



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 11:53 AM UTC

PDB ID : 7W9T / pdb_00007w9t
EMDB ID : EMD-32372
Title : Cryo-EM structure of human Nav1.7(E406K) in complex with auxiliary beta subunits, huwentoxin-IV and saxitoxin (S6IV alpha helix conformer)
Authors : Yan, N.; Huang, G.; Liu, D.; Wei, P.
Deposited on : 2021-12-10
Resolution : 3.00 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

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.dev132
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) : 2.49

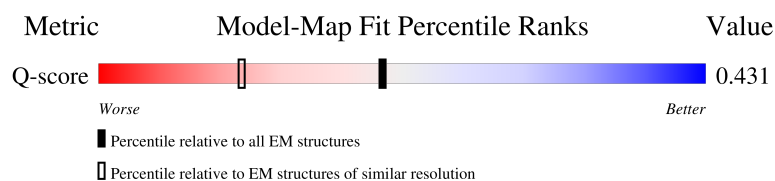
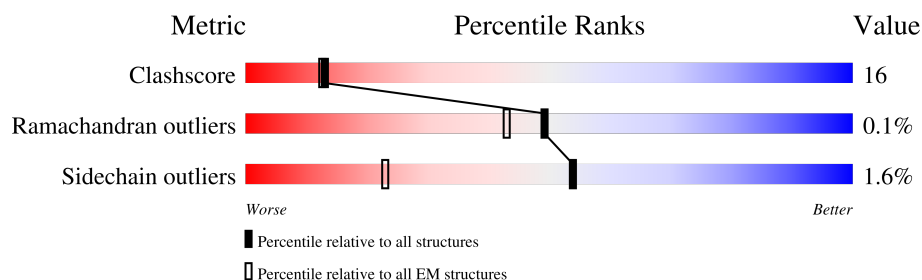
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

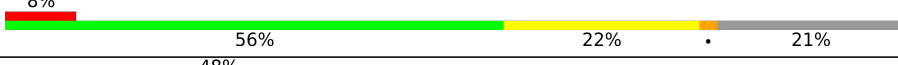
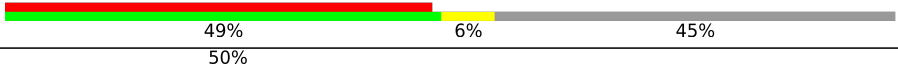
The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2031	
2	B	218	
3	C	215	
4	D	2	

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Mol	Chain	Length	Quality of chain
4	E	2	50% 100%
4	F	2	100%

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
11	PCW	A	2013	-	-	X	-
6	NAG	A	2008	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14841 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
1	A	1417	Total	C	N	O	S	0	0
			11419	7539	1798	1997	85		

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

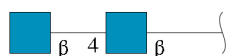
- Molecule 2 is a protein called Sodium channel subunit beta-1.

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

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

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

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



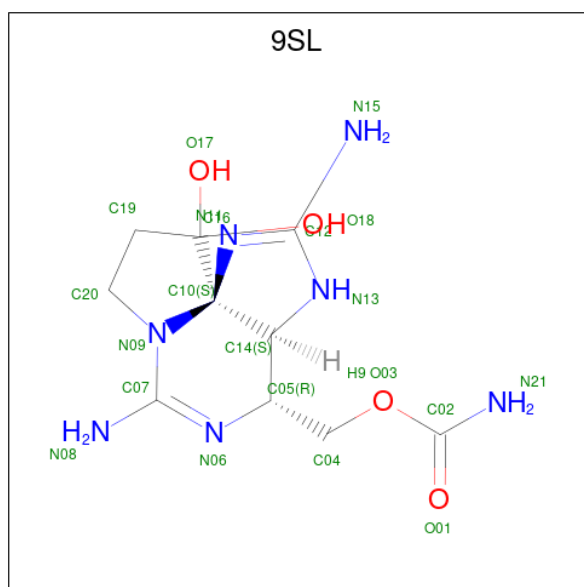
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

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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 [(3aS,4R,10aS)-2,6-diamino-10,10-dihydroxy-3a,4,9,10-tetrahydro-3H,8H-pyrrolo[1,2-c]purin-4-yl]methyl carbamate (CCD ID: 9SL) (formula: C₁₀H₁₇N₇O₄) (labeled as "Ligand of Interest" by depositor).



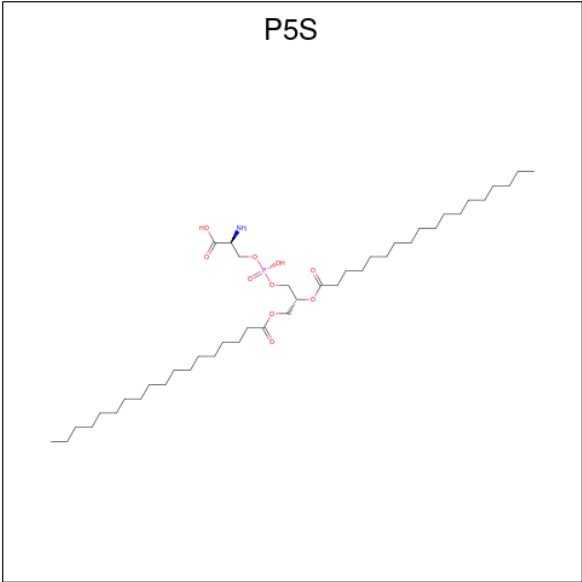
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	21	10	7	4	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



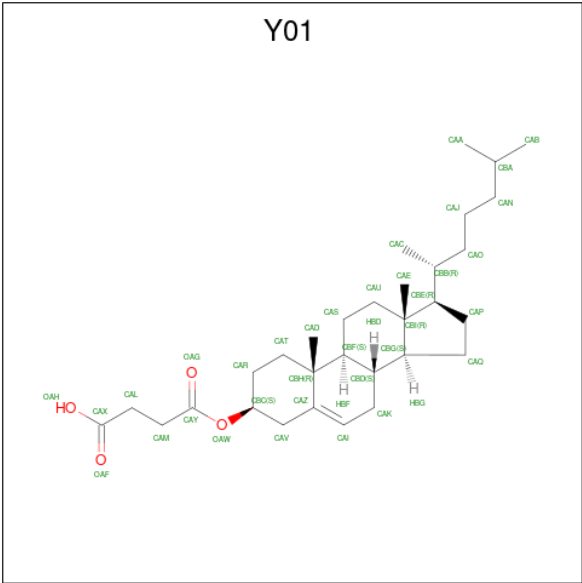
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			35	24	1	9	1	
7	A	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 8 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



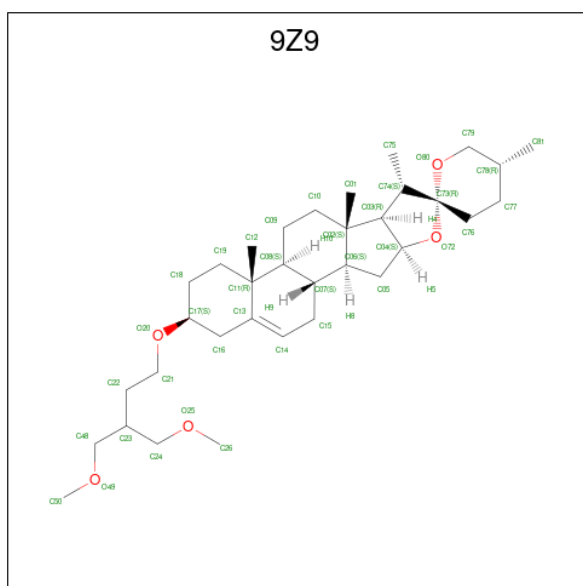
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	

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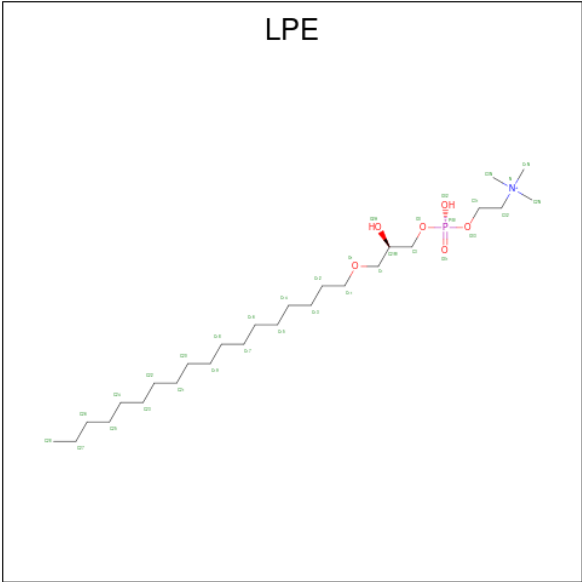
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	

- Molecule 9 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: C₃₄H₅₆O₅).



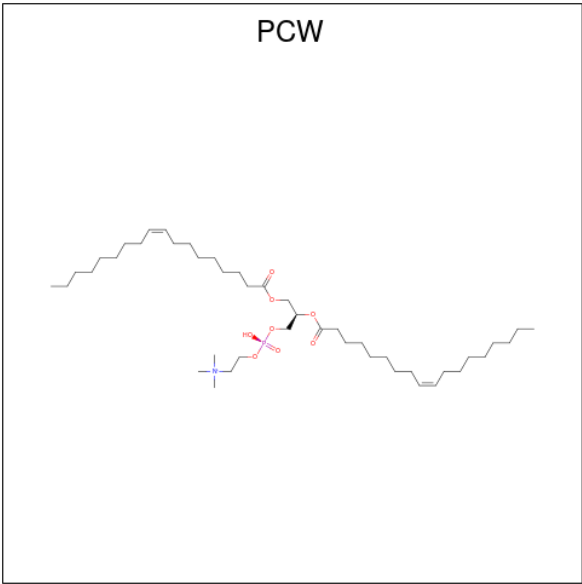
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			39	34	5	

- Molecule 10 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: LPE) (formula: C₂₆H₅₇NO₆P).



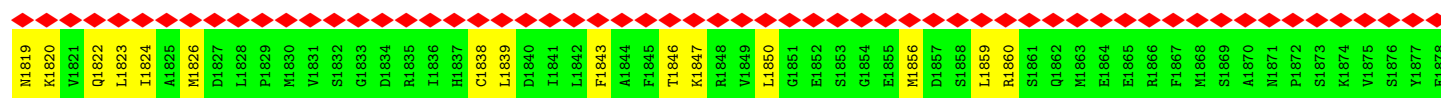
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			20	12	1	6	1	
10	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
10	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			17	9	1	6	1	
10	B	1	Total	C	N	O	P	0
			17	9	1	6	1	

- Molecule 11 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).

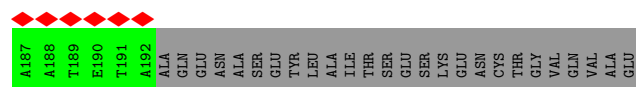
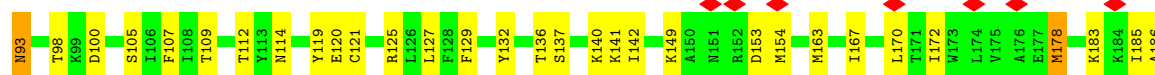
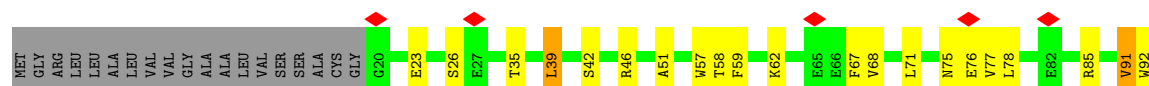


Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			53	43	1	8	1	
11	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

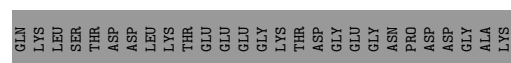
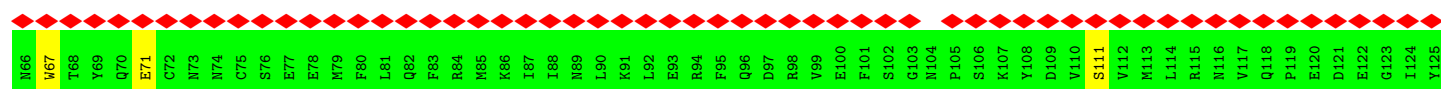
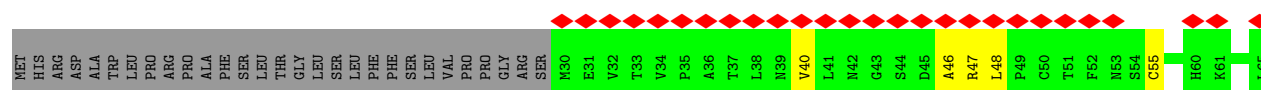
I1759	M1646	H1571	I1497	H1293	V1189	THR	HIS	F1009	M910	E802	ASN	HIS
L1760	L1649	Y1572	P1498	A1294	E1190	VAL	LEU	I1010	N911	Y803	CYS	LYS
E1761	L1650	Y1573	R1499	L1298	E1195	ASN	MET	L1011	N918	Y804	SER	LYS
M1762	P1500		G1501	L1301	I1216	PRO	LEU	K1012	L924	Q805	ARG	ARG
F1763	G1501		G1501	F1304	E1217	LEU	GLY	A1013	E927	G807	LYS	CYS
S1764	M1502	G1577	K1502	E1305	R1218	GLY	GLY	F1014		W808	TYR	SER
V1765	K1503	N1578	K1503	E1306	T1221	GLY	PHE	SER		W809	LEU	SER
F1766	I1504	N1580	I1504	M1307	I1225	GLY	ILE	LYS		W810	LEU	LEU
T1767	Y1657	D1582	Q1505	R1308	L1226	ALA	ASN	ILE		W811	SER	SER
E1768	F1583	F1583	G1506	V1309	D1230	GLU	PRO	SER		W812	ASP	ASP
E1769	V1584	V1584	C1507	V1310	I1232	GLU	ASN	ILE		W813	MET	GLU
S1770	V1585	V1585	I1508	N1311	D1230	ALA	PRO	ARG		W814	LEU	LEU
T1771	V1586	V1586	F1509	M1312	K1231	GLU	SER	GLY		W815	ASN	ASN
E1772	I1588	I1588	D1510	V1324	I1232	THR	THR	ILE		W816	ASP	ASP
P1773	S1589	S1589	G1512	L1325	Y1235	VAL	GLN	GLN		W817	PRO	PRO
L1774	I1590	I1590	V1512	L1326	E1240	THR	THR	ALA		W818	ASN	ASN
S1775	V1591	V1591	T1513	F1331	I1243	VAL	VAL	ALA		W819	LEU	LEU
E1776	G1592	G1592	M1514	L1332	K1244	ILE	PRO	GLU		W820	ARG	ARG
D1777	M1593	M1593	Q1515	L1333	W1245	GLU	ALA	LEU		W821	GLN	GLN
F1778	F1594	F1594	A1516	L1334	I1246	THR	THR	THR		W822	ALA	ALA
D1778	L1595	L1595	F1517	F1335	A1247	CYS	GLY	LYS		W823	MET	MET
F1779	A1596	A1596	D1518	F1336	Y1248	PHE	GLU	THR		W824	SER	SER
F1779	D1597	D1597	I1519	S1336	G1249	ASP	ASP	GLY		W825	ARG	ARG
E1780	S1697	S1697	S1520	L1337	Y1250	ASP	ASP	LEU		W826	ALA	ALA
M1781	I1689	I1689	I1521	M1338	Y1251	GLY	GLY	TYR		W827	SER	SER
F1782	W1700	W1700	M1522	G1339	I1252	CYS	ASN	ILE		W828	ILE	ILE
F1783	D1701	D1701	I1525	V1340	F1253	VAL	THR	ILE		W829	LEU	LEU
E1784	G1702	G1702	C1526	Y1348	Y1254	TRP	MET	ASN		W830	ASN	ASN
V1785	L1703	L1703	L1527	P1360	A1257	ARG	ALA	ASN		W831	THR	THR
W1786	P1706	P1706	L1528	Q1363	I1257	SER	GLU	THR		W832	VAL	VAL
E1787	I1707	I1707	M1529	V1364	W1260	CYS	GLU	LEU		W833	GLU	GLU
K1788	L1708	L1708	V1530	V1365	I1268	CYS	LEU	ALA		W834	LEU	LEU
F1789	M1709	M1709	M1531	N1366	V1268	GLN	SER	MET		W835	GLU	GLU
D1790	C1730	C1730	M1532	N1367	V1274	VAL	ASP	SER		W836	GLU	GLU
P1791	V1735	V1735	M1533	S1368	M1275	ILE	SER	LYS		W837	ARG	ARG
D1792	V1736	V1736	E1537	E1369	A1276	GLU	ASP	GLY		W838	SER	SER
A1793	I1737	I1737	M1543	M1374	M1277	SER	GLU	ASN		W839	GLN	GLN
T1794	F1738	F1738	T1544	N1375	T1277	THR	TYR	PHE		W840	LYS	LYS
Q1795	V1739	V1739	E1545	V1376	L1278	LEU	LEU	LEU		W841	CYS	CYS
F1796	V1741	V1741	V1546	S1377	G1279	SER	SER	LEU		W842	PRO	PRO
I1797	I1744	I1744	W1549	Q1378	Y1280	VAL	VAL	GLU		W843	PRO	PRO
E1798	F1748	F1748	V1553	R1381	S1281	ARG	ARG	ASP		W844	TRP	TRP
F1799	V1752	V1752	F1558	N1384	D1282	LEU	ASN	LYS		W845	TYR	TYR
K1801	M1753	M1753	T1559	L1283	I1181	ASN	ILE	ILE		W846	ARG	ARG
L1802	M1754	M1754	G1560	G1284	R1182	GLY	ARG	GLY		W847	PHE	PHE
S1803	V1755	V1755	E1561	N1388	R1183	GLY	SER	GLY		W848	ALA	ALA
D1804	A1757	A1757	E1561	V1392	T1184	GLY	SER	PHE		W849	GLY	GLY
F1805	V1758	V1758	L1564	G1393	I1286	SER	GLU	GLY		W850	LYS	LYS
A1806			K1565	S1490	K1287	ASP	ASP	SER		W851	PHE	PHE
A1807			L1566	K1491	S1288	VAL	VAL	VAL		W852	LEU	LEU
A1808			L1566	K1492	R1289	ASP	ASP	ASP		W853	TRP	TRP
L1809			L1567	Q1493	R1290	LYS	LYS	LYS		W854	ARG	ARG
D1810			S1568	Q1494	T1291	THR	THR	THR		W855	ALA	ALA
P1811			L1569	K1495	L1292	THR	THR	THR		W856	ALA	ALA
P1812			R1570	P1496						W857	ALA	ALA
L1813										W858	ALA	ALA
L1814										W859	ALA	ALA
I1815										W860	ALA	ALA
A1816										W861	ALA	ALA
K1817										W862	ALA	ALA
P1818										W863	ALA	ALA



• Molecule 2: Sodium channel subunit beta-1



• Molecule 3: Sodium channel subunit beta-2



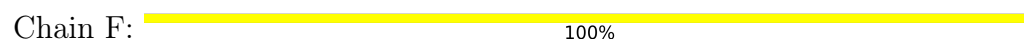
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	165021	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	2.876	Depositor
Minimum map value	-1.308	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.63	Depositor
Map size (Å)	261.84, 261.84, 261.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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: 9SL, P5S, Y01, NAG, LPE, 9Z9, PCW

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	0.45	2/11693 (0.0%)	0.65	16/15834 (0.1%)
2	B	0.37	0/1442	0.48	0/1949
3	C	0.35	0/1011	0.58	0/1367
All	All	0.43	2/14146 (0.0%)	0.63	16/19150 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1658	TYR	C-O	-5.34	1.17	1.24
1	A	1528	ASN	C-O	-5.08	1.18	1.24

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1418	SER	N-CA-C	8.82	122.34	108.67
1	A	1419	VAL	N-CA-C	8.58	118.59	110.53
1	A	1769	GLU	N-CA-C	7.68	122.53	110.32
1	A	1421	VAL	N-CA-C	7.51	118.28	110.62
1	A	1249	GLY	CA-C-O	-6.21	117.94	122.23

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	11419	0	11645	378	0
2	B	1416	0	1380	43	0
3	C	980	0	935	4	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
5	A	21	0	0	3	0
6	A	28	0	26	9	0
6	B	42	0	39	0	0
7	A	76	0	96	21	0
8	A	175	0	245	48	0
9	A	39	0	0	9	0
10	A	312	0	426	84	0
10	B	17	0	19	9	0
11	A	232	0	321	35	0
All	All	14841	0	15207	493	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 16.

The worst 5 of 493 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:A:1602:TYR:CE2	1:A:1603:PHE:CE1	1.76	1.65
1:A:1602:TYR:CE2	1:A:1603:PHE:HE1	1.04	1.64
1:A:1602:TYR:CD2	1:A:1603:PHE:CE1	1.92	1.53
2:B:178:MET:HE1	10:B:304:LPE:C1	1.55	1.35
1:A:1602:TYR:CD2	1:A:1603:PHE:CD1	2.18	1.28

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	1409/2031 (69%)	1337 (95%)	71 (5%)	1 (0%)	48 80
2	B	171/218 (78%)	156 (91%)	14 (8%)	1 (1%)	21 56
3	C	120/215 (56%)	116 (97%)	4 (3%)	0	100 100
All	All	1700/2464 (69%)	1609 (95%)	89 (5%)	2 (0%)	49 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1492	LYS
2	B	76	GLU

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	1266/1809 (70%)	1251 (99%)	15 (1%)	63 82
2	B	157/190 (83%)	152 (97%)	5 (3%)	34 67
3	C	114/193 (59%)	109 (96%)	5 (4%)	25 60
All	All	1537/2192 (70%)	1512 (98%)	25 (2%)	54 79

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1595	LEU
2	B	93	ASN
3	C	147	LEU
2	B	91	VAL
2	B	167	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1539	GLN

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Mol	Chain	Res	Type
3	C	53	ASN
1	A	1721	HIS
1	A	1871	ASN
3	C	145	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	0.25	0	17,19,21	0.48	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.40	0
4	NAG	E	1	1,4	14,14,15	0.17	0	17,19,21	0.48	0
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.68	0
4	NAG	F	1	4,2	14,14,15	0.56	0	17,19,21	1.18	2 (11%)
4	NAG	F	2	4	14,14,15	0.66	0	17,19,21	1.22	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,2	-	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.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	2.75	115.87	112.19
4	F	1	NAG	C3-C4-C5	-2.60	105.52	110.23
4	F	2	NAG	C4-C3-C2	-2.42	107.47	111.02

There are no chirality outliers.

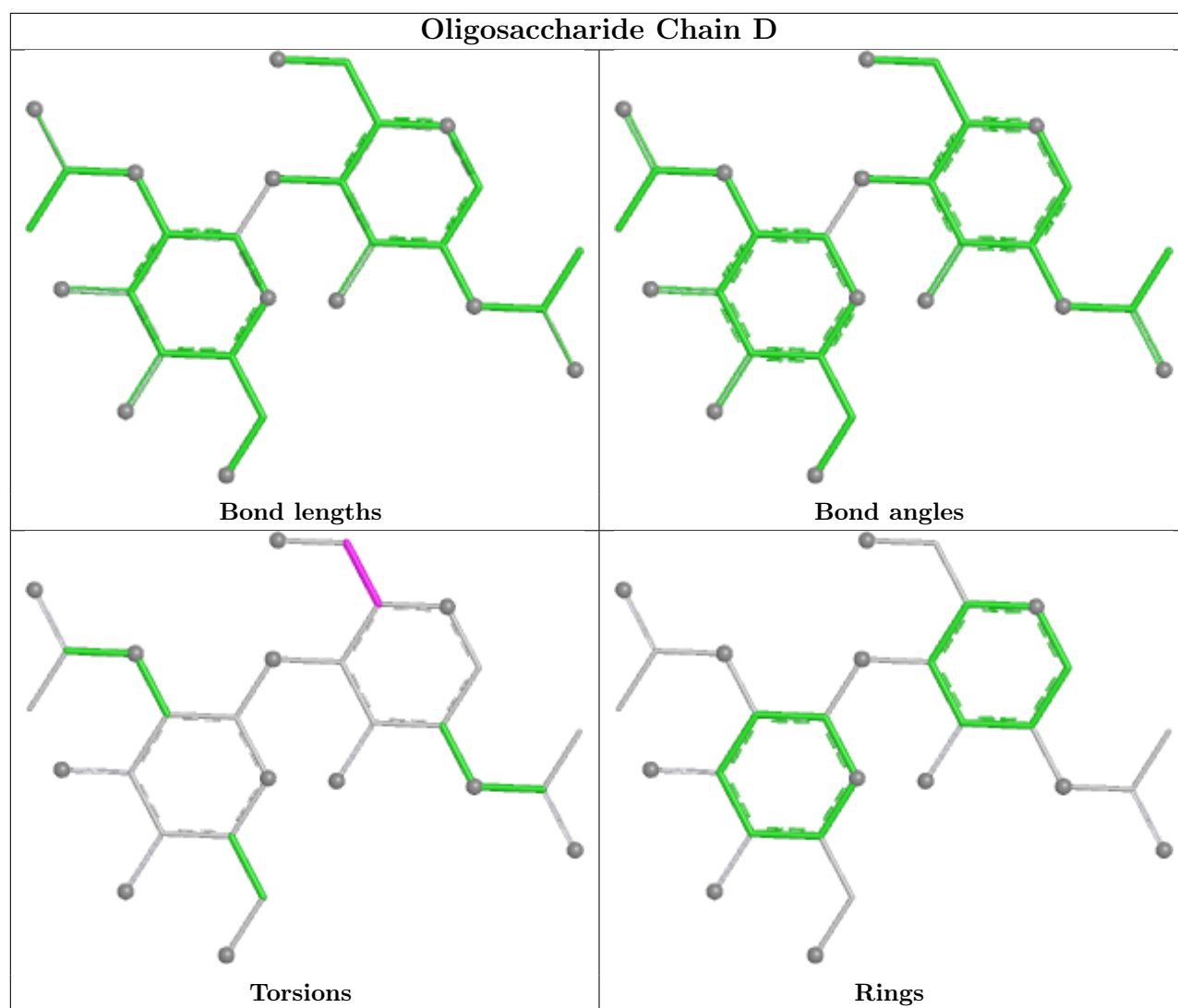
5 of 10 torsion outliers are listed below:

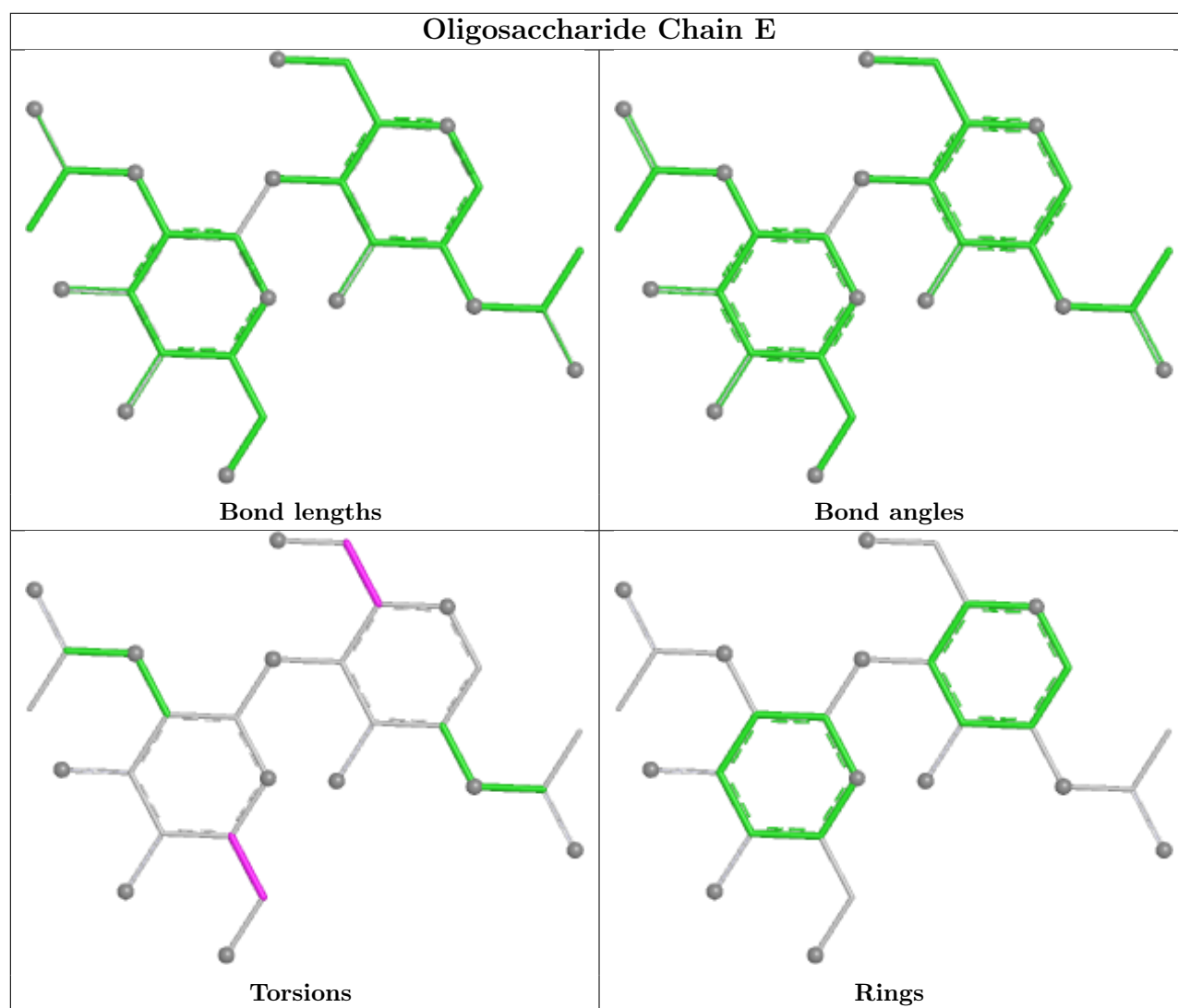
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6

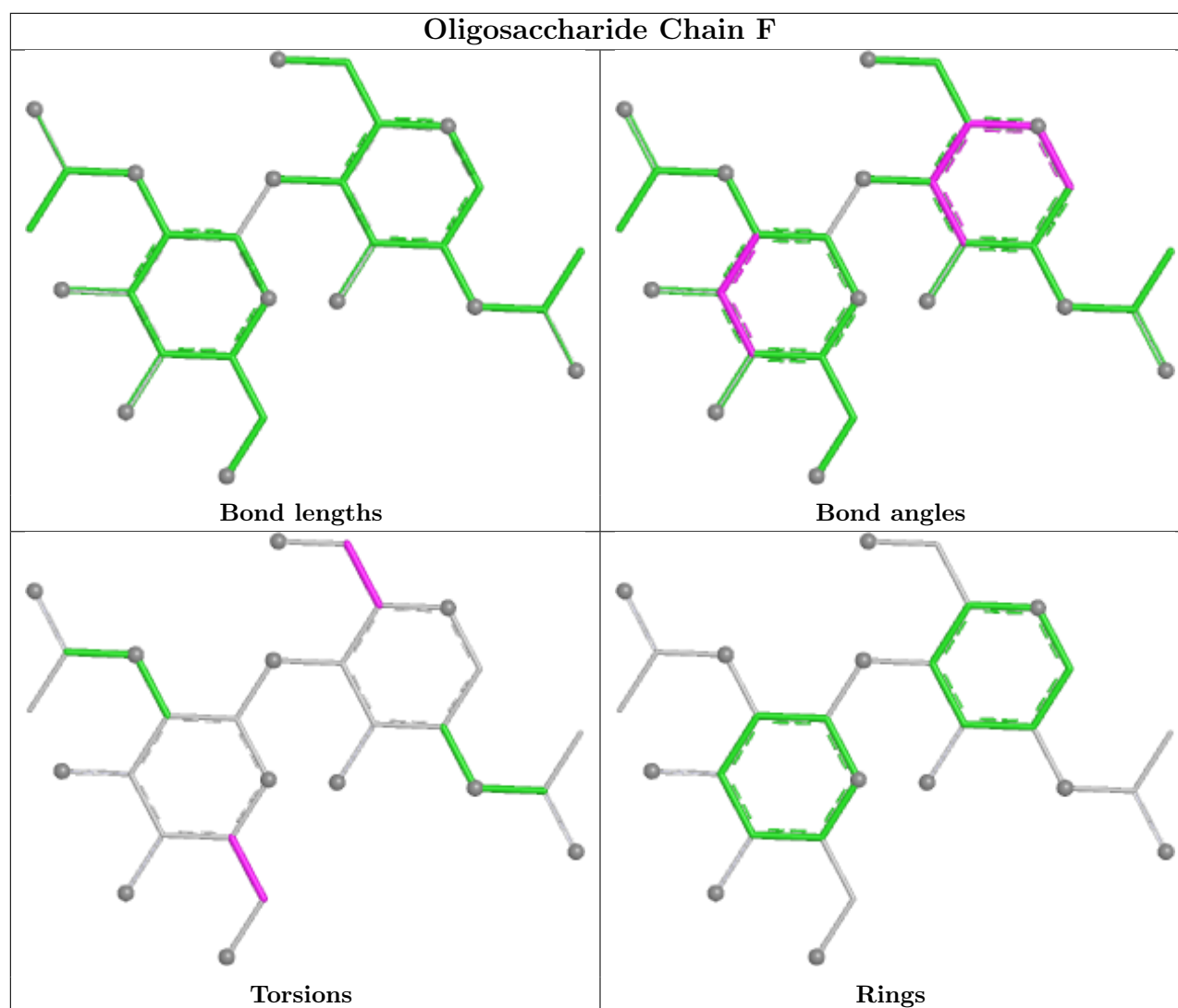
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

33 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	$\# Z > 2$
10	LPE	A	2025	-	24,24,33	0.55	0	28,30,39	0.50	0
6	NAG	B	303	2	14,14,15	0.27	0	17,19,21	0.44	0
6	NAG	B	301	2	14,14,15	0.64	0	17,19,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	P5S	A	2003	-	33,34,53	0.77	1 (3%)	34,40,60	1.79	4 (11%)
10	LPE	A	2021	-	24,24,33	0.55	0	28,30,39	0.69	1 (3%)
10	LPE	A	2011	-	24,24,33	0.33	0	25,27,39	0.61	0
11	PCW	A	2018	-	43,43,53	1.02	2 (4%)	49,51,61	1.13	6 (12%)
6	NAG	A	2008	1	14,14,15	0.31	0	17,19,21	0.99	1 (5%)
10	LPE	A	2015	-	27,27,33	0.55	0	31,33,39	0.62	0
8	Y01	A	2005	-	38,38,38	0.68	1 (2%)	57,57,57	1.83	13 (22%)
10	LPE	A	2023	-	24,24,33	0.54	0	28,30,39	0.54	0
11	PCW	A	2028	-	43,43,53	1.00	2 (4%)	49,51,61	2.88	6 (12%)
10	LPE	A	2010	-	24,24,33	0.53	0	28,30,39	0.61	0
10	LPE	A	2012	-	19,19,33	0.64	0	23,25,39	0.52	0
6	NAG	B	302	2	14,14,15	0.19	0	17,19,21	0.43	0
7	P5S	A	2017	-	40,40,53	1.18	3 (7%)	43,45,60	1.38	3 (6%)
8	Y01	A	2006	-	38,38,38	1.17	4 (10%)	57,57,57	1.79	12 (21%)
8	Y01	A	2009	-	38,38,38	1.17	4 (10%)	57,57,57	1.79	12 (21%)
10	LPE	A	2024	-	24,24,33	0.52	0	28,30,39	0.63	0
10	LPE	B	304	-	16,16,33	0.68	0	20,22,39	0.61	0
8	Y01	A	2004	-	38,38,38	0.69	1 (2%)	57,57,57	1.83	12 (21%)
11	PCW	A	2016	-	46,46,53	1.00	3 (6%)	52,54,61	1.19	4 (7%)
10	LPE	A	2019	-	24,24,33	0.61	0	28,30,39	0.90	1 (3%)
11	PCW	A	2013	-	52,52,53	0.94	2 (3%)	58,60,61	0.98	2 (3%)
8	Y01	A	2029	-	38,38,38	1.66	7 (18%)	57,57,57	1.68	12 (21%)
10	LPE	A	2022	-	24,24,33	0.54	0	28,30,39	0.65	0
10	LPE	A	2026	-	16,16,33	0.70	0	20,22,39	0.69	0
5	9SL	A	2001	-	17,23,23	3.66	9 (52%)	14,37,37	2.99	7 (50%)
10	LPE	A	2020	-	24,24,33	0.88	0	28,30,39	0.91	1 (3%)
9	9Z9	A	2007	-	44,44,44	0.73	1 (2%)	64,68,68	1.51	11 (17%)
6	NAG	A	2002	1	14,14,15	0.35	0	17,19,21	0.46	0
10	LPE	A	2014	-	21,21,33	0.70	0	25,27,39	1.05	2 (8%)
11	PCW	A	2027	-	43,43,53	1.04	2 (4%)	49,51,61	0.95	2 (4%)

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
10	LPE	A	2025	-	-	10/25/25/34	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	303	2	-	0/6/23/26	0/1/1/1
6	NAG	B	301	2	-	0/6/23/26	0/1/1/1
7	P5S	A	2003	-	-	27/39/39/59	-
10	LPE	A	2021	-	-	2/25/25/34	-
10	LPE	A	2011	-	-	8/25/25/34	-
11	PCW	A	2018	-	-	10/47/47/57	-
6	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
10	LPE	A	2015	-	-	8/28/28/34	-
8	Y01	A	2005	-	-	0/19/77/77	0/4/4/4
10	LPE	A	2023	-	-	7/25/25/34	-
11	PCW	A	2028	-	-	10/47/47/57	-
10	LPE	A	2010	-	-	8/25/25/34	-
10	LPE	A	2012	-	-	8/20/20/34	-
6	NAG	B	302	2	-	0/6/23/26	0/1/1/1
7	P5S	A	2017	-	-	8/44/44/59	-
8	Y01	A	2006	-	-	4/19/77/77	0/4/4/4
8	Y01	A	2009	-	-	4/19/77/77	0/4/4/4
10	LPE	A	2024	-	-	4/25/25/34	-
10	LPE	B	304	-	-	9/17/17/34	-
8	Y01	A	2004	-	-	0/19/77/77	0/4/4/4
11	PCW	A	2016	-	-	12/50/50/57	-
10	LPE	A	2019	-	-	5/25/25/34	-
11	PCW	A	2013	-	-	16/56/56/57	-
8	Y01	A	2029	-	-	7/19/77/77	0/4/4/4
10	LPE	A	2022	-	-	3/25/25/34	-
10	LPE	A	2026	-	-	6/17/17/34	-
5	9SL	A	2001	-	-	4/5/53/53	0/3/3/3
10	LPE	A	2020	-	-	11/25/25/34	-
9	9Z9	A	2007	-	-	0/12/100/100	0/6/6/6
6	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
10	LPE	A	2014	-	-	15/22/22/34	-
11	PCW	A	2027	-	-	15/47/47/57	-

The worst 5 of 42 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	9SL	C12-N13	8.85	1.49	1.35
5	A	2001	9SL	C07-N08	6.30	1.45	1.34
5	A	2001	9SL	C02-N21	6.16	1.44	1.33
5	A	2001	9SL	C12-N15	4.65	1.45	1.34
8	A	2029	Y01	CBB-CBE	-4.44	1.46	1.54

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2028	PCW	C8-N-C6	-11.84	77.88	108.98
11	A	2028	PCW	C8-N-C7	-11.78	78.04	108.98
11	A	2028	PCW	C8-N-C5	-8.04	77.97	109.91
5	A	2001	9SL	O03-C02-N21	7.78	120.78	111.11
7	A	2003	P5S	OG-CB-CA	7.06	114.22	108.06

There are no chirality outliers.

5 of 225 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2001	9SL	O01-C02-O03-C04
5	A	2001	9SL	N21-C02-O03-C04
5	A	2001	9SL	O03-C04-C05-N06
5	A	2001	9SL	O03-C04-C05-C14
7	A	2003	P5S	C-CA-CB-OG

There are no ring outliers.

29 monomers are involved in 189 short contacts:

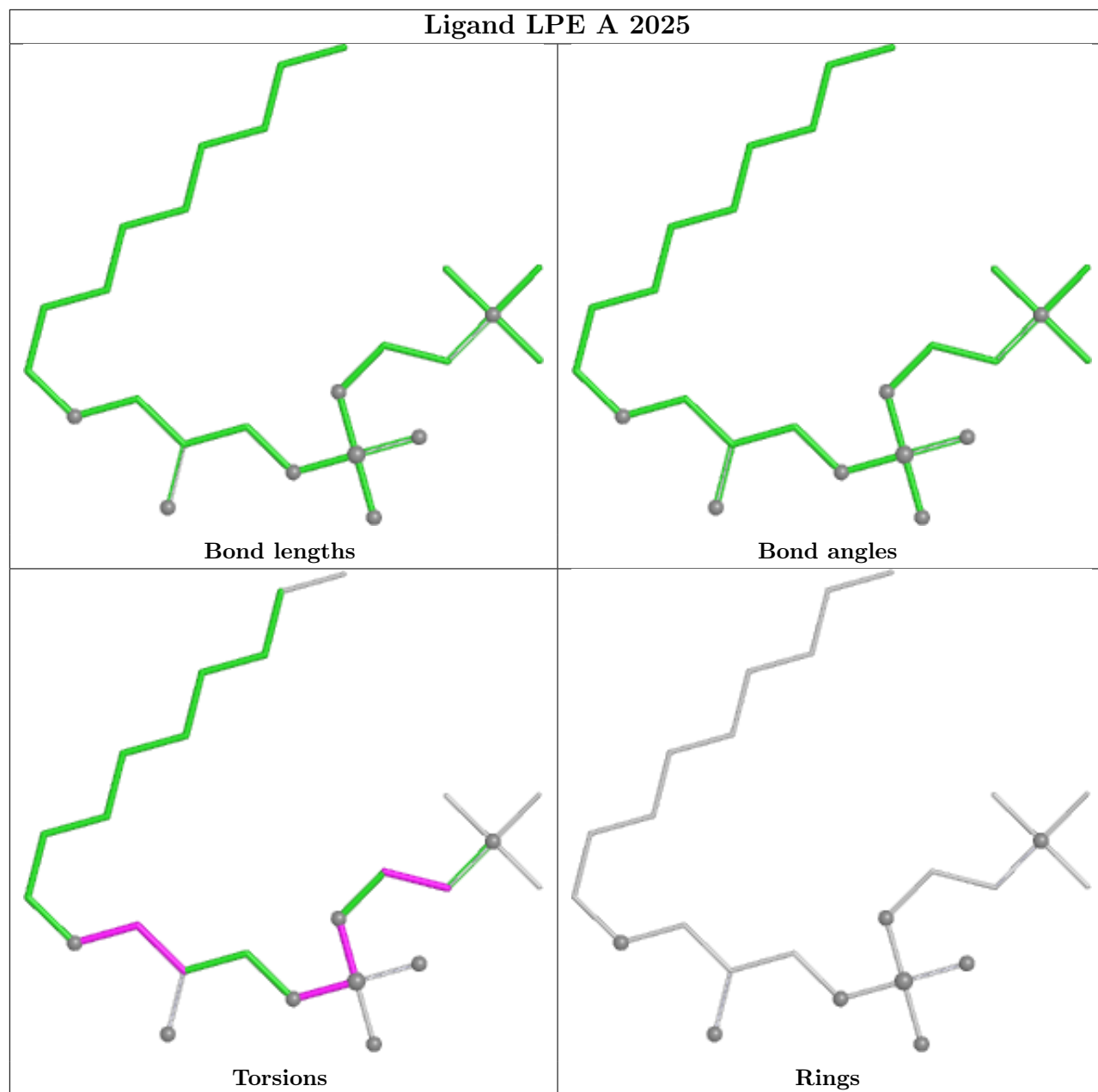
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2025	LPE	11	0
7	A	2003	P5S	12	0
10	A	2021	LPE	11	0
10	A	2011	LPE	2	0
11	A	2018	PCW	6	0
6	A	2008	NAG	9	0
10	A	2015	LPE	6	0
8	A	2005	Y01	3	0
10	A	2023	LPE	8	0
11	A	2028	PCW	2	0

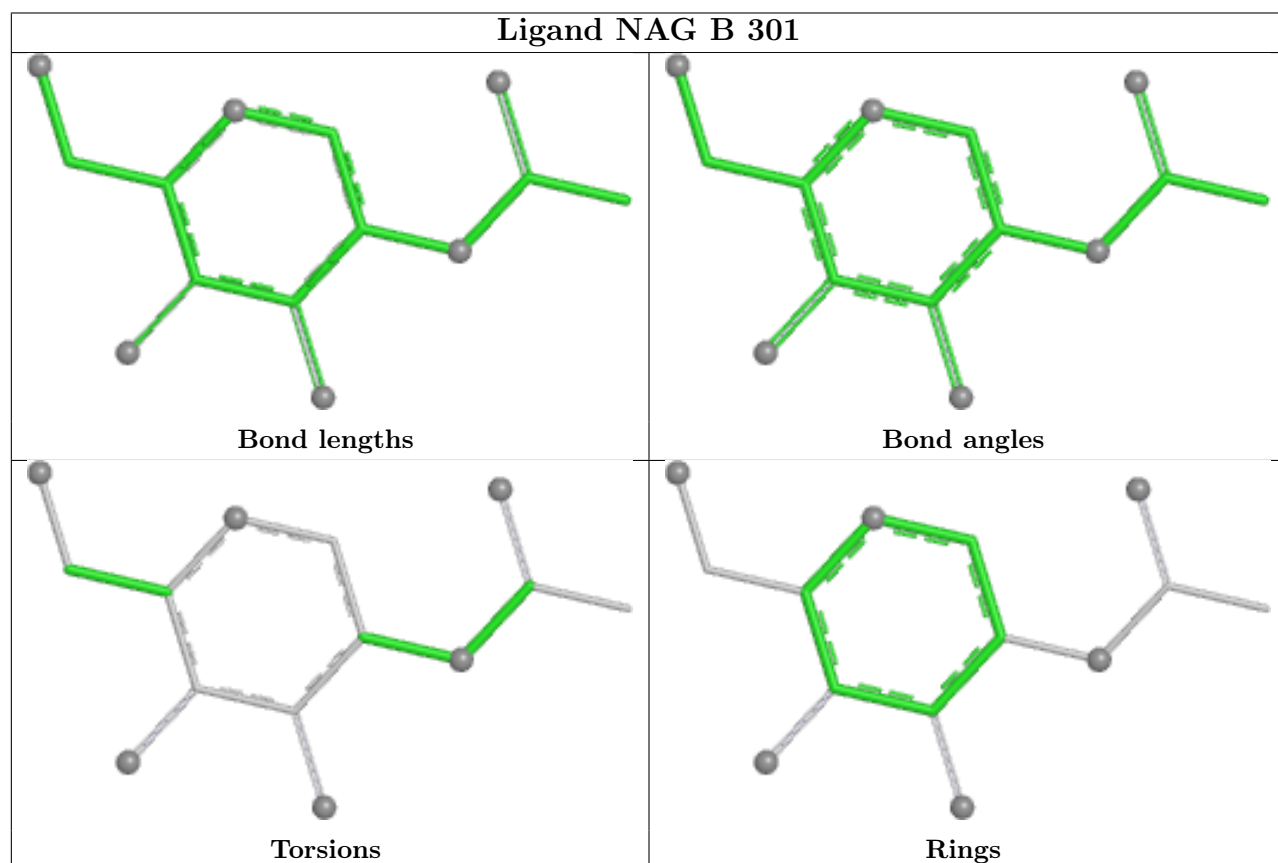
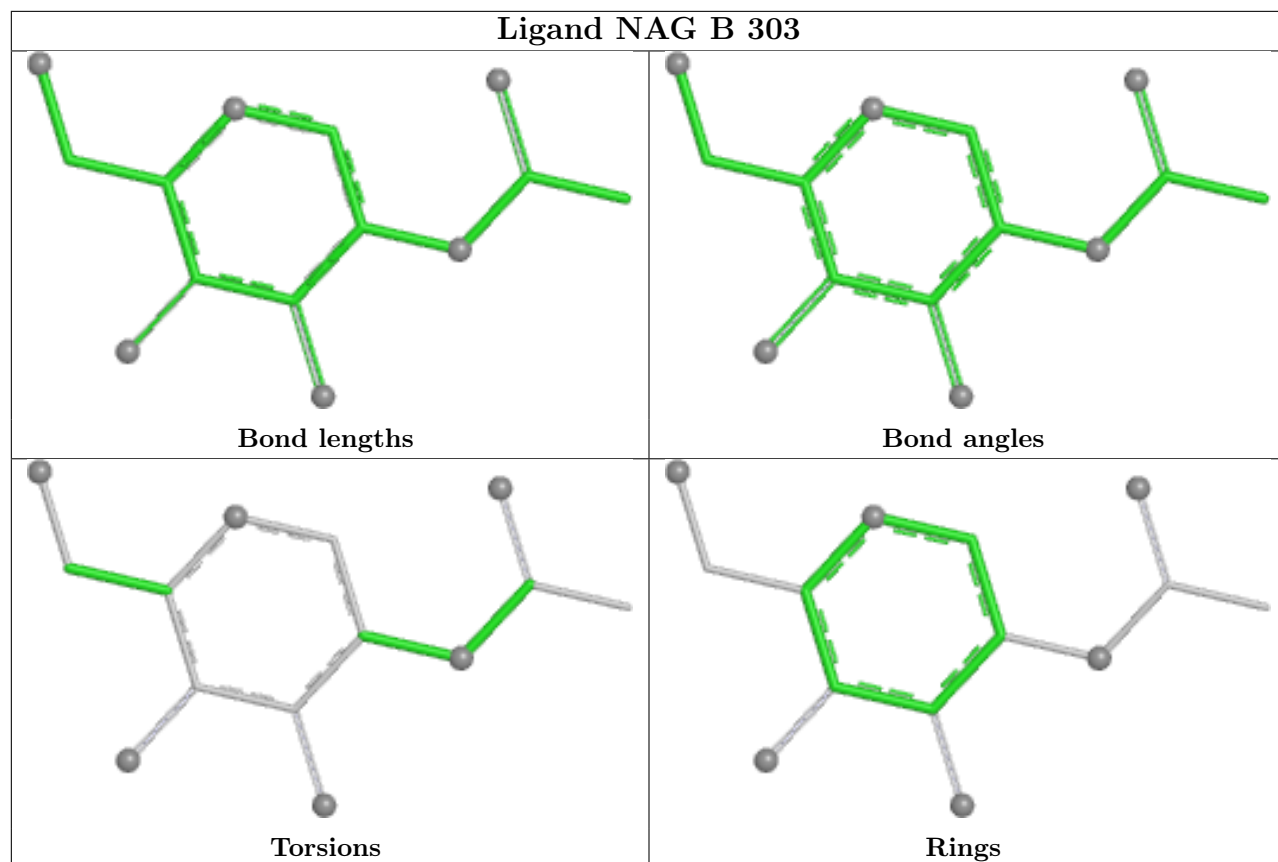
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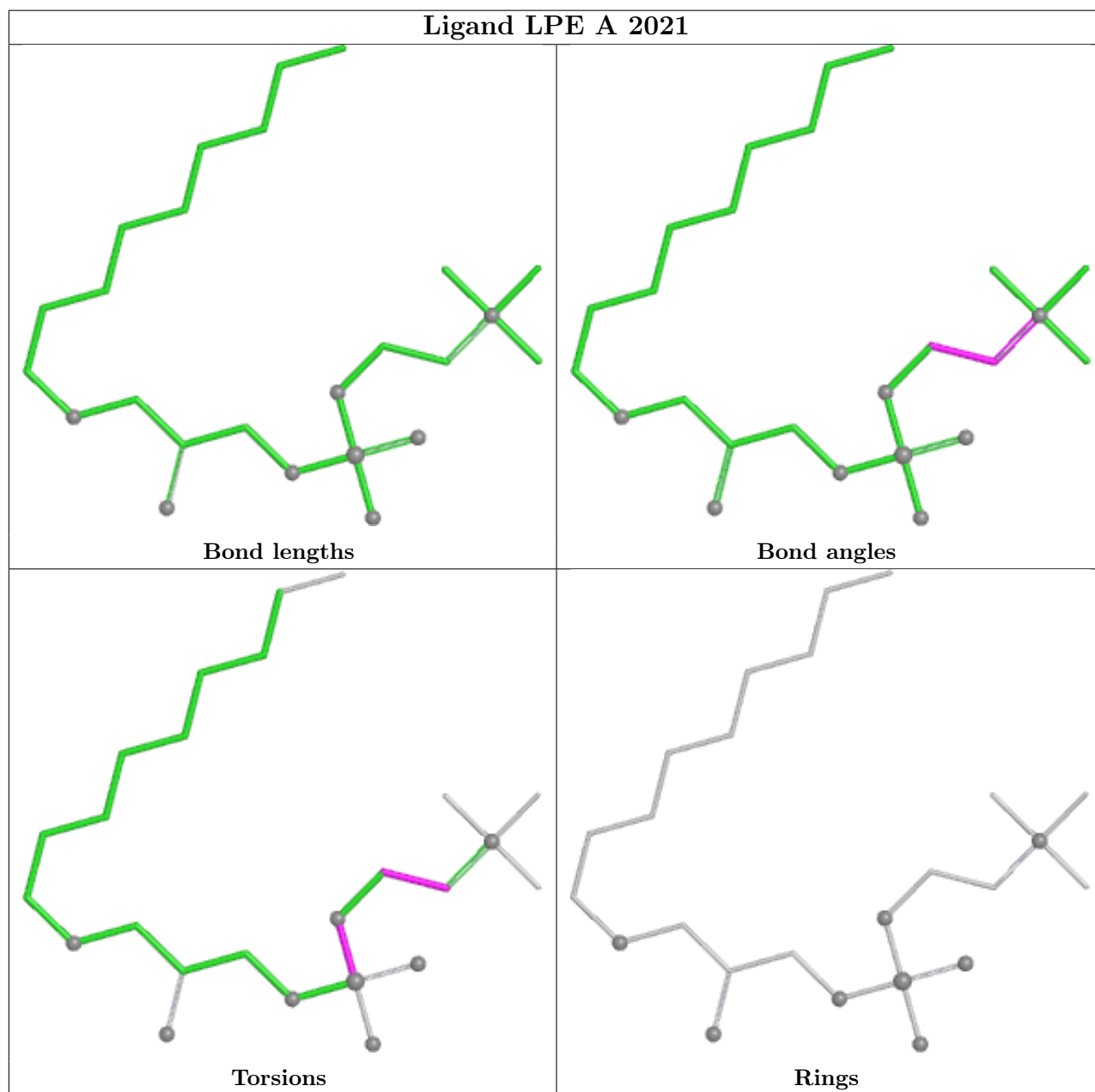
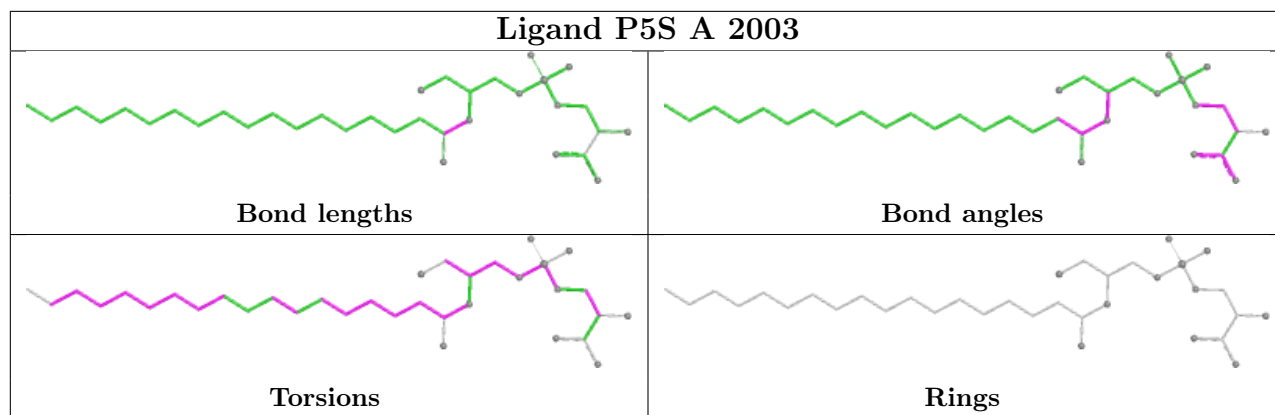
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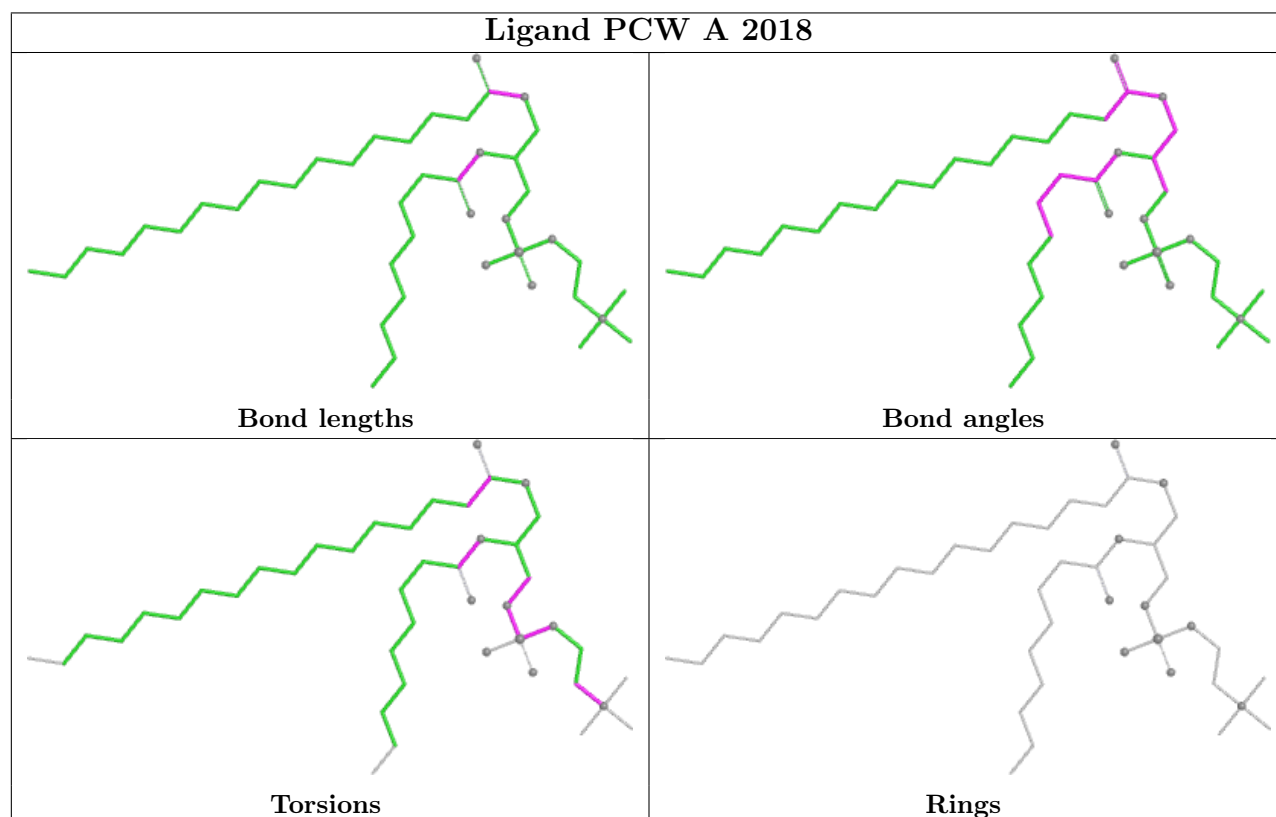
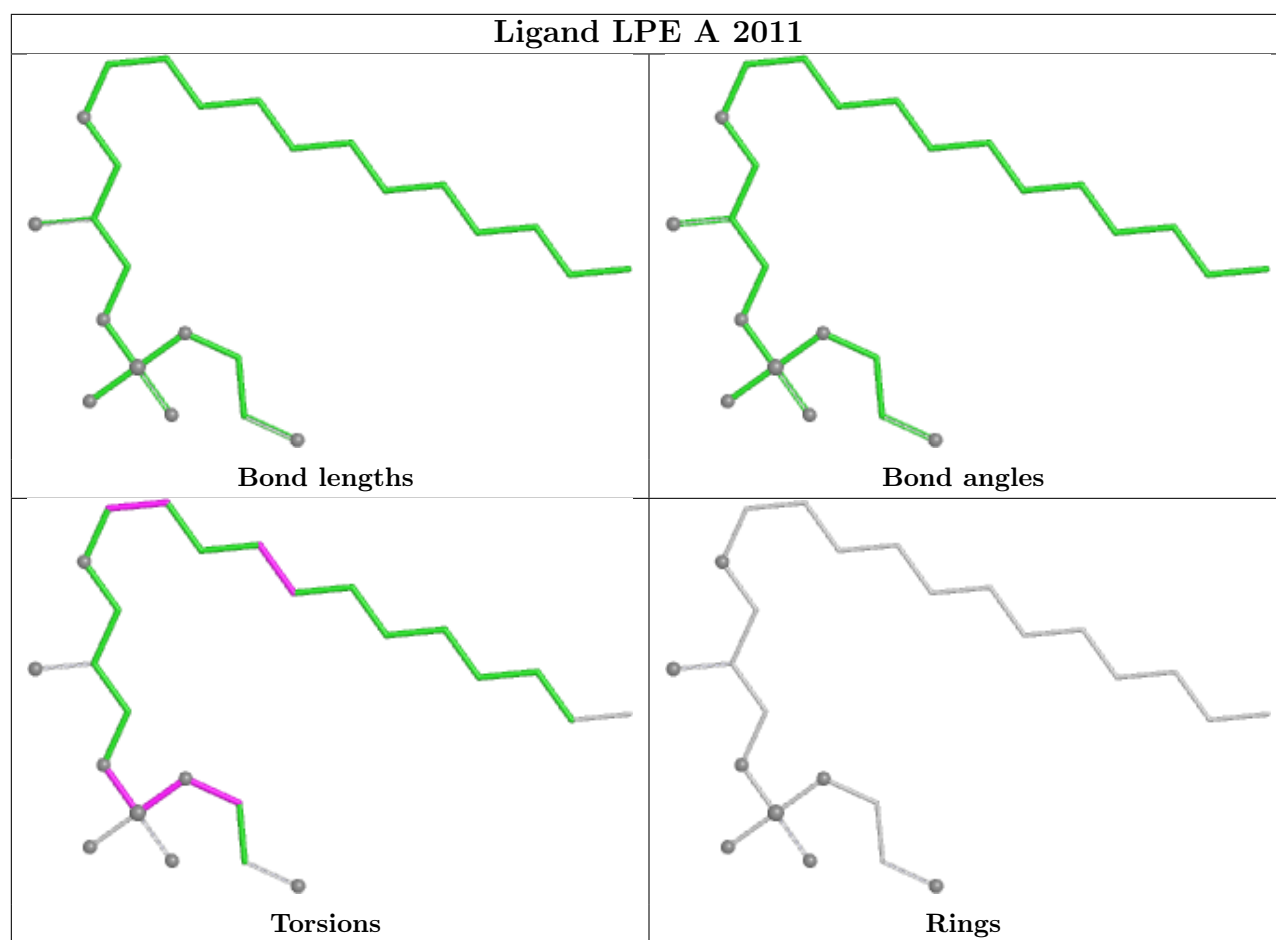
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2010	LPE	2	0
10	A	2012	LPE	9	0
7	A	2017	P5S	9	0
8	A	2006	Y01	16	0
8	A	2009	Y01	5	0
10	A	2024	LPE	1	0
10	B	304	LPE	9	0
8	A	2004	Y01	6	0
11	A	2016	PCW	1	0
10	A	2019	LPE	9	0
11	A	2013	PCW	22	0
8	A	2029	Y01	18	0
10	A	2022	LPE	7	0
10	A	2026	LPE	10	0
5	A	2001	9SL	3	0
10	A	2020	LPE	1	0
9	A	2007	9Z9	9	0
10	A	2014	LPE	17	0
11	A	2027	PCW	8	0

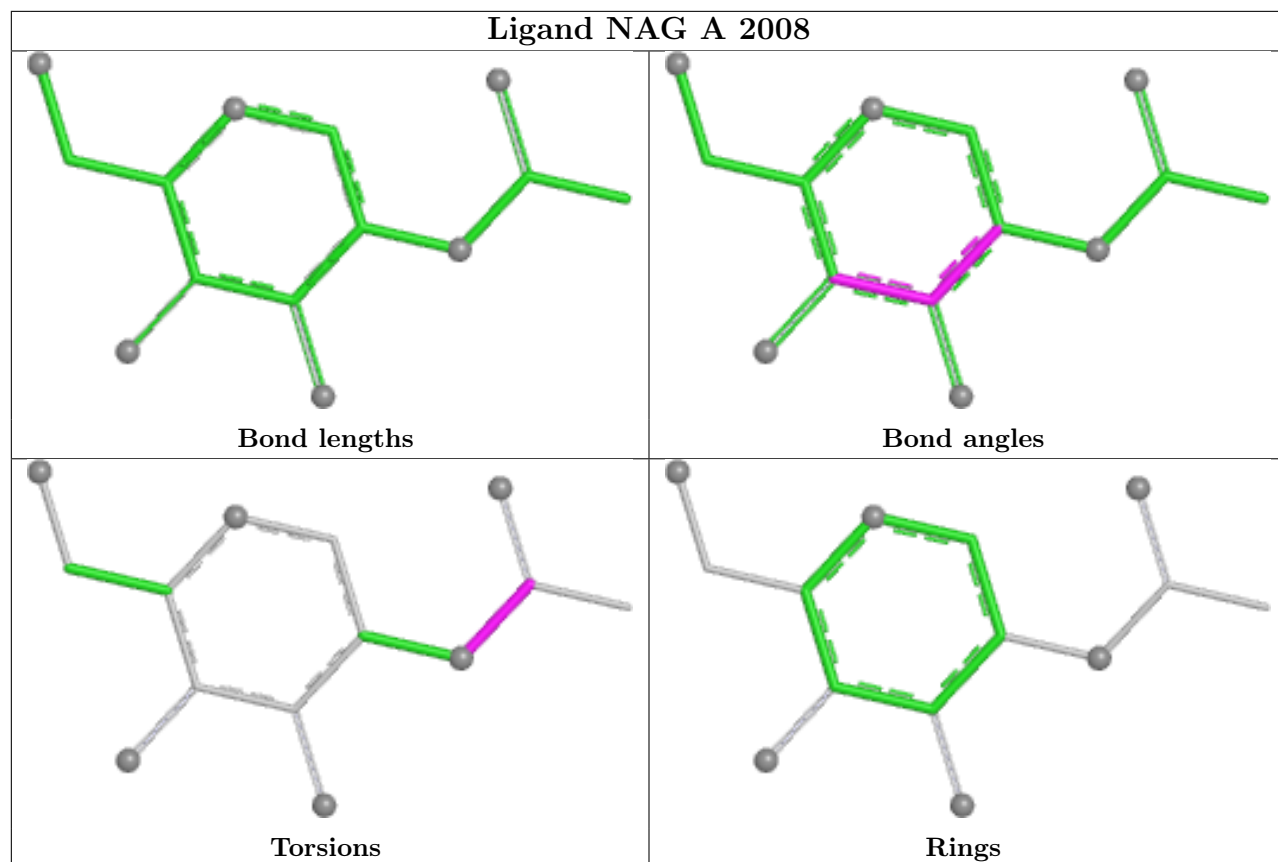
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

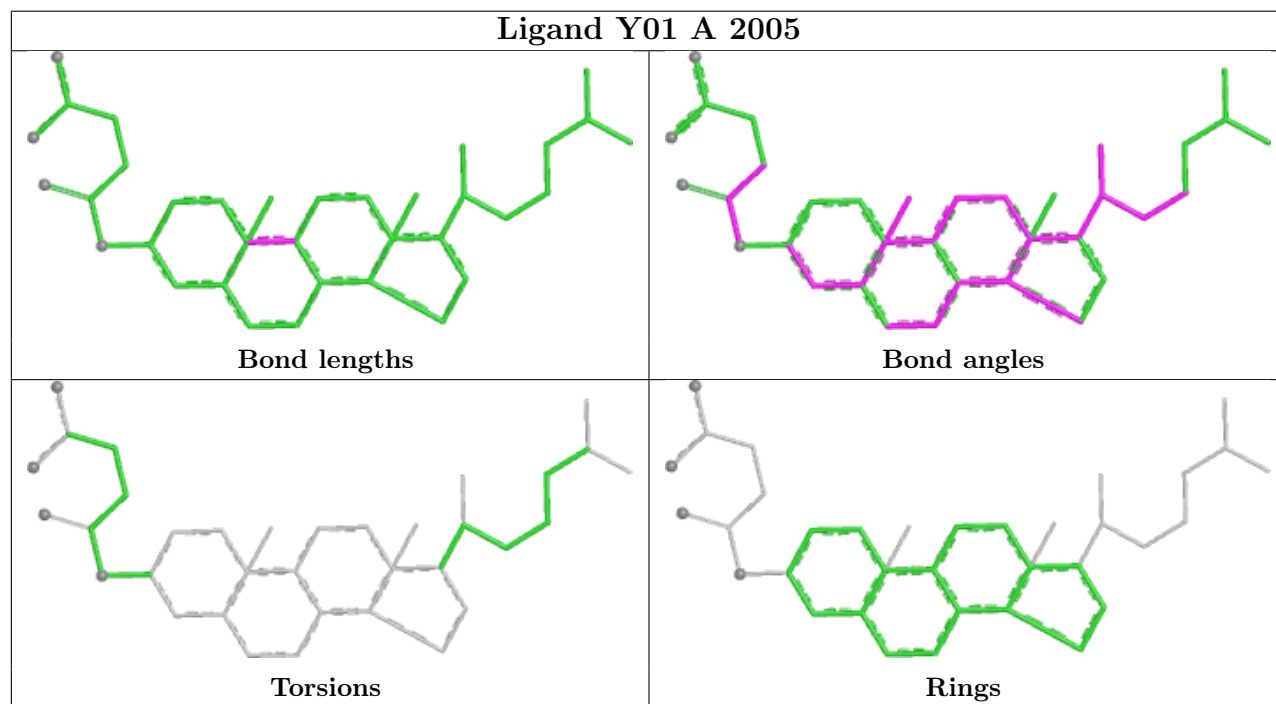
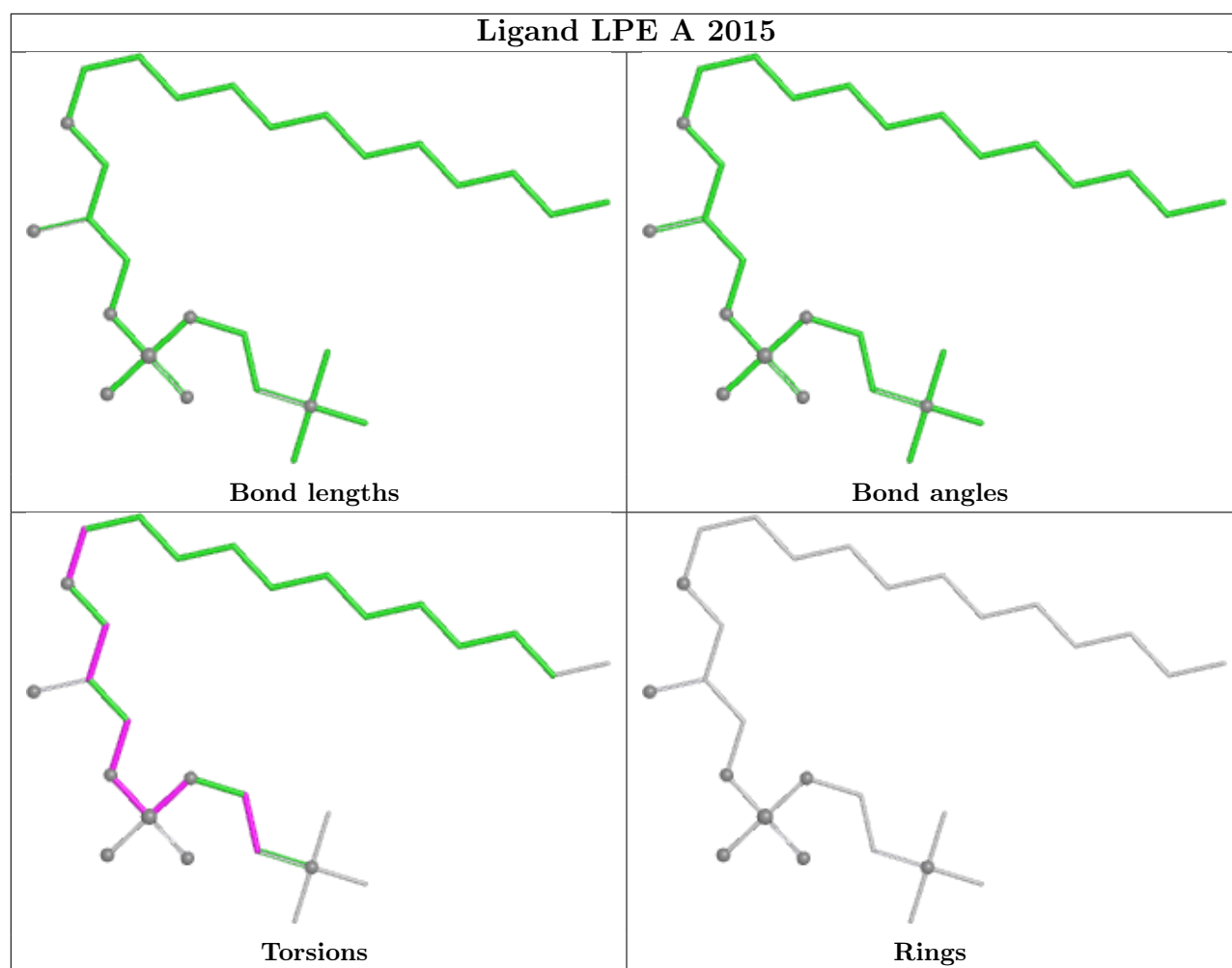


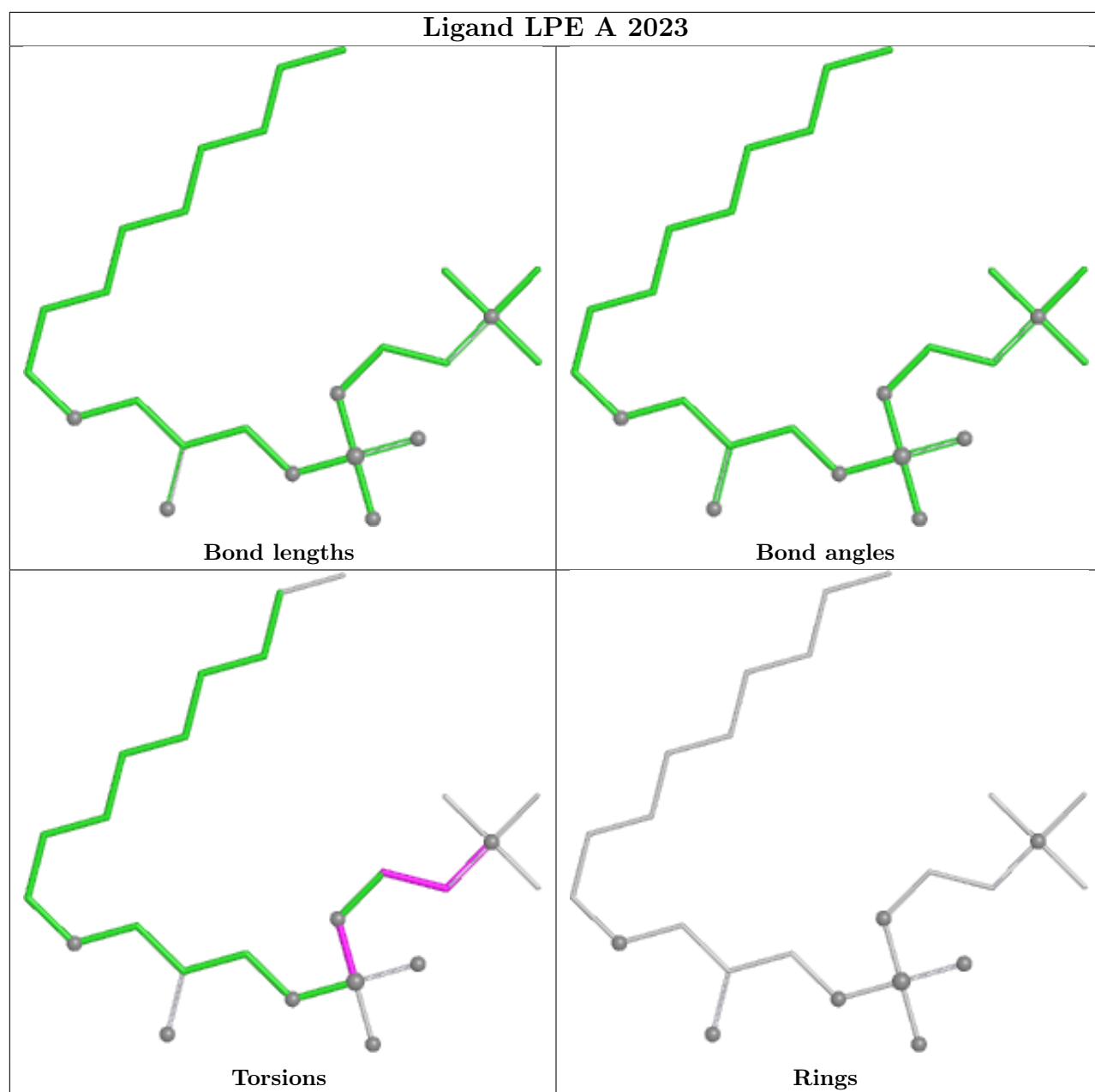


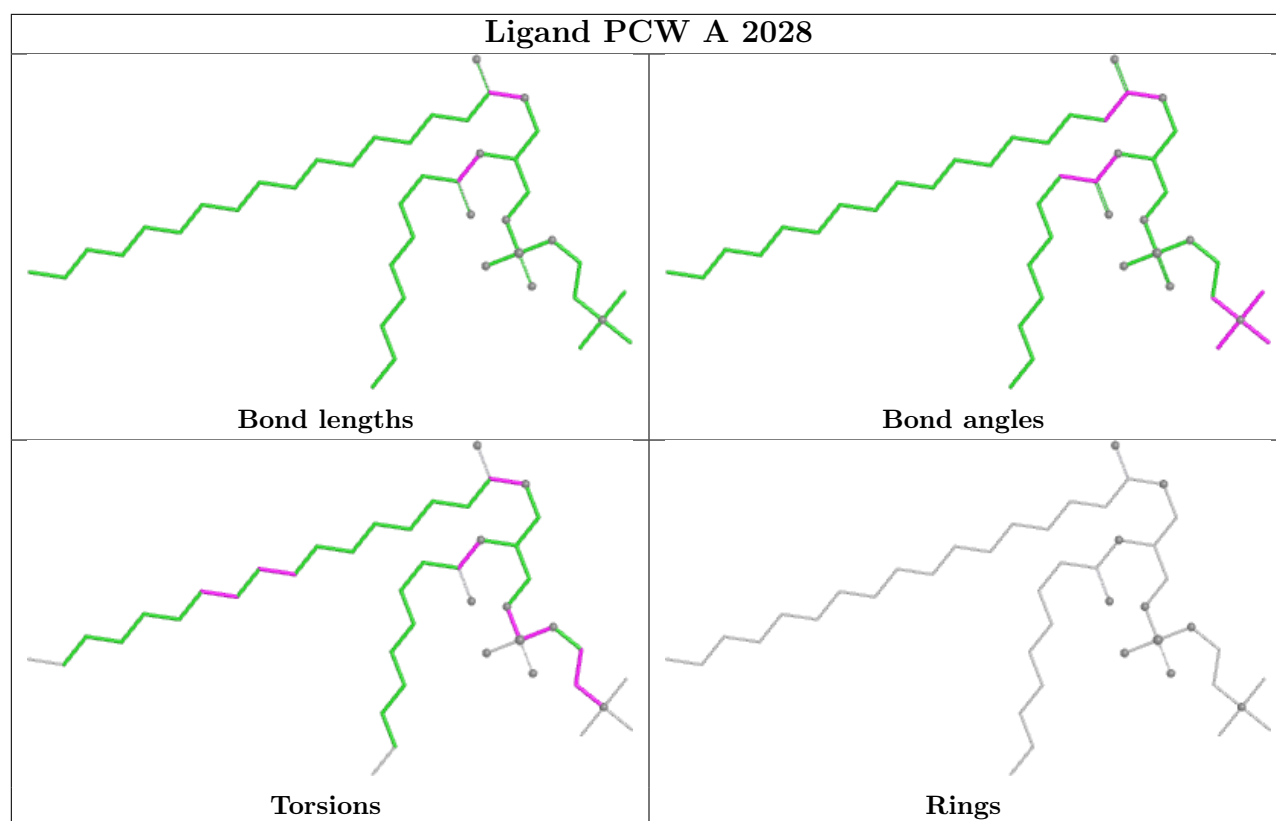


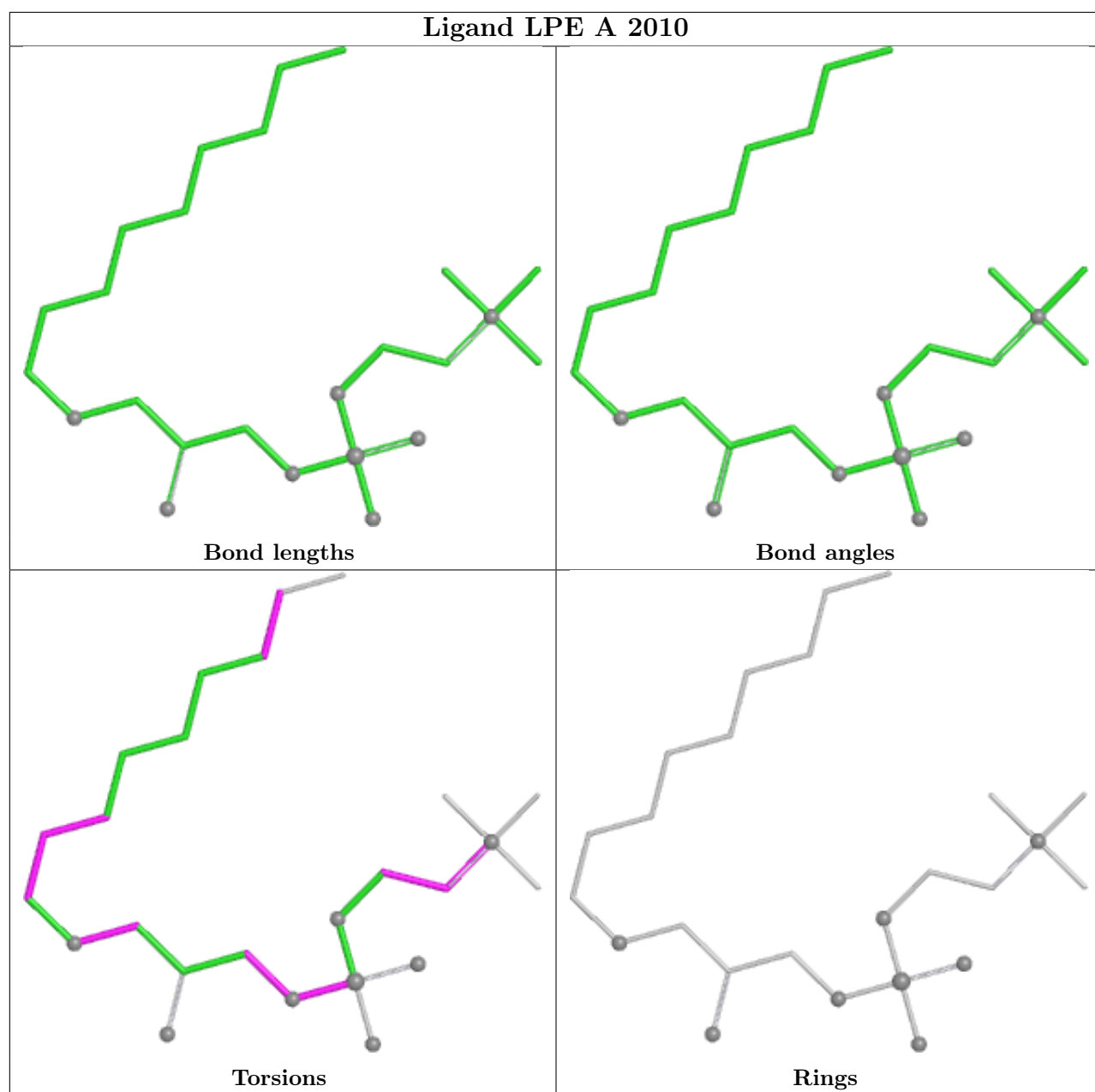


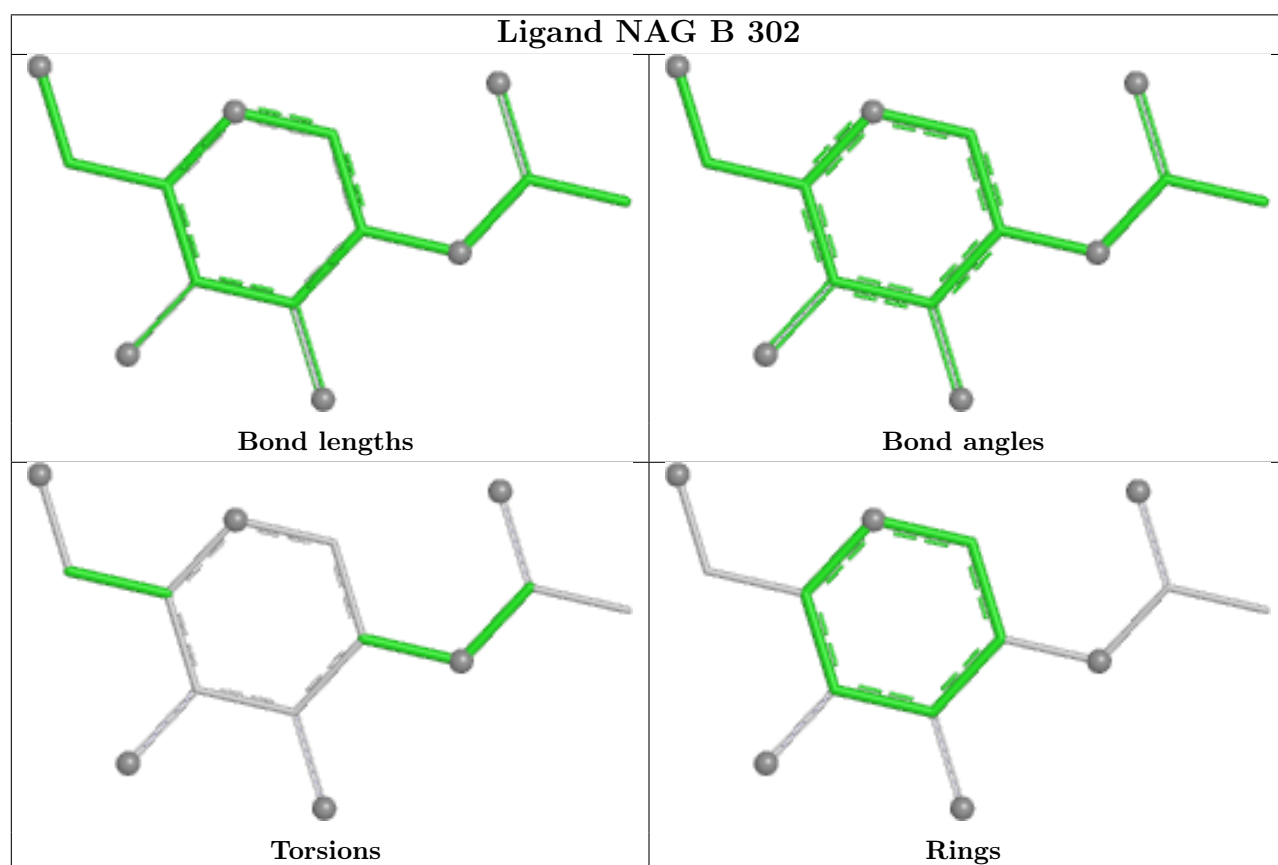
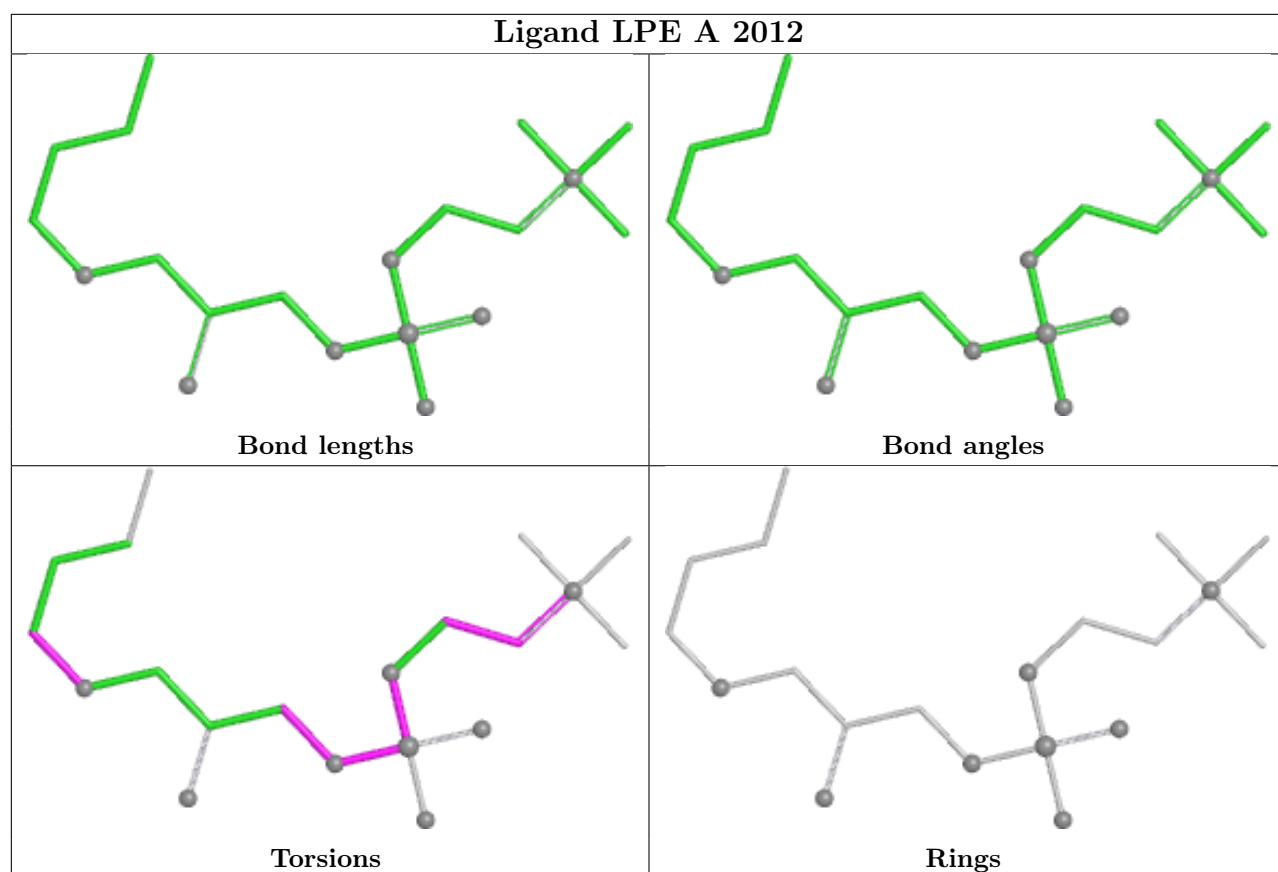


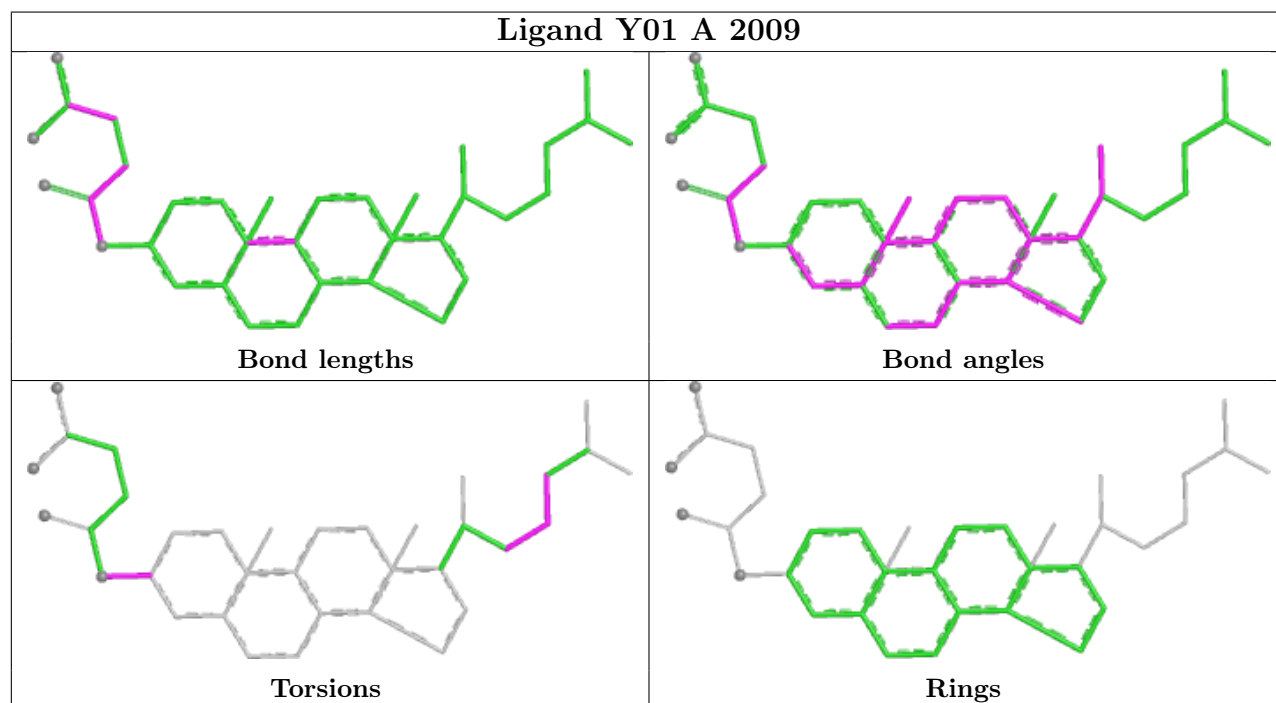
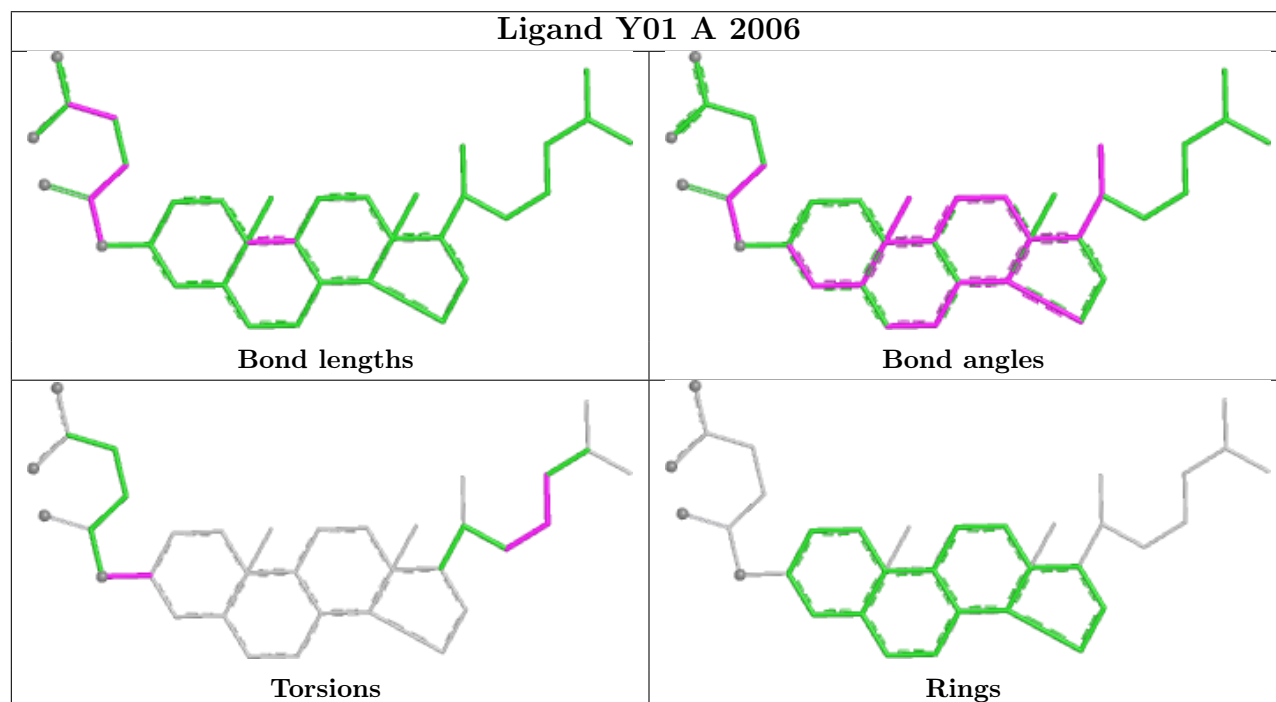
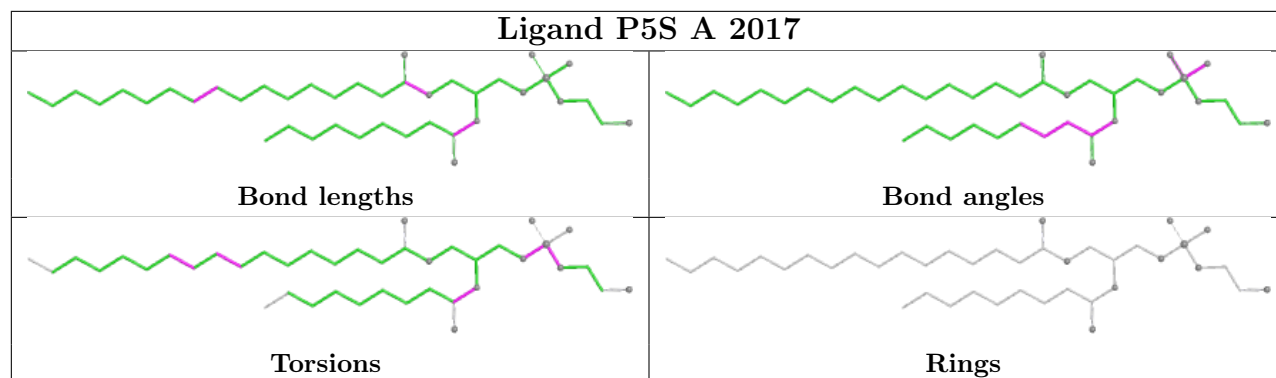


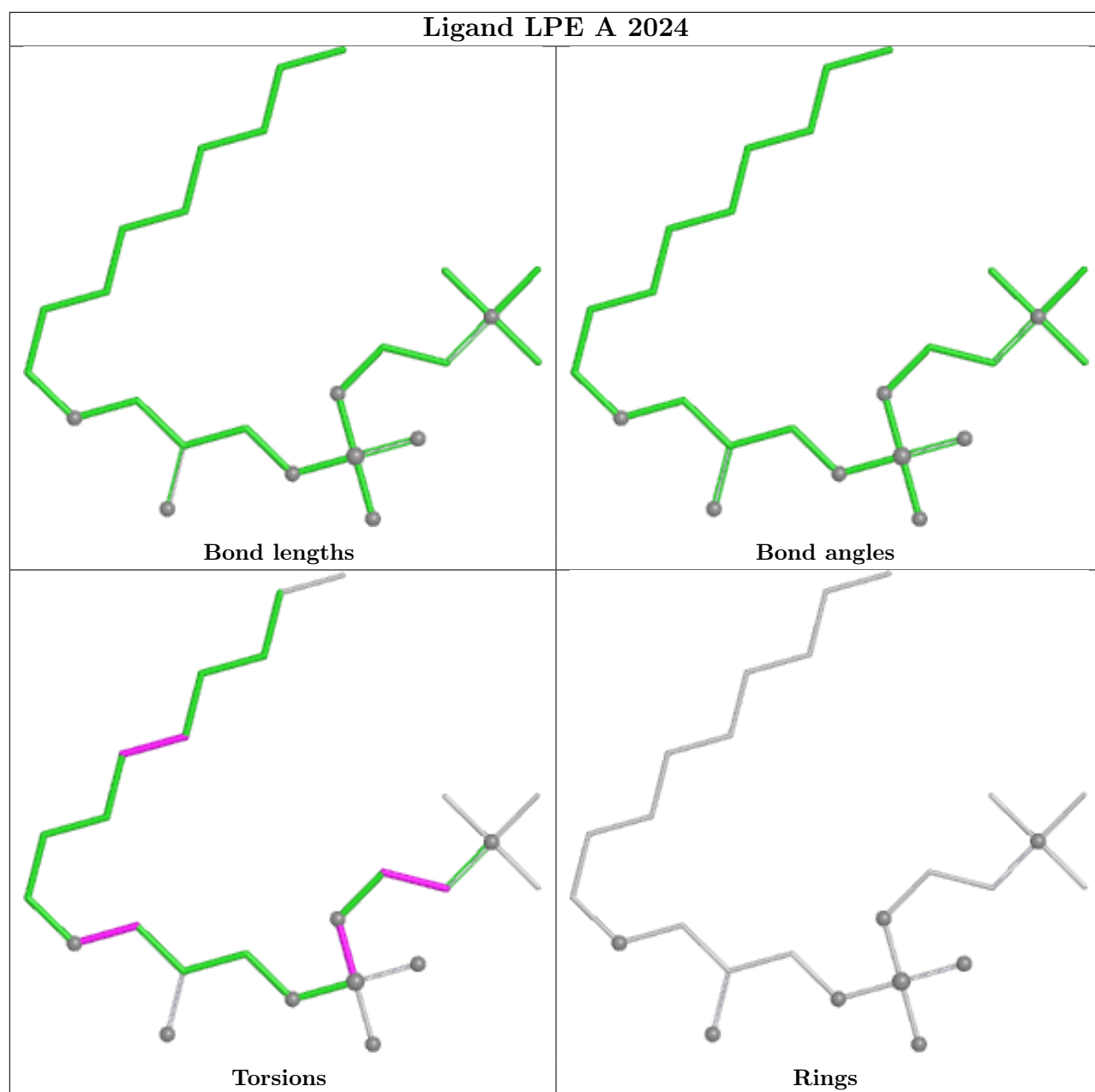


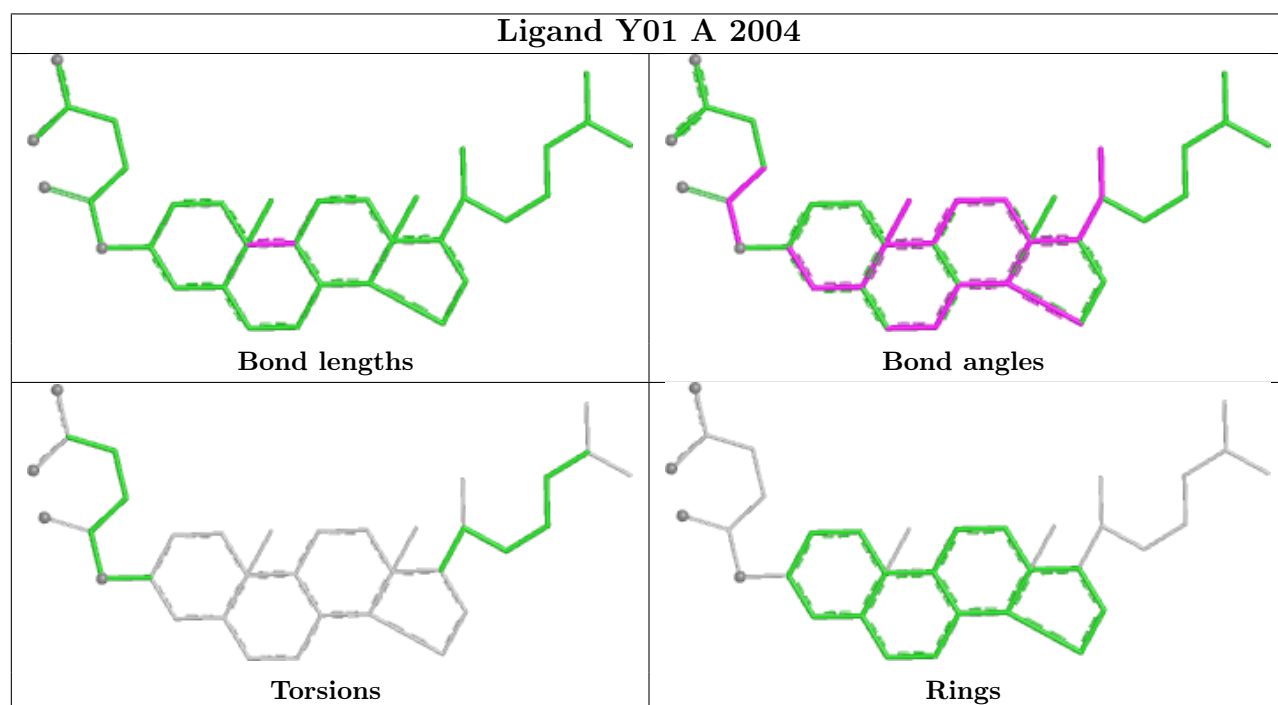
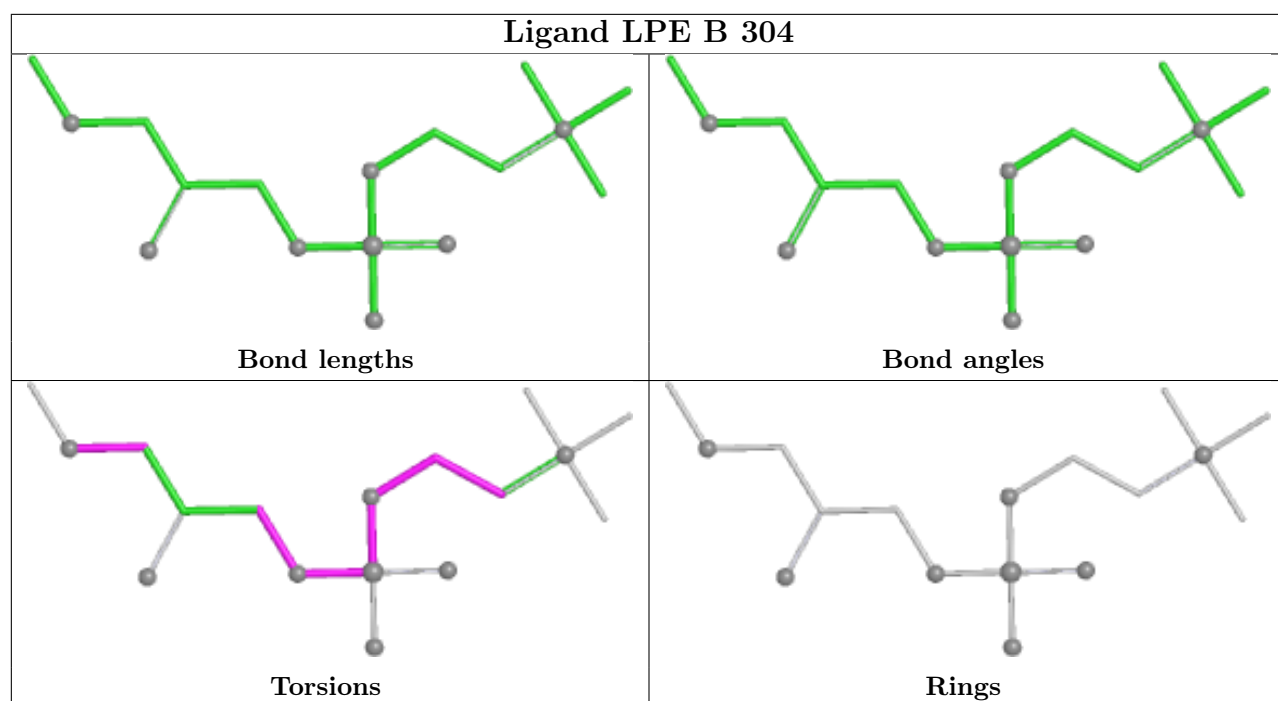


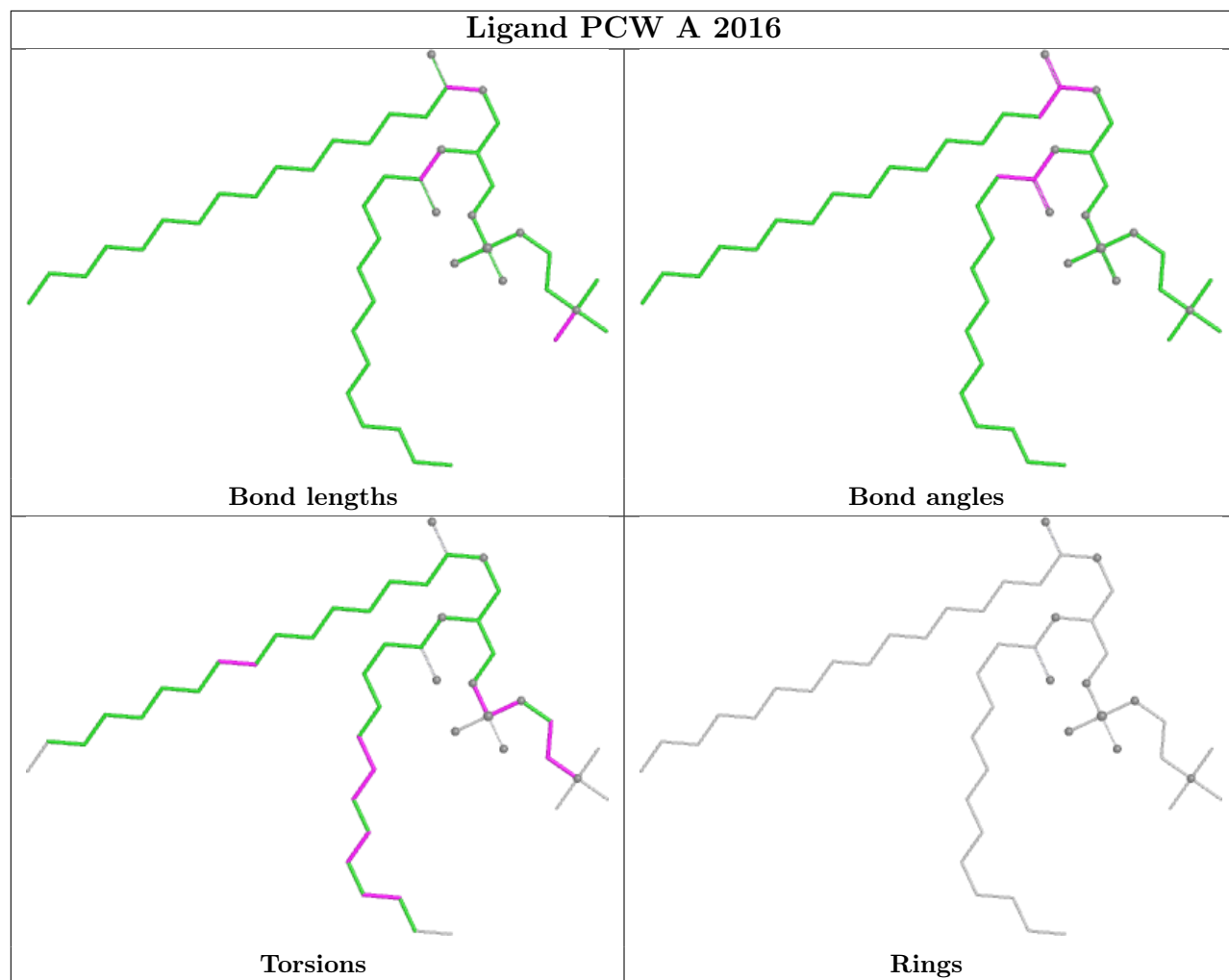


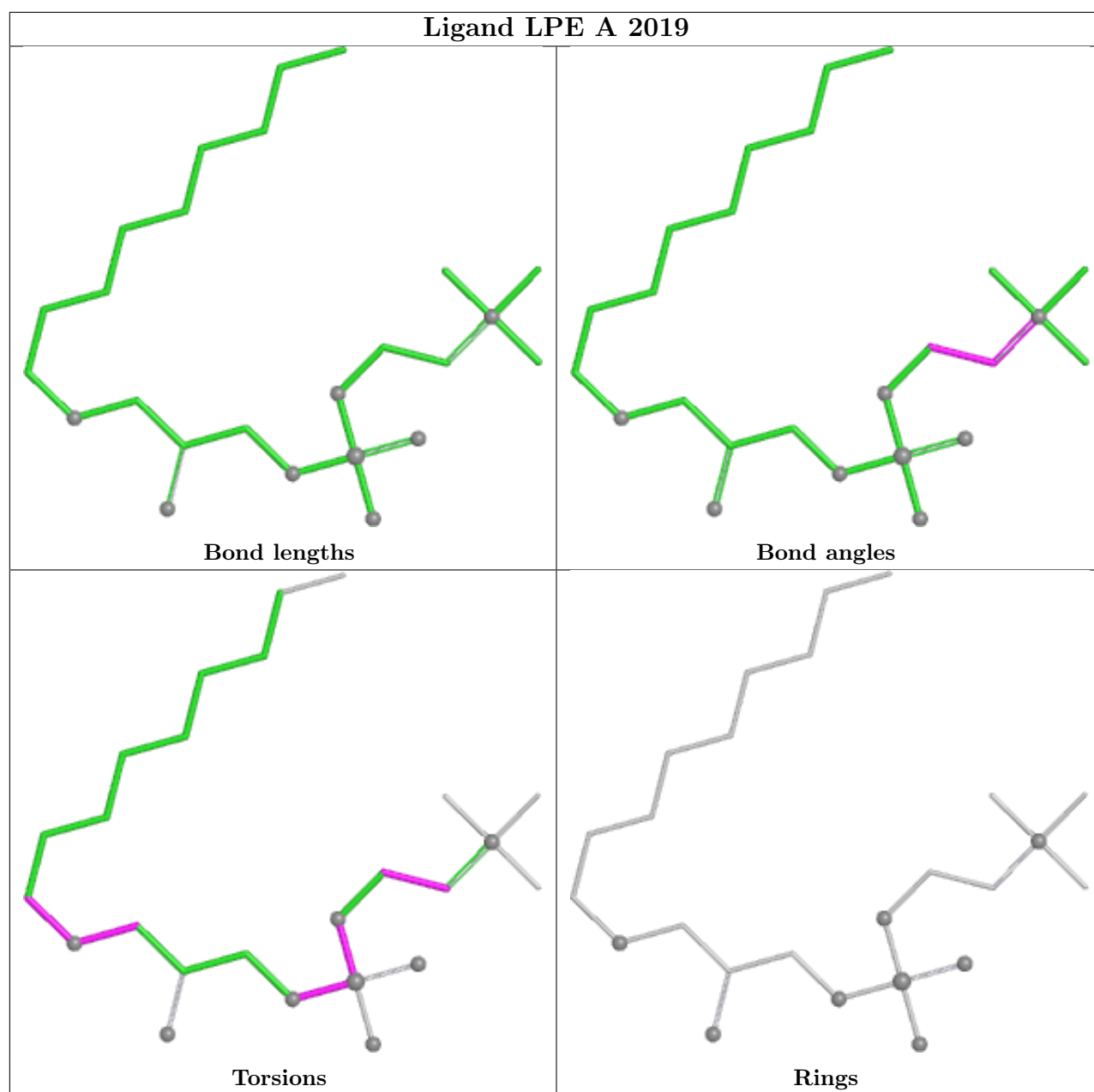


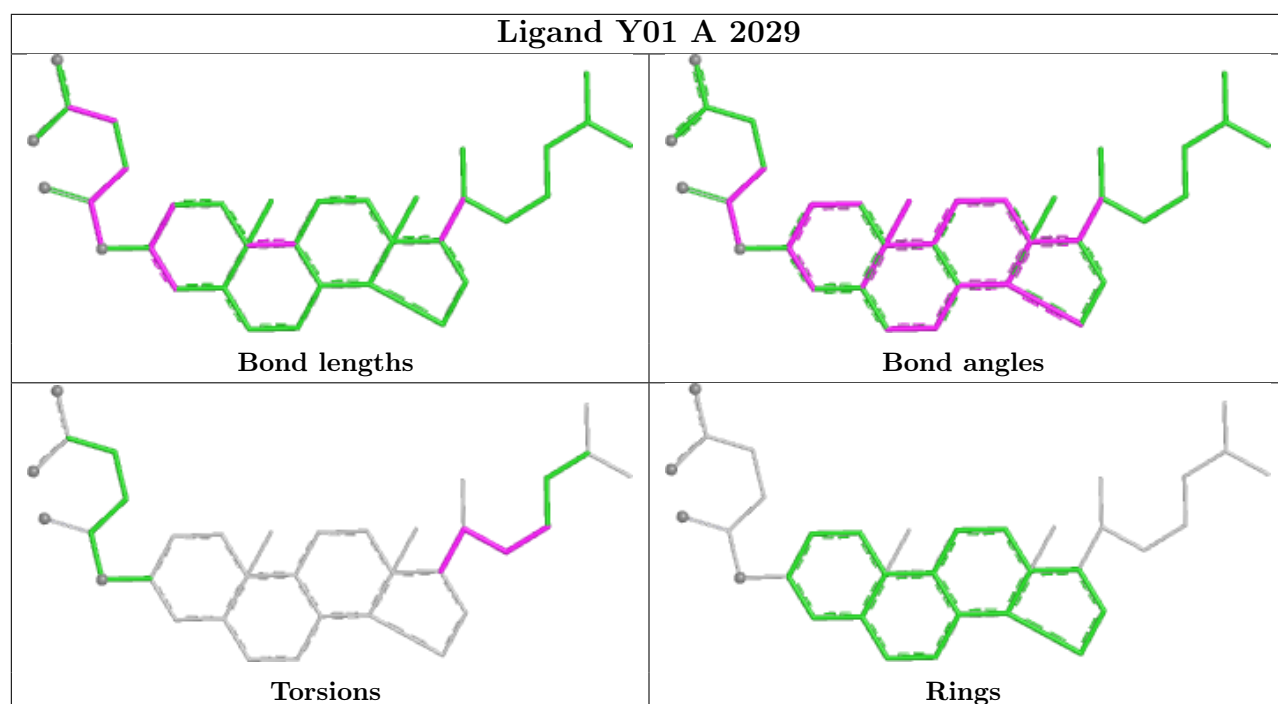
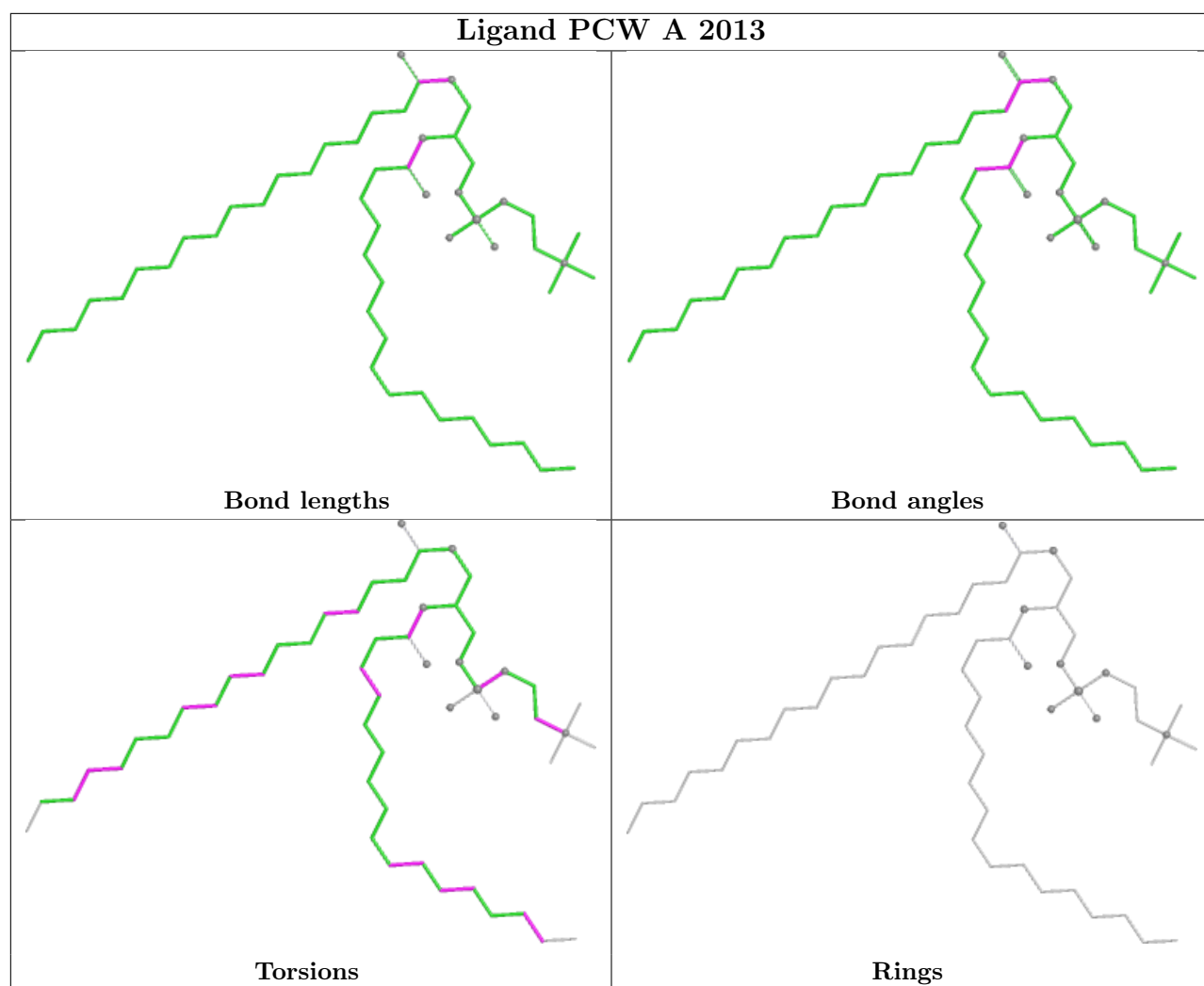


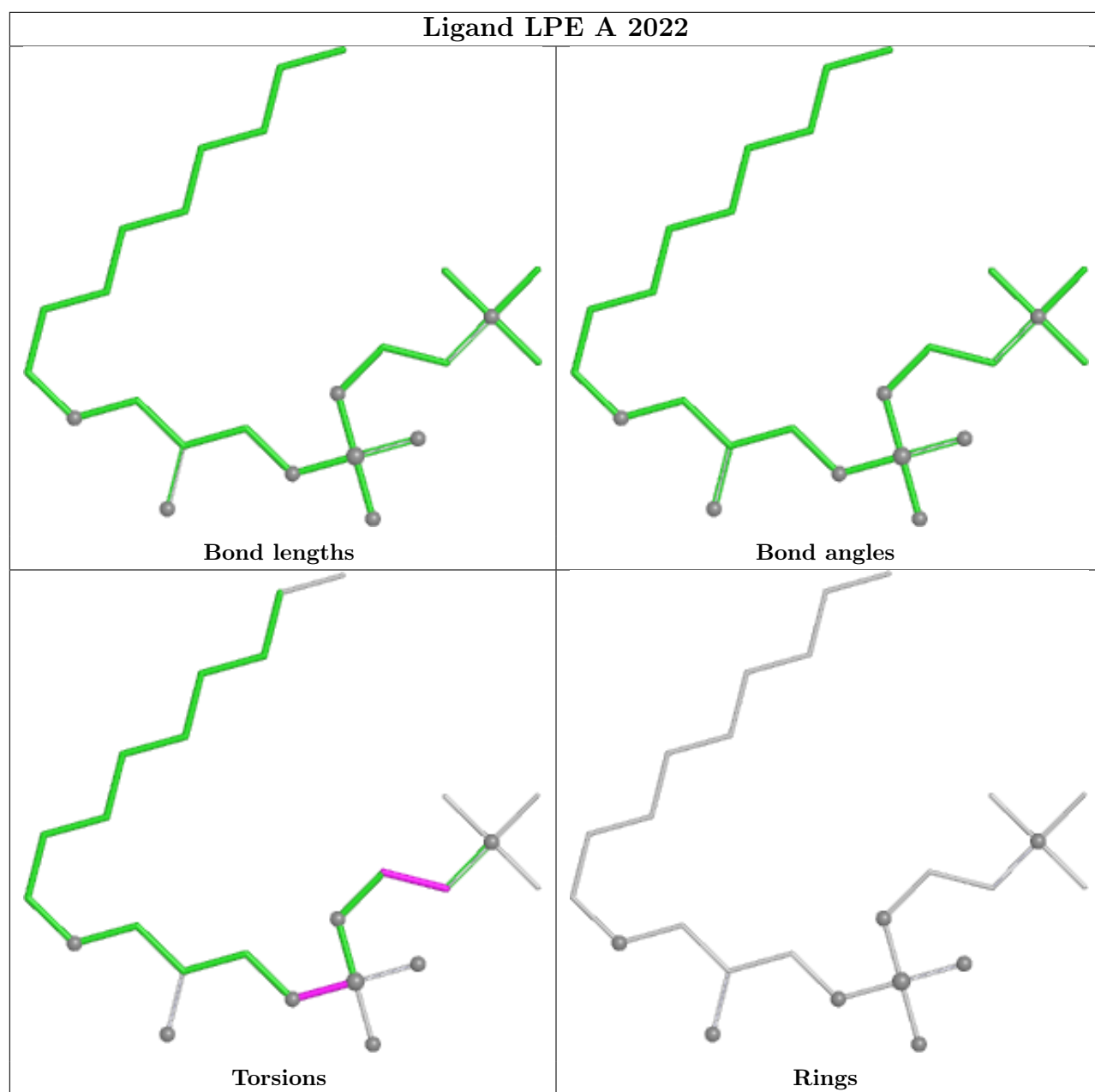


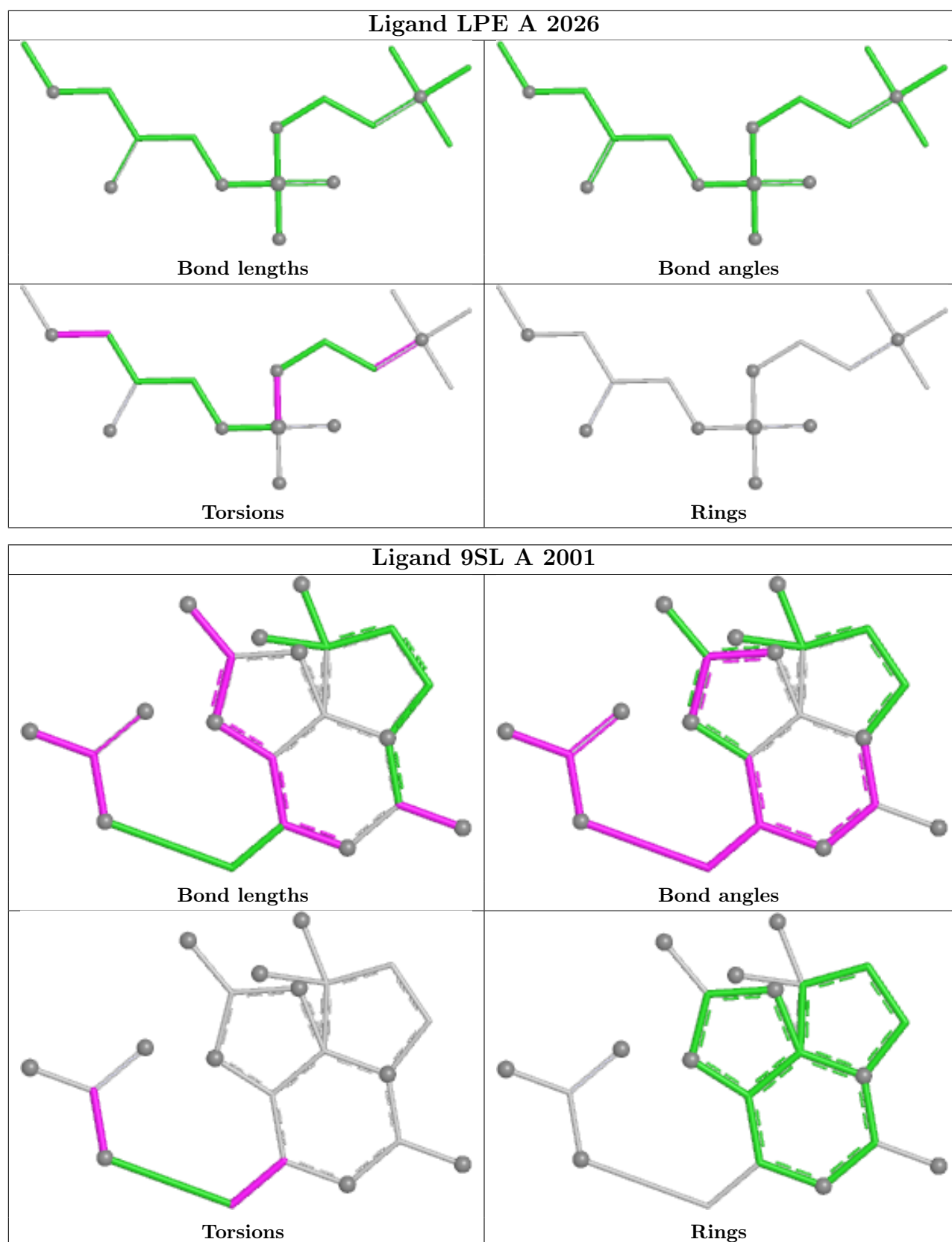












Ligand LPE A 2020

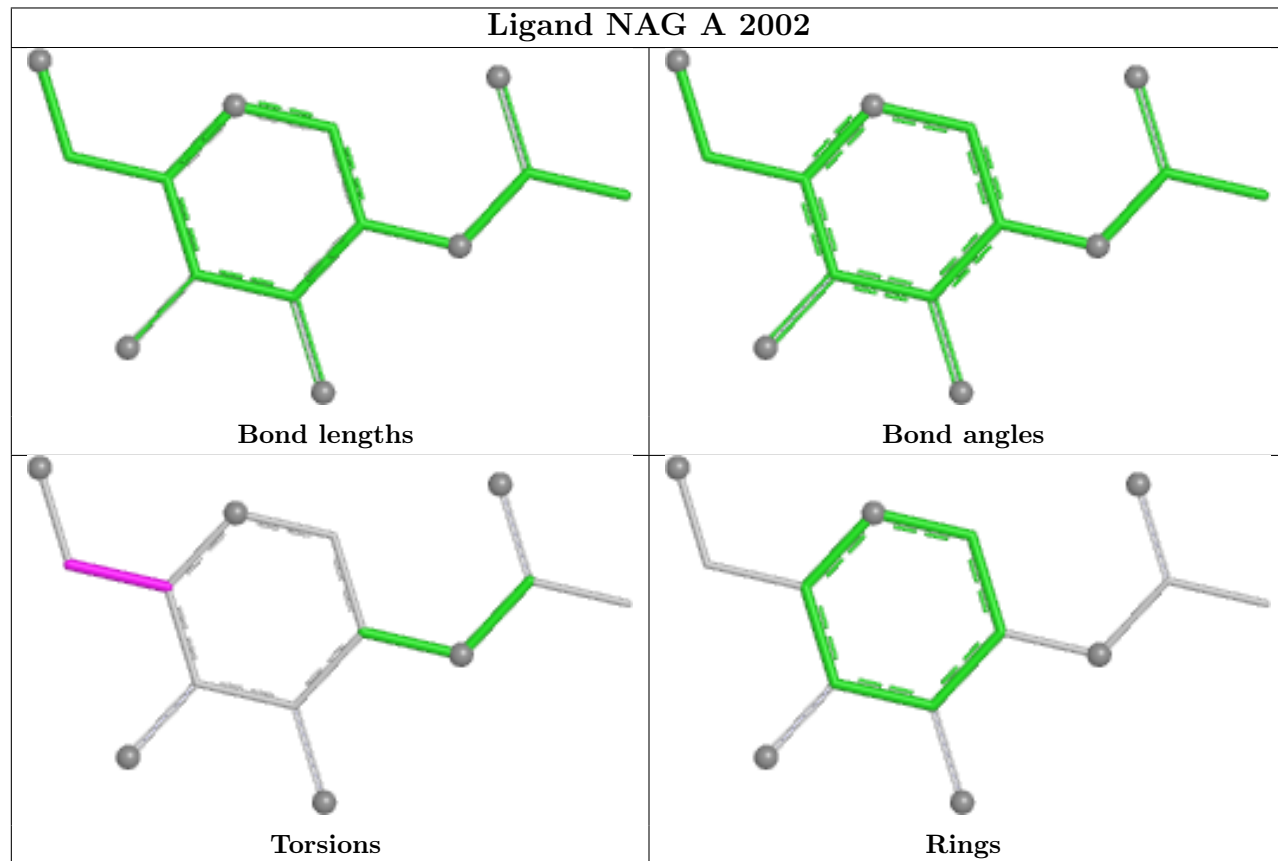
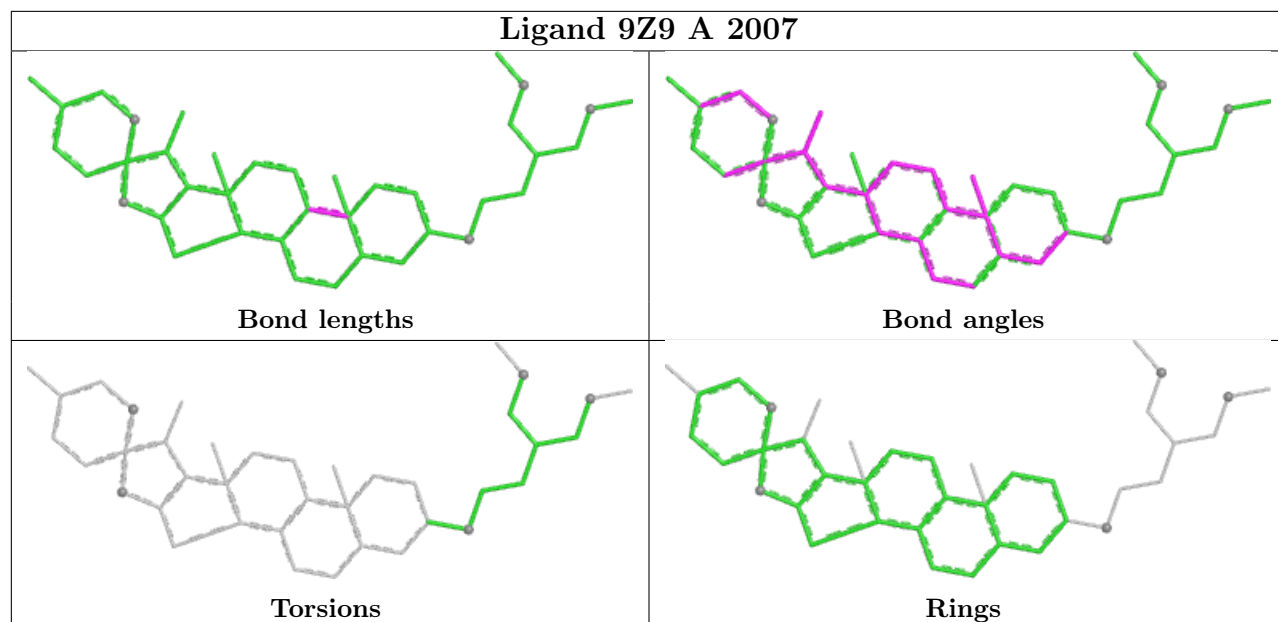
The figure displays four panels of structural analysis for Ligand LPE A 2020. The panels are arranged in a 2x2 grid. The top-left panel shows bond lengths, the top-right panel shows bond angles, the bottom-left panel shows torsions, and the bottom-right panel shows rings. Each panel features a 3D ball-and-stick model of the ligand, with atoms represented by grey spheres and bonds by colored lines. The ligand is a complex organic molecule with a long, flexible chain and a central ring system. The bond lengths are shown in green, the bond angles in magenta, the torsions in green, and the rings in grey.

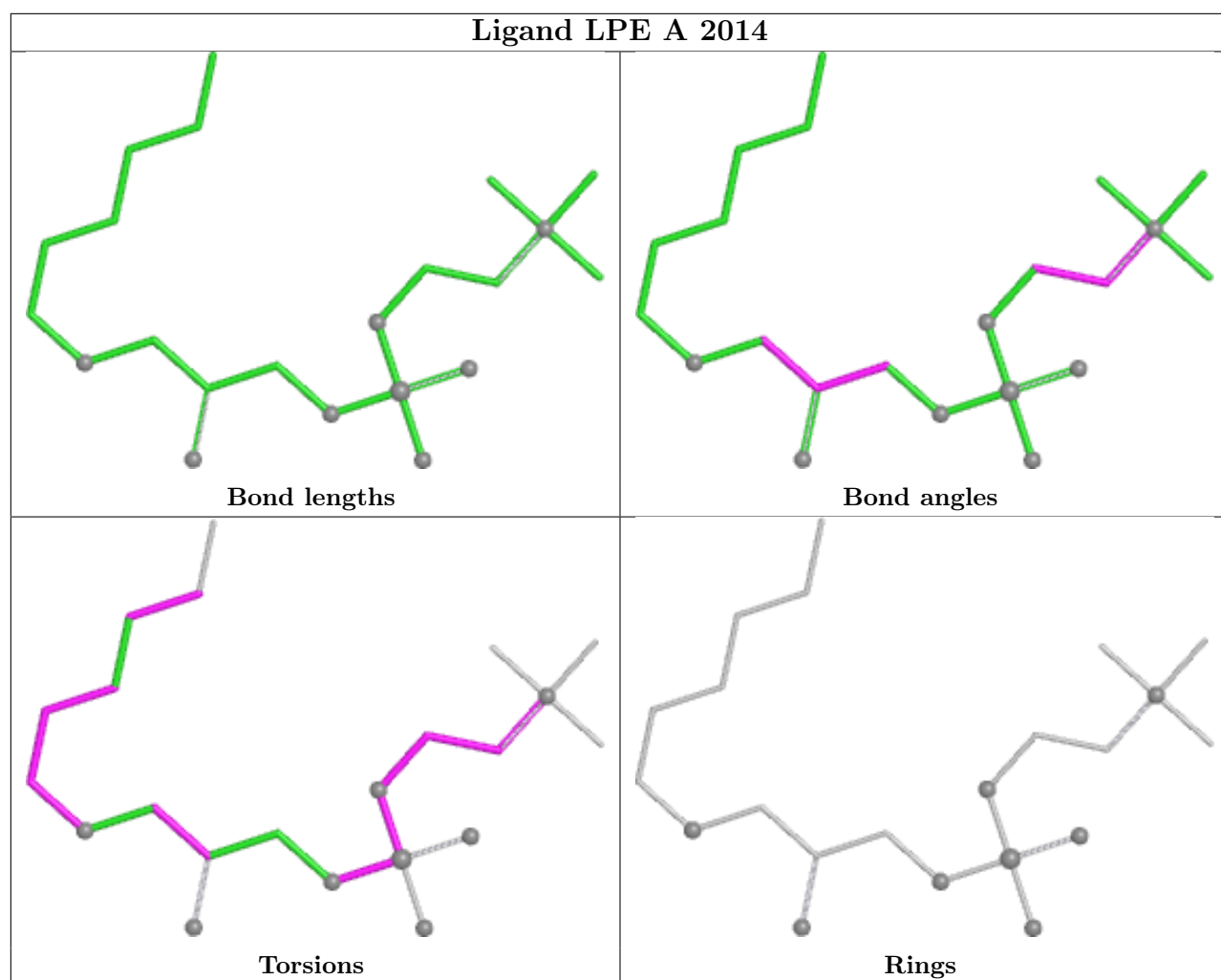
Bond lengths

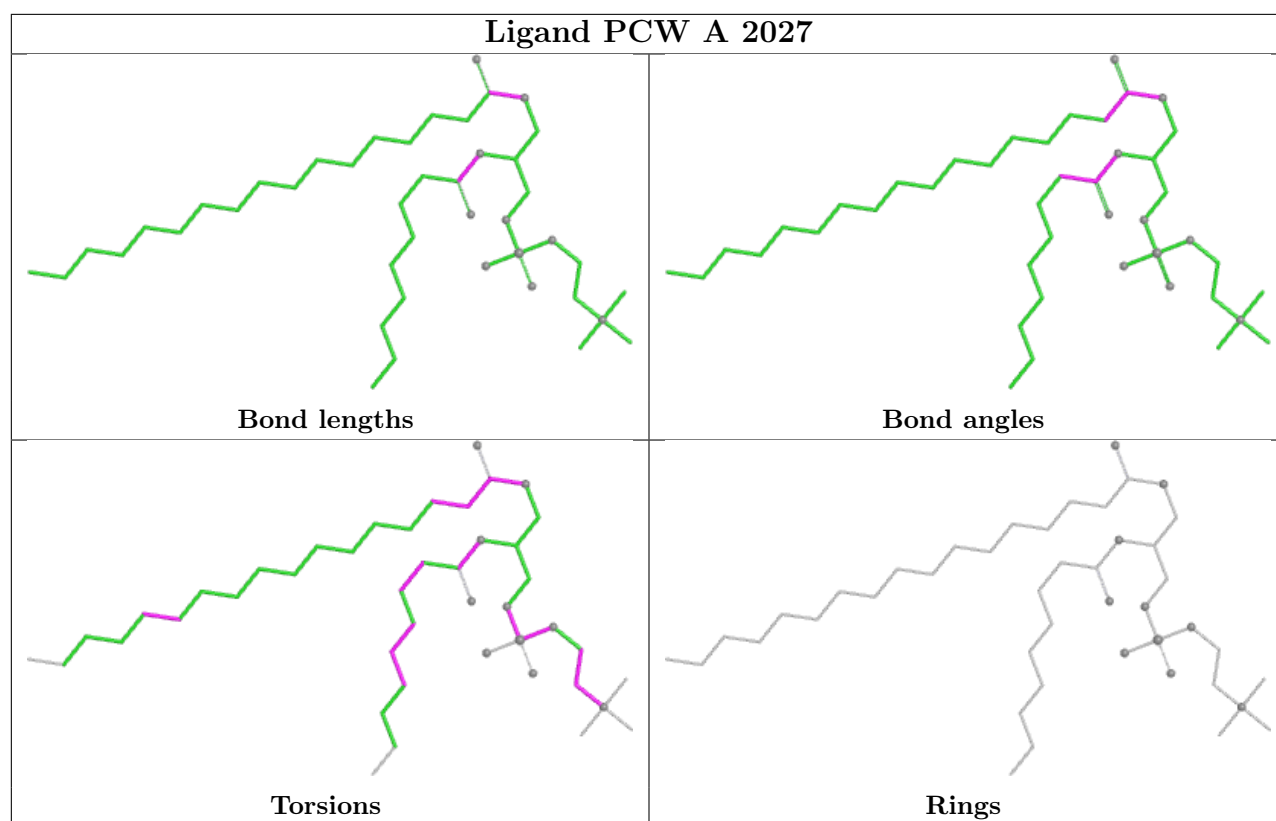
Bond angles

Torsions

Rings







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.

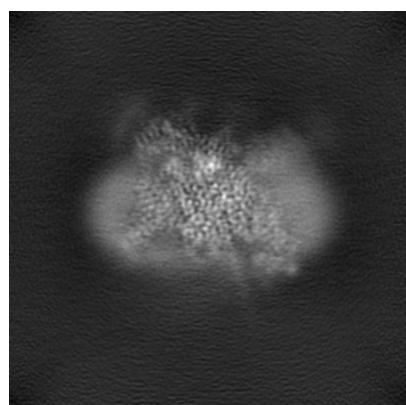
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32372. These allow visual inspection of the internal detail of the map and identification of artifacts.

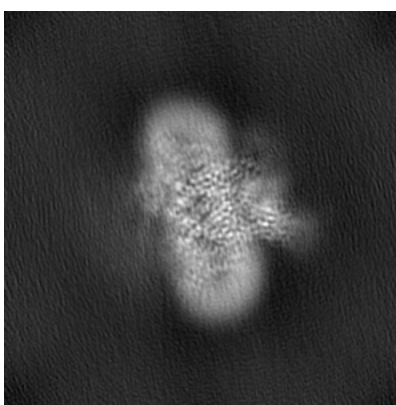
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

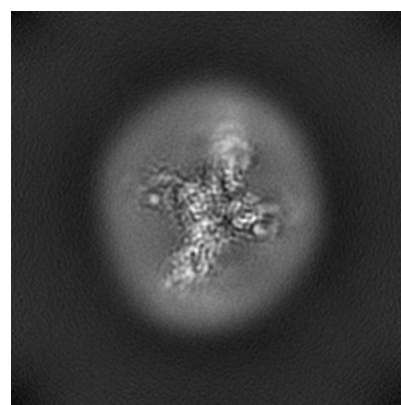
6.1.1 Primary map



X



Y

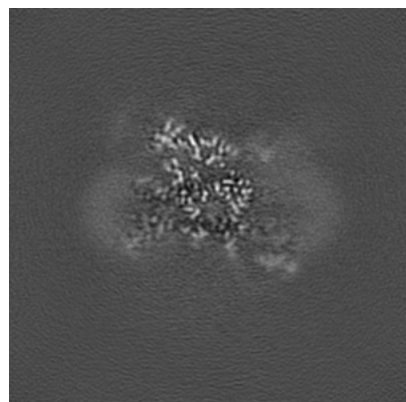


Z

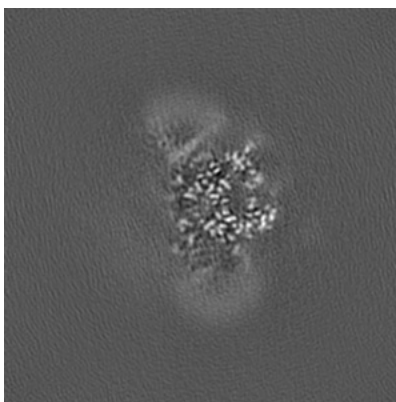
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

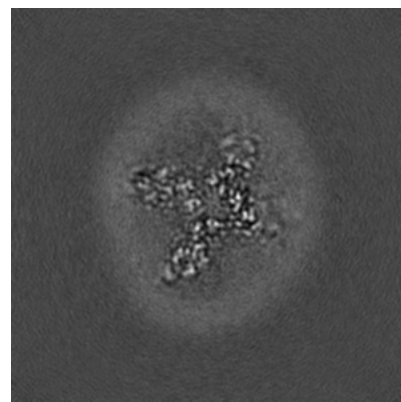
6.2.1 Primary map



X Index: 120



Y Index: 120

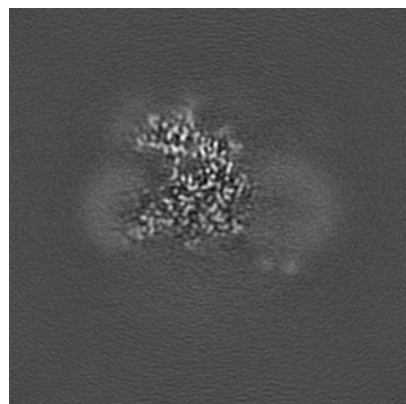


Z Index: 120

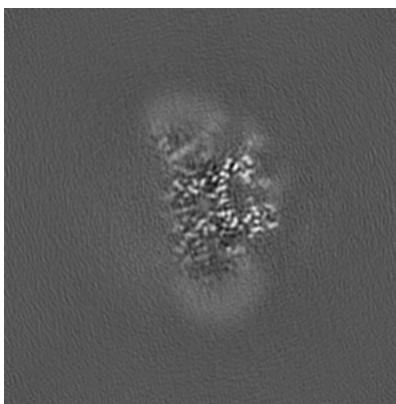
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

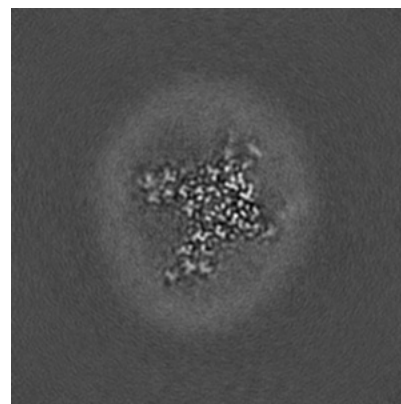
6.3.1 Primary map



X Index: 112



Y Index: 122

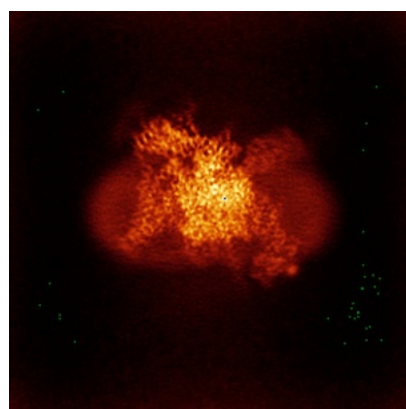


Z Index: 126

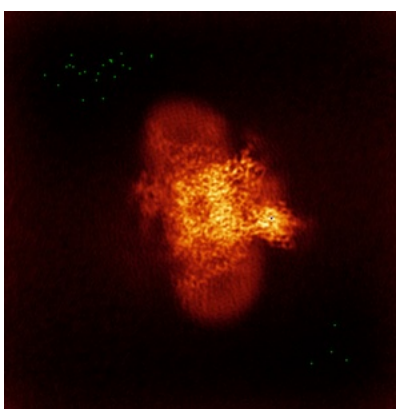
The images above show the largest variance slices of the map in three orthogonal directions.

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

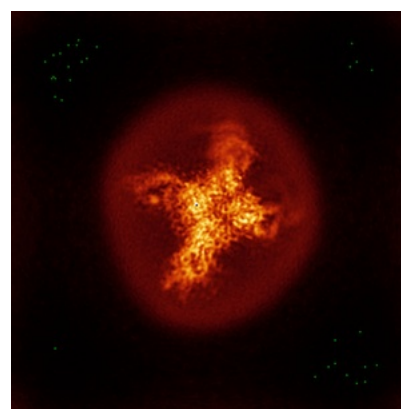
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

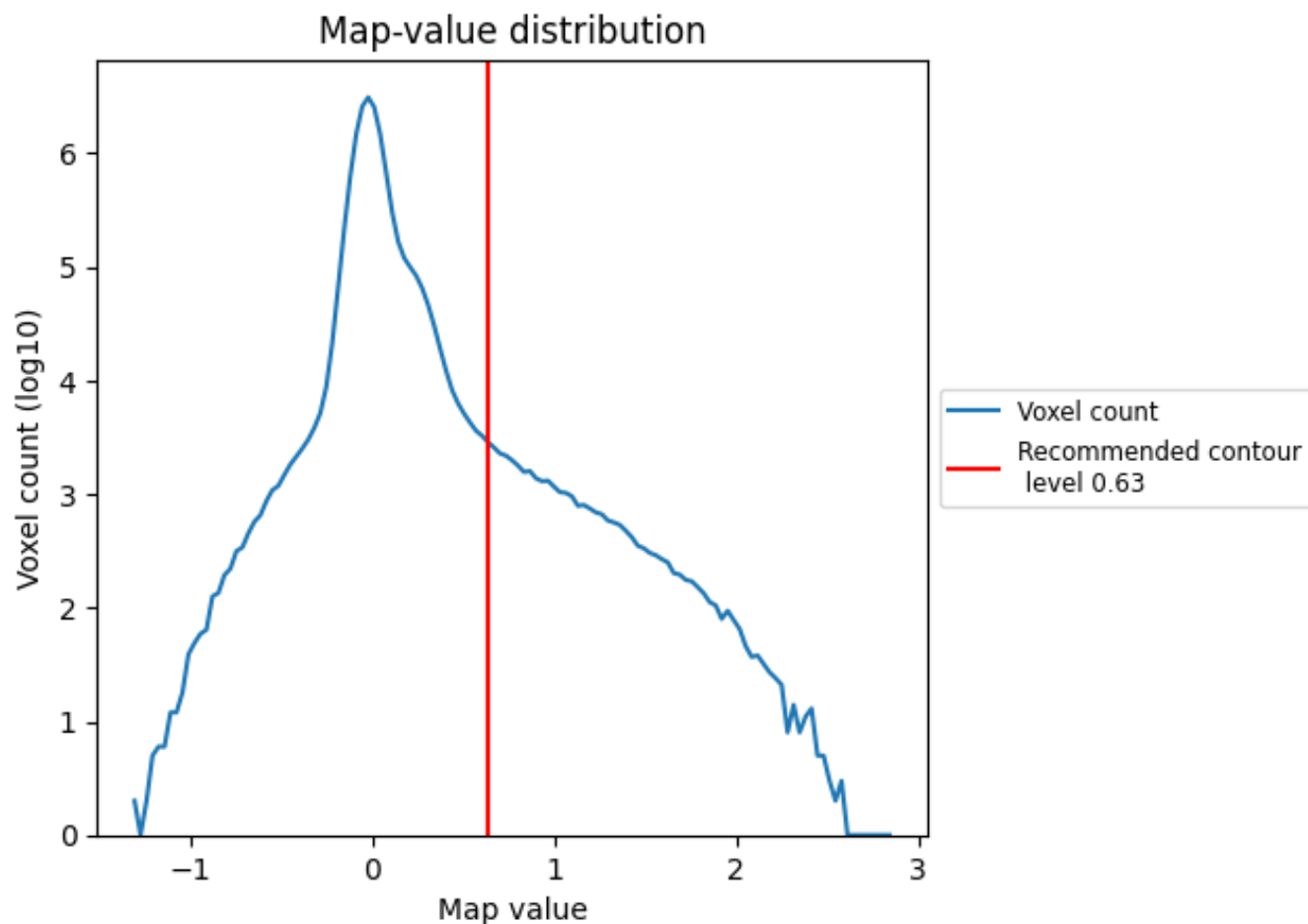
6.6 Mask visualisation

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

7 Map analysis [i](#)

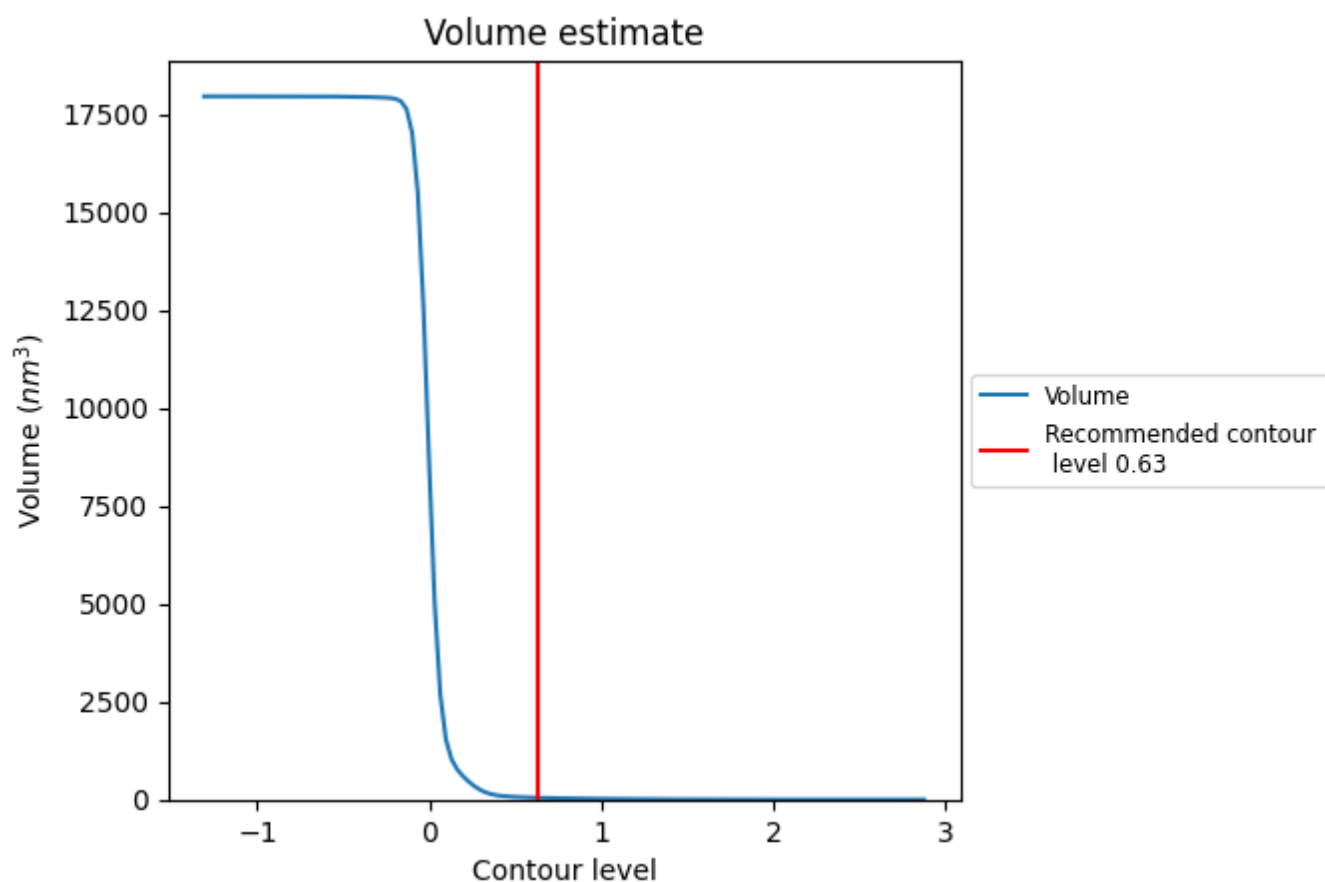
This section contains the results of statistical analysis of the map.

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.

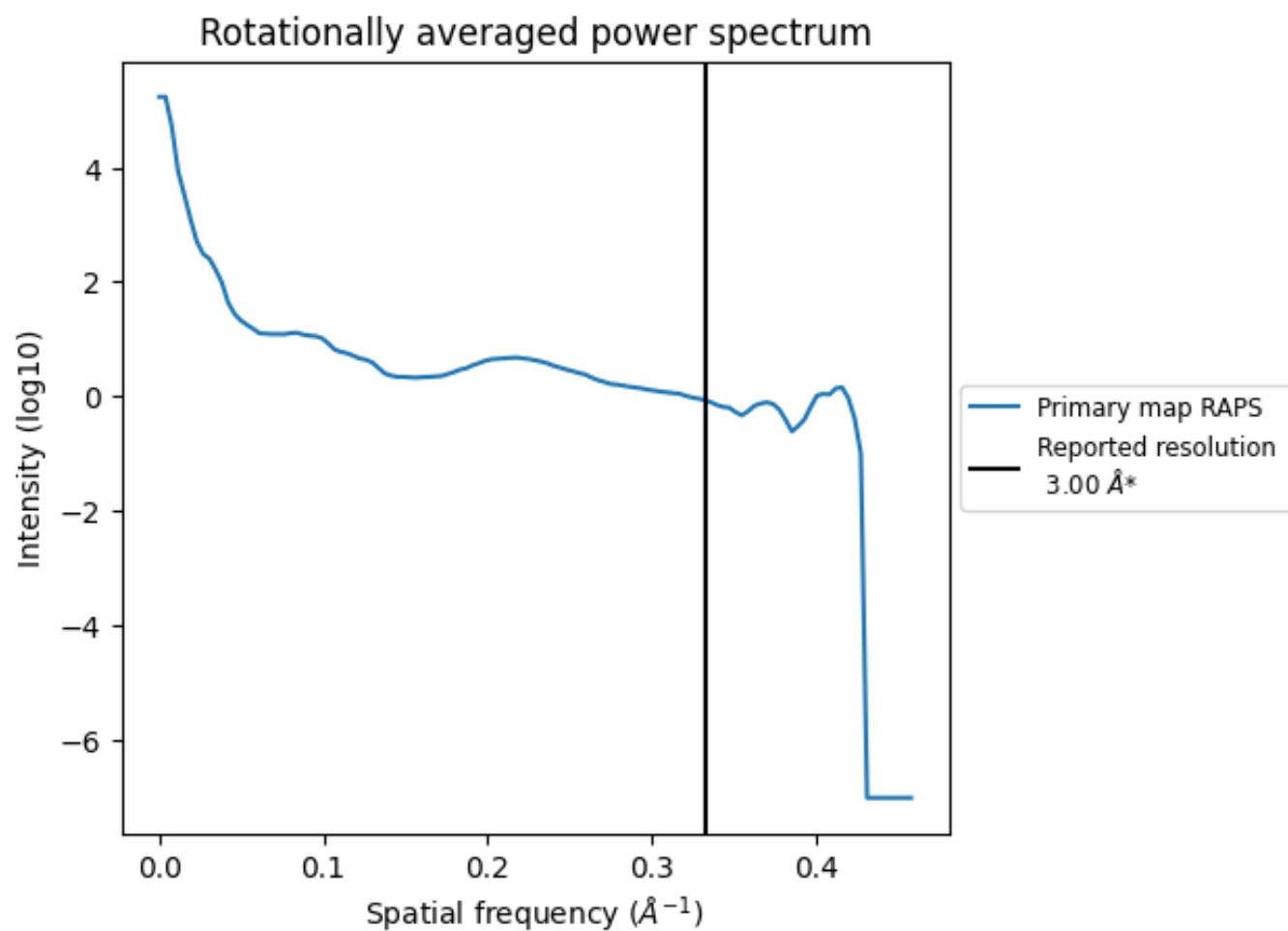
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm^3 ; this corresponds to an approximate mass of 42 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation

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

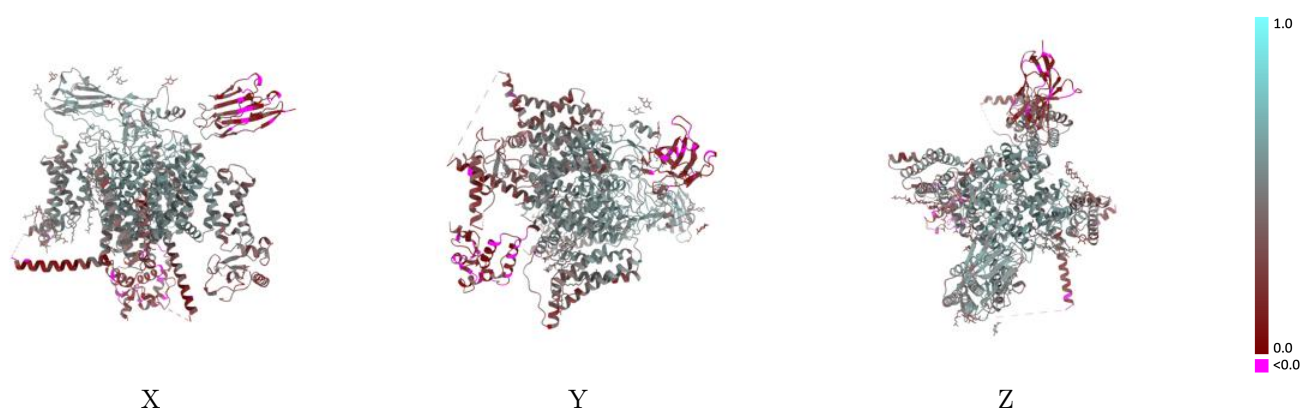
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32372 and PDB model 7W9T. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)

This section was not generated.

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

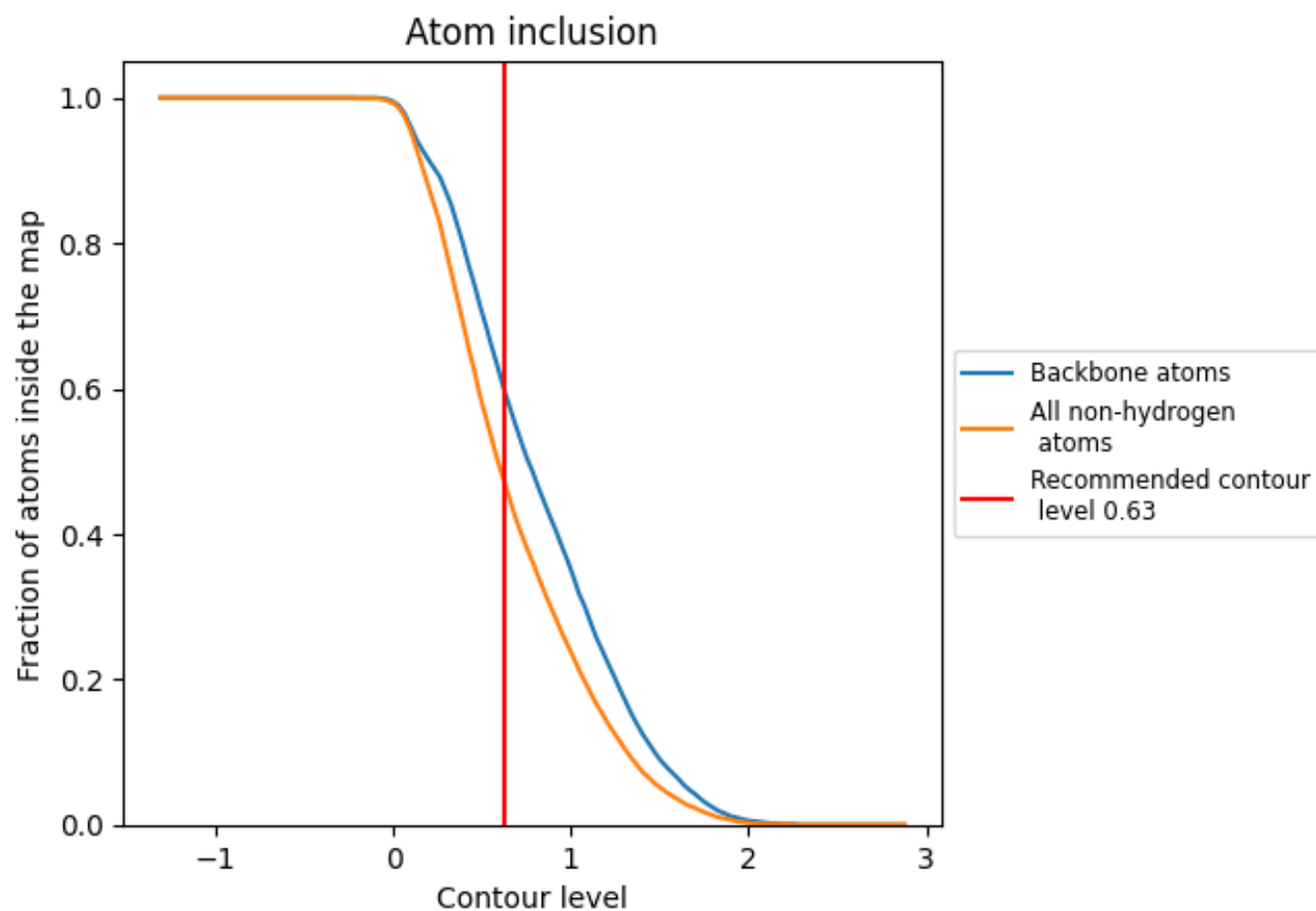


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 47% 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 (0.63) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4680	0.4310
A	0.4680	0.4410
B	0.6940	0.5070
C	0.1130	0.1840
D	0.4640	0.4680
E	0.5710	0.4350
F	0.6790	0.4410

1.0

0.0

<0.0