



# wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 10:35 AM JST

PDB ID : 7W9L  
EMDB ID : EMD-32369  
Title : Cryo-EM structure of human Nav1.7(E406K)-beta1-beta2 complex  
Authors : Yan, N.; Huang, G.; Liu, D.; Wei, P.; Shen, H.  
Deposited on : 2021-12-10  
Resolution : 3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

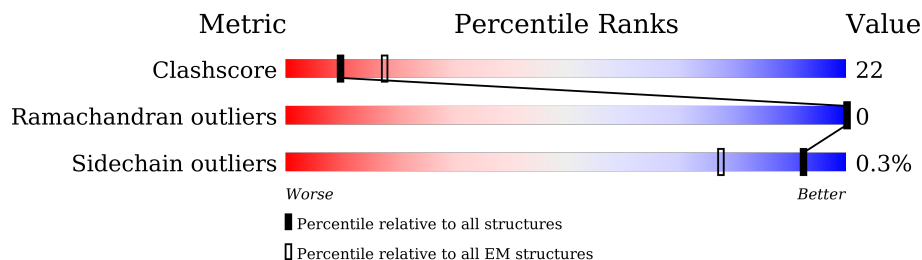
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	2031	
2	B	218	
3	C	215	
4	D	2	
4	E	2	
4	F	2	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
10	PCW	A	2018	-	-	X	-
7	Y01	A	2005	-	-	X	-
8	9Z9	A	2006	-	-	X	-

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 14915 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 Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1420	11445	7554	1802	2004	85	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	expression tag	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858
A	406	LYS	GLU	engineered mutation	UNP Q15858

- Molecule 2 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	173	1416	902	232	272	10	0	0

- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	119	980	615	172	183	10	4	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



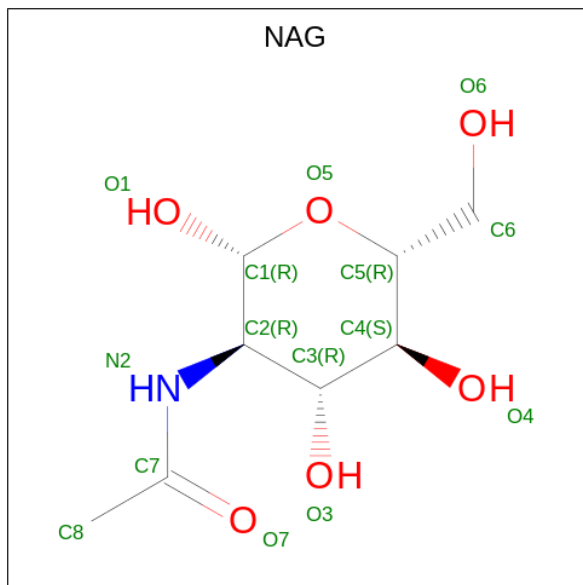
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	E	2	28	16	2	10	0	0

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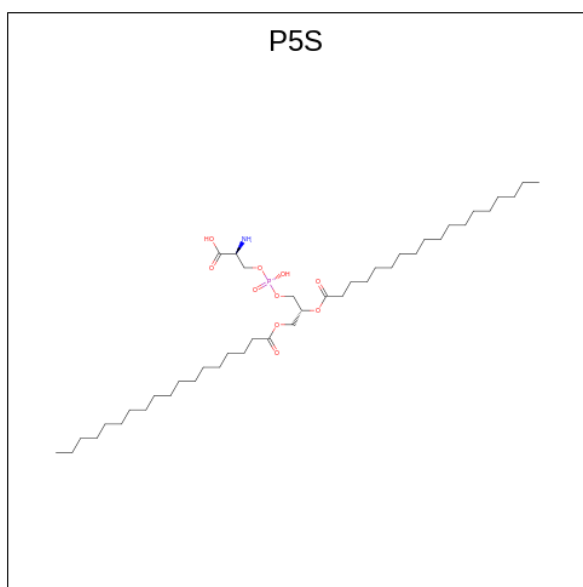
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	F	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



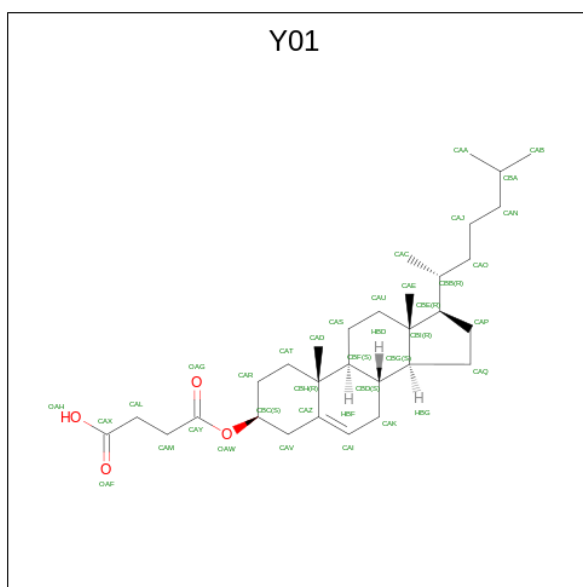
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	28	16	2	10	0
5	A	1	28	16	2	10	0
5	B	1	42	24	3	15	0
5	B	1	42	24	3	15	0
5	B	1	42	24	3	15	0

- Molecule 6 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy} (hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula:  $C_{42}H_{82}NO_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf	
6	A	1	Total	C	N	O	P	0
			110	77	3	27	3	
6	A	1	Total	C	N	O	P	0
			110	77	3	27	3	
6	A	1	Total	C	N	O	P	0
			110	77	3	27	3	

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ).



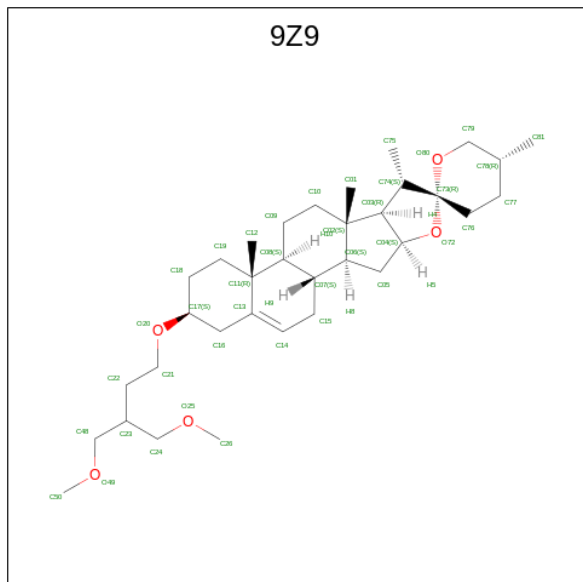
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	
			210	186	24	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	A	1	210	186	24	0
7	A	1	210	186	24	0
7	A	1	210	186	24	0
7	A	1	210	186	24	0
7	A	1	210	186	24	0

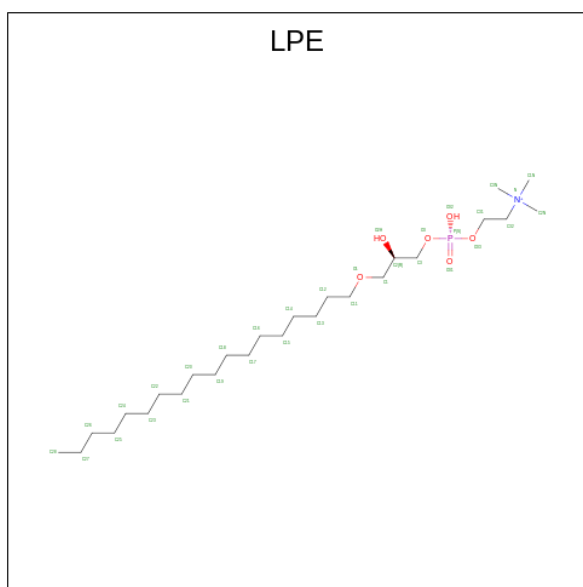
- Molecule 8 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: C<sub>34</sub>H<sub>56</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	A	1	39	34	5	0

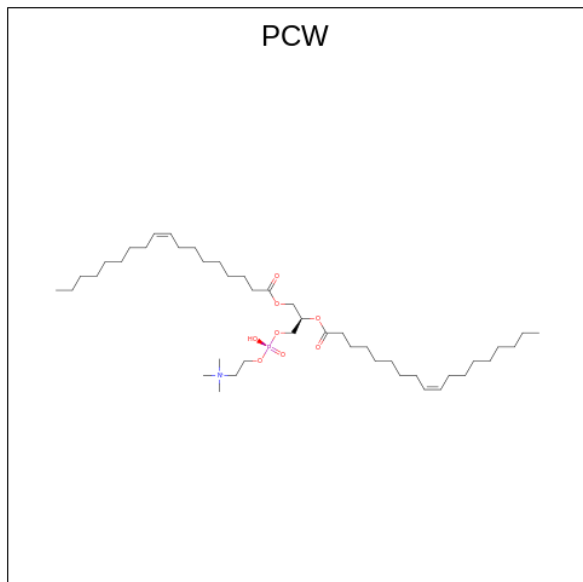
- Molecule 9 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: C<sub>26</sub>H<sub>57</sub>NO<sub>6</sub>P).





Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	A	1	Total 312	208	13	78	13	0
9	A	1	Total 312	208	13	78	13	0
9	A	1	Total 312	208	13	78	13	0
9	A	1	Total 312	208	13	78	13	0
9	A	1	Total 312	208	13	78	13	0
9	A	1	Total 312	208	13	78	13	0
9	A	1	Total 312	208	13	78	13	0
9	A	1	Total 312	208	13	78	13	0
9	A	1	Total 312	208	13	78	13	0
9	A	1	Total 312	208	13	78	13	0
9	A	1	Total 312	208	13	78	13	0
9	A	1	Total 312	208	13	78	13	0
9	B	1	Total 17	9	1	6	1	0

- Molecule 10 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula:  $C_{44}H_{85}NO_8P$ ).

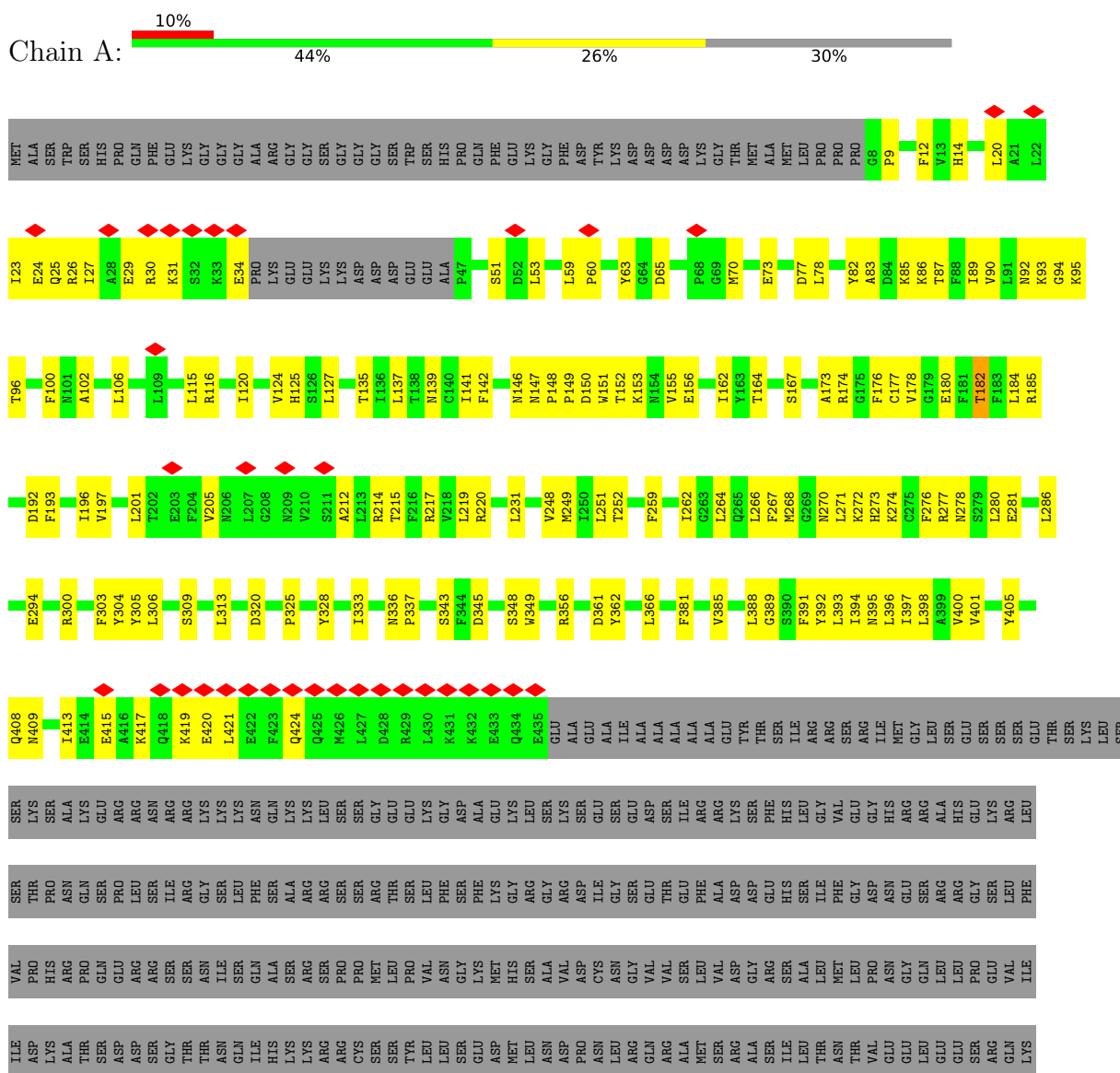


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
10	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
10	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
10	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
10	A	1	Total	C	N	O	P	0
			232	182	5	40	5	

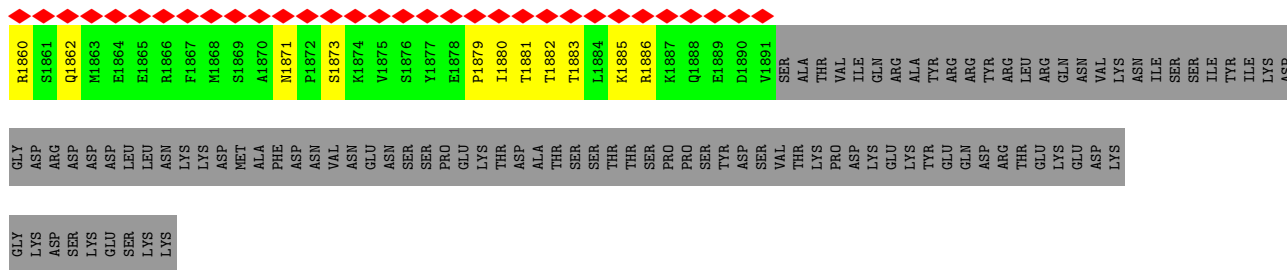
### 3 Residue-property plots i

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

- Molecule 1: Sodium channel protein type 9 subunit alpha

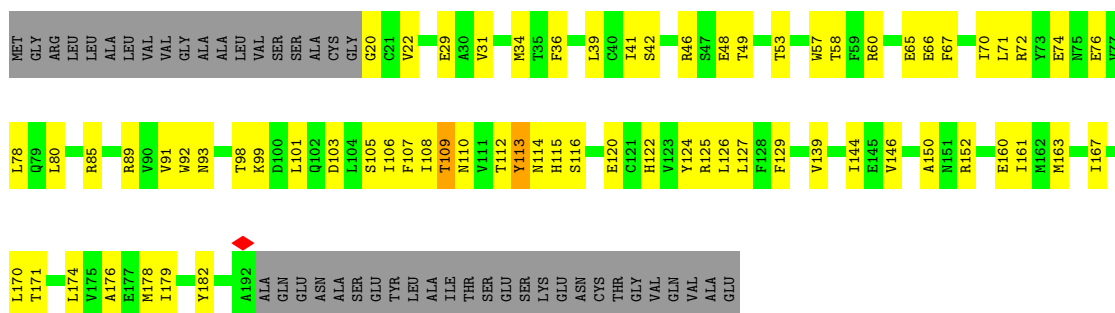


S1800	P1717	I1630	V1530	V1434	F1343	M1258	CYS	H986	H987	Y892	F787	CYS
K1901	H1721	I1631	E1537	V1438	A1344	C1259	GLN	N987	N988	K893	L988	PRO
L1802	P1722	T1632	M1543	V1439	K1346	M1260	ASN	Q989	Q990	E790	TRP	PRO
S1803	M1732	L1633	M1546	F1440	F1347	L1264	ILE	H991	H992	C896	TRP	TRP
D1804	M1735	L1634	V1546	I1441	Y1348	Y1271	GLU	ASN	ASN	V897	TYR	TYR
F1805	G1736	L1635	V1552	I1442	E1349	V1274	SER	PHE	PHE	K998	ARG	ARG
A1806	M1638	L1636	V1552	F1443	C1359	V1274	GLY	LEU	LEU	C903	ALA	ALA
A1807	M1639	S1445	V1552	F1444	I1351	V1274	LYS	TYR	TYR	G995	HIS	HIS
A1808	S1640	G1446	I1557	F1446	R1358	T1277	VAL	GLU	GLU	L905	LYS	LYS
L1809	L1641	F1447	L1557	F1447	M1366	D1282	ARG	ASP	ASP	H909	PHE	PHE
D1810	I1647	T1448	F1558	T1448	R1367	D1282	LEU	ILE	ILE	I919	TRP	TRP
P1811	G1648	L1449	E1561	L1449	R1373	P1285	ASN	ASN	ASN	I999	TRP	TRP
F1812	L1649	V1455	E1561	V1455	L1373	I1286	ARG	GLY	GLY	H1000	ASN	ASN
L1813	L1650	I1456	L1564	I1456	M1374	K1287	SER	PHE	PHE	I1001	ASN	ASN
L1814	L1653	I1457	H1571	I1457	N1375	S1288	SER	GLY	GLY	S820	CYS	CYS
I1815	F1656	D1458	H1571	D1458	V1376	L1289	SER	SER	SER	L924	CYS	CYS
A1816	F1656	M1459	G1577	M1459	Q1378	R1291	SER	VAL	VAL	Y928	ASP	ASP
K1817	I1657	F1460	V1578	F1460	M1379	L1292	CYS	ASP	ASP	D934	ASP	ASP
F1818	A1659	M1461	N1579	M1461	V1380	R1293	THR	LYS	LYS	C935	ASP	ASP
M1819	I1660	Q1470	I1580	Q1470	R1381	A1294	VAL	HIS	HIS	N936	ASP	ASP
K1820	F1661	T1475	F1581	T1475	M1382	L1295	ASP	LEU	LEU	F937	GLY	GLY
V1821	Y1668	G1489	D1582	G1489	K1383	R1296	MET	MET	MET	V938	GLN	GLN
Q1822	E1768	S1490	V1584	S1490	M1384	F1297	GLU	GLU	GLU	V933	VAL	VAL
L1823	E1769	K1491	V1585	K1491	L1385	L1298	ASN	ASN	ASN	L834	GLU	GLU
I1824	S1770	L1492	V1586	L1492	L1386	R1299	PRO	PRO	PRO	G940	ASP	ASP
A1825	T1771	P1493	I1587	P1493	A1300	A1300	PRO	PRO	PRO	Q941	ASP	ASP
M1826	E1772	Q1494	I1587	Q1494	L1301	L1301	GLY	GLY	GLY	I946	GLY	GLY
D1827	P1773	K1495	L1588	K1495	S1302	S1302	GLY	GLY	GLY	M950	GLN	GLN
L1828	L1774	I1496	I1589	I1496	R1303	R1303	GLY	GLY	GLY	V951	SER	SER
P1829	S1775	P1497	E1600	P1497	F1305	F1305	ALA	ALA	ALA	R841	PHE	PHE
M1830	E1776	F1498	T1601	F1498	E1306	E1306	ALA	ALA	ALA	M952	ILE	ILE
I1831	D1777	R1499	T1606	R1499	M1307	M1307	GLU	GLU	GLU	G955	LYS	LYS
S1832	F1778	P1500	P1606	P1500	R1308	R1308	ALA	ALA	ALA	N956	PRO	PRO
C1833	E1780	G1501	T1607	G1501	V1309	V1309	GLU	GLU	GLU	F963	LEU	LEU
D1834	M1781	M1502	R1610	M1502	M1312	M1312	PRO	PRO	PRO	L964	LEU	LEU
I1835	F1782	K1503	V1611	K1503	I1321	I1321	VAL	VAL	VAL	L965	THR	THR
I1836	Y1783	I1504	V1612	I1504	V1324	V1324	ASP	ASP	ASP	L968	THR	THR
C1838	E1784	Q1505	R1613	Q1505	L1325	L1325	GLU	GLU	GLU	S969	ARG	ARG
L1839	V1785	I1508	R1614	I1508	L1326	L1326	PRO	PRO	PRO	S972	ILE	ILE
D1840	W1786	F1509	R1616	F1509	V1327	V1327	ALA	ALA	ALA	S973	ALA	ALA
I1841	W1786	V1512	R1617	V1512	C1328	C1328	ALA	ALA	ALA	D974	GLY	GLY
L1842	K1788	V1517	G1618	V1517	L1329	L1329	PHE	PHE	PHE	N975	GLU	GLU
F1843	F1789	F1517	I1619	F1517	I1330	I1330	THR	THR	THR	L976	SER	SER
A1844	D1790	M1709	L1620	M1709	L1333	L1333	ASP	ASP	ASP	T977	ASP	ASP
F1845	P1791	L1708	L1621	L1708	I1334	I1334	GLY	GLY	GLY	A978	LYS	LYS
T1846	D1792	P1712	L1623	P1712	I1337	I1337	VAL	VAL	VAL	I979	ASN	ASN
K1847	A1793	C1526	L1624	C1526	V1340	V1340	TRP	TRP	TRP	E980	GLN	GLN
R1848	T1794	L1527	V1624	L1527	M1433	M1433	ARG	ARG	ARG	E981	ASN	ASN
V1849	Q1795				Y1263	Y1263	TRP	TRP	TRP	F878	GLY	GLY
L1850	F1796				F1254	F1254	ARG	ARG	ARG	I979	ASN	ASN
G1851	I1797				L1255	L1255	PHE	PHE	PHE	F880	ILE	ILE
E1852	E1798				M1256	M1256	SER	SER	SER	E981	GLY	GLY
G1854	F1799				L1342	L1342	GLU	GLU	GLU	F883	ALA	ALA
E1855							CYS	CYS	CYS	T784	GLY	GLY
M1856							GLU	GLU	GLU	I786	ALA	ALA
D1857							LEU	LEU	LEU			
S1858							ALA	ALA	ALA			
L1859							GLU	GLU	GLU			



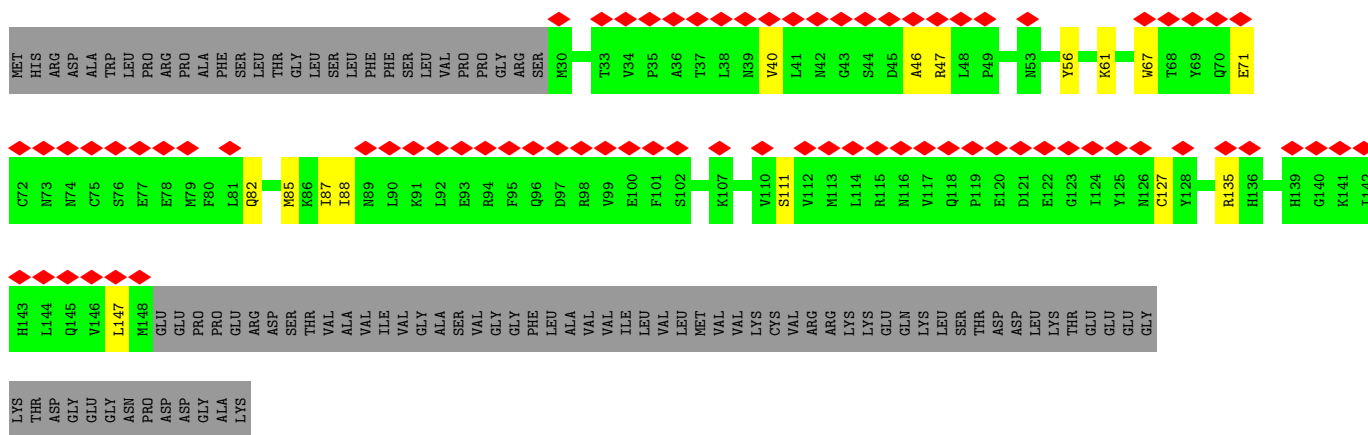
- Molecule 2: Sodium channel subunit beta-1

Chain B: 48% 31% 21%



- Molecule 3: Sodium channel subunit beta-2

Chain C: 36% 48% 7% 45%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1  
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1197096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.345	Depositor
Minimum map value	-3.549	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.116	Depositor
Recommended contour level	0.43	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: NAG, LPE, 9Z9, PCW, P5S, Y01

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	0.48	0/11719	0.52	0/15869
2	B	0.53	0/1442	0.55	0/1949
3	C	0.36	0/1011	0.59	0/1367
All	All	0.48	0/14172	0.53	0/19185

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1712	PRO	Peptide

### 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	11445	0	11662	539	0
2	B	1416	0	1379	78	0
3	C	980	0	935	17	0
4	D	28	0	25	1	0
4	E	28	0	25	5	0
4	F	28	0	25	6	0
5	A	28	0	26	0	0
5	B	42	0	39	6	0
6	A	110	0	130	24	0
7	A	210	0	294	74	0
8	A	39	0	0	33	0
9	A	312	0	426	58	0
9	B	17	0	19	9	0
10	A	232	0	323	50	0
All	All	14915	0	15308	666	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 22.

The worst 5 of 666 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)
2:B:178:MET:CE	9:B:304:LPE:H12	1.51	1.41
1:A:1330:ILE:CD1	7:A:2005:Y01:HAB2	1.60	1.32
1:A:1653:LEU:HB3	9:A:2014:LPE:C16	1.60	1.29
1:A:398:LEU:HD23	8:A:2006:9Z9:C75	1.61	1.28
1:A:212:ALA:HB1	7:A:2007:Y01:OAG	1.31	1.27

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	1412/2031 (70%)	1300 (92%)	112 (8%)	0	100	100
2	B	171/218 (78%)	153 (90%)	18 (10%)	0	100	100
3	C	120/215 (56%)	116 (97%)	4 (3%)	0	100	100
All	All	1703/2464 (69%)	1569 (92%)	134 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1268/1809 (70%)	1267 (100%)	1 (0%)	93	98
2	B	157/190 (83%)	155 (99%)	2 (1%)	69	86
3	C	114/193 (59%)	112 (98%)	2 (2%)	59	81
All	All	1539/2192 (70%)	1534 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	THR
2	B	109	THR
2	B	113	TYR
3	C	71	GLU
3	C	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	115	HIS
3	C	70	GLN
3	C	118	GLN
3	C	82	GLN
1	A	780	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	1	1,4	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	D	2	4	14,14,15	0.30	0	17,19,21	0.71	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.31	0	17,19,21	0.89	1 (5%)
4	NAG	E	2	4	14,14,15	0.27	0	17,19,21	0.90	1 (5%)
4	NAG	F	1	2,4	14,14,15	0.57	0	17,19,21	1.19	2 (11%)
4	NAG	F	2	4	14,14,15	0.66	0	17,19,21	1.19	1 (5%)

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
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C4-C3-C2	-2.91	106.75	111.02
4	E	2	NAG	C4-C3-C2	-2.83	106.87	111.02
4	F	1	NAG	C1-O5-C5	2.73	115.89	112.19
4	F	1	NAG	C3-C4-C5	-2.63	105.55	110.24
4	F	2	NAG	C4-C3-C2	-2.40	107.50	111.02

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

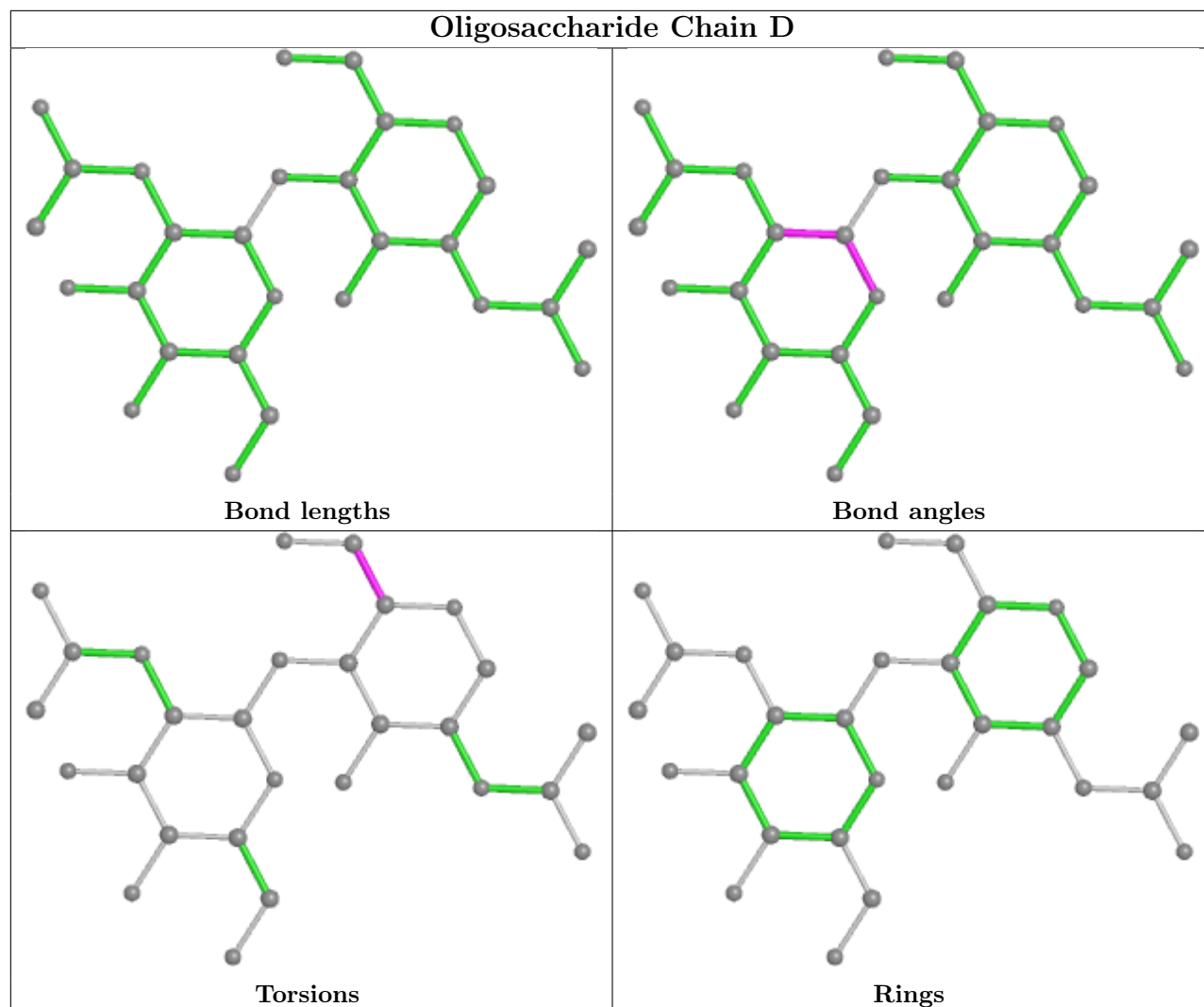
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	F	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6

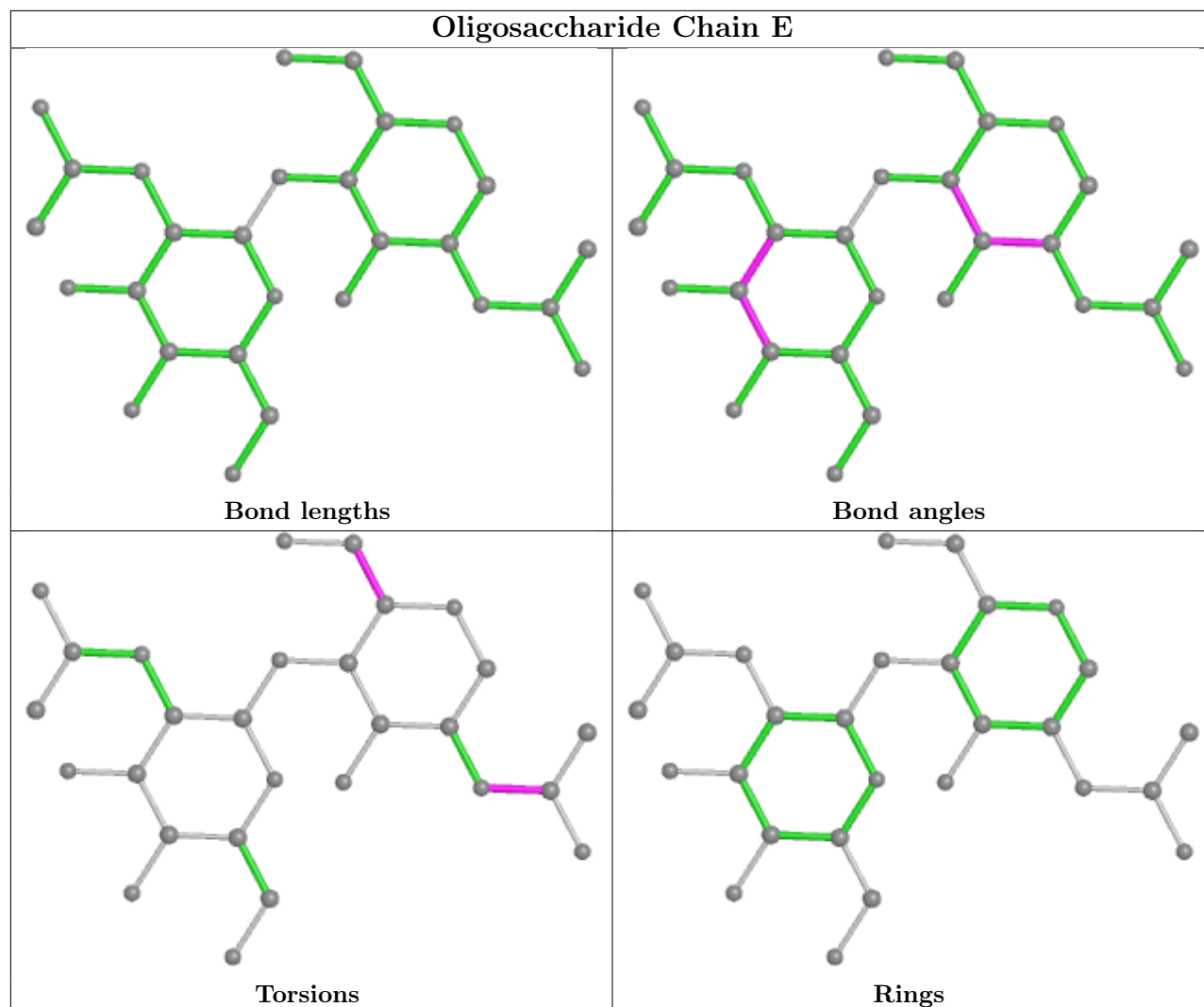
There are no ring outliers.

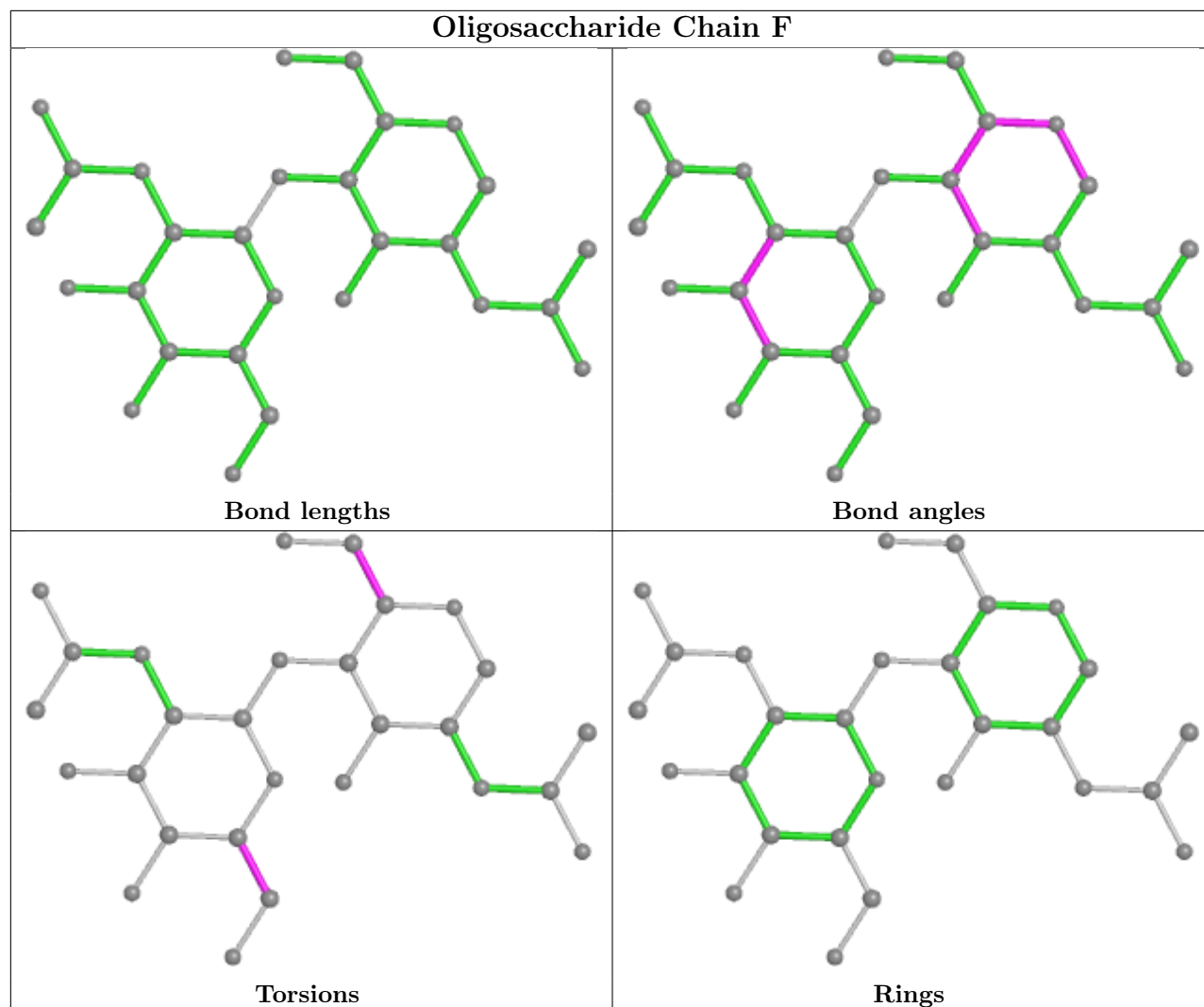
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	5	0
4	F	2	NAG	4	0
4	F	1	NAG	2	0
4	D	1	NAG	1	0
4	E	2	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







## 5.6 Ligand geometry [i](#)

34 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
8	9Z9	A	2006	-	44,44,44	0.70	1 (2%)	66,68,68	1.45	12 (18%)
5	NAG	A	2008	1	14,14,15	0.29	0	17,19,21	1.04	1 (5%)
6	P5S	A	2017	-	40,40,53	1.13	3 (7%)	43,45,60	1.37	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	303	2	14,14,15	0.27	0	17,19,21	0.43	0
6	P5S	A	2029	-	32,33,53	1.16	4 (12%)	36,40,60	1.04	3 (8%)
7	Y01	A	2007	-	38,38,38	0.67	1 (2%)	57,57,57	1.79	11 (19%)
9	LPE	A	2026	-	16,16,33	0.69	0	20,22,39	0.67	0
10	PCW	A	2018	-	43,43,53	1.01	2 (4%)	49,51,61	1.12	5 (10%)
7	Y01	A	2003	-	38,38,38	0.66	1 (2%)	57,57,57	1.78	12 (21%)
9	LPE	A	2015	-	27,27,33	0.54	0	31,33,39	0.60	0
9	LPE	A	2019	-	24,24,33	0.57	0	28,30,39	0.67	0
10	PCW	A	2013	-	52,52,53	0.93	2 (3%)	58,60,61	1.03	3 (5%)
9	LPE	A	2021	-	24,24,33	0.60	0	28,30,39	0.87	0
9	LPE	A	2011	-	24,24,33	0.33	0	25,27,39	0.60	0
5	NAG	B	301	2	14,14,15	0.65	0	17,19,21	0.99	0
7	Y01	A	2004	-	38,38,38	0.65	1 (2%)	57,57,57	1.78	11 (19%)
9	LPE	A	2012	-	19,19,33	0.62	0	23,25,39	0.51	0
10	PCW	A	2016	-	46,46,53	0.99	3 (6%)	52,54,61	1.18	4 (7%)
10	PCW	A	2028	-	43,43,53	0.99	2 (4%)	49,51,61	2.91	7 (14%)
5	NAG	A	2001	1	14,14,15	0.35	0	17,19,21	0.44	0
9	LPE	A	2020	-	24,24,33	0.85	0	28,30,39	0.92	1 (3%)
9	LPE	A	2025	-	24,24,33	0.54	0	28,30,39	0.50	0
9	LPE	A	2023	-	24,24,33	0.53	0	28,30,39	0.54	0
7	Y01	A	2005	-	38,38,38	1.16	4 (10%)	57,57,57	1.74	11 (19%)
9	LPE	A	2024	-	24,24,33	0.51	0	28,30,39	0.62	0
9	LPE	A	2014	-	21,21,33	0.67	0	25,27,39	1.03	2 (8%)
7	Y01	A	2030	-	38,38,38	1.62	7 (18%)	57,57,57	1.63	10 (17%)
9	LPE	A	2022	-	24,24,33	0.53	0	28,30,39	0.64	0
6	P5S	A	2002	-	33,34,53	0.86	1 (3%)	36,40,60	1.66	5 (13%)
7	Y01	A	2009	-	38,38,38	1.15	4 (10%)	57,57,57	1.74	12 (21%)
5	NAG	B	302	2	14,14,15	0.37	0	17,19,21	0.96	1 (5%)
9	LPE	B	304	-	16,16,33	0.66	0	20,22,39	0.60	0
10	PCW	A	2027	-	43,43,53	1.03	2 (4%)	49,51,61	0.94	2 (4%)
9	LPE	A	2010	-	24,24,33	0.51	0	28,30,39	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	9Z9	A	2006	-	-	0/12/100/100	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
6	P5S	A	2017	-	-	8/44/44/59	-
5	NAG	B	303	2	-	0/6/23/26	0/1/1/1
6	P5S	A	2029	-	-	16/39/39/59	-
7	Y01	A	2007	-	-	0/19/77/77	0/4/4/4
9	LPE	A	2026	-	-	7/17/17/34	-
10	PCW	A	2018	-	-	12/47/47/57	-
7	Y01	A	2003	-	-	0/19/77/77	0/4/4/4
9	LPE	A	2015	-	-	10/28/28/34	-
9	LPE	A	2019	-	-	5/25/25/34	-
10	PCW	A	2013	-	-	10/56/56/57	-
9	LPE	A	2021	-	-	3/25/25/34	-
9	LPE	A	2011	-	-	8/25/25/34	-
5	NAG	B	301	2	-	0/6/23/26	0/1/1/1
7	Y01	A	2004	-	-	0/19/77/77	0/4/4/4
9	LPE	A	2012	-	-	10/20/20/34	-
10	PCW	A	2016	-	-	13/50/50/57	-
10	PCW	A	2028	-	-	10/47/47/57	-
5	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
9	LPE	A	2020	-	-	12/25/25/34	-
9	LPE	A	2025	-	-	10/25/25/34	-
9	LPE	A	2023	-	-	8/25/25/34	-
7	Y01	A	2005	-	-	4/19/77/77	0/4/4/4
9	LPE	A	2024	-	-	6/25/25/34	-
9	LPE	A	2014	-	-	15/22/22/34	-
7	Y01	A	2030	-	-	7/19/77/77	0/4/4/4
9	LPE	A	2022	-	-	3/25/25/34	-
6	P5S	A	2002	-	-	7/39/39/59	-
7	Y01	A	2009	-	-	4/19/77/77	0/4/4/4
5	NAG	B	302	2	-	2/6/23/26	0/1/1/1
9	LPE	B	304	-	-	9/17/17/34	-
10	PCW	A	2027	-	-	16/47/47/57	-
9	LPE	A	2010	-	-	10/25/25/34	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2017	P5S	O37-C38	4.40	1.46	1.34
10	A	2027	PCW	O3-C11	4.39	1.46	1.33
7	A	2030	Y01	CBB-CBE	-4.36	1.46	1.54
6	A	2002	P5S	O37-C38	4.27	1.46	1.34
10	A	2028	PCW	O3-C11	4.25	1.45	1.33

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2028	PCW	C8-N-C6	-12.05	77.99	108.97
10	A	2028	PCW	C8-N-C7	-12.04	78.02	108.97
10	A	2028	PCW	C8-N-C5	-7.82	77.94	109.92
6	A	2002	P5S	O37-C38-C39	6.69	125.92	111.50
7	A	2009	Y01	CBI-CBE-CBB	-5.95	110.16	119.49

There are no chirality outliers.

5 of 229 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	302	NAG	C8-C7-N2-C2
5	B	302	NAG	O7-C7-N2-C2
6	A	2002	P5S	N-CA-CB-OG
6	A	2002	P5S	C39-C38-O37-C2
6	A	2002	P5S	O47-C38-O37-C2

There are no ring outliers.

29 monomers are involved in 247 short contacts:

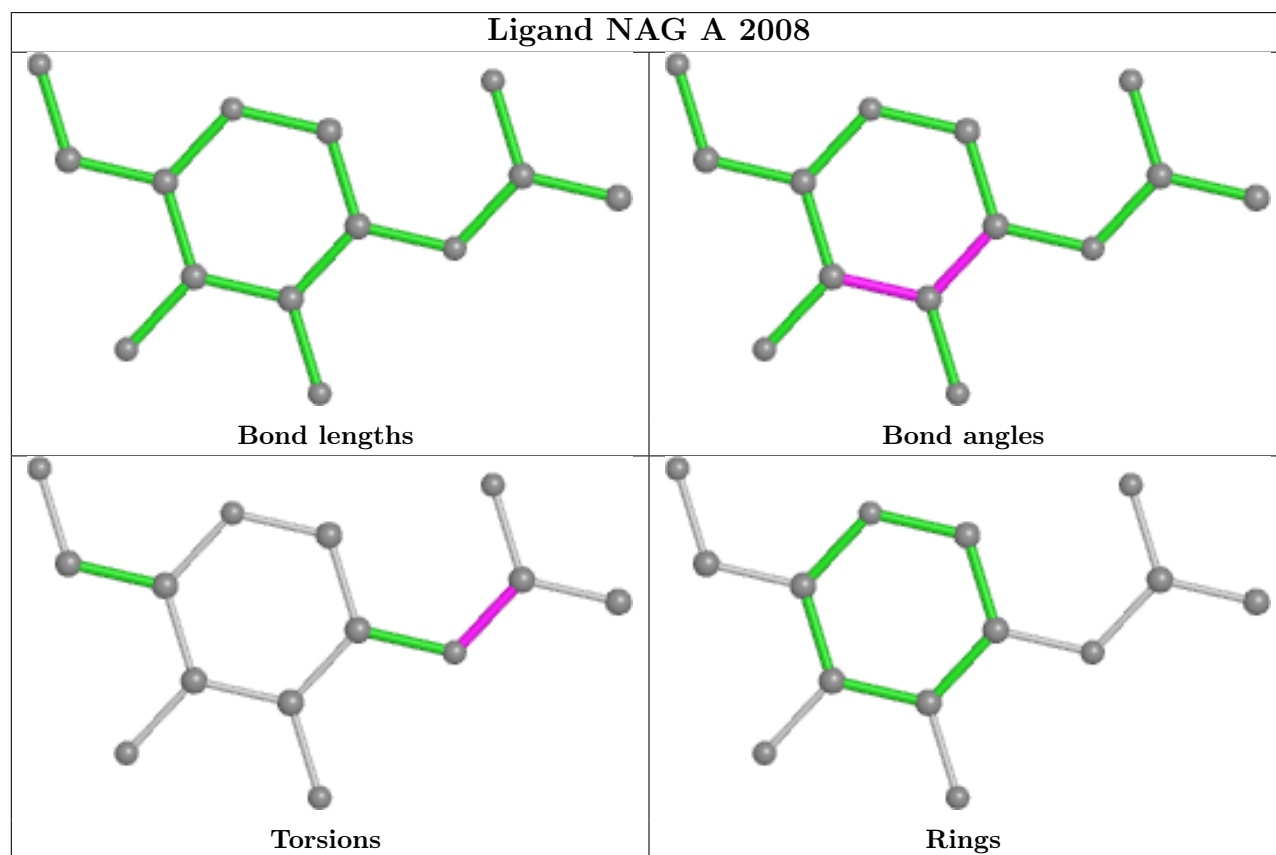
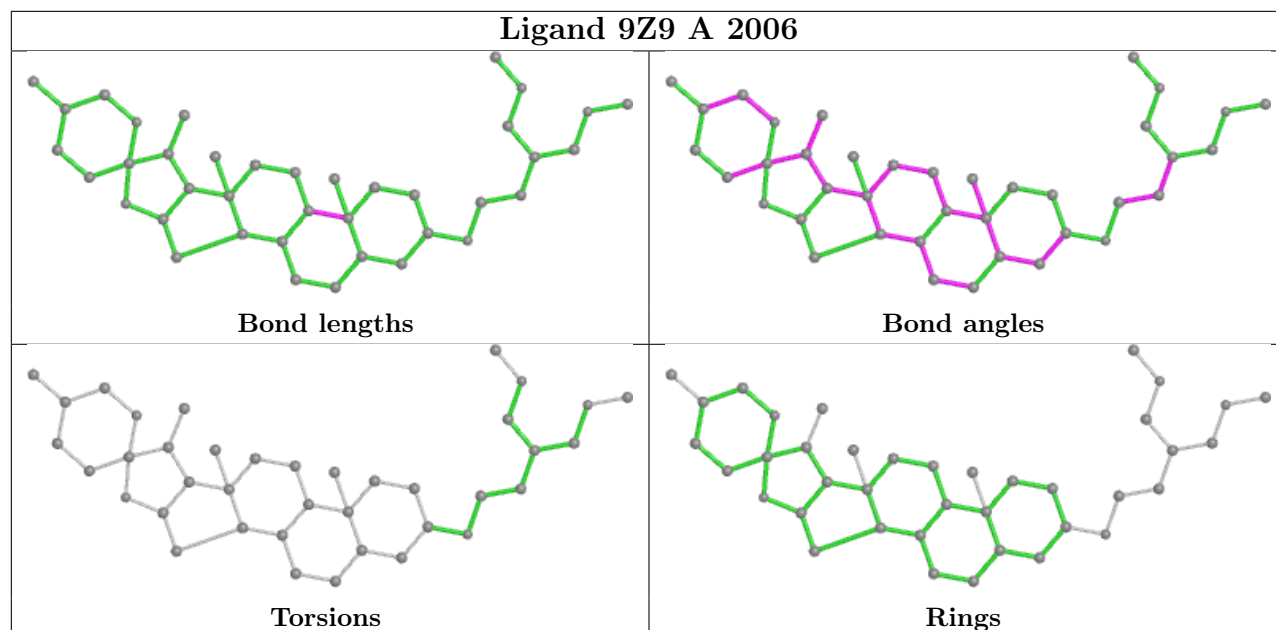
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2006	9Z9	33	0
6	A	2017	P5S	17	0
6	A	2029	P5S	2	0
7	A	2007	Y01	19	0
9	A	2026	LPE	2	0
10	A	2018	PCW	22	0
7	A	2003	Y01	5	0
9	A	2015	LPE	5	0
9	A	2019	LPE	1	0
10	A	2013	PCW	7	0
9	A	2021	LPE	4	0
9	A	2011	LPE	1	0
7	A	2004	Y01	8	0

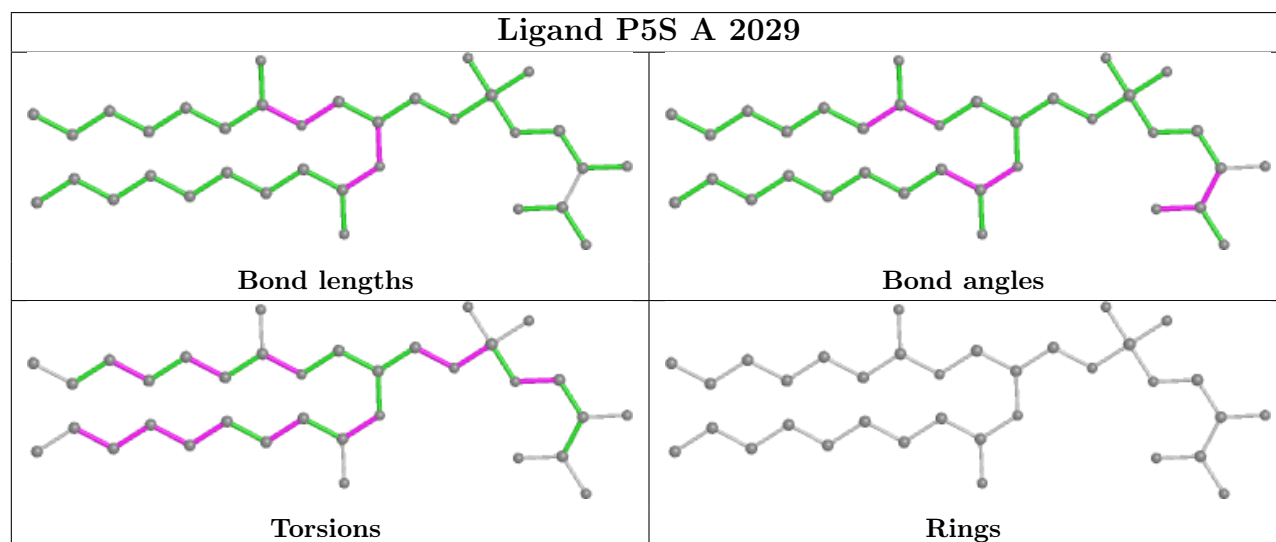
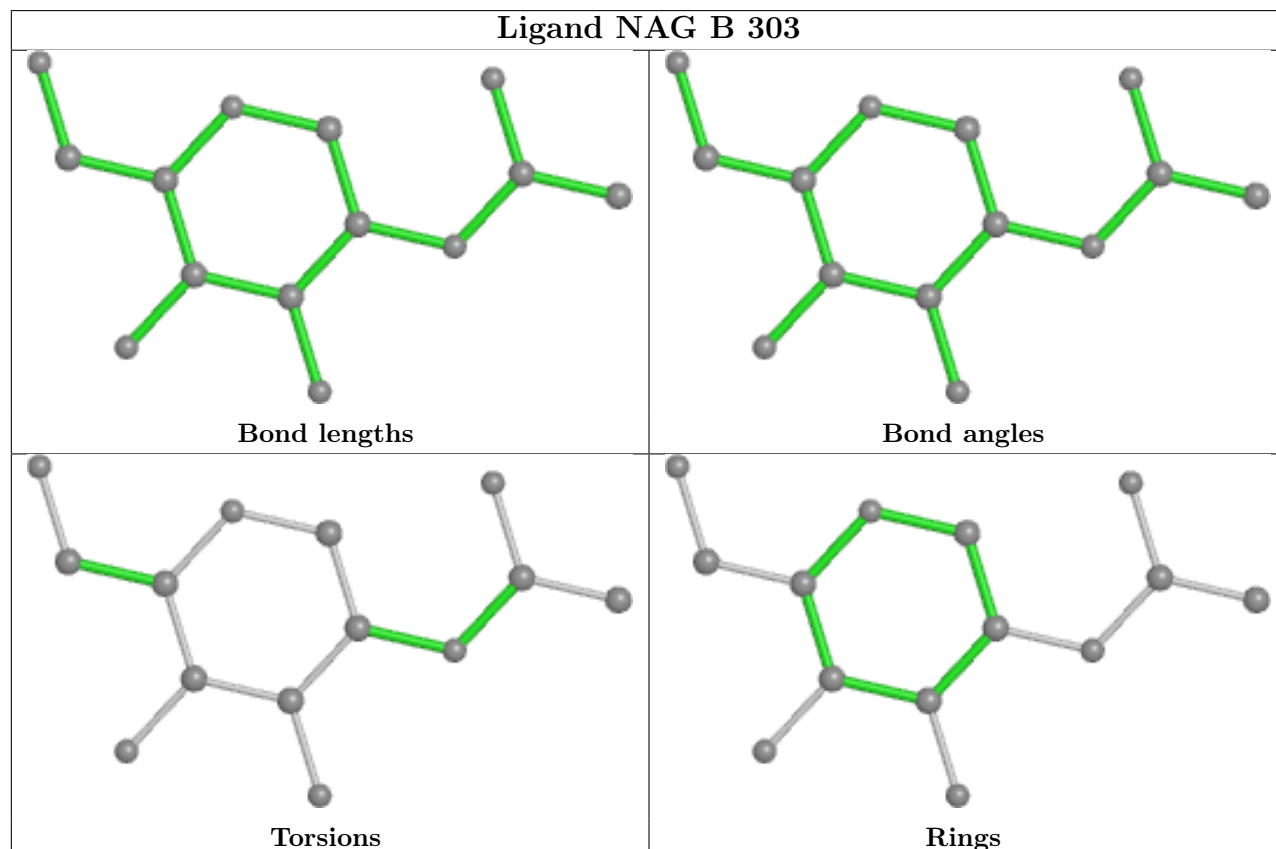
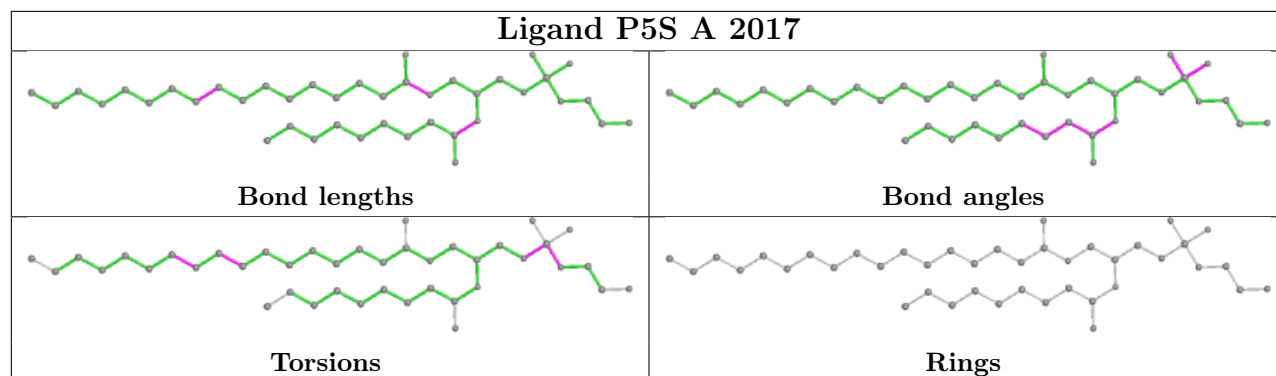
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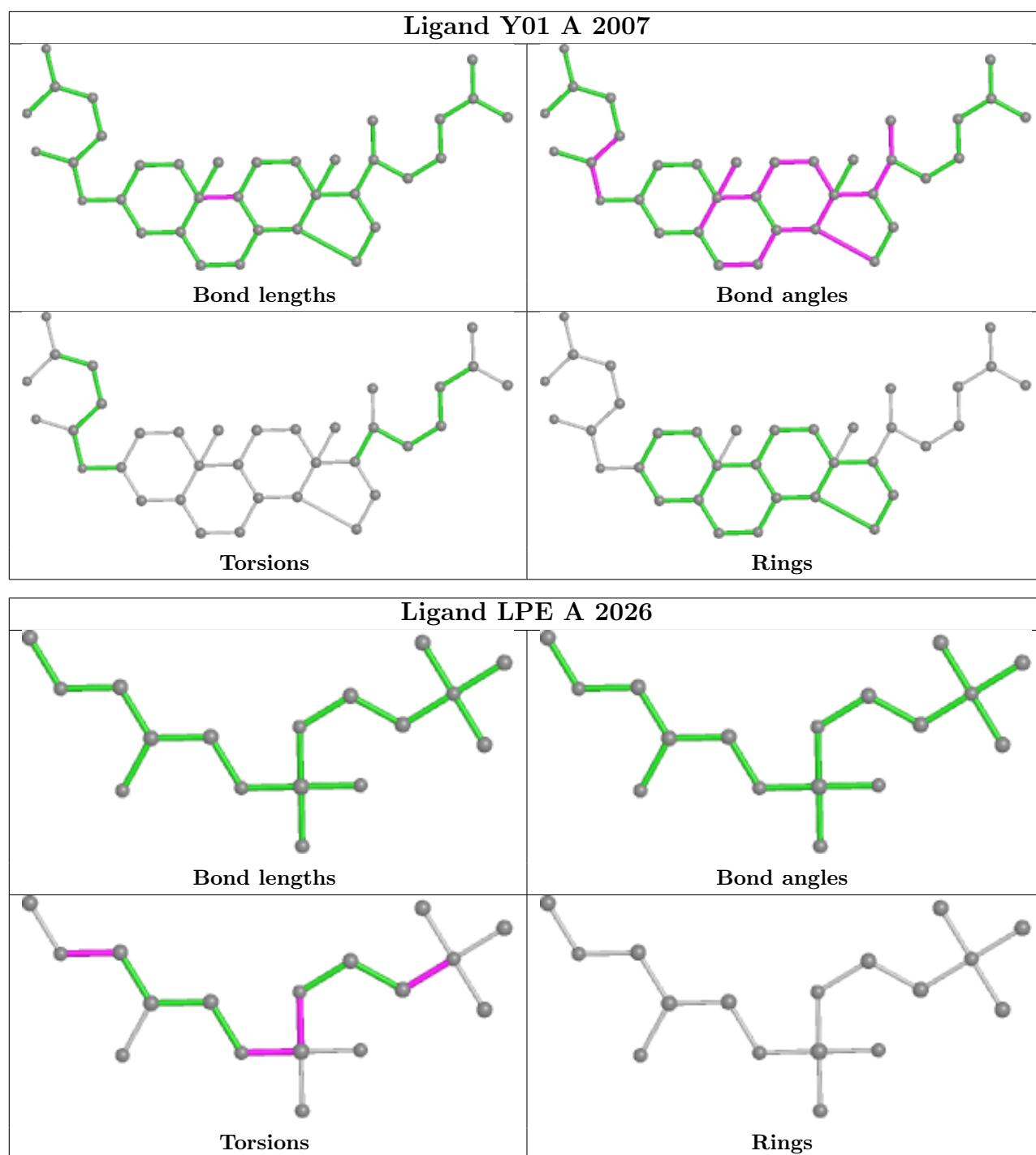
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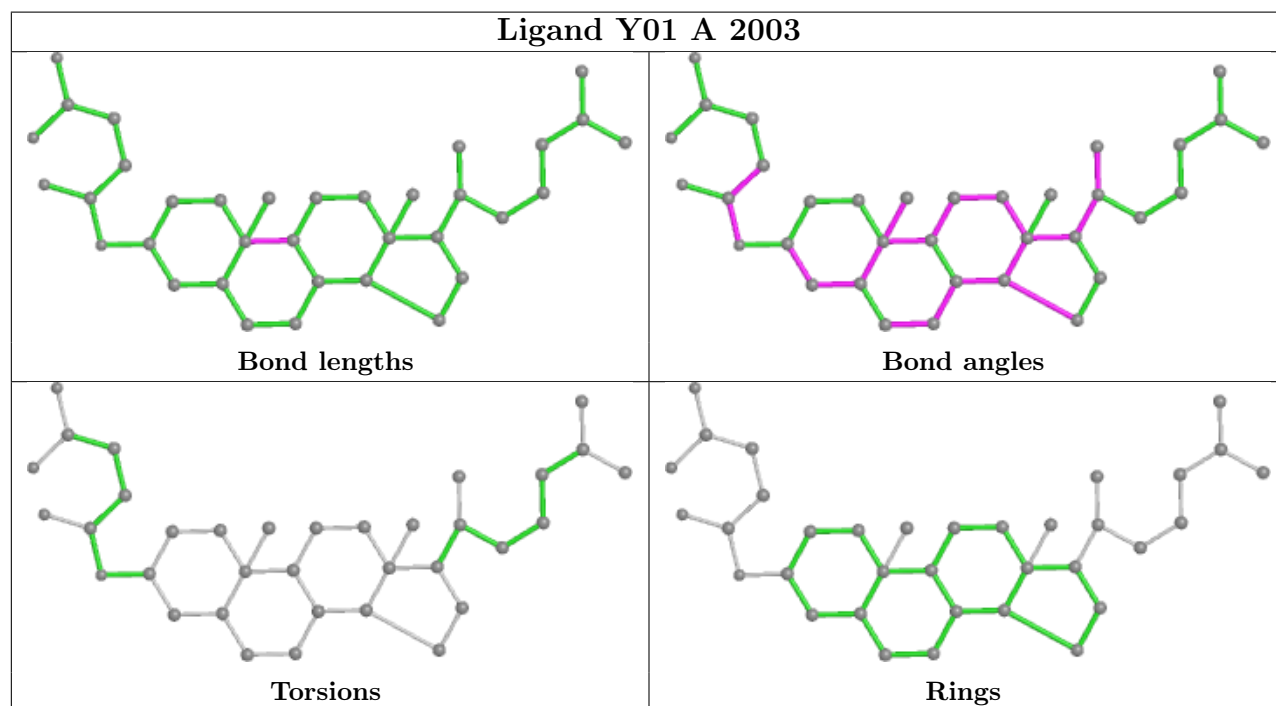
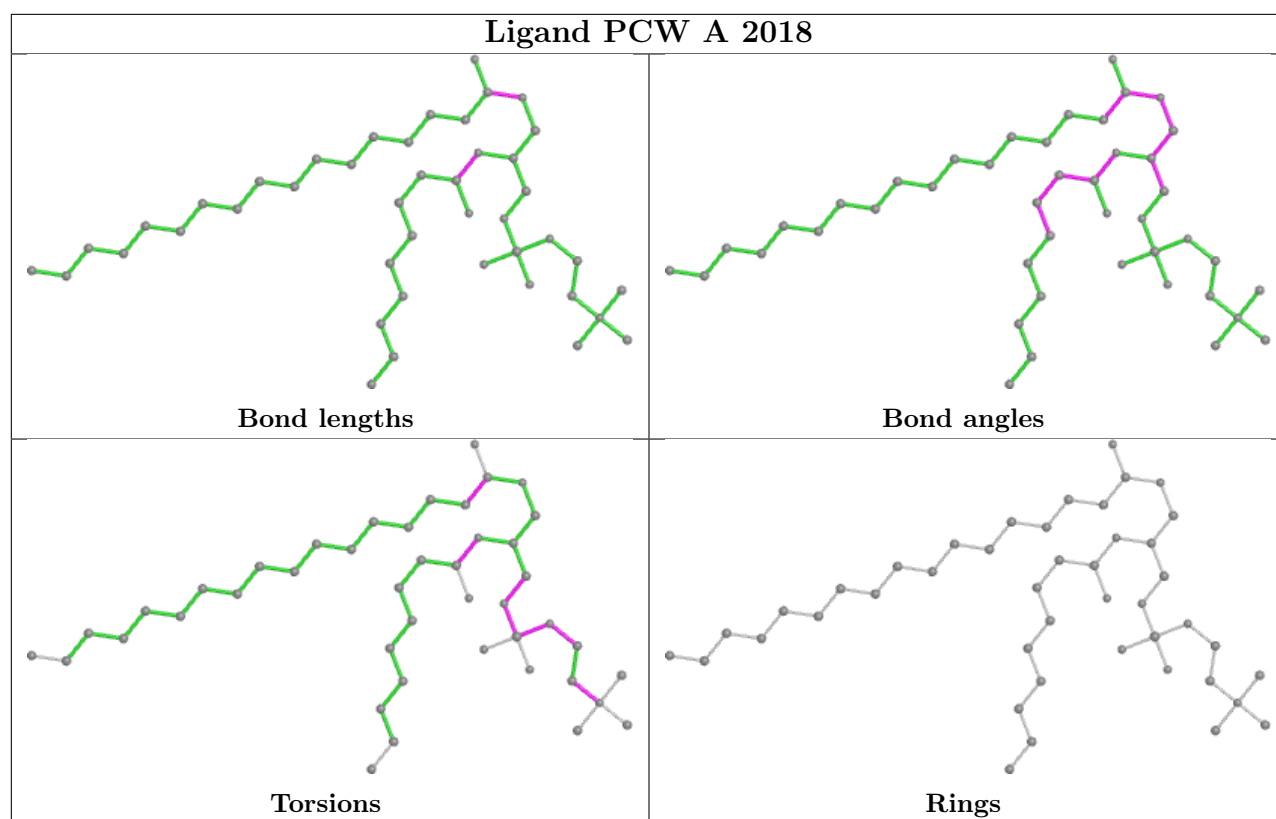
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2012	LPE	4	0
10	A	2016	PCW	16	0
10	A	2028	PCW	1	0
9	A	2020	LPE	2	0
9	A	2025	LPE	1	0
9	A	2023	LPE	14	0
7	A	2005	Y01	27	0
9	A	2014	LPE	18	0
7	A	2030	Y01	9	0
9	A	2022	LPE	8	0
6	A	2002	P5S	5	0
7	A	2009	Y01	6	0
5	B	302	NAG	6	0
9	B	304	LPE	9	0
10	A	2027	PCW	5	0
9	A	2010	LPE	4	0

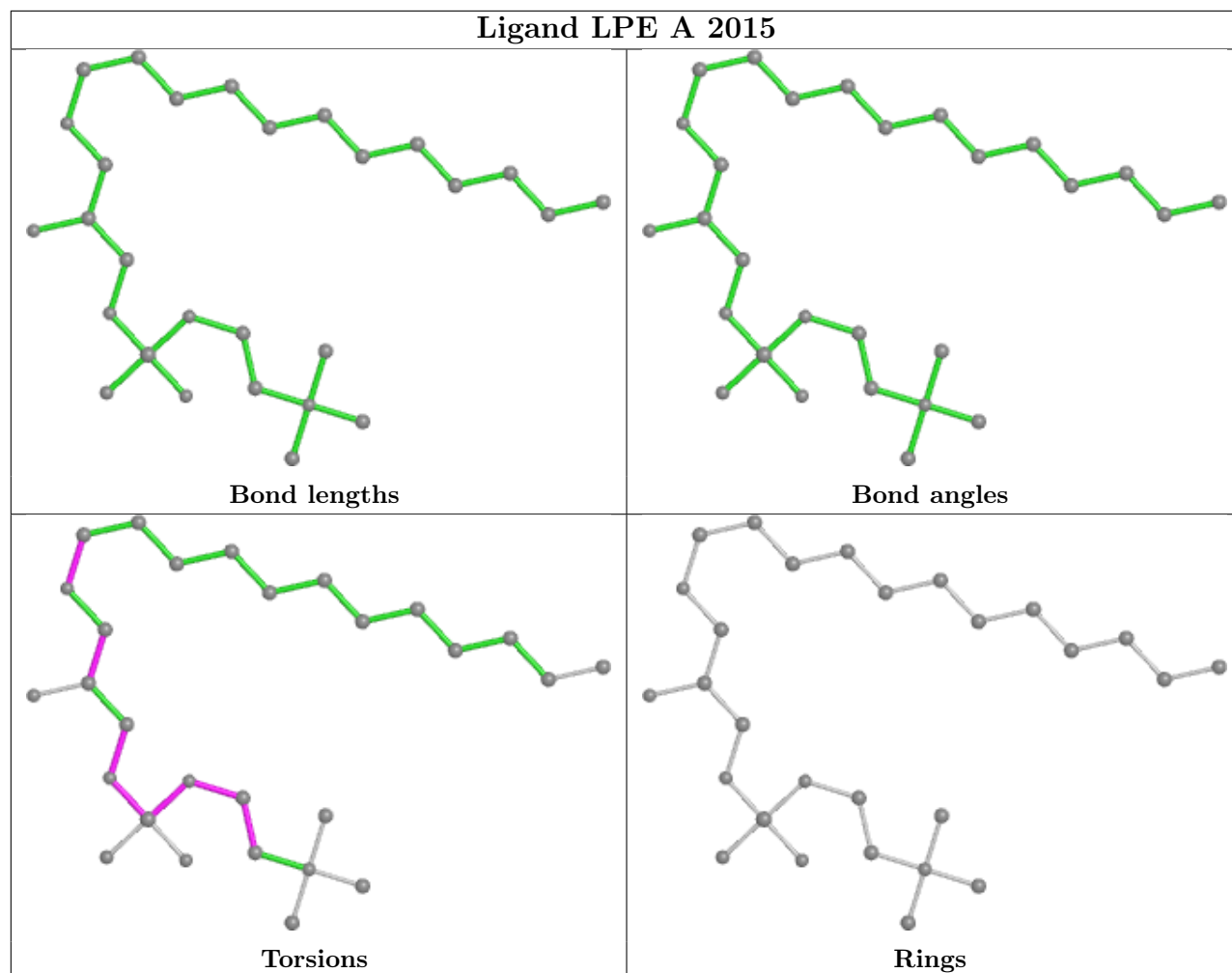
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



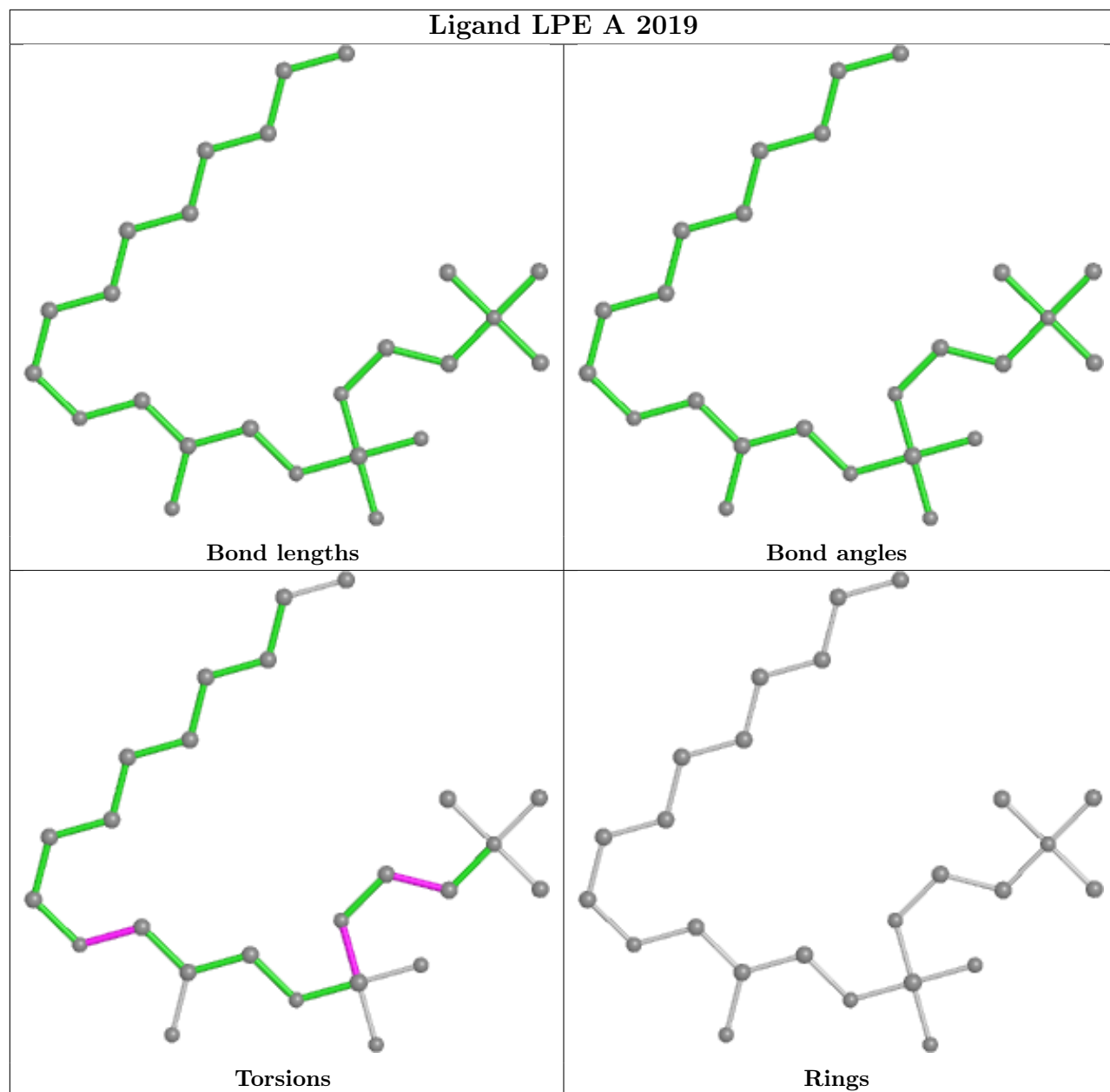


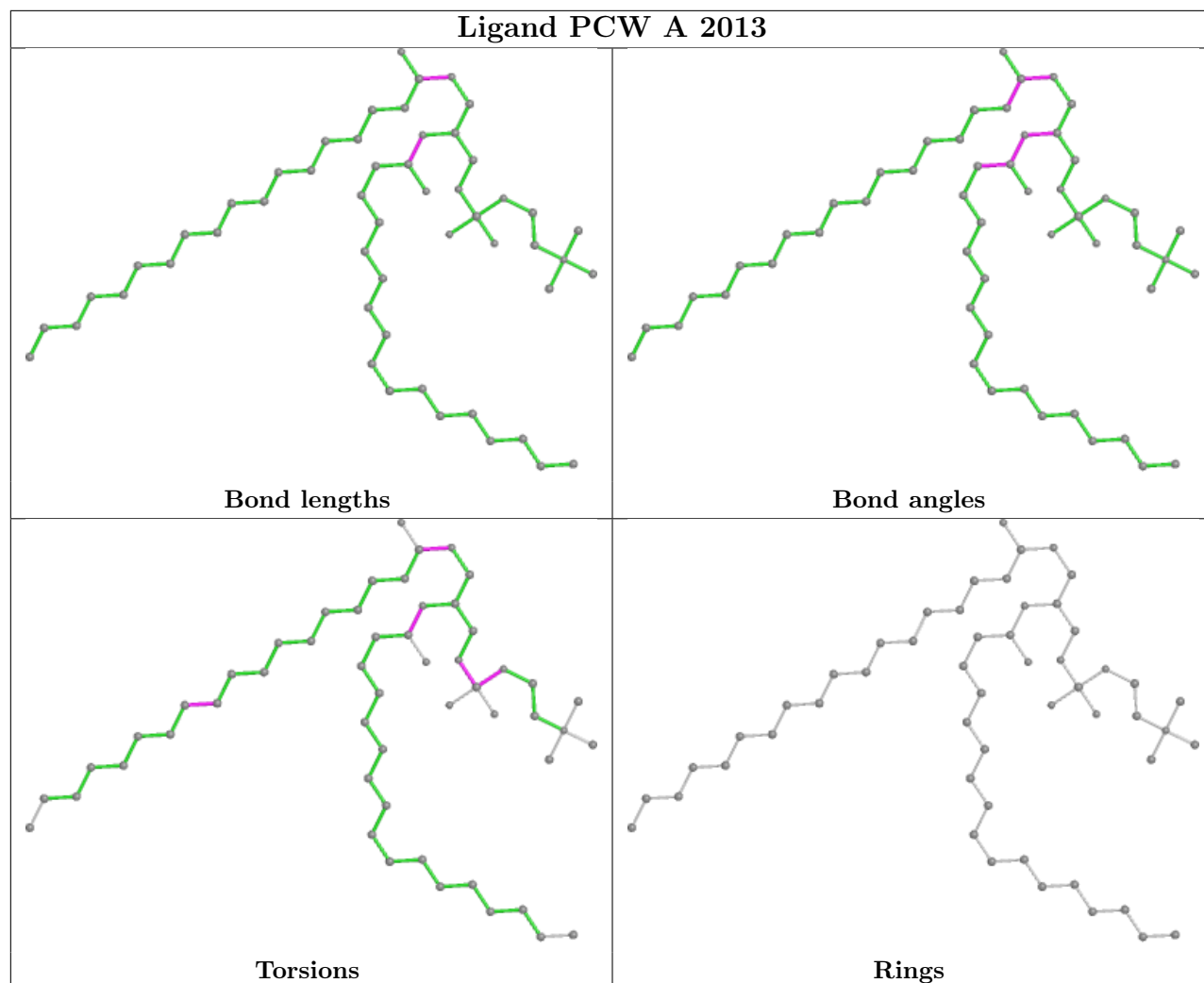


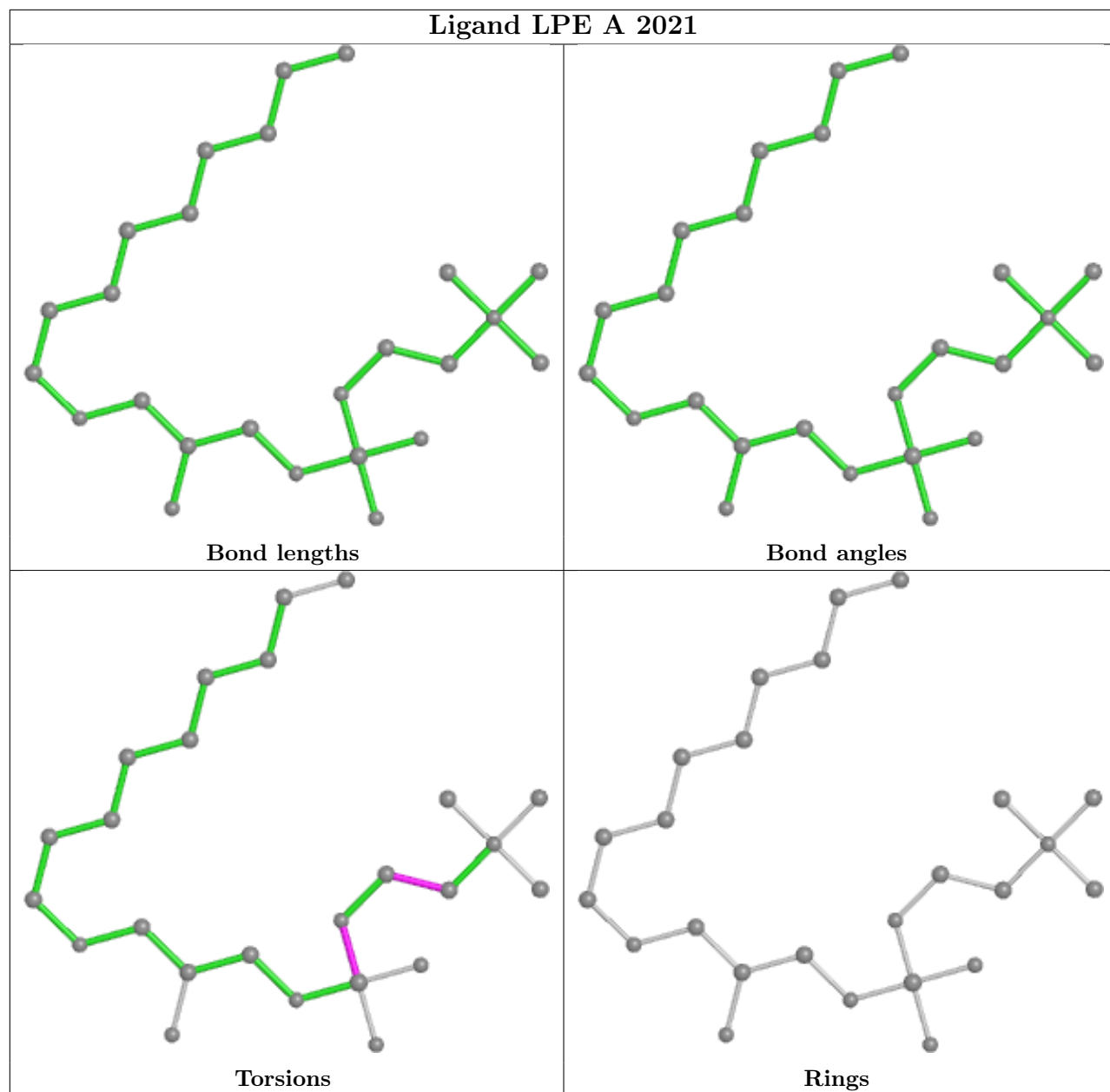


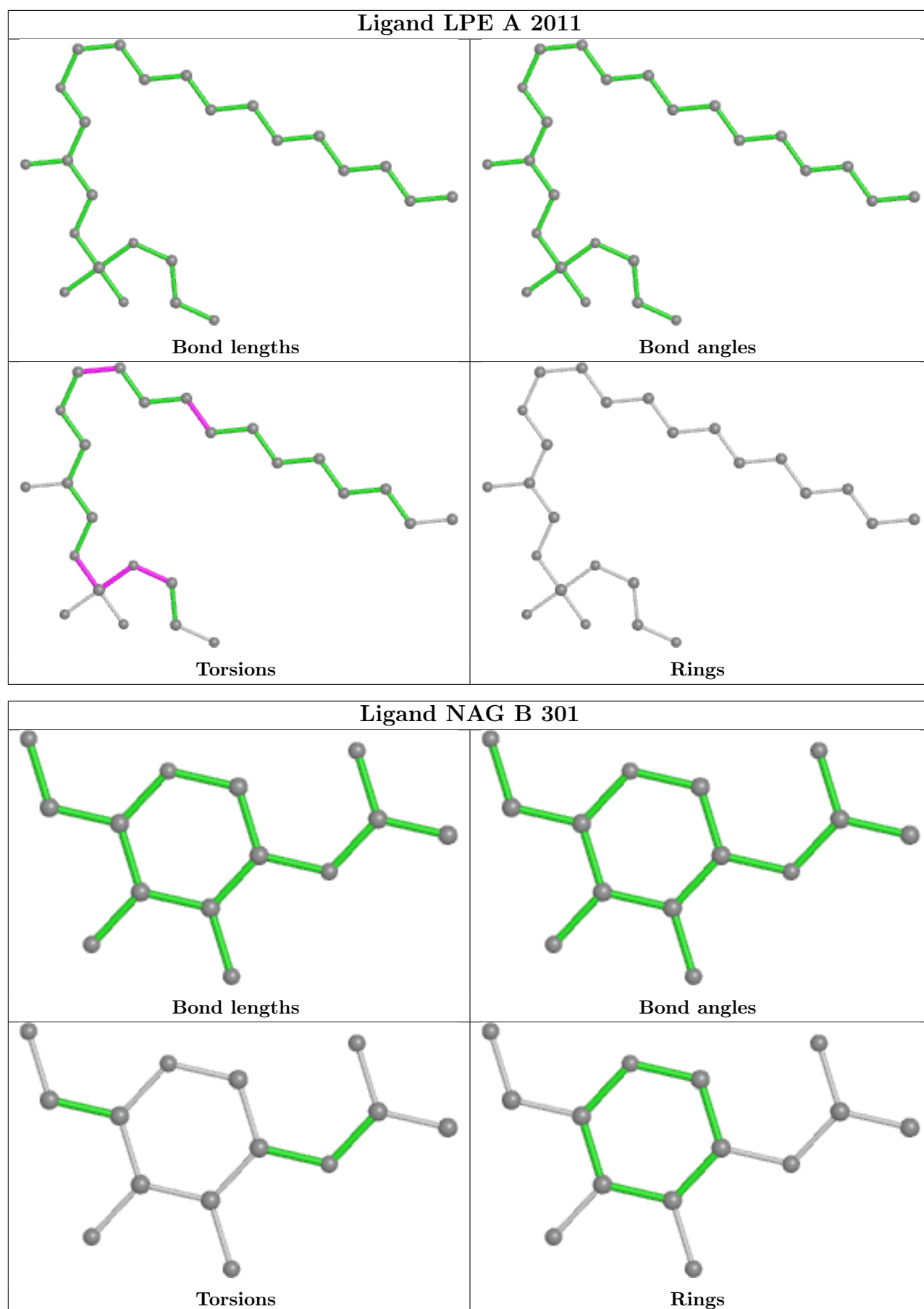


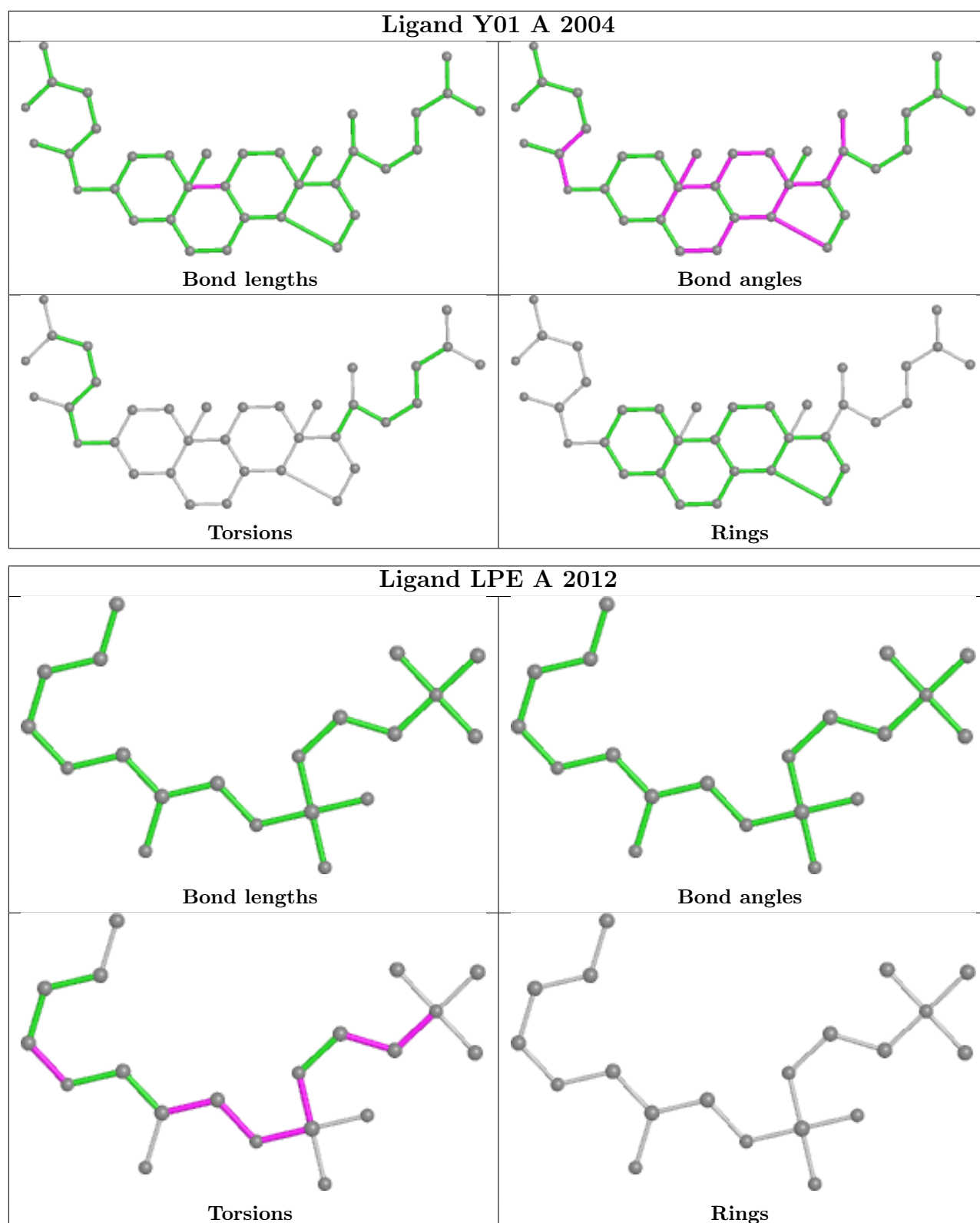


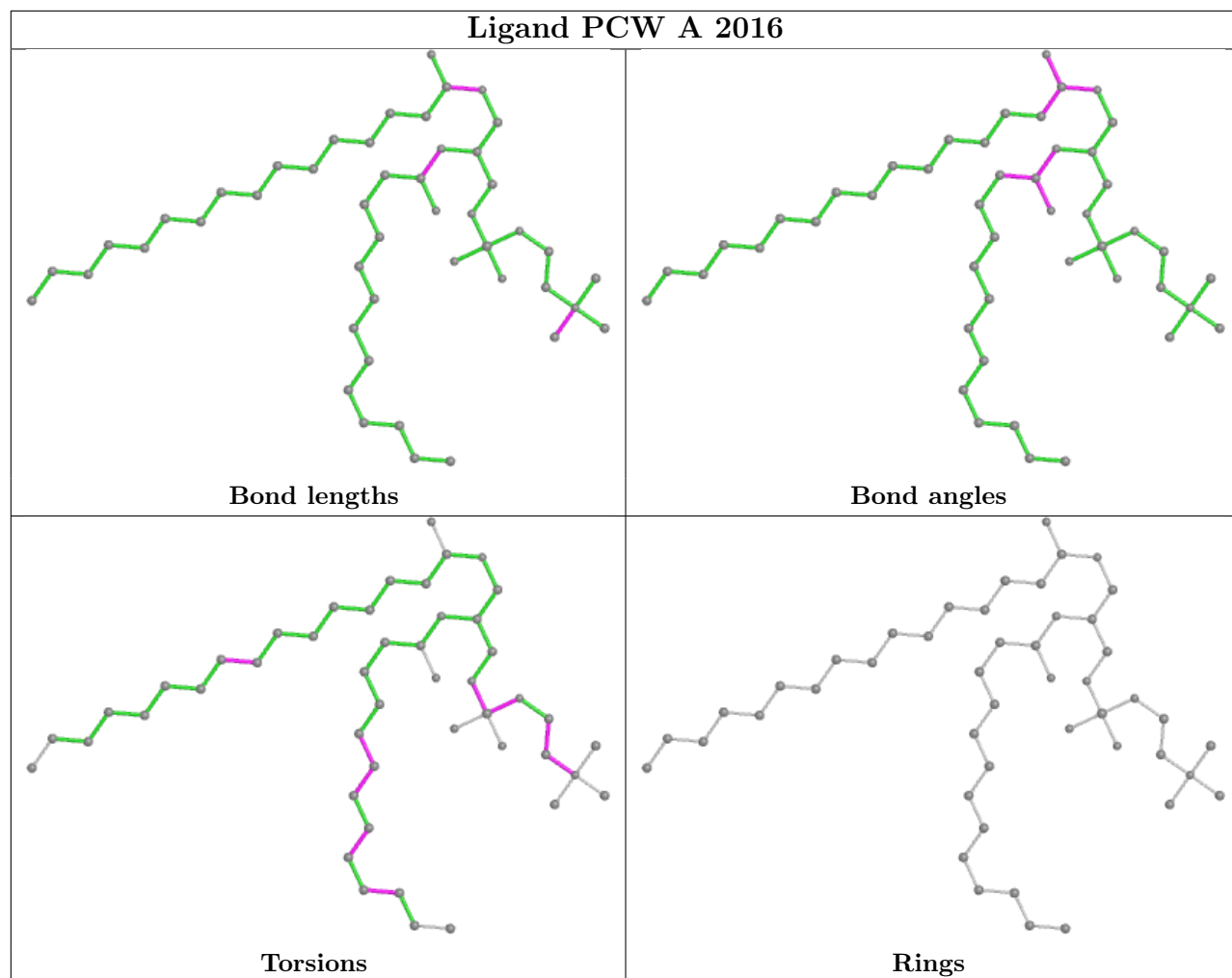


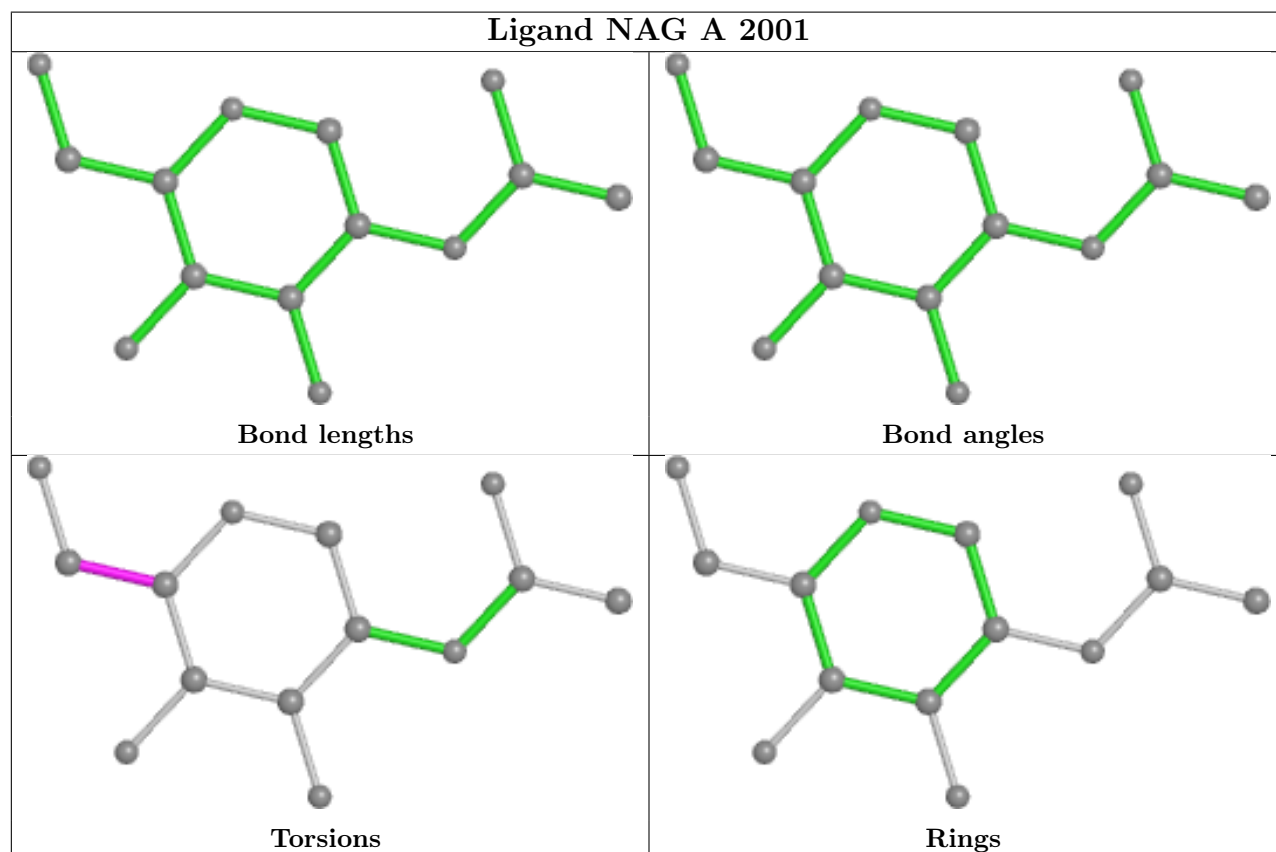
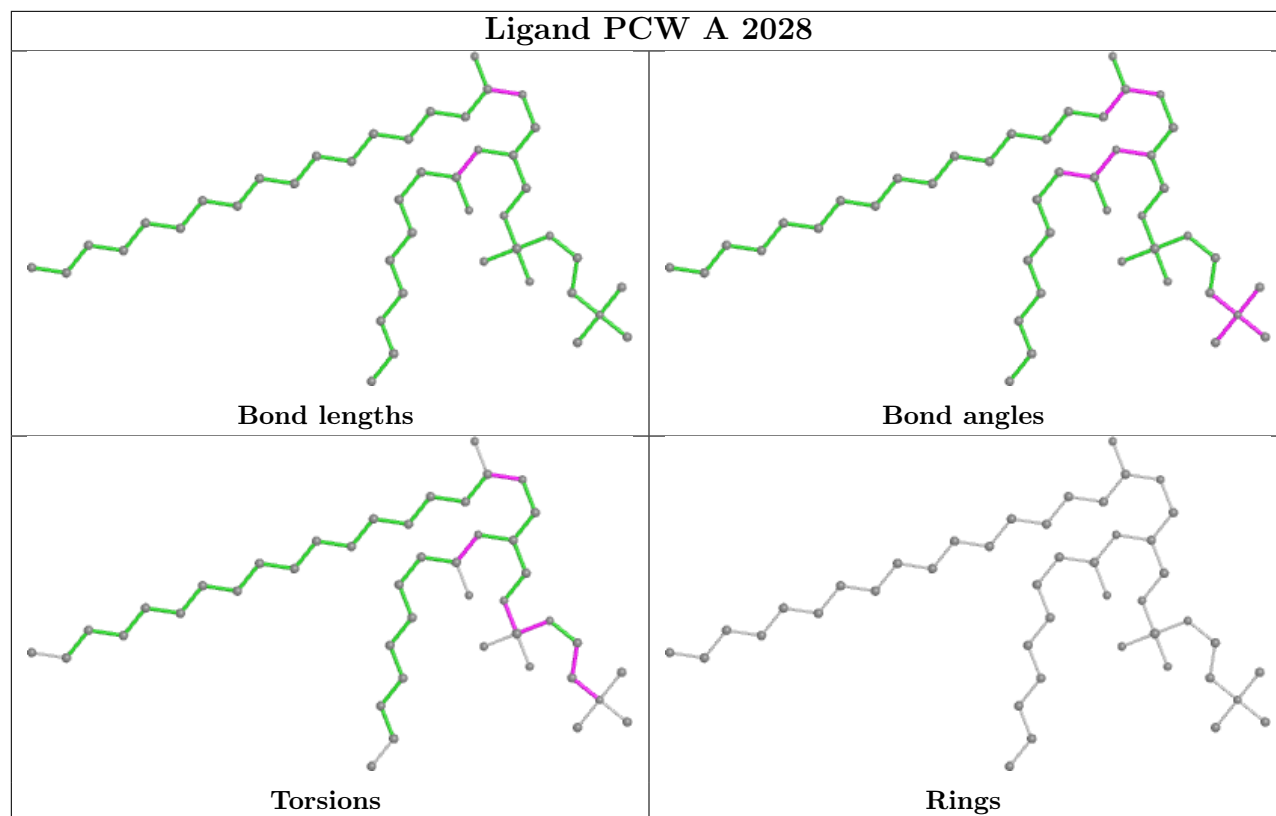


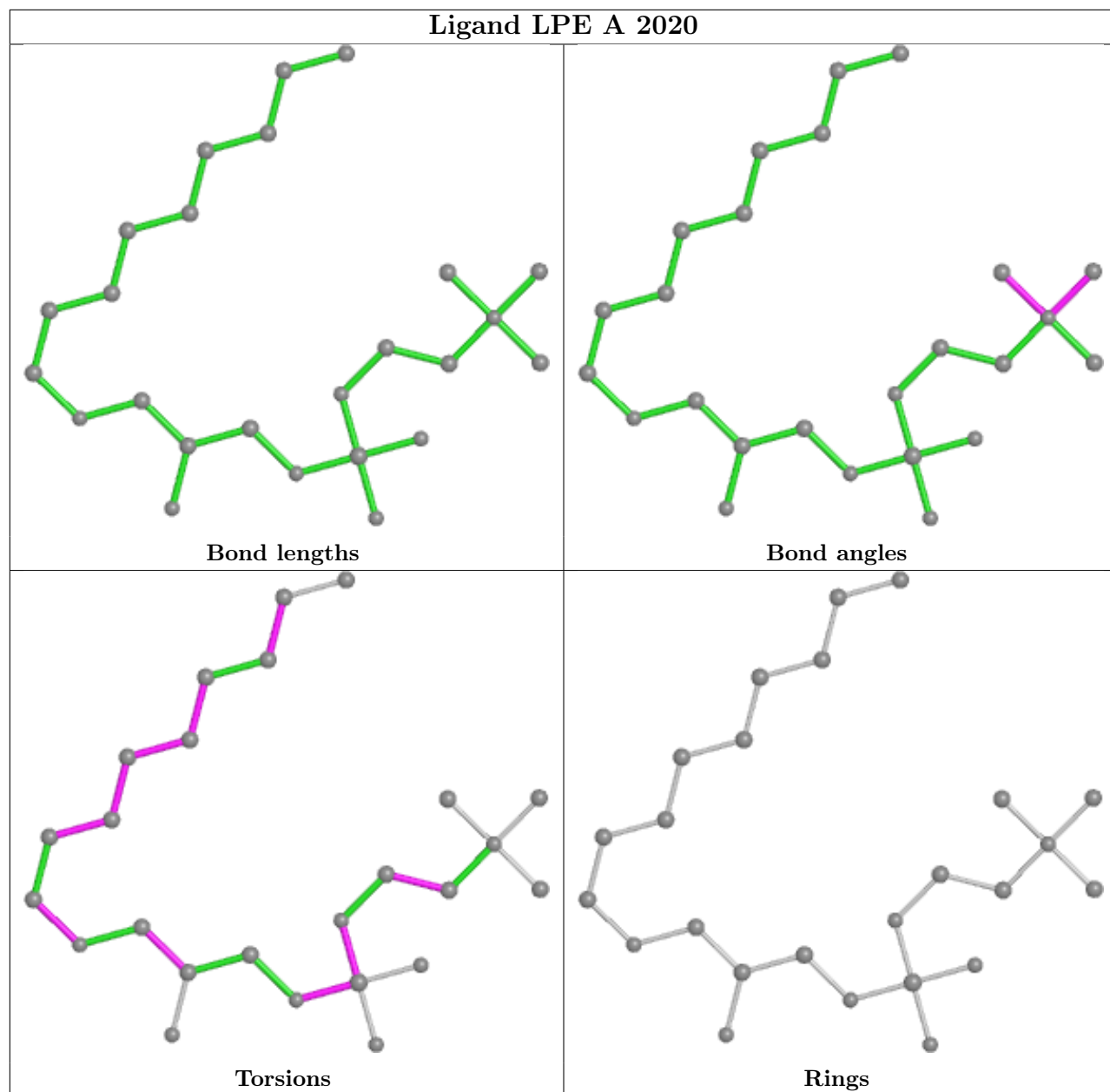




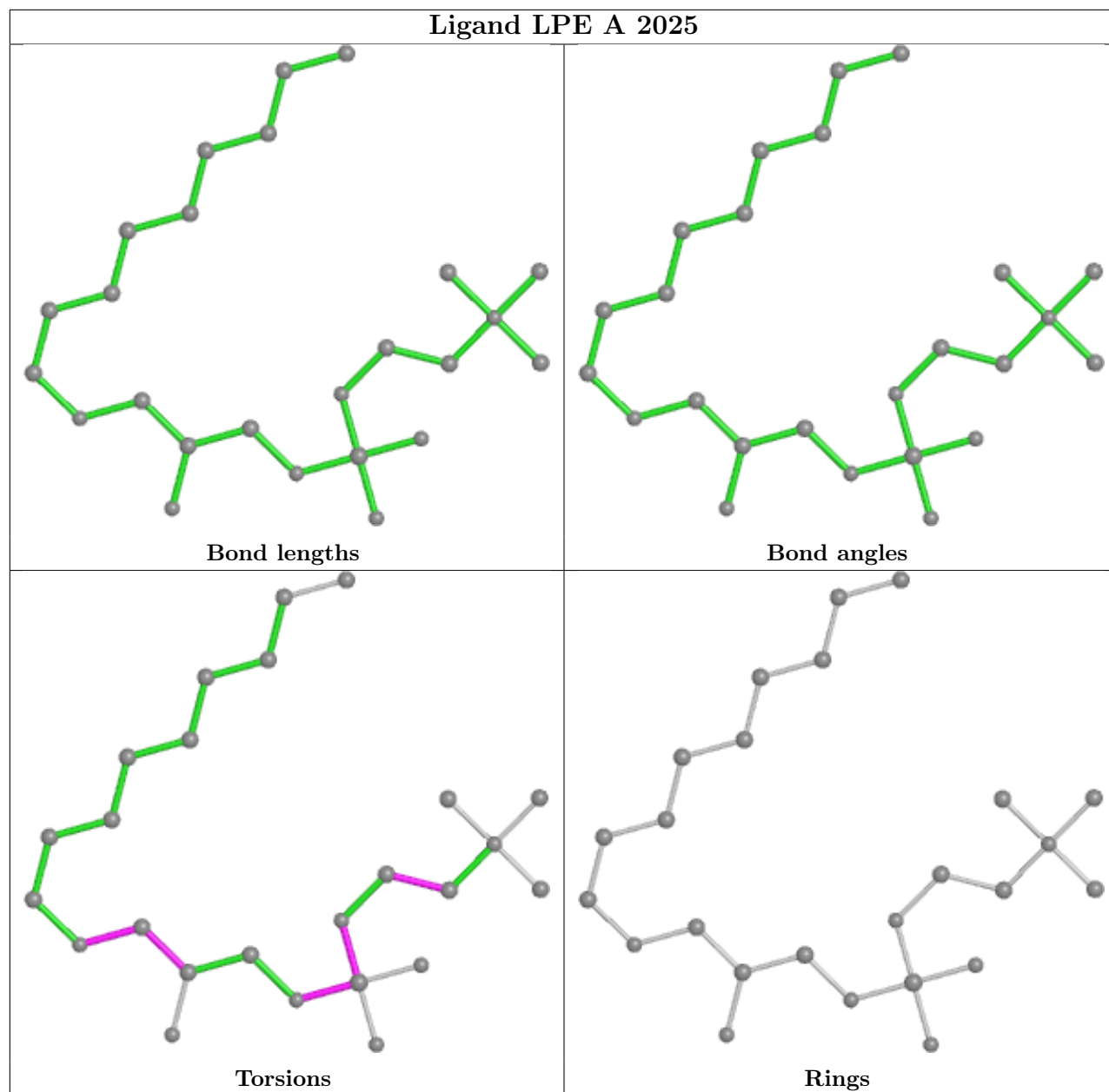


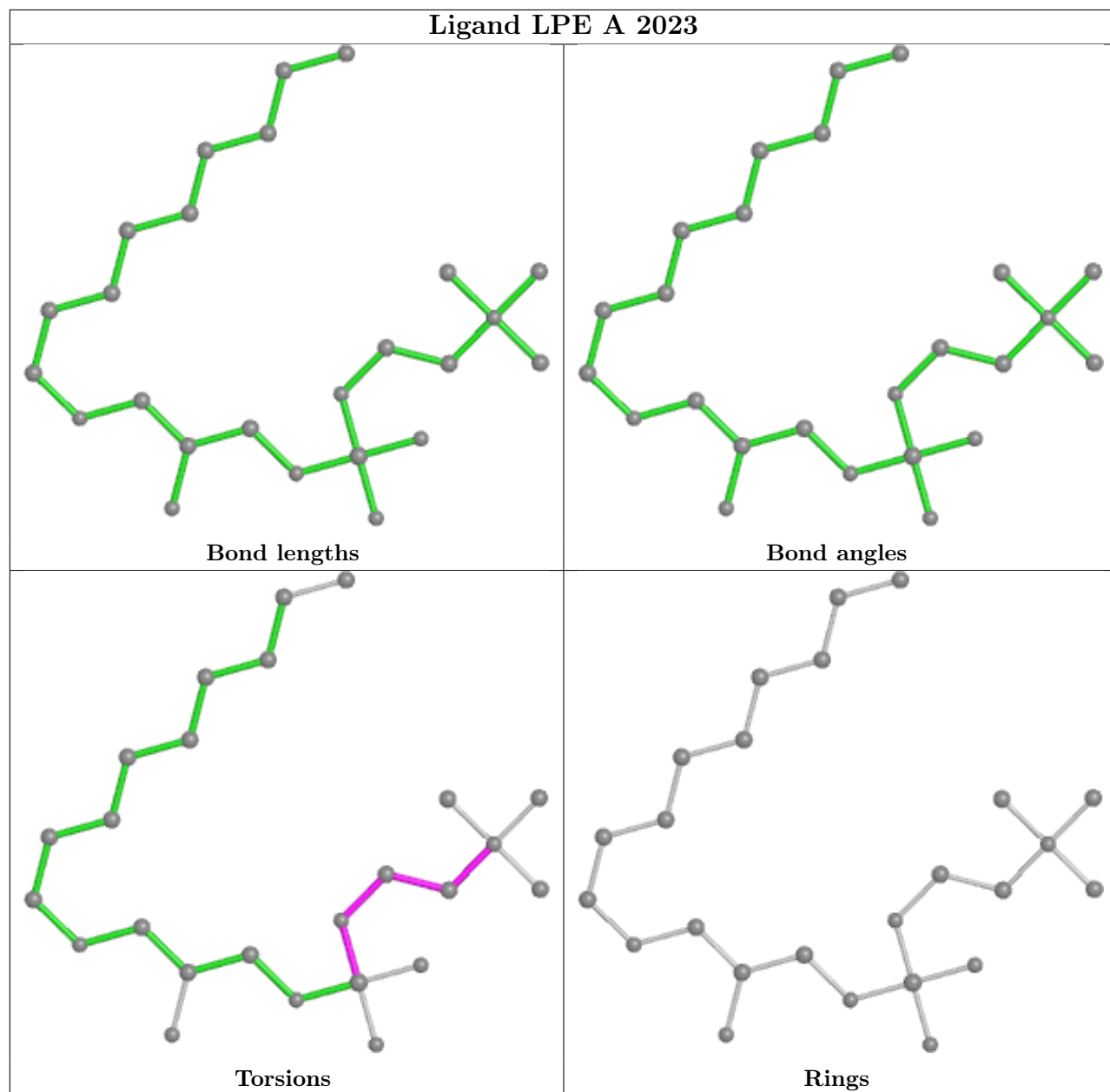


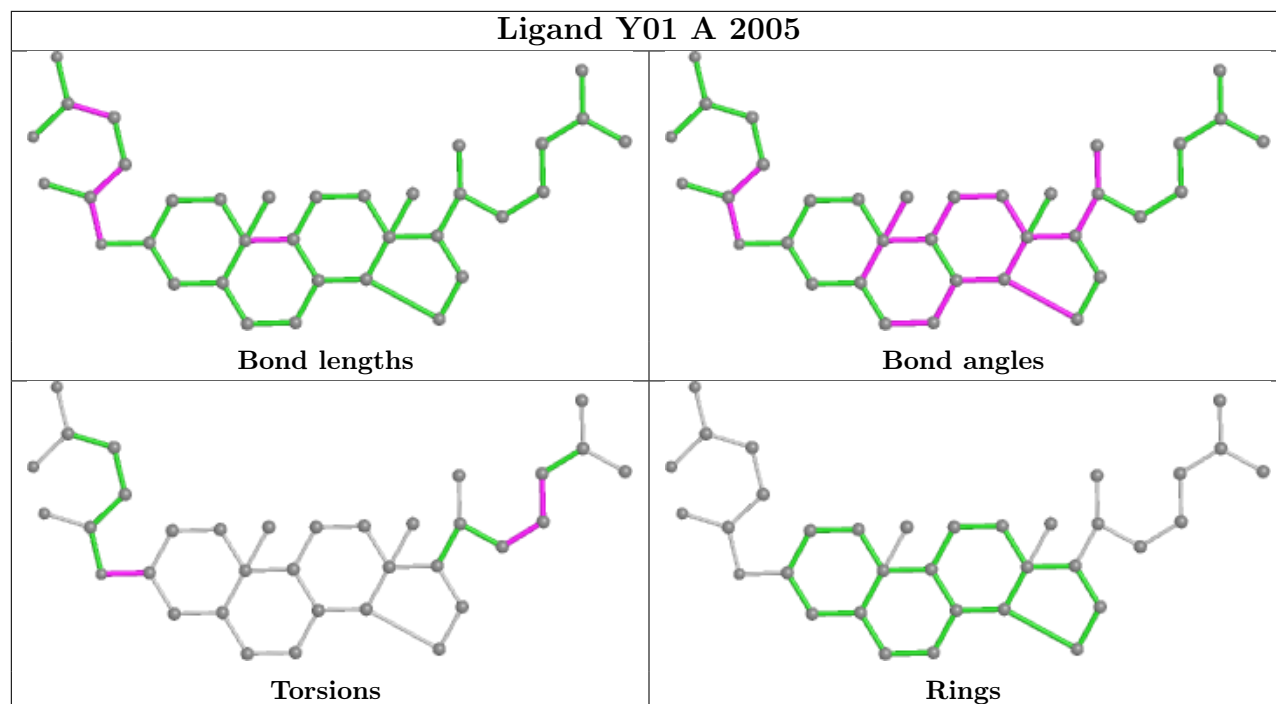


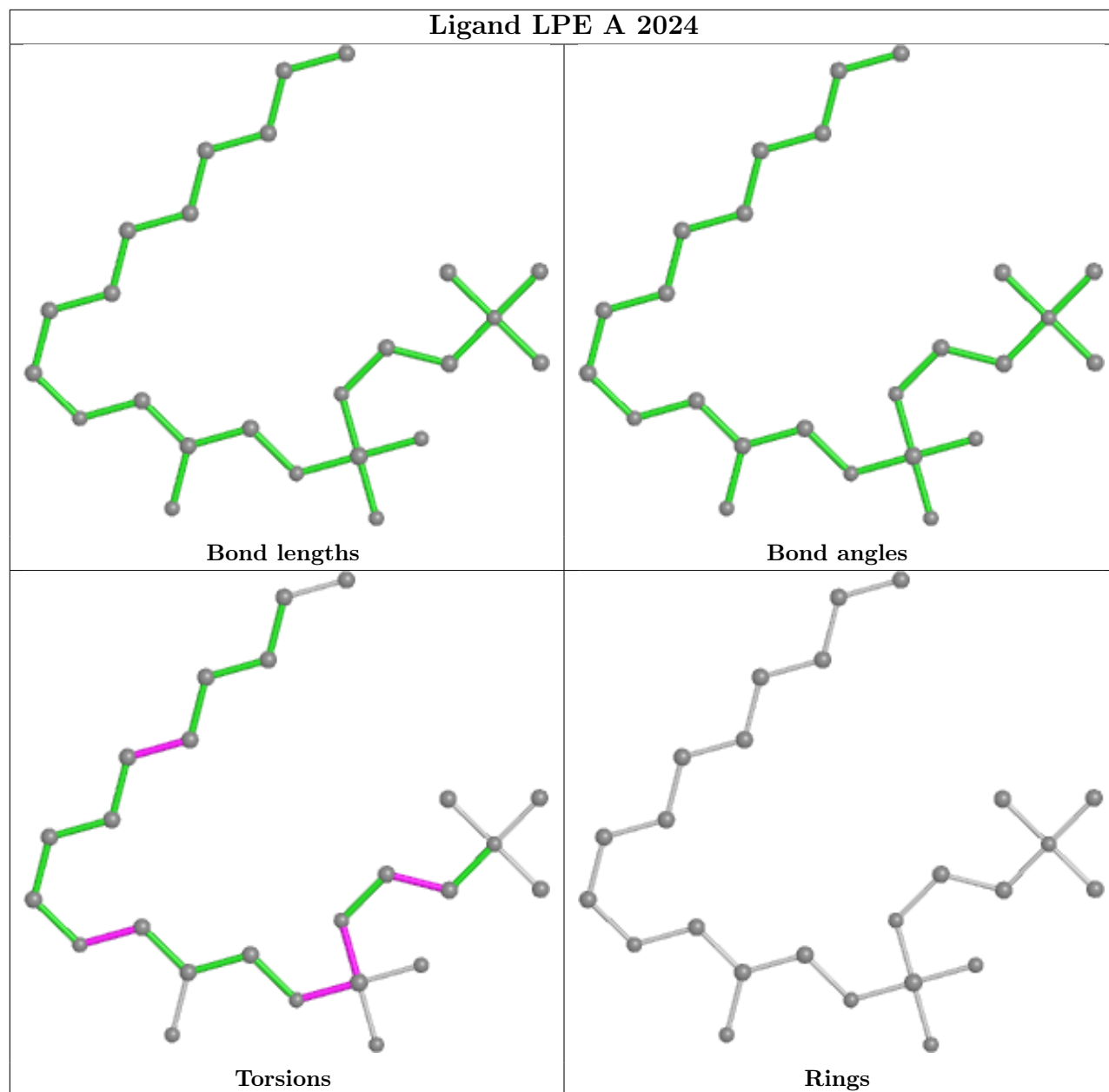


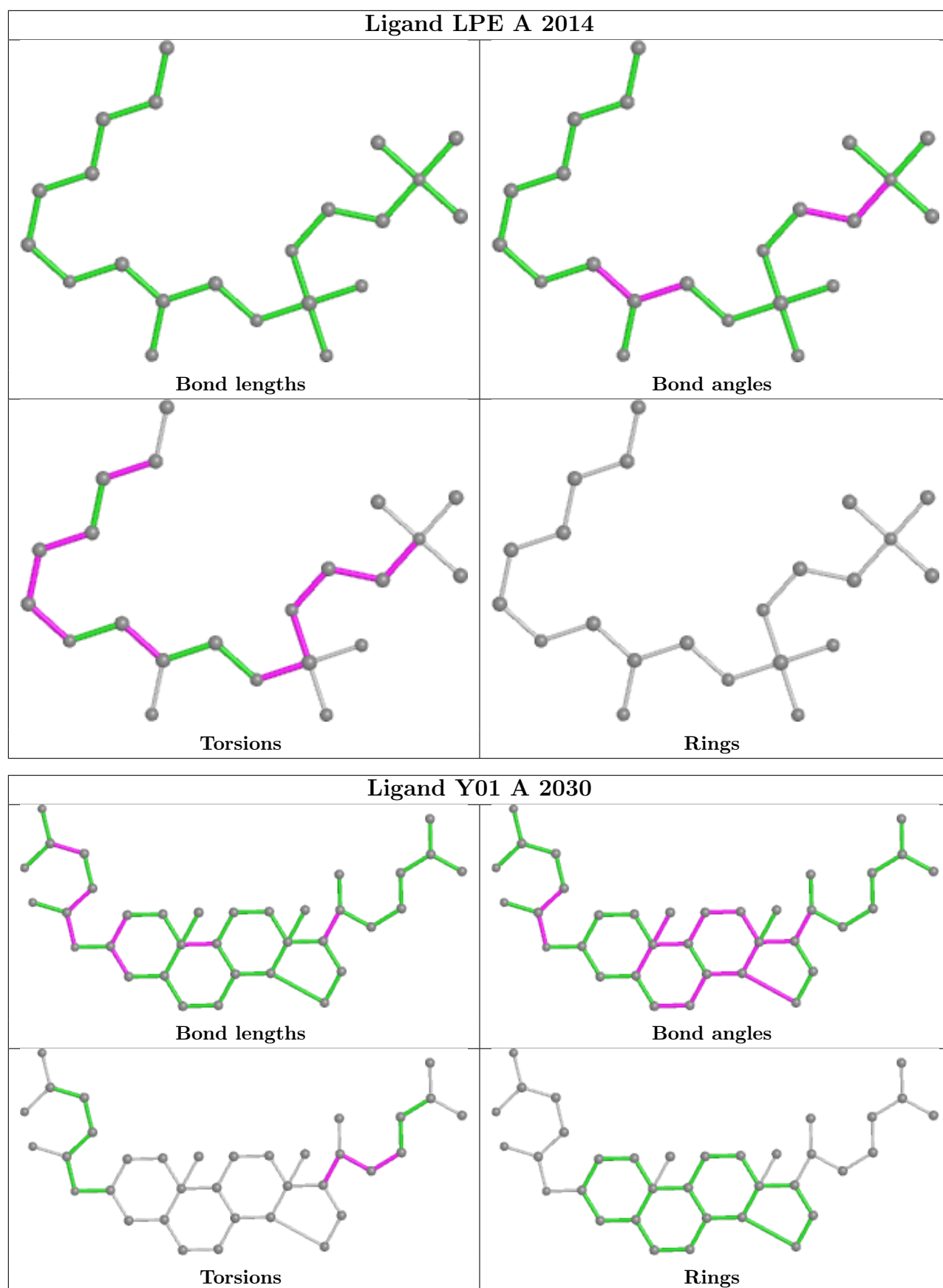


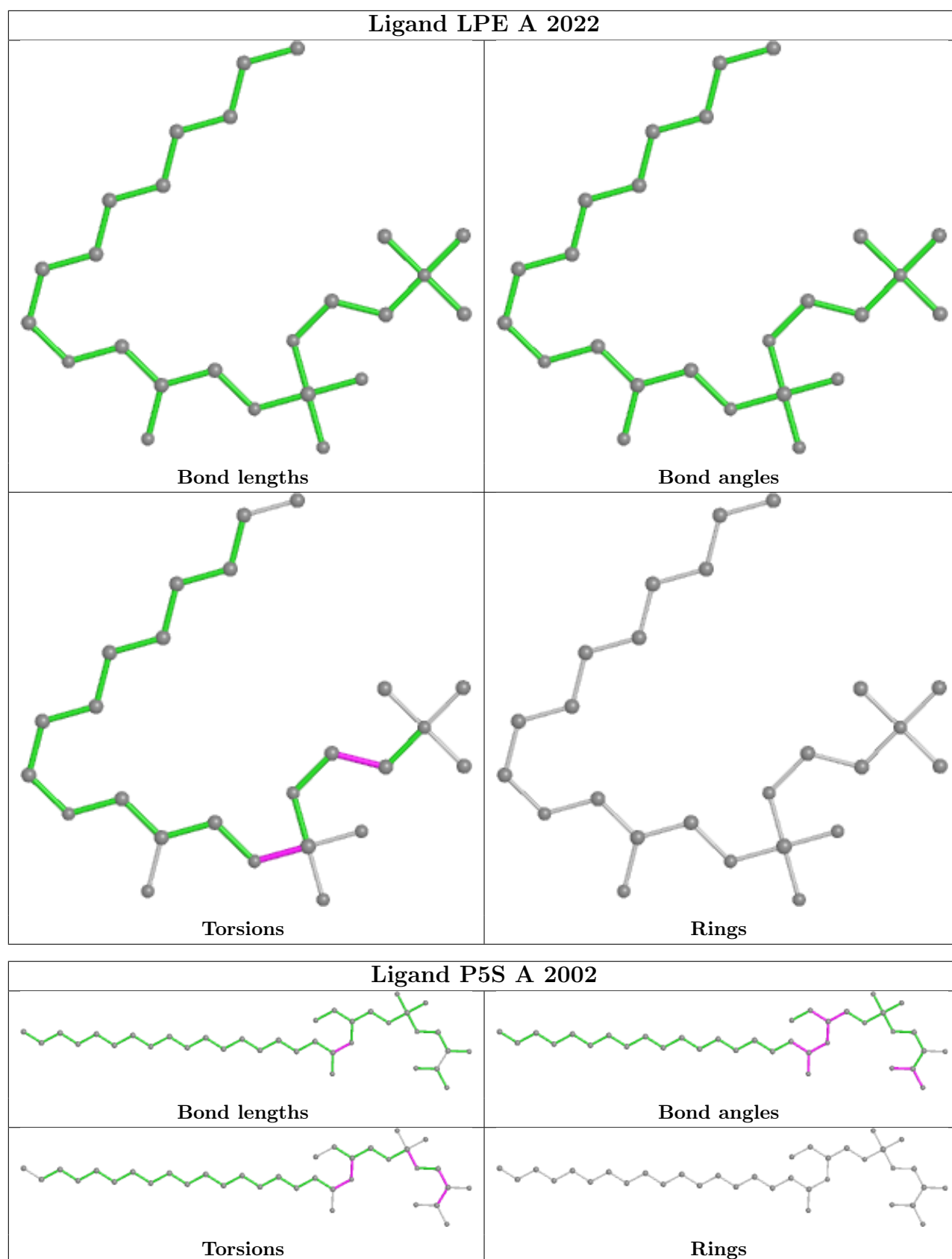


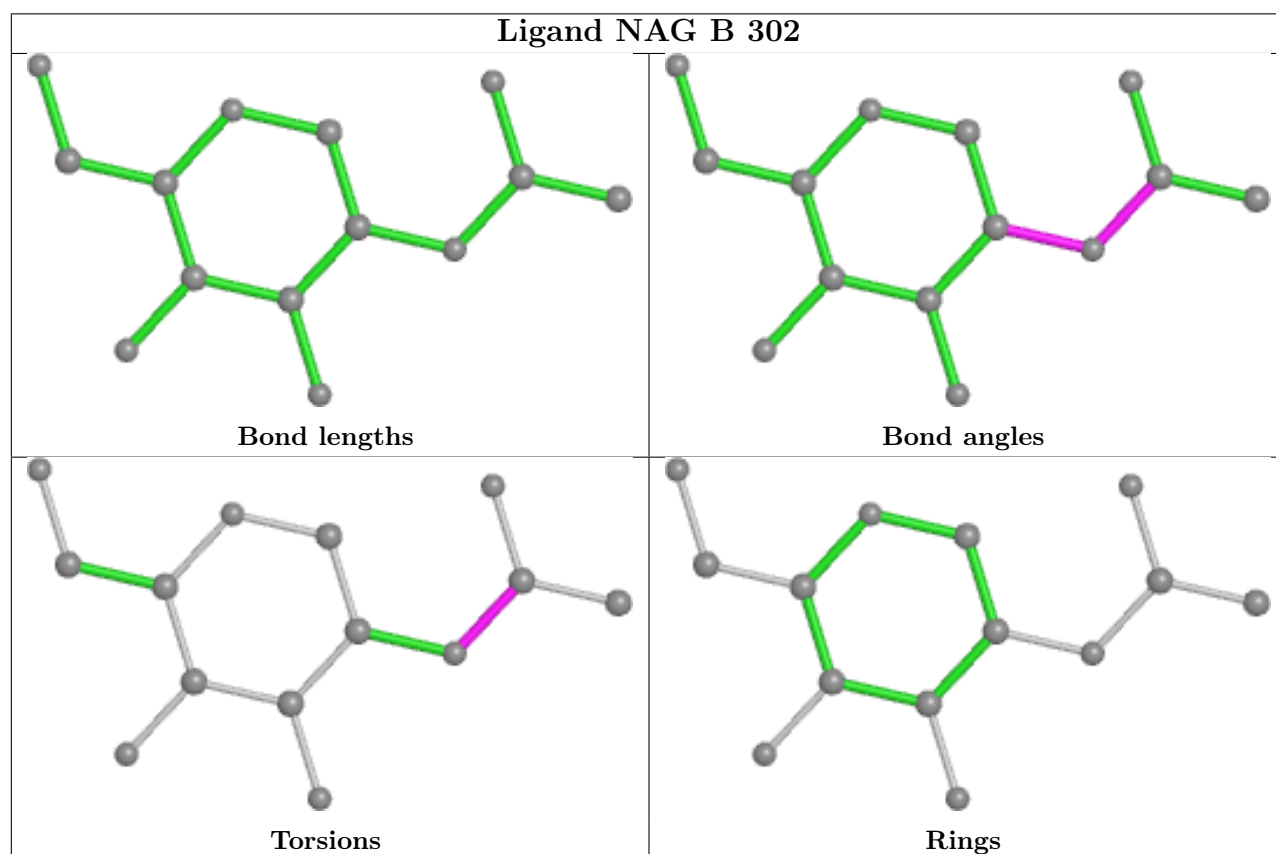
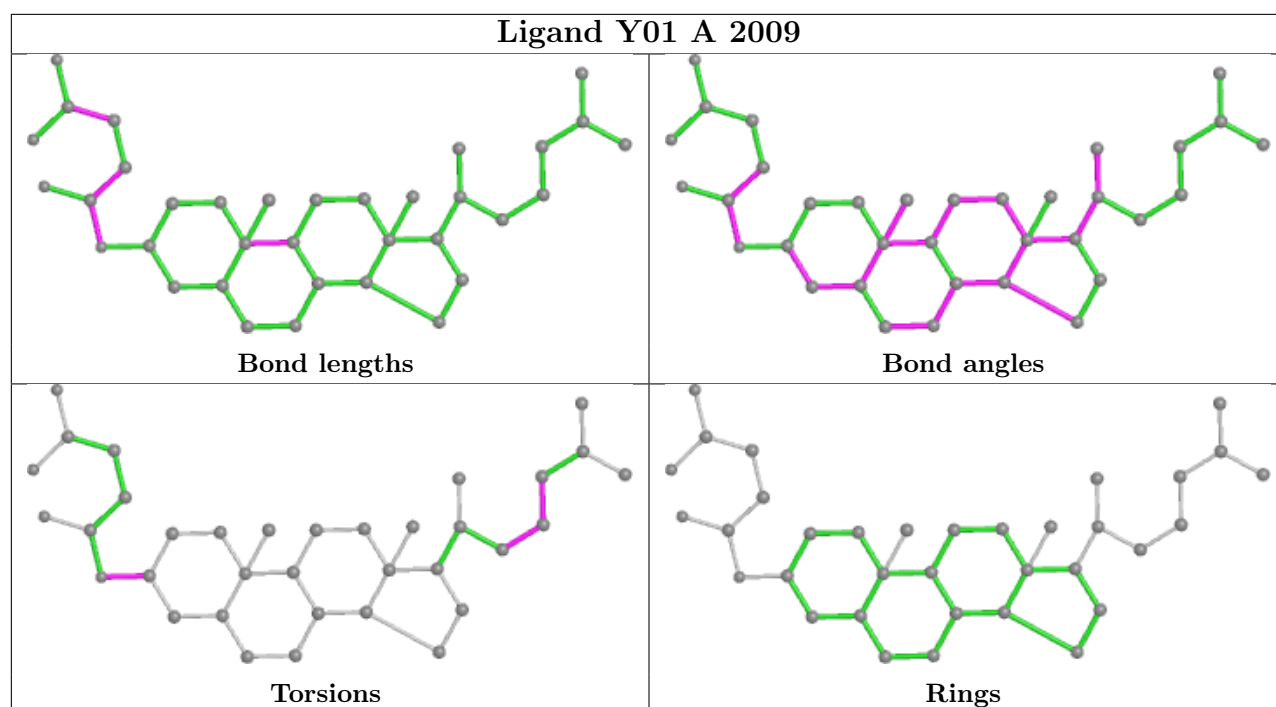


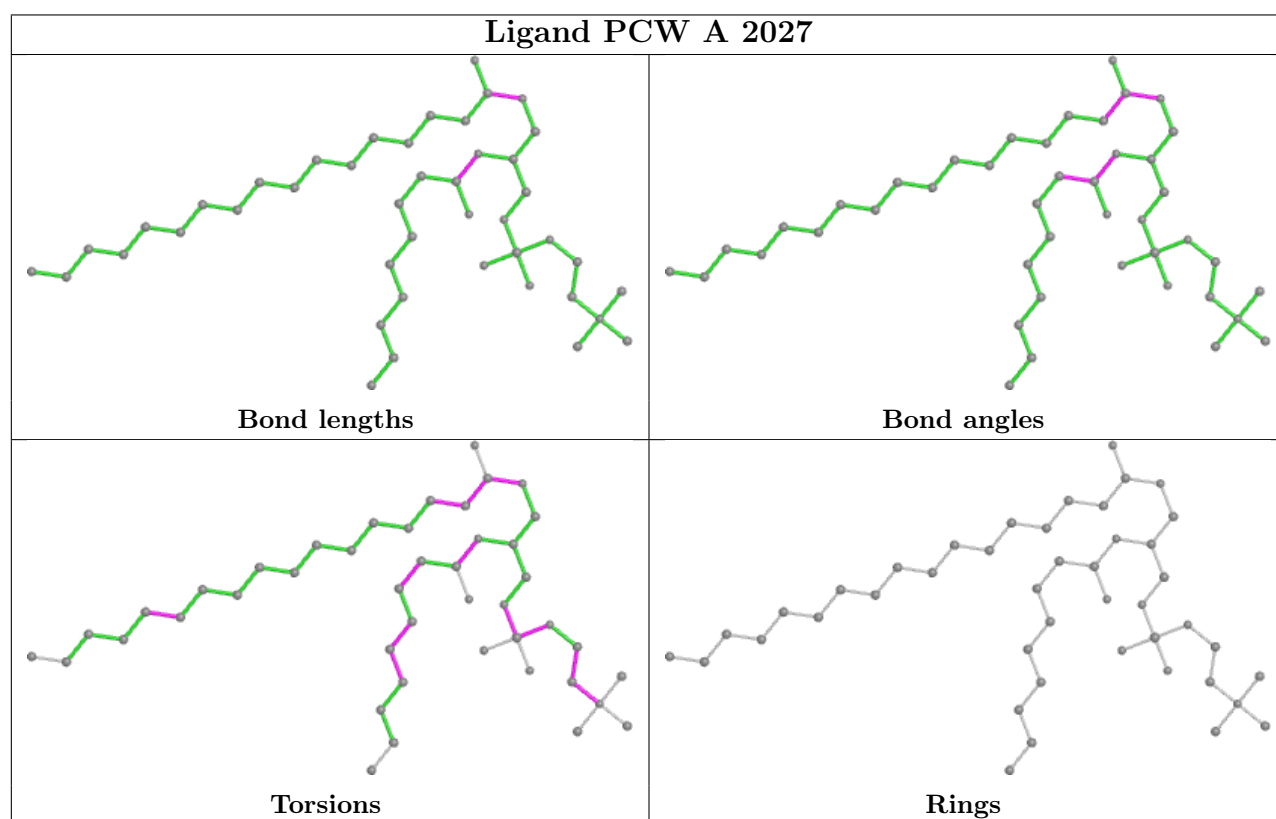
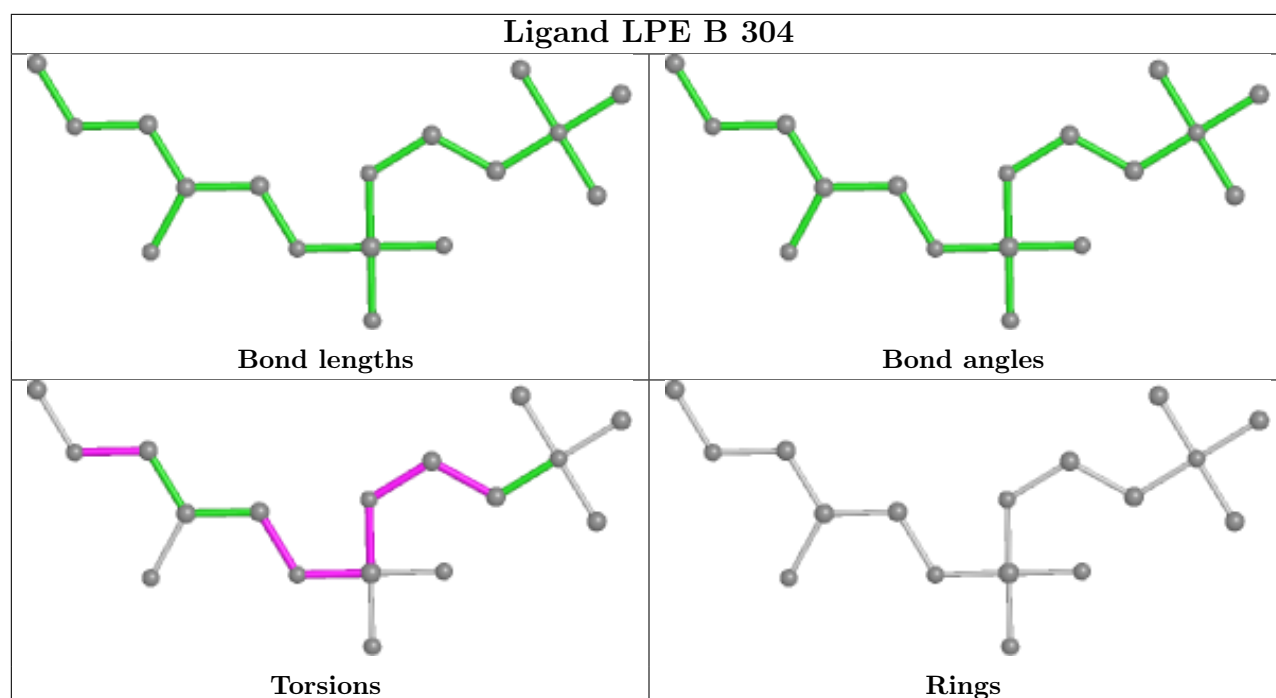




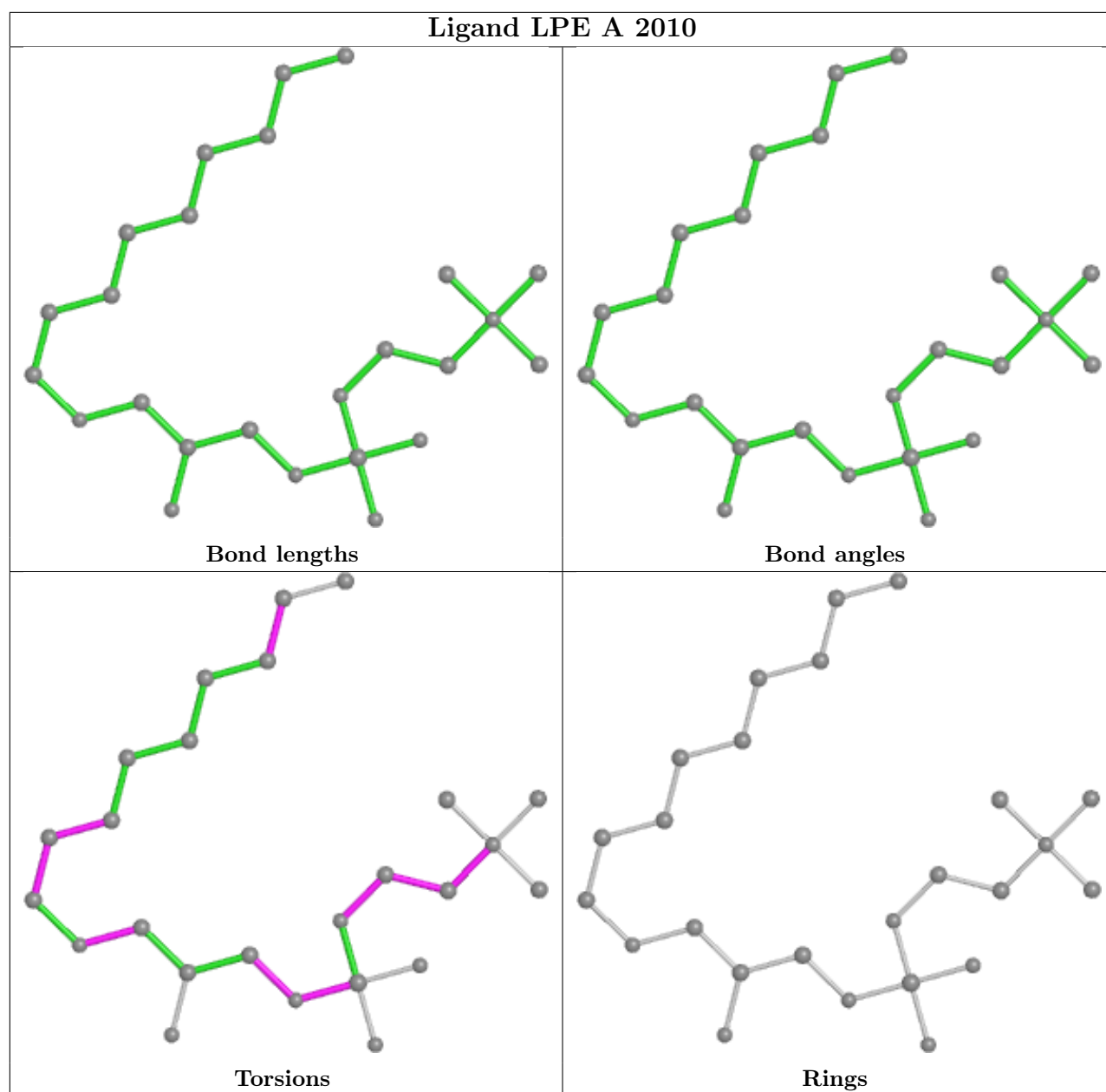












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

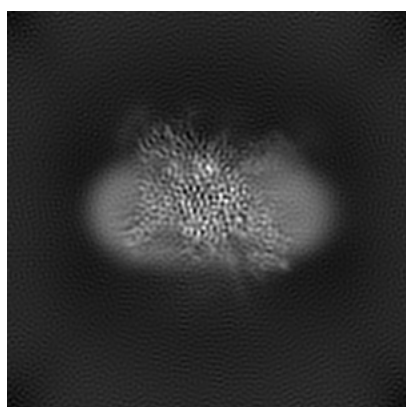
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32369. These allow visual inspection of the internal detail of the map and identification of artifacts.

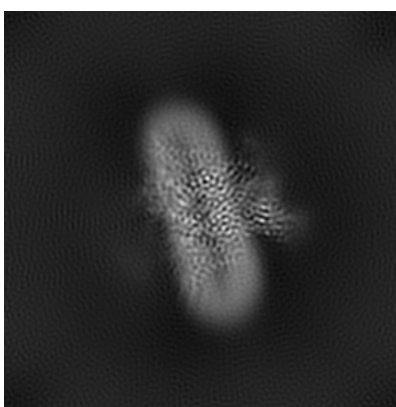
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

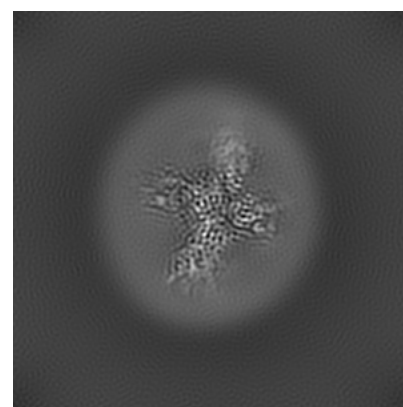
#### 6.1.1 Primary map



X



Y

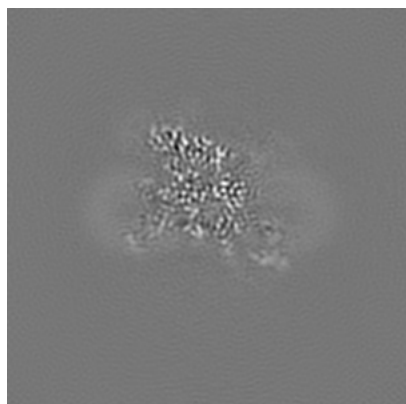


Z

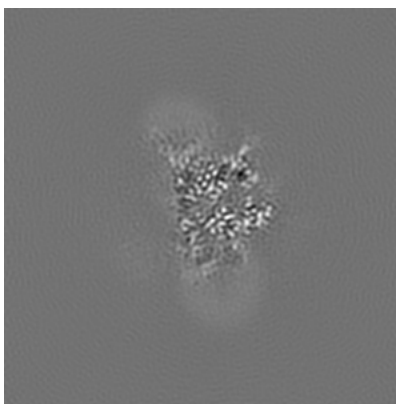
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

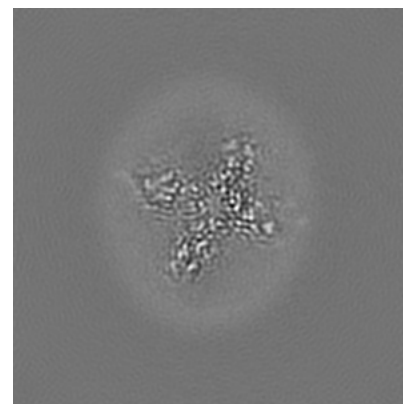
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

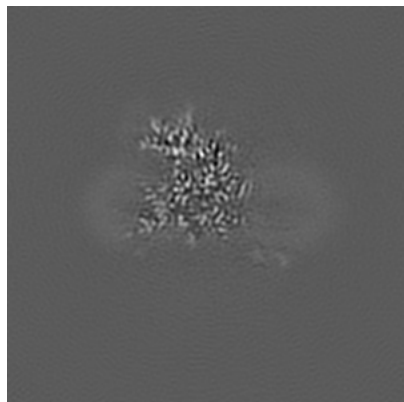


Z Index: 128

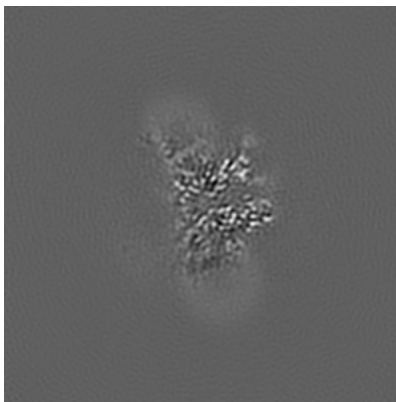
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

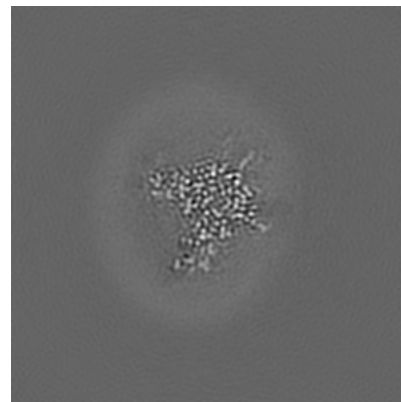
### 6.3.1 Primary map



X Index: 122



Y Index: 130



Z Index: 138

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.43. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

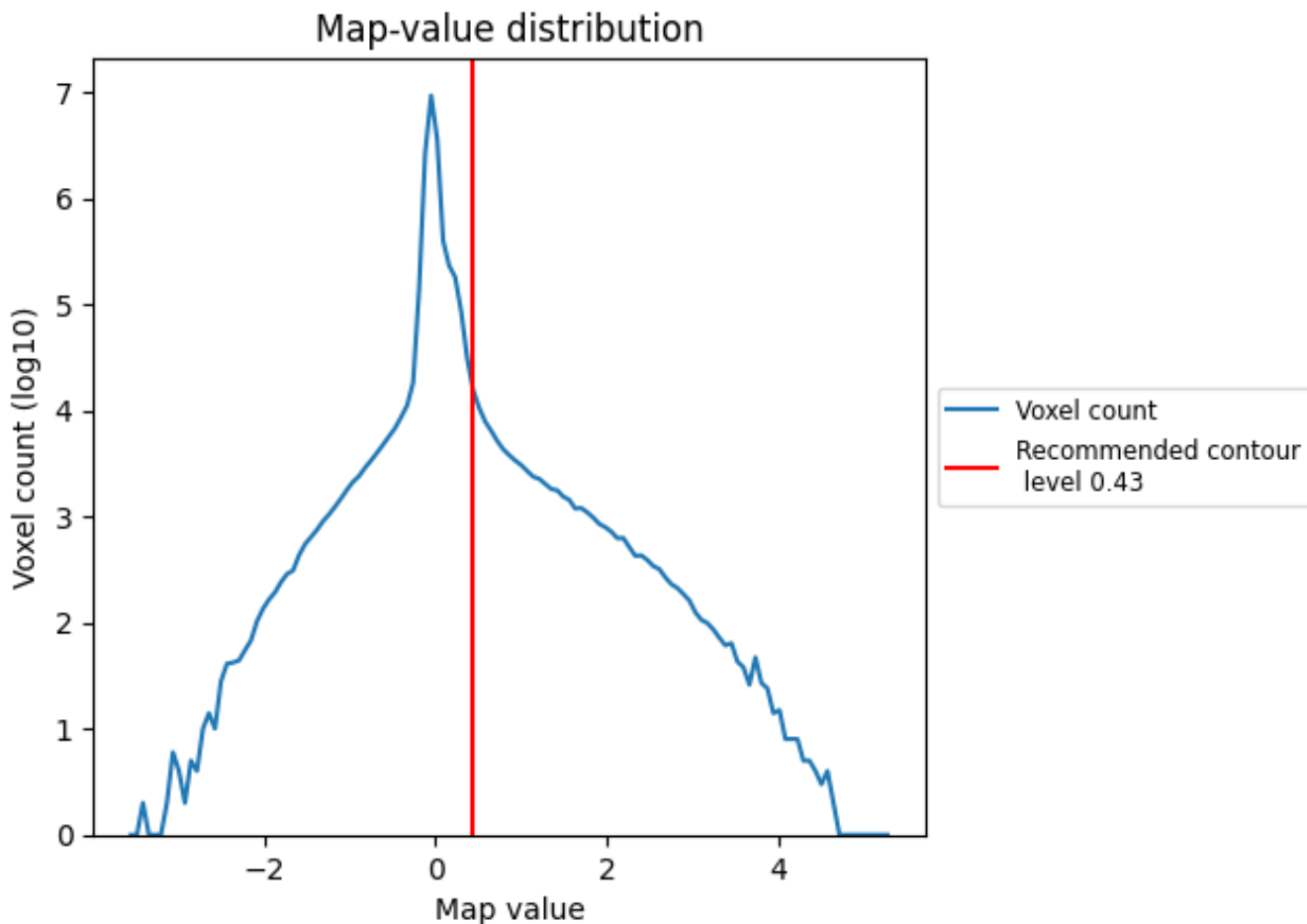
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

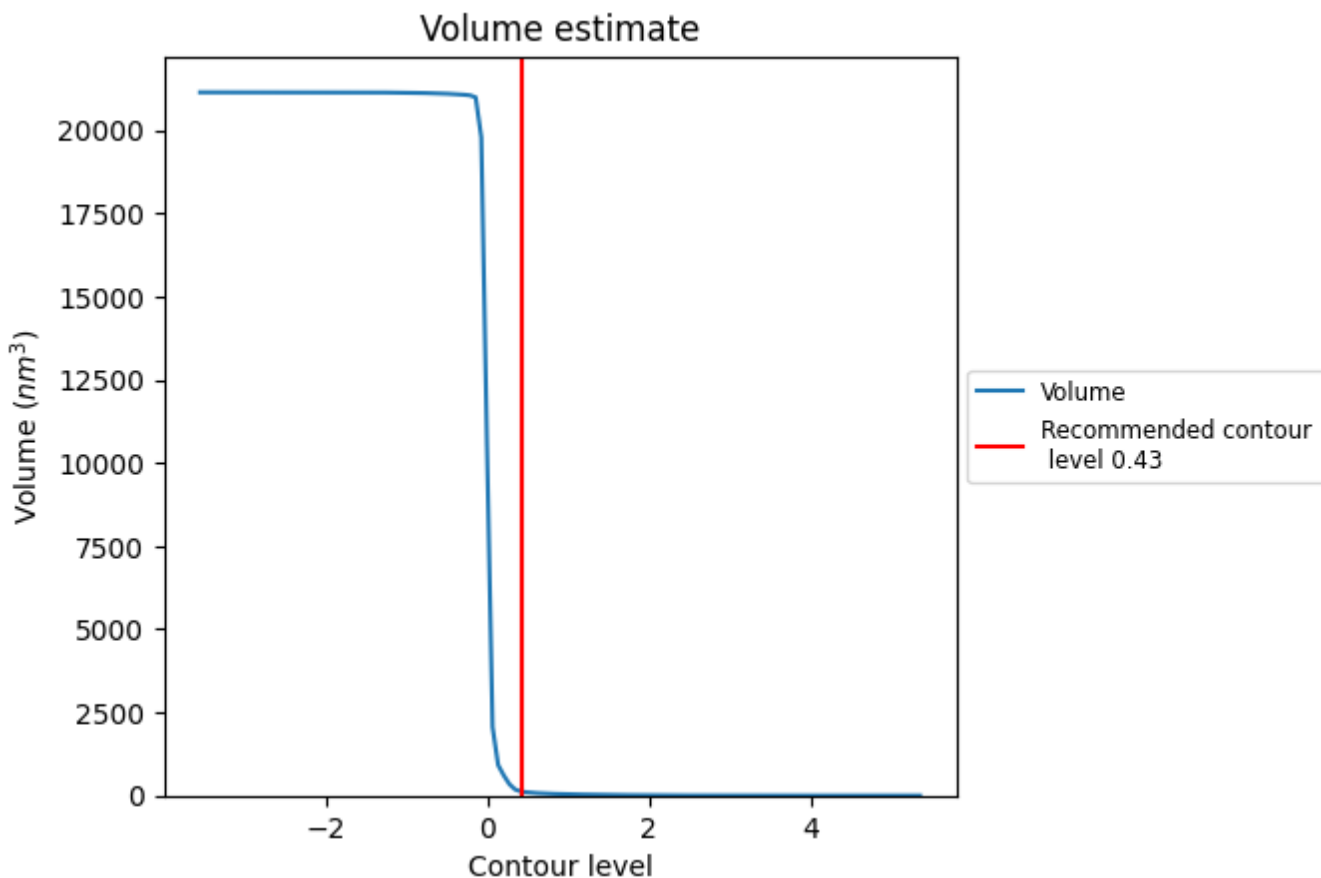
This section contains the results of statistical analysis of the map.

### 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.

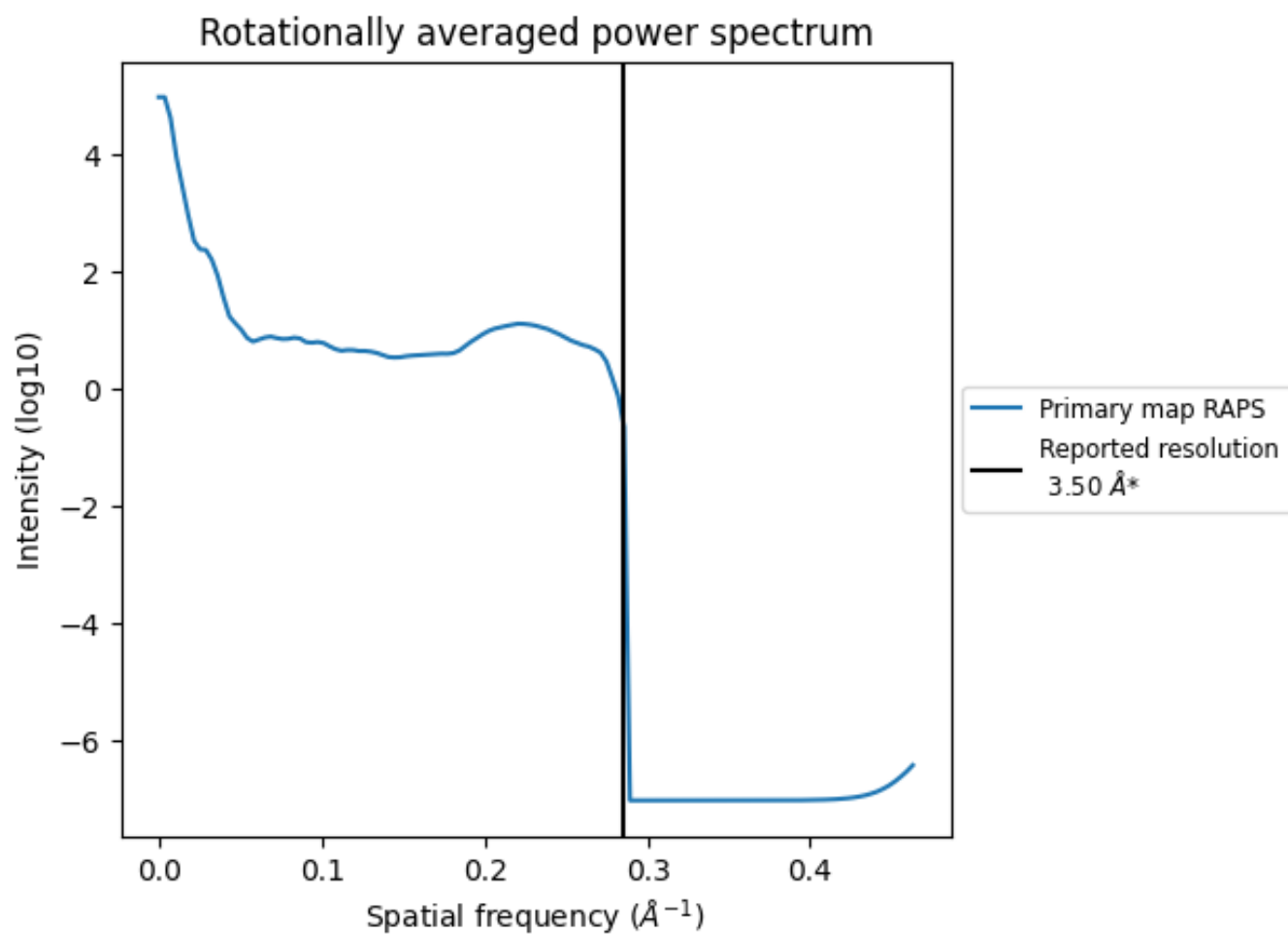
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm<sup>3</sup>; this corresponds to an approximate mass of 106 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 i



\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

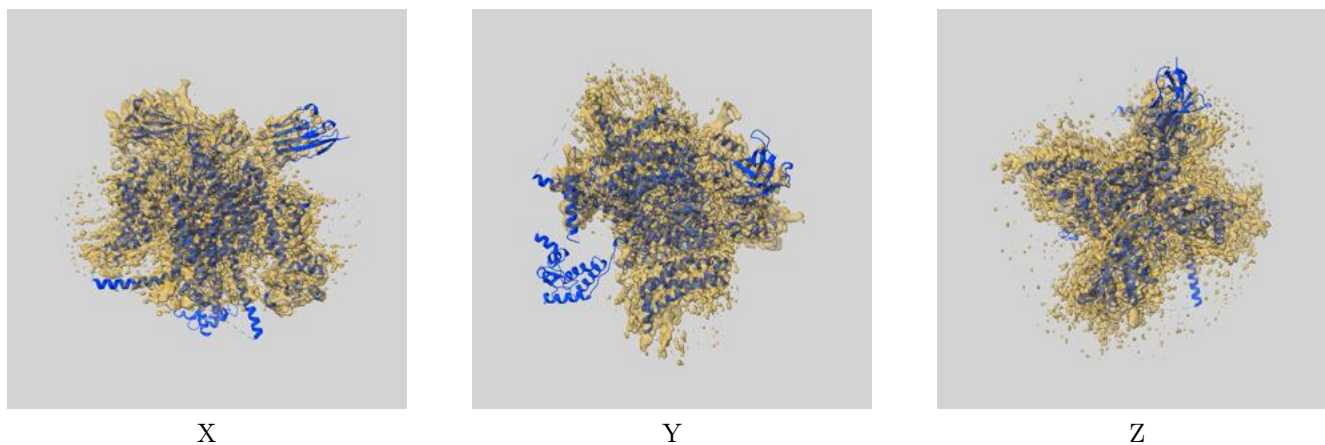
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

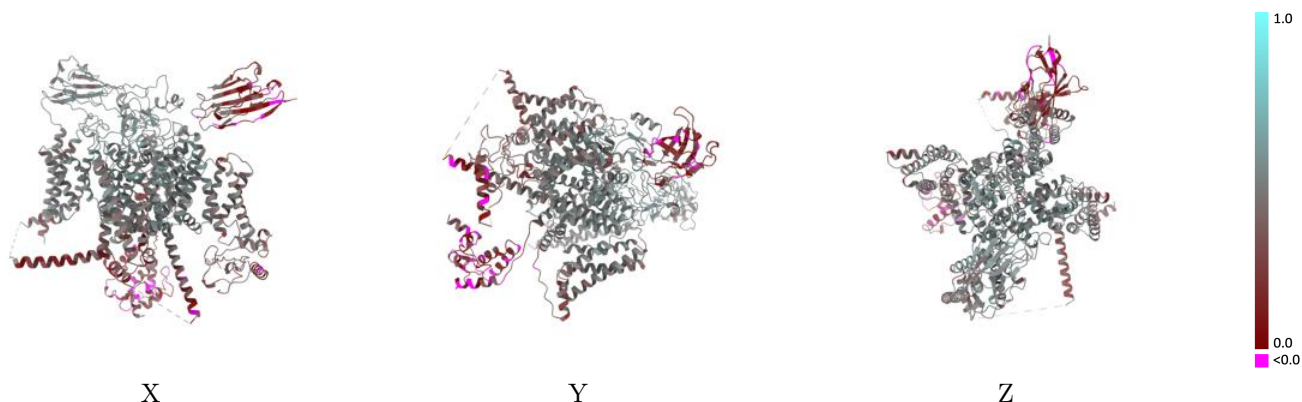
This section contains information regarding the fit between EMDB map EMD-32369 and PDB model 7W9L. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



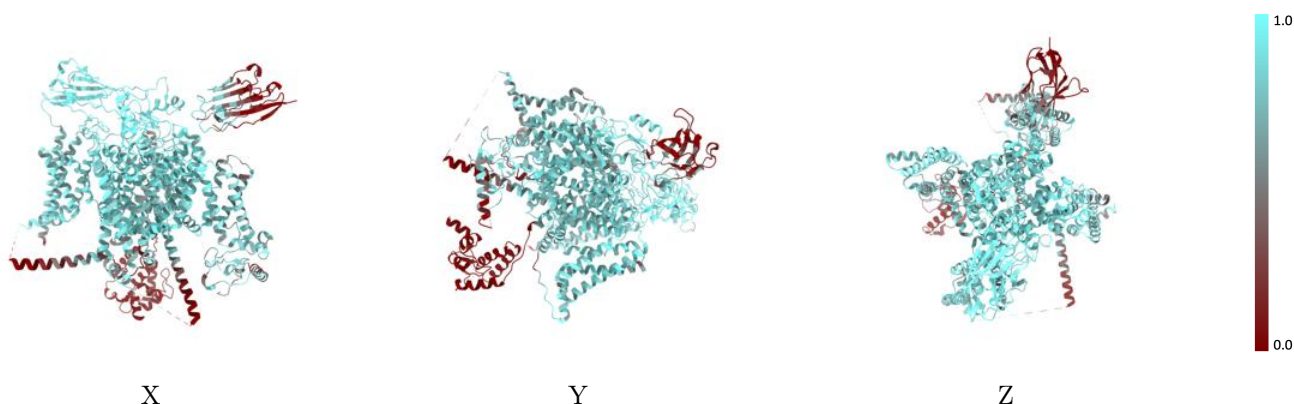
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



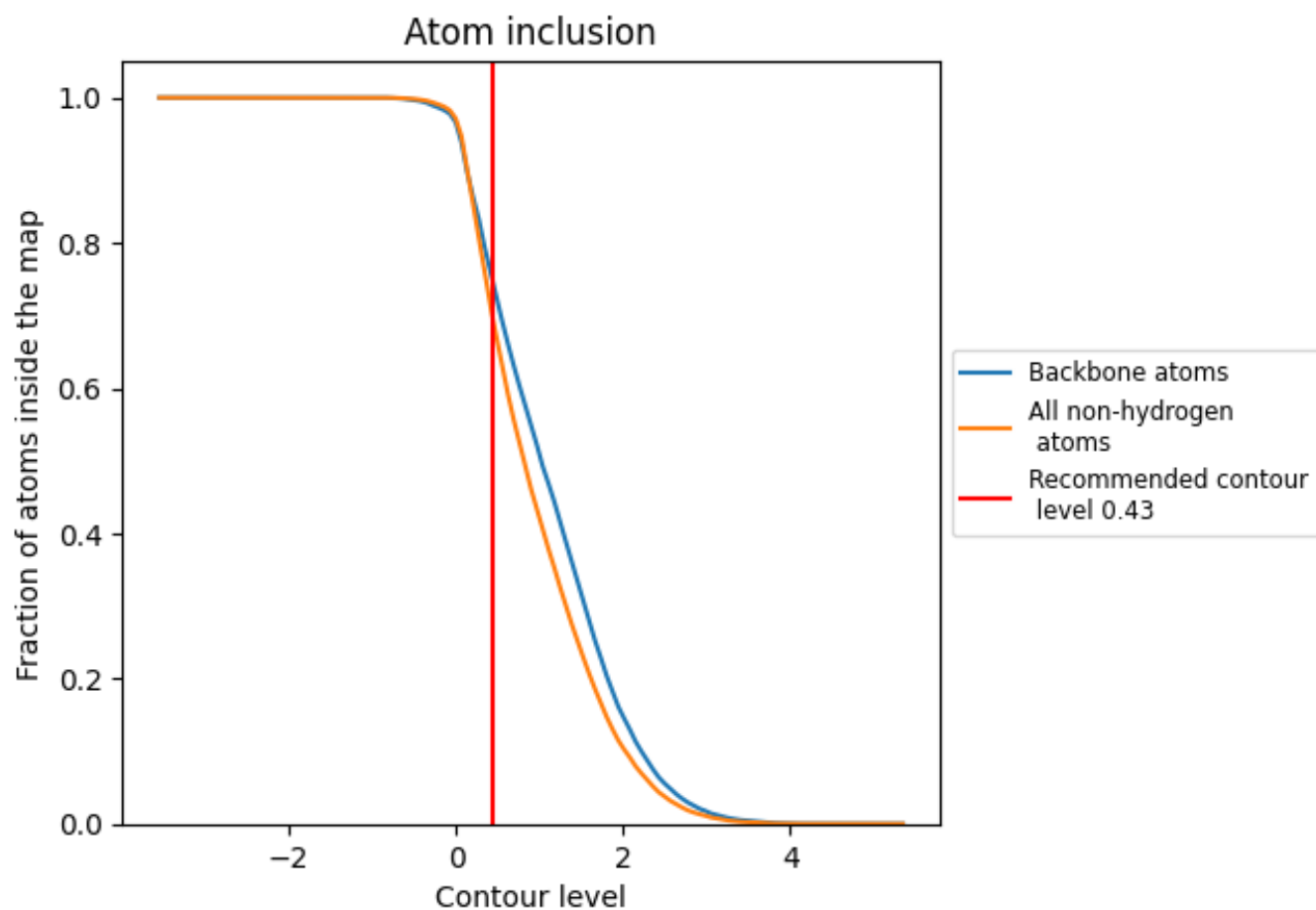
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.43).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7008	 0.4140
A	 0.7109	 0.4230
B	 0.8601	 0.4750
C	 0.3260	 0.2170
D	 0.7500	 0.3970
E	 0.6429	 0.2600
F	 0.8571	 0.4420

