



Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 05:53 AM EDT

PDB ID : 11DC / pdb_000011dc
EMDB ID : EMD-75630
Title : Human Slo1-PenitremA complex under divalent chelated condition - gating-ring masked out
Authors : Chowdhury, S.; Pal, K.; Kallure, G.S.
Deposited on : 2026-02-18
Resolution : 2.58 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

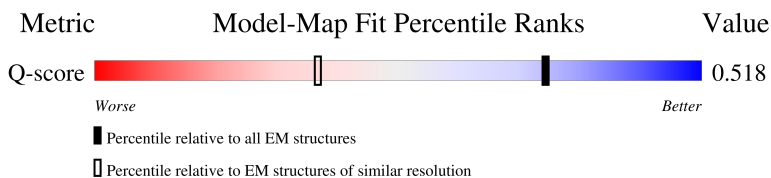
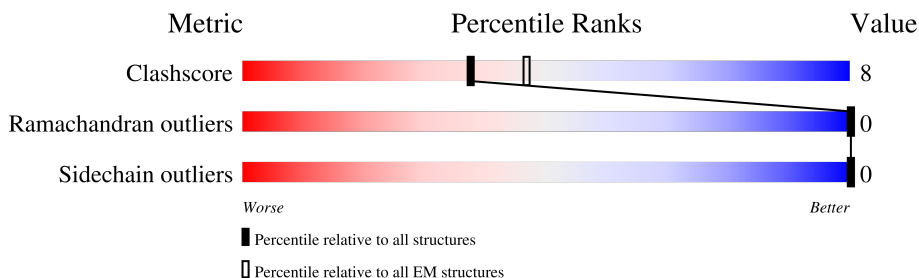
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.58 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	7675 (2.08 - 3.08)

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	1106	X	-	-	-
3	LBN	A	1107	X	-	-	-
3	LBN	A	1108	X	-	-	-
3	LBN	A	1109	X	-	-	-
3	LBN	A	1110	X	-	-	-
3	LBN	A	1119	X	-	-	-
3	LBN	A	1120	X	-	-	-
3	LBN	A	1121	X	-	-	-
3	LBN	A	1122	X	-	-	-
3	LBN	B	1101	X	-	-	-
3	LBN	B	1102	X	-	-	-
3	LBN	B	1103	X	-	-	-
3	LBN	B	1112	X	-	-	-
3	LBN	B	1113	X	-	-	-
3	LBN	B	1114	X	-	-	-
3	LBN	B	1115	X	-	-	-
3	LBN	C	1101	X	-	-	-
3	LBN	C	1102	X	-	-	-
3	LBN	C	1103	X	-	-	-
3	LBN	C	1104	X	-	-	-
3	LBN	C	1113	X	-	-	-
3	LBN	C	1114	X	-	-	-
3	LBN	C	1115	X	-	-	-
3	LBN	C	1116	X	-	-	-
3	LBN	D	1101	X	-	-	-
3	LBN	D	1102	X	-	-	-
3	LBN	D	1103	X	-	-	-
3	LBN	D	1104	X	-	-	-
3	LBN	D	1113	X	-	-	-
3	LBN	D	1114	X	-	-	-
3	LBN	D	1115	X	-	-	-
3	LBN	D	1116	X	-	-	-
5	CLR	A	1112	X	-	-	-
5	CLR	A	1113	X	-	-	-
5	CLR	A	1114	X	-	-	-
5	CLR	A	1115	X	-	-	-
5	CLR	A	1116	X	-	-	-
5	CLR	A	1117	X	-	-	-
5	CLR	A	1118	X	-	-	-
5	CLR	B	1105	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLR	B	1106	X	-	-	-
5	CLR	B	1107	X	-	-	-
5	CLR	B	1108	X	-	-	-
5	CLR	B	1109	X	-	-	-
5	CLR	B	1110	X	-	-	-
5	CLR	B	1111	X	-	-	-
5	CLR	C	1106	X	-	-	-
5	CLR	C	1107	X	-	-	-
5	CLR	C	1108	X	-	-	-
5	CLR	C	1109	X	-	-	-
5	CLR	C	1110	X	-	-	-
5	CLR	C	1111	X	-	-	-
5	CLR	C	1112	X	-	-	-
5	CLR	D	1106	X	-	-	-
5	CLR	D	1107	X	-	-	-
5	CLR	D	1108	X	-	-	-
5	CLR	D	1109	X	-	-	-
5	CLR	D	1110	X	-	-	-
5	CLR	D	1111	X	-	-	-
5	CLR	D	1112	X	-	-	-
6	A1C9J	A	1130	X	-	-	-
6	A1C9J	B	1123	X	-	-	-
6	A1C9J	C	1124	X	-	-	-
6	A1C9J	D	1124	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12327 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 Isoform 5 of Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	274	Total	C	N	O	S	0	0
			2251	1515	352	373	11		
1	B	274	Total	C	N	O	S	0	0
			2251	1515	352	373	11		
1	C	274	Total	C	N	O	S	0	0
			2251	1515	352	373	11		
1	D	274	Total	C	N	O	S	0	0
			2251	1515	352	373	11		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	513	ILE	MET	engineered mutation	UNP Q12791
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	513	ILE	MET	engineered mutation	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	513	ILE	MET	engineered mutation	UNP Q12791

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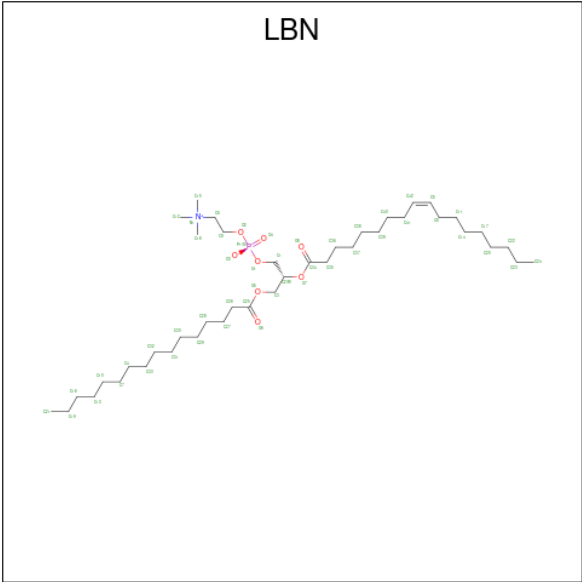
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	SER	-	expression tag	UNP Q12791
C	1058	ASN	-	expression tag	UNP Q12791
C	1059	SER	-	expression tag	UNP Q12791
C	1060	LEU	-	expression tag	UNP Q12791
C	1061	GLU	-	expression tag	UNP Q12791
C	1062	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	513	ILE	MET	engineered mutation	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).

Mol	Chain	Residues	Atoms	AltConf
2	A	5	Total K 5 5	0

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



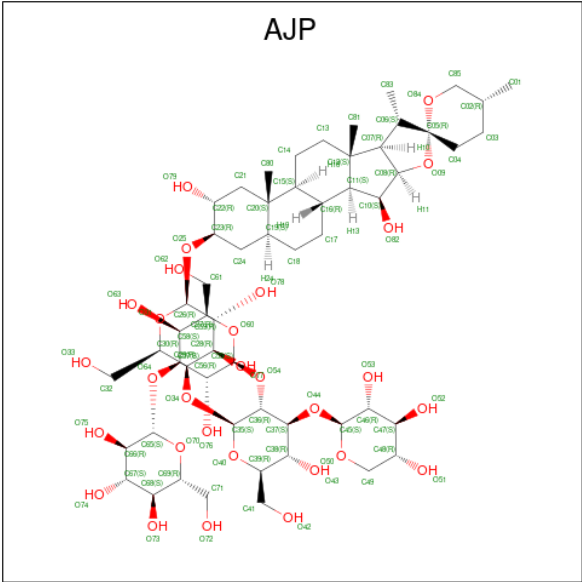
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			22	14	7	1	
3	A	1	Total	C	O	P	0
			22	14	7	1	
3	A	1	Total	C	O	P	0
			22	14	7	1	
3	A	1	Total	C	O	P	0
			24	15	8	1	
3	A	1	Total	C	O	P	0
			36	27	8	1	
3	A	1	Total	C	O	P	0
			31	22	8	1	
3	A	1	Total	C	O	P	0
			20	12	7	1	
3	A	1	Total	C	O	P	0
			29	20	8	1	
3	A	1	Total	C	O	P	0
			27	18	8	1	
3	B	1	Total	C	O	P	0
			22	14	7	1	
3	B	1	Total	C	O	P	0
			24	15	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	

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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	O	P	0
			20	12	7	1	
3	B	1	Total	C	O	P	0
			27	18	8	1	
3	C	1	Total	C	O	P	0
			22	14	7	1	
3	C	1	Total	C	O	P	0
			22	14	7	1	
3	C	1	Total	C	O	P	0
			24	15	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	C	1	Total	C	O	P	0
			27	18	8	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
			24	15	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	
3	D	1	Total	C	O	P	0
			27	18	8	1	

- Molecule 4 is Digitonin (CCD ID: AJP) (formula: C₅₆H₉₂O₂₉).



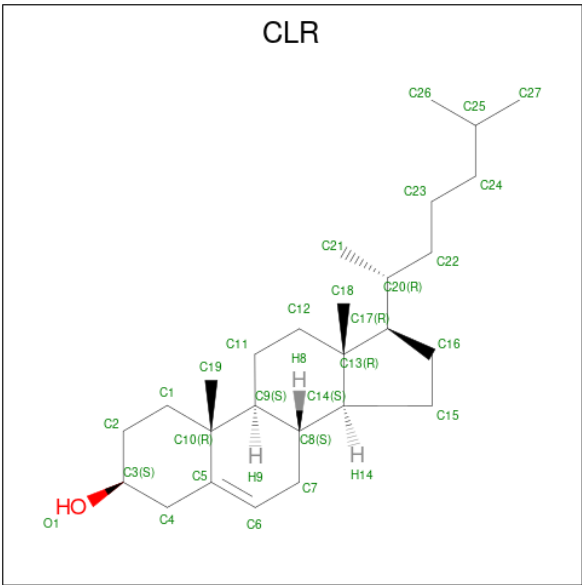
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			54	39	15	
			Total	C	O	
			43	33	10	
			Total	C	O	
4	A	1	43	33	10	0
			Total	C	O	
			43	33	10	
			Total	C	O	
			43	33	10	
4	A	1	Total	C	O	0
			43	33	10	
			Total	C	O	
			65	45	20	
			Total	C	O	
4	A	1	43	33	10	0
			Total	C	O	
			43	33	10	
			Total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

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

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



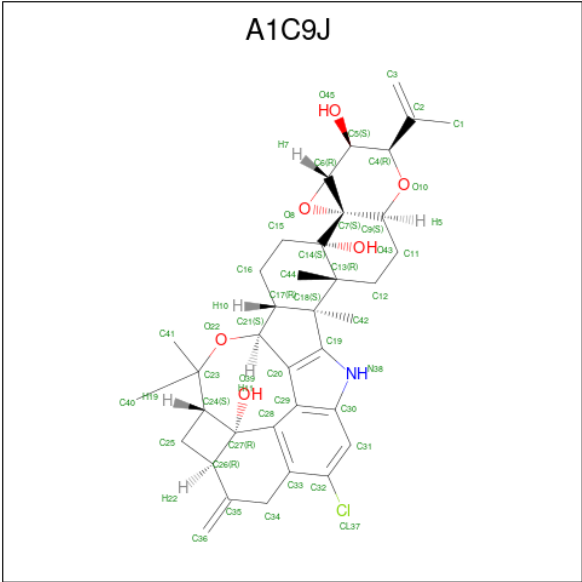
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27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

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

- Molecule 6 is Penitrem A (CCD ID: A1C9J) (formula: $C_{37}H_{44}ClNO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Cl	N	O	0
			45	37	1	1	6	
6	B	1	Total	C	Cl	N	O	0
			45	37	1	1	6	
6	C	1	Total	C	Cl	N	O	0
			45	37	1	1	6	
6	D	1	Total	C	Cl	N	O	0
			45	37	1	1	6	

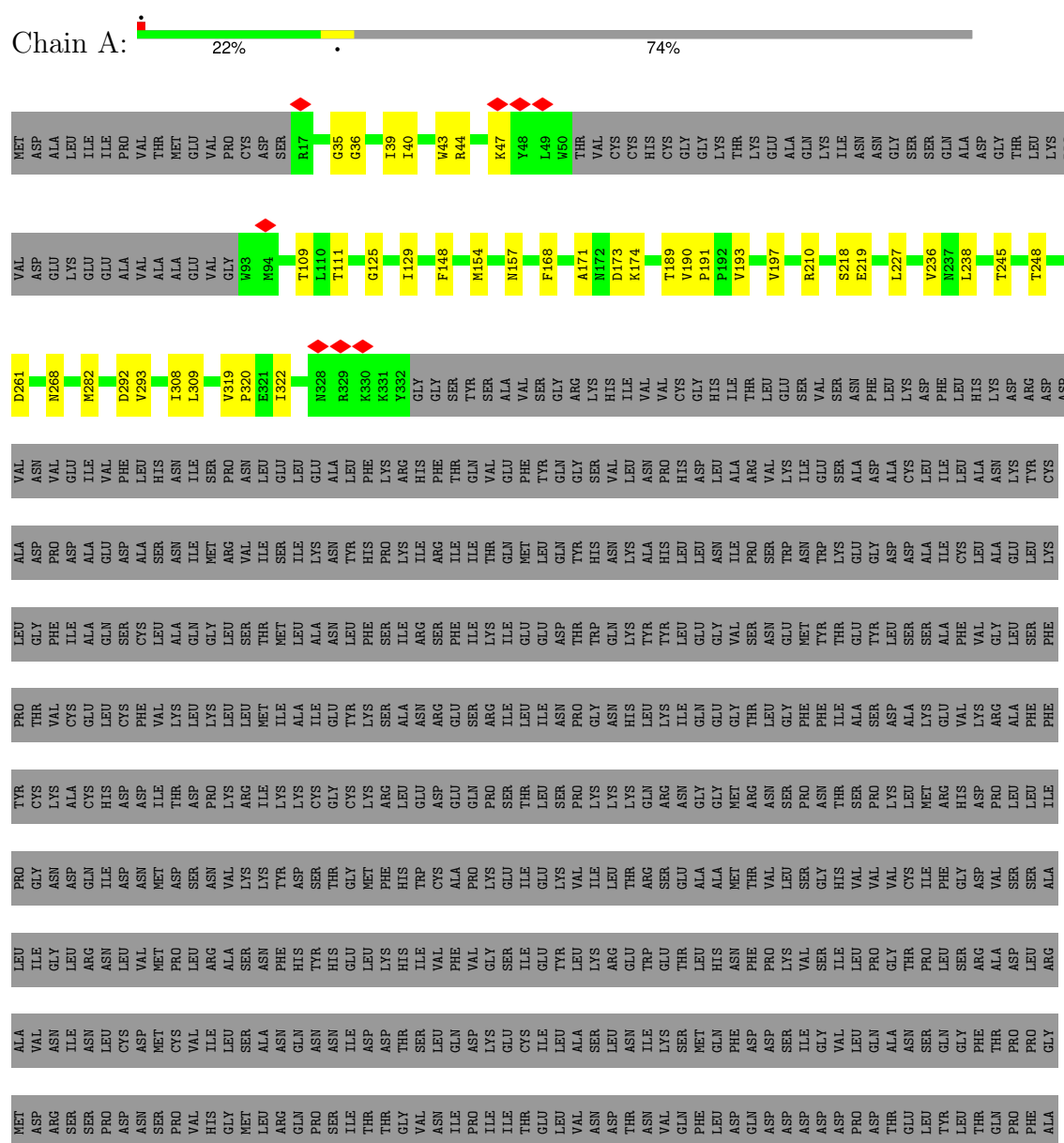
- Molecule 7 is water.

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

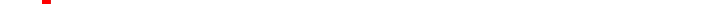
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Isoform 5 of Calcium-activated potassium channel subunit alpha-1



ARG	TYR	VAL	ILE	THR	ASN	PRO	PRO	TYR	GLU	PHE	GLU	LEU	VAL	PRO	THR	ASP	LEU	ILE	PHE	CYS	LEU	MET	GLN	PHE	ASP	SER	ASN	SER	LEU	GLU	VAL	LEU	PHE	GLN
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- Molecule 1: Isoform 5 of Calcium-activated potassium channel subunit alpha-1

Chain B:  22% 74%

THR	LEU	LYS	PRO	VAL	ASP	GLU	GLU	GLU	GLU	ALA	VAL	ALA	ALA	GLU	VAL	GLY	W93	W94	W100	T109	L110	T111	G125	I129	F148	M154	F168	A171	N172	D173	K174	T189	V190	P191	P192	V193	V197	R210	S218	E219	L227	V236	N237	L238
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T245
T248
D261
N268
M282
D292
V293
L308
L309
V319
P320
E321
L322
N328
R329
K330
K331
Y332
GLY
GLY
SER
TYR
SER
SER
ALA
ALA
VAL
SER
GLY
ARG
HIS
HIS
ILE
ILE
VAL
VAL
CYS
GLY
HIS
HIS
ILE
THR
LEU
LEU
GLU
SER
VAL
SER
ASN
PHE
LEU
HIS
LYS
ASP
PHE
LEU
HIS
LYS

ASP ARG ASP ASP VAL ASN VAL GLU LEU HIS ASN SER PRO ASN LEU GLU LEU GLU ALA LEU PHE LYS ARG HIS PHE THR GLN VAL GLU PHE TYR GLN GLY SER VAL VAL LEU ASN PRO HIS ASP LEU ALA ALA ARG VAL LYS LEU GLU SER ALA ASP ALA CYS LEU LEU LEU LEU

ASN	LYS	TYR	CYS	ALA	ASP	PRO	ASP	ALA	GLU	ASP	ALA	ALA	SER	ASN	ILE	ILE	VAL	ARG	MET	GLN	ILE	ILE	ILE	THR	GLN	LEU	GLN	TYR	HIS	ASN	LYS	ALA	HIS	LEU	LEU	ASP	ASN	GLY	GLU	TRP	TRP	LYS	LYS	ASP	ASP	ALA	ALA	CYS	LEU
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ALA	GLU	LEU	LYS	GLY	PHE	ILE	ALA	GLN	SER	CYS	LEU	ALA	GLN	GLY	SER	THR	MET	LEU	ALA	ASN	LEU	PHE	SER	ILE	ARG	SER	PHE	ILE	LYS	ILE	GLU	GLU	ASP	THR	TRP	GLN	LYS	TYR	TYR	LEU	GLU	GLY	VAL	SER	ASN	GLU	MET	TYR	THR	GLU	TYR	LEU	SER	SER	ALA	PHE	VAL
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GLY LEU SER SER PHE PRO THR VAL CYS LEU LEU PHE VAL LYS LYS LYS LEU LEU LEU LEU MET ILE ILE ALA ALA GLU TYR LYS SER SER ASN ASN ARG ARG GLU SER ARG ILE ILE ILE ASN PRO PRO GLY GLY ASN ASN HIS HIS LEU LEU LYS ILE ILE GLN GLY GLY GLY THR LEU LEU GLY PHE PHE PHE ILE ILE ALA ALA SER ASP ALA LYS LYS GLU VAL VAL

ARG	ALA	PHE	PHE	TYR	CYS	LYS	ALA	CYS	HIS	ASP	ASP	ILE	THR	ASP	PRO	LYS	ARG	LYS	GLY	CYS	LYS	ARG	LEU	GLU	ASP	GLU	GLN	PRO	SER	THR	SER	LEU	SER	PRO	LYS	LYS	LYS	GLN	GLN	ARG	ASN	GLY	GLY	MET	MET	ARG	ASN	SER	SER	PRO	ASN	THR	THR	PRO	LYS	LEU	LYS	MET	MET	ARG	HIS	ASP
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PRO	LEU	LEU	ILE	ILE	PRO	GLY	ASN	ASP	ASN	GLN	ILE	ILE	ASP	ASN	MET	ASP	SER	ASN	VAL	LYS	LYS	TYR	ASP	SER	SER	THR	GLY	MET	PHE	HIS	TRP	CYS	ALA	ALA	PRO	LYS	GLU	ILE	ILE	LYS	VAL	LEU	THR	THR	ARG	SER	GLU	ALA	ALA	ALA	MET	MET	THR	THR	VAL	LEU	SER	GLY	HIS	VAL	VAL	VAL	CYS	ILE	PHE	GLY	ASP
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VAL	SER	SER	SER	ALA	ALA	LEU	ILE	GLY	LEU	ARG	ASN	LEU	VAL	MET	PRO	LEU	ARG	ALA	SER	ASN	PHE	HIS	TYR	HIS	GLU	LEU	LYS	HIS	ILE	VAL	PHE	VAL	GLY	SER	ILE	GLU	TYR	LEU	LYS	ARG	GLU	TRP	GLU	THR	LEU	HIS	ASN	PHE	PRO	LYS	VAL	SER	ILE	LEU	PRO	GLY	THR	PRO	LEU	SER	ARG
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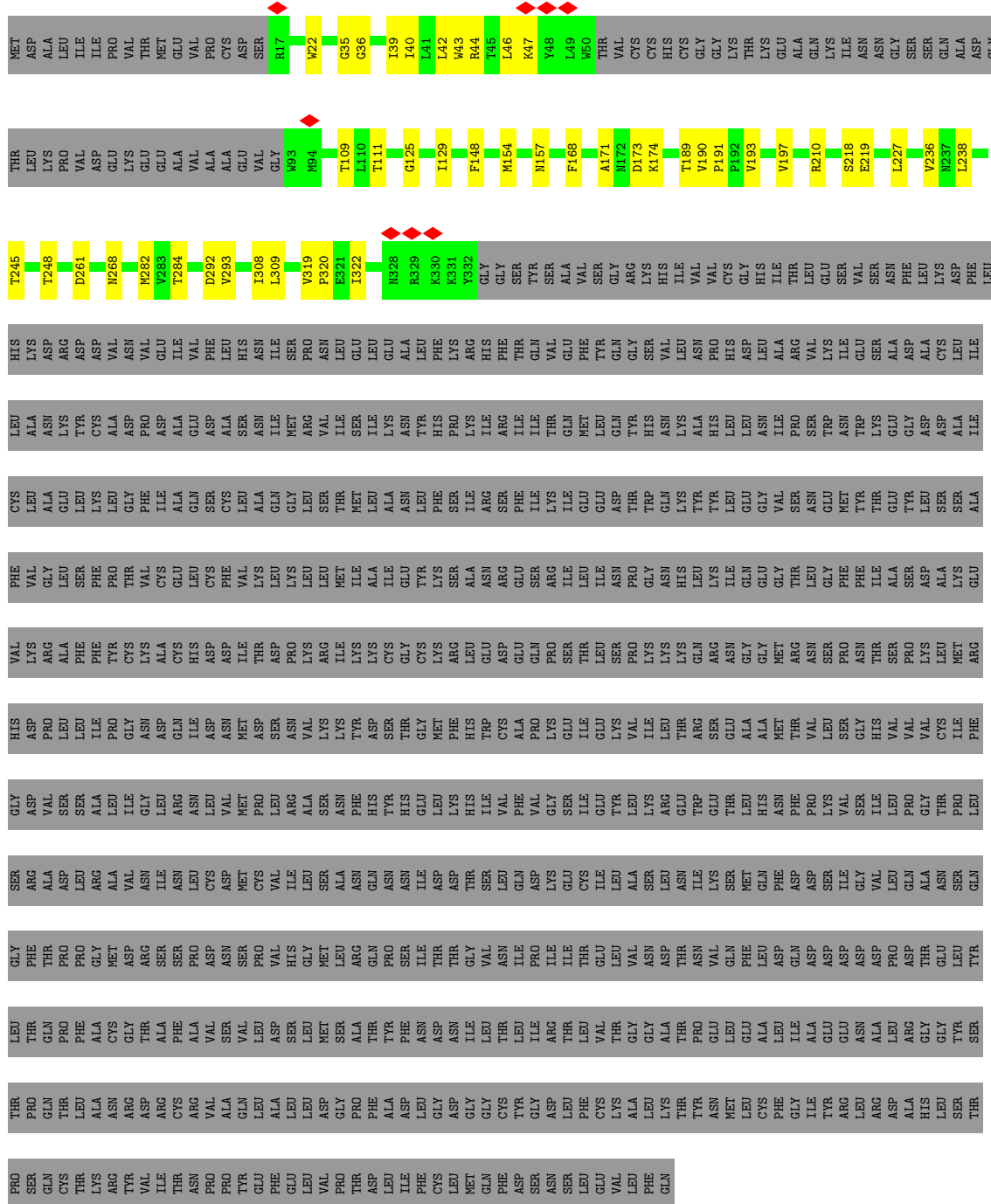
ALA ASP LEU LEU ARG ALA VAL ASN ASN ILE LEU LEU CYS ASP MET CYS VAL VAL ILE ILE LEU SER ALA ALA ASN GLN ASN ASN ASN ILE ASP ASP LYS GLU CYS ILE LEU ALA SER SER LEU LEU ASN ASN LYS SER MET GLN PHE ASP ASP SER ILE GLY VAL VAL GLN ALA ASN SER GLN GLY PHE

[illegible]

GLN PRO PHE PRO CYS GLY THR ALA ALA PHE VAL SER VAL ASP SER THR TYR PHE ASN ASP ASN THR LEU LEU LEU LEU LEU LEU ARG THR VAL THR GLY ALA ALA THR THR PRO GLU LEU GLU ALA LEU ILE ALA GLU ASN THR LEU ARG GLY TYR SER THR PRO

GLN THR LEU LEU ALA ALA ASN ARG ASP ARG ARG CYS VAL VAL GLN LEU ALA ALA LEU LEU LEU LEU GLY GLY PRO PRO PHE PHE ASP ASP LEU LEU GLY GLY CYS CYS TYR TYR GLY ASP LEU LEU PHE PHE CYS CYS LYS LYS ALA ALA LEU LEU LYS TYR THR TYR TYR ASN ASN MET MET LEU LEU CYS CYS PHE PHE GLY GLY ILE TYR TYR ARG ARG LEU LEU ARG ARG ASP ASP ALA ALA HIS HIS LEU LEU SER SER THR THR PRO PRO PHE PHE

Chain C: 22% . 74%



Chain D: 22% 0% 74%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	235323	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	0.494	Depositor
Minimum map value	-0.202	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.08	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: CLR, AJP, A1C9J, K, LBN

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	0.14	0/2317	0.31	0/3151
1	B	0.14	0/2317	0.31	0/3151
1	C	0.14	0/2317	0.31	0/3151
1	D	0.14	0/2317	0.31	0/3151
All	All	0.14	0/9268	0.31	0/12604

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	2251	0	2274	28	0
1	B	2251	0	2274	31	0
1	C	2251	0	2274	31	0
1	D	2251	0	2274	28	0
2	A	5	0	0	0	0
3	A	233	0	0	1	0
3	B	188	0	0	1	0
3	C	210	0	0	0	0
3	D	211	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	377	0	0	1	0
4	B	377	0	0	1	0
4	C	377	0	0	1	0
4	D	377	0	0	1	0
5	A	196	0	320	16	0
5	B	196	0	320	18	0
5	C	196	0	320	18	0
5	D	196	0	318	16	0
6	A	45	0	0	0	0
6	B	45	0	0	0	0
6	C	45	0	0	0	0
6	D	45	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	12327	0	10374	171	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 8.

All (171) 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:168:PHE:O	1:B:174:LYS:NZ	2.20	0.74
1:D:168:PHE:O	1:D:174:LYS:NZ	2.20	0.74
1:C:168:PHE:O	1:C:174:LYS:NZ	2.20	0.73
1:A:168:PHE:O	1:A:174:LYS:NZ	2.20	0.73
1:A:44:ARG:NH2	1:A:173:ASP:OD2	2.23	0.71
1:C:44:ARG:NH2	1:C:173:ASP:OD2	2.23	0.71
1:D:44:ARG:NH2	1:D:173:ASP:OD2	2.23	0.70
1:B:44:ARG:NH2	1:B:173:ASP:OD2	2.23	0.68
1:B:174:LYS:HG3	5:B:1111:CLR:H191	1.77	0.64
1:D:174:LYS:HG3	5:D:1112:CLR:H111	1.83	0.60
1:D:154:MET:HE2	1:D:197:VAL:HG22	1.84	0.60
1:C:154:MET:HE2	1:C:197:VAL:HG22	1.84	0.59
3:B:1102:LBN:O2	4:B:1104:AJP:O78	2.20	0.59
1:A:154:MET:HE2	1:A:197:VAL:HG22	1.84	0.59
1:B:154:MET:HE2	1:B:197:VAL:HG22	1.84	0.58
1:D:157:ASN:ND2	1:D:193:VAL:HG21	2.21	0.55
3:A:1109:LBN:O2	4:A:1111:AJP:O78	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1120:AJP:O34	4:D:1120:AJP:O33	2.25	0.54
1:D:218:SER:OG	1:D:219:GLU:OE2	2.27	0.53
1:B:218:SER:OG	1:B:219:GLU:OE2	2.27	0.53
1:A:174:LYS:HG3	5:A:1118:CLR:H111	1.91	0.52
1:A:218:SER:OG	1:A:219:GLU:OE2	2.27	0.52
1:C:218:SER:OG	1:C:219:GLU:OE2	2.27	0.52
1:C:36:GLY:O	1:C:40:ILE:HG12	2.11	0.51
1:C:245:THR:HA	1:C:248:THR:HG22	1.92	0.51
1:D:245:THR:HA	1:D:248:THR:HG22	1.92	0.51
1:A:245:THR:HA	1:A:248:THR:HG22	1.92	0.51
1:B:36:GLY:O	1:B:40:ILE:HG12	2.11	0.51
1:A:36:GLY:O	1:A:40:ILE:HG12	2.11	0.50
1:B:245:THR:HA	1:B:248:THR:HG22	1.92	0.50
1:D:36:GLY:O	1:D:40:ILE:HG12	2.10	0.50
1:A:190:VAL:HB	1:A:191:PRO:HD3	1.95	0.49
1:B:190:VAL:HB	1:B:191:PRO:HD3	1.95	0.48
5:D:1108:CLR:H20	5:D:1108:CLR:H183	1.49	0.48
5:A:1114:CLR:H183	5:A:1114:CLR:H20	1.52	0.48
5:A:1118:CLR:H152	5:A:1118:CLR:H181	1.66	0.48
5:A:1113:CLR:H20	5:A:1113:CLR:H183	1.44	0.48
1:A:189:THR:HG21	1:A:210:ARG:HE	1.79	0.48
5:A:1113:CLR:H152	5:A:1113:CLR:H181	1.67	0.48
5:C:1108:CLR:H183	5:C:1108:CLR:H20	1.49	0.48
5:D:1109:CLR:H20	5:D:1109:CLR:H183	1.56	0.48
5:B:1106:CLR:H20	5:B:1106:CLR:H183	1.53	0.48
1:D:190:VAL:HB	1:D:191:PRO:HD3	1.95	0.48
1:C:174:LYS:HG3	5:C:1112:CLR:H111	1.94	0.48
1:C:309:LEU:HG	1:D:282:MET:HE2	1.96	0.48
5:D:1112:CLR:H183	5:D:1112:CLR:H20	1.40	0.48
5:C:1112:CLR:H232	5:C:1112:CLR:H211	1.67	0.47
1:C:189:THR:HG21	1:C:210:ARG:HE	1.79	0.47
1:C:190:VAL:HB	1:C:191:PRO:HD3	1.95	0.47
1:D:189:THR:HG21	1:D:210:ARG:HE	1.79	0.47
5:D:1111:CLR:H20	5:D:1111:CLR:H183	1.43	0.47
5:B:1110:CLR:H183	5:B:1110:CLR:H20	1.43	0.47
1:C:238:LEU:HD21	1:C:322:ILE:HG22	1.96	0.47
1:B:189:THR:HG21	1:B:210:ARG:HE	1.79	0.47
1:B:238:LEU:HD21	1:B:322:ILE:HG22	1.96	0.47
5:D:1106:CLR:H111	5:D:1106:CLR:H182	1.64	0.47
1:A:308:ILE:HG22	1:B:282:MET:HE3	1.97	0.47
5:D:1112:CLR:H211	5:D:1112:CLR:H232	1.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD21	1:A:322:ILE:HG22	1.96	0.46
5:A:1115:CLR:H183	5:A:1115:CLR:H20	1.49	0.46
1:B:308:ILE:HG22	1:C:282:MET:HE3	1.97	0.46
1:D:238:LEU:HD21	1:D:322:ILE:HG22	1.96	0.46
5:C:1110:CLR:H111	5:C:1110:CLR:H182	1.87	0.46
1:C:308:ILE:HG22	1:D:282:MET:HE3	1.97	0.46
1:A:282:MET:HE3	1:D:308:ILE:HG22	1.98	0.46
5:D:1112:CLR:H152	5:D:1112:CLR:H181	1.67	0.46
1:A:35:GLY:O	1:A:39:ILE:HG12	2.16	0.46
1:D:35:GLY:O	1:D:39:ILE:HG12	2.16	0.46
5:D:1110:CLR:H111	5:D:1110:CLR:H182	1.88	0.46
5:B:1111:CLR:H211	5:B:1111:CLR:H232	1.66	0.45
1:A:282:MET:HE2	1:D:309:LEU:HG	1.98	0.45
1:D:219:GLU:OE2	1:D:219:GLU:N	2.50	0.45
1:B:35:GLY:O	1:B:39:ILE:HG12	2.16	0.45
1:A:171:ALA:HB3	1:A:174:LYS:NZ	2.32	0.45
1:A:319:VAL:HG12	1:A:320:PRO:HD3	1.99	0.45
1:B:219:GLU:OE2	1:B:219:GLU:N	2.50	0.45
5:D:1110:CLR:H211	5:D:1110:CLR:H231	1.74	0.45
1:A:309:LEU:HG	1:B:282:MET:HE2	1.99	0.45
1:C:171:ALA:HB3	1:C:174:LYS:NZ	2.32	0.45
5:A:1115:CLR:H152	5:A:1115:CLR:H181	1.68	0.45
5:B:1111:CLR:H20	5:B:1111:CLR:H183	1.37	0.45
1:D:319:VAL:HG12	1:D:320:PRO:HD3	1.99	0.44
1:C:35:GLY:O	1:C:39:ILE:HG12	2.16	0.44
1:A:292:ASP:OD1	1:A:293:VAL:N	2.51	0.44
5:B:1111:CLR:H273	5:B:1111:CLR:H231	1.82	0.44
1:C:219:GLU:OE2	1:C:219:GLU:N	2.50	0.44
5:C:1108:CLR:H111	5:C:1108:CLR:H182	1.91	0.44
5:C:1112:CLR:H152	5:C:1112:CLR:H181	1.67	0.44
1:B:309:LEU:HG	1:C:282:MET:HE2	2.00	0.44
5:B:1108:CLR:H183	5:B:1108:CLR:H20	1.56	0.44
1:D:171:ALA:HB3	1:D:174:LYS:NZ	2.32	0.44
5:A:1118:CLR:H211	5:A:1118:CLR:H232	1.66	0.44
1:A:219:GLU:OE2	1:A:219:GLU:N	2.50	0.44
5:A:1114:CLR:H152	5:A:1114:CLR:H181	1.69	0.44
1:C:261:ASP:OD2	1:C:268:ASN:ND2	2.35	0.44
5:C:1108:CLR:H152	5:C:1108:CLR:H181	1.68	0.44
1:D:292:ASP:OD1	1:D:293:VAL:N	2.51	0.44
5:B:1110:CLR:H111	5:B:1110:CLR:H182	1.92	0.43
1:A:43:TRP:CH2	1:A:47:LYS:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ALA:HB3	1:B:174:LYS:NZ	2.32	0.43
1:C:319:VAL:HG12	1:C:320:PRO:HD3	1.99	0.43
1:C:109:THR:HG22	1:C:111:THR:H	1.84	0.43
1:C:292:ASP:OD1	1:C:293:VAL:N	2.51	0.43
5:C:1109:CLR:H152	5:C:1109:CLR:H181	1.69	0.43
1:D:43:TRP:CH2	1:D:47:LYS:HG3	2.54	0.43
5:C:1106:CLR:H211	5:C:1106:CLR:H231	1.66	0.43
1:A:261:ASP:OD2	1:A:268:ASN:ND2	2.35	0.43
1:B:125:GLY:O	1:B:129:ILE:HG12	2.19	0.43
5:D:1107:CLR:H111	5:D:1107:CLR:H182	1.93	0.43
1:A:109:THR:HG22	1:A:111:THR:H	1.84	0.43
1:A:125:GLY:O	1:A:129:ILE:HG12	2.19	0.43
1:B:319:VAL:HG12	1:B:320:PRO:HD3	1.99	0.43
1:A:148:PHE:CE1	5:A:1115:CLR:H9	2.53	0.43
5:A:1117:CLR:H263	5:A:1117:CLR:H231	1.76	0.43
5:C:1107:CLR:H273	5:C:1107:CLR:H231	1.79	0.43
5:C:1108:CLR:H162	5:C:1108:CLR:H221	1.76	0.43
5:A:1113:CLR:H111	5:A:1113:CLR:H182	1.91	0.43
1:B:148:PHE:CE1	5:B:1107:CLR:H9	2.53	0.43
1:C:43:TRP:CH2	1:C:47:LYS:HG3	2.54	0.43
1:B:43:TRP:CH2	1:B:47:LYS:HG3	2.53	0.42
1:B:261:ASP:OD2	1:B:268:ASN:ND2	2.35	0.42
5:C:1106:CLR:H221	5:C:1106:CLR:C12	2.49	0.42
1:B:109:THR:HG22	1:B:111:THR:H	1.84	0.42
5:C:1111:CLR:H111	5:C:1111:CLR:H182	1.91	0.42
5:A:1115:CLR:H111	5:A:1115:CLR:H182	1.90	0.42
5:A:1116:CLR:H213	5:A:1116:CLR:H231	1.79	0.42
1:D:148:PHE:CE1	5:D:1108:CLR:H9	2.54	0.42
1:B:292:ASP:OD1	1:B:293:VAL:N	2.51	0.42
5:C:1112:CLR:H183	5:C:1112:CLR:H20	1.41	0.42
5:C:1109:CLR:H20	5:C:1109:CLR:H183	1.56	0.42
1:D:125:GLY:O	1:D:129:ILE:HG12	2.19	0.42
5:D:1107:CLR:H20	5:D:1107:CLR:H183	1.53	0.42
5:D:1112:CLR:H222	5:D:1112:CLR:H162	1.94	0.42
1:D:109:THR:HG22	1:D:111:THR:H	1.84	0.42
1:C:125:GLY:O	1:C:129:ILE:HG12	2.19	0.42
1:D:261:ASP:OD2	1:D:268:ASN:ND2	2.35	0.42
5:D:1106:CLR:H162	5:D:1106:CLR:H181	1.66	0.42
1:B:227:LEU:HD11	1:B:236:VAL:HG21	2.02	0.42
5:C:1112:CLR:H111	5:C:1112:CLR:H182	1.88	0.41
5:B:1109:CLR:H211	5:B:1109:CLR:H231	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1105:AJP:O34	4:C:1105:AJP:O33	2.37	0.41
1:D:227:LEU:HD11	1:D:236:VAL:HG21	2.02	0.41
1:C:227:LEU:HD11	1:C:236:VAL:HG21	2.02	0.41
1:C:284:THR:OG1	1:D:290:TYR:OH	2.21	0.41
5:A:1115:CLR:H162	5:A:1115:CLR:H221	1.76	0.41
1:D:193:VAL:O	1:D:197:VAL:HG23	2.21	0.41
5:B:1107:CLR:H183	5:B:1107:CLR:H20	1.49	0.41
5:A:1112:CLR:H111	5:A:1112:CLR:H182	1.94	0.41
5:D:1108:CLR:H111	5:D:1108:CLR:H182	1.91	0.41
1:A:227:LEU:HD11	1:A:236:VAL:HG21	2.02	0.41
1:B:43:TRP:CZ3	1:B:47:LYS:HG3	2.56	0.41
1:B:193:VAL:O	1:B:197:VAL:HG23	2.21	0.41
5:B:1106:CLR:H162	5:B:1106:CLR:H221	1.89	0.41
5:B:1107:CLR:H111	5:B:1107:CLR:H182	1.91	0.41
5:B:1109:CLR:H231	5:B:1109:CLR:H263	1.75	0.41
1:C:22:TRP:CZ3	5:C:1106:CLR:H3	2.56	0.41
1:C:148:PHE:CE1	5:C:1108:CLR:H9	2.55	0.41
1:C:193:VAL:O	1:C:197:VAL:HG23	2.21	0.41
5:B:1105:CLR:H211	5:B:1105:CLR:H231	1.63	0.41
1:A:193:VAL:O	1:A:197:VAL:HG23	2.21	0.40
1:B:42:LEU:HD23	1:B:46:LEU:HD23	2.04	0.40
1:C:43:TRP:CZ3	1:C:47:LYS:HG3	2.56	0.40
1:B:100:TRP:CD1	1:B:100:TRP:C	2.99	0.40
1:C:42:LEU:HD23	1:C:46:LEU:HD23	2.03	0.40
1:B:319:VAL:HG23	1:B:322:ILE:HD11	2.03	0.40
5:B:1106:CLR:H231	5:B:1106:CLR:H213	1.76	0.40
1:A:157:ASN:OD1	1:A:193:VAL:HG21	2.21	0.40
1:A:319:VAL:HG23	1:A:322:ILE:HD11	2.03	0.40
5:B:1109:CLR:H152	5:B:1109:CLR:H181	1.75	0.40
1:B:26:LEU:HD21	5:B:1105:CLR:H8	2.02	0.40
1:C:157:ASN:OD1	1:C:193:VAL:HG21	2.21	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	270/1065 (25%)	264 (98%)	6 (2%)	0	100	100
1	B	270/1065 (25%)	265 (98%)	5 (2%)	0	100	100
1	C	270/1065 (25%)	264 (98%)	6 (2%)	0	100	100
1	D	270/1065 (25%)	264 (98%)	6 (2%)	0	100	100
All	All	1080/4260 (25%)	1057 (98%)	23 (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	242/937 (26%)	242 (100%)	0	100	100
1	B	242/937 (26%)	242 (100%)	0	100	100
1	C	242/937 (26%)	242 (100%)	0	100	100
1	D	242/937 (26%)	242 (100%)	0	100	100
All	All	968/3748 (26%)	968 (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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	B	267	GLN
1	C	267	GLN
1	D	157	ASN
1	D	267	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 101 ligands modelled in this entry, 5 are monoatomic - leaving 96 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	D	1101	-	21,21,51	0.52	0	23,25,59	0.66	1 (4%)
4	AJP	A	1125	-	49,49,95	0.13	0	75,80,149	0.33	0
4	AJP	A	1111	-	61,61,95	0.15	0	93,98,149	0.42	0
4	AJP	B	1117	-	49,49,95	0.17	0	75,80,149	0.49	0
5	CLR	A	1113	-	31,31,31	4.50	12 (38%)	48,48,48	4.90	19 (39%)
6	A1C9J	D	1124	-	46,54,54	2.14	14 (30%)	57,98,98	4.90	31 (54%)
4	AJP	B	1119	-	49,49,95	0.17	0	75,80,149	0.42	0
4	AJP	A	1124	-	49,49,95	0.16	0	75,80,149	0.43	0
4	AJP	D	1117	-	49,49,95	0.15	0	75,80,149	0.35	0
6	A1C9J	A	1130	-	46,54,54	2.14	14 (30%)	57,98,98	4.89	31 (54%)
3	LBN	C	1102	-	21,21,51	0.52	0	23,25,59	0.65	1 (4%)
3	LBN	C	1113	-	28,28,51	0.46	0	31,33,59	0.59	1 (3%)
3	LBN	B	1113	-	30,30,51	0.45	0	33,35,59	0.61	1 (3%)
3	LBN	B	1101	-	21,21,51	0.52	0	23,25,59	0.68	1 (4%)
4	AJP	D	1118	-	49,49,95	0.15	0	75,80,149	0.39	0
5	CLR	B	1110	-	31,31,31	4.51	12 (38%)	48,48,48	4.91	19 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AJP	D	1105	-	61,61,95	0.17	0	93,98,149	0.43	0
6	A1C9J	B	1123	-	46,54,54	2.15	14 (30%)	57,98,98	4.91	31 (54%)
3	LBN	B	1112	-	28,28,51	0.46	0	31,33,59	0.58	1 (3%)
3	LBN	D	1103	-	23,23,51	0.50	0	26,28,59	0.66	1 (3%)
4	AJP	C	1123	-	49,49,95	0.14	0	75,80,149	0.34	0
4	AJP	B	1121	-	49,49,95	0.14	0	75,80,149	0.33	0
4	AJP	C	1122	-	49,49,95	0.15	0	75,80,149	0.34	0
4	AJP	A	1129	-	49,49,95	0.15	0	75,80,149	0.36	0
4	AJP	C	1120	-	49,49,95	0.15	0	75,80,149	0.36	0
3	LBN	A	1106	-	21,21,51	0.52	0	23,25,59	0.66	1 (4%)
4	AJP	C	1117	-	49,49,95	0.14	0	75,80,149	0.46	0
4	AJP	B	1104	-	61,61,95	0.17	0	93,98,149	0.46	0
5	CLR	C	1110	-	31,31,31	4.51	12 (38%)	48,48,48	5.01	18 (37%)
5	CLR	C	1109	-	31,31,31	4.52	12 (38%)	48,48,48	4.90	17 (35%)
4	AJP	C	1118	-	49,49,95	0.16	0	75,80,149	0.40	0
4	AJP	B	1118	-	49,49,95	0.13	0	75,80,149	0.33	0
5	CLR	A	1115	-	31,31,31	4.52	12 (38%)	48,48,48	4.91	15 (31%)
5	CLR	B	1107	-	31,31,31	4.51	12 (38%)	48,48,48	4.91	15 (31%)
5	CLR	D	1109	-	31,31,31	4.52	12 (38%)	48,48,48	4.90	17 (35%)
5	CLR	B	1108	-	31,31,31	4.51	12 (38%)	48,48,48	4.89	17 (35%)
3	LBN	A	1121	-	28,28,51	0.47	0	31,33,59	0.64	1 (3%)
5	CLR	A	1117	-	31,31,31	4.51	12 (38%)	48,48,48	5.01	18 (37%)
5	CLR	D	1107	-	31,31,31	4.52	12 (38%)	48,48,48	4.91	16 (33%)
3	LBN	C	1115	-	19,19,51	0.90	1 (5%)	21,23,59	0.85	1 (4%)
3	LBN	C	1101	-	21,21,51	0.52	0	23,25,59	0.66	1 (4%)
5	CLR	A	1118	-	31,31,31	4.55	12 (38%)	48,48,48	4.87	17 (35%)
5	CLR	C	1112	-	31,31,31	4.54	12 (38%)	48,48,48	4.88	18 (37%)
4	AJP	A	1128	-	49,49,95	0.15	0	75,80,149	0.34	0
4	AJP	D	1122	-	49,49,95	0.16	0	75,80,149	0.40	0
5	CLR	B	1109	-	31,31,31	4.51	12 (38%)	48,48,48	5.01	18 (37%)
5	CLR	A	1112	-	31,31,31	4.51	12 (38%)	48,48,48	5.00	21 (43%)
4	AJP	C	1119	-	49,49,95	0.13	0	75,80,149	0.33	0
4	AJP	C	1105	-	61,61,95	0.15	0	93,98,149	0.48	0
5	CLR	D	1111	-	31,31,31	4.51	12 (38%)	48,48,48	4.91	18 (37%)
4	AJP	B	1116	-	49,49,95	0.14	0	75,80,149	0.35	0
5	CLR	C	1108	-	31,31,31	4.52	12 (38%)	48,48,48	4.91	14 (29%)
4	AJP	A	1127	-	73,73,95	0.14	0	111,116,149	0.40	0
3	LBN	C	1116	-	26,26,51	0.47	0	29,31,59	0.65	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AJP	B	1120	-	73,73,95	0.14	0	111,116,149	0.40	0
3	LBN	A	1109	-	23,23,51	0.51	0	26,28,59	0.65	1 (3%)
3	LBN	D	1113	-	28,28,51	0.46	0	31,33,59	0.65	1 (3%)
4	AJP	D	1120	-	49,49,95	0.16	0	75,80,149	0.47	0
4	AJP	D	1121	-	73,73,95	0.14	0	111,116,149	0.40	0
3	LBN	A	1119	-	30,30,51	0.45	0	33,35,59	0.61	1 (3%)
5	CLR	A	1116	-	31,31,31	4.52	12 (38%)	48,48,48	4.89	17 (35%)
3	LBN	B	1115	-	26,26,51	0.48	0	29,31,59	0.62	1 (3%)
4	AJP	D	1119	-	49,49,95	0.13	0	75,80,149	0.34	0
3	LBN	C	1114	-	30,30,51	0.44	0	33,35,59	0.61	1 (3%)
3	LBN	A	1122	-	26,26,51	0.47	0	29,31,59	0.62	1 (3%)
3	LBN	A	1120	-	19,19,51	0.90	1 (5%)	21,23,59	0.85	1 (4%)
3	LBN	A	1108	-	21,21,51	0.52	0	23,25,59	0.68	1 (4%)
5	CLR	B	1111	-	31,31,31	4.56	12 (38%)	48,48,48	4.90	18 (37%)
3	LBN	B	1114	-	19,19,51	0.54	0	21,23,59	0.68	1 (4%)
4	AJP	A	1123	-	49,49,95	0.14	0	75,80,149	0.37	0
5	CLR	D	1110	-	31,31,31	4.51	12 (38%)	48,48,48	5.01	18 (37%)
3	LBN	D	1104	-	35,35,51	0.42	0	38,40,59	0.60	1 (2%)
4	AJP	D	1123	-	49,49,95	0.15	0	75,80,149	0.41	0
3	LBN	B	1103	-	34,34,51	0.43	0	37,39,59	0.62	1 (2%)
3	LBN	C	1103	-	23,23,51	0.50	0	26,28,59	0.73	1 (3%)
3	LBN	B	1102	-	23,23,51	0.50	0	26,28,59	0.66	1 (3%)
4	AJP	A	1126	-	49,49,95	0.15	0	75,80,149	0.36	0
5	CLR	D	1108	-	31,31,31	4.51	12 (38%)	48,48,48	4.91	14 (29%)
3	LBN	D	1102	-	21,21,51	0.52	0	23,25,59	0.65	1 (4%)
3	LBN	D	1116	-	26,26,51	0.48	0	29,31,59	0.62	1 (3%)
4	AJP	C	1121	-	73,73,95	0.14	0	111,116,149	0.40	0
3	LBN	A	1110	-	35,35,51	0.43	0	38,40,59	0.61	1 (2%)
6	A1C9J	C	1124	-	46,54,54	2.14	14 (30%)	57,98,98	4.91	31 (54%)
5	CLR	C	1106	-	31,31,31	4.51	12 (38%)	48,48,48	5.00	18 (37%)
3	LBN	A	1107	-	21,21,51	0.52	0	23,25,59	0.67	1 (4%)
5	CLR	D	1112	-	31,31,31	4.53	12 (38%)	48,48,48	4.85	17 (35%)
5	CLR	B	1106	-	31,31,31	4.53	12 (38%)	48,48,48	4.91	16 (33%)
4	AJP	B	1122	-	49,49,95	0.14	0	75,80,149	0.34	0
3	LBN	D	1115	-	19,19,51	0.90	1 (5%)	21,23,59	0.85	1 (4%)
5	CLR	B	1105	-	31,31,31	4.51	12 (38%)	48,48,48	4.97	21 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CLR	C	1107	-	31,31,31	4.52	12 (38%)	48,48,48	4.91	17 (35%)
3	LBN	D	1114	-	30,30,51	0.45	0	33,35,59	0.60	1 (3%)
5	CLR	D	1106	-	31,31,31	4.48	12 (38%)	48,48,48	5.32	23 (47%)
5	CLR	A	1114	-	31,31,31	4.53	12 (38%)	48,48,48	4.90	15 (31%)
3	LBN	C	1104	-	34,34,51	0.43	0	37,39,59	0.61	1 (2%)
5	CLR	C	1111	-	31,31,31	4.50	12 (38%)	48,48,48	4.89	19 (39%)

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	D	1101	-	1/1/3/7	0/21/21/55	-
4	AJP	A	1125	-	-	1/6/121/220	0/7/7/11
4	AJP	A	1111	-	-	4/12/147/220	1/8/8/11
4	AJP	B	1117	-	-	1/6/121/220	0/7/7/11
5	CLR	A	1113	-	2/2/10/11	8/10/68/68	0/4/4/4
6	A1C9J	D	1124	-	1/1/16/16	0/4/130/130	-
4	AJP	B	1119	-	-	1/6/121/220	0/7/7/11
4	AJP	A	1124	-	-	1/6/121/220	0/7/7/11
4	AJP	D	1117	-	-	0/6/121/220	0/7/7/11
6	A1C9J	A	1130	-	1/1/16/16	0/4/130/130	-
3	LBN	C	1102	-	1/1/3/7	0/21/21/55	-
3	LBN	C	1113	-	1/1/4/7	3/30/30/55	-
3	LBN	B	1113	-	1/1/4/7	2/32/32/55	-
3	LBN	B	1101	-	1/1/3/7	0/21/21/55	-
4	AJP	D	1118	-	-	2/6/121/220	0/7/7/11
5	CLR	B	1110	-	2/2/10/11	8/10/68/68	0/4/4/4
4	AJP	D	1105	-	-	6/12/147/220	0/8/8/11
6	A1C9J	B	1123	-	1/1/16/16	0/4/130/130	-
3	LBN	B	1112	-	1/1/4/7	3/30/30/55	-
3	LBN	D	1103	-	1/1/4/7	1/25/25/55	-
4	AJP	C	1123	-	-	3/6/121/220	0/7/7/11
4	AJP	B	1121	-	-	2/6/121/220	0/7/7/11
4	AJP	C	1122	-	-	3/6/121/220	0/7/7/11
4	AJP	A	1129	-	-	0/6/121/220	0/7/7/11
4	AJP	C	1120	-	-	1/6/121/220	0/7/7/11
3	LBN	A	1106	-	1/1/3/7	0/21/21/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AJP	C	1117	-	-	0/6/121/220	0/7/7/11
4	AJP	B	1104	-	-	3/12/147/220	0/8/8/11
5	CLR	C	1110	-	2/2/10/11	7/10/68/68	0/4/4/4
5	CLR	C	1109	-	2/2/10/11	2/10/68/68	0/4/4/4
4	AJP	C	1118	-	-	1/6/121/220	0/7/7/11
4	AJP	B	1118	-	-	0/6/121/220	0/7/7/11
5	CLR	A	1115	-	2/2/10/11	6/10/68/68	0/4/4/4
5	CLR	B	1107	-	2/2/10/11	6/10/68/68	0/4/4/4
5	CLR	D	1109	-	2/2/10/11	2/10/68/68	0/4/4/4
5	CLR	B	1108	-	2/2/10/11	2/10/68/68	0/4/4/4
3	LBN	A	1121	-	1/1/4/7	5/30/30/55	-
5	CLR	A	1117	-	2/2/10/11	7/10/68/68	0/4/4/4
5	CLR	D	1107	-	2/2/10/11	3/10/68/68	0/4/4/4
3	LBN	C	1115	-	1/1/3/7	0/19/19/55	-
3	LBN	C	1101	-	1/1/3/7	0/21/21/55	-
5	CLR	A	1118	-	2/2/10/11	8/10/68/68	0/4/4/4
5	CLR	C	1112	-	2/2/10/11	8/10/68/68	0/4/4/4
5	CLR	B	1109	-	2/2/10/11	7/10/68/68	0/4/4/4
4	AJP	A	1128	-	-	1/6/121/220	0/7/7/11
4	AJP	D	1122	-	-	0/6/121/220	0/7/7/11
5	CLR	A	1112	-	2/2/10/11	9/10/68/68	0/4/4/4
4	AJP	C	1119	-	-	1/6/121/220	0/7/7/11
4	AJP	C	1105	-	-	6/12/147/220	1/8/8/11
5	CLR	D	1111	-	2/2/10/11	8/10/68/68	0/4/4/4
4	AJP	B	1116	-	-	0/6/121/220	0/7/7/11
5	CLR	C	1108	-	2/2/10/11	6/10/68/68	0/4/4/4
4	AJP	A	1127	-	-	5/18/173/220	0/9/9/11
3	LBN	C	1116	-	1/1/4/7	3/28/28/55	-
4	AJP	B	1120	-	-	5/18/173/220	0/9/9/11
3	LBN	A	1109	-	1/1/4/7	0/25/25/55	-
3	LBN	D	1113	-	1/1/4/7	4/30/30/55	-
4	AJP	D	1120	-	-	1/6/121/220	0/7/7/11
4	AJP	D	1121	-	-	5/18/173/220	0/9/9/11
3	LBN	A	1119	-	1/1/4/7	2/32/32/55	-
5	CLR	A	1116	-	2/2/10/11	2/10/68/68	0/4/4/4
3	LBN	B	1115	-	1/1/4/7	3/28/28/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AJP	D	1119	-	-	1/6/121/220	0/7/7/11
3	LBN	C	1114	-	1/1/4/7	2/32/32/55	-
3	LBN	A	1122	-	1/1/4/7	3/28/28/55	-
3	LBN	A	1120	-	1/1/3/7	0/19/19/55	-
3	LBN	A	1108	-	1/1/3/7	0/21/21/55	-
5	CLR	B	1111	-	2/2/10/11	7/10/68/68	0/4/4/4
3	LBN	B	1114	-	1/1/3/7	0/19/19/55	-
4	AJP	A	1123	-	-	0/6/121/220	0/7/7/11
5	CLR	D	1110	-	2/2/10/11	7/10/68/68	0/4/4/4
3	LBN	D	1104	-	1/1/4/7	5/37/37/55	-
4	AJP	D	1123	-	-	4/6/121/220	1/7/7/11
3	LBN	B	1103	-	1/1/4/7	4/36/36/55	-
3	LBN	C	1103	-	1/1/4/7	2/25/25/55	-
3	LBN	B	1102	-	1/1/4/7	1/25/25/55	-
4	AJP	A	1126	-	-	1/6/121/220	0/7/7/11
5	CLR	D	1108	-	2/2/10/11	6/10/68/68	0/4/4/4
3	LBN	D	1102	-	1/1/3/7	0/21/21/55	-
3	LBN	D	1116	-	1/1/4/7	3/28/28/55	-
4	AJP	C	1121	-	-	4/18/173/220	0/9/9/11
3	LBN	A	1110	-	1/1/4/7	5/37/37/55	-
6	A1C9J	C	1124	-	1/1/16/16	0/4/130/130	-
5	CLR	C	1106	-	2/2/10/11	8/10/68/68	0/4/4/4
3	LBN	A	1107	-	1/1/3/7	0/21/21/55	-
5	CLR	D	1112	-	2/2/10/11	8/10/68/68	0/4/4/4
5	CLR	B	1106	-	2/2/10/11	3/10/68/68	0/4/4/4
4	AJP	B	1122	-	-	3/6/121/220	0/7/7/11
3	LBN	D	1115	-	1/1/3/7	0/19/19/55	-
5	CLR	B	1105	-	2/2/10/11	6/10/68/68	0/4/4/4
5	CLR	C	1107	-	2/2/10/11	3/10/68/68	0/4/4/4
3	LBN	D	1114	-	1/1/4/7	2/32/32/55	-
5	CLR	D	1106	-	2/2/10/11	5/10/68/68	0/4/4/4
5	CLR	A	1114	-	2/2/10/11	4/10/68/68	0/4/4/4
3	LBN	C	1104	-	1/1/4/7	5/36/36/55	-
5	CLR	C	1111	-	2/2/10/11	8/10/68/68	0/4/4/4

All (395) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1114	CLR	C6-C5	12.79	1.59	1.33
5	C	1108	CLR	C6-C5	12.77	1.59	1.33
5	C	1110	CLR	C6-C5	12.75	1.59	1.33
5	B	1107	CLR	C6-C5	12.74	1.59	1.33
5	A	1117	CLR	C6-C5	12.73	1.59	1.33
5	B	1106	CLR	C6-C5	12.73	1.59	1.33
5	D	1107	CLR	C6-C5	12.73	1.59	1.33
5	D	1110	CLR	C6-C5	12.73	1.59	1.33
5	D	1106	CLR	C6-C5	12.73	1.59	1.33
5	B	1109	CLR	C6-C5	12.72	1.59	1.33
5	A	1115	CLR	C6-C5	12.72	1.59	1.33
5	D	1108	CLR	C6-C5	12.72	1.59	1.33
5	C	1106	CLR	C6-C5	12.70	1.59	1.33
5	A	1116	CLR	C6-C5	12.70	1.59	1.33
5	C	1107	CLR	C6-C5	12.70	1.59	1.33
5	A	1112	CLR	C6-C5	12.69	1.59	1.33
5	D	1109	CLR	C6-C5	12.68	1.59	1.33
5	B	1108	CLR	C6-C5	12.66	1.59	1.33
5	C	1109	CLR	C6-C5	12.66	1.59	1.33
5	B	1110	CLR	C6-C5	12.64	1.59	1.33
5	D	1111	CLR	C6-C5	12.64	1.59	1.33
5	A	1113	CLR	C6-C5	12.64	1.59	1.33
5	B	1105	CLR	C6-C5	12.63	1.59	1.33
5	A	1118	CLR	C6-C5	12.63	1.59	1.33
5	C	1112	CLR	C6-C5	12.62	1.59	1.33
5	C	1111	CLR	C6-C5	12.62	1.59	1.33
5	D	1112	CLR	C6-C5	12.58	1.58	1.33
5	B	1111	CLR	C6-C5	12.54	1.58	1.33
5	B	1111	CLR	C7-C8	10.46	1.70	1.53
5	A	1118	CLR	C7-C8	10.23	1.69	1.53
5	D	1112	CLR	C7-C8	10.22	1.69	1.53
5	C	1112	CLR	C7-C8	10.14	1.69	1.53
5	B	1105	CLR	C7-C8	10.08	1.69	1.53
5	C	1106	CLR	C7-C8	10.07	1.69	1.53
5	D	1111	CLR	C7-C8	10.06	1.69	1.53
5	B	1110	CLR	C7-C8	10.05	1.69	1.53
5	C	1110	CLR	C7-C8	10.04	1.69	1.53
5	A	1112	CLR	C7-C8	10.04	1.69	1.53
5	D	1110	CLR	C7-C8	10.03	1.69	1.53
5	B	1106	CLR	C7-C8	10.03	1.69	1.53
5	D	1109	CLR	C7-C8	10.02	1.69	1.53
5	A	1116	CLR	C7-C8	10.02	1.69	1.53
5	C	1109	CLR	C7-C8	10.02	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1111	CLR	C7-C8	10.02	1.69	1.53
5	D	1107	CLR	C7-C8	10.01	1.69	1.53
5	A	1115	CLR	C7-C8	10.01	1.69	1.53
5	B	1107	CLR	C7-C8	10.01	1.69	1.53
5	A	1113	CLR	C7-C8	10.00	1.69	1.53
5	B	1108	CLR	C7-C8	10.00	1.69	1.53
5	D	1108	CLR	C7-C8	9.99	1.69	1.53
5	A	1117	CLR	C7-C8	9.99	1.69	1.53
5	B	1109	CLR	C7-C8	9.98	1.69	1.53
5	A	1114	CLR	C7-C8	9.97	1.69	1.53
5	C	1108	CLR	C7-C8	9.97	1.69	1.53
5	C	1107	CLR	C7-C8	9.97	1.69	1.53
5	B	1111	CLR	C8-C14	9.91	1.72	1.53
5	A	1118	CLR	C8-C14	9.86	1.72	1.53
5	C	1112	CLR	C8-C14	9.83	1.72	1.53
5	D	1112	CLR	C8-C14	9.76	1.72	1.53
5	D	1106	CLR	C7-C8	9.71	1.68	1.53
5	C	1106	CLR	C8-C14	9.71	1.71	1.53
5	A	1117	CLR	C8-C14	9.67	1.71	1.53
5	C	1109	CLR	C8-C14	9.67	1.71	1.53
5	D	1109	CLR	C8-C14	9.66	1.71	1.53
5	A	1112	CLR	C8-C14	9.66	1.71	1.53
5	D	1106	CLR	C8-C14	9.65	1.71	1.53
5	D	1110	CLR	C8-C14	9.65	1.71	1.53
5	B	1109	CLR	C8-C14	9.64	1.71	1.53
5	A	1116	CLR	C8-C14	9.63	1.71	1.53
5	C	1110	CLR	C8-C14	9.62	1.71	1.53
5	B	1108	CLR	C8-C14	9.62	1.71	1.53
5	B	1105	CLR	C8-C14	9.61	1.71	1.53
5	C	1108	CLR	C8-C14	9.60	1.71	1.53
5	B	1107	CLR	C8-C14	9.60	1.71	1.53
5	A	1115	CLR	C8-C14	9.60	1.71	1.53
5	C	1107	CLR	C8-C14	9.60	1.71	1.53
5	B	1110	CLR	C8-C14	9.56	1.71	1.53
5	A	1114	CLR	C8-C14	9.56	1.71	1.53
5	D	1111	CLR	C8-C14	9.54	1.71	1.53
5	D	1108	CLR	C8-C14	9.54	1.71	1.53
5	D	1107	CLR	C8-C14	9.52	1.71	1.53
5	B	1106	CLR	C8-C14	9.52	1.71	1.53
5	A	1113	CLR	C8-C14	9.52	1.71	1.53
5	C	1111	CLR	C8-C14	9.49	1.71	1.53
5	B	1111	CLR	C10-C9	9.35	1.70	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1118	CLR	C10-C9	9.07	1.70	1.56
5	C	1112	CLR	C10-C9	9.02	1.70	1.56
5	B	1109	CLR	C10-C9	8.96	1.70	1.56
5	B	1108	CLR	C10-C9	8.95	1.70	1.56
5	C	1107	CLR	C10-C9	8.94	1.70	1.56
5	D	1112	CLR	C10-C9	8.94	1.70	1.56
5	B	1110	CLR	C10-C9	8.93	1.70	1.56
5	B	1105	CLR	C10-C9	8.93	1.70	1.56
5	D	1109	CLR	C10-C9	8.93	1.70	1.56
5	C	1109	CLR	C10-C9	8.92	1.70	1.56
5	A	1117	CLR	C10-C9	8.91	1.70	1.56
5	D	1106	CLR	C10-C9	8.91	1.70	1.56
5	C	1110	CLR	C10-C9	8.91	1.70	1.56
5	D	1110	CLR	C10-C9	8.91	1.70	1.56
5	C	1111	CLR	C10-C9	8.91	1.70	1.56
5	A	1114	CLR	C10-C9	8.90	1.70	1.56
5	A	1116	CLR	C10-C9	8.89	1.70	1.56
5	D	1107	CLR	C10-C9	8.89	1.70	1.56
5	A	1113	CLR	C10-C9	8.88	1.70	1.56
5	B	1106	CLR	C10-C9	8.87	1.70	1.56
5	C	1106	CLR	C10-C9	8.86	1.70	1.56
5	D	1111	CLR	C10-C9	8.85	1.70	1.56
5	A	1112	CLR	C10-C9	8.85	1.70	1.56
5	C	1108	CLR	C10-C9	8.81	1.70	1.56
5	D	1108	CLR	C10-C9	8.81	1.70	1.56
5	A	1115	CLR	C10-C9	8.79	1.70	1.56
5	B	1107	CLR	C10-C9	8.78	1.70	1.56
5	B	1106	CLR	C8-C9	-7.74	1.39	1.53
5	D	1107	CLR	C8-C9	-7.74	1.39	1.53
5	A	1114	CLR	C8-C9	-7.73	1.39	1.53
5	A	1115	CLR	C8-C9	-7.68	1.39	1.53
5	B	1107	CLR	C8-C9	-7.68	1.39	1.53
5	B	1105	CLR	C8-C9	-7.68	1.39	1.53
5	A	1112	CLR	C8-C9	-7.66	1.39	1.53
5	C	1107	CLR	C8-C9	-7.65	1.39	1.53
5	C	1108	CLR	C8-C9	-7.65	1.39	1.53
5	D	1108	CLR	C8-C9	-7.65	1.39	1.53
5	C	1109	CLR	C8-C9	-7.63	1.39	1.53
5	D	1111	CLR	C8-C9	-7.62	1.39	1.53
5	C	1111	CLR	C8-C9	-7.62	1.39	1.53
5	A	1116	CLR	C8-C9	-7.61	1.39	1.53
5	B	1110	CLR	C8-C9	-7.61	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1113	CLR	C8-C9	-7.61	1.39	1.53
5	B	1108	CLR	C8-C9	-7.60	1.39	1.53
5	D	1109	CLR	C8-C9	-7.60	1.39	1.53
5	C	1106	CLR	C8-C9	-7.59	1.39	1.53
5	B	1109	CLR	C8-C9	-7.55	1.39	1.53
5	C	1110	CLR	C8-C9	-7.51	1.39	1.53
5	D	1110	CLR	C8-C9	-7.51	1.39	1.53
5	A	1117	CLR	C8-C9	-7.50	1.39	1.53
5	D	1112	CLR	C8-C9	-7.46	1.39	1.53
5	A	1118	CLR	C8-C9	-7.45	1.39	1.53
5	C	1112	CLR	C8-C9	-7.38	1.39	1.53
5	B	1111	CLR	C8-C9	-7.19	1.40	1.53
5	D	1106	CLR	C8-C9	-6.92	1.40	1.53
5	D	1106	CLR	C13-C14	-6.81	1.42	1.55
5	B	1111	CLR	C13-C14	-6.52	1.43	1.55
5	C	1112	CLR	C13-C14	-6.49	1.43	1.55
5	A	1118	CLR	C13-C14	-6.49	1.43	1.55
5	C	1111	CLR	C13-C14	-6.48	1.43	1.55
5	C	1108	CLR	C13-C14	-6.47	1.43	1.55
5	D	1111	CLR	C13-C14	-6.45	1.43	1.55
5	A	1113	CLR	C13-C14	-6.44	1.43	1.55
5	B	1106	CLR	C13-C14	-6.44	1.43	1.55
5	D	1112	CLR	C13-C14	-6.44	1.43	1.55
5	A	1114	CLR	C13-C14	-6.43	1.43	1.55
5	D	1108	CLR	C13-C14	-6.43	1.43	1.55
5	A	1115	CLR	C13-C14	-6.42	1.43	1.55
5	C	1109	CLR	C13-C14	-6.41	1.43	1.55
5	D	1107	CLR	C13-C14	-6.41	1.43	1.55
5	C	1107	CLR	C13-C14	-6.41	1.43	1.55
5	D	1109	CLR	C13-C14	-6.41	1.43	1.55
5	B	1107	CLR	C13-C14	-6.40	1.43	1.55
5	B	1110	CLR	C13-C14	-6.40	1.43	1.55
5	A	1116	CLR	C13-C14	-6.38	1.43	1.55
5	B	1109	CLR	C13-C14	-6.38	1.43	1.55
5	C	1110	CLR	C13-C14	-6.38	1.43	1.55
5	D	1110	CLR	C13-C14	-6.38	1.43	1.55
5	B	1108	CLR	C13-C14	-6.37	1.43	1.55
5	A	1117	CLR	C13-C14	-6.36	1.43	1.55
5	A	1112	CLR	C13-C14	-6.35	1.43	1.55
5	C	1106	CLR	C13-C14	-6.34	1.43	1.55
6	D	1124	A1C9J	C7-C6	6.31	1.54	1.47
5	B	1105	CLR	C13-C14	-6.29	1.43	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1124	A1C9J	C7-C6	6.29	1.54	1.47
6	B	1123	A1C9J	C7-C6	6.27	1.54	1.47
6	A	1130	A1C9J	C7-C6	6.23	1.54	1.47
6	B	1123	A1C9J	O8-C6	-6.13	1.37	1.45
6	A	1130	A1C9J	O8-C6	-6.11	1.37	1.45
6	C	1124	A1C9J	O8-C6	-6.11	1.37	1.45
6	D	1124	A1C9J	O8-C6	-6.07	1.37	1.45
6	C	1124	A1C9J	C5-C4	5.15	1.61	1.53
6	D	1124	A1C9J	C5-C4	5.14	1.61	1.53
6	B	1123	A1C9J	C5-C4	5.14	1.61	1.53
6	A	1130	A1C9J	C5-C4	5.11	1.61	1.53
5	B	1106	CLR	C20-C17	-4.61	1.46	1.54
5	A	1114	CLR	C20-C17	-4.58	1.46	1.54
5	A	1113	CLR	C20-C17	-4.57	1.46	1.54
5	C	1107	CLR	C20-C17	-4.56	1.46	1.54
5	D	1107	CLR	C20-C17	-4.54	1.46	1.54
5	C	1108	CLR	C20-C17	-4.54	1.46	1.54
5	C	1111	CLR	C20-C17	-4.53	1.46	1.54
5	A	1115	CLR	C20-C17	-4.52	1.46	1.54
5	D	1108	CLR	C20-C17	-4.52	1.46	1.54
5	B	1110	CLR	C20-C17	-4.51	1.46	1.54
5	D	1111	CLR	C20-C17	-4.49	1.46	1.54
5	B	1107	CLR	C20-C17	-4.48	1.46	1.54
5	C	1109	CLR	C20-C17	-4.38	1.46	1.54
5	A	1116	CLR	C20-C17	-4.38	1.46	1.54
5	D	1109	CLR	C20-C17	-4.38	1.46	1.54
5	B	1108	CLR	C20-C17	-4.34	1.47	1.54
5	D	1112	CLR	C20-C17	-4.25	1.47	1.54
5	D	1106	CLR	C15-C14	4.25	1.63	1.54
5	C	1112	CLR	C20-C17	-4.21	1.47	1.54
5	A	1118	CLR	C20-C17	-4.18	1.47	1.54
6	C	1124	A1C9J	C27-C28	-4.13	1.49	1.52
5	D	1106	CLR	C20-C17	-4.12	1.47	1.54
6	B	1123	A1C9J	C27-C28	-4.11	1.49	1.52
6	A	1130	A1C9J	C27-C28	-4.09	1.49	1.52
6	D	1124	A1C9J	C27-C28	-4.08	1.49	1.52
5	A	1117	CLR	C13-C17	4.08	1.62	1.55
5	B	1109	CLR	C13-C17	4.06	1.62	1.55
5	C	1106	CLR	C13-C17	4.05	1.62	1.55
5	D	1110	CLR	C13-C17	4.03	1.62	1.55
5	B	1105	CLR	C13-C17	4.03	1.62	1.55
5	C	1110	CLR	C13-C17	4.02	1.62	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1111	CLR	C20-C17	-4.00	1.47	1.54
5	A	1112	CLR	C13-C17	3.99	1.62	1.55
5	B	1109	CLR	C15-C14	3.94	1.62	1.54
5	C	1110	CLR	C15-C14	3.93	1.62	1.54
5	D	1110	CLR	C15-C14	3.92	1.62	1.54
5	A	1117	CLR	C15-C14	3.89	1.62	1.54
5	A	1112	CLR	C16-C17	3.85	1.62	1.54
5	A	1115	CLR	C16-C17	3.85	1.62	1.54
5	C	1106	CLR	C15-C14	3.85	1.62	1.54
5	D	1106	CLR	C16-C17	3.84	1.62	1.54
5	B	1105	CLR	C16-C17	3.84	1.62	1.54
5	D	1108	CLR	C16-C17	3.83	1.62	1.54
5	C	1106	CLR	C16-C17	3.82	1.62	1.54
5	B	1108	CLR	C16-C17	3.81	1.62	1.54
5	C	1110	CLR	C16-C17	3.81	1.62	1.54
5	B	1107	CLR	C16-C17	3.81	1.62	1.54
5	A	1116	CLR	C16-C17	3.80	1.62	1.54
5	C	1109	CLR	C16-C17	3.80	1.62	1.54
5	B	1109	CLR	C16-C17	3.80	1.62	1.54
5	A	1112	CLR	C15-C14	3.80	1.62	1.54
5	B	1106	CLR	C16-C17	3.79	1.62	1.54
5	C	1108	CLR	C16-C17	3.79	1.62	1.54
5	D	1107	CLR	C16-C17	3.78	1.62	1.54
5	D	1112	CLR	C16-C15	-3.78	1.43	1.54
5	C	1107	CLR	C16-C17	3.78	1.62	1.54
5	C	1107	CLR	C15-C14	3.78	1.62	1.54
5	B	1105	CLR	C15-C14	3.77	1.62	1.54
5	D	1109	CLR	C16-C17	3.77	1.62	1.54
5	B	1111	CLR	C16-C15	-3.77	1.43	1.54
5	C	1112	CLR	C16-C17	3.77	1.62	1.54
5	D	1110	CLR	C16-C17	3.77	1.62	1.54
5	A	1117	CLR	C16-C17	3.76	1.62	1.54
5	A	1113	CLR	C16-C15	-3.76	1.43	1.54
5	A	1114	CLR	C16-C17	3.76	1.62	1.54
5	D	1112	CLR	C16-C17	3.76	1.62	1.54
5	B	1110	CLR	C16-C17	3.76	1.62	1.54
5	C	1112	CLR	C16-C15	-3.75	1.43	1.54
5	D	1108	CLR	C15-C14	3.75	1.62	1.54
5	C	1108	CLR	C15-C14	3.75	1.62	1.54
5	A	1118	CLR	C16-C15	-3.74	1.43	1.54
5	C	1109	CLR	C15-C14	3.74	1.62	1.54
5	D	1111	CLR	C16-C15	-3.74	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1110	CLR	C16-C15	-3.74	1.43	1.54
5	A	1118	CLR	C16-C17	3.74	1.62	1.54
5	B	1105	CLR	C16-C15	-3.73	1.43	1.54
5	D	1111	CLR	C16-C17	3.73	1.62	1.54
5	C	1111	CLR	C16-C15	-3.73	1.43	1.54
5	D	1107	CLR	C15-C14	3.73	1.62	1.54
5	A	1113	CLR	C16-C17	3.72	1.62	1.54
5	B	1108	CLR	C15-C14	3.72	1.62	1.54
5	D	1109	CLR	C15-C14	3.71	1.62	1.54
5	C	1111	CLR	C16-C17	3.71	1.62	1.54
5	A	1115	CLR	C15-C14	3.70	1.61	1.54
5	A	1114	CLR	C16-C15	-3.70	1.43	1.54
5	A	1114	CLR	C15-C14	3.70	1.61	1.54
5	A	1116	CLR	C15-C14	3.70	1.61	1.54
5	B	1111	CLR	C16-C17	3.70	1.61	1.54
5	B	1106	CLR	C15-C14	3.70	1.61	1.54
5	B	1107	CLR	C15-C14	3.69	1.61	1.54
5	B	1106	CLR	C16-C15	-3.69	1.44	1.54
5	A	1116	CLR	C16-C15	-3.69	1.44	1.54
5	C	1109	CLR	C16-C15	-3.68	1.44	1.54
5	A	1118	CLR	C15-C14	3.67	1.61	1.54
5	C	1107	CLR	C16-C15	-3.67	1.44	1.54
5	D	1109	CLR	C16-C15	-3.67	1.44	1.54
5	A	1112	CLR	C16-C15	-3.67	1.44	1.54
5	C	1112	CLR	C15-C14	3.66	1.61	1.54
5	B	1107	CLR	C16-C15	-3.66	1.44	1.54
5	C	1106	CLR	C16-C15	-3.66	1.44	1.54
5	B	1108	CLR	C16-C15	-3.66	1.44	1.54
5	D	1107	CLR	C16-C15	-3.66	1.44	1.54
5	C	1108	CLR	C16-C15	-3.66	1.44	1.54
5	C	1110	CLR	C16-C15	-3.65	1.44	1.54
5	D	1108	CLR	C16-C15	-3.65	1.44	1.54
5	A	1117	CLR	C16-C15	-3.64	1.44	1.54
5	A	1115	CLR	C16-C15	-3.64	1.44	1.54
5	D	1112	CLR	C15-C14	3.64	1.61	1.54
5	B	1109	CLR	C16-C15	-3.63	1.44	1.54
5	B	1110	CLR	C15-C14	3.63	1.61	1.54
5	D	1110	CLR	C16-C15	-3.63	1.44	1.54
5	D	1111	CLR	C15-C14	3.63	1.61	1.54
5	B	1111	CLR	C15-C14	3.61	1.61	1.54
5	A	1113	CLR	C15-C14	3.59	1.61	1.54
5	C	1111	CLR	C15-C14	3.57	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1115	LBN	P1-O4	3.40	1.61	1.50
3	C	1115	LBN	P1-O4	3.39	1.61	1.50
3	A	1120	LBN	P1-O4	3.39	1.61	1.50
5	D	1106	CLR	C16-C15	-3.36	1.44	1.54
5	C	1106	CLR	C10-C5	-3.29	1.46	1.52
5	B	1105	CLR	C10-C5	-3.28	1.46	1.52
5	D	1106	CLR	C10-C5	-3.24	1.46	1.52
5	A	1112	CLR	C10-C5	-3.24	1.46	1.52
5	B	1111	CLR	C13-C17	3.22	1.60	1.55
5	B	1108	CLR	C10-C5	-3.20	1.46	1.52
5	C	1112	CLR	C13-C17	3.20	1.60	1.55
5	A	1118	CLR	C10-C5	-3.20	1.46	1.52
5	B	1110	CLR	C10-C5	-3.19	1.46	1.52
5	D	1109	CLR	C10-C5	-3.19	1.46	1.52
5	D	1112	CLR	C13-C17	3.19	1.60	1.55
5	A	1115	CLR	C10-C5	-3.18	1.46	1.52
5	A	1118	CLR	C13-C17	3.18	1.60	1.55
5	A	1116	CLR	C10-C5	-3.18	1.46	1.52
5	C	1108	CLR	C10-C5	-3.18	1.46	1.52
5	C	1109	CLR	C10-C5	-3.17	1.46	1.52
5	A	1114	CLR	C10-C5	-3.16	1.46	1.52
5	A	1113	CLR	C10-C5	-3.16	1.46	1.52
5	D	1107	CLR	C10-C5	-3.16	1.46	1.52
5	C	1112	CLR	C10-C5	-3.16	1.46	1.52
5	D	1111	CLR	C10-C5	-3.16	1.46	1.52
5	A	1117	CLR	C10-C5	-3.15	1.46	1.52
5	D	1109	CLR	C13-C17	3.15	1.60	1.55
5	B	1107	CLR	C10-C5	-3.15	1.46	1.52
5	B	1106	CLR	C10-C5	-3.15	1.46	1.52
5	D	1110	CLR	C10-C5	-3.15	1.46	1.52
5	D	1108	CLR	C10-C5	-3.14	1.46	1.52
5	C	1109	CLR	C13-C17	3.14	1.60	1.55
5	D	1112	CLR	C10-C5	-3.13	1.46	1.52
5	C	1110	CLR	C10-C5	-3.13	1.46	1.52
5	C	1107	CLR	C10-C5	-3.13	1.46	1.52
5	A	1116	CLR	C13-C17	3.13	1.60	1.55
5	C	1111	CLR	C10-C5	-3.12	1.46	1.52
5	B	1109	CLR	C10-C5	-3.10	1.47	1.52
5	B	1108	CLR	C13-C17	3.10	1.60	1.55
5	B	1111	CLR	C10-C5	-3.08	1.47	1.52
5	B	1106	CLR	C13-C17	3.06	1.60	1.55
5	C	1107	CLR	C13-C17	3.05	1.60	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1114	CLR	C13-C17	3.04	1.60	1.55
5	D	1107	CLR	C13-C17	3.03	1.60	1.55
5	C	1111	CLR	C13-C17	2.95	1.60	1.55
5	D	1111	CLR	C13-C17	2.92	1.60	1.55
5	A	1115	CLR	C13-C17	2.90	1.60	1.55
5	C	1108	CLR	C13-C17	2.90	1.60	1.55
5	D	1108	CLR	C13-C17	2.89	1.60	1.55
5	A	1113	CLR	C13-C17	2.86	1.60	1.55
5	B	1107	CLR	C13-C17	2.86	1.60	1.55
5	D	1106	CLR	C13-C17	2.86	1.60	1.55
5	B	1110	CLR	C13-C17	2.83	1.60	1.55
5	B	1109	CLR	C20-C17	-2.75	1.49	1.54
5	A	1117	CLR	C20-C17	-2.74	1.49	1.54
5	C	1110	CLR	C20-C17	-2.72	1.49	1.54
6	D	1124	A1C9J	O39-C27	-2.70	1.39	1.43
5	D	1110	CLR	C20-C17	-2.69	1.49	1.54
6	C	1124	A1C9J	O39-C27	-2.69	1.39	1.43
6	B	1123	A1C9J	O39-C27	-2.69	1.39	1.43
6	A	1130	A1C9J	O39-C27	-2.67	1.39	1.43
5	A	1112	CLR	C20-C17	-2.62	1.49	1.54
5	B	1105	CLR	C20-C17	-2.62	1.49	1.54
5	C	1106	CLR	C20-C17	-2.60	1.49	1.54
6	B	1123	A1C9J	C44-C13	2.59	1.57	1.53
6	A	1130	A1C9J	C44-C13	2.55	1.57	1.53
6	D	1124	A1C9J	C44-C13	2.55	1.57	1.53
6	D	1124	A1C9J	C14-C13	-2.50	1.53	1.57
6	C	1124	A1C9J	C44-C13	2.50	1.57	1.53
6	C	1124	A1C9J	C34-C33	-2.50	1.46	1.51
6	A	1130	A1C9J	C14-C13	-2.49	1.53	1.57
6	B	1123	A1C9J	C34-C33	-2.48	1.46	1.51
6	C	1124	A1C9J	C14-C13	-2.47	1.53	1.57
6	B	1123	A1C9J	C14-C13	-2.47	1.53	1.57
6	D	1124	A1C9J	C34-C33	-2.46	1.46	1.51
6	A	1130	A1C9J	C34-C33	-2.45	1.46	1.51
6	C	1124	A1C9J	C4-C2	2.37	1.53	1.50
6	A	1130	A1C9J	C12-C11	2.37	1.58	1.53
6	B	1123	A1C9J	C4-C2	2.37	1.53	1.50
6	D	1124	A1C9J	C4-C2	2.36	1.53	1.50
6	B	1123	A1C9J	C12-C11	2.35	1.58	1.53
6	A	1130	A1C9J	C4-C2	2.34	1.53	1.50
6	D	1124	A1C9J	C12-C11	2.32	1.58	1.53
6	C	1124	A1C9J	C12-C11	2.31	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1124	A1C9J	C5-C6	2.29	1.57	1.53
6	B	1123	A1C9J	C5-C6	2.27	1.57	1.53
6	D	1124	A1C9J	C5-C6	2.26	1.57	1.53
6	A	1130	A1C9J	C5-C6	2.25	1.57	1.53
6	C	1124	A1C9J	C42-C18	-2.20	1.49	1.53
6	A	1130	A1C9J	C42-C18	-2.20	1.49	1.53
6	A	1130	A1C9J	C18-C19	-2.20	1.46	1.51
6	D	1124	A1C9J	C18-C19	-2.19	1.46	1.51
6	D	1124	A1C9J	C42-C18	-2.19	1.49	1.53
6	B	1123	A1C9J	C42-C18	-2.18	1.49	1.53
6	B	1123	A1C9J	C18-C19	-2.18	1.46	1.51
6	A	1130	A1C9J	C16-C17	-2.17	1.50	1.53
6	B	1123	A1C9J	C16-C17	-2.14	1.50	1.53
6	C	1124	A1C9J	C18-C19	-2.13	1.46	1.51
6	D	1124	A1C9J	C16-C17	-2.13	1.50	1.53
6	C	1124	A1C9J	C16-C17	-2.12	1.50	1.53

All (646) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1106	CLR	C18-C13-C12	-24.10	75.08	110.61
5	C	1110	CLR	C18-C13-C12	-24.02	75.19	110.61
5	B	1109	CLR	C18-C13-C12	-23.99	75.23	110.61
5	A	1117	CLR	C18-C13-C12	-23.99	75.25	110.61
5	D	1110	CLR	C18-C13-C12	-23.98	75.26	110.61
5	C	1106	CLR	C18-C13-C12	-23.75	75.59	110.61
5	A	1112	CLR	C18-C13-C12	-23.59	75.83	110.61
5	B	1105	CLR	C18-C13-C12	-23.51	75.96	110.61
5	D	1107	CLR	C18-C13-C12	-23.08	76.59	110.61
5	B	1106	CLR	C18-C13-C12	-23.06	76.61	110.61
5	B	1107	CLR	C18-C13-C12	-23.03	76.65	110.61
5	D	1108	CLR	C18-C13-C12	-23.02	76.67	110.61
5	A	1115	CLR	C18-C13-C12	-23.02	76.67	110.61
5	C	1107	CLR	C18-C13-C12	-23.01	76.69	110.61
5	C	1108	CLR	C18-C13-C12	-23.00	76.70	110.61
5	A	1114	CLR	C18-C13-C12	-22.99	76.72	110.61
5	A	1113	CLR	C18-C13-C12	-22.68	77.17	110.61
5	C	1111	CLR	C18-C13-C12	-22.66	77.20	110.61
5	D	1111	CLR	C18-C13-C12	-22.63	77.25	110.61
5	B	1110	CLR	C18-C13-C12	-22.62	77.26	110.61
5	D	1109	CLR	C18-C13-C12	-22.60	77.29	110.61
5	B	1108	CLR	C18-C13-C12	-22.59	77.31	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1116	CLR	C18-C13-C12	-22.57	77.33	110.61
5	C	1109	CLR	C18-C13-C12	-22.57	77.33	110.61
5	D	1112	CLR	C18-C13-C12	-21.74	78.55	110.61
5	C	1112	CLR	C18-C13-C12	-21.64	78.70	110.61
5	A	1118	CLR	C18-C13-C12	-21.54	78.85	110.61
5	B	1111	CLR	C18-C13-C12	-21.12	79.47	110.61
6	B	1123	A1C9J	C13-C18-C19	-18.01	104.83	119.93
6	C	1124	A1C9J	C13-C18-C19	-17.97	104.86	119.93
6	A	1130	A1C9J	C13-C18-C19	-17.97	104.86	119.93
6	D	1124	A1C9J	C13-C18-C19	-17.96	104.88	119.93
6	B	1123	A1C9J	C42-C18-C13	15.53	128.75	113.13
6	A	1130	A1C9J	C42-C18-C13	15.52	128.75	113.13
6	C	1124	A1C9J	C42-C18-C13	15.48	128.71	113.13
6	D	1124	A1C9J	C42-C18-C13	15.45	128.68	113.13
5	D	1106	CLR	C12-C13-C14	13.33	127.19	107.25
5	B	1111	CLR	C18-C13-C17	-13.32	87.52	111.68
5	D	1112	CLR	C18-C13-C17	-13.10	87.93	111.68
5	A	1118	CLR	C18-C13-C17	-13.07	87.97	111.68
5	C	1112	CLR	C18-C13-C17	-13.06	87.99	111.68
5	C	1111	CLR	C18-C13-C17	-12.84	88.39	111.68
5	D	1109	CLR	C18-C13-C17	-12.82	88.42	111.68
5	C	1109	CLR	C18-C13-C17	-12.81	88.45	111.68
5	B	1110	CLR	C18-C13-C17	-12.81	88.45	111.68
5	D	1111	CLR	C18-C13-C17	-12.80	88.45	111.68
5	A	1113	CLR	C18-C13-C17	-12.79	88.48	111.68
5	A	1116	CLR	C18-C13-C17	-12.78	88.50	111.68
5	B	1108	CLR	C18-C13-C17	-12.78	88.50	111.68
5	C	1107	CLR	C18-C13-C17	-12.77	88.51	111.68
5	D	1107	CLR	C18-C13-C17	-12.67	88.70	111.68
5	B	1106	CLR	C18-C13-C17	-12.67	88.71	111.68
5	A	1114	CLR	C18-C13-C17	-12.66	88.71	111.68
5	C	1108	CLR	C18-C13-C17	-12.65	88.74	111.68
5	D	1108	CLR	C18-C13-C17	-12.64	88.75	111.68
5	B	1107	CLR	C18-C13-C17	-12.64	88.76	111.68
5	A	1115	CLR	C18-C13-C17	-12.63	88.77	111.68
5	B	1107	CLR	C12-C13-C14	12.45	125.87	107.25
5	C	1108	CLR	C12-C13-C14	12.44	125.87	107.25
5	A	1115	CLR	C12-C13-C14	12.43	125.85	107.25
5	D	1108	CLR	C12-C13-C14	12.41	125.81	107.25
5	D	1111	CLR	C12-C13-C14	12.40	125.80	107.25
5	A	1113	CLR	C12-C13-C14	12.39	125.79	107.25
5	B	1110	CLR	C12-C13-C14	12.37	125.76	107.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1111	CLR	C12-C13-C14	12.34	125.71	107.25
5	B	1106	CLR	C12-C13-C14	12.18	125.48	107.25
5	A	1114	CLR	C12-C13-C14	12.16	125.44	107.25
5	D	1107	CLR	C12-C13-C14	12.15	125.43	107.25
5	C	1107	CLR	C12-C13-C14	12.13	125.39	107.25
5	D	1109	CLR	C12-C13-C14	12.03	125.25	107.25
5	C	1109	CLR	C12-C13-C14	12.01	125.21	107.25
5	A	1116	CLR	C12-C13-C14	11.99	125.19	107.25
5	B	1108	CLR	C12-C13-C14	11.99	125.18	107.25
5	A	1117	CLR	C12-C13-C14	11.98	125.17	107.25
5	C	1110	CLR	C12-C13-C14	11.97	125.15	107.25
5	D	1110	CLR	C12-C13-C14	11.95	125.13	107.25
5	B	1109	CLR	C12-C13-C14	11.95	125.12	107.25
5	A	1112	CLR	C12-C13-C14	11.74	124.82	107.25
5	C	1106	CLR	C12-C13-C14	11.74	124.81	107.25
5	B	1105	CLR	C12-C13-C14	11.66	124.69	107.25
5	C	1112	CLR	C12-C13-C14	11.65	124.68	107.25
5	D	1112	CLR	C12-C13-C14	11.59	124.58	107.25
5	A	1118	CLR	C12-C13-C14	11.54	124.51	107.25
5	D	1106	CLR	C18-C13-C17	-11.52	90.79	111.68
5	B	1111	CLR	C12-C13-C14	11.29	124.13	107.25
5	B	1105	CLR	C18-C13-C17	-11.12	91.50	111.68
5	A	1112	CLR	C18-C13-C17	-11.11	91.53	111.68
5	C	1106	CLR	C18-C13-C17	-11.02	91.68	111.68
5	D	1110	CLR	C18-C13-C17	-10.98	91.76	111.68
5	A	1117	CLR	C18-C13-C17	-10.97	91.79	111.68
5	C	1110	CLR	C18-C13-C17	-10.96	91.80	111.68
5	B	1109	CLR	C18-C13-C17	-10.95	91.81	111.68
6	C	1124	A1C9J	C17-C18-C19	10.85	106.03	97.19
6	D	1124	A1C9J	C17-C18-C19	10.85	106.03	97.19
6	B	1123	A1C9J	C17-C18-C19	10.79	105.97	97.19
6	A	1130	A1C9J	C17-C18-C19	10.75	105.95	97.19
6	C	1124	A1C9J	C7-O8-C6	10.35	66.70	60.96
6	B	1123	A1C9J	C7-O8-C6	10.31	66.68	60.96
6	D	1124	A1C9J	C7-O8-C6	10.30	66.68	60.96
6	A	1130	A1C9J	C7-O8-C6	10.25	66.65	60.96
5	A	1118	CLR	C18-C13-C14	-9.99	93.56	111.68
5	C	1112	CLR	C18-C13-C14	-9.95	93.64	111.68
5	D	1112	CLR	C18-C13-C14	-9.92	93.68	111.68
5	B	1111	CLR	C18-C13-C14	-9.90	93.72	111.68
6	D	1124	A1C9J	C18-C19-C20	-9.85	105.75	112.87
6	C	1124	A1C9J	C18-C19-C20	-9.82	105.77	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1123	A1C9J	C18-C19-C20	-9.78	105.80	112.87
6	A	1130	A1C9J	C18-C19-C20	-9.73	105.84	112.87
5	C	1106	CLR	C18-C13-C14	-9.63	94.21	111.68
5	B	1105	CLR	C18-C13-C14	-9.60	94.27	111.68
5	A	1112	CLR	C18-C13-C14	-9.59	94.28	111.68
5	A	1117	CLR	C18-C13-C14	-9.52	94.40	111.68
5	C	1110	CLR	C18-C13-C14	-9.52	94.41	111.68
5	D	1110	CLR	C18-C13-C14	-9.52	94.41	111.68
5	B	1109	CLR	C18-C13-C14	-9.52	94.42	111.68
5	B	1110	CLR	C18-C13-C14	-9.31	94.79	111.68
5	D	1111	CLR	C18-C13-C14	-9.28	94.84	111.68
5	A	1113	CLR	C18-C13-C14	-9.26	94.88	111.68
5	A	1115	CLR	C18-C13-C14	-9.26	94.88	111.68
5	A	1114	CLR	C18-C13-C14	-9.26	94.88	111.68
5	C	1111	CLR	C18-C13-C14	-9.25	94.91	111.68
5	B	1108	CLR	C18-C13-C14	-9.24	94.91	111.68
5	C	1109	CLR	C18-C13-C14	-9.23	94.93	111.68
5	D	1108	CLR	C18-C13-C14	-9.23	94.94	111.68
5	A	1116	CLR	C18-C13-C14	-9.22	94.95	111.68
5	B	1107	CLR	C18-C13-C14	-9.22	94.95	111.68
5	C	1108	CLR	C18-C13-C14	-9.22	94.96	111.68
5	D	1109	CLR	C18-C13-C14	-9.21	94.98	111.68
5	B	1106	CLR	C18-C13-C14	-9.18	95.03	111.68
5	D	1107	CLR	C18-C13-C14	-9.13	95.13	111.68
5	D	1106	CLR	C18-C13-C14	-9.11	95.15	111.68
5	C	1107	CLR	C18-C13-C14	-9.08	95.21	111.68
5	D	1110	CLR	C12-C13-C17	8.63	129.31	116.60
5	A	1117	CLR	C12-C13-C17	8.62	129.30	116.60
5	B	1109	CLR	C12-C13-C17	8.62	129.30	116.60
5	C	1110	CLR	C12-C13-C17	8.58	129.24	116.60
6	B	1123	A1C9J	O8-C7-C6	-8.48	54.38	59.27
6	A	1130	A1C9J	O8-C7-C6	-8.45	54.39	59.27
6	C	1124	A1C9J	O8-C7-C6	-8.45	54.39	59.27
6	D	1124	A1C9J	O8-C7-C6	-8.45	54.39	59.27
5	A	1112	CLR	C12-C13-C17	8.38	128.94	116.60
5	B	1105	CLR	C12-C13-C17	8.37	128.92	116.60
5	B	1111	CLR	C17-C13-C14	8.36	109.69	100.10
5	C	1106	CLR	C12-C13-C17	8.36	128.91	116.60
6	C	1124	A1C9J	C18-C19-N38	8.25	142.23	135.51
6	D	1124	A1C9J	C18-C19-N38	8.21	142.20	135.51
6	B	1123	A1C9J	C18-C19-N38	8.17	142.17	135.51
6	A	1130	A1C9J	C18-C19-N38	8.13	142.14	135.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1118	CLR	C17-C13-C14	7.76	109.00	100.10
5	D	1106	CLR	C12-C13-C17	7.69	127.92	116.60
5	D	1112	CLR	C17-C13-C14	7.63	108.86	100.10
5	C	1112	CLR	C17-C13-C14	7.59	108.81	100.10
6	D	1124	A1C9J	C42-C18-C17	-7.03	95.90	112.65
6	A	1130	A1C9J	C42-C18-C17	-7.02	95.92	112.65
6	C	1124	A1C9J	C42-C18-C17	-7.02	95.92	112.65
6	B	1123	A1C9J	C42-C18-C17	-7.02	95.93	112.65
5	D	1107	CLR	C12-C13-C17	6.74	126.53	116.60
5	B	1106	CLR	C12-C13-C17	6.70	126.47	116.60
5	C	1107	CLR	C12-C13-C17	6.69	126.46	116.60
5	A	1114	CLR	C12-C13-C17	6.63	126.37	116.60
5	A	1116	CLR	C12-C13-C17	6.60	126.32	116.60
5	B	1108	CLR	C12-C13-C17	6.56	126.27	116.60
5	B	1110	CLR	C17-C13-C14	6.55	107.61	100.10
5	C	1109	CLR	C12-C13-C17	6.54	126.24	116.60
5	D	1109	CLR	C12-C13-C17	6.54	126.24	116.60
5	D	1111	CLR	C17-C13-C14	6.46	107.51	100.10
5	D	1108	CLR	C12-C13-C17	6.38	125.99	116.60
5	B	1107	CLR	C12-C13-C17	6.36	125.96	116.60
5	A	1115	CLR	C12-C13-C17	6.34	125.95	116.60
5	C	1111	CLR	C17-C13-C14	6.34	107.37	100.10
5	C	1108	CLR	C12-C13-C17	6.33	125.92	116.60
5	A	1113	CLR	C17-C13-C14	6.32	107.35	100.10
5	C	1109	CLR	C17-C13-C14	6.28	107.31	100.10
5	B	1108	CLR	C17-C13-C14	6.28	107.30	100.10
5	D	1109	CLR	C17-C13-C14	6.24	107.26	100.10
5	A	1116	CLR	C17-C13-C14	6.24	107.26	100.10
6	B	1123	A1C9J	C30-C31-C32	-6.19	110.28	120.05
6	D	1124	A1C9J	C30-C31-C32	-6.15	110.35	120.05
5	B	1111	CLR	C7-C8-C9	6.14	116.82	109.72
6	C	1124	A1C9J	C30-C31-C32	-6.14	110.36	120.05
5	C	1111	CLR	C12-C13-C17	6.13	125.64	116.60
6	A	1130	A1C9J	C30-C31-C32	-6.12	110.40	120.05
5	A	1113	CLR	C12-C13-C17	6.10	125.58	116.60
5	D	1111	CLR	C12-C13-C17	5.99	125.42	116.60
5	B	1110	CLR	C12-C13-C17	5.95	125.36	116.60
5	D	1106	CLR	C14-C8-C9	5.90	116.80	109.09
5	C	1108	CLR	C17-C13-C14	5.90	106.87	100.10
5	D	1112	CLR	C12-C13-C17	5.90	125.29	116.60
5	C	1112	CLR	C12-C13-C17	5.89	125.28	116.60
5	A	1118	CLR	C12-C13-C17	5.89	125.28	116.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1108	CLR	C17-C13-C14	5.88	106.84	100.10
5	A	1115	CLR	C17-C13-C14	5.88	106.84	100.10
5	A	1114	CLR	C17-C13-C14	5.86	106.82	100.10
5	B	1107	CLR	C17-C13-C14	5.85	106.81	100.10
5	C	1107	CLR	C17-C13-C14	5.83	106.79	100.10
5	D	1106	CLR	C7-C8-C9	5.79	116.41	109.72
5	B	1111	CLR	C12-C13-C17	5.75	125.07	116.60
5	B	1106	CLR	C17-C13-C14	5.74	106.68	100.10
5	D	1107	CLR	C17-C13-C14	5.73	106.68	100.10
5	B	1106	CLR	C7-C6-C5	-5.43	115.85	125.02
5	D	1111	CLR	C7-C6-C5	-5.42	115.87	125.02
5	A	1114	CLR	C7-C6-C5	-5.41	115.88	125.02
5	D	1107	CLR	C7-C6-C5	-5.40	115.90	125.02
5	A	1115	CLR	C7-C6-C5	-5.38	115.93	125.02
5	C	1108	CLR	C7-C6-C5	-5.38	115.93	125.02
5	B	1110	CLR	C7-C6-C5	-5.37	115.94	125.02
5	D	1106	CLR	C16-C17-C20	5.37	120.30	112.18
5	B	1107	CLR	C7-C6-C5	-5.36	115.97	125.02
5	D	1108	CLR	C7-C6-C5	-5.35	115.98	125.02
5	D	1106	CLR	C21-C20-C17	-5.33	104.88	112.88
5	C	1107	CLR	C7-C6-C5	-5.30	116.08	125.02
6	B	1123	A1C9J	C31-C30-C29	5.27	129.02	123.15
6	C	1124	A1C9J	C31-C30-C29	5.23	128.97	123.15
6	D	1124	A1C9J	C31-C30-C29	5.22	128.96	123.15
5	A	1113	CLR	C7-C6-C5	-5.22	116.21	125.02
6	A	1130	A1C9J	C31-C30-C29	5.21	128.95	123.15
5	C	1111	CLR	C7-C6-C5	-5.20	116.23	125.02
5	A	1116	CLR	C7-C6-C5	-5.18	116.28	125.02
5	B	1109	CLR	C7-C6-C5	-5.17	116.29	125.02
5	B	1108	CLR	C7-C6-C5	-5.16	116.31	125.02
5	B	1105	CLR	C7-C6-C5	-5.15	116.32	125.02
5	C	1109	CLR	C7-C6-C5	-5.15	116.33	125.02
5	A	1117	CLR	C7-C6-C5	-5.14	116.33	125.02
5	D	1110	CLR	C7-C6-C5	-5.14	116.34	125.02
5	C	1110	CLR	C7-C6-C5	-5.13	116.35	125.02
5	D	1106	CLR	C11-C9-C10	-5.13	106.76	113.08
5	D	1109	CLR	C7-C6-C5	-5.12	116.37	125.02
5	C	1106	CLR	C10-C5-C6	-5.10	115.48	122.93
5	B	1111	CLR	C7-C6-C5	-5.10	116.41	125.02
5	C	1106	CLR	C7-C6-C5	-5.09	116.42	125.02
5	D	1112	CLR	C7-C6-C5	-5.04	116.51	125.02
5	C	1112	CLR	C7-C6-C5	-5.00	116.57	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1118	CLR	C7-C6-C5	-4.98	116.62	125.02
5	A	1112	CLR	C7-C6-C5	-4.95	116.66	125.02
5	B	1105	CLR	C13-C17-C20	4.95	127.14	119.50
5	B	1106	CLR	C10-C5-C6	-4.92	115.75	122.93
6	B	1123	A1C9J	O10-C9-C7	4.89	118.41	110.37
6	C	1124	A1C9J	O10-C9-C7	4.89	118.40	110.37
5	C	1112	CLR	C10-C5-C6	-4.89	115.79	122.93
6	D	1124	A1C9J	O10-C9-C7	4.89	118.40	110.37
6	A	1130	A1C9J	O10-C9-C7	4.88	118.40	110.37
5	C	1108	CLR	C10-C5-C6	-4.87	115.81	122.93
5	D	1107	CLR	C10-C5-C6	-4.87	115.82	122.93
5	A	1117	CLR	C10-C5-C6	-4.86	115.83	122.93
5	D	1108	CLR	C10-C5-C6	-4.85	115.84	122.93
5	D	1111	CLR	C7-C8-C9	4.85	115.33	109.72
5	A	1112	CLR	C10-C5-C6	-4.85	115.85	122.93
5	B	1107	CLR	C10-C5-C6	-4.85	115.85	122.93
5	B	1109	CLR	C10-C5-C6	-4.85	115.85	122.93
5	A	1112	CLR	C13-C17-C20	4.84	126.97	119.50
5	C	1110	CLR	C10-C5-C6	-4.84	115.86	122.93
5	D	1110	CLR	C10-C5-C6	-4.84	115.86	122.93
5	B	1105	CLR	C10-C5-C6	-4.83	115.88	122.93
5	A	1115	CLR	C10-C5-C6	-4.83	115.88	122.93
5	B	1110	CLR	C7-C8-C9	4.83	115.30	109.72
5	D	1106	CLR	C7-C6-C5	-4.82	116.87	125.02
5	A	1114	CLR	C10-C5-C6	-4.82	115.89	122.93
5	D	1109	CLR	C10-C5-C6	-4.81	115.91	122.93
5	C	1109	CLR	C10-C5-C6	-4.79	115.93	122.93
5	A	1116	CLR	C10-C5-C6	-4.79	115.94	122.93
5	D	1111	CLR	C10-C5-C6	-4.78	115.94	122.93
5	B	1108	CLR	C10-C5-C6	-4.78	115.95	122.93
5	C	1107	CLR	C10-C5-C6	-4.78	115.95	122.93
5	A	1113	CLR	C7-C8-C9	4.77	115.24	109.72
5	B	1110	CLR	C10-C5-C6	-4.75	116.00	122.93
5	C	1111	CLR	C7-C8-C9	4.70	115.16	109.72
5	C	1106	CLR	C13-C17-C20	4.70	126.75	119.50
5	B	1105	CLR	C7-C8-C9	4.63	115.08	109.72
5	A	1117	CLR	C7-C8-C9	4.61	115.05	109.72
5	C	1106	CLR	C7-C8-C9	4.60	115.04	109.72
5	B	1109	CLR	C7-C8-C9	4.59	115.03	109.72
5	D	1110	CLR	C7-C8-C9	4.58	115.01	109.72
5	C	1110	CLR	C7-C8-C9	4.58	115.01	109.72
5	A	1112	CLR	C7-C8-C9	4.56	114.99	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1124	A1C9J	C21-C20-C19	4.54	119.44	108.31
6	D	1124	A1C9J	C29-C20-C19	-4.53	103.89	107.12
5	A	1118	CLR	C10-C5-C6	-4.52	116.33	122.93
6	A	1130	A1C9J	C21-C20-C19	4.52	119.39	108.31
6	C	1124	A1C9J	C21-C20-C19	4.52	119.39	108.31
6	B	1123	A1C9J	C21-C20-C19	4.52	119.39	108.31
5	D	1112	CLR	C7-C8-C9	4.51	114.93	109.72
5	D	1106	CLR	C22-C20-C17	4.50	119.67	110.33
6	B	1123	A1C9J	C29-C20-C19	-4.50	103.92	107.12
5	C	1107	CLR	C7-C8-C9	4.46	114.88	109.72
5	B	1105	CLR	C17-C13-C14	4.46	105.22	100.10
6	A	1130	A1C9J	C29-C20-C19	-4.44	103.96	107.12
5	C	1112	CLR	C7-C8-C9	4.43	114.84	109.72
5	D	1109	CLR	C7-C8-C9	4.43	114.84	109.72
5	C	1109	CLR	C7-C8-C9	4.42	114.83	109.72
6	C	1124	A1C9J	C29-C20-C19	-4.42	103.97	107.12
5	A	1113	CLR	C10-C5-C6	-4.40	116.50	122.93
5	C	1110	CLR	C13-C17-C20	4.39	126.28	119.50
5	D	1110	CLR	C13-C17-C20	4.38	126.26	119.50
5	A	1118	CLR	C7-C8-C9	4.37	114.78	109.72
5	C	1111	CLR	C10-C5-C6	-4.37	116.55	122.93
5	A	1117	CLR	C13-C17-C20	4.37	126.24	119.50
5	A	1116	CLR	C7-C8-C9	4.36	114.77	109.72
5	B	1108	CLR	C7-C8-C9	4.35	114.75	109.72
6	B	1123	A1C9J	C13-C18-C17	4.35	115.59	109.34
5	C	1106	CLR	C11-C9-C10	-4.34	107.73	113.08
5	B	1109	CLR	C13-C17-C20	4.34	126.20	119.50
5	C	1112	CLR	C11-C9-C10	-4.33	107.74	113.08
6	D	1124	A1C9J	C13-C18-C17	4.33	115.57	109.34
6	A	1130	A1C9J	C13-C18-C17	4.32	115.56	109.34
6	C	1124	A1C9J	C13-C18-C17	4.31	115.55	109.34
5	D	1107	CLR	C7-C8-C9	4.31	114.71	109.72
5	A	1112	CLR	C17-C13-C14	4.31	105.05	100.10
5	C	1106	CLR	C17-C13-C14	4.31	105.05	100.10
5	A	1112	CLR	C11-C9-C10	-4.28	107.81	113.08
5	D	1112	CLR	C10-C5-C6	-4.26	116.70	122.93
5	A	1114	CLR	C7-C8-C9	4.26	114.64	109.72
5	B	1109	CLR	C11-C9-C10	-4.25	107.85	113.08
5	A	1118	CLR	C11-C9-C10	-4.24	107.86	113.08
5	A	1117	CLR	C11-C9-C10	-4.23	107.86	113.08
5	C	1110	CLR	C11-C9-C10	-4.23	107.88	113.08
5	B	1106	CLR	C7-C8-C9	4.21	114.59	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1110	CLR	C11-C9-C10	-4.18	107.93	113.08
5	A	1115	CLR	C7-C8-C9	4.16	114.53	109.72
5	B	1107	CLR	C7-C8-C9	4.15	114.52	109.72
5	C	1109	CLR	C11-C9-C10	-4.14	107.98	113.08
5	D	1108	CLR	C7-C8-C9	4.14	114.50	109.72
5	C	1108	CLR	C7-C8-C9	4.14	114.50	109.72
5	B	1111	CLR	C14-C8-C9	4.09	114.42	109.09
5	B	1108	CLR	C11-C9-C10	-4.09	108.05	113.08
5	A	1116	CLR	C11-C9-C10	-4.08	108.06	113.08
5	D	1109	CLR	C11-C9-C10	-4.06	108.08	113.08
5	B	1111	CLR	C11-C9-C10	-4.05	108.09	113.08
5	B	1111	CLR	C10-C5-C6	-4.03	117.04	122.93
5	C	1112	CLR	C14-C8-C9	4.03	114.35	109.09
5	A	1118	CLR	C14-C8-C9	3.96	114.26	109.09
5	B	1111	CLR	C9-C10-C5	3.94	115.42	109.65
5	D	1106	CLR	C11-C9-C8	3.86	117.16	111.78
5	D	1112	CLR	C11-C9-C10	-3.79	108.41	113.08
5	B	1110	CLR	C11-C9-C10	-3.75	108.46	113.08
6	A	1130	A1C9J	C27-C28-C33	3.75	133.68	119.67
6	D	1124	A1C9J	C27-C28-C33	3.74	133.66	119.67
6	B	1123	A1C9J	C27-C28-C33	3.74	133.66	119.67
5	B	1105	CLR	C11-C9-C10	-3.74	108.47	113.08
5	D	1111	CLR	C11-C9-C10	-3.73	108.48	113.08
6	C	1124	A1C9J	C27-C28-C33	3.72	133.58	119.67
5	A	1113	CLR	C11-C9-C10	-3.68	108.55	113.08
5	C	1110	CLR	C17-C13-C14	3.66	104.30	100.10
5	D	1106	CLR	C10-C5-C6	-3.66	117.59	122.93
5	B	1109	CLR	C17-C13-C14	3.65	104.29	100.10
5	D	1106	CLR	C21-C20-C22	-3.65	104.70	110.34
5	D	1110	CLR	C17-C13-C14	3.63	104.27	100.10
5	C	1111	CLR	C11-C9-C10	-3.61	108.63	113.08
5	A	1117	CLR	C17-C13-C14	3.61	104.24	100.10
5	C	1110	CLR	C14-C8-C9	3.59	113.78	109.09
5	C	1107	CLR	C11-C9-C10	-3.58	108.67	113.08
5	D	1106	CLR	C23-C22-C20	-3.57	105.10	115.08
5	D	1110	CLR	C14-C8-C9	3.54	113.72	109.09
5	A	1117	CLR	C14-C8-C9	3.54	113.71	109.09
5	A	1118	CLR	C9-C10-C5	3.54	114.83	109.65
5	D	1112	CLR	C14-C8-C9	3.51	113.68	109.09
5	D	1106	CLR	C15-C14-C8	3.50	124.68	119.10
5	B	1109	CLR	C14-C8-C9	3.49	113.64	109.09
5	A	1112	CLR	C22-C20-C17	3.43	117.44	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1112	CLR	C9-C10-C5	3.42	114.66	109.65
5	B	1111	CLR	C19-C10-C9	-3.40	107.85	111.66
5	A	1112	CLR	C4-C5-C10	-3.34	112.15	116.42
5	B	1105	CLR	C22-C20-C17	3.33	117.24	110.33
5	C	1108	CLR	C11-C9-C10	-3.33	108.98	113.08
5	D	1108	CLR	C11-C9-C10	-3.33	108.98	113.08
5	D	1106	CLR	C4-C5-C10	-3.33	112.16	116.42
5	A	1115	CLR	C11-C9-C10	-3.31	109.00	113.08
5	B	1107	CLR	C11-C9-C10	-3.31	109.00	113.08
3	A	1120	LBN	O3-P1-O2	3.26	120.01	107.80
5	C	1112	CLR	C4-C5-C10	-3.26	112.25	116.42
3	D	1115	LBN	O3-P1-O2	3.25	119.98	107.80
3	C	1115	LBN	O3-P1-O2	3.25	119.97	107.80
5	A	1118	CLR	C4-C5-C10	-3.22	112.30	116.42
5	C	1106	CLR	C14-C8-C9	3.18	113.24	109.09
5	C	1112	CLR	C9-C10-C5	3.17	114.30	109.65
5	D	1107	CLR	C11-C9-C10	-3.14	109.22	113.08
5	C	1109	CLR	C14-C8-C9	3.10	113.14	109.09
5	C	1107	CLR	C14-C8-C9	3.07	113.10	109.09
5	A	1112	CLR	C14-C8-C9	3.07	113.09	109.09
5	B	1105	CLR	C4-C5-C10	-3.05	112.52	116.42
5	A	1113	CLR	C4-C5-C10	-3.05	112.52	116.42
5	D	1109	CLR	C14-C8-C9	3.04	113.06	109.09
5	A	1116	CLR	C14-C8-C9	3.04	113.06	109.09
6	C	1124	A1C9J	C15-C14-C13	-3.04	105.24	110.21
5	B	1106	CLR	C11-C9-C10	-3.03	109.35	113.08
5	A	1114	CLR	C11-C9-C10	-3.02	109.36	113.08
5	B	1108	CLR	C4-C5-C10	-3.02	112.55	116.42
6	D	1124	A1C9J	C34-C35-C36	-3.02	118.54	122.62
5	D	1112	CLR	C4-C5-C10	-3.01	112.57	116.42
6	A	1130	A1C9J	C15-C14-C13	-3.01	105.30	110.21
5	B	1105	CLR	C14-C8-C9	3.01	113.01	109.09
6	D	1124	A1C9J	C15-C14-C13	-3.00	105.31	110.21
5	B	1107	CLR	C15-C14-C8	3.00	123.89	119.10
6	B	1123	A1C9J	C15-C14-C13	-3.00	105.31	110.21
5	C	1109	CLR	C4-C5-C10	-3.00	112.58	116.42
5	B	1108	CLR	C14-C8-C9	2.98	112.98	109.09
5	A	1115	CLR	C15-C14-C8	2.98	123.86	119.10
5	D	1109	CLR	C4-C5-C10	-2.98	112.61	116.42
5	C	1111	CLR	C14-C8-C9	2.98	112.98	109.09
5	A	1113	CLR	C14-C8-C9	2.98	112.98	109.09
5	A	1116	CLR	C4-C5-C10	-2.98	112.61	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1123	A1C9J	C34-C35-C36	-2.98	118.60	122.62
5	C	1111	CLR	C4-C5-C10	-2.97	112.62	116.42
6	A	1130	A1C9J	C34-C35-C36	-2.96	118.61	122.62
5	D	1108	CLR	C15-C14-C8	2.95	123.81	119.10
5	C	1108	CLR	C15-C14-C8	2.95	123.81	119.10
5	D	1106	CLR	C17-C13-C14	2.95	103.48	100.10
5	B	1111	CLR	C4-C5-C10	-2.93	112.66	116.42
5	B	1110	CLR	C4-C5-C10	-2.93	112.67	116.42
5	D	1111	CLR	C4-C5-C10	-2.92	112.68	116.42
6	C	1124	A1C9J	C34-C35-C36	-2.92	118.67	122.62
5	C	1106	CLR	C22-C20-C17	2.92	116.38	110.33
5	C	1106	CLR	C4-C5-C10	-2.90	112.71	116.42
5	A	1114	CLR	C15-C14-C8	2.86	123.66	119.10
6	A	1130	A1C9J	C26-C25-C24	2.84	91.51	87.20
5	B	1111	CLR	C12-C11-C9	2.84	117.97	113.14
6	B	1123	A1C9J	C26-C25-C24	2.83	91.49	87.20
5	B	1106	CLR	C15-C14-C8	2.83	123.62	119.10
6	D	1124	A1C9J	C26-C25-C24	2.82	91.47	87.20
5	B	1110	CLR	C14-C8-C9	2.81	112.76	109.09
6	C	1124	A1C9J	C26-C25-C24	2.81	91.45	87.20
5	B	1109	CLR	C4-C5-C10	-2.80	112.84	116.42
5	D	1111	CLR	C14-C8-C9	2.79	112.73	109.09
5	A	1117	CLR	C4-C5-C10	-2.77	112.87	116.42
5	D	1110	CLR	C4-C5-C10	-2.77	112.88	116.42
5	D	1107	CLR	C14-C8-C9	2.75	112.68	109.09
5	C	1110	CLR	C4-C5-C10	-2.75	112.90	116.42
5	D	1107	CLR	C15-C14-C8	2.75	123.48	119.10
5	C	1107	CLR	C4-C5-C10	-2.74	112.92	116.42
6	B	1123	A1C9J	C31-C30-N38	-2.74	125.03	130.65
6	D	1124	A1C9J	C34-C33-C28	-2.72	113.70	118.24
6	A	1130	A1C9J	C34-C33-C28	-2.72	113.70	118.24
6	C	1124	A1C9J	C34-C33-C28	-2.72	113.70	118.24
6	A	1130	A1C9J	C31-C30-N38	-2.71	125.09	130.65
6	C	1124	A1C9J	C31-C30-N38	-2.71	125.10	130.65
6	B	1123	A1C9J	C34-C33-C28	-2.70	113.74	118.24
6	D	1124	A1C9J	C31-C30-N38	-2.69	125.13	130.65
5	A	1115	CLR	C14-C8-C9	2.68	112.58	109.09
5	B	1106	CLR	C14-C8-C9	2.67	112.58	109.09
5	B	1107	CLR	C1-C10-C5	2.67	113.34	108.74
5	D	1108	CLR	C4-C5-C10	-2.66	113.01	116.42
5	D	1108	CLR	C1-C10-C5	2.66	113.32	108.74
5	B	1107	CLR	C14-C8-C9	2.66	112.56	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1115	CLR	C4-C5-C10	-2.65	113.03	116.42
5	B	1107	CLR	C4-C5-C10	-2.65	113.03	116.42
5	B	1108	CLR	C15-C14-C8	2.65	123.32	119.10
5	C	1108	CLR	C1-C10-C5	2.64	113.30	108.74
5	A	1115	CLR	C1-C10-C5	2.64	113.30	108.74
5	D	1108	CLR	C14-C8-C9	2.64	112.53	109.09
5	C	1108	CLR	C14-C8-C9	2.63	112.53	109.09
5	C	1108	CLR	C4-C5-C10	-2.63	113.05	116.42
5	B	1106	CLR	C1-C10-C5	2.63	113.27	108.74
5	A	1116	CLR	C15-C14-C8	2.62	123.27	119.10
5	C	1112	CLR	C11-C9-C8	2.61	115.42	111.78
5	D	1107	CLR	C4-C5-C10	-2.59	113.10	116.42
5	C	1107	CLR	C15-C14-C8	2.59	123.23	119.10
5	D	1109	CLR	C15-C14-C8	2.58	123.22	119.10
5	C	1109	CLR	C15-C14-C8	2.58	123.22	119.10
5	A	1113	CLR	C21-C20-C17	-2.58	109.02	112.88
5	A	1114	CLR	C4-C5-C10	-2.57	113.13	116.42
5	D	1107	CLR	C1-C10-C5	2.57	113.18	108.74
5	C	1111	CLR	C21-C20-C17	-2.57	109.02	112.88
6	B	1123	A1C9J	C44-C13-C12	2.57	111.59	108.07
5	D	1111	CLR	C21-C20-C17	-2.56	109.04	112.88
6	A	1130	A1C9J	C44-C13-C12	2.56	111.57	108.07
6	C	1124	A1C9J	C44-C13-C12	2.56	111.57	108.07
5	D	1106	CLR	C9-C10-C5	2.55	113.38	109.65
5	A	1114	CLR	C14-C8-C9	2.54	112.40	109.09
5	B	1106	CLR	C4-C5-C10	-2.54	113.17	116.42
5	A	1114	CLR	C1-C10-C5	2.53	113.11	108.74
6	D	1124	A1C9J	C40-C23-C24	2.53	118.90	113.21
6	B	1123	A1C9J	C40-C23-C24	2.52	118.88	113.21
6	D	1124	A1C9J	C44-C13-C12	2.52	111.51	108.07
6	C	1124	A1C9J	C40-C23-C24	2.51	118.87	113.21
6	A	1130	A1C9J	C40-C23-C24	2.51	118.85	113.21
5	A	1118	CLR	C11-C9-C8	2.50	115.27	111.78
5	D	1109	CLR	C23-C22-C20	-2.48	108.13	115.08
5	B	1110	CLR	C15-C14-C8	2.48	123.06	119.10
6	C	1124	A1C9J	C44-C13-C14	-2.48	106.90	110.23
5	B	1110	CLR	C21-C20-C17	-2.47	109.18	112.88
5	D	1110	CLR	C1-C10-C5	2.45	112.97	108.74
5	D	1111	CLR	C15-C14-C8	2.45	123.00	119.10
5	A	1116	CLR	C23-C22-C20	-2.44	108.25	115.08
5	B	1109	CLR	C1-C10-C5	2.44	112.94	108.74
6	C	1124	A1C9J	O43-C14-C15	-2.43	100.99	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1110	CLR	C1-C10-C5	2.43	112.94	108.74
6	D	1124	A1C9J	O43-C14-C15	-2.43	101.00	106.98
5	A	1112	CLR	C9-C10-C5	2.42	113.20	109.65
5	A	1117	CLR	C1-C10-C5	2.42	112.92	108.74
6	B	1123	A1C9J	O43-C14-C15	-2.41	101.04	106.98
5	C	1109	CLR	C23-C22-C20	-2.41	108.33	115.08
6	A	1130	A1C9J	O43-C14-C15	-2.41	101.06	106.98
5	B	1108	CLR	C23-C22-C20	-2.40	108.38	115.08
3	A	1119	LBN	O3-P1-O4	2.39	120.16	110.83
3	B	1113	LBN	O3-P1-O4	2.39	120.15	110.83
3	D	1114	LBN	O3-P1-O4	2.39	120.14	110.83
3	C	1114	LBN	O3-P1-O4	2.38	120.11	110.83
5	A	1113	CLR	C15-C14-C8	2.38	122.89	119.10
3	A	1121	LBN	O3-P1-O4	2.38	120.09	110.83
5	A	1117	CLR	C15-C14-C8	2.37	122.89	119.10
3	D	1113	LBN	O3-P1-O4	2.37	120.07	110.83
6	D	1124	A1C9J	C44-C13-C14	-2.37	107.05	110.23
5	C	1110	CLR	C15-C14-C8	2.37	122.88	119.10
3	A	1109	LBN	O3-P1-O4	2.37	120.05	110.83
5	B	1109	CLR	C22-C20-C17	2.36	115.23	110.33
5	A	1117	CLR	C22-C20-C17	2.36	115.22	110.33
3	A	1107	LBN	O3-P1-O4	2.36	120.02	110.83
3	A	1108	LBN	O3-P1-O4	2.35	120.01	110.83
3	D	1102	LBN	O3-P1-O4	2.35	120.00	110.83
3	B	1102	LBN	O3-P1-O4	2.35	120.00	110.83
3	C	1101	LBN	O3-P1-O4	2.35	120.00	110.83
5	D	1110	CLR	C22-C20-C17	2.35	115.20	110.33
5	D	1111	CLR	C1-C10-C5	2.35	112.79	108.74
3	B	1101	LBN	O3-P1-O4	2.35	119.98	110.83
3	D	1101	LBN	O3-P1-O4	2.35	119.97	110.83
3	C	1113	LBN	O3-P1-O4	2.34	119.96	110.83
3	C	1104	LBN	O3-P1-O4	2.34	119.96	110.83
3	C	1102	LBN	O3-P1-O4	2.34	119.96	110.83
5	C	1107	CLR	C1-C10-C5	2.34	112.78	108.74
3	C	1103	LBN	O3-P1-O4	2.34	119.95	110.83
5	B	1109	CLR	C15-C14-C8	2.34	122.83	119.10
5	D	1106	CLR	C8-C7-C6	-2.34	109.53	112.76
3	A	1106	LBN	O3-P1-O4	2.34	119.93	110.83
5	C	1111	CLR	C9-C10-C5	2.34	113.07	109.65
5	A	1113	CLR	C9-C10-C5	2.33	113.07	109.65
3	B	1112	LBN	O3-P1-O4	2.33	119.92	110.83
5	D	1110	CLR	C15-C14-C8	2.33	122.82	119.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1114	LBN	O3-P1-O4	2.33	119.92	110.83
3	D	1103	LBN	O3-P1-O4	2.33	119.91	110.83
5	C	1112	CLR	C15-C14-C8	2.33	122.82	119.10
3	A	1110	LBN	O3-P1-O4	2.33	119.91	110.83
5	C	1111	CLR	C15-C14-C8	2.33	122.82	119.10
3	D	1104	LBN	O3-P1-O4	2.33	119.91	110.83
6	A	1130	A1C9J	C44-C13-C14	-2.33	107.10	110.23
3	B	1103	LBN	O3-P1-O4	2.33	119.90	110.83
3	B	1115	LBN	O3-P1-O4	2.33	119.89	110.83
3	C	1116	LBN	O3-P1-O4	2.32	119.88	110.83
6	B	1123	A1C9J	C44-C13-C14	-2.32	107.11	110.23
3	D	1116	LBN	O3-P1-O4	2.32	119.86	110.83
6	C	1124	A1C9J	C1-C2-C4	2.32	121.32	116.98
3	A	1122	LBN	O3-P1-O4	2.31	119.85	110.83
5	B	1110	CLR	C1-C10-C5	2.31	112.73	108.74
6	B	1123	A1C9J	C1-C2-C4	2.30	121.30	116.98
5	A	1118	CLR	C12-C11-C9	2.30	117.05	113.14
6	D	1124	A1C9J	C1-C2-C4	2.30	121.29	116.98
5	C	1110	CLR	C22-C20-C17	2.30	115.10	110.33
5	A	1118	CLR	C15-C14-C8	2.30	122.77	119.10
5	B	1105	CLR	C9-C10-C5	2.29	113.00	109.65
5	A	1116	CLR	C21-C20-C22	-2.28	106.81	110.34
6	A	1130	A1C9J	C1-C2-C4	2.28	121.25	116.98
6	C	1124	A1C9J	C16-C17-C21	-2.28	107.00	114.62
5	D	1109	CLR	C21-C20-C22	-2.27	106.82	110.34
6	B	1123	A1C9J	C16-C17-C21	-2.27	107.03	114.62
6	D	1124	A1C9J	C16-C17-C21	-2.27	107.03	114.62
6	A	1130	A1C9J	C16-C17-C21	-2.27	107.03	114.62
5	D	1112	CLR	C15-C14-C8	2.25	122.69	119.10
5	D	1109	CLR	C1-C10-C5	2.25	112.62	108.74
5	A	1112	CLR	C15-C14-C8	2.25	122.69	119.10
5	C	1109	CLR	C21-C20-C22	-2.25	106.86	110.34
5	C	1106	CLR	C9-C10-C5	2.24	112.94	109.65
5	A	1116	CLR	C1-C10-C5	2.24	112.61	108.74
5	D	1112	CLR	C11-C9-C8	2.24	114.91	111.78
6	D	1124	A1C9J	O43-C14-C13	2.24	112.42	107.51
5	B	1111	CLR	C11-C9-C8	2.24	114.90	111.78
5	C	1109	CLR	C1-C10-C5	2.23	112.60	108.74
6	C	1124	A1C9J	O43-C14-C13	2.23	112.41	107.51
6	A	1130	A1C9J	O43-C14-C13	2.23	112.40	107.51
5	B	1108	CLR	C1-C10-C5	2.23	112.58	108.74
6	B	1123	A1C9J	O43-C14-C13	2.23	112.40	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1106	CLR	C12-C11-C9	2.22	116.92	113.14
6	B	1123	A1C9J	C34-C33-C32	-2.21	117.57	121.33
5	C	1106	CLR	C15-C14-C8	2.21	122.62	119.10
5	C	1112	CLR	C12-C11-C9	2.21	116.89	113.14
5	D	1109	CLR	C9-C10-C5	2.20	112.88	109.65
5	C	1109	CLR	C9-C10-C5	2.20	112.88	109.65
5	B	1105	CLR	C12-C11-C9	2.20	116.87	113.14
6	A	1130	A1C9J	C34-C33-C32	-2.19	117.61	121.33
5	A	1113	CLR	C1-C10-C5	2.19	112.51	108.74
5	B	1108	CLR	C21-C20-C22	-2.18	106.97	110.34
5	A	1112	CLR	C12-C11-C9	2.18	116.83	113.14
6	D	1124	A1C9J	C20-C19-N38	2.17	111.89	109.74
5	A	1116	CLR	C9-C10-C5	2.17	112.83	109.65
6	B	1123	A1C9J	C20-C19-N38	2.16	111.88	109.74
5	D	1112	CLR	C12-C11-C9	2.16	116.81	113.14
5	B	1111	CLR	C19-C10-C1	-2.16	106.14	109.43
5	B	1108	CLR	C9-C10-C5	2.16	112.82	109.65
6	C	1124	A1C9J	C34-C33-C32	-2.16	117.67	121.33
6	A	1130	A1C9J	C20-C19-N38	2.16	111.88	109.74
6	D	1124	A1C9J	C34-C33-C32	-2.16	117.67	121.33
5	C	1106	CLR	C1-C10-C5	2.15	112.44	108.74
6	A	1130	A1C9J	C33-C32-CL37	2.15	123.37	119.60
5	A	1112	CLR	C19-C10-C9	-2.14	109.25	111.66
5	B	1105	CLR	C19-C10-C9	-2.14	109.26	111.66
6	B	1123	A1C9J	C33-C32-CL37	2.13	123.36	119.60
5	B	1110	CLR	C9-C10-C5	2.13	112.78	109.65
5	A	1118	CLR	C15-C16-C17	2.13	109.31	105.14
6	D	1124	A1C9J	C33-C32-CL37	2.13	123.35	119.60
6	C	1124	A1C9J	C33-C32-CL37	2.13	123.34	119.60
5	B	1106	CLR	C23-C22-C20	-2.12	109.14	115.08
5	D	1106	CLR	C12-C11-C9	2.12	116.74	113.14
6	C	1124	A1C9J	C20-C19-N38	2.12	111.84	109.74
5	C	1111	CLR	C1-C10-C5	2.12	112.40	108.74
5	D	1111	CLR	C9-C10-C5	2.12	112.75	109.65
5	D	1112	CLR	C15-C16-C17	2.11	109.28	105.14
5	C	1107	CLR	C23-C22-C20	-2.11	109.17	115.08
5	D	1107	CLR	C23-C22-C20	-2.11	109.17	115.08
5	C	1112	CLR	C15-C16-C17	2.10	109.25	105.14
5	A	1114	CLR	C23-C22-C20	-2.09	109.24	115.08
5	C	1110	CLR	C11-C9-C8	2.09	114.69	111.78
5	C	1110	CLR	C9-C10-C5	2.08	112.70	109.65
5	D	1110	CLR	C9-C10-C5	2.08	112.70	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1117	CLR	C9-C10-C5	2.07	112.68	109.65
5	D	1110	CLR	C11-C9-C8	2.07	114.66	111.78
6	A	1130	A1C9J	O45-C5-C6	2.07	114.50	109.67
5	C	1111	CLR	C19-C10-C9	-2.07	109.34	111.66
5	A	1113	CLR	C19-C10-C9	-2.06	109.34	111.66
5	B	1109	CLR	C11-C9-C8	2.06	114.66	111.78
5	B	1111	CLR	C16-C17-C13	-2.06	101.42	103.84
6	B	1123	A1C9J	O45-C5-C6	2.06	114.49	109.67
5	B	1110	CLR	C11-C9-C8	2.06	114.65	111.78
6	D	1124	A1C9J	O45-C5-C6	2.06	114.49	109.67
5	B	1110	CLR	C19-C10-C9	-2.06	109.35	111.66
5	A	1112	CLR	C23-C22-C20	-2.06	109.33	115.08
5	B	1105	CLR	C23-C22-C20	-2.06	109.33	115.08
5	C	1112	CLR	C1-C10-C5	2.05	112.28	108.74
6	C	1124	A1C9J	O45-C5-C6	2.05	114.47	109.67
5	D	1106	CLR	C19-C10-C9	-2.05	109.36	111.66
5	C	1111	CLR	C11-C9-C8	2.05	114.64	111.78
5	B	1105	CLR	C15-C14-C13	2.05	106.25	103.84
5	A	1113	CLR	C11-C9-C8	2.05	114.64	111.78
5	B	1105	CLR	C1-C10-C5	2.05	112.27	108.74
5	A	1117	CLR	C11-C9-C8	2.04	114.62	111.78
5	B	1109	CLR	C9-C10-C5	2.04	112.64	109.65
5	A	1112	CLR	C15-C14-C13	2.04	106.23	103.84
5	A	1115	CLR	C21-C20-C17	-2.04	109.83	112.88
5	C	1107	CLR	C19-C10-C9	-2.03	109.38	111.66
5	D	1111	CLR	C11-C9-C8	2.03	114.61	111.78
5	A	1112	CLR	C1-C10-C5	2.03	112.24	108.74
5	B	1106	CLR	C21-C20-C22	-2.03	107.20	110.34
5	C	1111	CLR	C12-C11-C9	2.02	116.58	113.14
5	D	1111	CLR	C19-C10-C9	-2.02	109.39	111.66
5	B	1107	CLR	C21-C20-C17	-2.02	109.85	112.88
5	A	1113	CLR	C12-C11-C9	2.02	116.56	113.14
5	B	1110	CLR	C12-C11-C9	2.02	116.56	113.14
5	C	1107	CLR	C21-C20-C22	-2.01	107.22	110.34
5	B	1105	CLR	C15-C14-C8	2.01	122.31	119.10
5	D	1107	CLR	C21-C20-C22	-2.00	107.24	110.34

All (92) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1106	LBN	C2
3	A	1107	LBN	C2

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Mol	Chain	Res	Type	Atom
3	A	1108	LBN	C2
3	A	1109	LBN	C2
3	A	1110	LBN	C2
3	A	1119	LBN	C2
3	A	1120	LBN	C2
3	A	1121	LBN	C2
3	A	1122	LBN	C2
3	B	1101	LBN	C2
3	B	1102	LBN	C2
3	B	1103	LBN	C2
3	B	1112	LBN	C2
3	B	1113	LBN	C2
3	B	1114	LBN	C2
3	B	1115	LBN	C2
3	C	1101	LBN	C2
3	C	1102	LBN	C2
3	C	1103	LBN	C2
3	C	1104	LBN	C2
3	C	1113	LBN	C2
3	C	1114	LBN	C2
3	C	1115	LBN	C2
3	C	1116	LBN	C2
3	D	1101	LBN	C2
3	D	1102	LBN	C2
3	D	1103	LBN	C2
3	D	1104	LBN	C2
3	D	1113	LBN	C2
3	D	1114	LBN	C2
3	D	1115	LBN	C2
3	D	1116	LBN	C2
5	A	1112	CLR	C13
5	A	1112	CLR	C8
5	A	1113	CLR	C13
5	A	1113	CLR	C8
5	A	1114	CLR	C13
5	A	1114	CLR	C8
5	A	1115	CLR	C13
5	A	1115	CLR	C8
5	A	1116	CLR	C13
5	A	1116	CLR	C8
5	A	1117	CLR	C13
5	A	1117	CLR	C8

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Mol	Chain	Res	Type	Atom
5	A	1118	CLR	C13
5	A	1118	CLR	C8
5	B	1105	CLR	C13
5	B	1105	CLR	C8
5	B	1106	CLR	C13
5	B	1106	CLR	C8
5	B	1107	CLR	C13
5	B	1107	CLR	C8
5	B	1108	CLR	C13
5	B	1108	CLR	C8
5	B	1109	CLR	C13
5	B	1109	CLR	C8
5	B	1110	CLR	C13
5	B	1110	CLR	C8
5	B	1111	CLR	C13
5	B	1111	CLR	C8
5	C	1106	CLR	C13
5	C	1106	CLR	C8
5	C	1107	CLR	C13
5	C	1107	CLR	C8
5	C	1108	CLR	C13
5	C	1108	CLR	C8
5	C	1109	CLR	C13
5	C	1109	CLR	C8
5	C	1110	CLR	C13
5	C	1110	CLR	C8
5	C	1111	CLR	C13
5	C	1111	CLR	C8
5	C	1112	CLR	C13
5	C	1112	CLR	C8
5	D	1106	CLR	C13
5	D	1106	CLR	C8
5	D	1107	CLR	C13
5	D	1107	CLR	C8
5	D	1108	CLR	C13
5	D	1108	CLR	C8
5	D	1109	CLR	C13
5	D	1109	CLR	C8
5	D	1110	CLR	C13
5	D	1110	CLR	C8
5	D	1111	CLR	C13
5	D	1111	CLR	C8

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Mol	Chain	Res	Type	Atom
5	D	1112	CLR	C13
5	D	1112	CLR	C8
6	A	1130	A1C9J	C17
6	B	1123	A1C9J	C17
6	C	1124	A1C9J	C17
6	D	1124	A1C9J	C17

All (288) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1124	AJP	C22-C23-O25-C26
4	B	1117	AJP	C22-C23-O25-C26
4	B	1122	AJP	C24-C23-O25-C26
4	C	1118	AJP	C22-C23-O25-C26
4	C	1123	AJP	C24-C23-O25-C26
4	D	1118	AJP	C22-C23-O25-C26
4	D	1120	AJP	C24-C23-O25-C26
5	A	1112	CLR	C13-C17-C20-C22
5	A	1112	CLR	C16-C17-C20-C21
5	A	1117	CLR	C13-C17-C20-C22
5	A	1117	CLR	C16-C17-C20-C21
5	B	1105	CLR	C13-C17-C20-C22
5	B	1105	CLR	C16-C17-C20-C21
5	B	1109	CLR	C13-C17-C20-C22
5	B	1109	CLR	C16-C17-C20-C21
5	C	1106	CLR	C13-C17-C20-C22
5	C	1106	CLR	C16-C17-C20-C21
5	C	1110	CLR	C13-C17-C20-C22
5	C	1110	CLR	C16-C17-C20-C21
5	D	1110	CLR	C13-C17-C20-C22
5	D	1110	CLR	C16-C17-C20-C21
4	A	1111	AJP	O31-C26-O25-C23
4	B	1104	AJP	O40-C35-O34-C29
4	B	1120	AJP	O60-C55-O54-C36
4	C	1105	AJP	O31-C26-O25-C23
4	D	1121	AJP	O60-C55-O54-C36
4	A	1111	AJP	C27-C26-O25-C23
4	C	1105	AJP	C27-C26-O25-C23
4	D	1121	AJP	C56-C55-O54-C36
4	A	1111	AJP	O40-C35-O34-C29
4	C	1121	AJP	O60-C55-O54-C36
4	B	1104	AJP	C36-C35-O34-C29

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Mol	Chain	Res	Type	Atoms
4	B	1120	AJP	C56-C55-O54-C36
5	B	1111	CLR	C21-C20-C22-C23
5	A	1112	CLR	C13-C17-C20-C21
5	A	1117	CLR	C13-C17-C20-C21
5	B	1105	CLR	C13-C17-C20-C21
5	B	1109	CLR	C13-C17-C20-C21
5	C	1106	CLR	C13-C17-C20-C21
5	C	1110	CLR	C13-C17-C20-C21
5	D	1110	CLR	C13-C17-C20-C21
4	C	1121	AJP	C56-C55-O54-C36
5	A	1117	CLR	C21-C20-C22-C23
5	B	1109	CLR	C21-C20-C22-C23
5	C	1110	CLR	C21-C20-C22-C23
5	D	1110	CLR	C21-C20-C22-C23
4	A	1128	AJP	O31-C26-O25-C23
5	A	1113	CLR	C21-C20-C22-C23
5	D	1111	CLR	C21-C20-C22-C23
5	A	1112	CLR	C16-C17-C20-C22
4	A	1127	AJP	C56-C55-O54-C36
5	A	1117	CLR	C16-C17-C20-C22
5	B	1105	CLR	C16-C17-C20-C22
5	B	1109	CLR	C16-C17-C20-C22
5	C	1106	CLR	C16-C17-C20-C22
5	C	1110	CLR	C16-C17-C20-C22
5	D	1110	CLR	C16-C17-C20-C22
5	D	1106	CLR	C13-C17-C20-C22
4	B	1120	AJP	O60-C59-C61-O62
5	A	1117	CLR	C17-C20-C22-C23
5	B	1109	CLR	C17-C20-C22-C23
5	C	1110	CLR	C17-C20-C22-C23
5	D	1110	CLR	C17-C20-C22-C23
4	D	1121	AJP	O60-C59-C61-O62
4	A	1127	AJP	O60-C55-O54-C36
4	B	1121	AJP	O31-C26-O25-C23
5	B	1110	CLR	C21-C20-C22-C23
5	C	1106	CLR	C21-C20-C22-C23
5	C	1111	CLR	C21-C20-C22-C23
4	B	1121	AJP	C27-C26-O25-C23
5	A	1118	CLR	C21-C20-C22-C23
5	C	1112	CLR	C21-C20-C22-C23
4	D	1105	AJP	O40-C35-O34-C29
4	C	1105	AJP	C30-C29-O34-C35

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Mol	Chain	Res	Type	Atoms
4	A	1127	AJP	C58-C59-C61-O62
5	D	1106	CLR	C13-C17-C20-C21
5	D	1106	CLR	C16-C17-C20-C22
5	A	1114	CLR	C22-C23-C24-C25
5	B	1111	CLR	C20-C22-C23-C24
5	D	1107	CLR	C22-C23-C24-C25
5	B	1106	CLR	C22-C23-C24-C25
5	A	1113	CLR	C13-C17-C20-C21
5	B	1110	CLR	C13-C17-C20-C21
5	C	1111	CLR	C13-C17-C20-C21
5	D	1111	CLR	C13-C17-C20-C21
4	D	1105	AJP	C36-C35-O34-C29
4	B	1120	AJP	C58-C59-C61-O62
5	A	1117	CLR	C20-C22-C23-C24
5	B	1105	CLR	C20-C22-C23-C24
5	C	1107	CLR	C22-C23-C24-C25
5	C	1110	CLR	C20-C22-C23-C24
5	A	1112	CLR	C20-C22-C23-C24
5	A	1112	CLR	C17-C20-C22-C23
5	D	1106	CLR	C16-C17-C20-C21
4	D	1121	AJP	C58-C59-C61-O62
5	D	1112	CLR	C21-C20-C22-C23
4	C	1105	AJP	C28-C29-O34-C35
5	C	1106	CLR	C23-C24-C25-C27
5	A	1118	CLR	C23-C24-C25-C26
5	C	1106	CLR	C23-C24-C25-C26
5	B	1109	CLR	C20-C22-C23-C24
5	D	1106	CLR	C20-C22-C23-C24
5	C	1112	CLR	C23-C24-C25-C26
3	D	1104	LBN	C35-C36-C37-C38
5	A	1112	CLR	C23-C24-C25-C26
5	A	1118	CLR	C23-C24-C25-C27
5	D	1112	CLR	C23-C24-C25-C26
5	B	1105	CLR	C21-C20-C22-C23
5	C	1112	CLR	C23-C24-C25-C27
5	D	1110	CLR	C20-C22-C23-C24
5	D	1111	CLR	C13-C17-C20-C22
5	B	1108	CLR	C23-C24-C25-C26
5	A	1113	CLR	C13-C17-C20-C22
5	B	1110	CLR	C13-C17-C20-C22
5	C	1111	CLR	C13-C17-C20-C22
3	C	1104	LBN	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
5	A	1113	CLR	C16-C17-C20-C21
5	B	1110	CLR	C16-C17-C20-C21
5	C	1111	CLR	C16-C17-C20-C21
5	D	1111	CLR	C16-C17-C20-C21
5	A	1116	CLR	C23-C24-C25-C26
5	A	1115	CLR	C17-C20-C22-C23
5	A	1112	CLR	C23-C24-C25-C27
5	A	1116	CLR	C23-C24-C25-C27
5	C	1109	CLR	C23-C24-C25-C26
5	C	1109	CLR	C23-C24-C25-C27
5	D	1109	CLR	C23-C24-C25-C27
5	D	1112	CLR	C23-C24-C25-C27
4	D	1118	AJP	O31-C30-C32-O33
5	C	1108	CLR	C17-C20-C22-C23
3	D	1104	LBN	C35-C34-O7-C2
4	A	1111	AJP	O31-C30-C32-O33
4	C	1119	AJP	O31-C30-C32-O33
4	C	1121	AJP	O40-C39-C41-O42
4	D	1119	AJP	O31-C30-C32-O33
4	A	1127	AJP	O31-C30-C32-O33
4	D	1105	AJP	O40-C39-C41-O42
5	B	1107	CLR	C17-C20-C22-C23
5	D	1108	CLR	C17-C20-C22-C23
5	B	1108	CLR	C23-C24-C25-C27
5	D	1109	CLR	C23-C24-C25-C26
4	C	1105	AJP	O40-C39-C41-O42
4	A	1125	AJP	O31-C30-C32-O33
4	B	1120	AJP	O31-C30-C32-O33
4	D	1121	AJP	O31-C30-C32-O33
4	D	1123	AJP	O31-C30-C32-O33
3	B	1103	LBN	C36-C37-C38-C39
3	D	1114	LBN	O1-C1-C2-C3
4	C	1121	AJP	O31-C30-C32-O33
3	B	1103	LBN	C35-C36-C37-C38
5	B	1111	CLR	C17-C20-C22-C23
3	D	1104	LBN	O8-C34-O7-C2
4	B	1104	AJP	O31-C30-C32-O33
4	C	1105	AJP	O31-C30-C32-O33
4	A	1127	AJP	O60-C59-C61-O62
4	C	1122	AJP	O31-C30-C32-O33
4	D	1105	AJP	O31-C30-C32-O33
3	D	1113	LBN	C35-C34-O7-C2

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Mol	Chain	Res	Type	Atoms
5	A	1118	CLR	C13-C17-C20-C21
5	B	1111	CLR	C13-C17-C20-C21
5	C	1112	CLR	C13-C17-C20-C21
5	D	1112	CLR	C13-C17-C20-C21
5	A	1118	CLR	C20-C22-C23-C24
3	C	1104	LBN	C35-C34-O7-C2
5	A	1115	CLR	C13-C17-C20-C21
5	C	1112	CLR	C20-C22-C23-C24
3	A	1110	LBN	C36-C37-C38-C39
3	A	1119	LBN	O1-C1-C2-C3
3	B	1113	LBN	O1-C1-C2-C3
3	C	1103	LBN	O1-C1-C2-C3
3	C	1104	LBN	O8-C34-O7-C2
5	B	1111	CLR	C13-C17-C20-C22
5	C	1108	CLR	C13-C17-C20-C21
5	B	1107	CLR	C13-C17-C20-C21
5	D	1108	CLR	C13-C17-C20-C21
3	B	1113	LBN	O1-C1-C2-O7
3	C	1103	LBN	O1-C1-C2-O7
5	A	1113	CLR	C16-C17-C20-C22
5	C	1111	CLR	C16-C17-C20-C22
5	D	1112	CLR	C20-C22-C23-C24
5	A	1115	CLR	C21-C20-C22-C23
3	B	1115	LBN	O7-C34-C35-C36
3	C	1116	LBN	O7-C34-C35-C36
3	A	1121	LBN	O7-C2-C3-O5
5	C	1108	CLR	C21-C20-C22-C23
5	B	1110	CLR	C16-C17-C20-C22
5	D	1111	CLR	C16-C17-C20-C22
3	A	1122	LBN	O7-C34-C35-C36
3	A	1121	LBN	C35-C36-C37-C38
5	D	1111	CLR	C17-C20-C22-C23
5	D	1112	CLR	C13-C17-C20-C22
5	B	1107	CLR	C21-C20-C22-C23
5	D	1108	CLR	C21-C20-C22-C23
5	A	1113	CLR	C17-C20-C22-C23
5	C	1112	CLR	C13-C17-C20-C22
3	B	1112	LBN	C26-C25-O5-C3
5	B	1111	CLR	C16-C17-C20-C21
3	C	1114	LBN	O1-C1-C2-C3
5	A	1118	CLR	C13-C17-C20-C22
3	D	1113	LBN	O8-C34-O7-C2

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Mol	Chain	Res	Type	Atoms
3	D	1116	LBN	O7-C34-C35-C36
5	D	1112	CLR	C16-C17-C20-C21
3	A	1119	LBN	O1-C1-C2-O7
3	D	1114	LBN	O1-C1-C2-O7
5	C	1112	CLR	C16-C17-C20-C21
3	B	1112	LBN	O6-C25-O5-C3
5	C	1106	CLR	C20-C22-C23-C24
4	C	1122	AJP	O31-C26-O25-C23
5	A	1113	CLR	C23-C24-C25-C27
5	B	1110	CLR	C23-C24-C25-C27
5	C	1111	CLR	C23-C24-C25-C27
5	D	1111	CLR	C23-C24-C25-C27
5	A	1118	CLR	C16-C17-C20-C21
4	C	1122	AJP	C27-C26-O25-C23
3	D	1113	LBN	C35-C36-C37-C38
5	A	1115	CLR	C16-C17-C20-C21
3	A	1110	LBN	O8-C34-O7-C2
5	B	1110	CLR	C17-C20-C22-C23
3	C	1114	LBN	O1-C1-C2-O7
5	C	1108	CLR	C16-C17-C20-C21
3	C	1113	LBN	O7-C2-C3-O5
3	A	1121	LBN	C1-C2-C3-O5
5	B	1111	CLR	C16-C17-C20-C22
5	C	1111	CLR	C17-C20-C22-C23
5	B	1107	CLR	C16-C17-C20-C21
5	D	1108	CLR	C16-C17-C20-C21
5	A	1114	CLR	C13-C17-C20-C21
5	A	1113	CLR	C23-C24-C25-C26
5	B	1110	CLR	C23-C24-C25-C26
5	C	1111	CLR	C23-C24-C25-C26
5	D	1111	CLR	C23-C24-C25-C26
3	C	1113	LBN	O6-C25-O5-C3
3	C	1113	LBN	C26-C25-O5-C3
5	A	1115	CLR	C13-C17-C20-C22
3	C	1104	LBN	C36-C37-C38-C39
4	B	1122	AJP	O31-C26-O25-C23
3	D	1116	LBN	C2-C1-O1-P1
5	C	1108	CLR	C13-C17-C20-C22
5	B	1106	CLR	C13-C17-C20-C21
5	D	1107	CLR	C13-C17-C20-C21
3	A	1121	LBN	C26-C25-O5-C3
3	A	1121	LBN	O6-C25-O5-C3

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Mol	Chain	Res	Type	Atoms
5	C	1112	CLR	C16-C17-C20-C22
5	D	1112	CLR	C16-C17-C20-C22
4	D	1123	AJP	C22-C23-O25-C26
5	A	1118	CLR	C16-C17-C20-C22
4	C	1123	AJP	O31-C26-O25-C23
5	B	1107	CLR	C13-C17-C20-C22
5	D	1108	CLR	C13-C17-C20-C22
3	C	1104	LBN	C3-C2-O7-C34
4	D	1105	AJP	O31-C26-O25-C23
5	C	1107	CLR	C13-C17-C20-C21
4	B	1119	AJP	C24-C23-O25-C26
3	B	1103	LBN	C40-C41-C42-C5
5	A	1114	CLR	C17-C20-C22-C23
4	B	1122	AJP	C27-C26-O25-C23
3	D	1103	LBN	O7-C2-C3-O5
3	A	1122	LBN	C2-C1-O1-P1
3	A	1110	LBN	C35-C34-O7-C2
3	D	1104	LBN	C36-C37-C38-C39
4	C	1123	AJP	C27-C26-O25-C23
3	B	1115	LBN	C2-C1-O1-P1
3	C	1116	LBN	C2-C1-O1-P1
5	C	1107	CLR	C17-C20-C22-C23
3	B	1102	LBN	C2-C3-O5-C25
3	B	1103	LBN	C3-C2-O7-C34
3	D	1104	LBN	C3-C2-O7-C34
5	A	1115	CLR	C16-C17-C20-C22
3	C	1116	LBN	O8-C34-C35-C36
3	A	1122	LBN	O8-C34-C35-C36
3	B	1115	LBN	O8-C34-C35-C36
5	C	1108	CLR	C16-C17-C20-C22
4	D	1105	AJP	C27-C26-O25-C23
3	A	1110	LBN	C40-C41-C42-C5
5	D	1108	CLR	C16-C17-C20-C22
5	B	1107	CLR	C16-C17-C20-C22
4	D	1123	AJP	O31-C26-O25-C23
5	D	1107	CLR	C17-C20-C22-C23
3	A	1110	LBN	C3-C2-O7-C34
5	A	1112	CLR	C21-C20-C22-C23
3	D	1116	LBN	O8-C34-C35-C36
4	A	1126	AJP	C22-C23-O25-C26
4	C	1120	AJP	C22-C23-O25-C26
5	B	1106	CLR	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
3	D	1113	LBN	O6-C25-O5-C3
5	A	1114	CLR	C21-C20-C22-C23
4	D	1123	AJP	C27-C26-O25-C23
3	B	1112	LBN	O7-C34-C35-C36

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1105	AJP	C19-C20-C21-C22-C23-C24
4	A	1111	AJP	C19-C20-C21-C22-C23-C24
4	D	1123	AJP	C19-C20-C21-C22-C23-C24

34 monomers are involved in 72 short contacts:

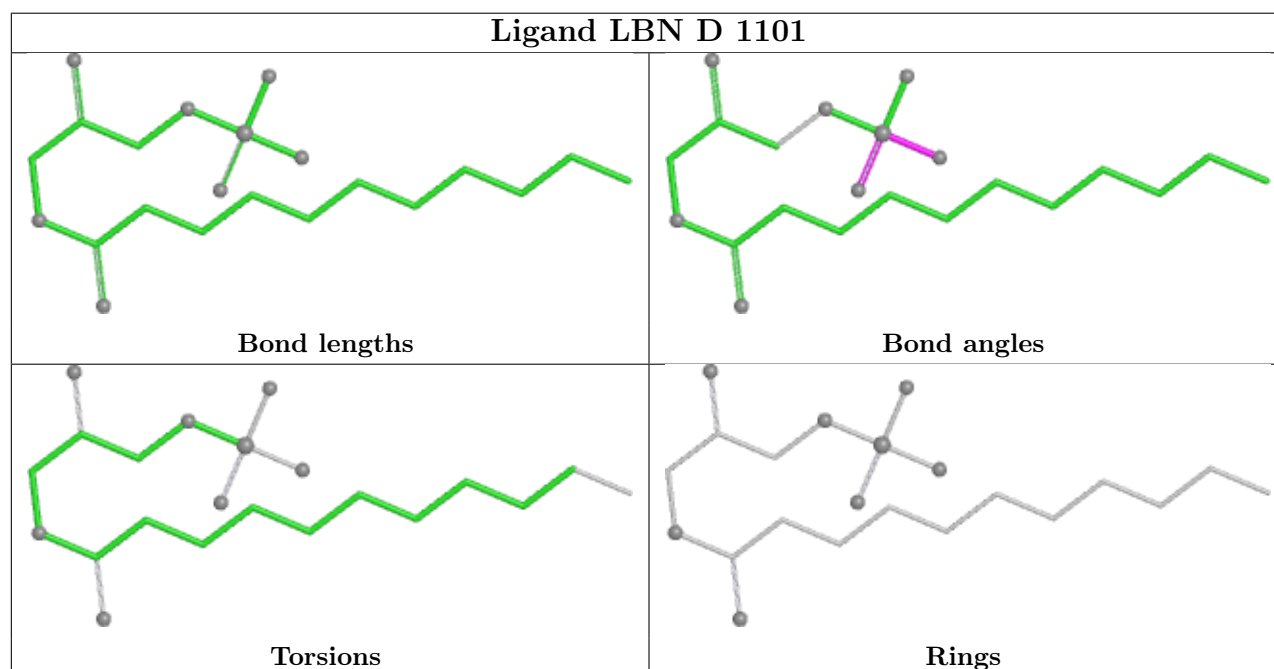
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1111	AJP	1	0
5	A	1113	CLR	3	0
5	B	1110	CLR	2	0
4	B	1104	AJP	1	0
5	C	1110	CLR	1	0
5	C	1109	CLR	2	0
5	A	1115	CLR	5	0
5	B	1107	CLR	3	0
5	D	1109	CLR	1	0
5	B	1108	CLR	1	0
5	A	1117	CLR	1	0
5	D	1107	CLR	2	0
5	A	1118	CLR	3	0
5	C	1112	CLR	5	0
5	B	1109	CLR	3	0
5	A	1112	CLR	1	0
4	C	1105	AJP	1	0
5	D	1111	CLR	1	0
5	C	1108	CLR	5	0
3	A	1109	LBN	1	0
4	D	1120	AJP	1	0
5	A	1116	CLR	1	0
5	B	1111	CLR	4	0
5	D	1110	CLR	2	0
3	B	1102	LBN	1	0
5	D	1108	CLR	3	0
5	C	1106	CLR	3	0

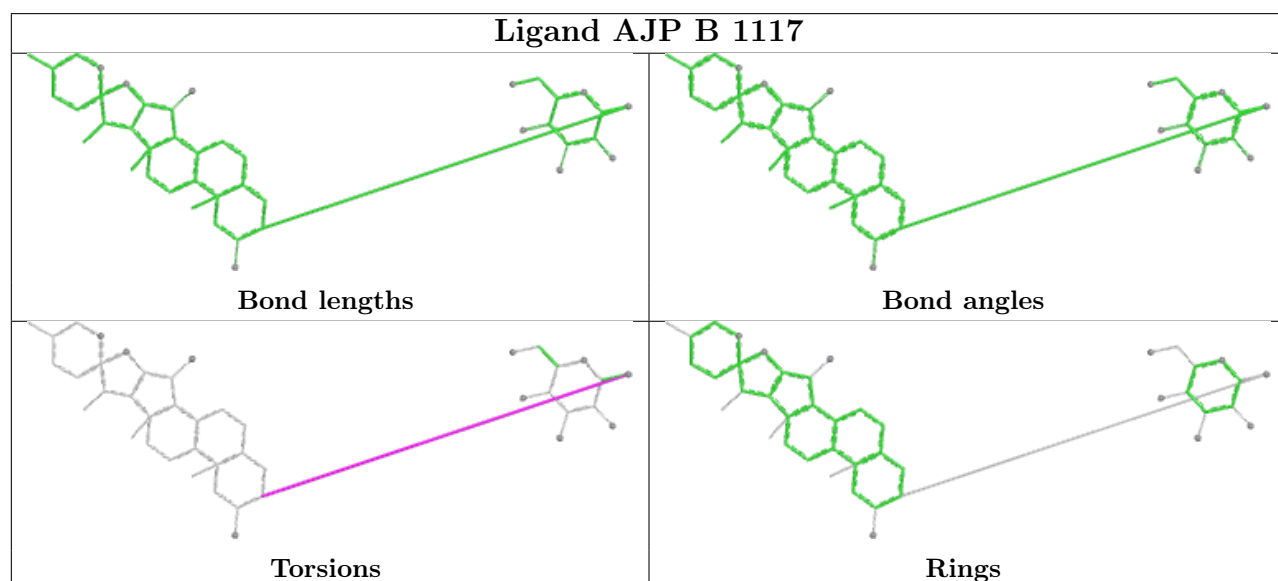
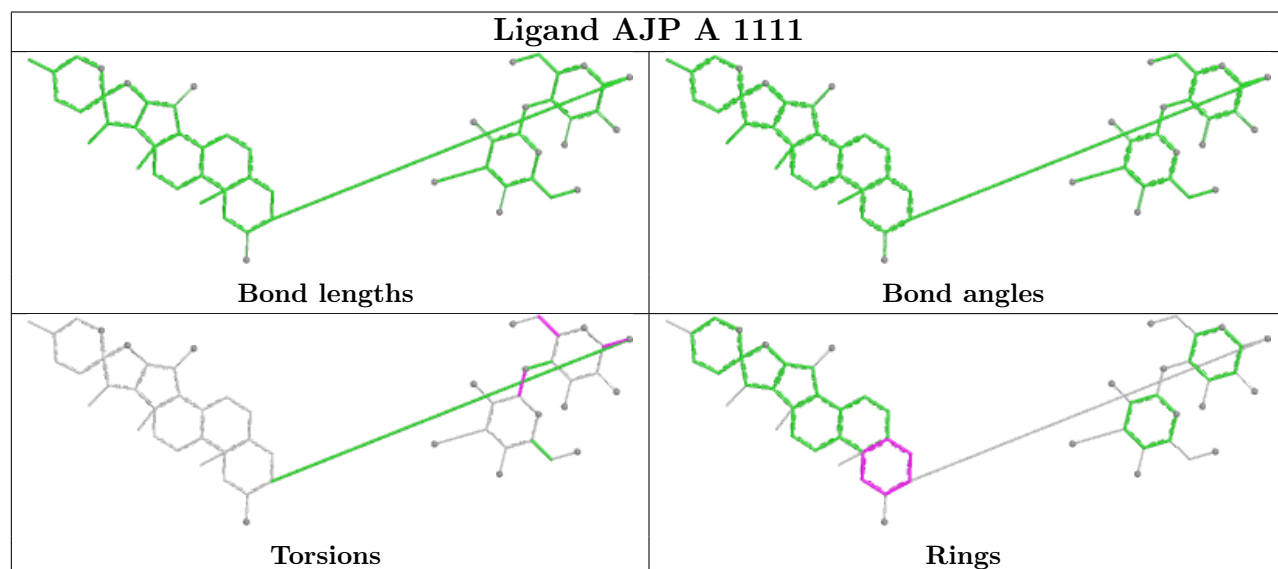
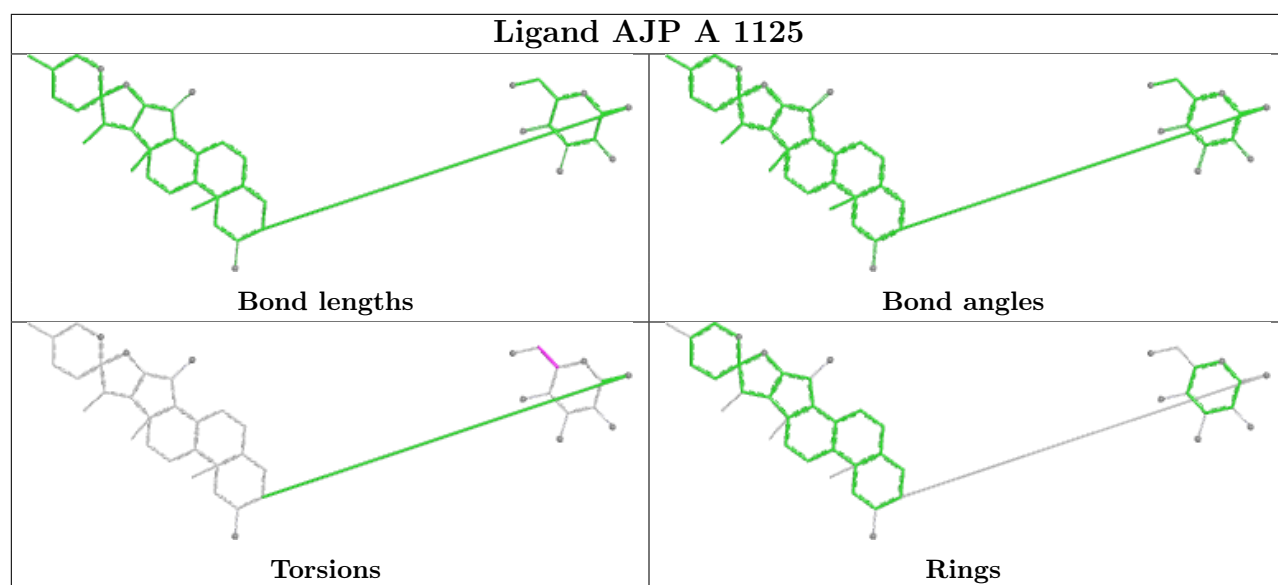
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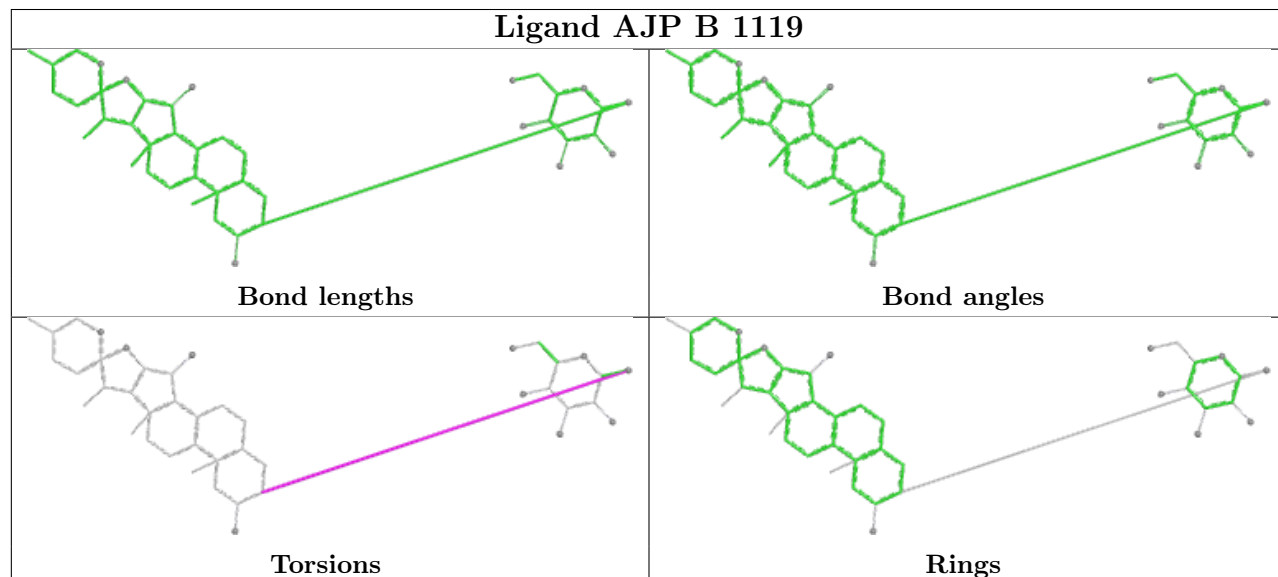
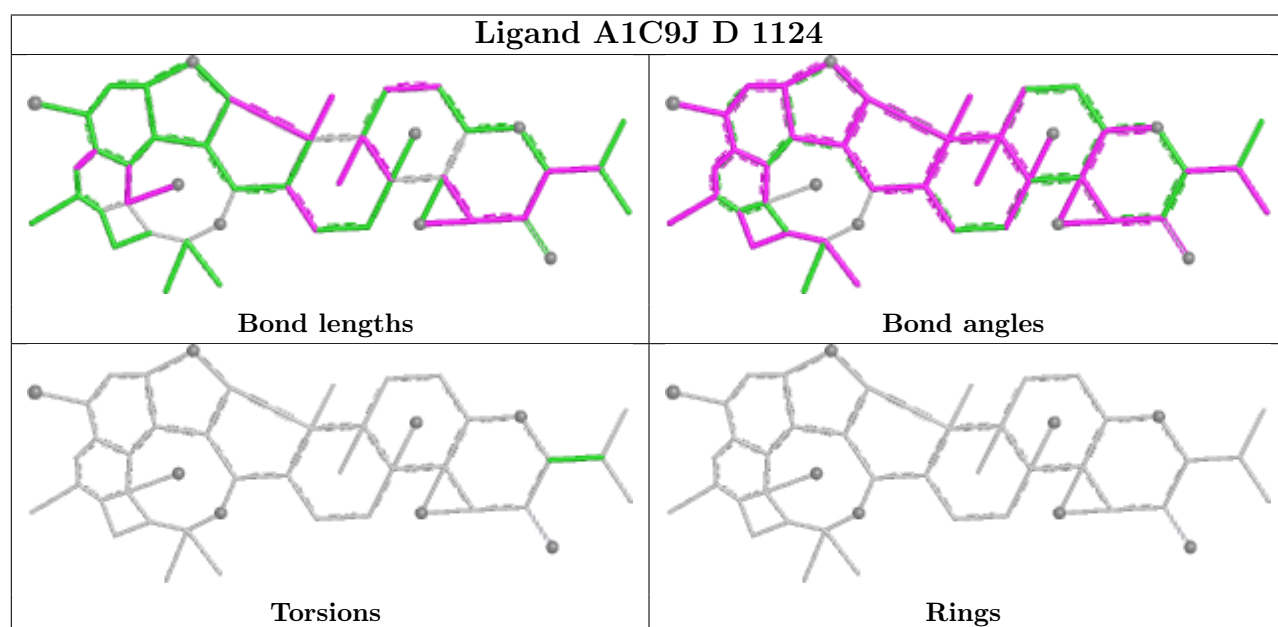
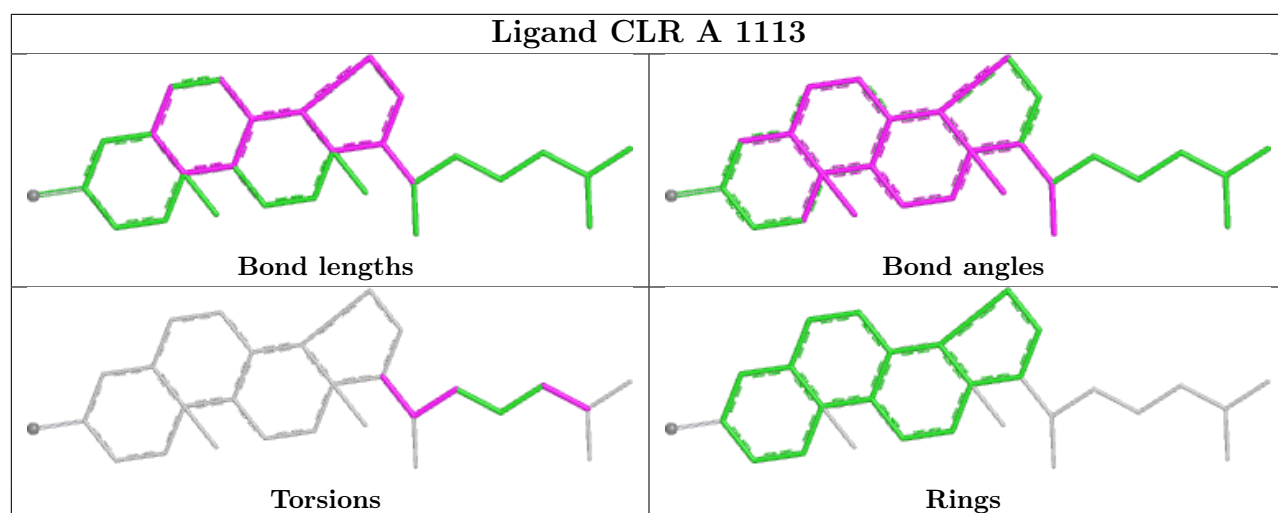
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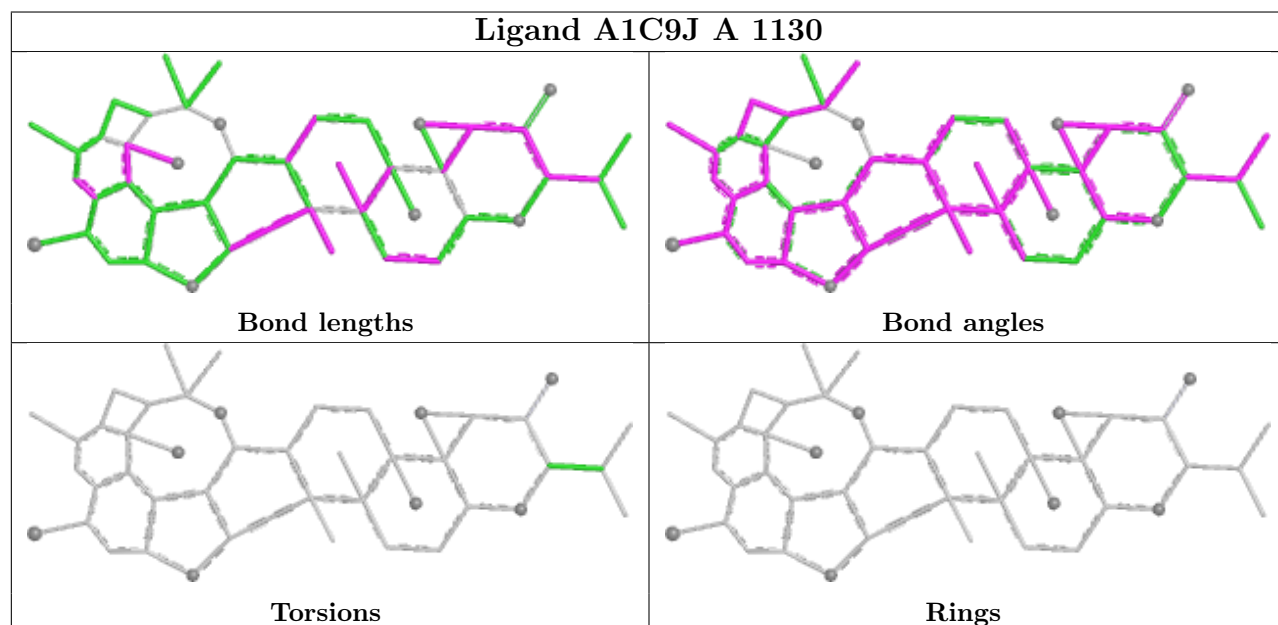
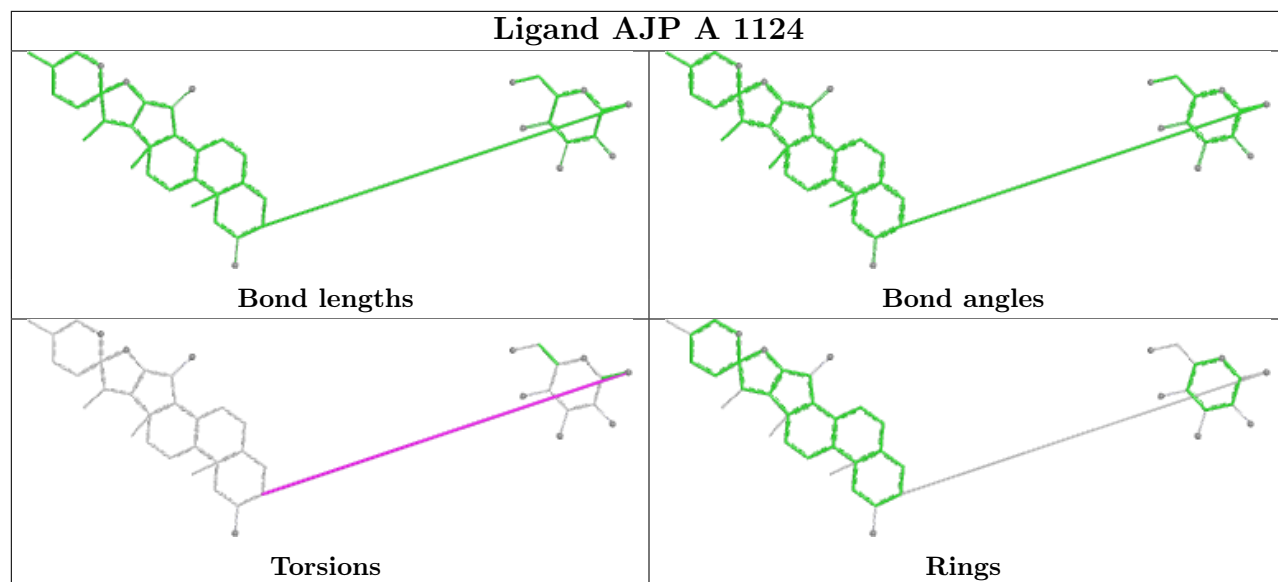
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1112	CLR	5	0
5	B	1106	CLR	3	0
5	B	1105	CLR	2	0
5	C	1107	CLR	1	0
5	D	1106	CLR	2	0
5	A	1114	CLR	2	0
5	C	1111	CLR	1	0

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.

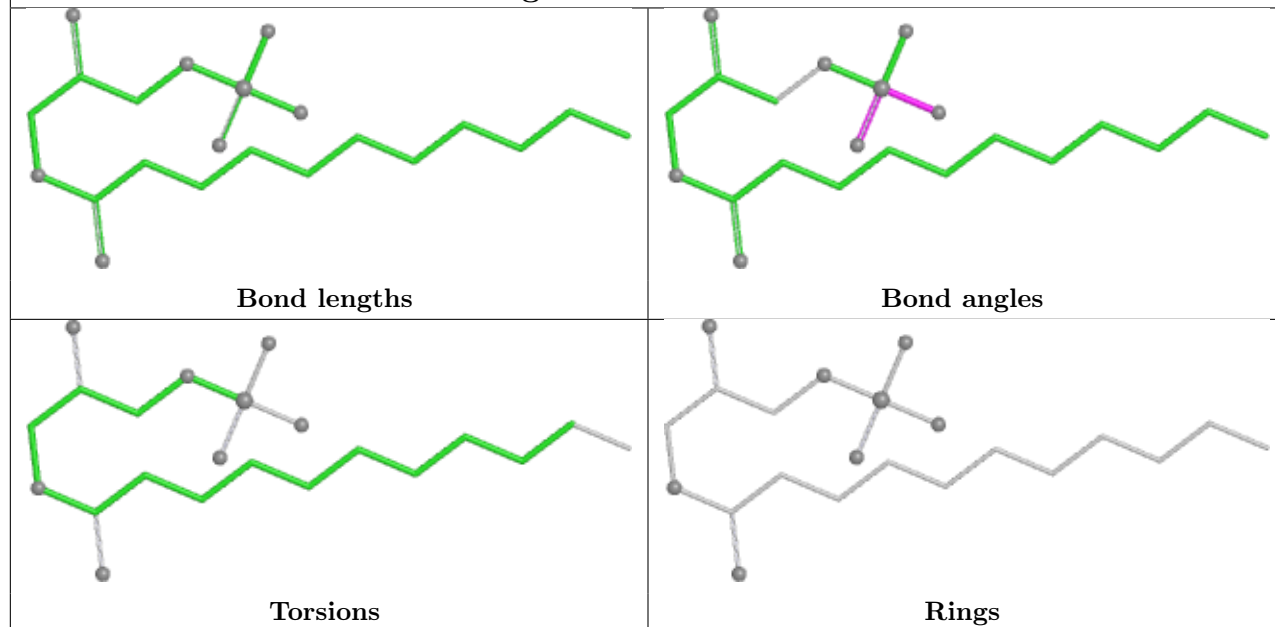




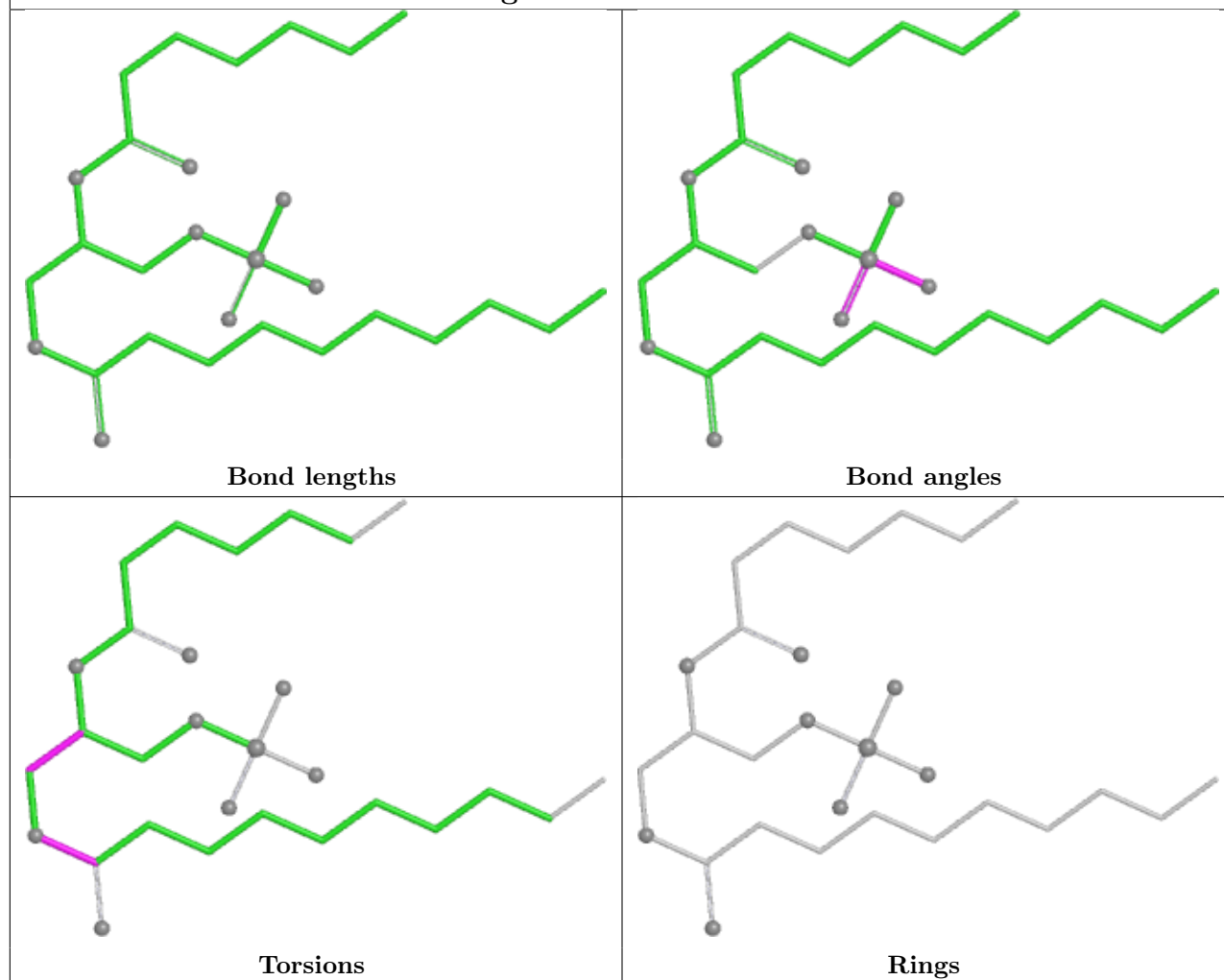


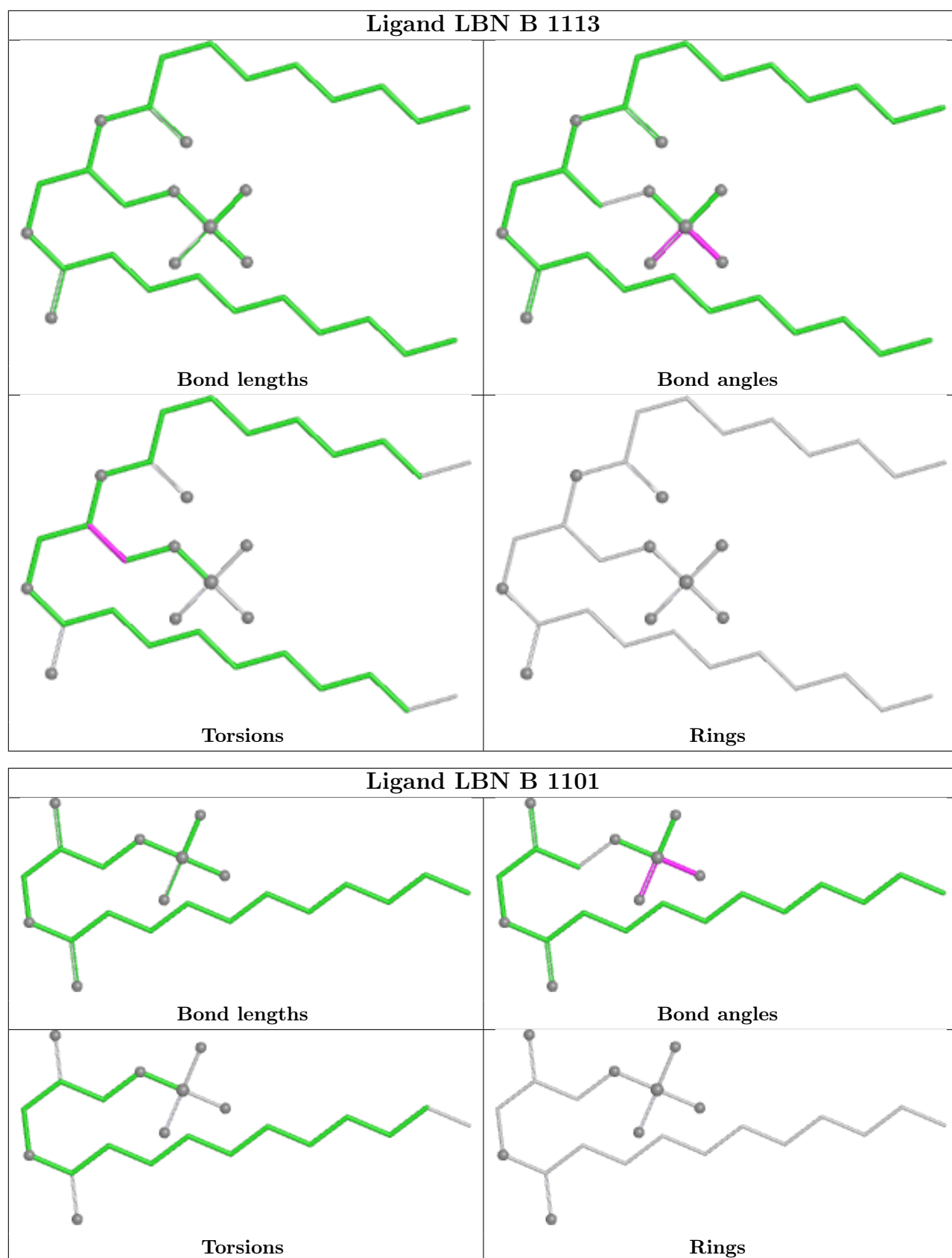


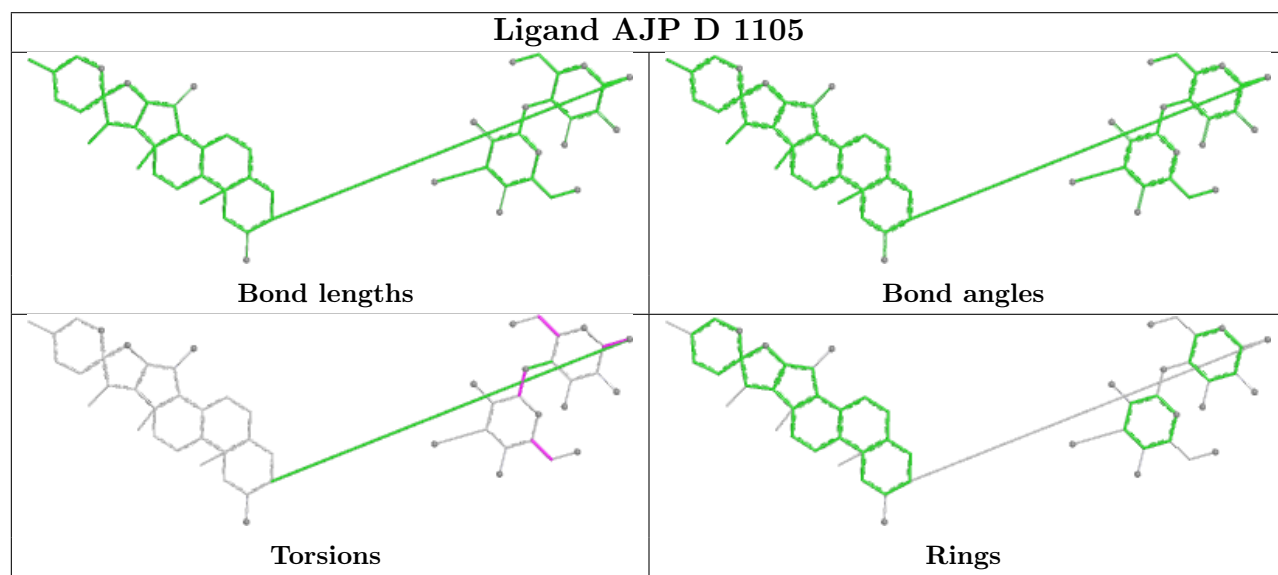
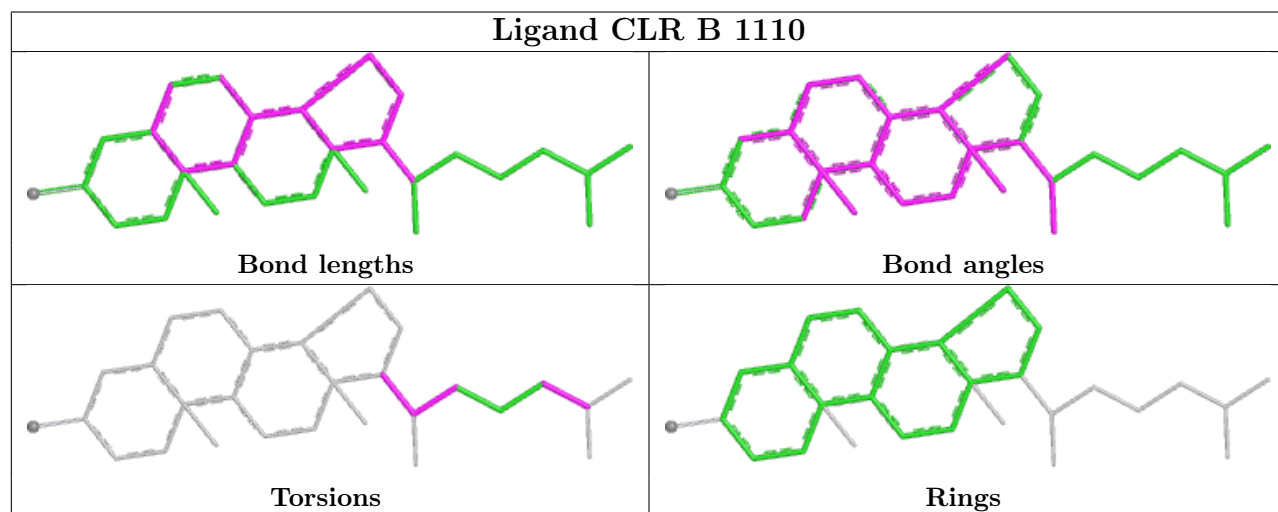
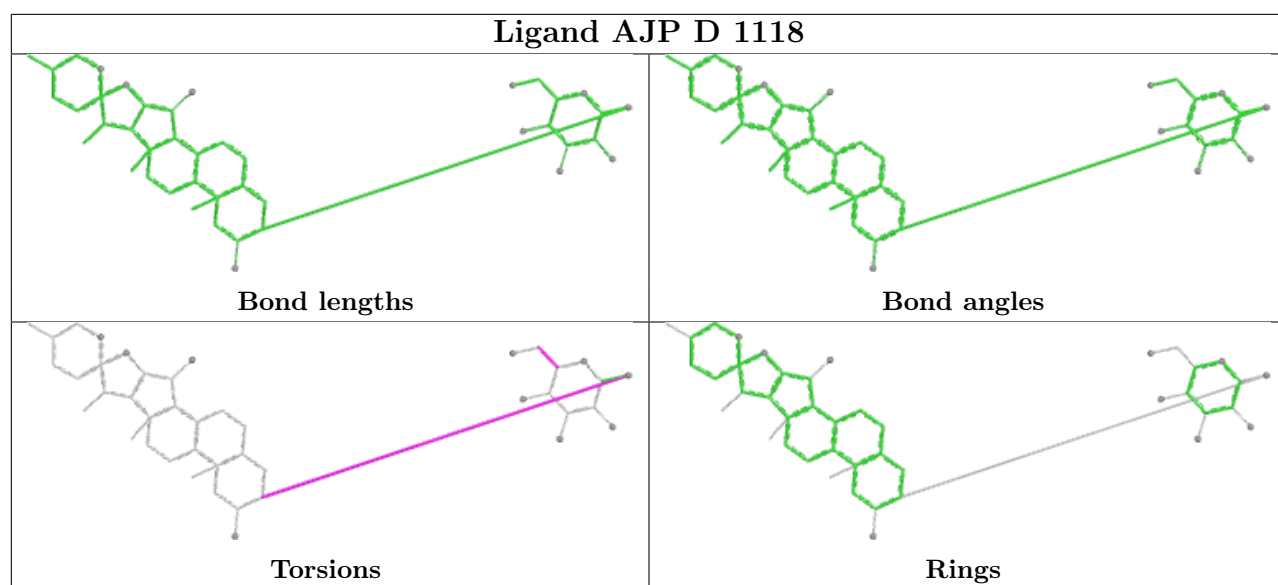
Ligand LBN C 1102



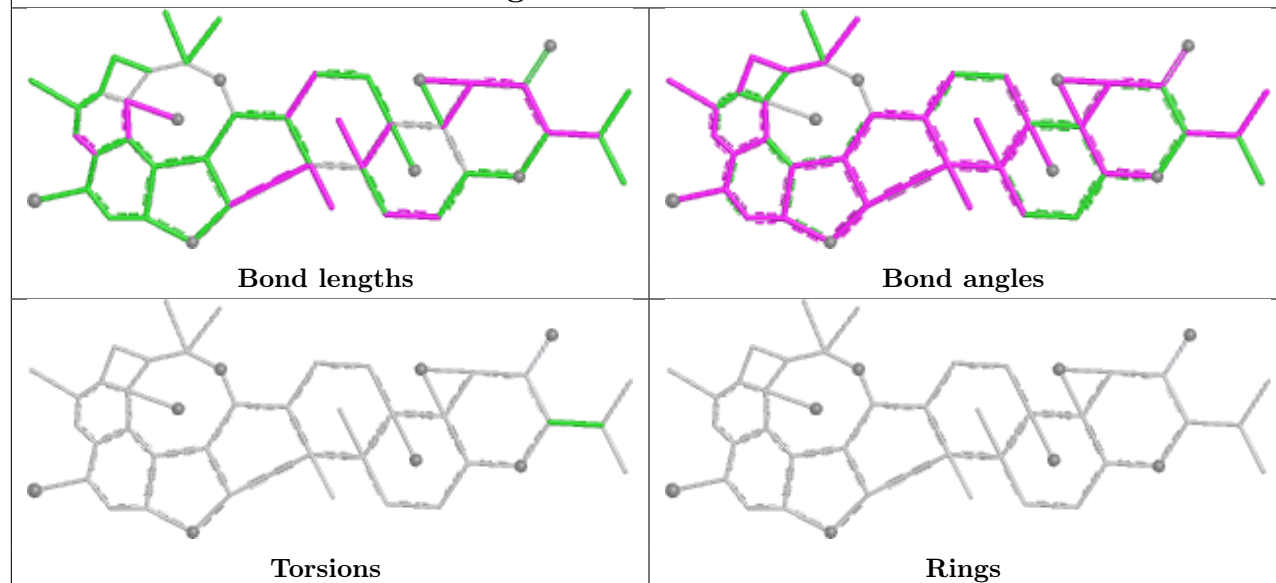
Ligand LBN C 1113



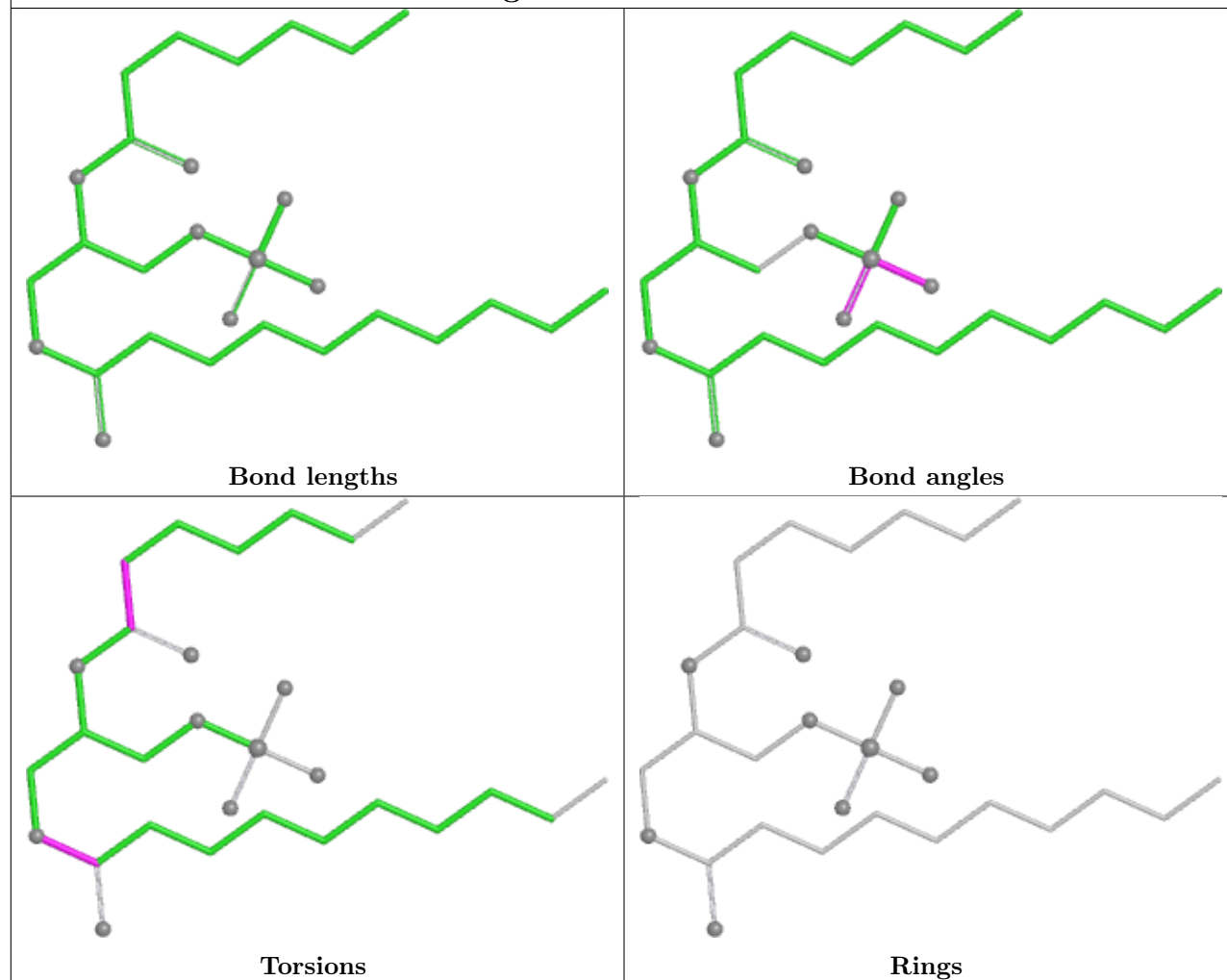


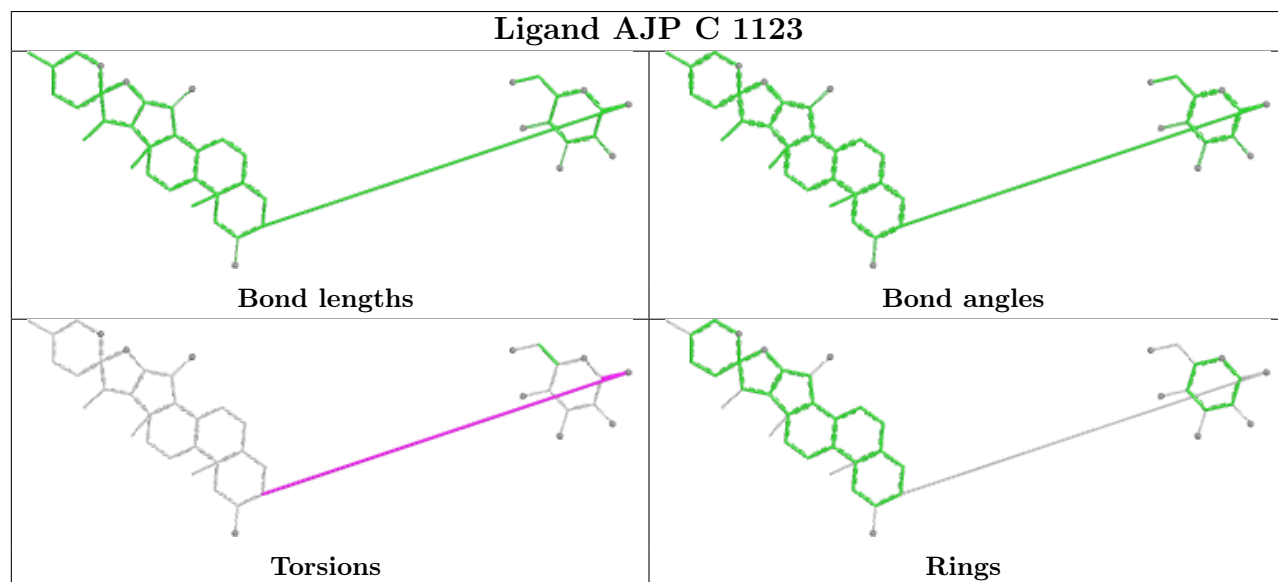
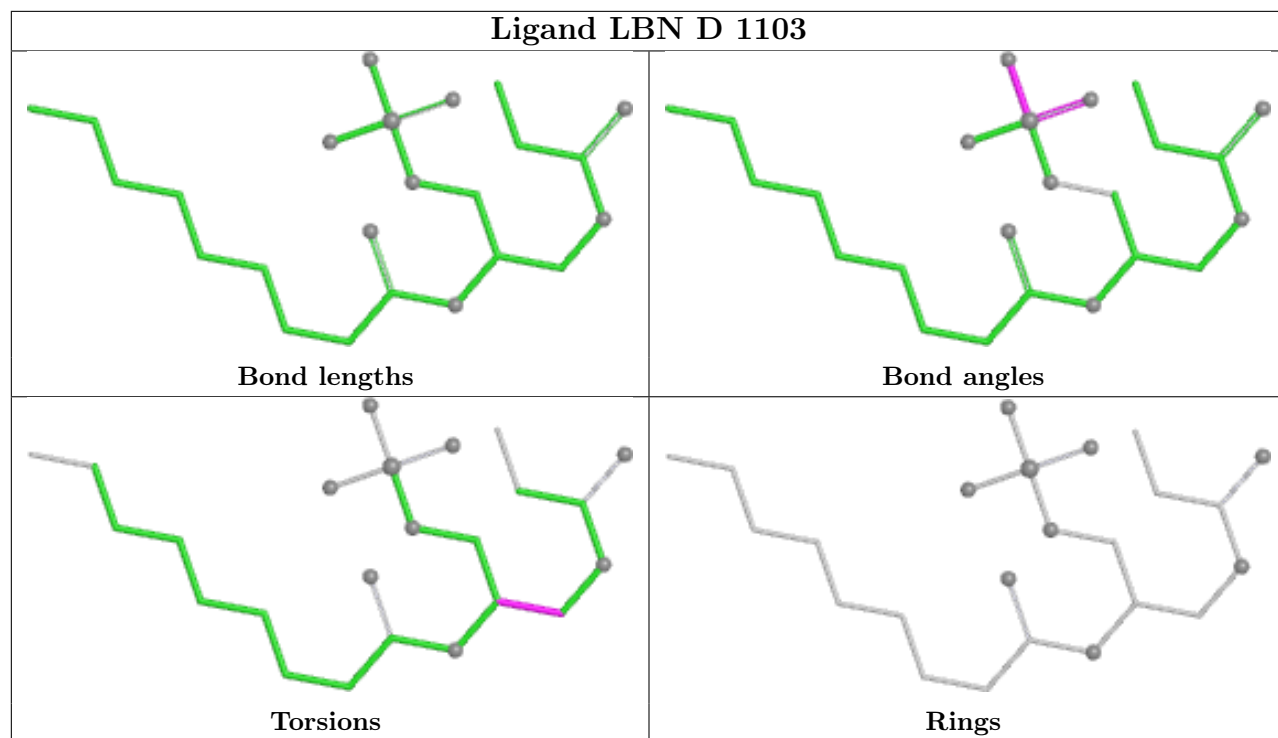


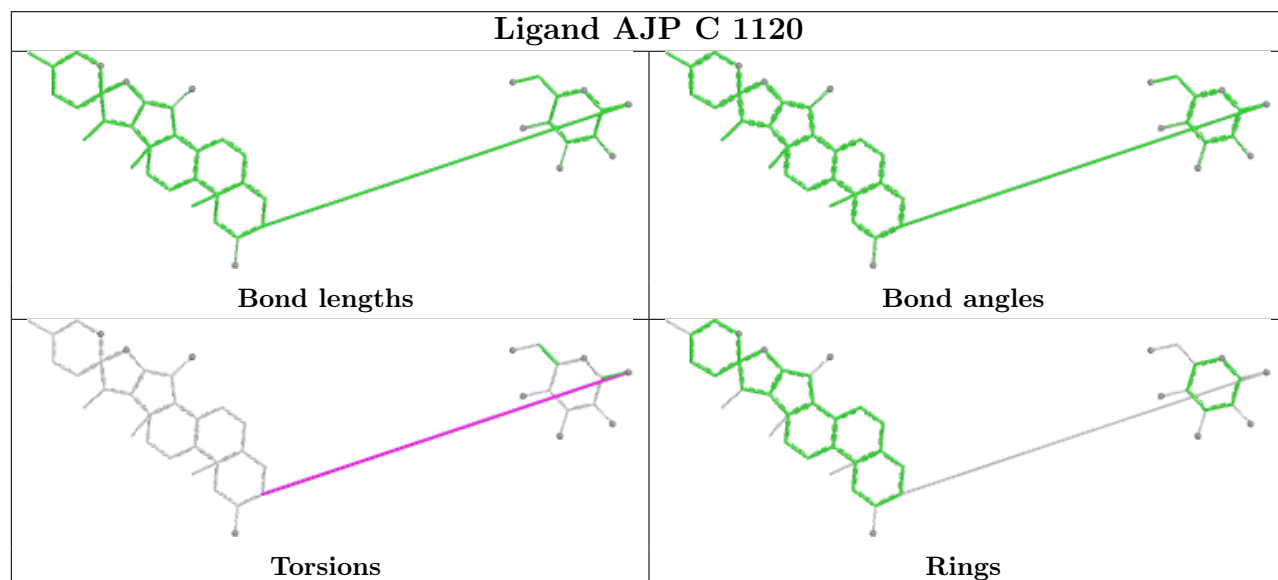
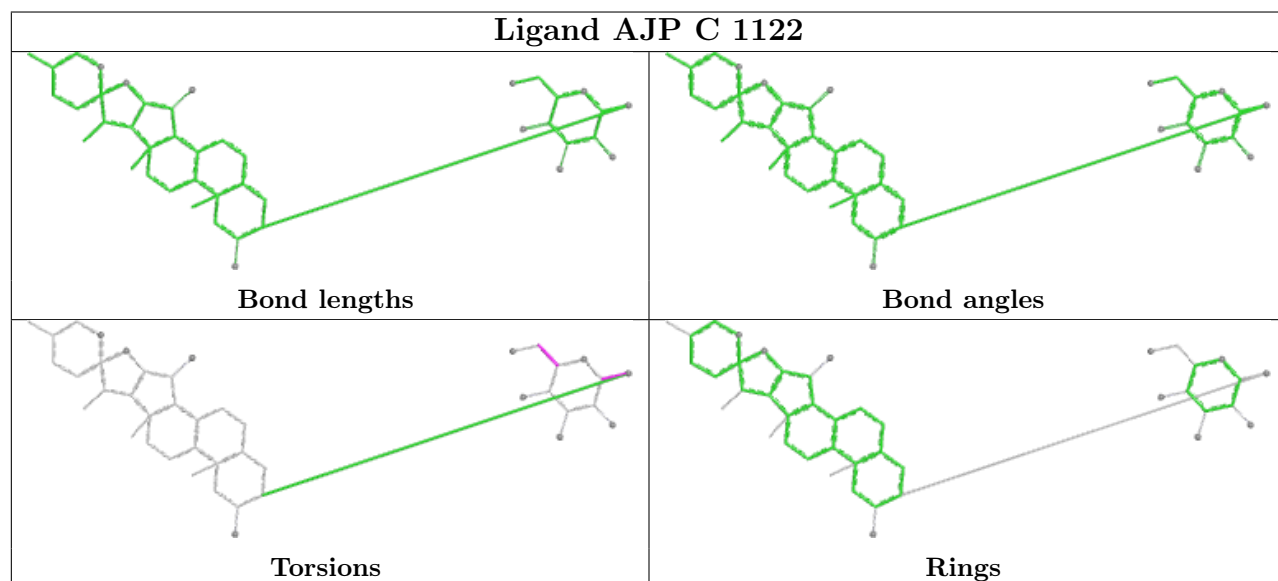
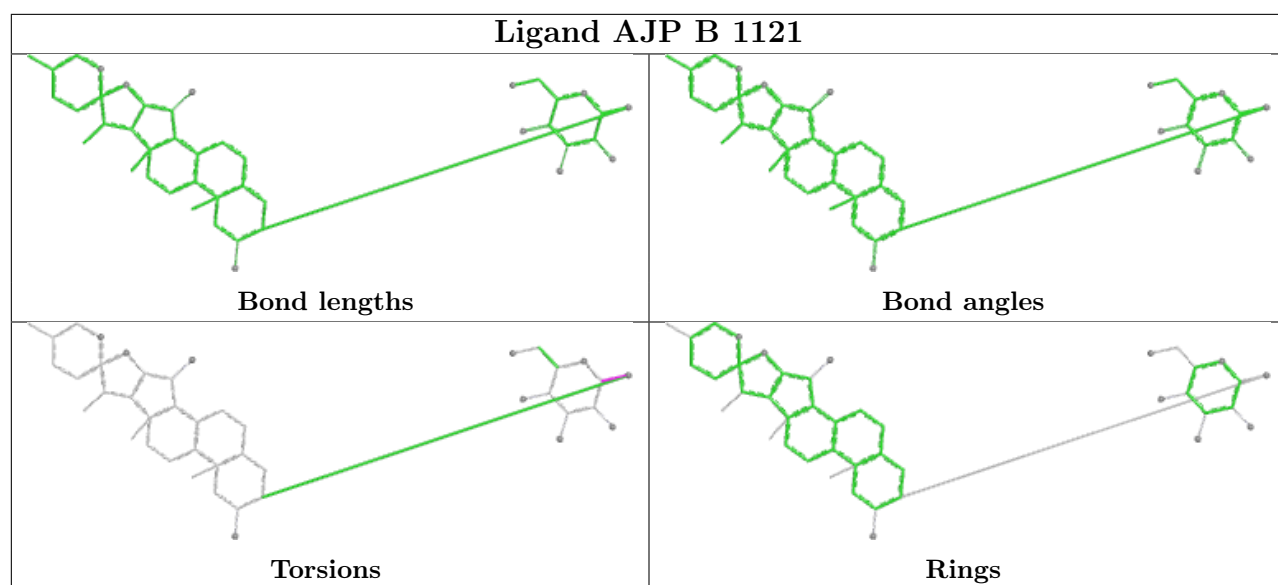
Ligand A1C9J B 1123

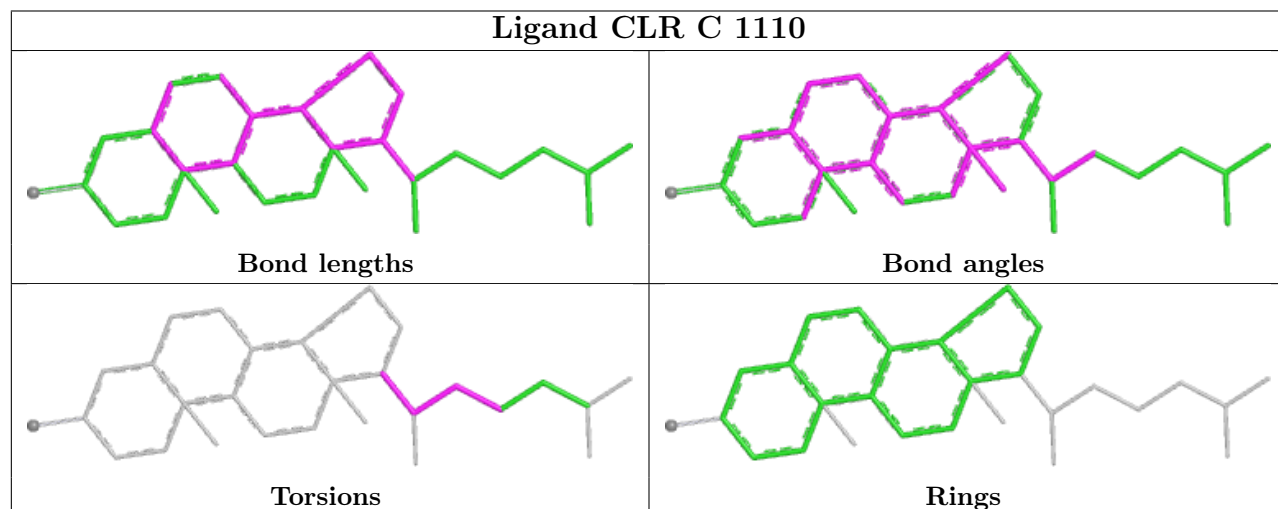
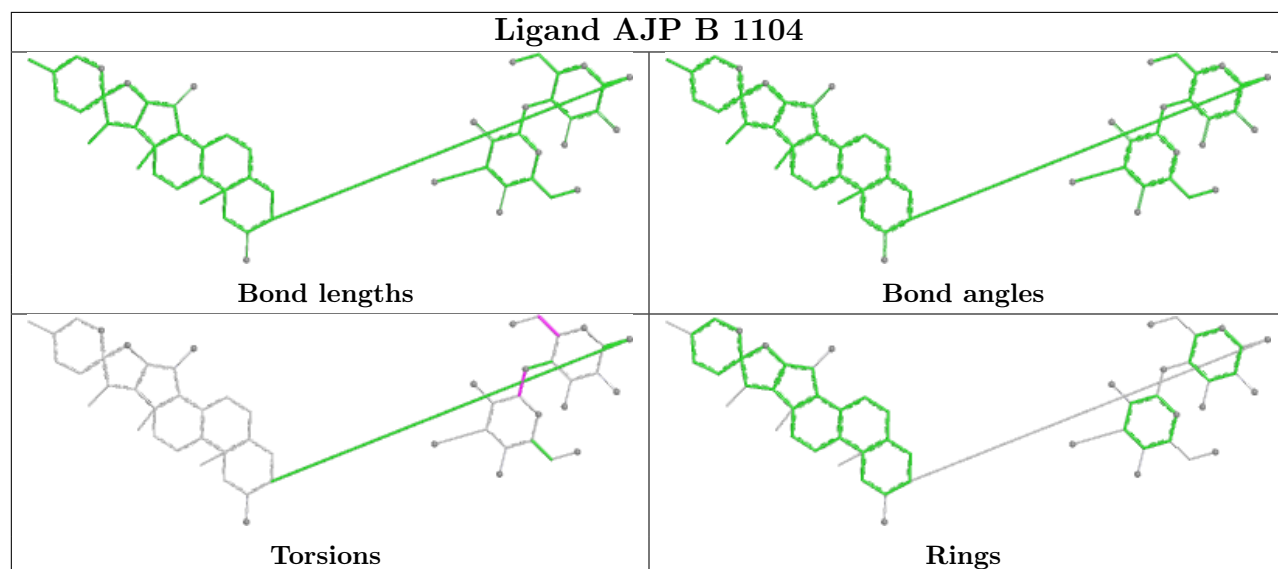
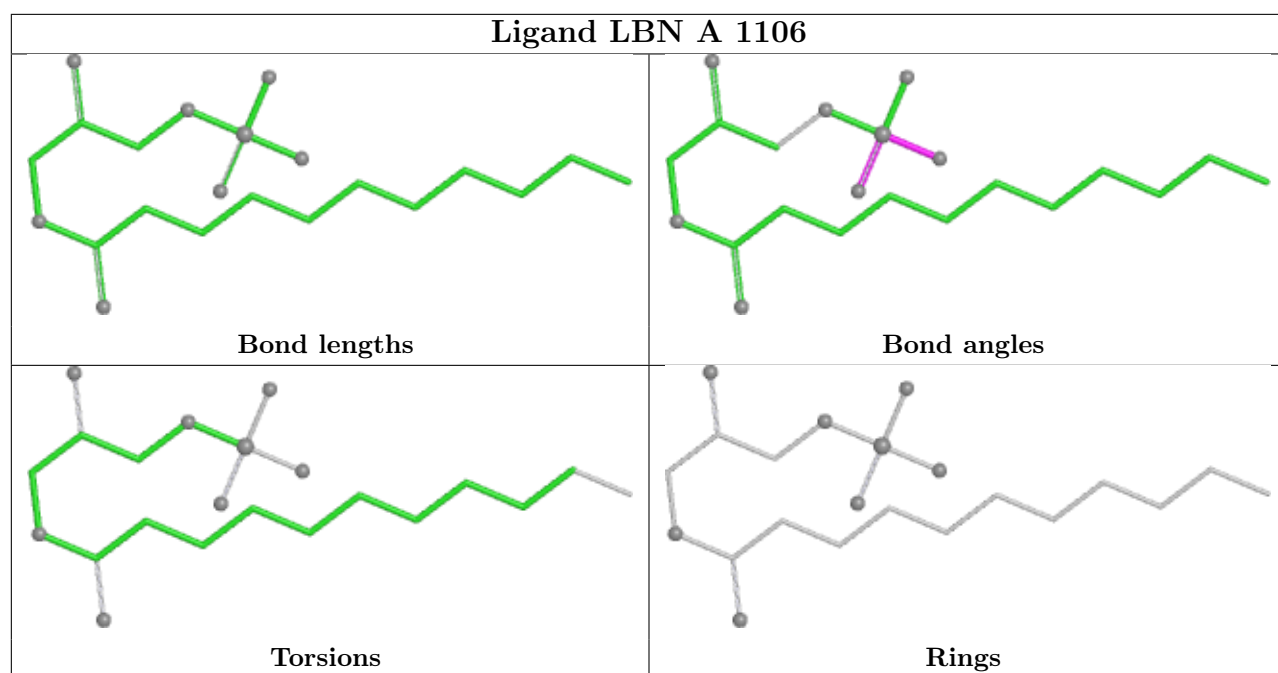


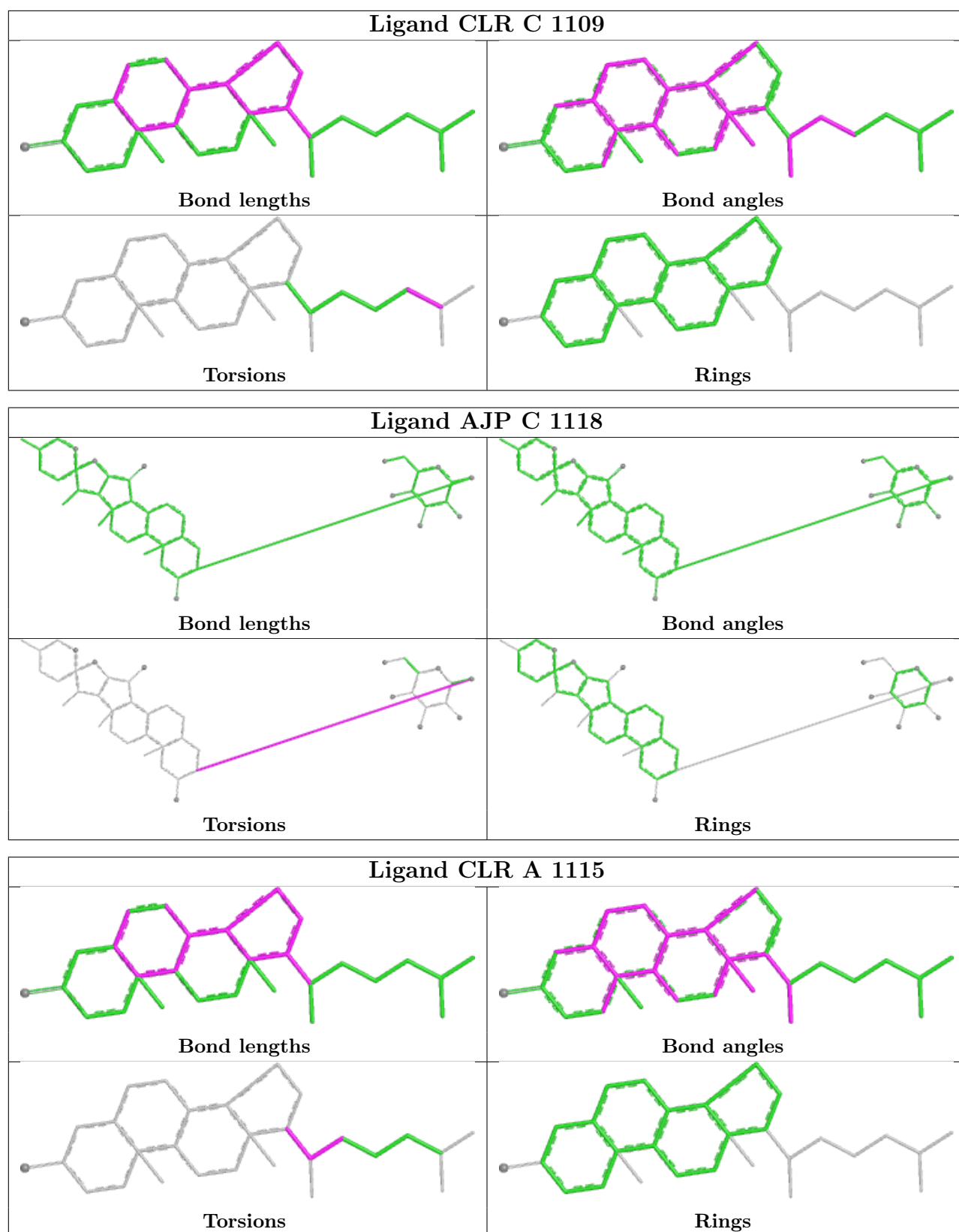
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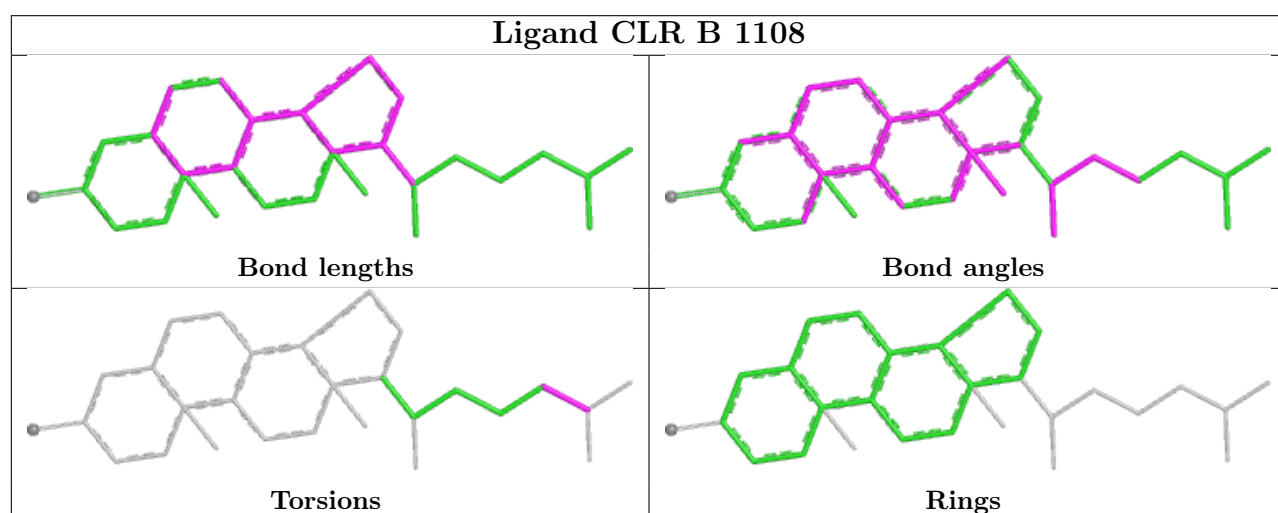
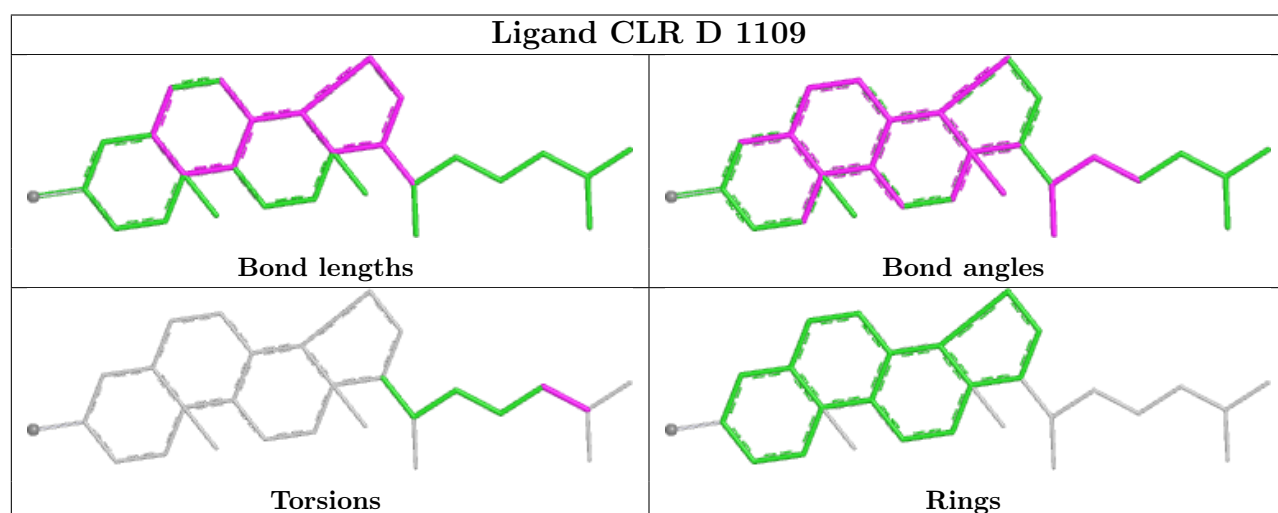
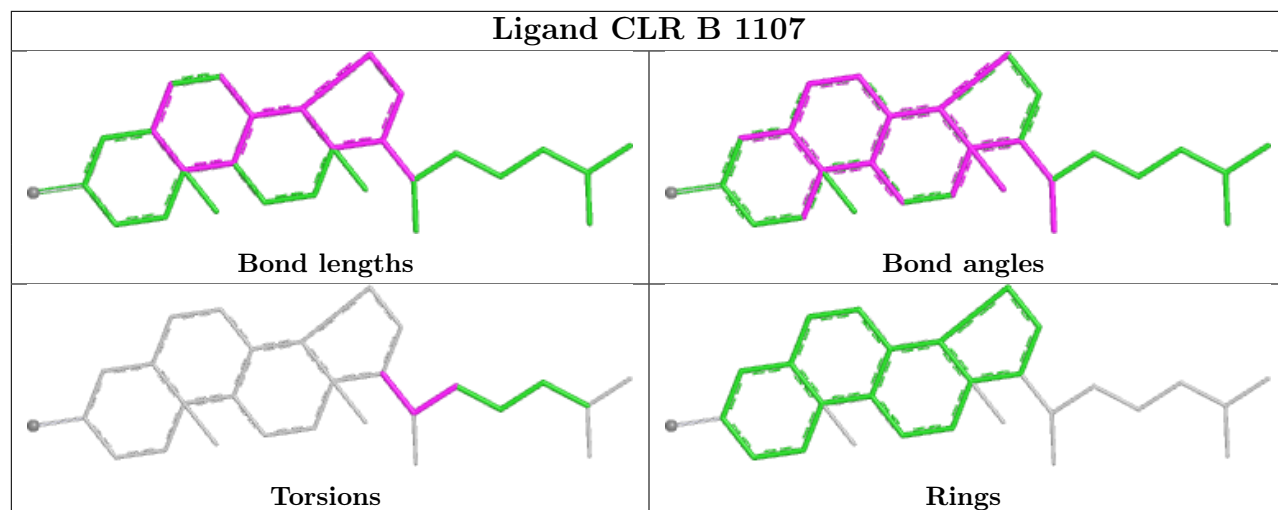




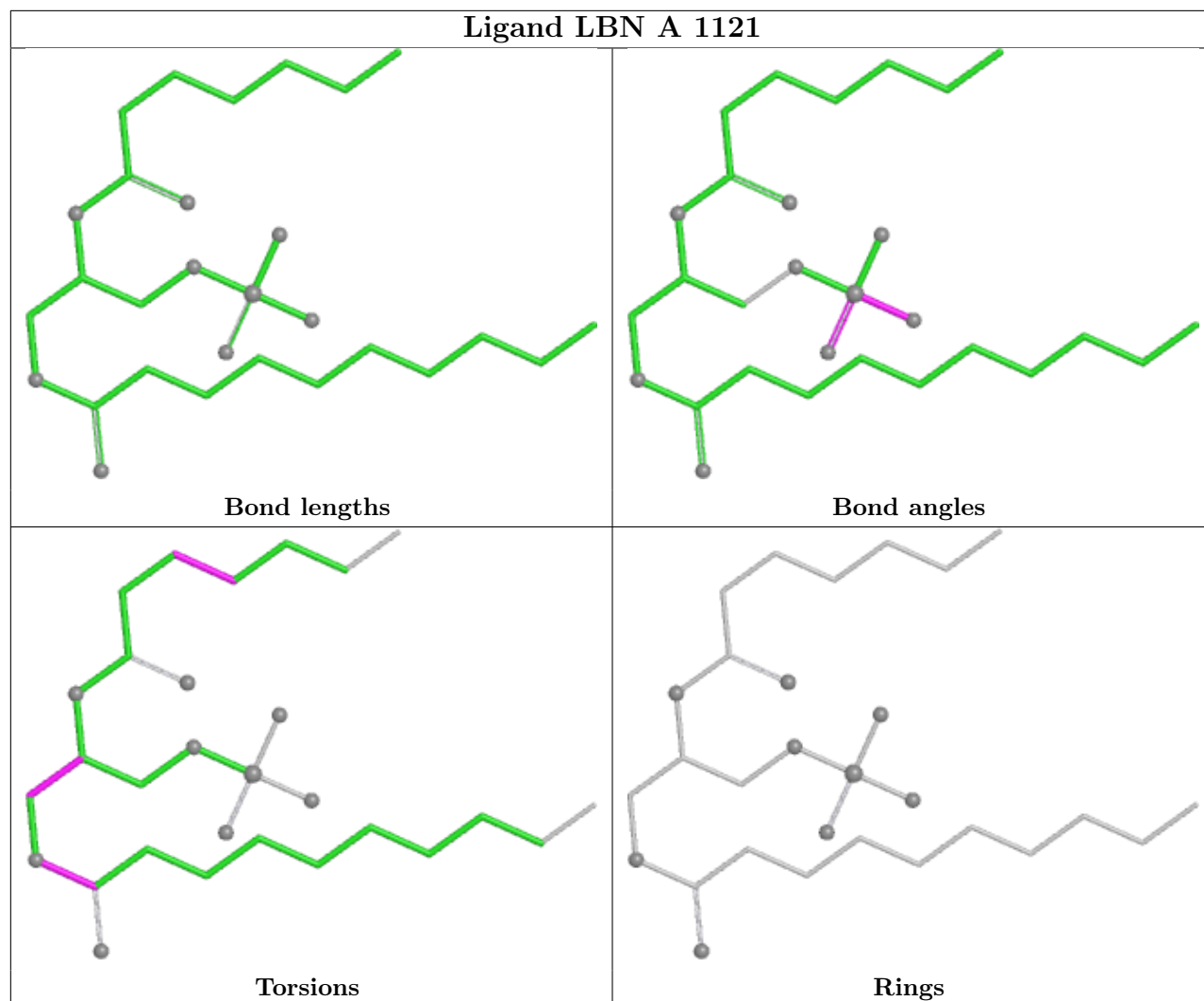




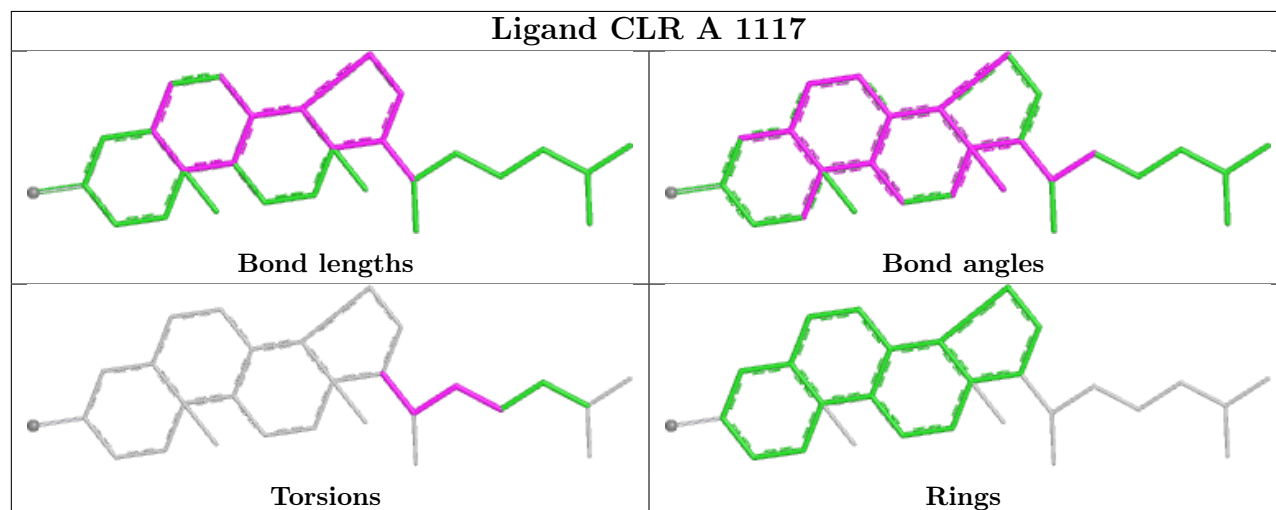


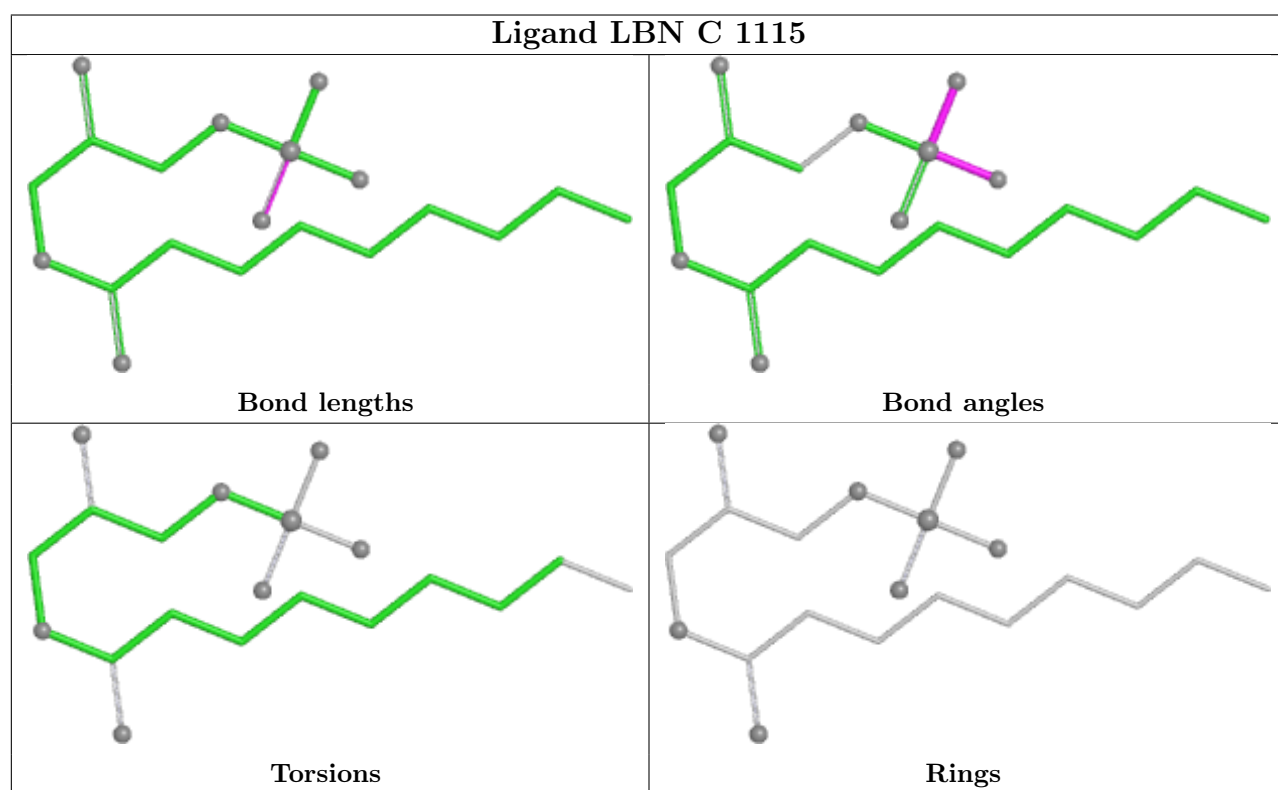
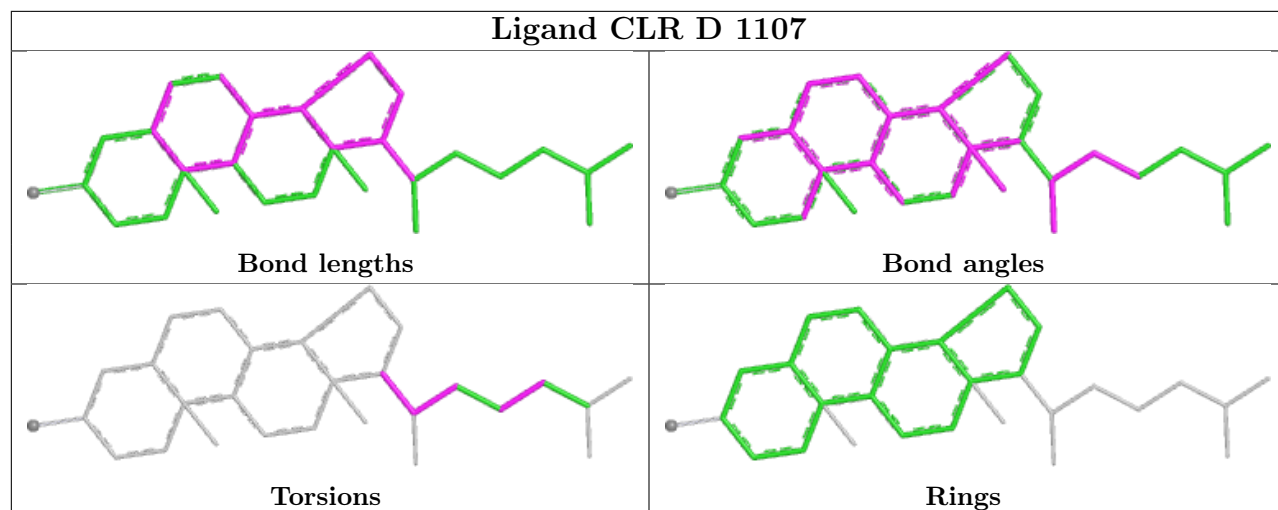


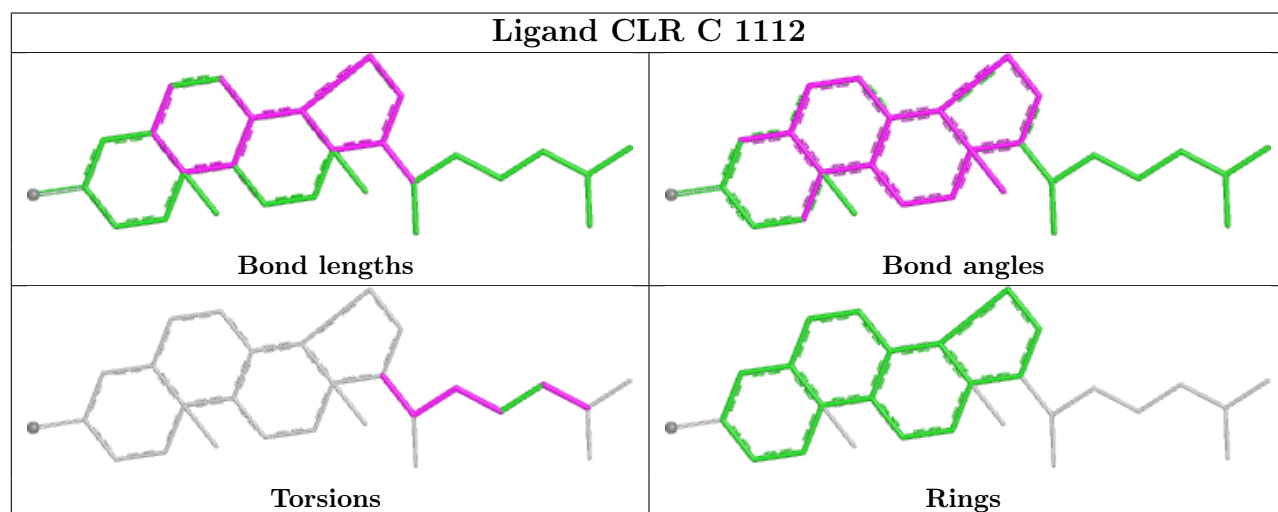
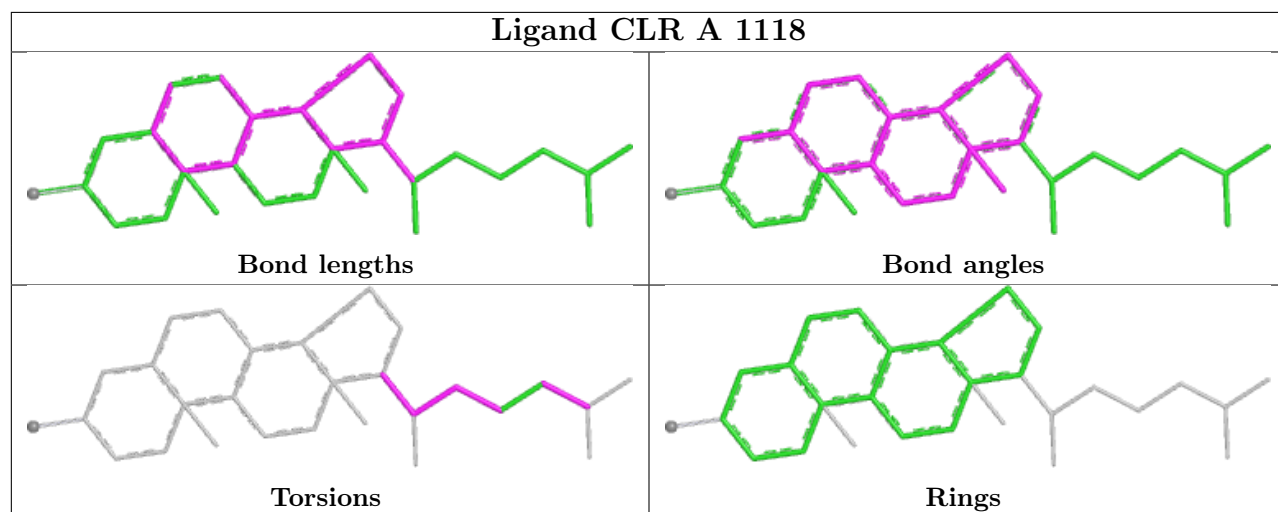
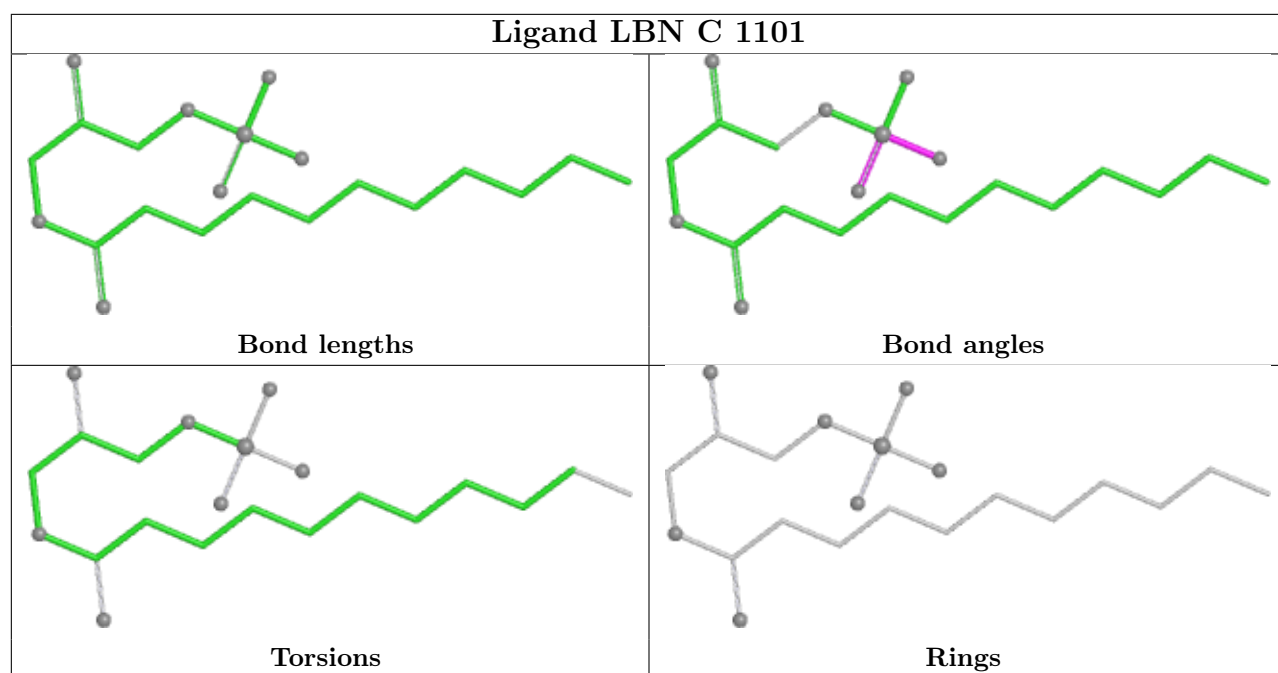
Ligand LBN A 1121

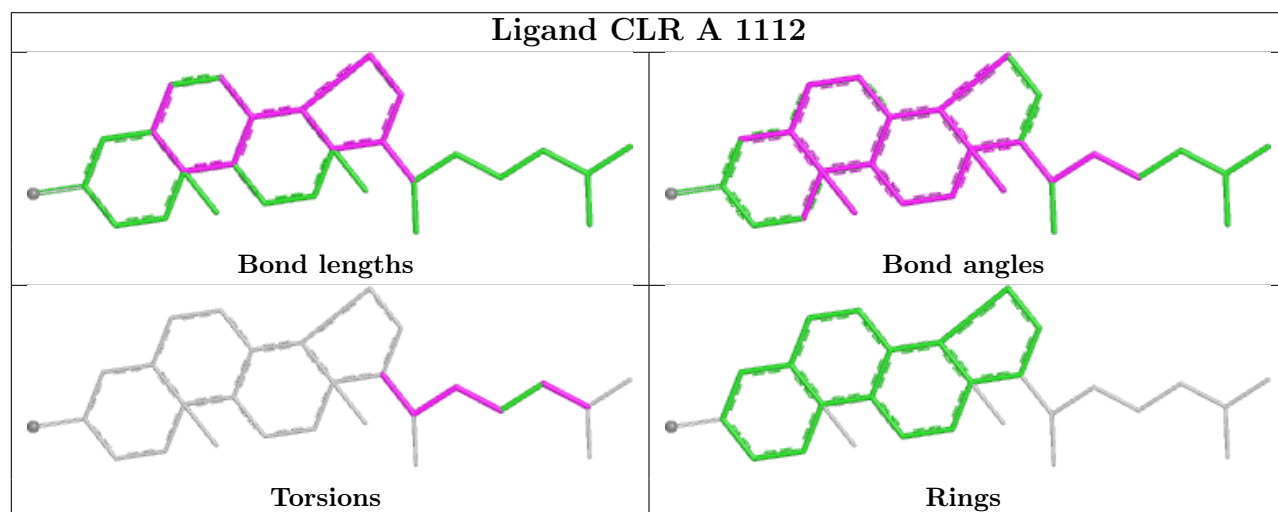
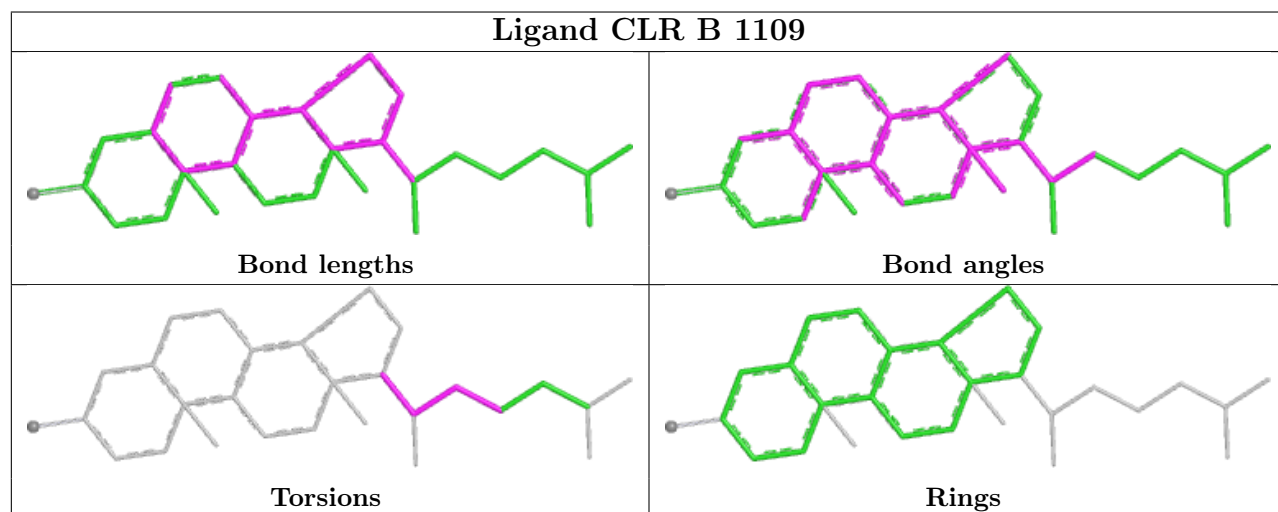
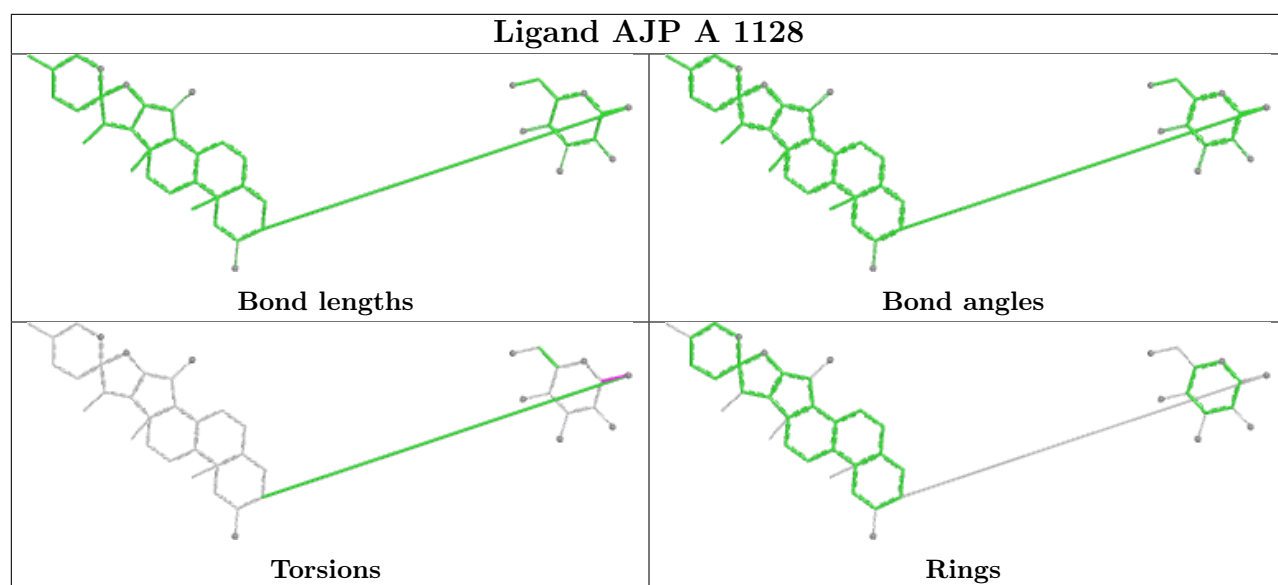


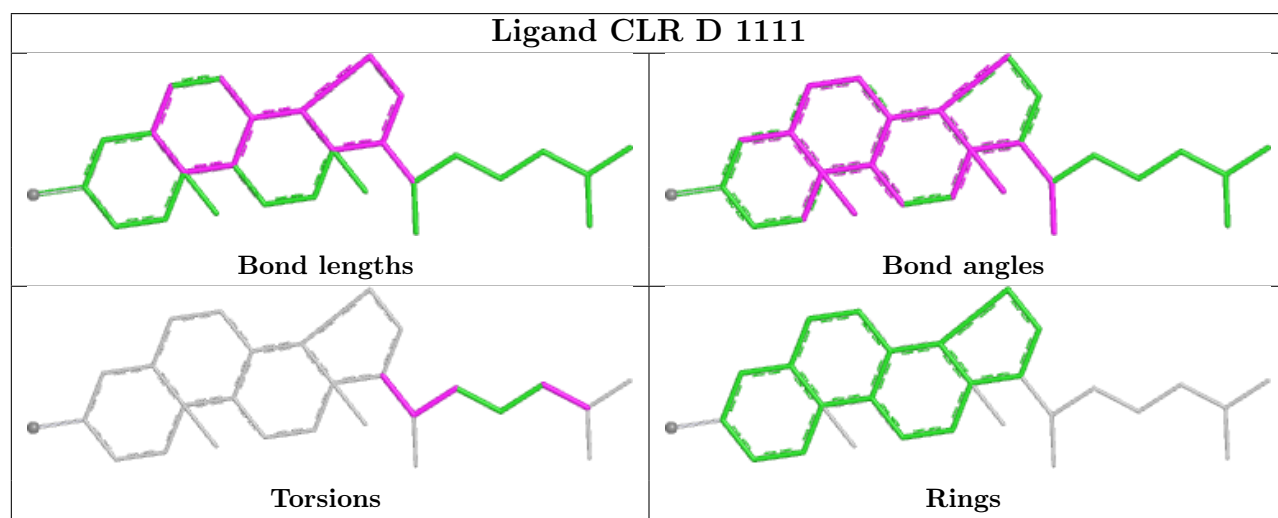
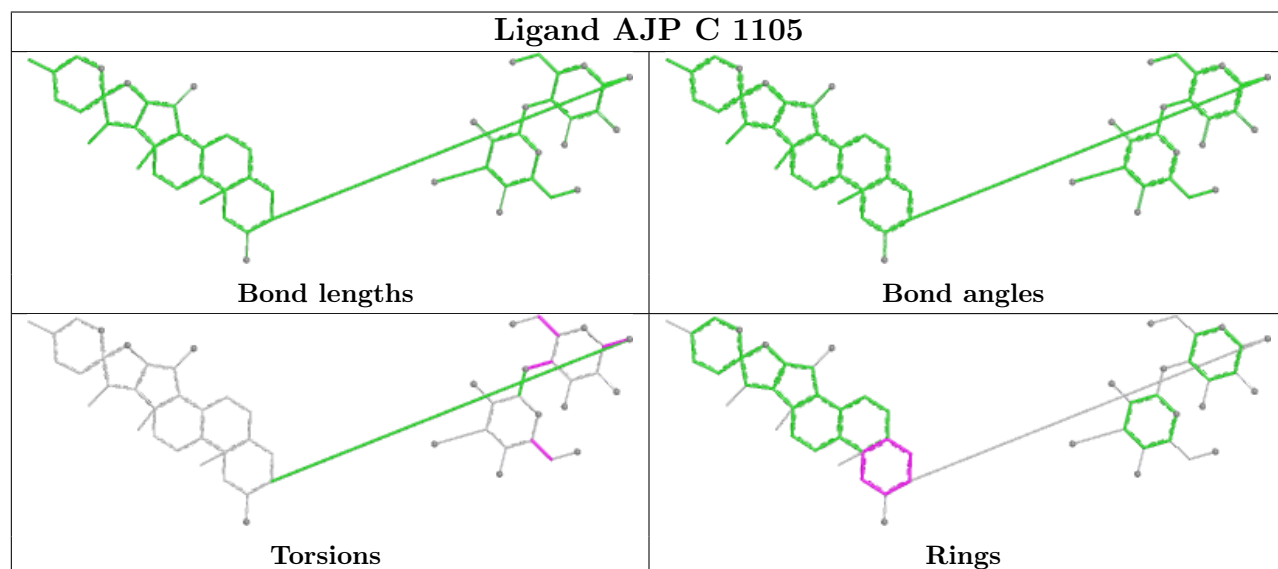
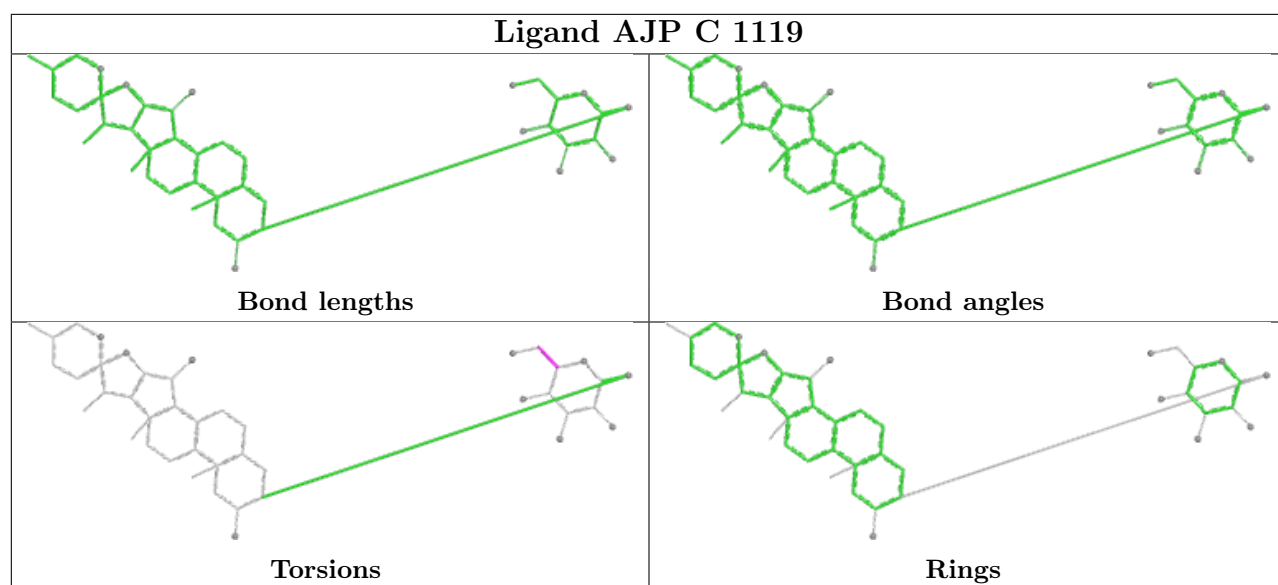
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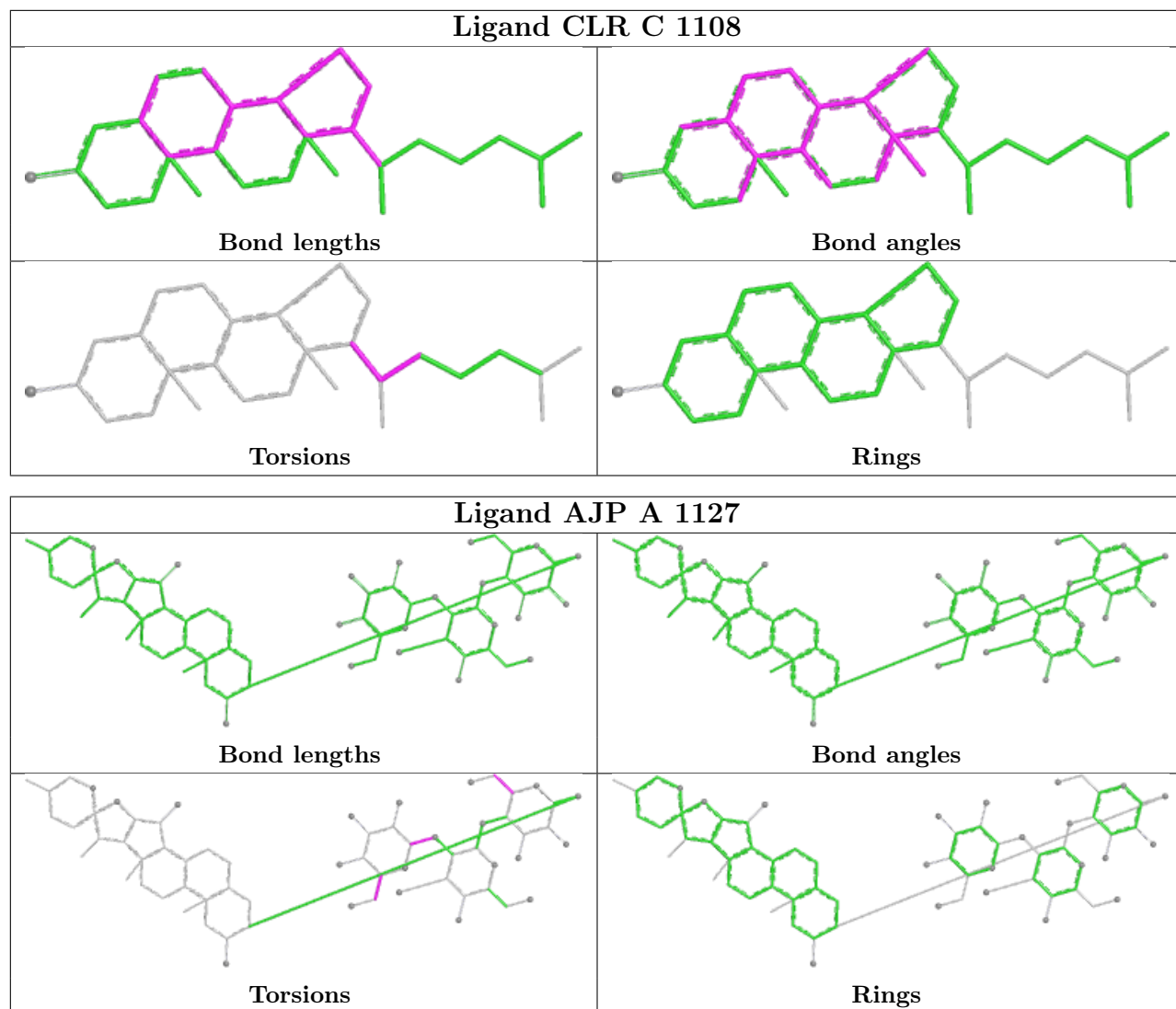




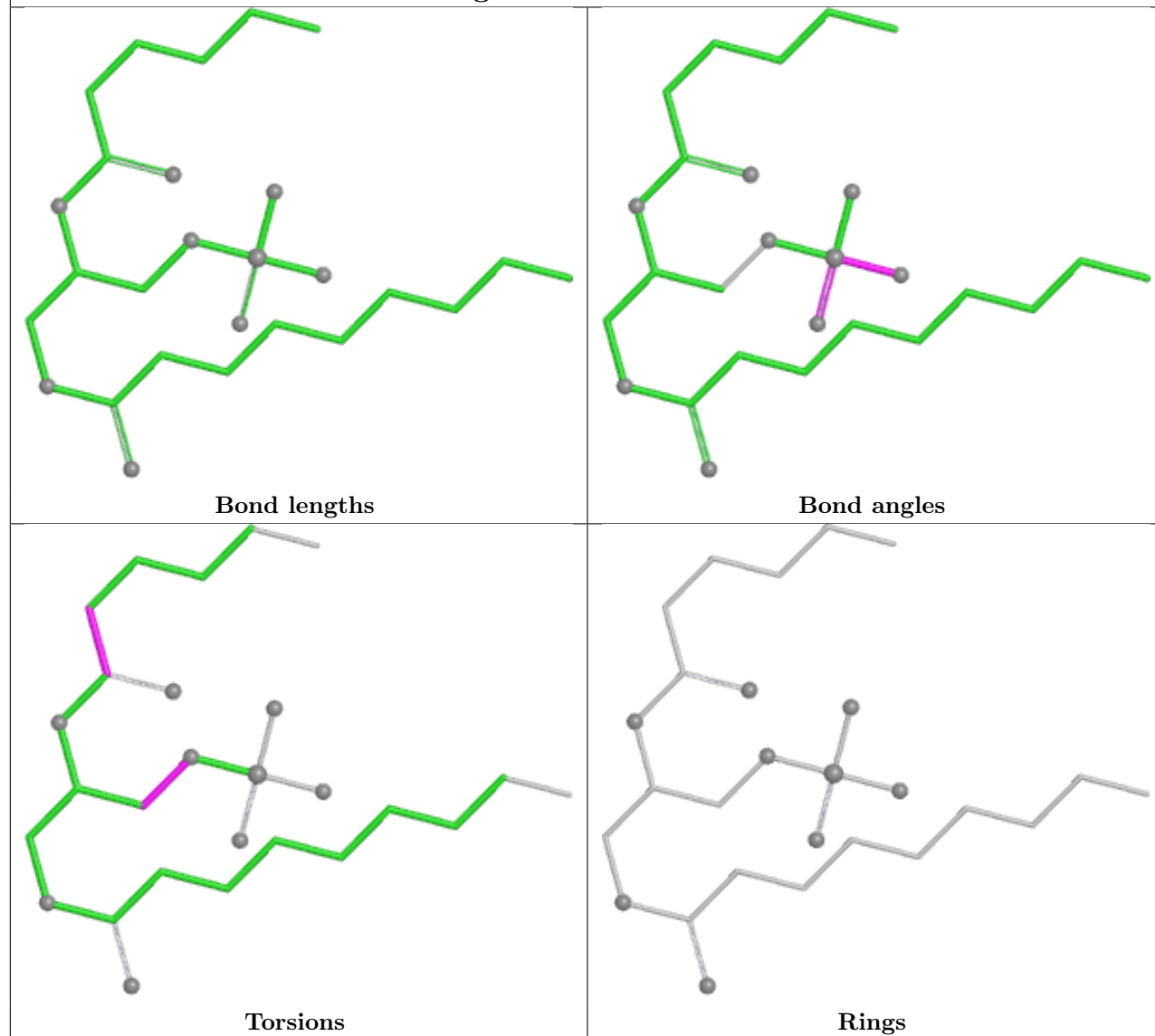




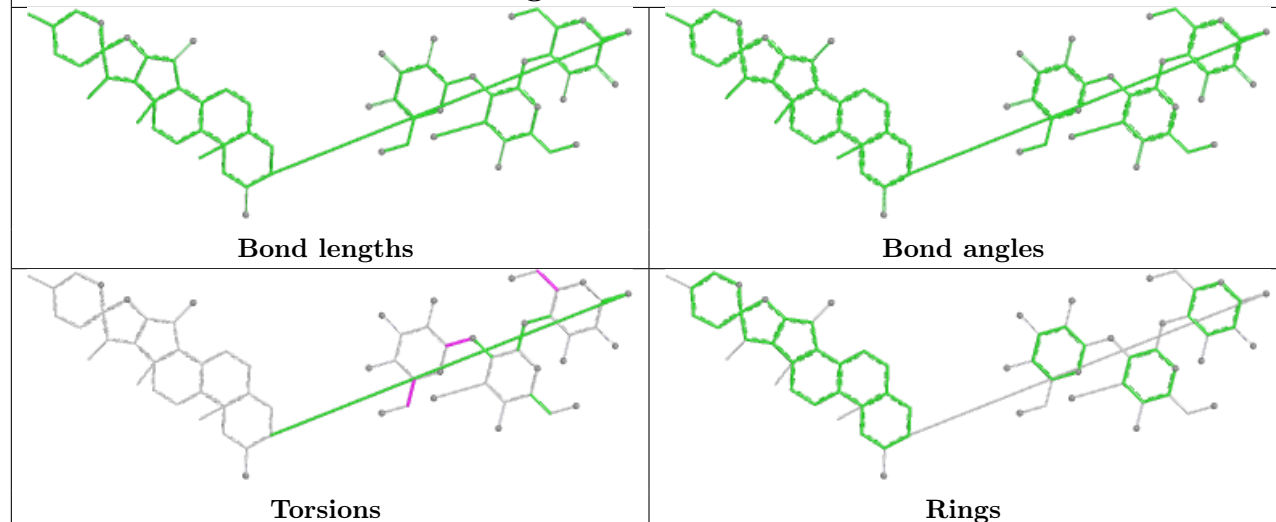


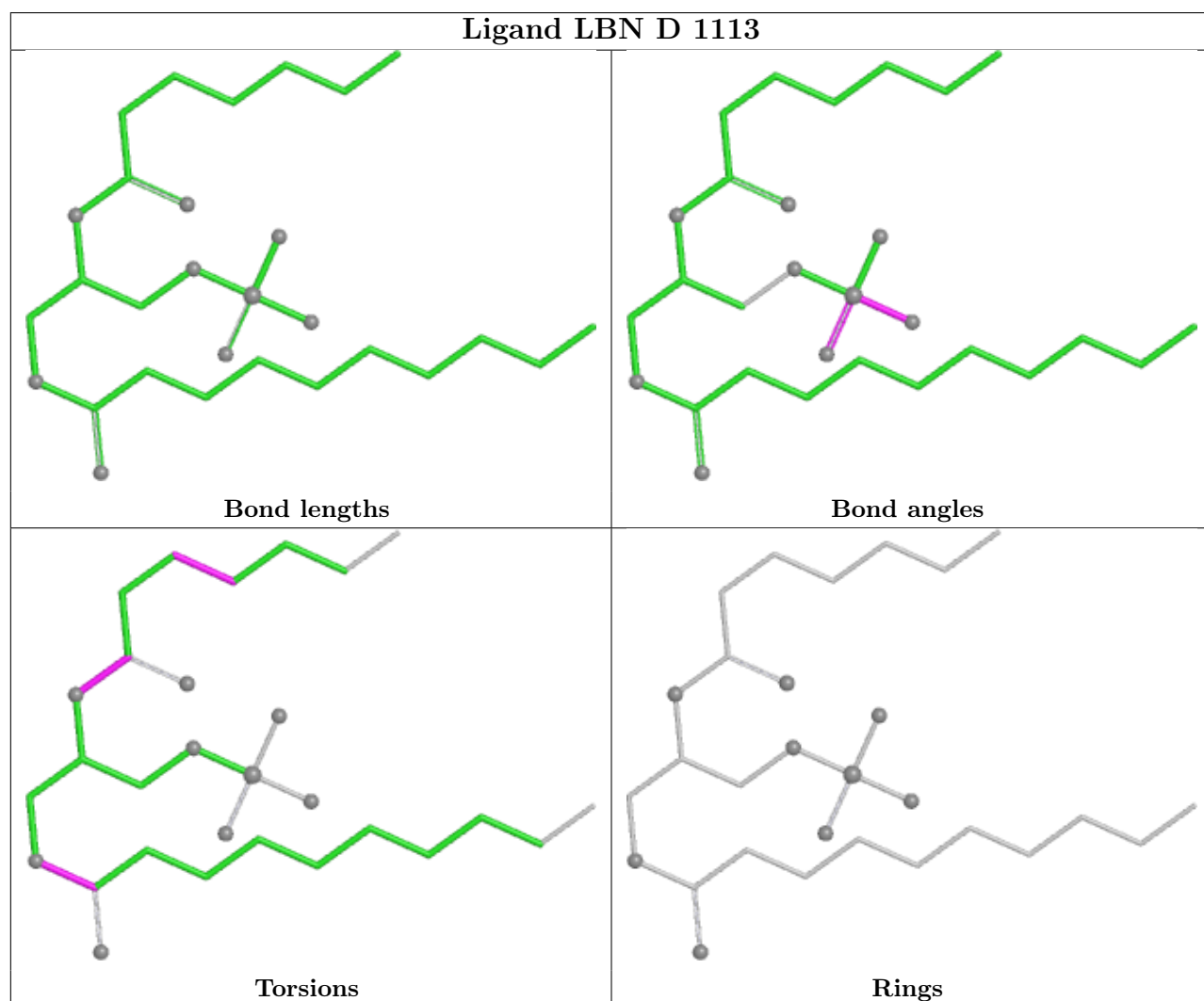
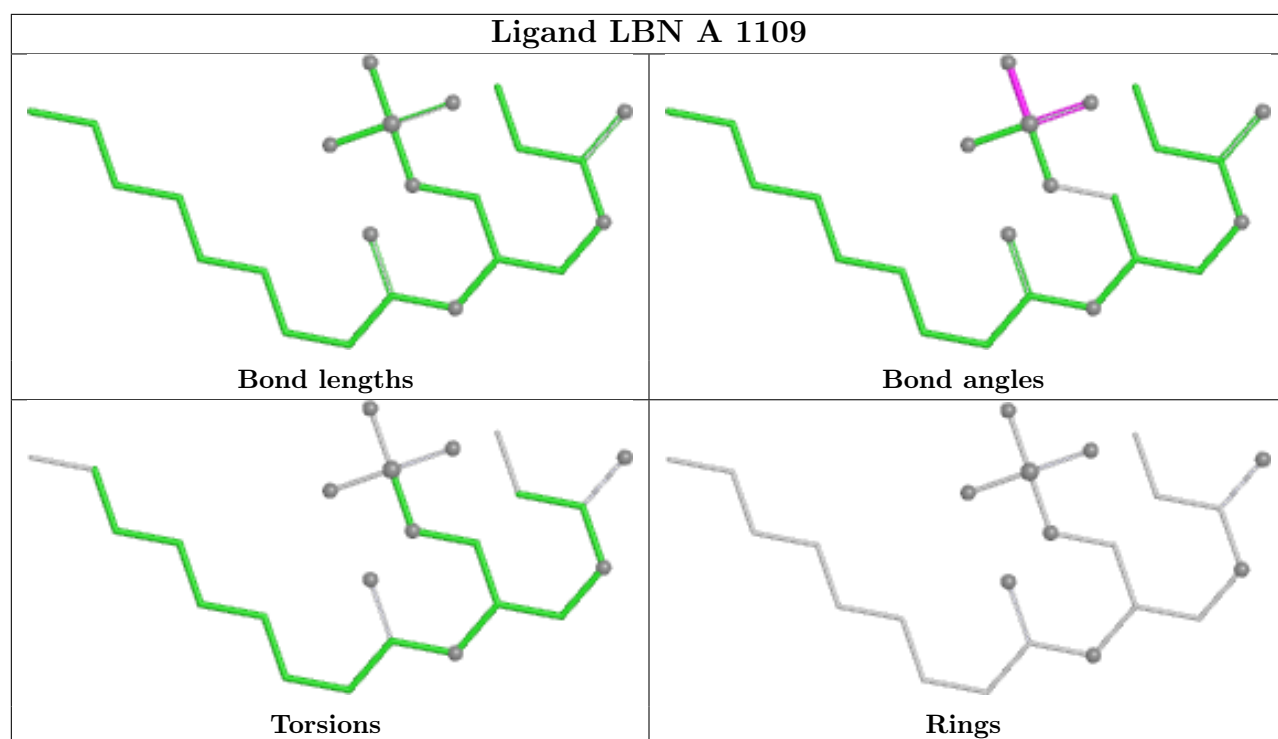


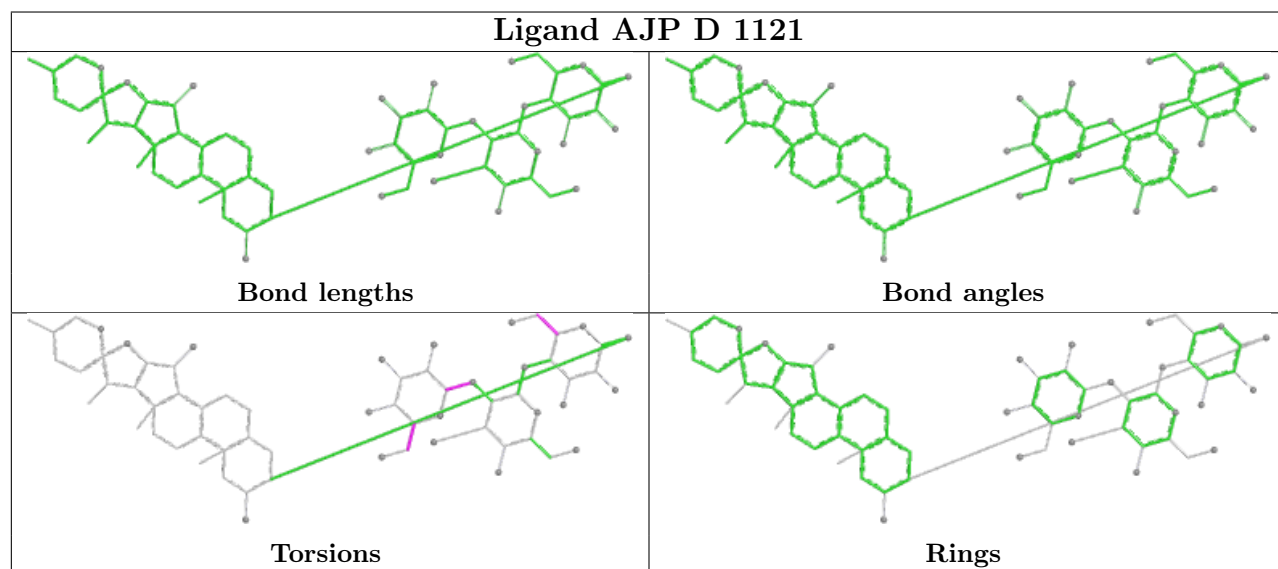
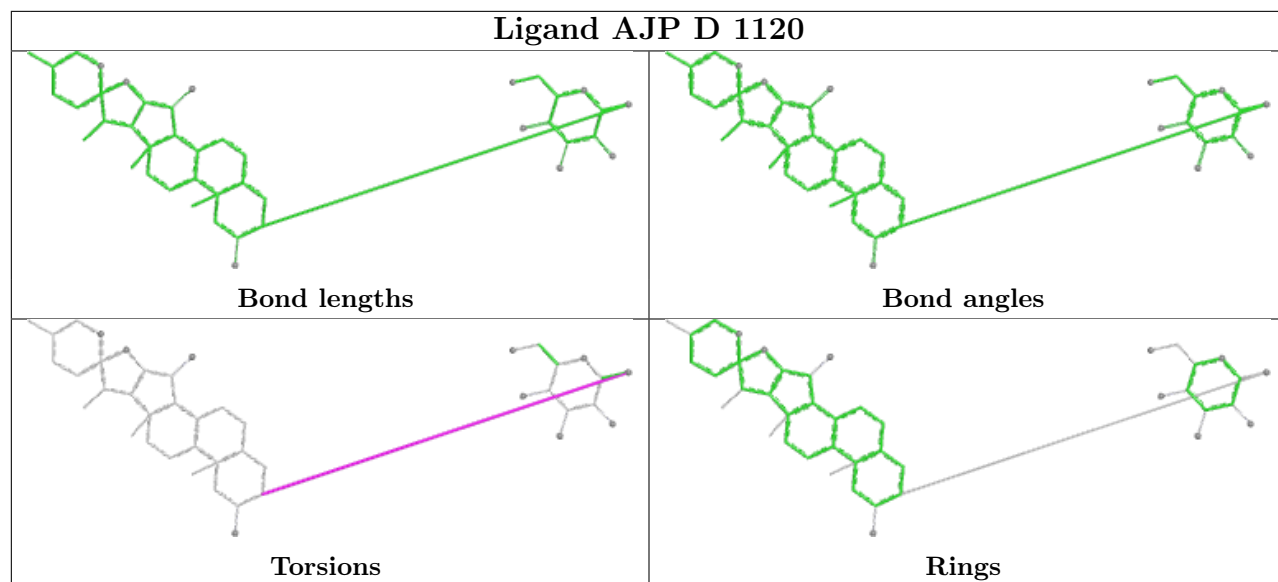
Ligand LBN C 1116

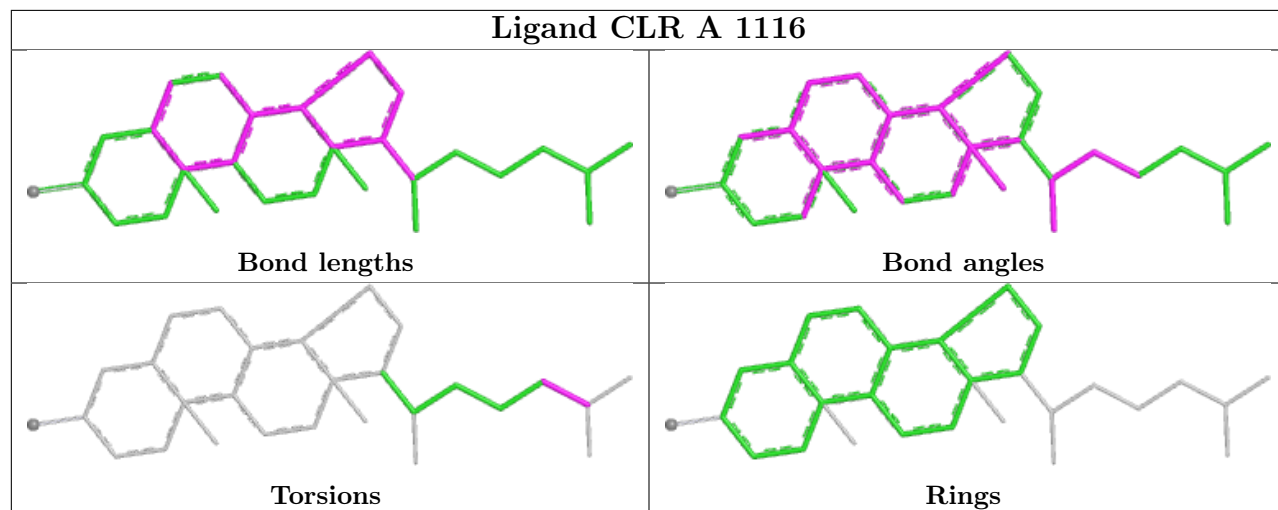
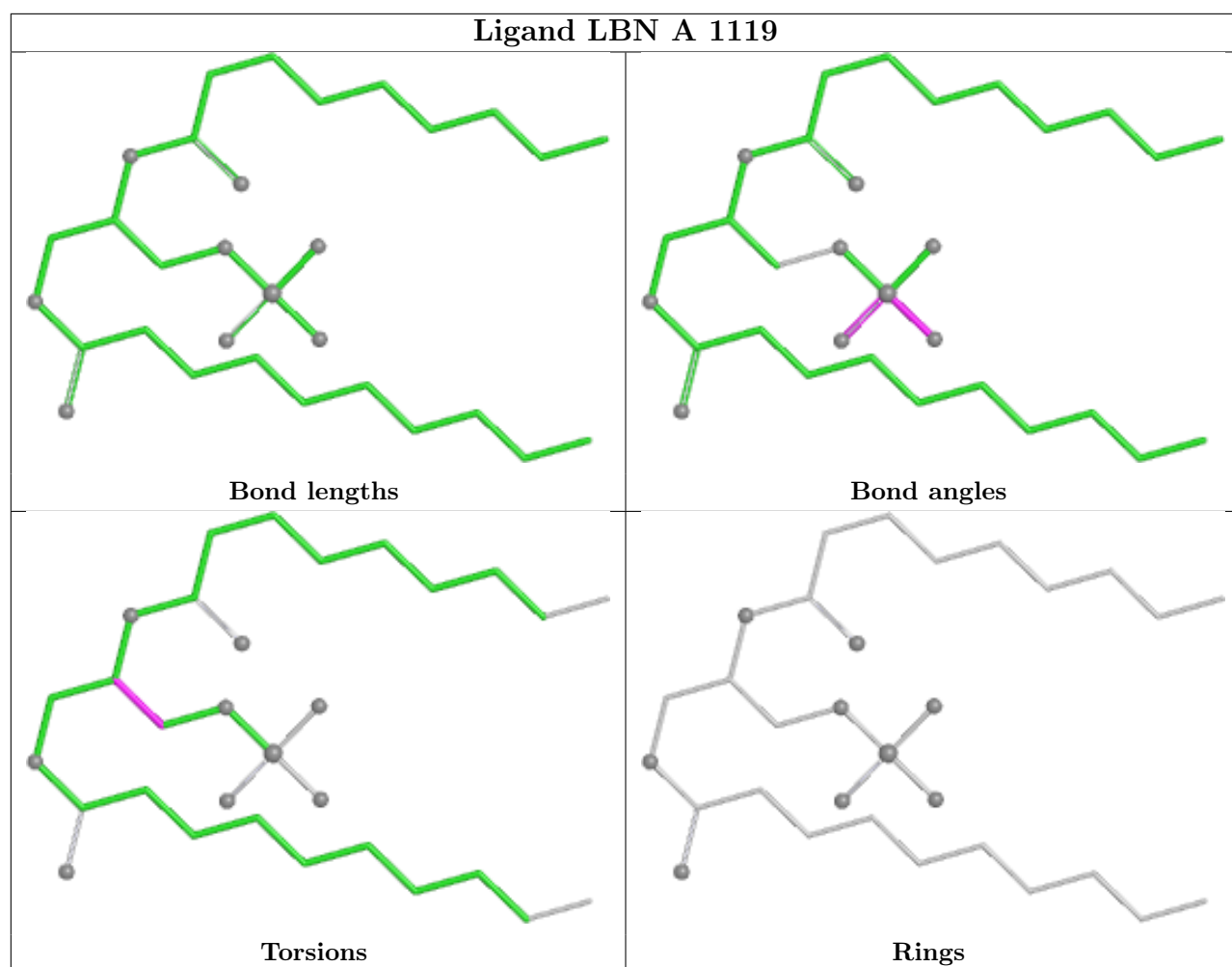


Ligand AJP B 1120

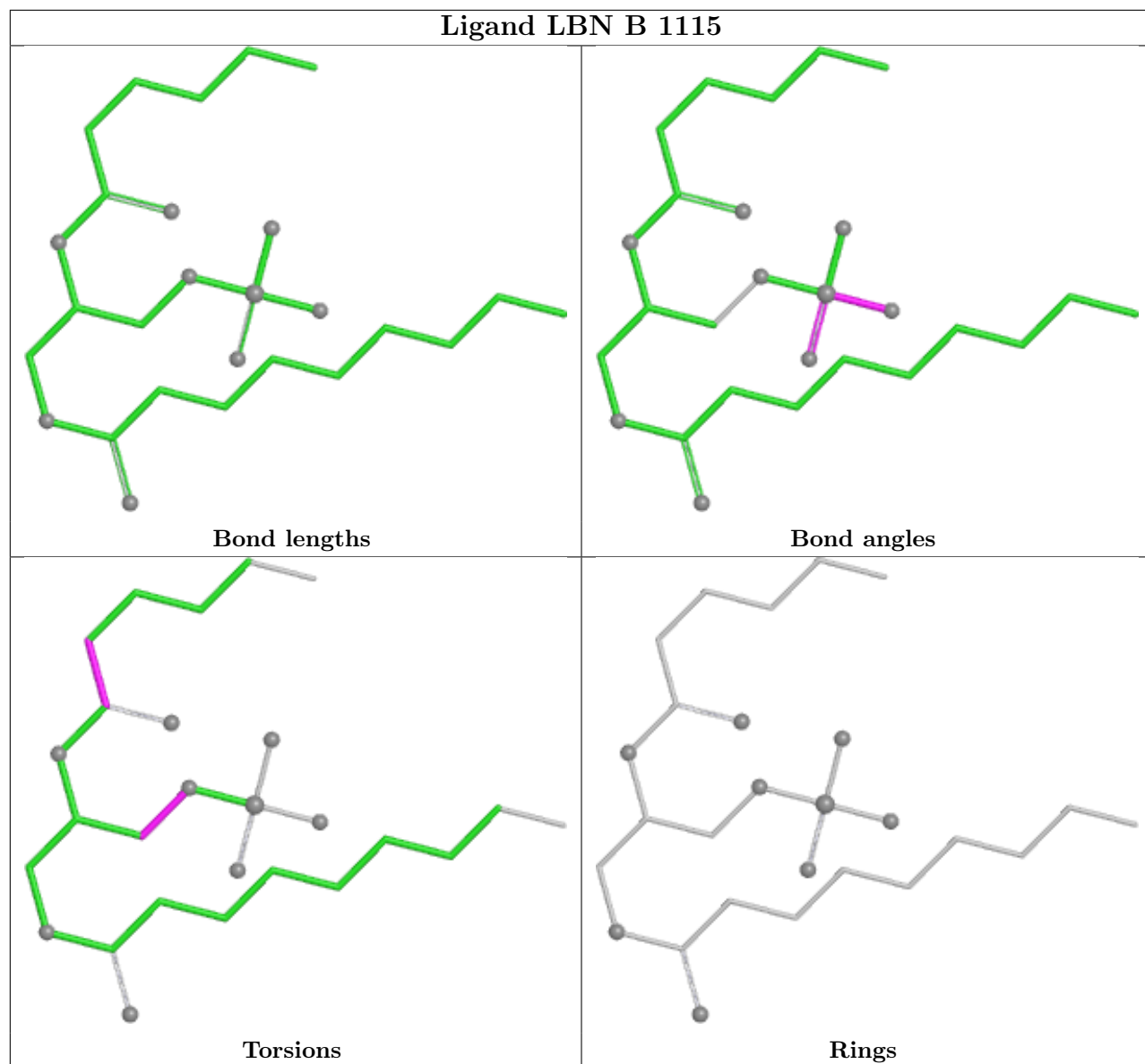




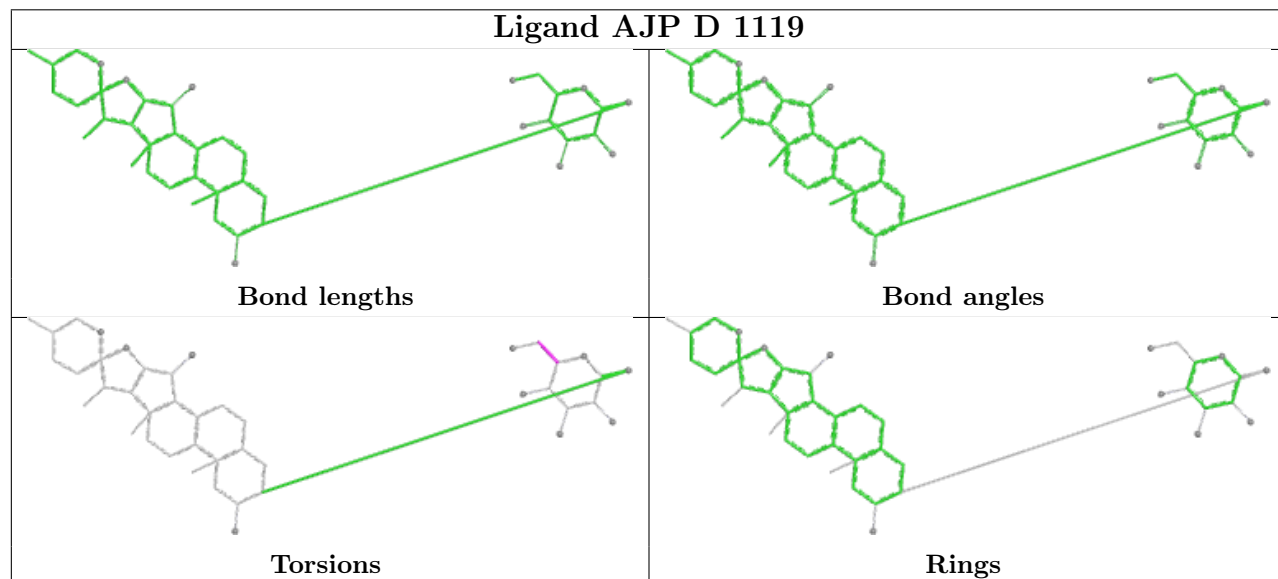


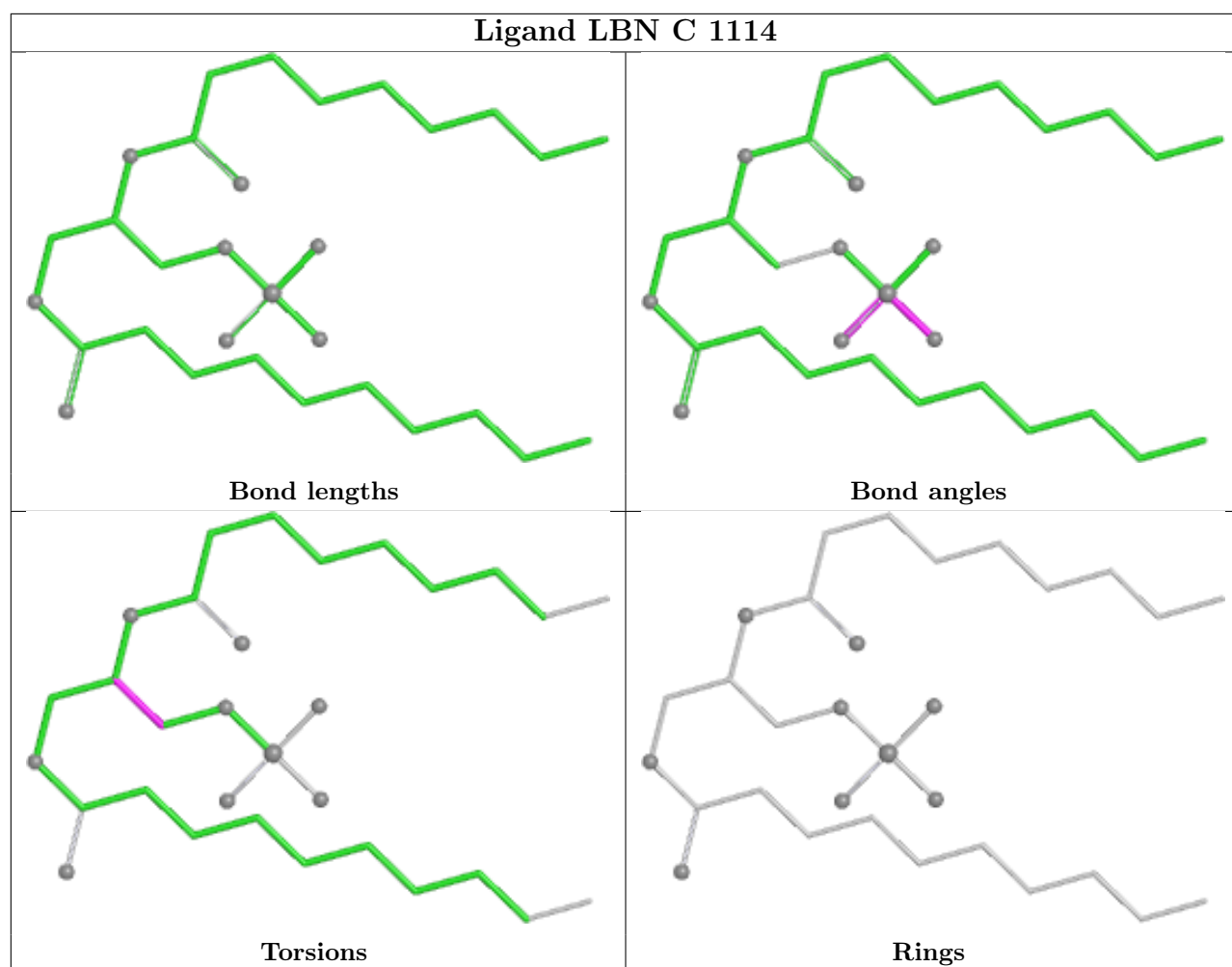


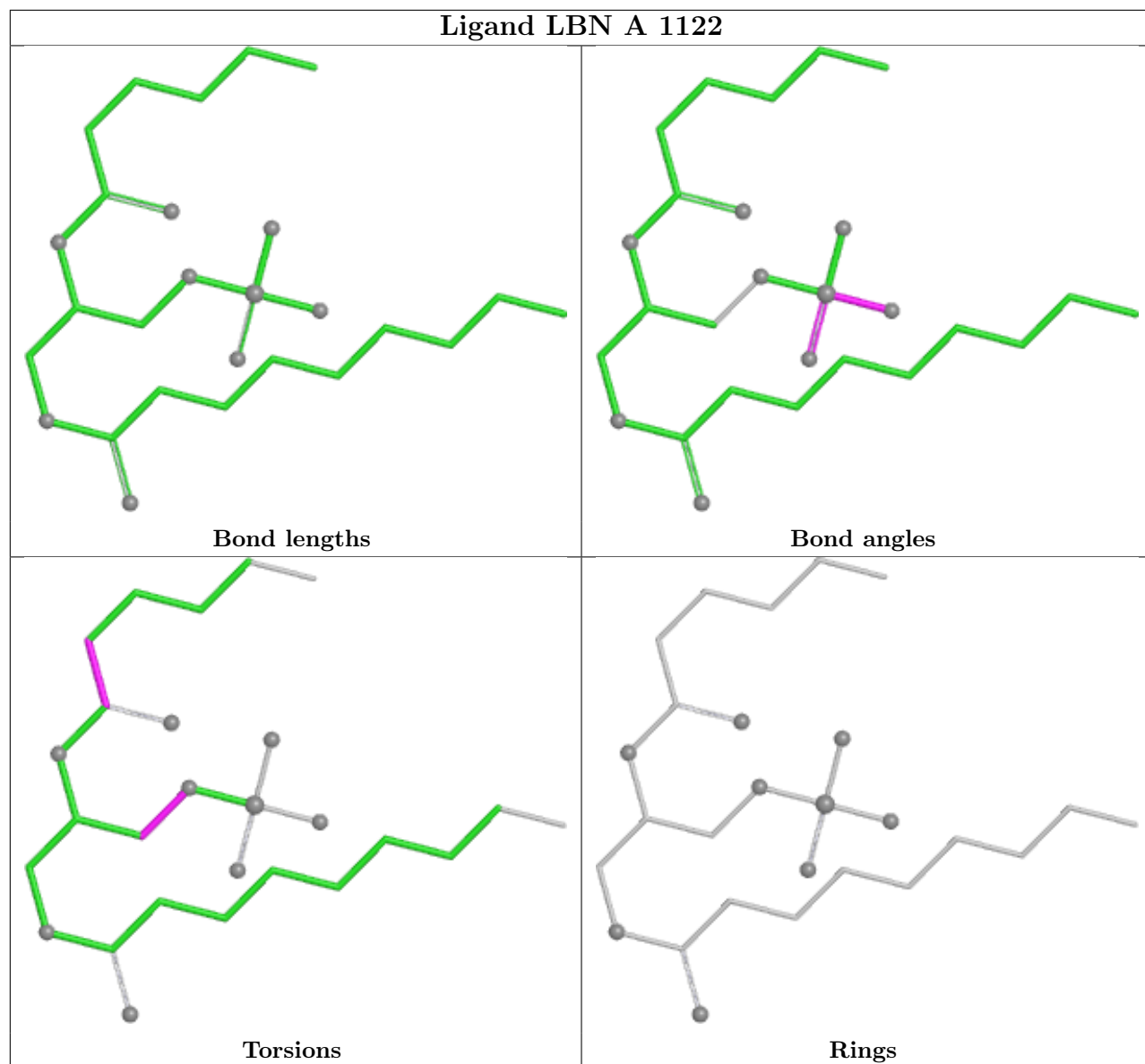
Ligand LBN B 1115

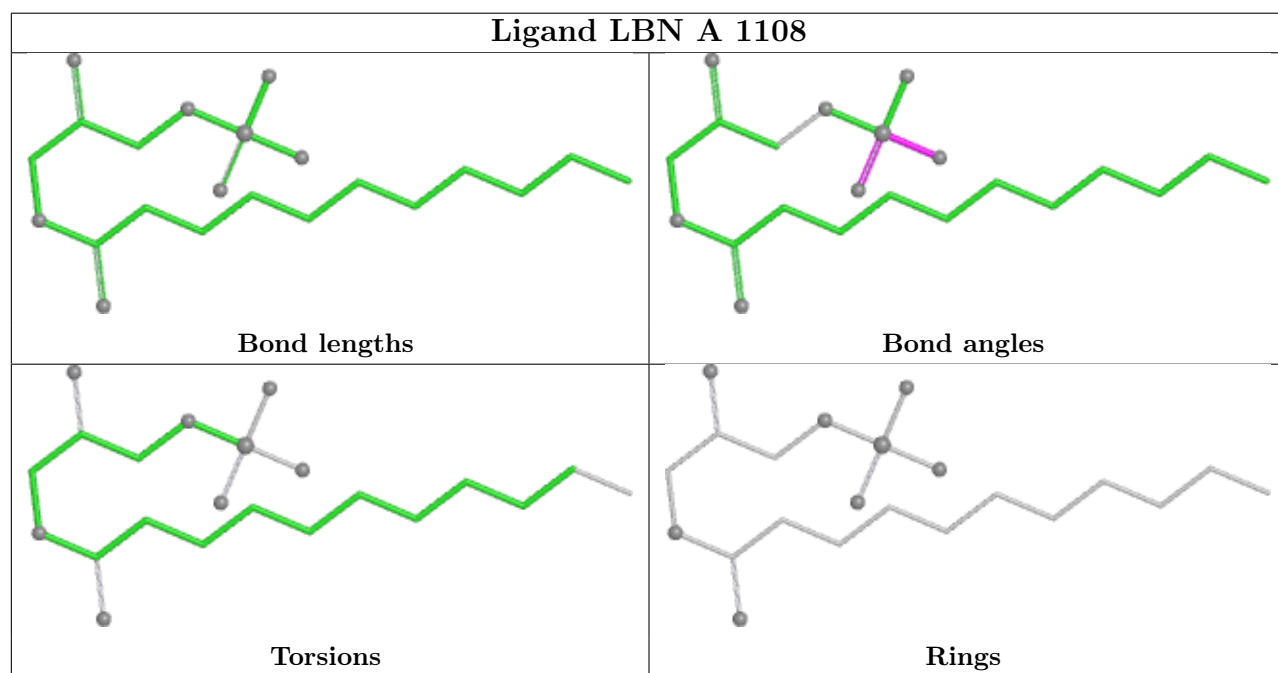
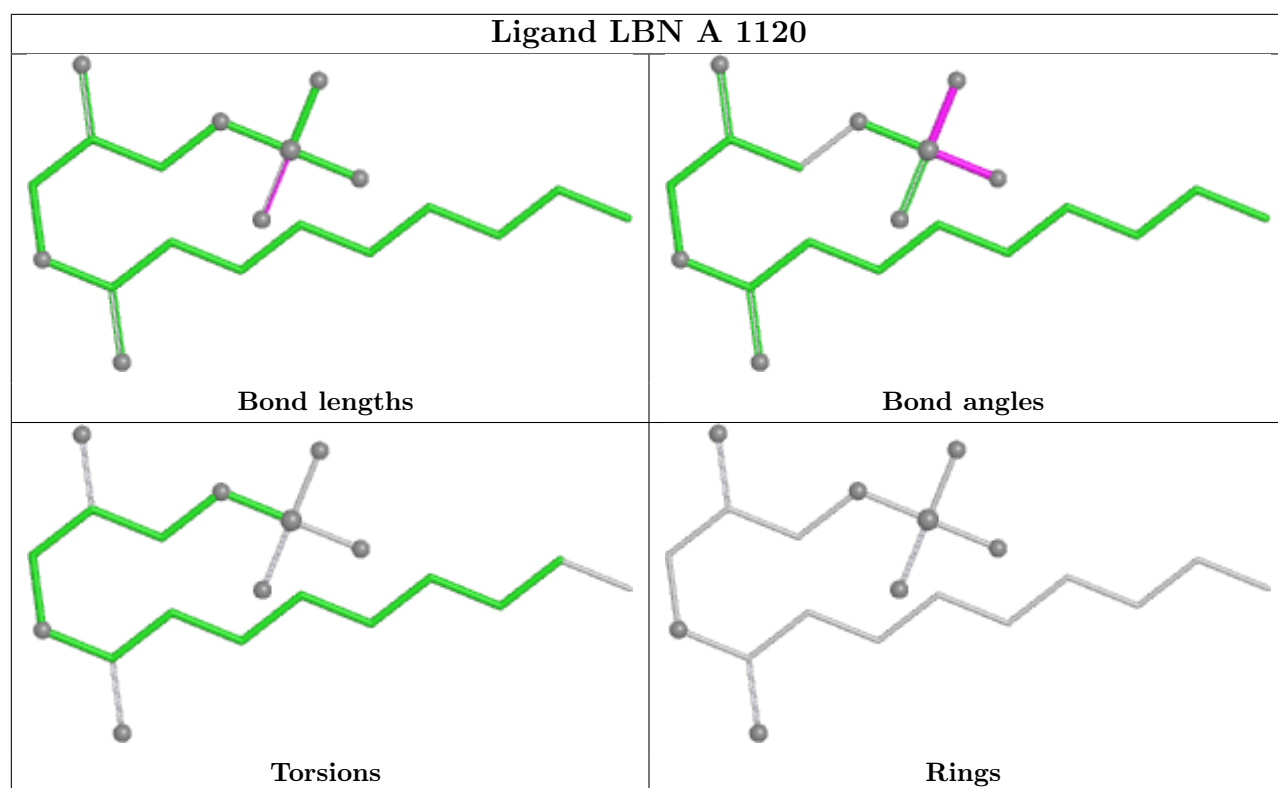


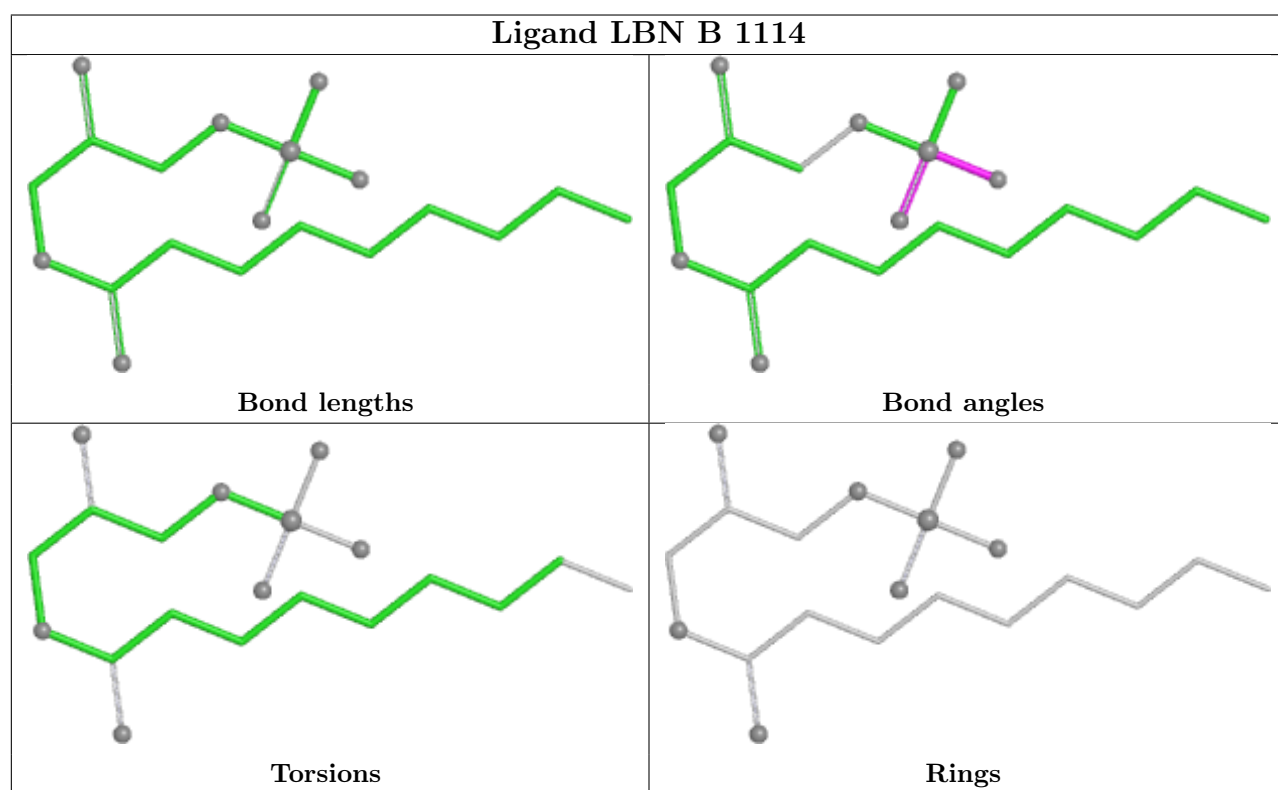
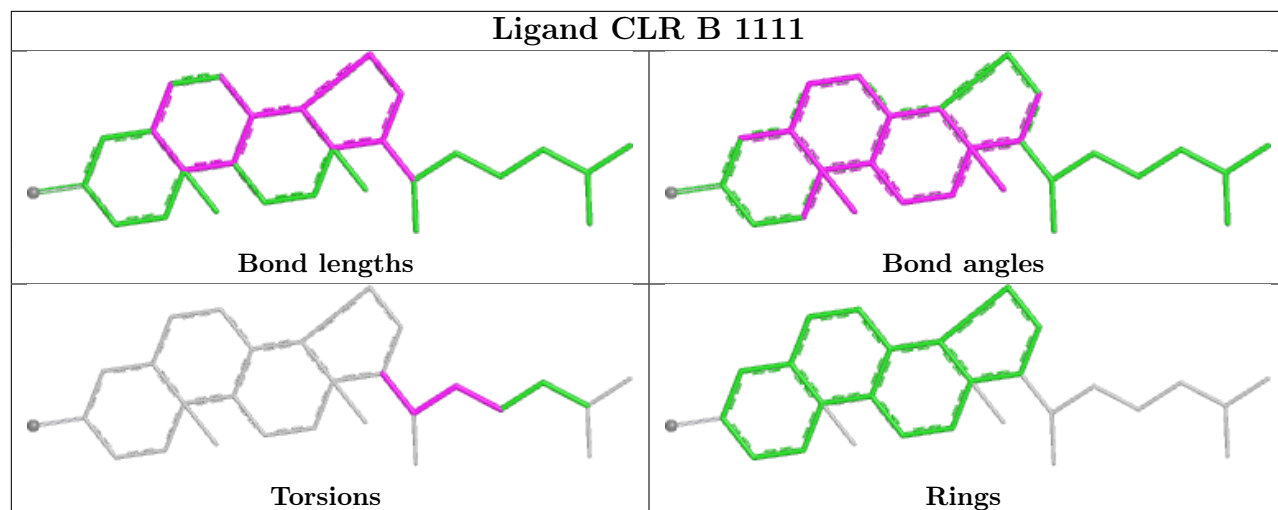
Ligand AJP D 1119

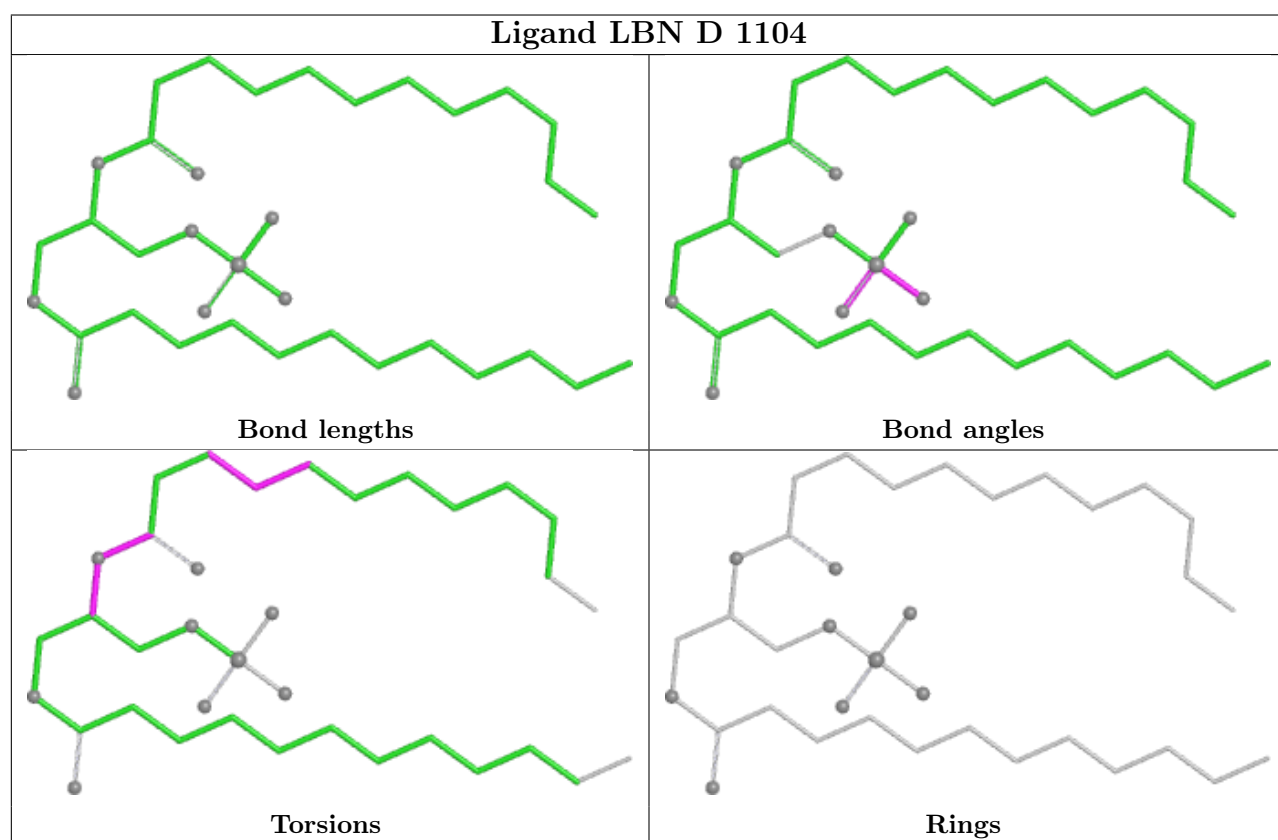
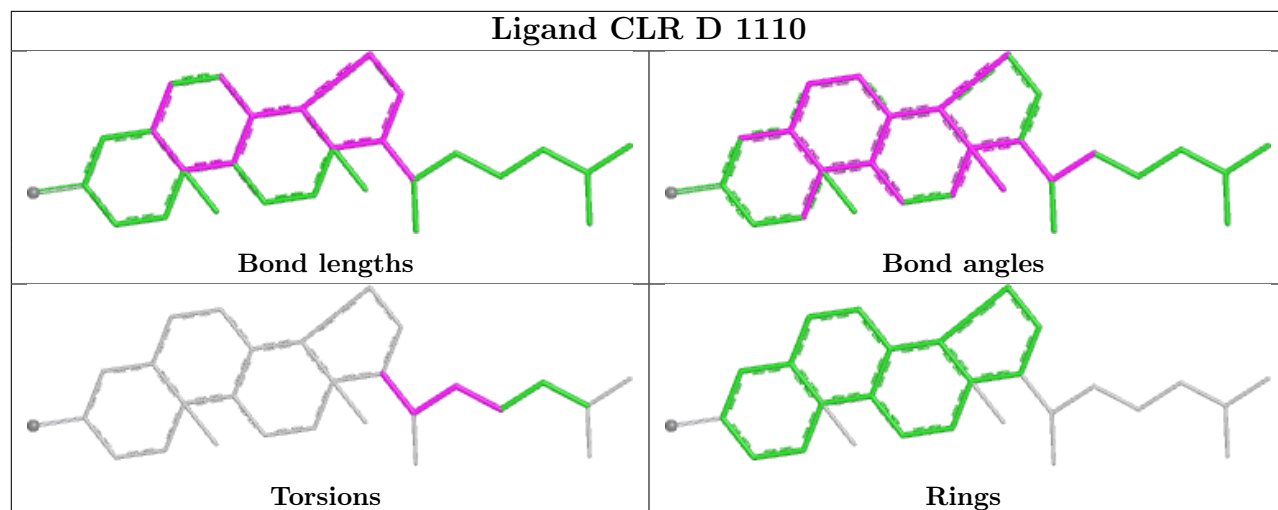


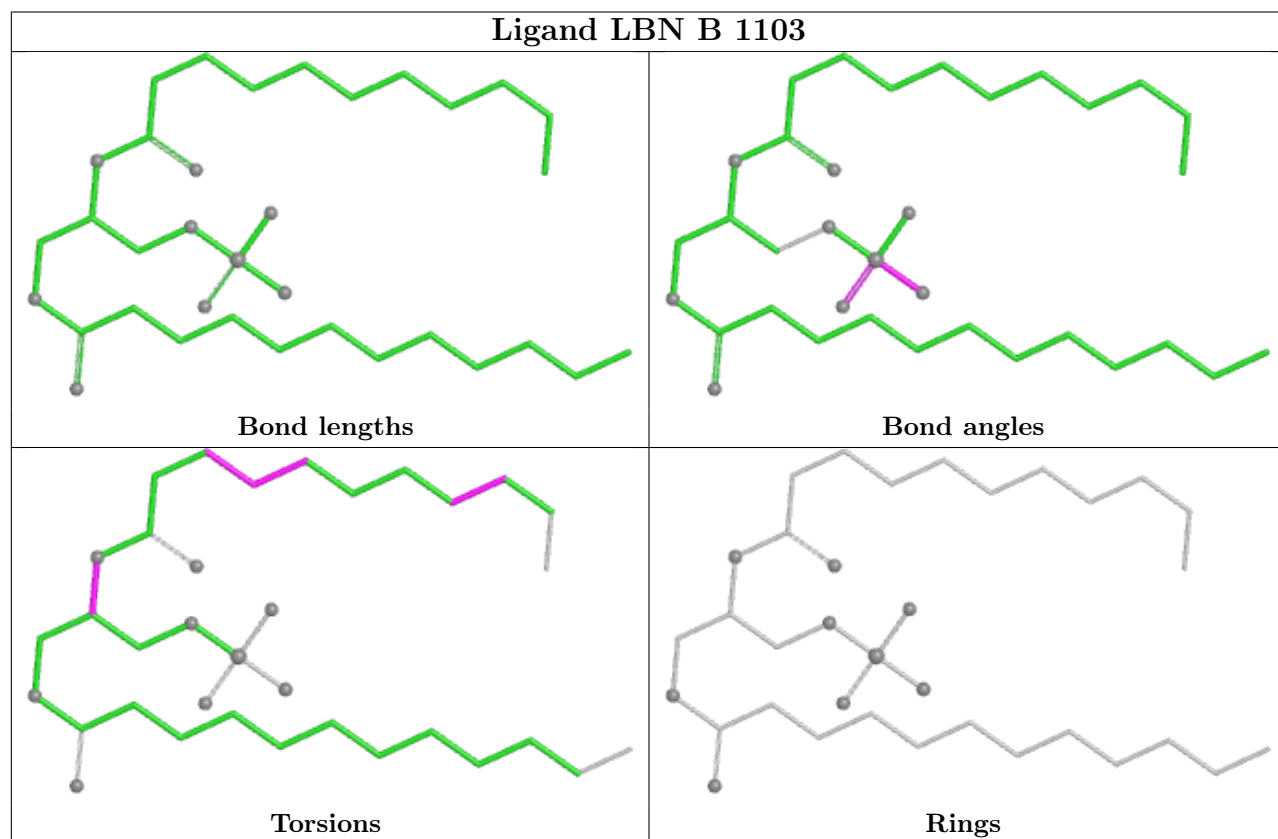
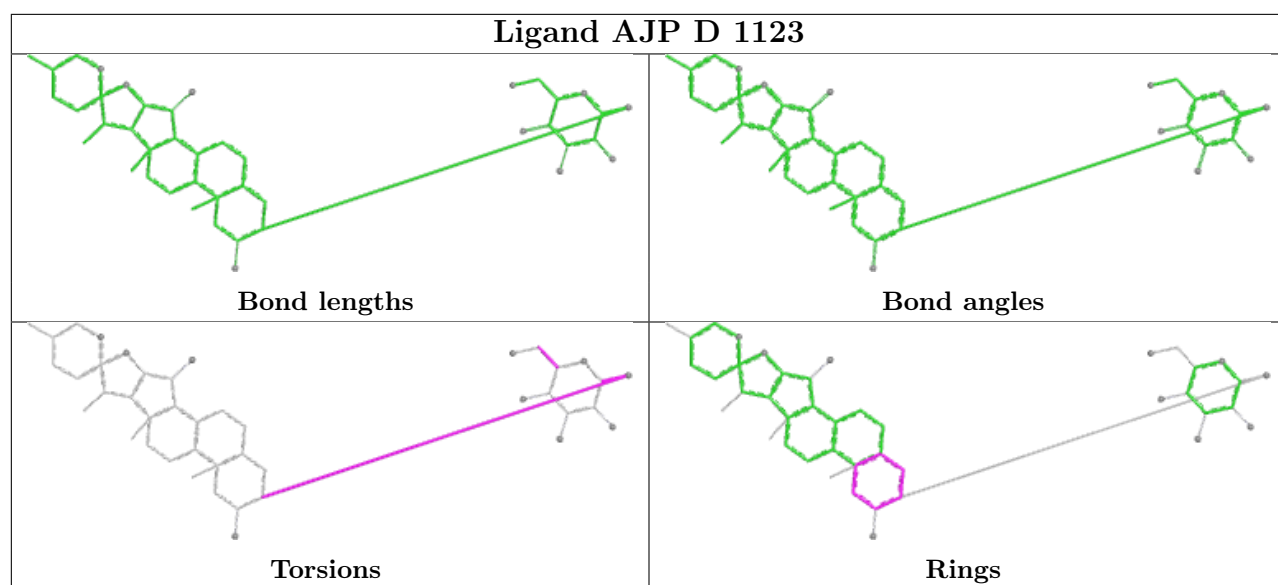


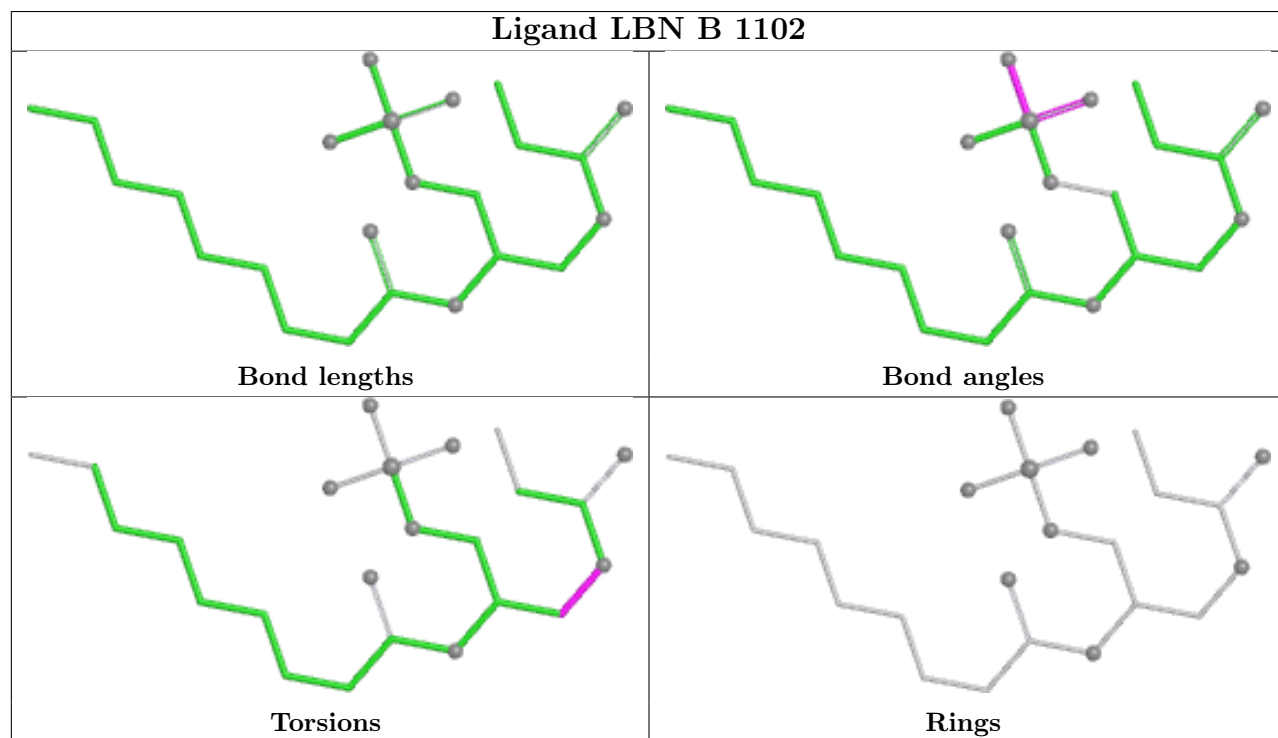
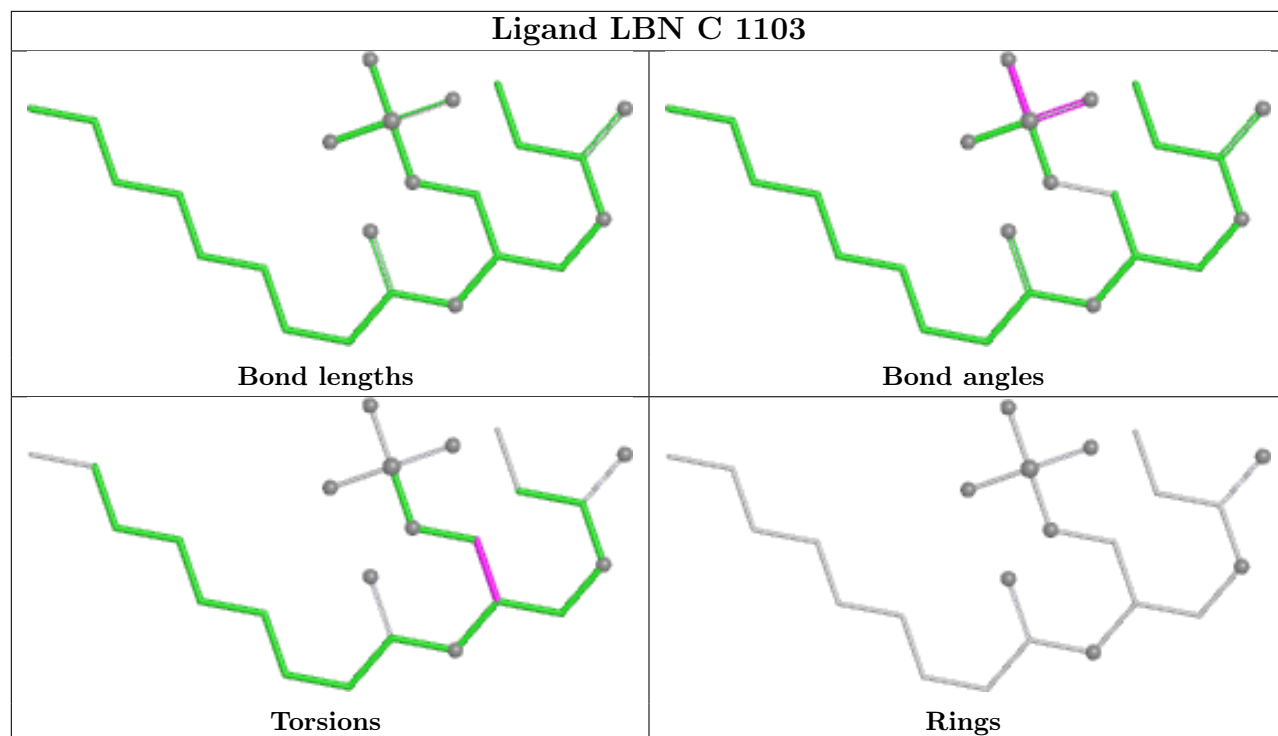


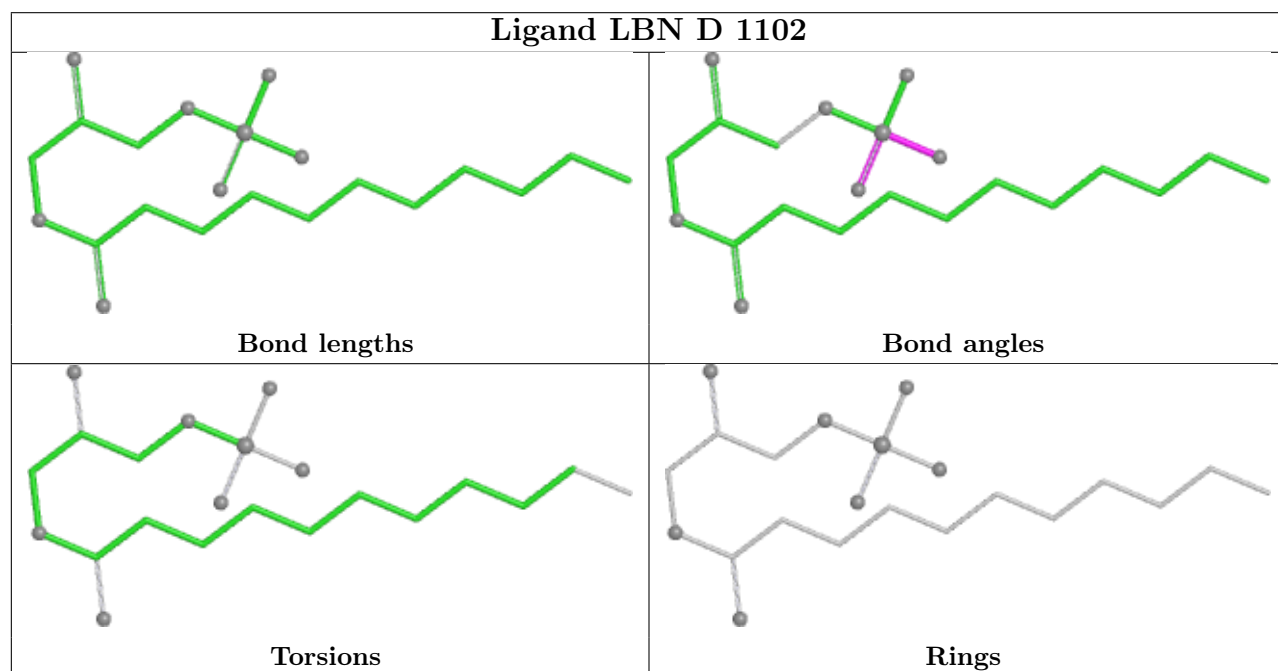
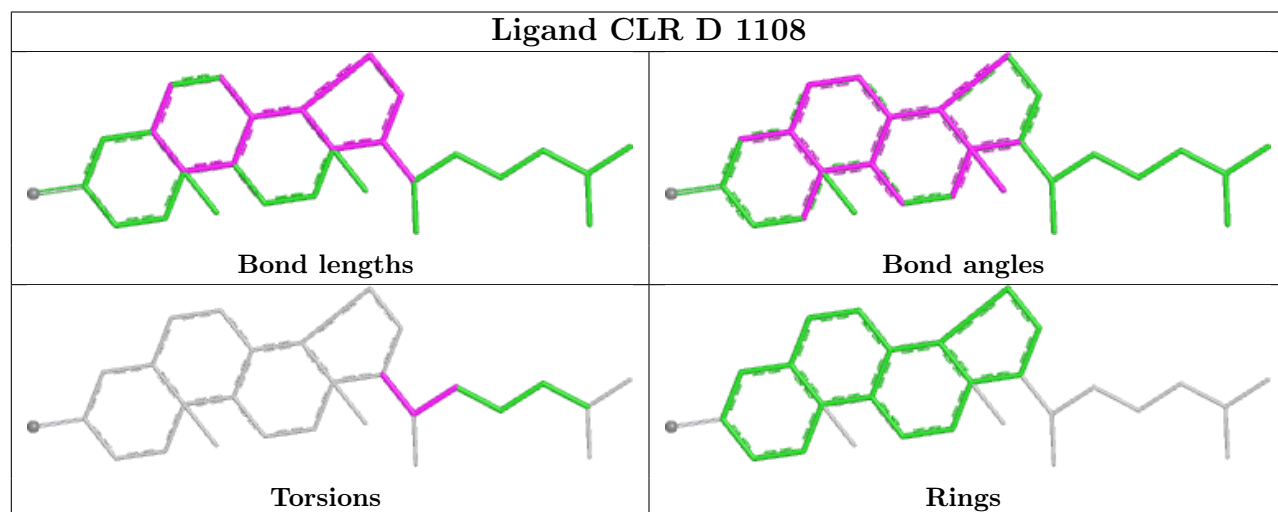
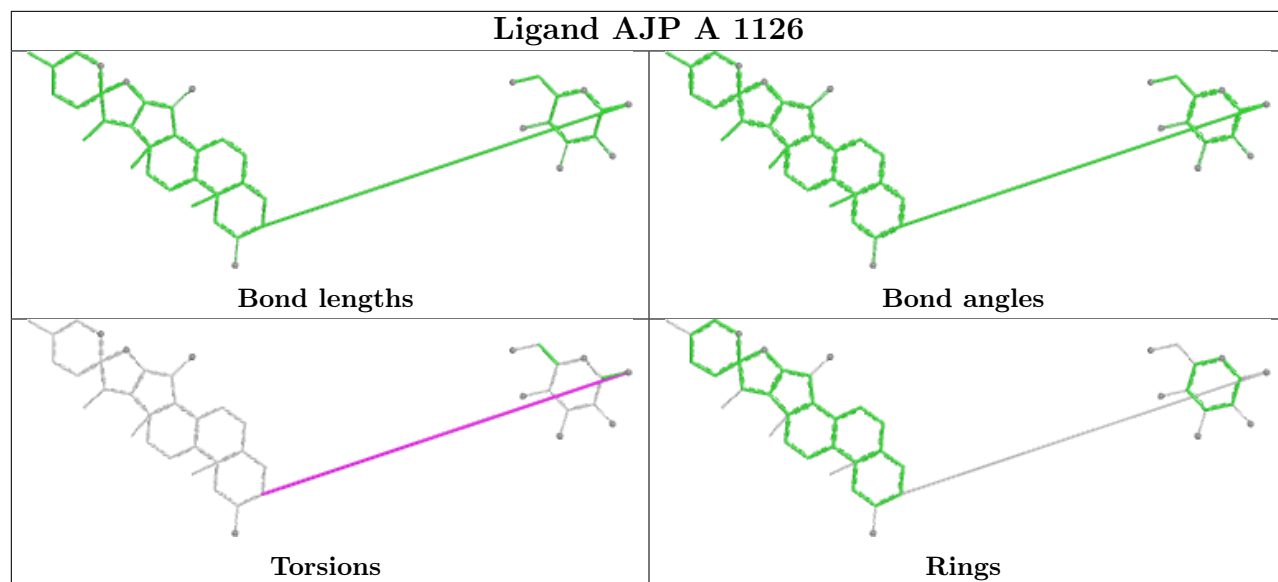




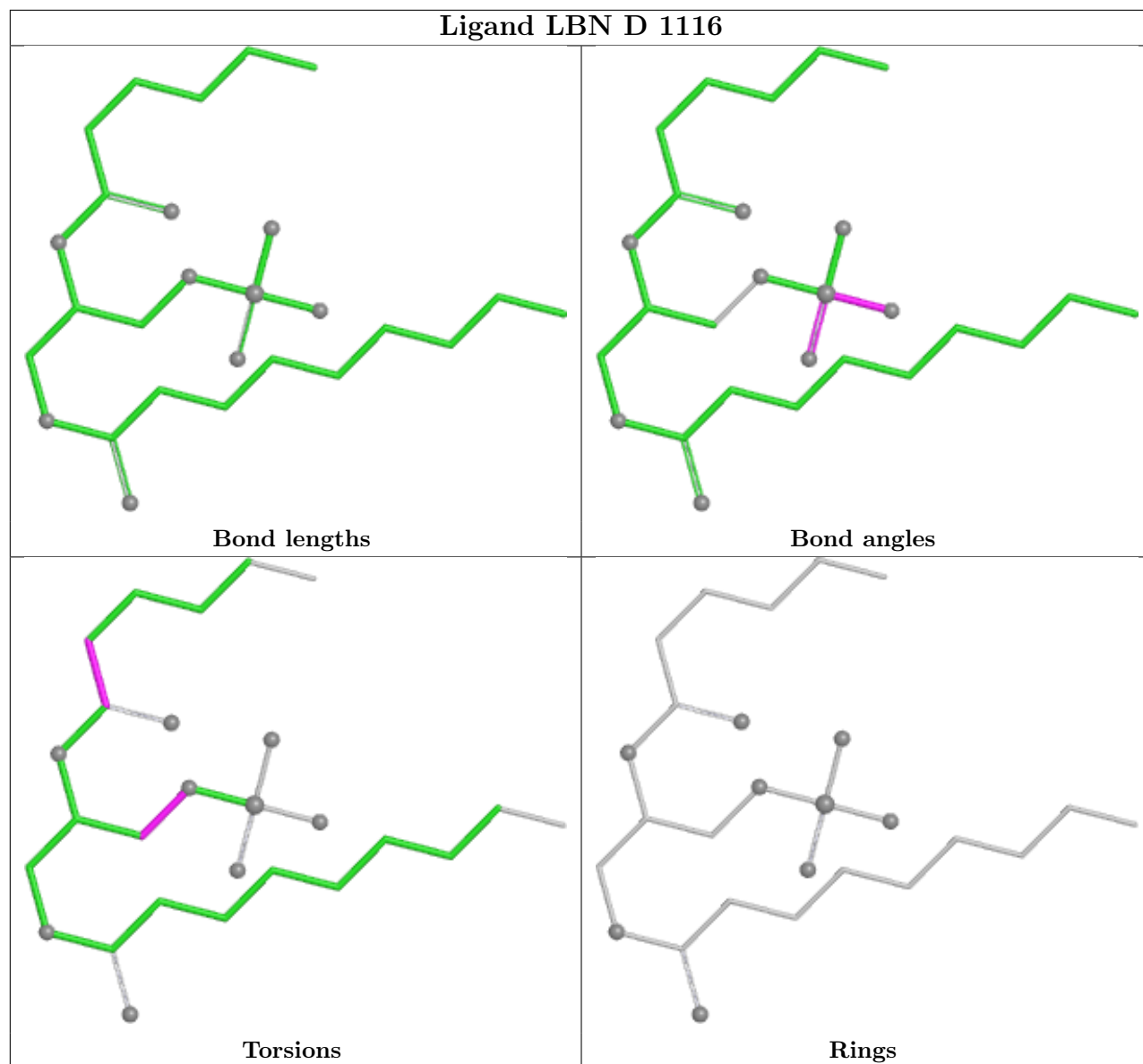




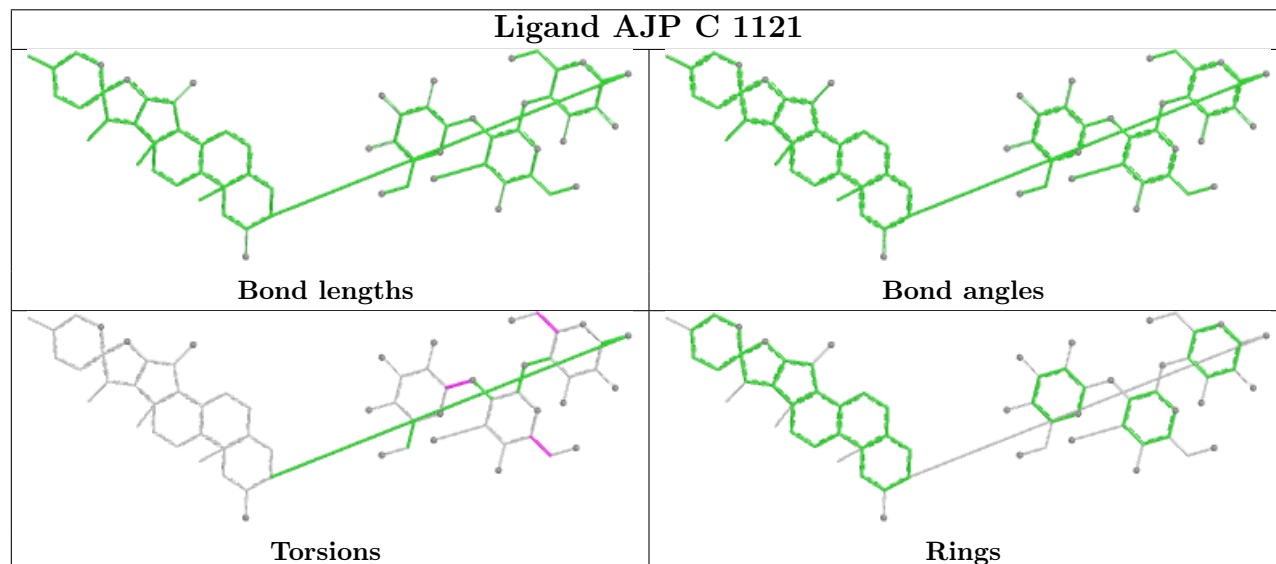


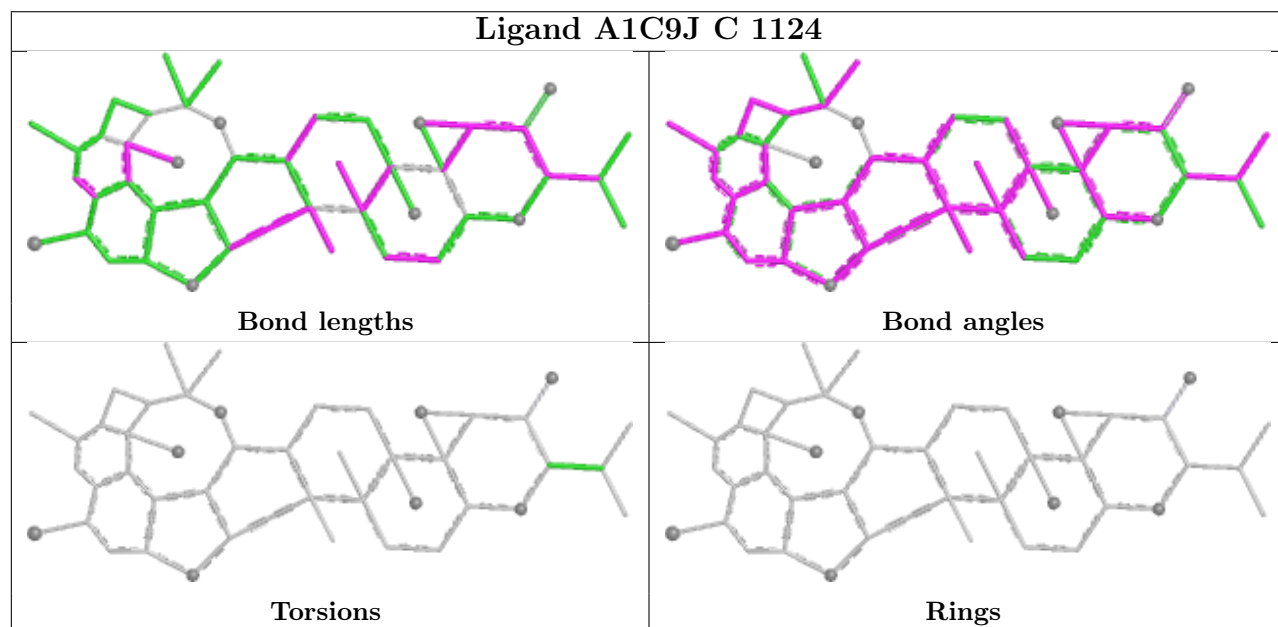
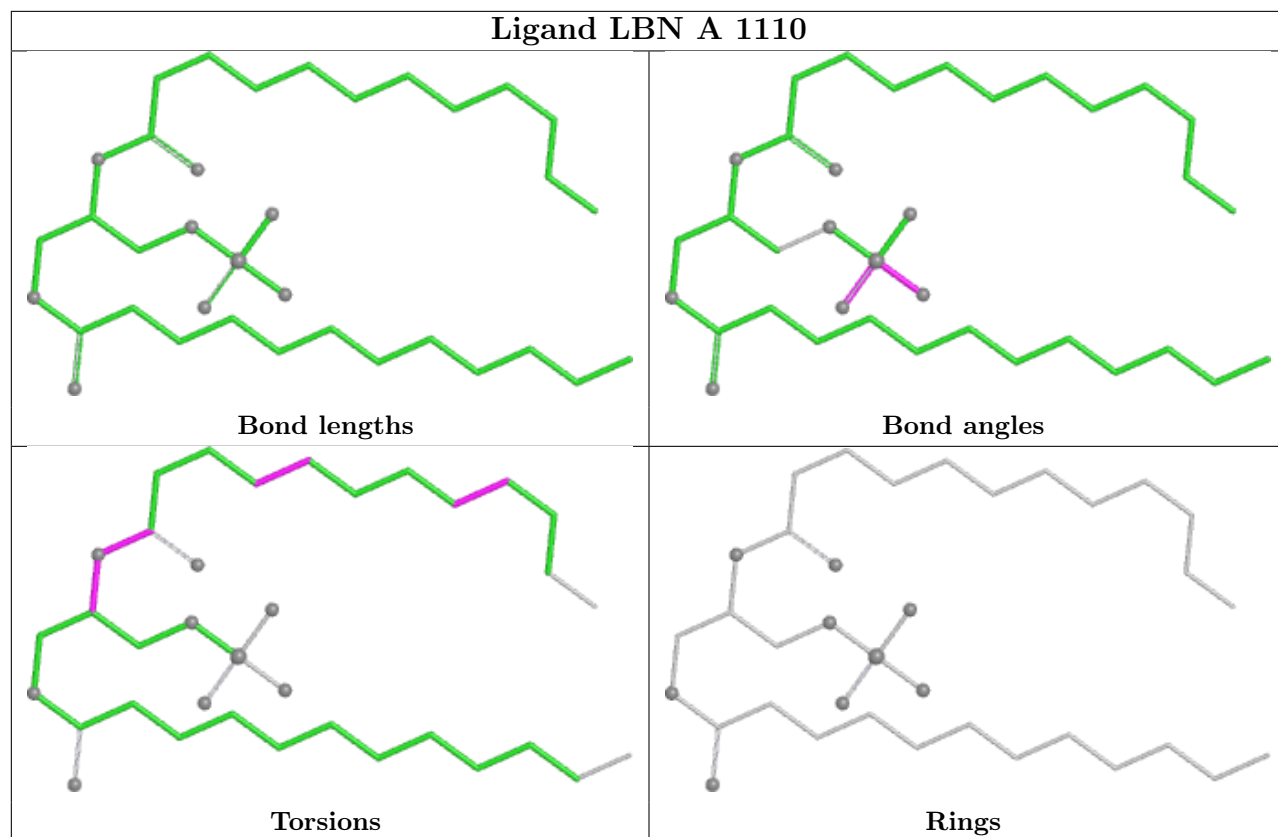


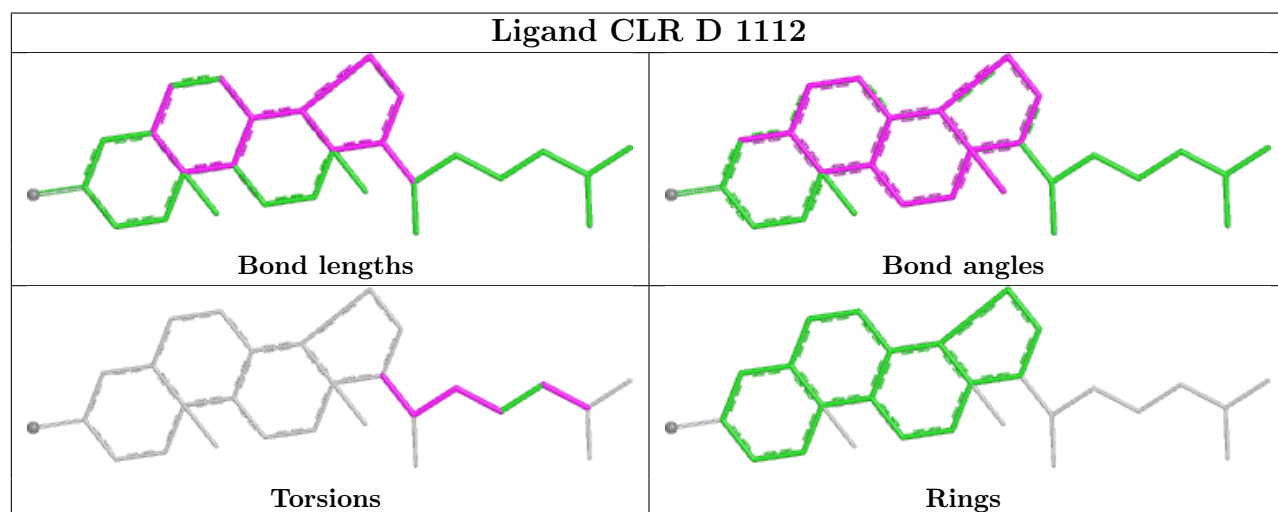
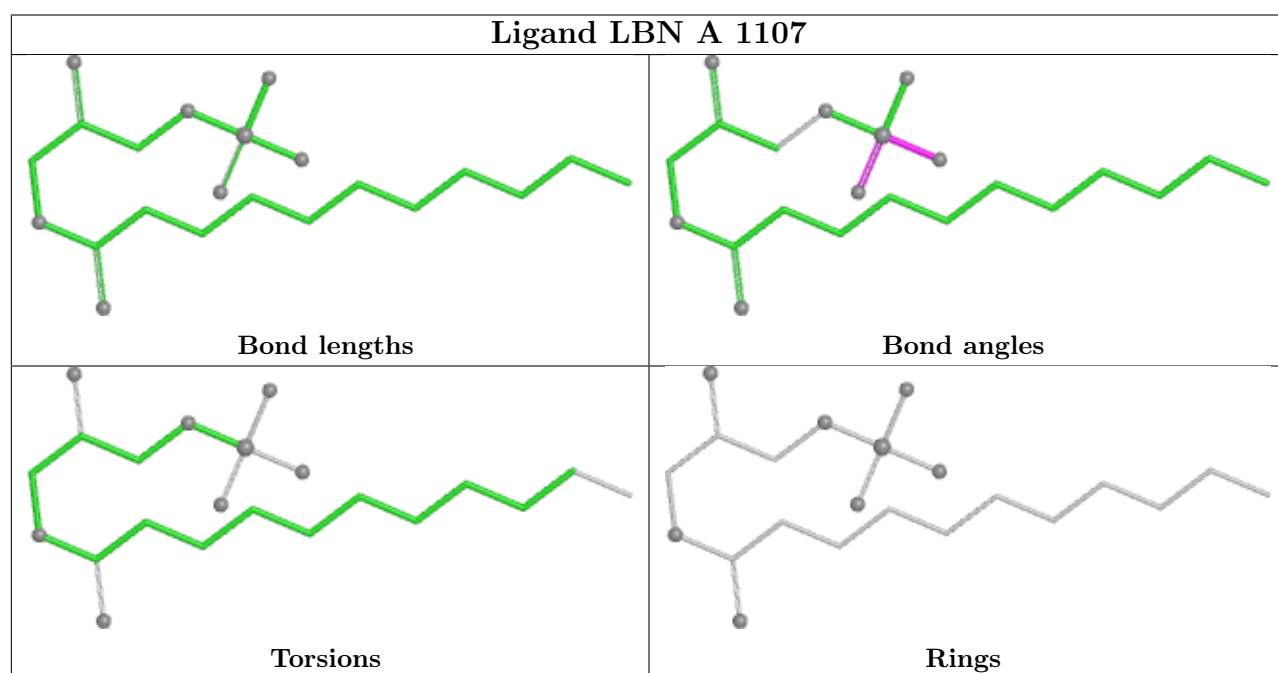
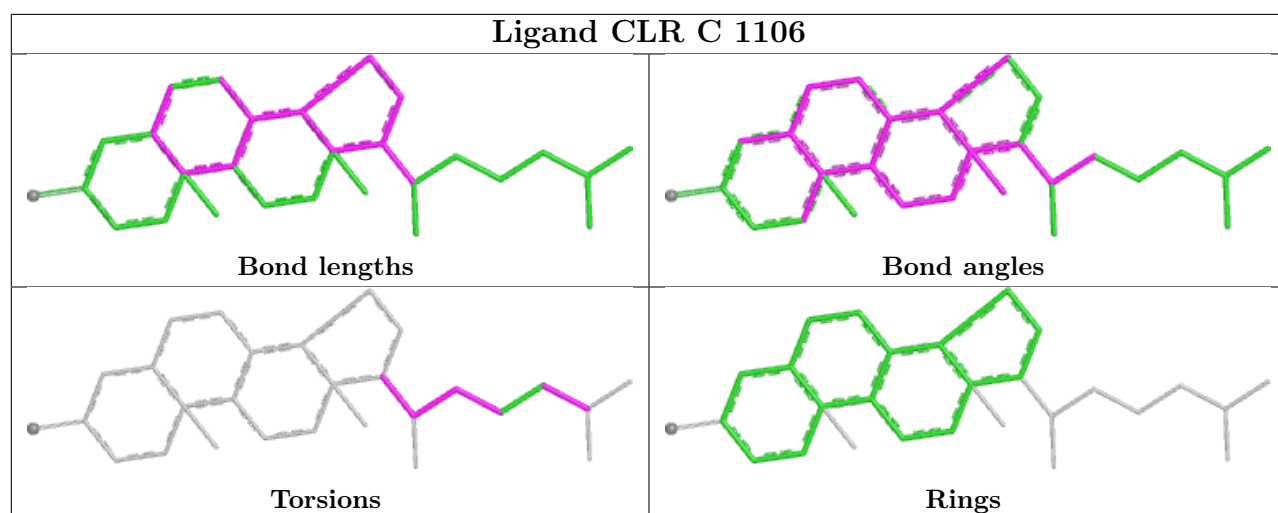
Ligand LBN D 1116

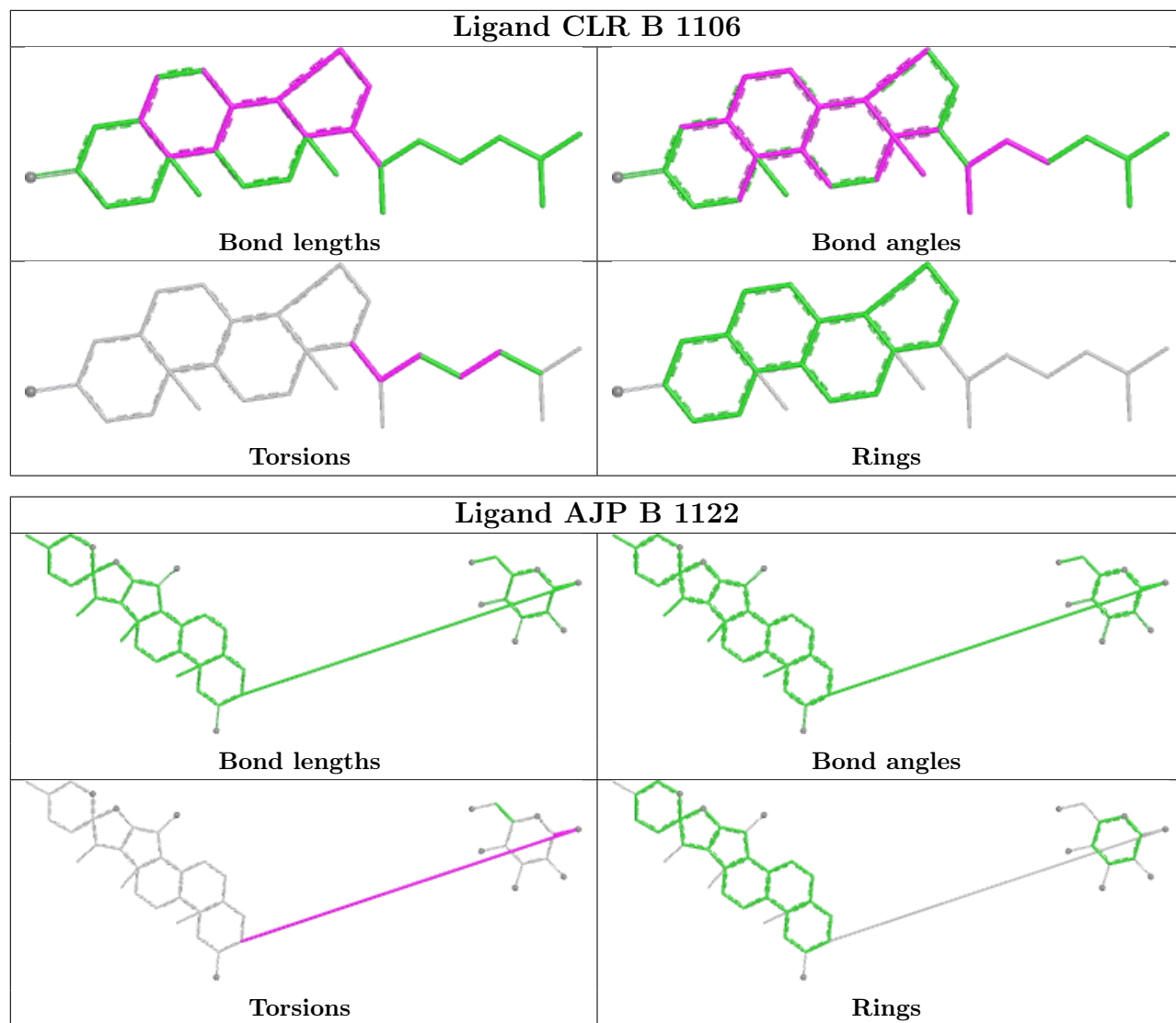


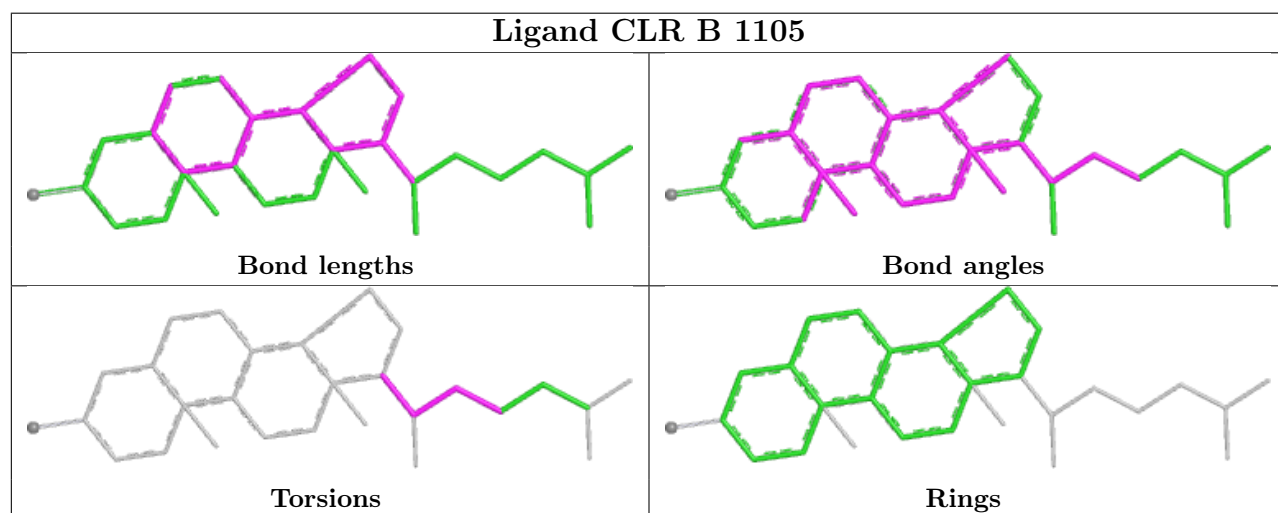
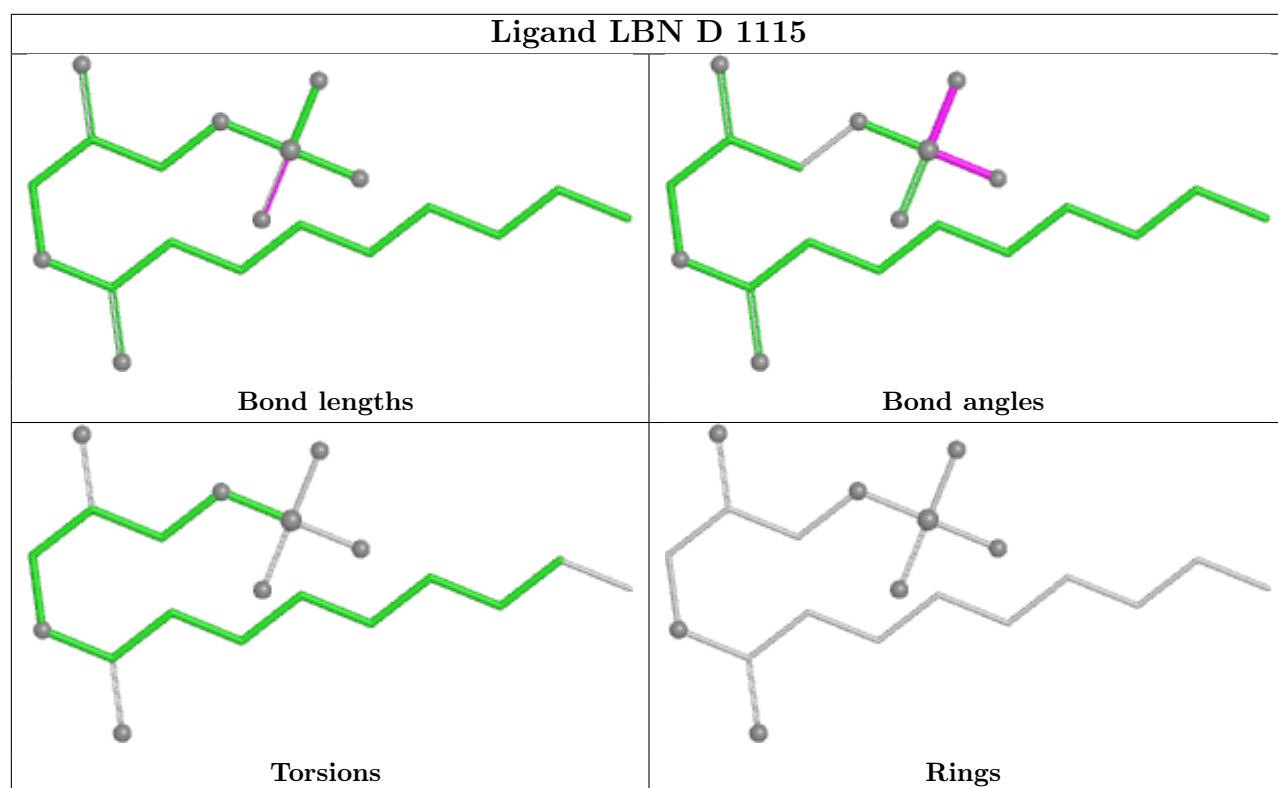
Ligand AJP C 1121

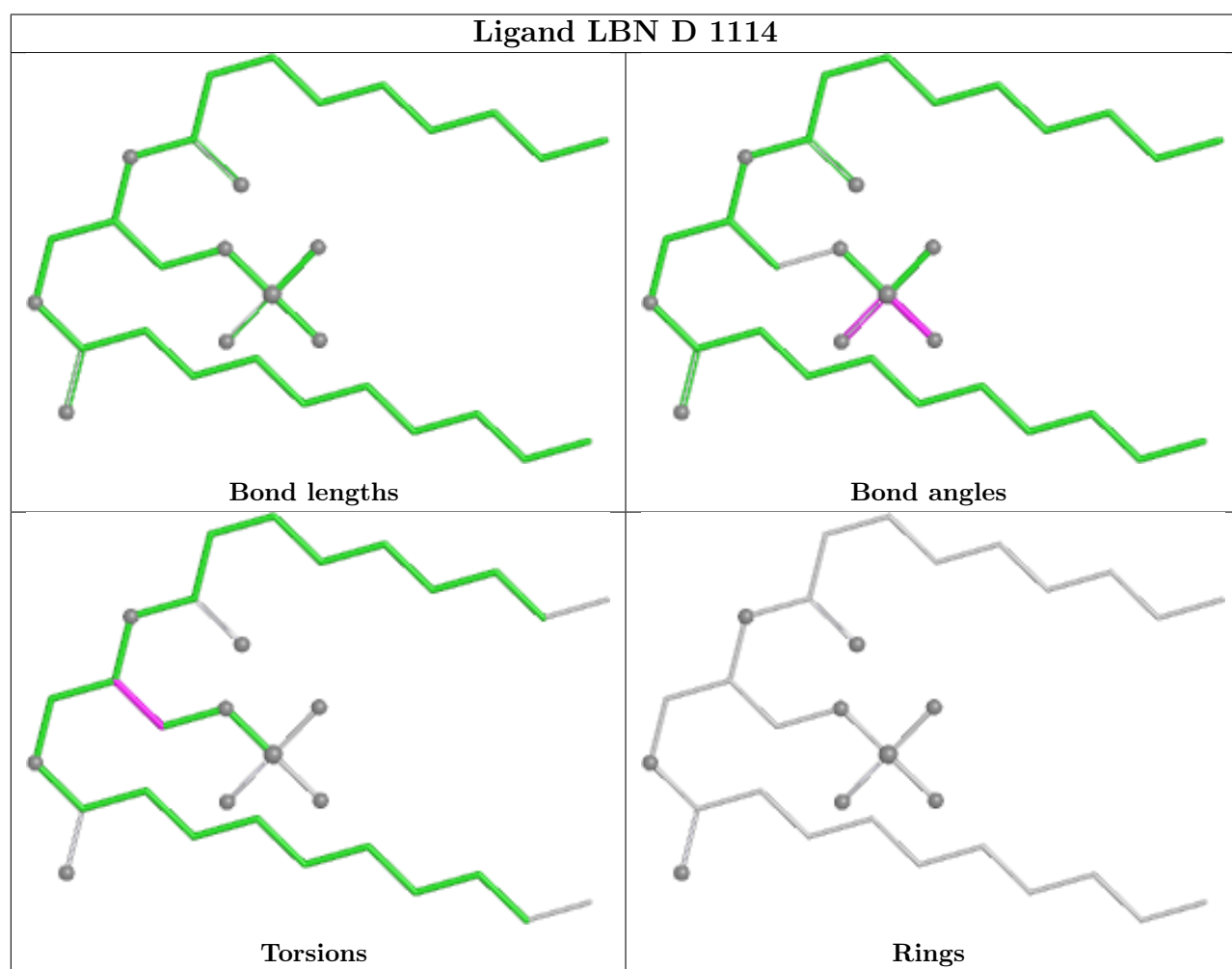
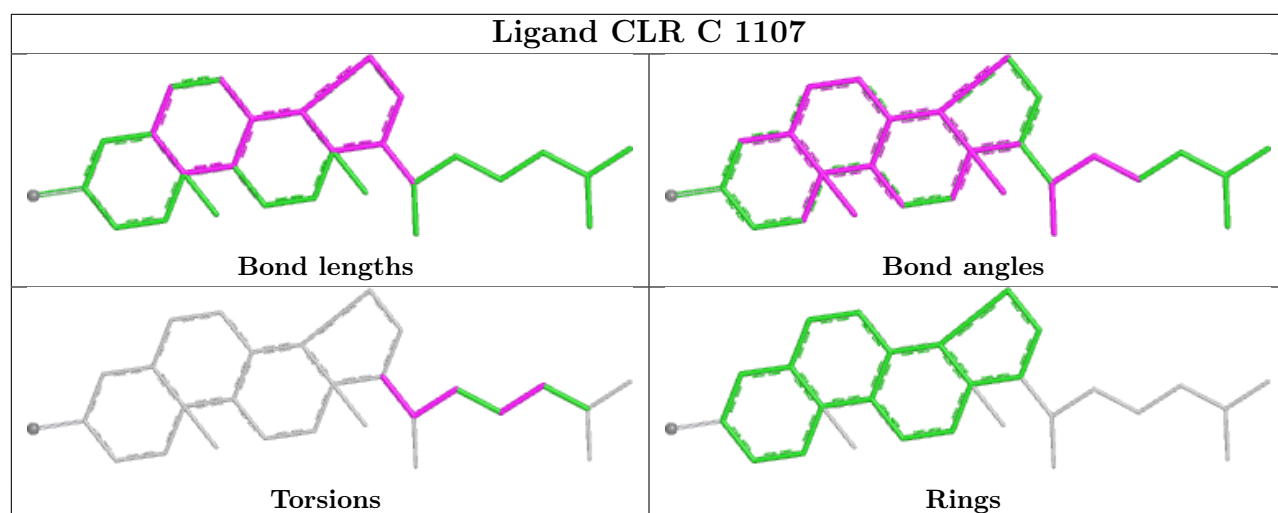


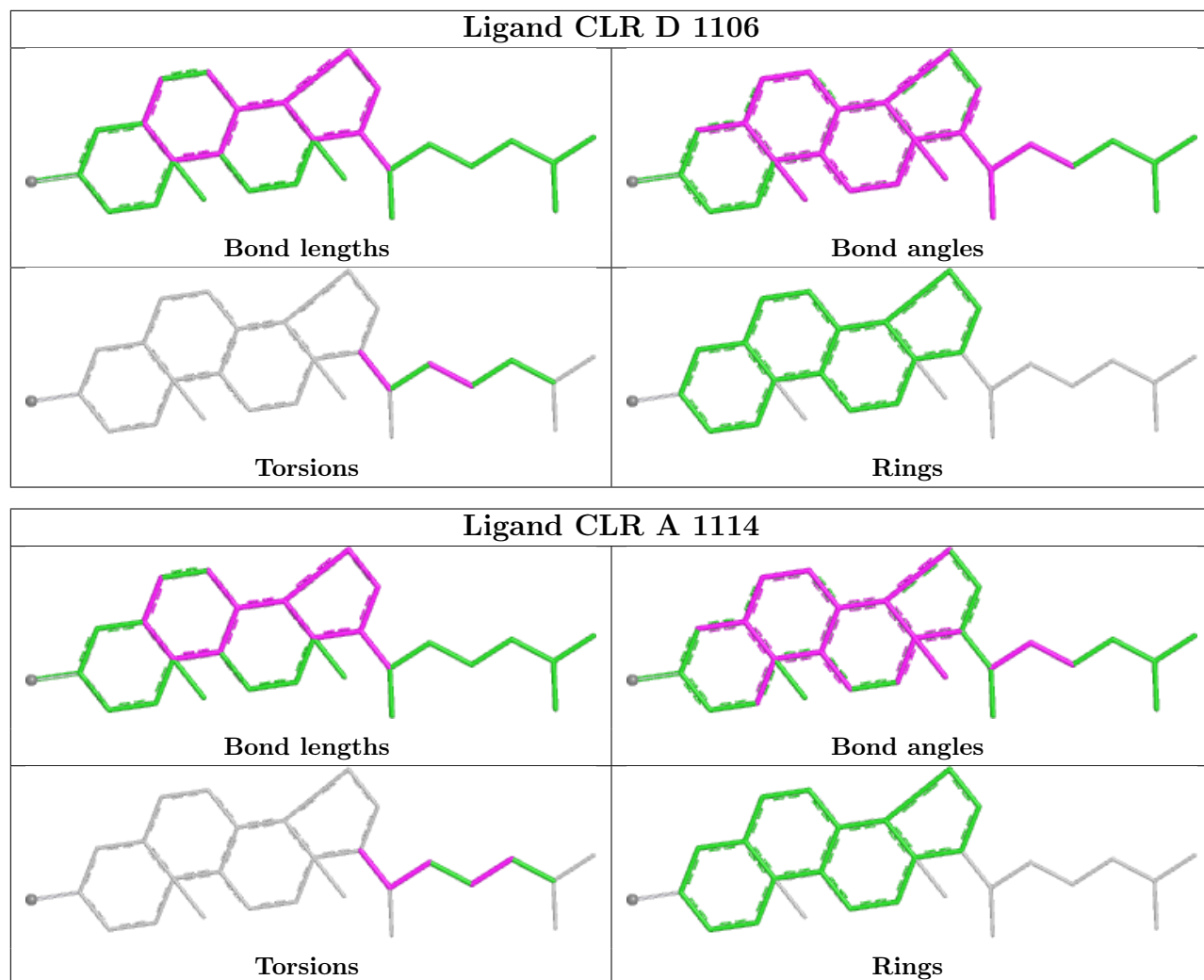


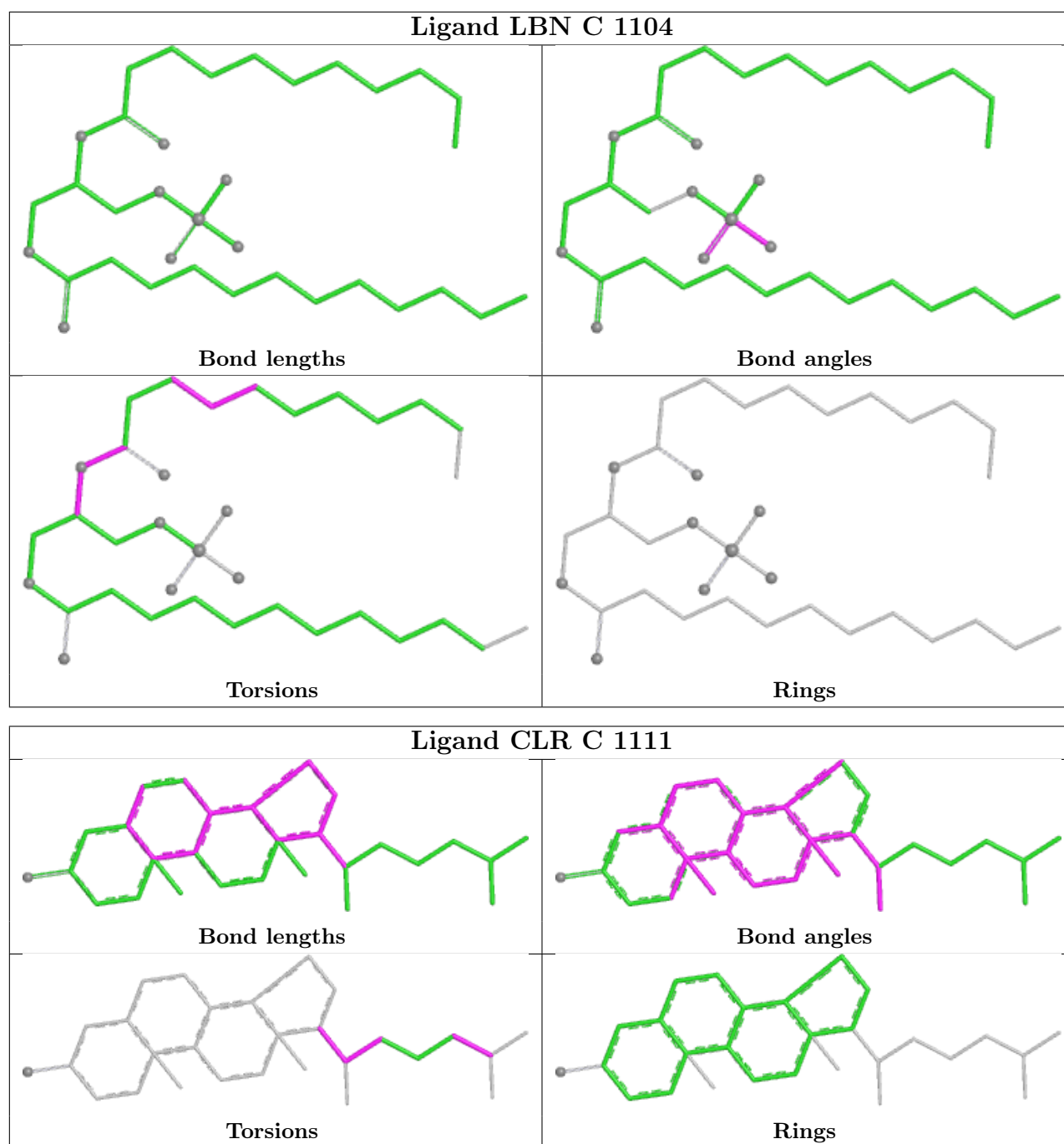












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

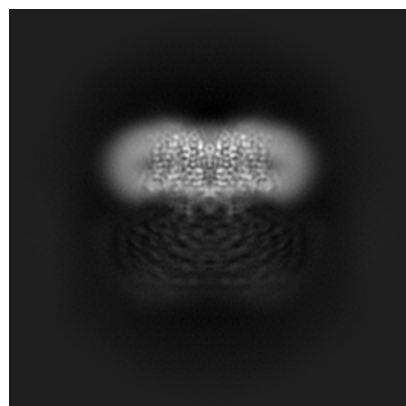
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75630. These allow visual inspection of the internal detail of the map and identification of artifacts.

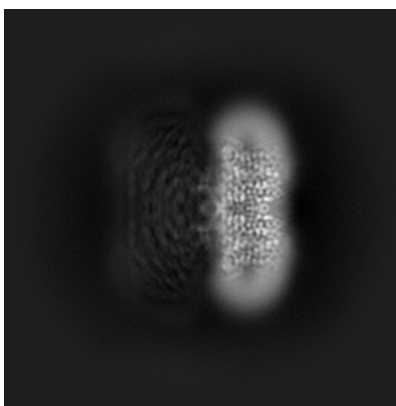
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

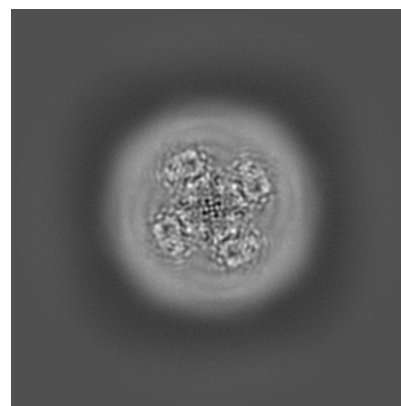
6.1.1 Primary map



X

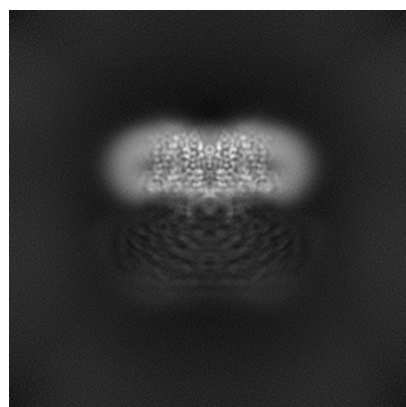


Y

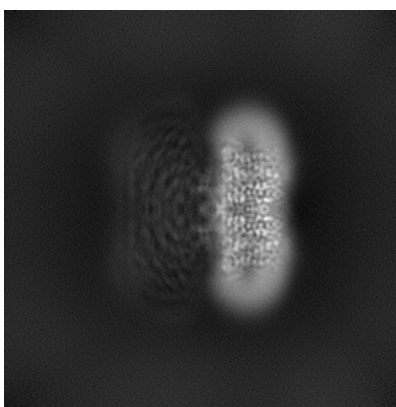


Z

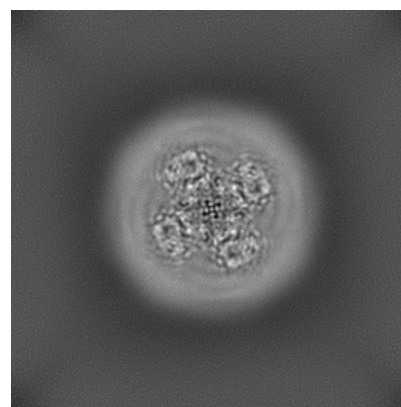
6.1.2 Raw map



X



Y

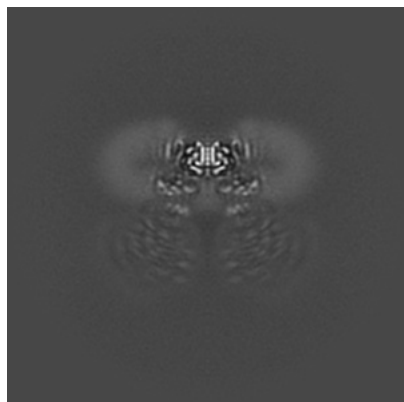


Z

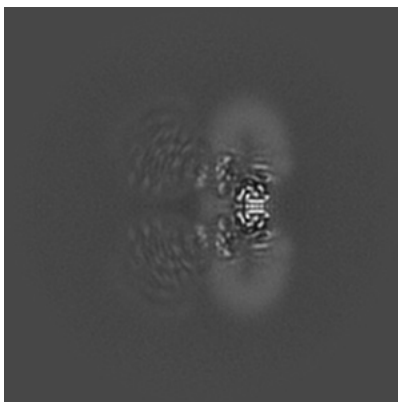
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

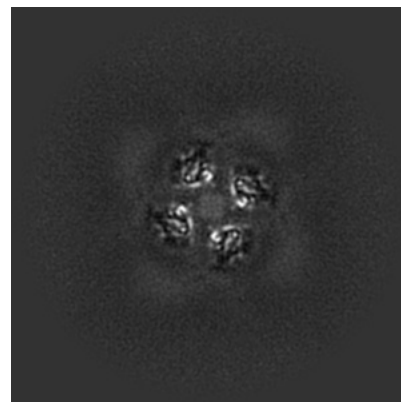
6.2.1 Primary map



X Index: 140

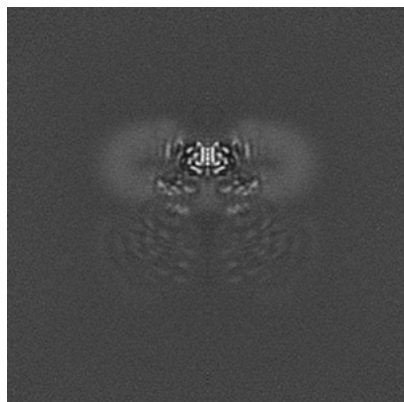


Y Index: 140

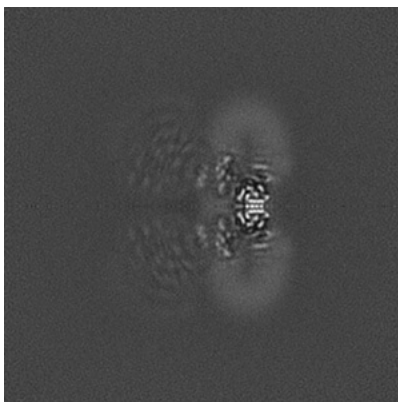


Z Index: 140

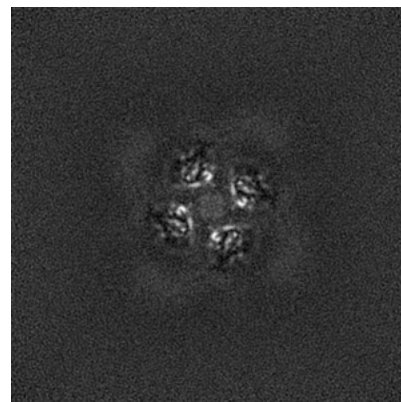
6.2.2 Raw map



X Index: 140



Y Index: 140

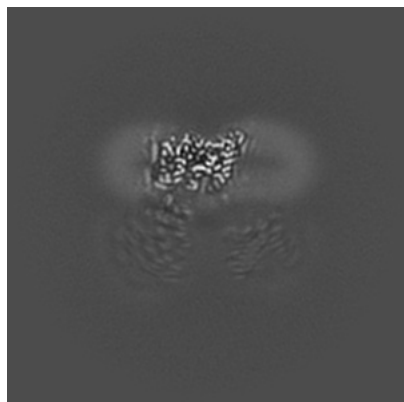


Z Index: 140

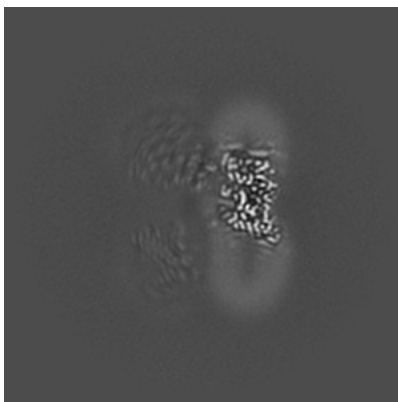
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

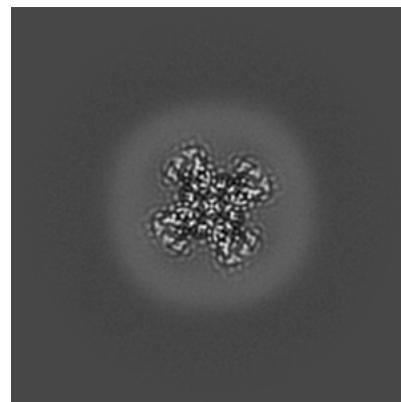
6.3.1 Primary map



X Index: 147

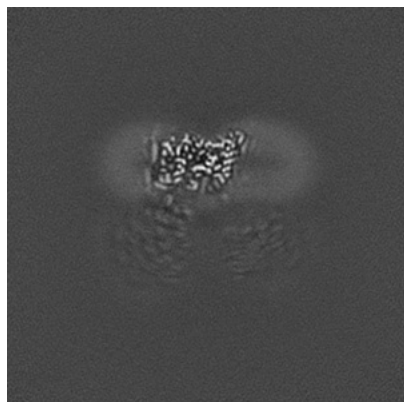


Y Index: 147

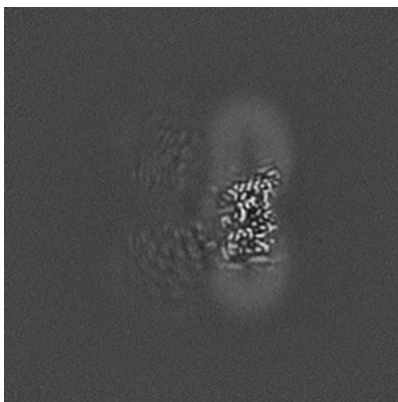


Z Index: 180

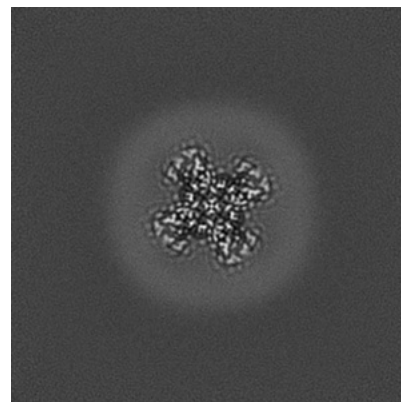
6.3.2 Raw map



X Index: 147



Y Index: 133

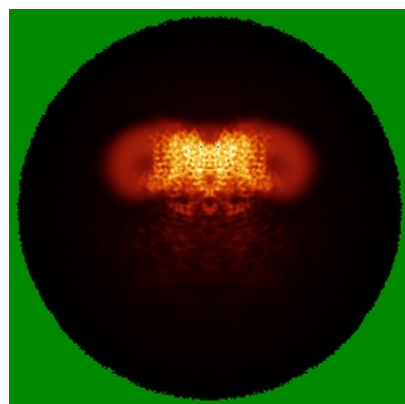


Z Index: 180

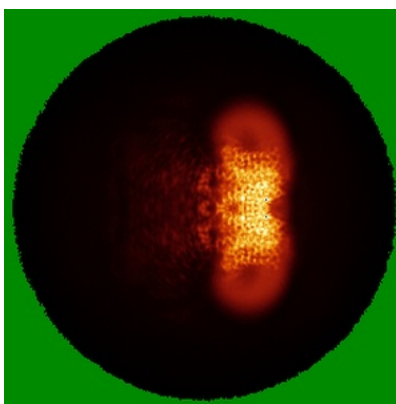
The images above show the largest variance slices of the map in three orthogonal directions.

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

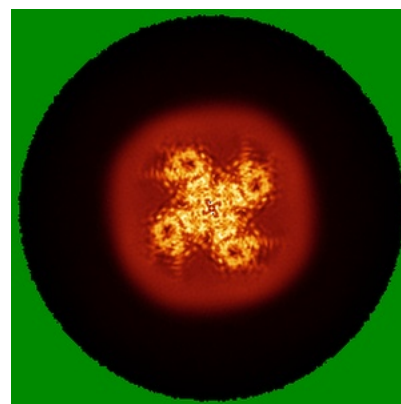
6.4.1 Primary map



X

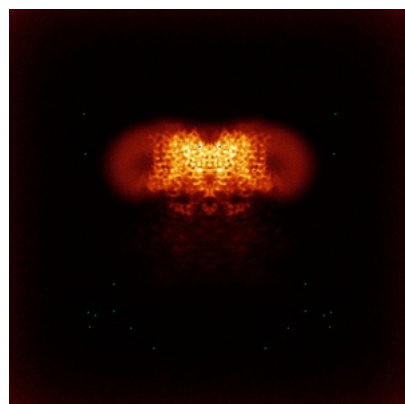


Y

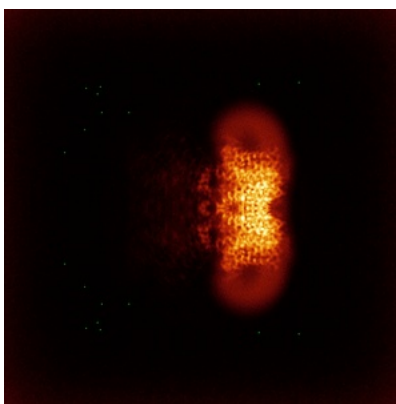


Z

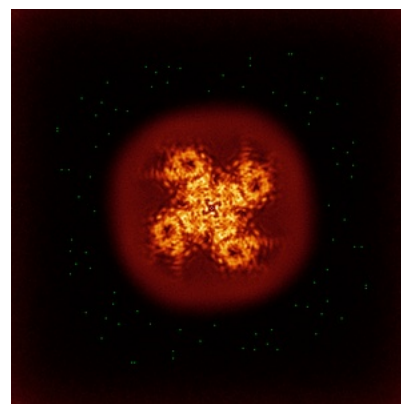
6.4.2 Raw map



X



Y

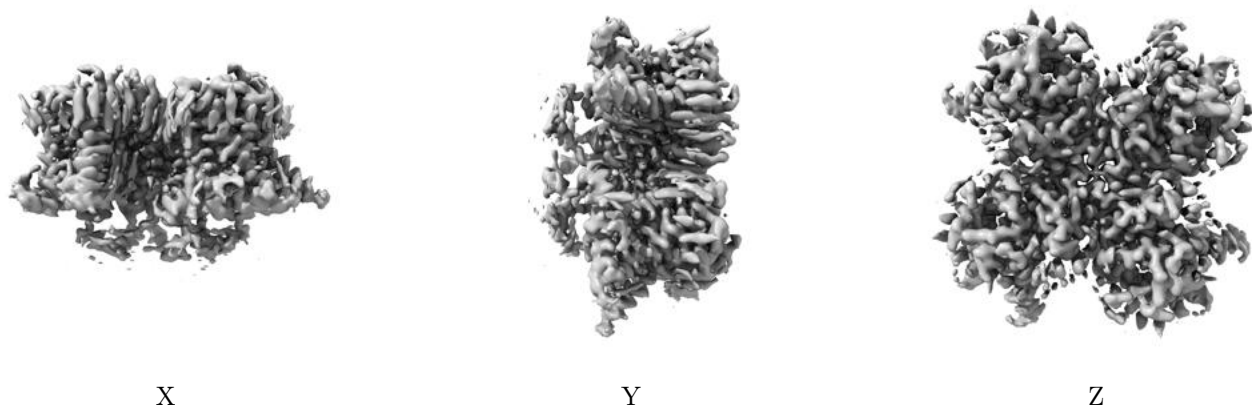


Z

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 0.08. 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.

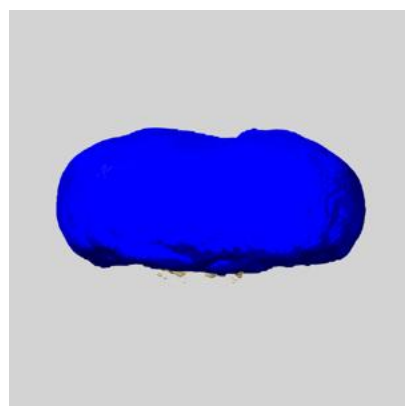
6.6 Mask visualisation [i](#)

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

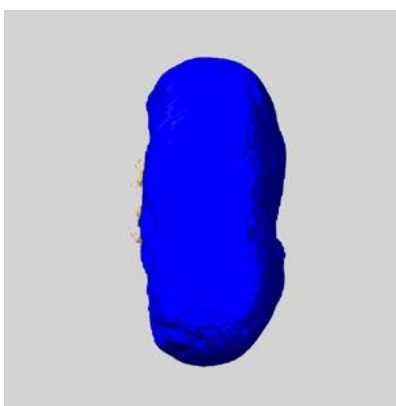
A mask typically either:

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

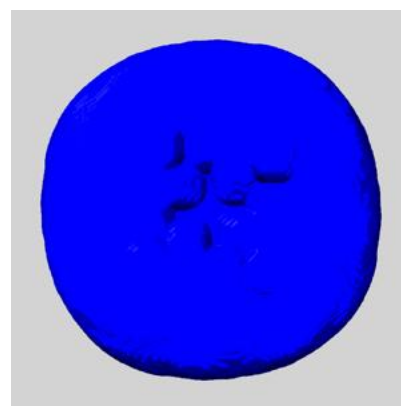
6.6.1 emd_75630_msk_1.map [i](#)



X



Y

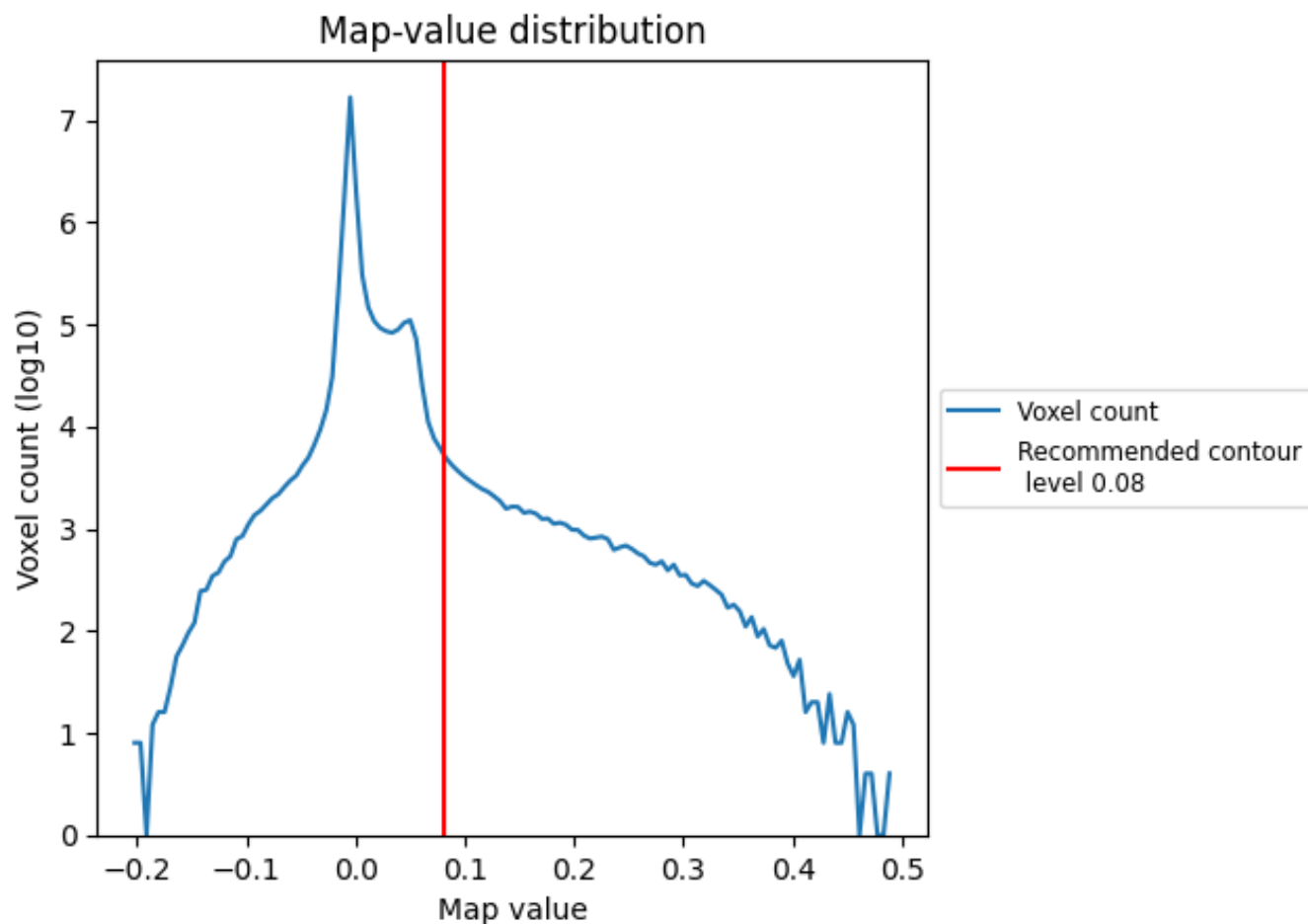


Z

7 Map analysis [i](#)

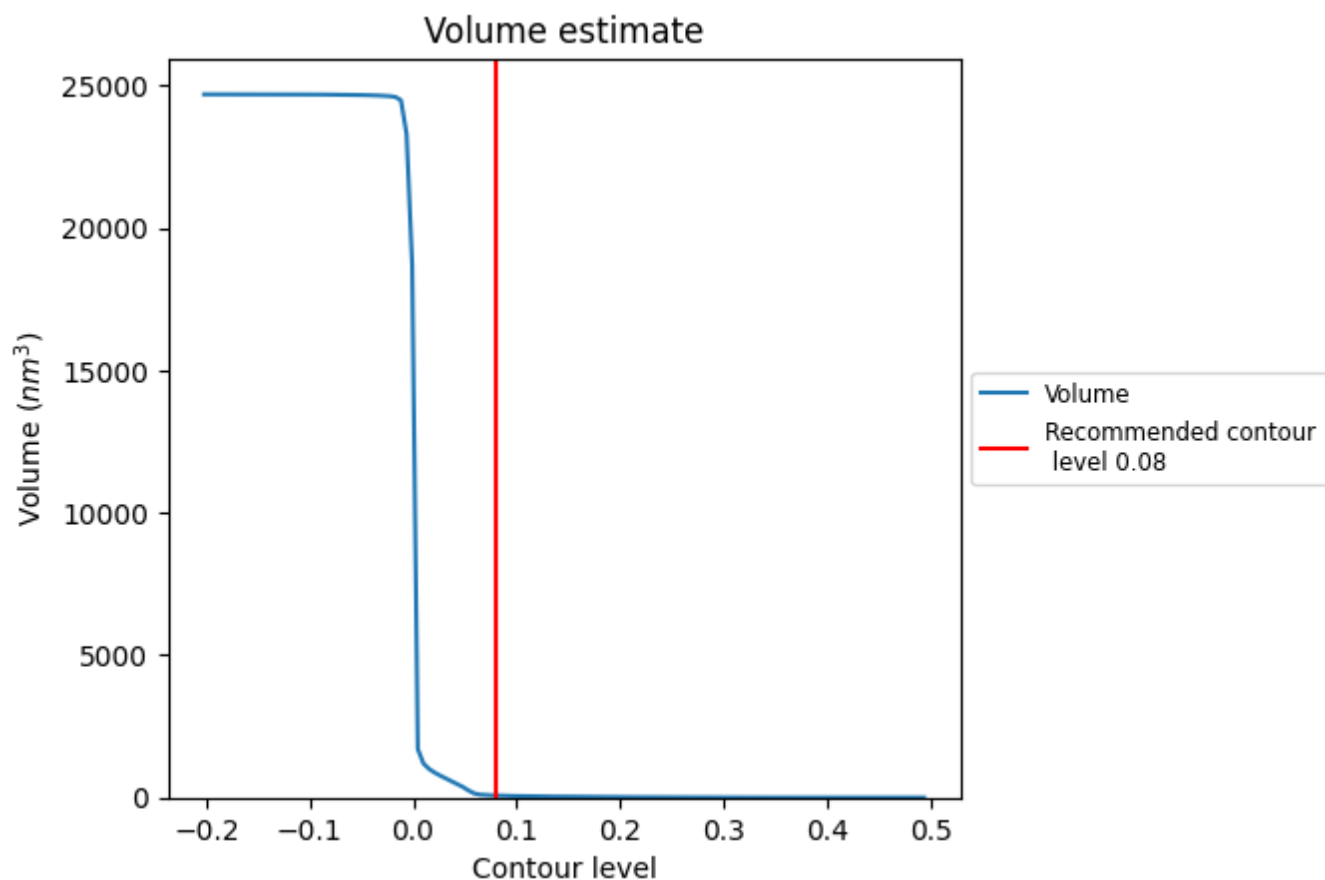
This section contains the results of statistical analysis of the map.

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.

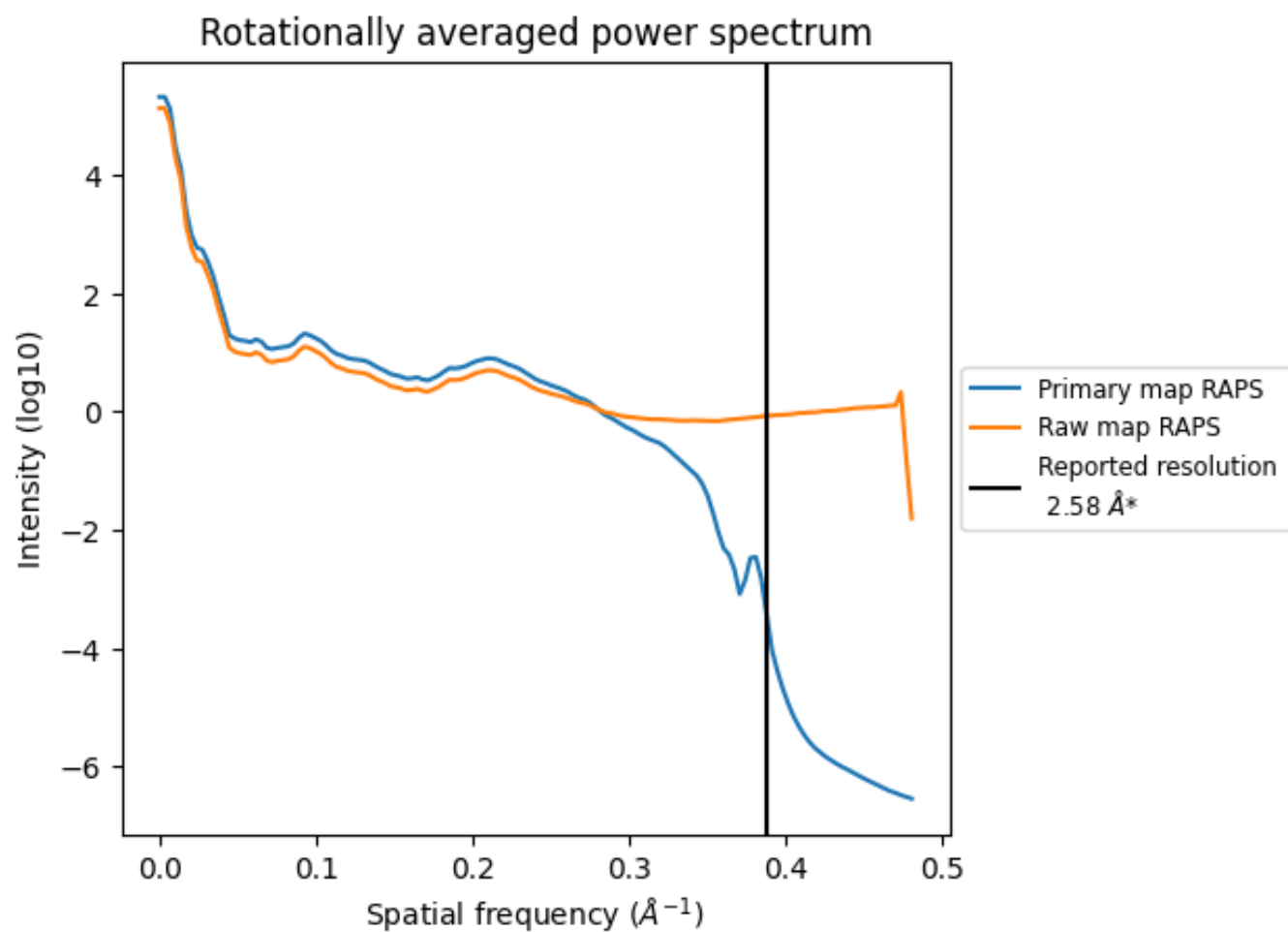
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 72 nm^3 ; this corresponds to an approximate mass of 65 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 ⓘ

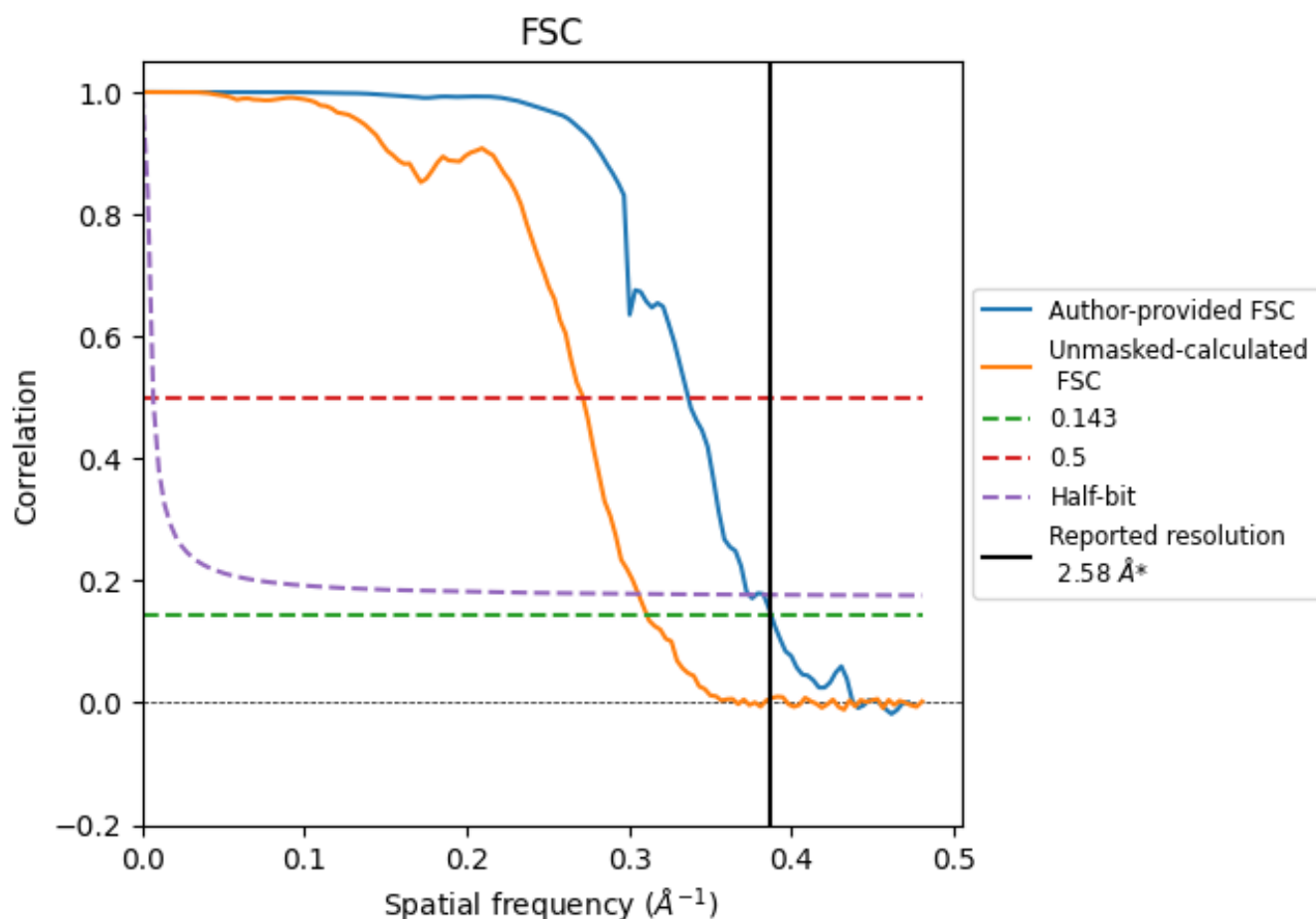


*Reported resolution corresponds to spatial frequency of 0.388 Å⁻¹

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 0.388 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

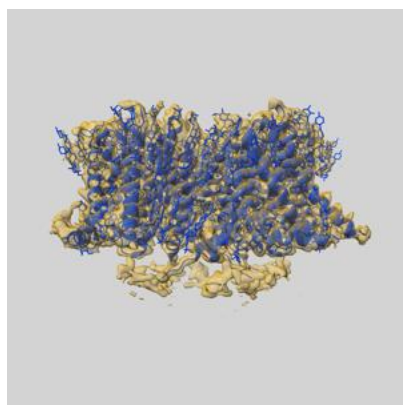
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.58	2.97	2.67
Unmasked-calculated*	3.21	3.68	3.27

*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 3.21 differs from the reported value 2.58 by more than 10 %

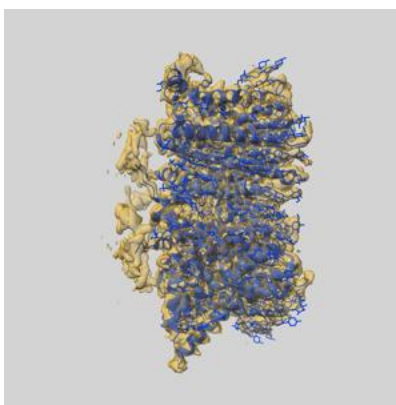
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75630 and PDB model 11DC. Per-residue inclusion information can be found in section [3](#) on page [14](#).

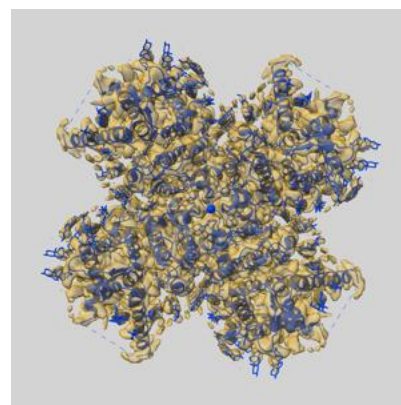
9.1 Map-model overlay [i](#)



X



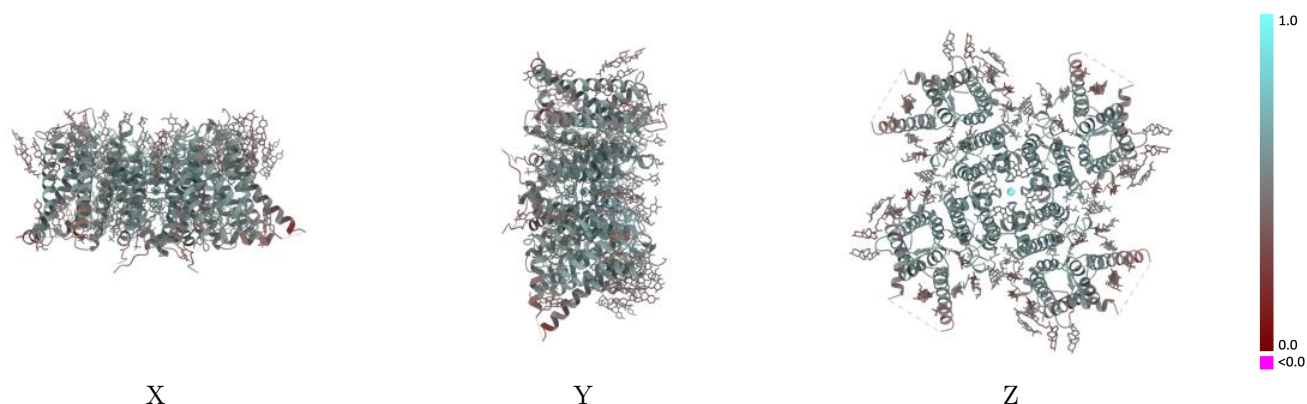
Y



Z

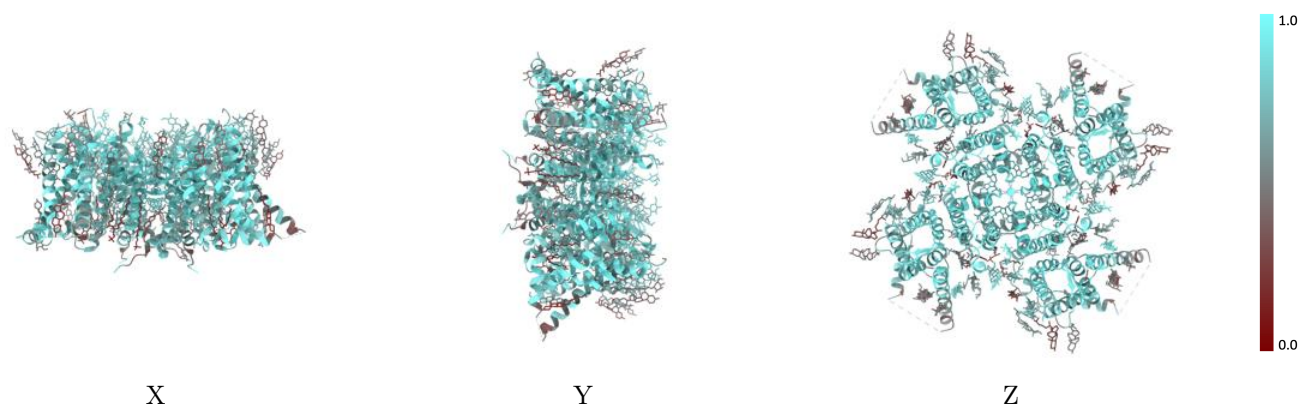
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



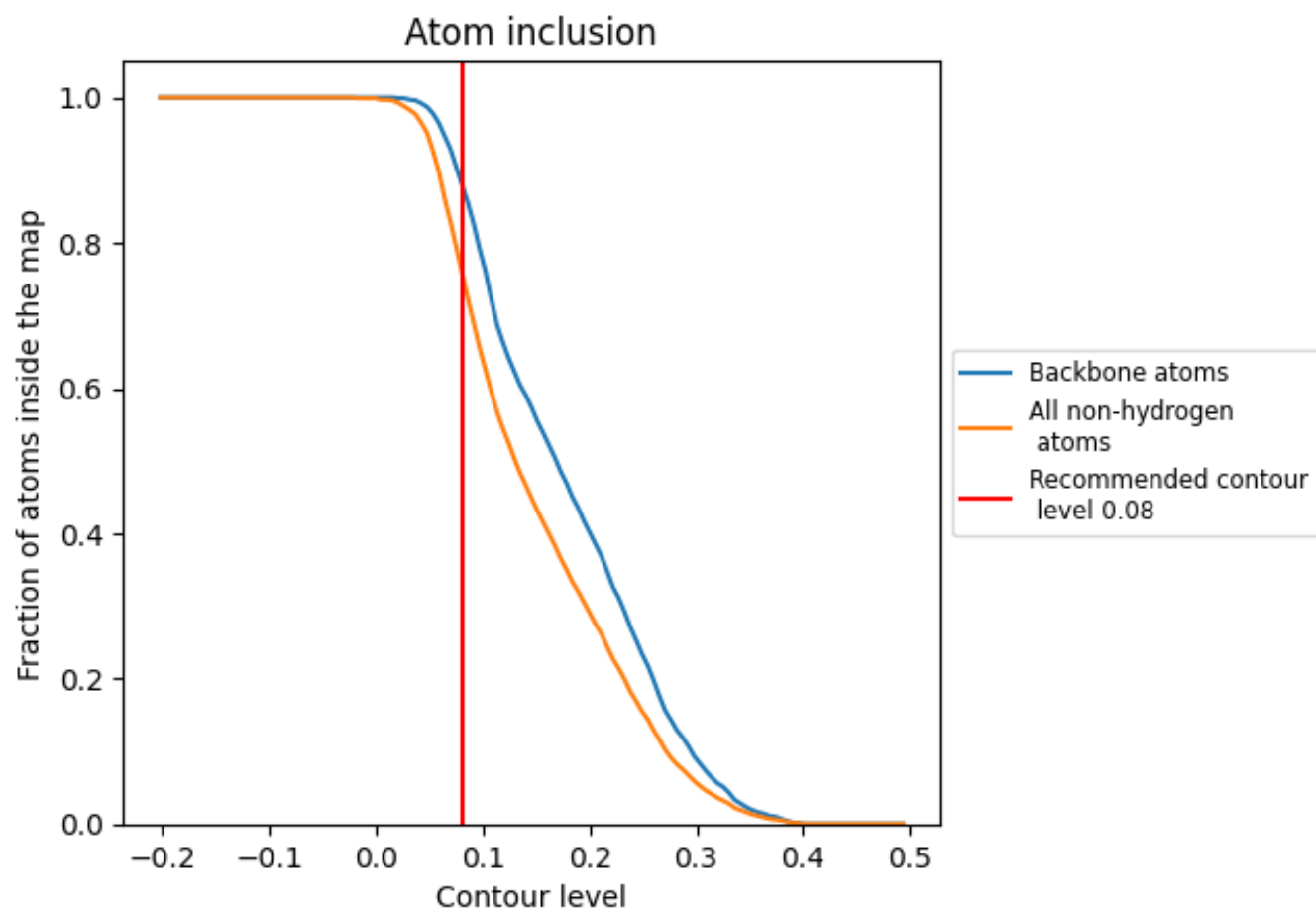
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 76% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7620	0.5180
A	0.7620	0.5200
B	0.7660	0.5190
C	0.7660	0.5190
D	0.7660	0.5170

