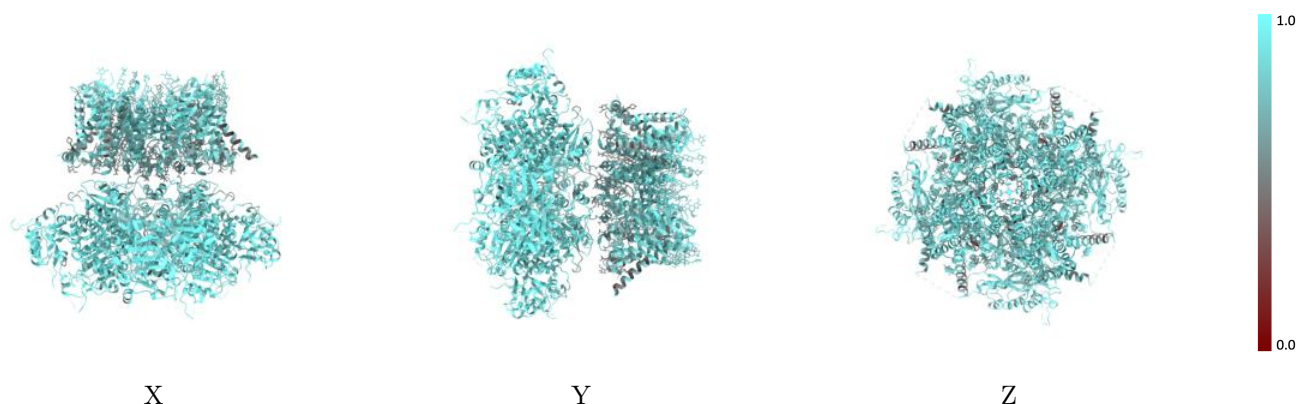
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



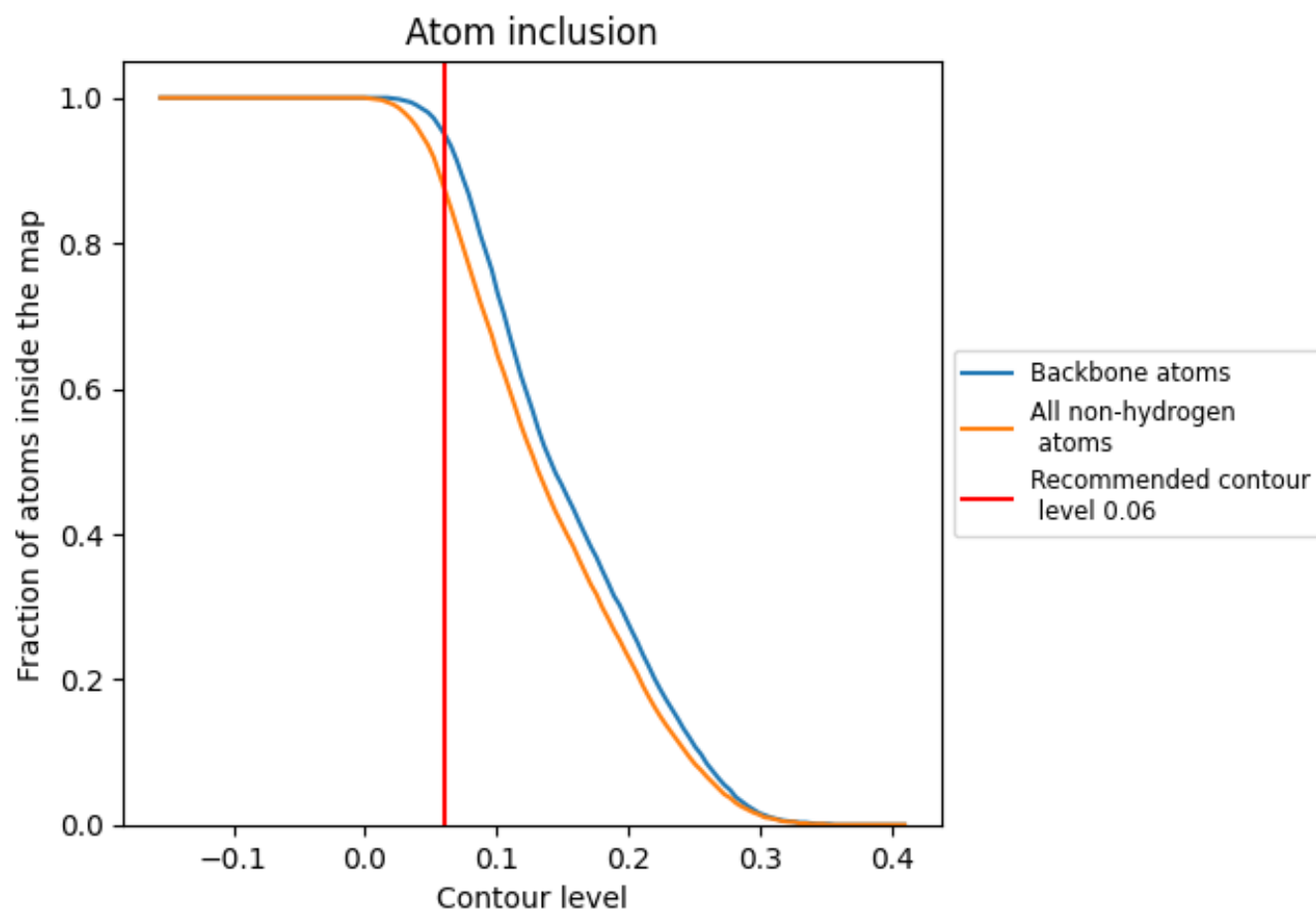
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8770	0.5410
A	0.8800	0.5410
B	0.8800	0.5410
C	0.8820	0.5410
D	0.8800	0.5410

