



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 03:37 PM JST

PDB ID : 7W9T
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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

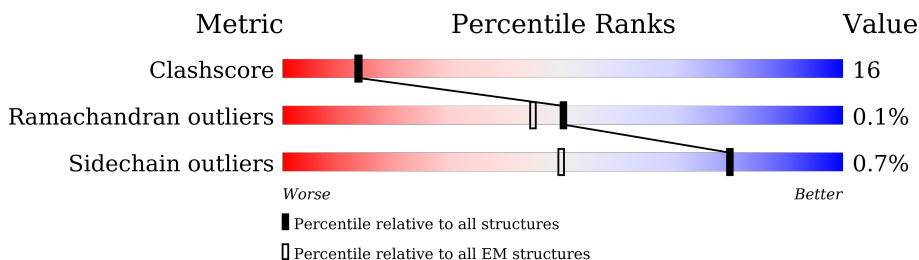
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>25%</div> <div>50%</div> <div>20%</div> <div>30%</div> </div>
2	B	218	<div> <div>8%</div> <div>56%</div> <div>22%</div> <div>•</div> <div>21%</div> </div>
3	C	215	<div> <div>48%</div> <div>51%</div> <div>5%</div> <div>45%</div> </div>
4	D	2	<div> <div>50%</div> <div>100%</div> </div>
4	E	2	<div> <div>50%</div> <div>100%</div> </div>
4	F	2	<div> <div>100%</div> </div>

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

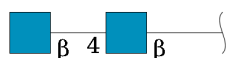
- Molecule 2 is a protein called Sodium channel subunit beta-1.

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.



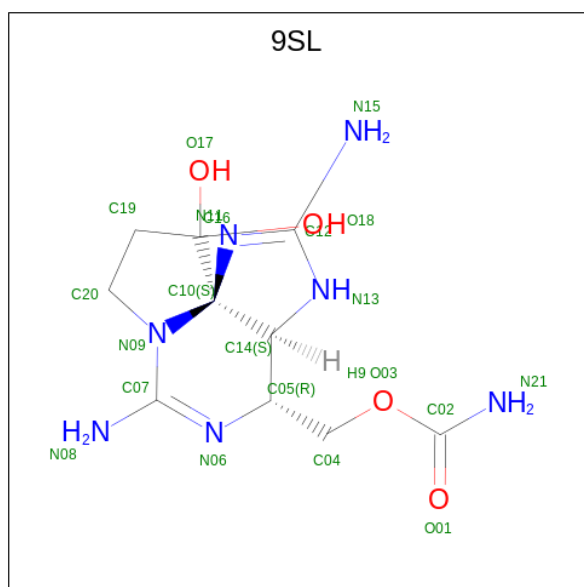
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

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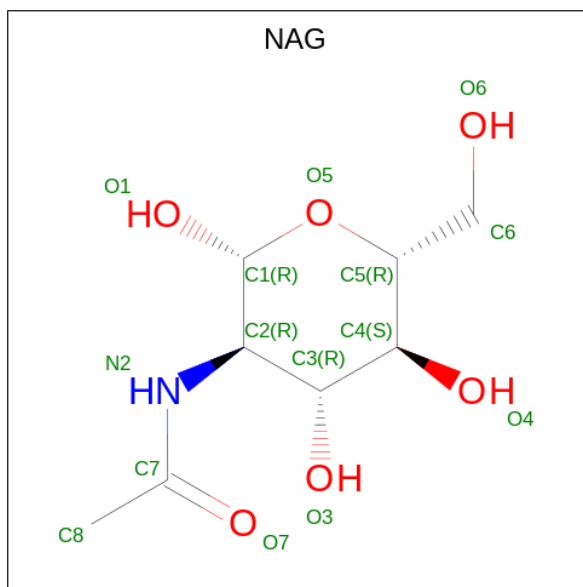
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	F	2	28	16	2	10	0	0

- 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 (three-letter code: 9SL) (formula: C₁₀H₁₇N₇O₄) (labeled as "Ligand of Interest" by depositor).



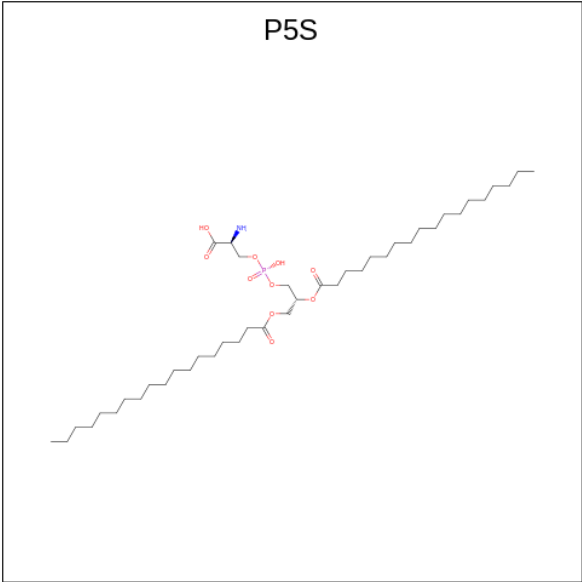
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	21	10	7	4	0

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



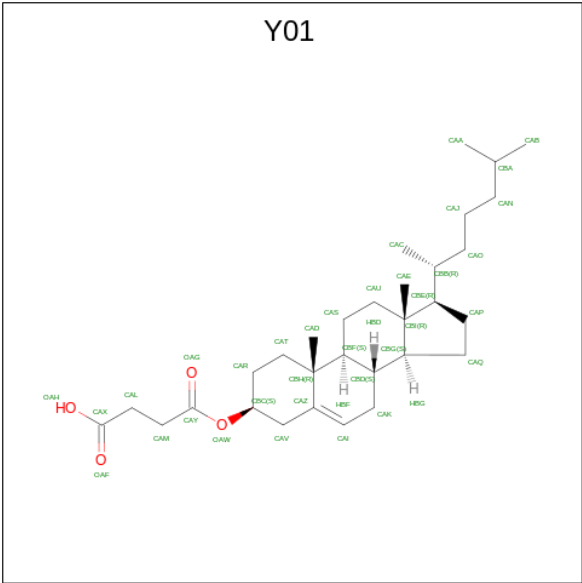
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: 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 (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



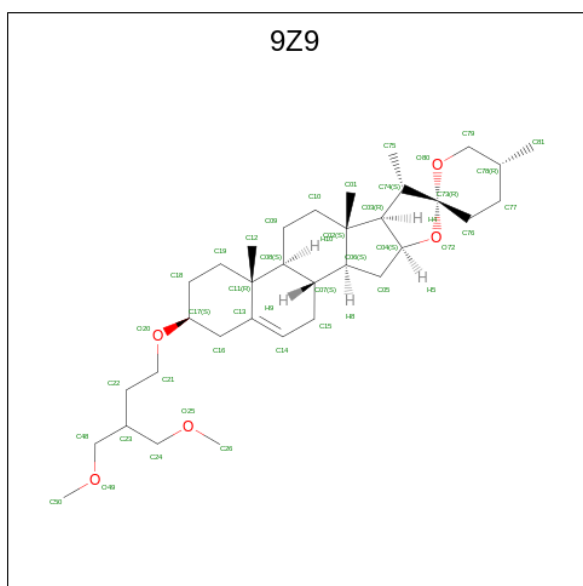
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	

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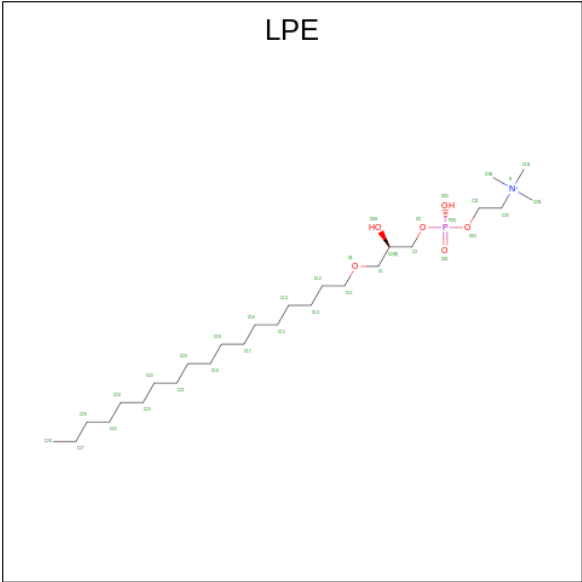
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	

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



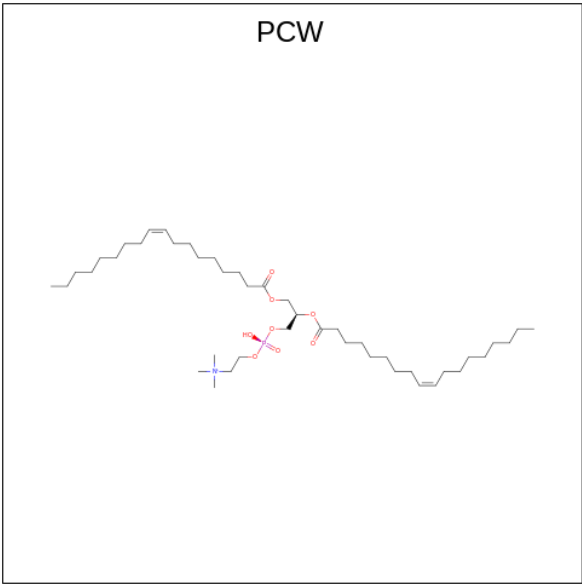
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			39	34	5	

- Molecule 10 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: C₂₆H₅₇NO₆P).



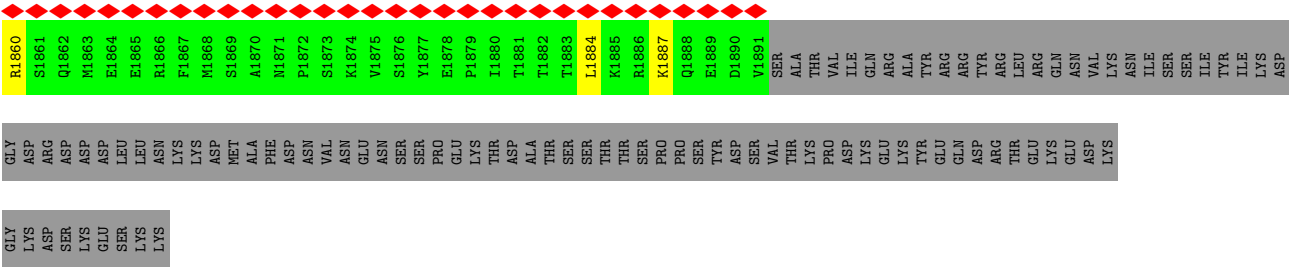
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			20	12	1	6	1	
10	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
10	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	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 (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).

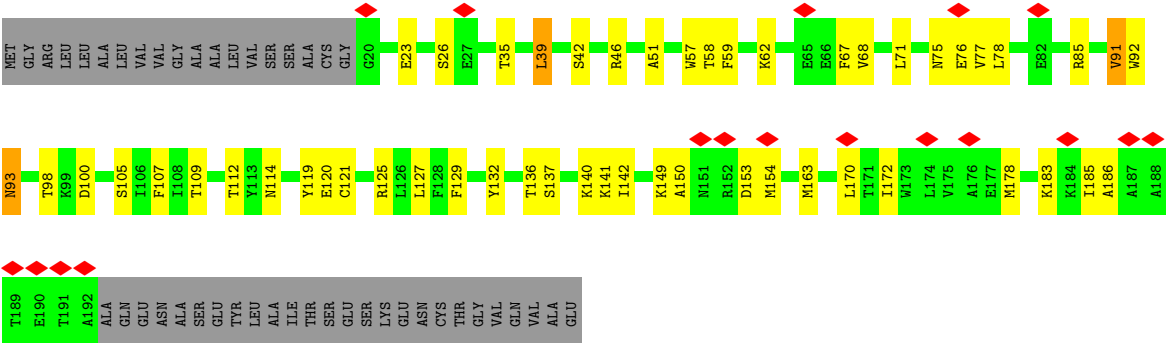


Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			53	43	1	8	1	
11	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

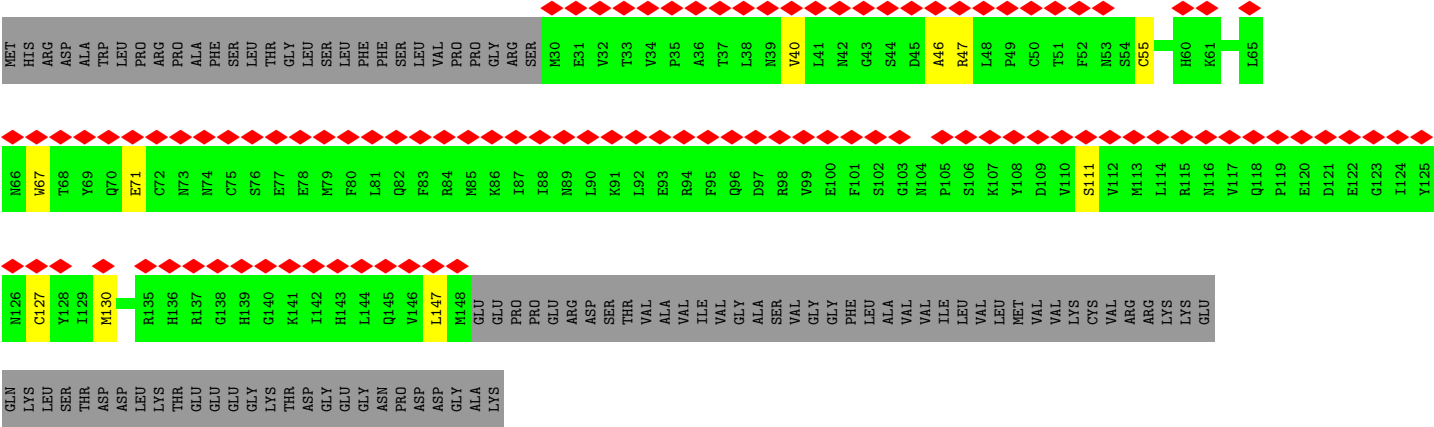
S1800	V1735	T1607	T1531	M1461	F1331	L1243	PRO	ALA	ASN	SER	V816	C736	GLU	SER
K1801	G1736	L1608	M1532	Q1462	W1332	K1244	GLU	ALA	THR	GLU	T817	I737	ASP	GLU
L1802	F1609	L1609	E1537	K1466	L1333	W1246	CYS	GLY	LYS	LYS	L818	Y738	MET	ASP
S1803	R1610	R1610	E1537	L1467	S1336	A1247	PHE	GLU	GLU	ASN	S819	F739	LEU	LEU
D1804	V1611	V1611	M1543	L1468	V1340	Y1248	THR	ASP	TVR	ASN	V821	I740	ASN	ASN
F1805	I1612	I1612	T1544	G1468	V1340	G1249	GLY	ASP	ILE	TRP	V821	V741	ASP	PRO
A1806	R1613	R1613	E1545	G1469	Y1348	Y1250	CYS	LEU	LEU	ASN	E822	M742	ASN	ASN
A1807	L1614	L1614	V1546	Q1470	Y1348	T1251	VAL	ASN	ASN	HIS	L823	D743	LEU	ARG
A1808	A1615	A1615	W1549	Q1471	P1360	Y1253	TRP	MET	HIS	THR	F824	F744	GLN	GLN
A1809	R1616	R1616	W1549	D1471	P1360	F1254	ARG	ASN	THR	LEU	L825	F745	ARG	ARG
D1810	R1619	R1619	V1553	E1477	Q1363	A1257	PHE	ALA	ALA	ALA	A826	V746	ALA	ALA
P1811	R1622	R1622	F1558	Q1478	Y1384	A1257	SER	GLU	GLU	GLU	D827	D747	MET	MET
L1812	L1623	L1623	T1559	K1480	M1366	W1260	CYS	LEU	LEU	GLU	V828	L748	SER	SER
P1813	V1624	V1624	G1560	K1481	R1367	V1268	GLN	SER	SER	LYS	E829	L748	ARG	ARG
L1814	A1757	A1757	E1561	Y1481	S1368	V1268	VAL	SER	LYS	LYS	G830	A749	ALA	ALA
I1815	K1628	K1628	E1561	Y1481	E1369	F1254	ASN	ASP	GLY	ASN	G830	I750	SER	SER
I1816	G1629	G1629	M1485	M1485	E1369	F1254	ILE	SER	HIS	ILE	T751	I751	ILE	ILE
A1817	I1630	I1630	K1486	K1486	Y1384	A1257	GLU	ASP	ASN	LEU	E770	E770	THR	THR
K1817	L1637	L1637	K1487	K1487	M1366	W1260	SER	SER	PHE	LEU	E771	E771	ASN	ASN
P1818	L1641	L1641	L1488	L1488	R1367	V1268	GLY	GLU	LEU	LYS	F772	F772	THR	THR
I1819	M1646	M1646	G1489	G1489	E1369	F1254	LYS	SER	GLY	LYS	K773	K773	VAL	VAL
K1820	V1765	V1765	K1491	K1491	M1384	V1274	LYS	LYS	LYS	LYS	N774	N774	GLU	GLU
V1821	A1766	A1766	K1492	K1492	M1388	A1275	VAL	VAL	ASP	ASP	V775	V775	GLU	GLU
Q1822	L1649	L1649	P1493	P1493	V1392	M1276	ARG	ARG	LYS	LYS	L776	L776	LEU	LEU
L1823	L1650	L1650	Q1494	Q1494	G1393	T1277	ASN	ASN	ILE	ILE	A777	A777	GLU	GLU
I1824	L1653	L1653	K1495	K1495	L1394	L1278	SER	SER	PHE	PHE	I778	I778	SER	SER
A1825	I1657	I1657	P1496	P1496	S1398	G1279	SER	SER	GLY	GLY	G779	G779	ARG	ARG
M1826	F1666	F1666	I1497	I1497	L1398	Y1280	GLU	GLU	VAL	VAL	N780	N780	GLN	GLN
D1827	F1666	F1666	P1498	P1498	M1412	Y1280	CYS	CYS	ASP	ASP	K847	K847	CYS	CYS
L1828	P1773	P1773	R1499	R1499	Y1413	L1289	SER	SER	LYS	LYS	G885	G885	PRO	PRO
M1830	L1774	L1774	P1500	P1500	Y1413	L1289	THR	THR	HIS	HIS	A788	A788	TRP	TRP
V1831	S1775	S1775	Q1501	Q1501	D1417	R1291	VAL	VAL	LYS	LYS	A789	A789	TRP	TRP
S1832	E1776	E1776	K1502	K1502	D1417	L1292	ASN	ASN	GLU	GLU	E790	E790	ARG	ARG
A1833	D1777	D1777	K1503	K1503	Y1427	A1294	PRO	PRO	ASP	ASP	M791	M791	PHE	PHE
D1834	I1689	I1689	I1504	I1504	S1430	L1298	LEU	LEU	SER	SER	V792	V792	ALA	ALA
R1835	I1694	I1694	Q1505	Q1505	M1433	L1298	PRO	PRO	ASP	ASP	L793	L793	LYS	LYS
I1836	S1697	S1697	G1506	G1506	M1433	L1301	GLY	GLY	GLY	GLY	K794	K794	PHE	PHE
C1838	G1592	G1592	C1507	C1507	M1433	L1301	GLY	GLY	GLY	GLY	L795	L795	ILE	ILE
L1839	M1593	M1593	I1508	I1508	F1443	F1304	ALA	ALA	ALA	ALA	I796	I796	TRP	TRP
D1840	F1594	F1594	F1509	F1509	G1444	E1306	ALA	ALA	PRO	PRO	A797	A797	ASN	ASN
L1841	L1595	L1595	D1510	D1510	S1445	M1307	GLY	GLY	ILE	ILE	M798	M798	CYS	CYS
L1842	L1596	L1596	L1511	L1511	I1453	R1308	GLY	GLY	HIS	HIS	D799	D799	SER	SER
F1843	D1597	D1597	T1513	T1513	G1454	V1309	PRO	PRO	ASN	ASN	P800	P800	Y729	Y729
A1844	L1598	L1598	M1514	M1514	V1455	V1310	LEU	LEU	PRO	PRO	L924	L924	W730	W730
F1845	L1707	L1707	Q1515	Q1515	V1456	V1311	MET	MET	THR	THR	E802	E802	I731	I731
L1846	M1709	M1709	A1516	A1516	I1457	V1312	ASN	ASN	VAL	VAL	N803	N803	K732	K732
K1847	C1730	C1730	F1517	F1517	D1458	V1324	ASP	ASP	THR	THR	F804	F804	F733	F733
R1848	T1791	T1791	D1518	D1518	N1459	L1326	PRO	PRO	VAL	VAL	Q805	Q805	K734	K734
V1849	D1792	D1792	I1519	I1519	L1528	L1326	LYS	LYS	PRO	PRO	V806	V806	W735	W735
L1850	A1793	A1793	S1520	S1520	M1522	I1330	LYS	LYS	PRO	PRO	Q807	Q807	W735	W735
G1851	T1794	T1794	I1521	I1521	M1522	I1330	ILE	ILE	LYS	LYS	W808	W808	W735	W735
E1852	Q1795	Q1795	M1522	M1522	F1460	I1330	ARG	ARG	SER	SER	N809	N809	W735	W735
G1853	F1796	F1796	I1525	I1525	F1460	I1330	GLU	GLU	ARG	ARG	I810	I810	W735	W735
S1854	E1798	E1798	L1527	L1527	F1460	I1330	GLN	GLN	ARG	ARG	F811	F811	W735	W735
E1855	F1799	F1799	M1528	M1528	F1460	I1330	ALA	ALA	GLN	GLN	D812	D812	W735	W735
M1856							GLU	GLU	ALA	ALA	S813	S813	W735	W735
S1858							LEU	LEU	ASP	ASP	L814	L814	W735	W735
L1859									LEU	LEU	I815	I815	W735	W735



• Molecule 2: Sodium channel subunit beta-1



• Molecule 3: Sodium channel subunit beta-2



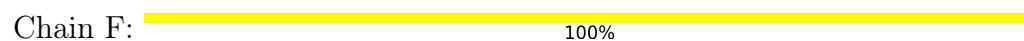
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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: NAG, Y01, 9Z9, 9SL, LPE, PCW, P5S

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	0.41	0/11693	0.52	1/15834 (0.0%)
2	B	0.41	0/1442	0.50	0/1949
3	C	0.36	0/1011	0.58	0/1367
All	All	0.40	0/14146	0.53	1/19150 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	CYS	CA-CB-SG	5.84	124.52	114.00

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	357	0
2	B	1416	0	1380	45	0
3	C	980	0	935	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	79	0
10	B	17	0	19	10	0
11	A	232	0	321	35	0
All	All	14841	0	15207	473	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 473 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
1:A:1602:TYR:CD2	1:A:1603:PHE:CD1	2.18	1.28
1:A:1602:TYR:HD2	1:A:1603:PHE:CD1	1.52	1.26

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1409/2031 (69%)	1337 (95%)	71 (5%)	1 (0%)	48	81
2	B	171/218 (78%)	156 (91%)	14 (8%)	1 (1%)	22	57
3	C	120/215 (56%)	116 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1700/2464 (69%)	1609 (95%)	89 (5%)	2 (0%)	50 81

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%)	1262 (100%)	4 (0%)	91 96
2	B	157/190 (83%)	154 (98%)	3 (2%)	52 79
3	C	114/193 (59%)	110 (96%)	4 (4%)	31 65
All	All	1537/2192 (70%)	1526 (99%)	11 (1%)	80 91

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	55	CYS
3	C	71	GLU
3	C	147	LEU
3	C	130	MET
2	B	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	941	GLN
2	B	115	HIS
1	A	987	ASN
3	C	82	GLN
1	A	1721	HIS

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 ⓘ

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	4,1	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	D	2	4	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	E	1	4,1	14,14,15	0.18	0	17,19,21	0.46	0
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.66	0
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	0.65	0	17,19,21	1.20	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	4,1	-	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	4,1	-	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	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.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	2.72	115.87	112.19
4	F	1	NAG	C3-C4-C5	-2.65	105.52	110.24
4	F	2	NAG	C4-C3-C2	-2.42	107.47	111.02

There are no chirality outliers.

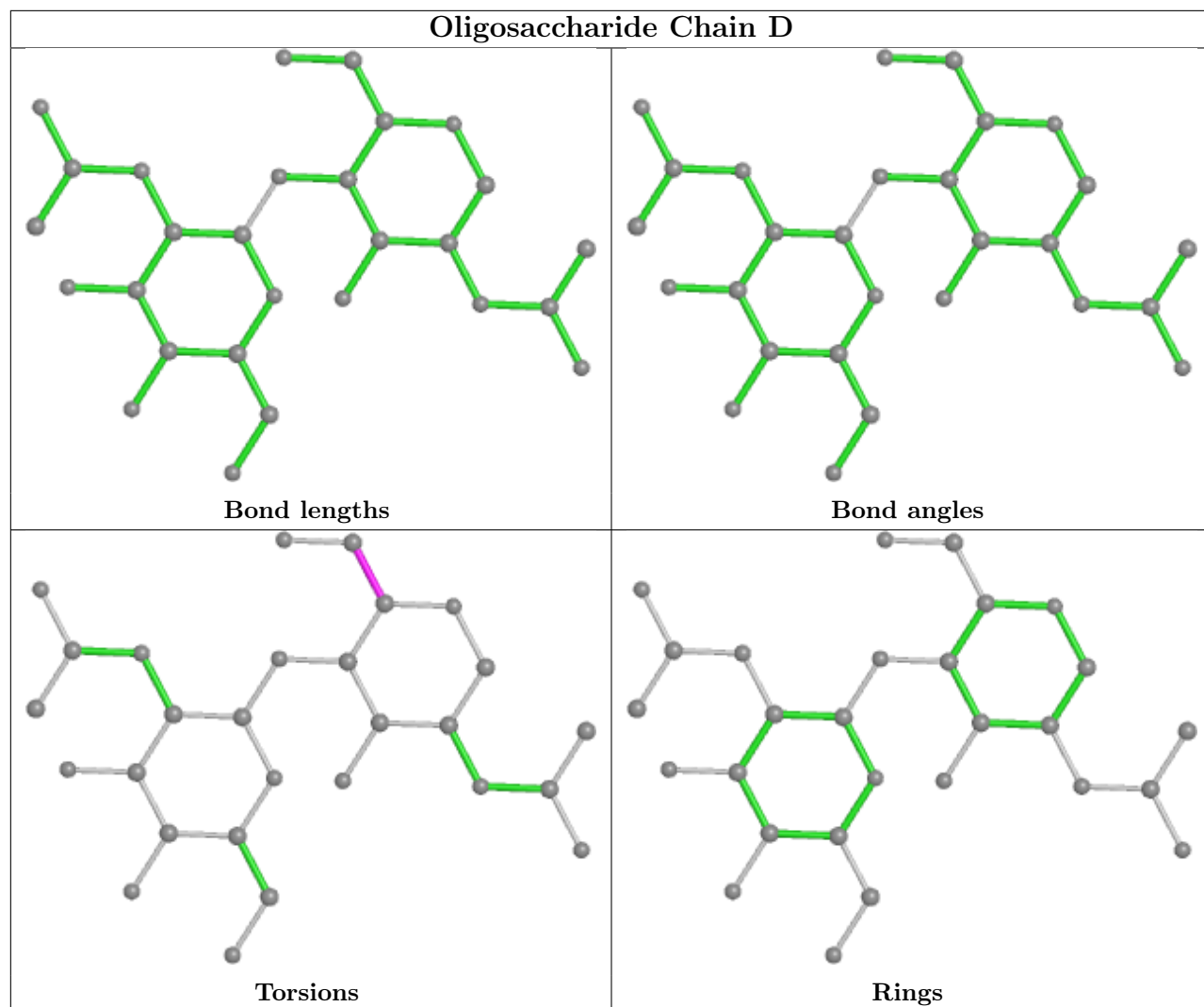
5 of 10 torsion outliers are listed below:

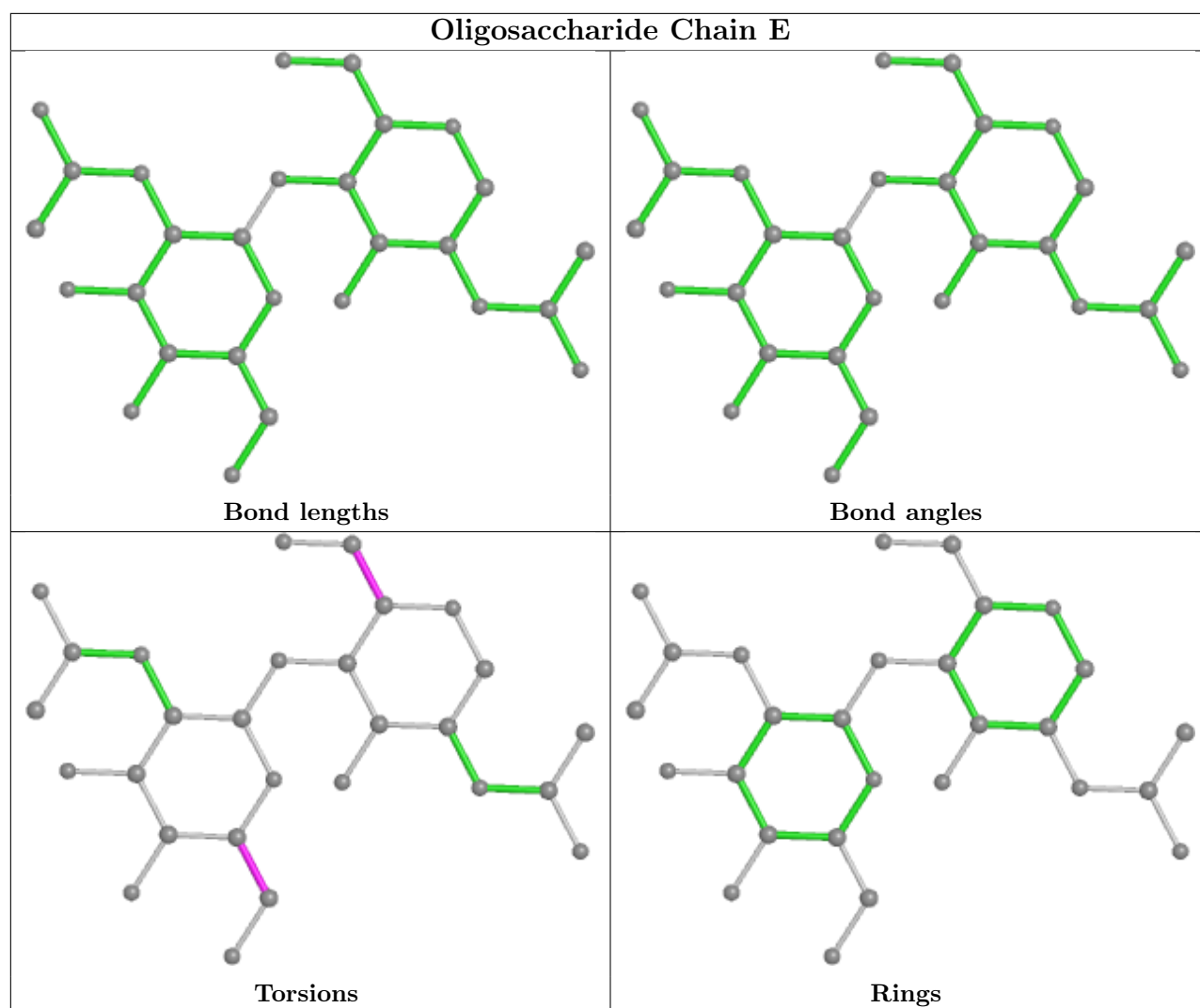
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6

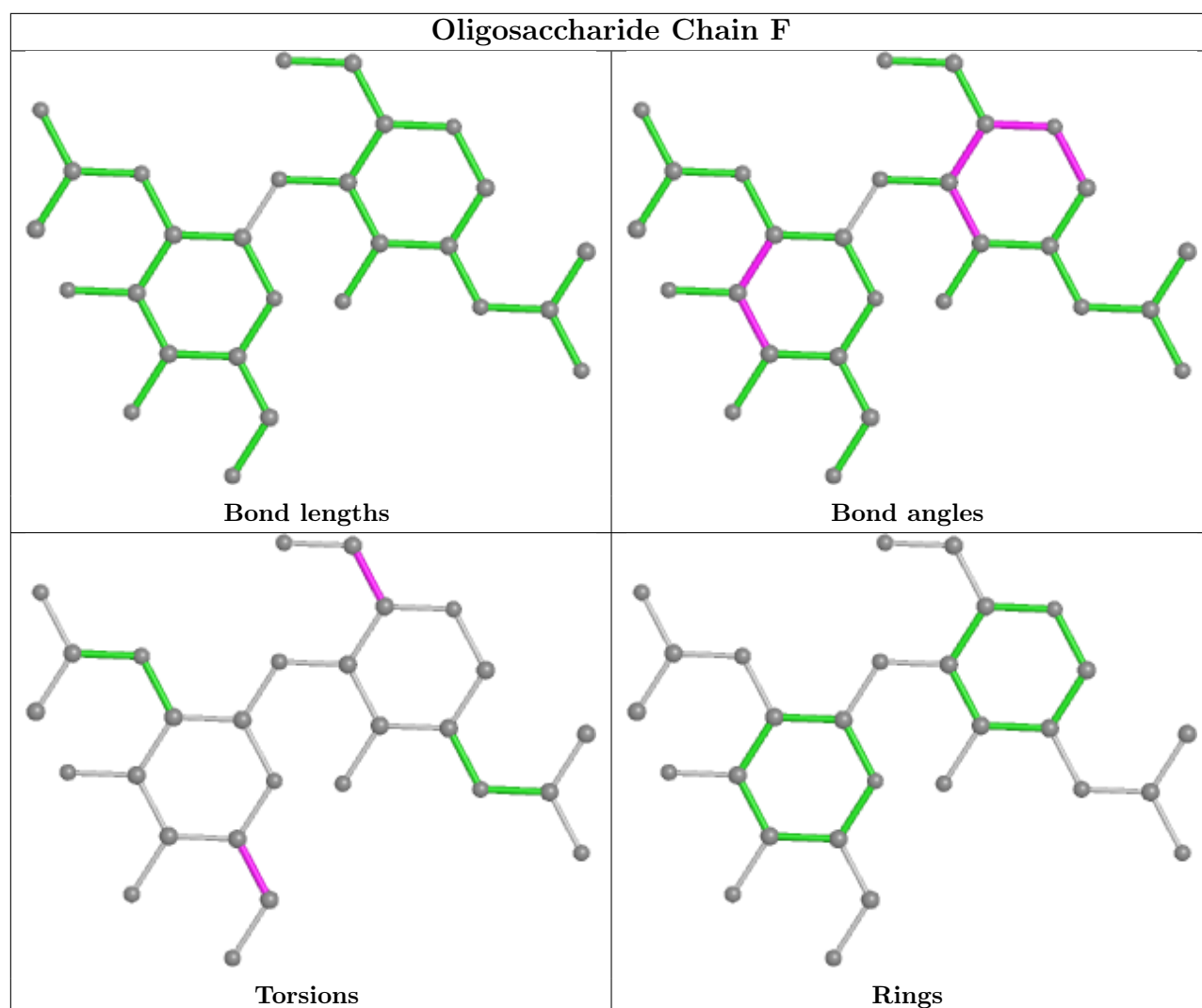
There are no ring outliers.

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	$\# Z > 2$
5	9SL	A	2001	-	17,23,23	3.61	8 (47%)	13,37,37	3.02	6 (46%)
8	Y01	A	2004	-	38,38,38	0.66	1 (2%)	57,57,57	1.79	11 (19%)
10	LPE	A	2015	-	27,27,33	0.54	0	31,33,39	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PCW	A	2027	-	43,43,53	1.03	2 (4%)	49,51,61	0.94	2 (4%)
11	PCW	A	2016	-	46,46,53	0.99	3 (6%)	52,54,61	1.18	4 (7%)
10	LPE	A	2022	-	24,24,33	0.53	0	28,30,39	0.63	0
10	LPE	A	2025	-	24,24,33	0.54	0	28,30,39	0.50	0
6	NAG	B	302	2	14,14,15	0.18	0	17,19,21	0.41	0
9	9Z9	A	2007	-	44,44,44	0.70	1 (2%)	66,68,68	1.45	12 (18%)
6	NAG	B	301	2	14,14,15	0.64	0	17,19,21	0.98	0
10	LPE	A	2010	-	24,24,33	0.52	0	28,30,39	0.60	0
11	PCW	A	2028	-	43,43,53	0.99	2 (4%)	49,51,61	2.90	6 (12%)
11	PCW	A	2013	-	52,52,53	0.93	2 (3%)	58,60,61	0.97	2 (3%)
6	NAG	A	2002	1	14,14,15	0.34	0	17,19,21	0.44	0
8	Y01	A	2029	-	38,38,38	1.62	7 (18%)	57,57,57	1.63	10 (17%)
10	LPE	A	2019	-	24,24,33	0.60	0	28,30,39	0.89	1 (3%)
10	LPE	A	2021	-	24,24,33	0.54	0	28,30,39	0.68	1 (3%)
10	LPE	A	2024	-	24,24,33	0.52	0	28,30,39	0.62	0
7	P5S	A	2003	-	33,34,53	0.76	1 (3%)	36,40,60	1.80	5 (13%)
10	LPE	A	2011	-	24,24,33	0.33	0	25,27,39	0.60	0
7	P5S	A	2017	-	40,40,53	1.14	3 (7%)	43,45,60	1.37	3 (6%)
8	Y01	A	2005	-	38,38,38	0.66	1 (2%)	57,57,57	1.79	11 (19%)
11	PCW	A	2018	-	43,43,53	1.01	2 (4%)	49,51,61	1.12	5 (10%)
6	NAG	B	303	2	14,14,15	0.25	0	17,19,21	0.42	0
8	Y01	A	2009	-	38,38,38	1.15	4 (10%)	57,57,57	1.74	10 (17%)
10	LPE	A	2020	-	24,24,33	0.85	0	28,30,39	0.92	1 (3%)
6	NAG	A	2008	1	14,14,15	0.30	0	17,19,21	1.00	1 (5%)
10	LPE	A	2012	-	19,19,33	0.62	0	23,25,39	0.51	0
10	LPE	A	2026	-	16,16,33	0.68	0	20,22,39	0.67	0
10	LPE	B	304	-	16,16,33	0.67	0	20,22,39	0.60	0
8	Y01	A	2006	-	38,38,38	1.15	4 (10%)	57,57,57	1.74	12 (21%)
10	LPE	A	2023	-	24,24,33	0.53	0	28,30,39	0.54	0
10	LPE	A	2014	-	21,21,33	0.68	0	25,27,39	1.03	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	9SL	A	2001	-	-	4/5/53/53	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	Y01	A	2004	-	-	0/19/77/77	0/4/4/4
10	LPE	A	2015	-	-	10/28/28/34	-
11	PCW	A	2027	-	-	16/47/47/57	-
11	PCW	A	2016	-	-	13/50/50/57	-
10	LPE	A	2022	-	-	3/25/25/34	-
10	LPE	A	2025	-	-	10/25/25/34	-
6	NAG	B	302	2	-	0/6/23/26	0/1/1/1
9	9Z9	A	2007	-	-	0/12/100/100	0/6/6/6
6	NAG	B	301	2	-	0/6/23/26	0/1/1/1
10	LPE	A	2010	-	-	10/25/25/34	-
11	PCW	A	2028	-	-	12/47/47/57	-
11	PCW	A	2013	-	-	16/56/56/57	-
6	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
8	Y01	A	2029	-	-	7/19/77/77	0/4/4/4
10	LPE	A	2019	-	-	7/25/25/34	-
10	LPE	A	2021	-	-	3/25/25/34	-
10	LPE	A	2024	-	-	6/25/25/34	-
7	P5S	A	2003	-	-	28/39/39/59	-
10	LPE	A	2011	-	-	8/25/25/34	-
7	P5S	A	2017	-	-	8/44/44/59	-
8	Y01	A	2005	-	-	0/19/77/77	0/4/4/4
11	PCW	A	2018	-	-	12/47/47/57	-
6	NAG	B	303	2	-	0/6/23/26	0/1/1/1
8	Y01	A	2009	-	-	4/19/77/77	0/4/4/4
10	LPE	A	2020	-	-	12/25/25/34	-
6	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
10	LPE	A	2012	-	-	10/20/20/34	-
10	LPE	A	2026	-	-	7/17/17/34	-
10	LPE	B	304	-	-	9/17/17/34	-
8	Y01	A	2006	-	-	4/19/77/77	0/4/4/4
10	LPE	A	2023	-	-	8/25/25/34	-
10	LPE	A	2014	-	-	15/22/22/34	-

The worst 5 of 41 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	6.10	1.45	1.34
5	A	2001	9SL	C02-N21	5.95	1.44	1.33
5	A	2001	9SL	C12-N15	4.57	1.45	1.34
7	A	2017	P5S	O37-C38	4.42	1.46	1.34

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2028	PCW	C8-N-C6	-12.10	77.88	108.97
11	A	2028	PCW	C8-N-C7	-12.03	78.04	108.97
5	A	2001	9SL	O03-C02-N21	7.82	120.78	111.08
11	A	2028	PCW	C8-N-C5	-7.81	77.97	109.92
7	A	2003	P5S	OG-CB-CA	7.06	114.22	108.06

There are no chirality outliers.

5 of 246 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.

27 monomers are involved in 185 short contacts:

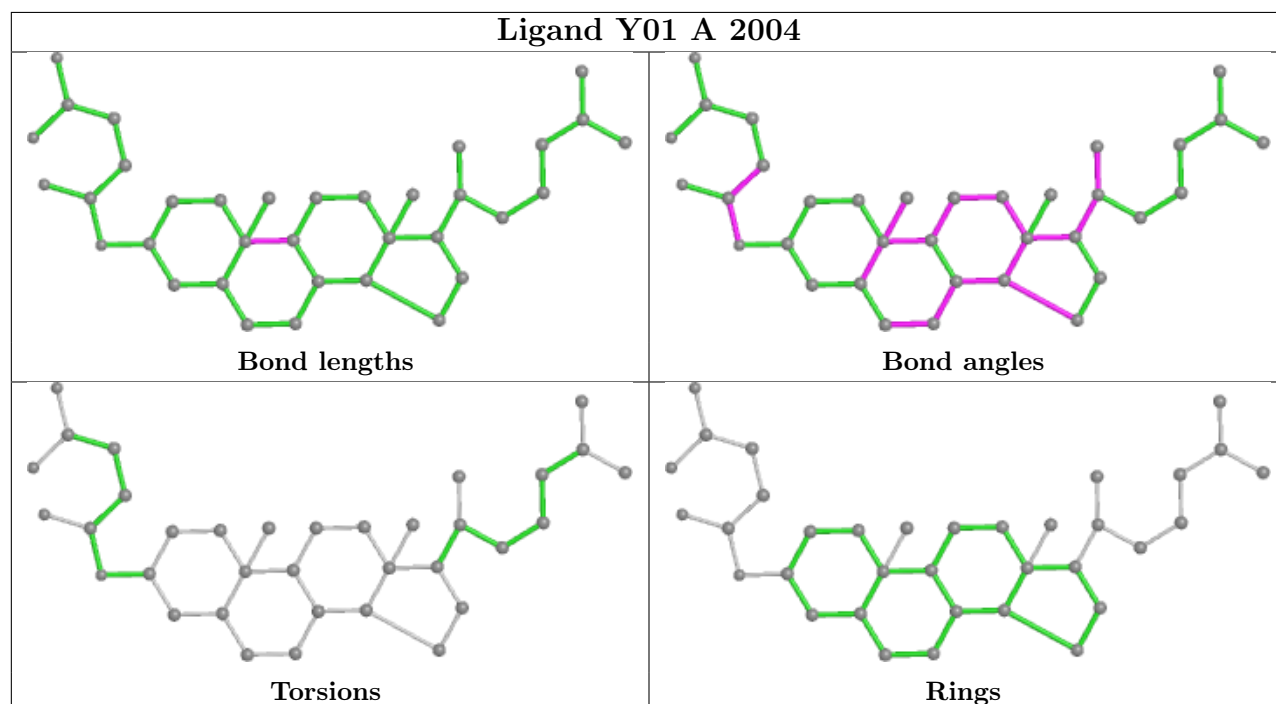
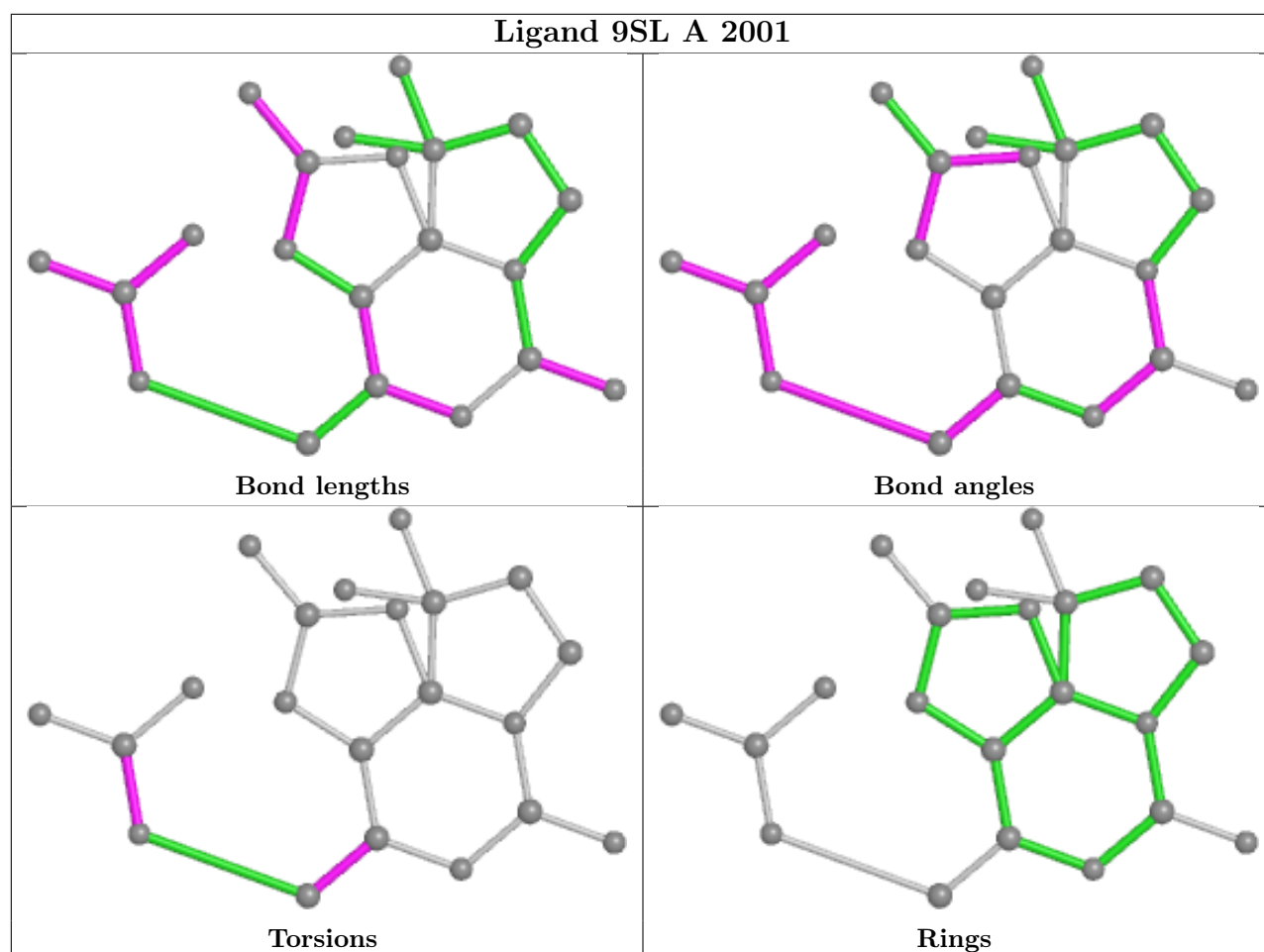
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2001	9SL	3	0
8	A	2004	Y01	6	0
10	A	2015	LPE	6	0
11	A	2027	PCW	8	0
11	A	2016	PCW	1	0
10	A	2022	LPE	7	0
10	A	2025	LPE	11	0
9	A	2007	9Z9	9	0
10	A	2010	LPE	2	0
11	A	2028	PCW	2	0

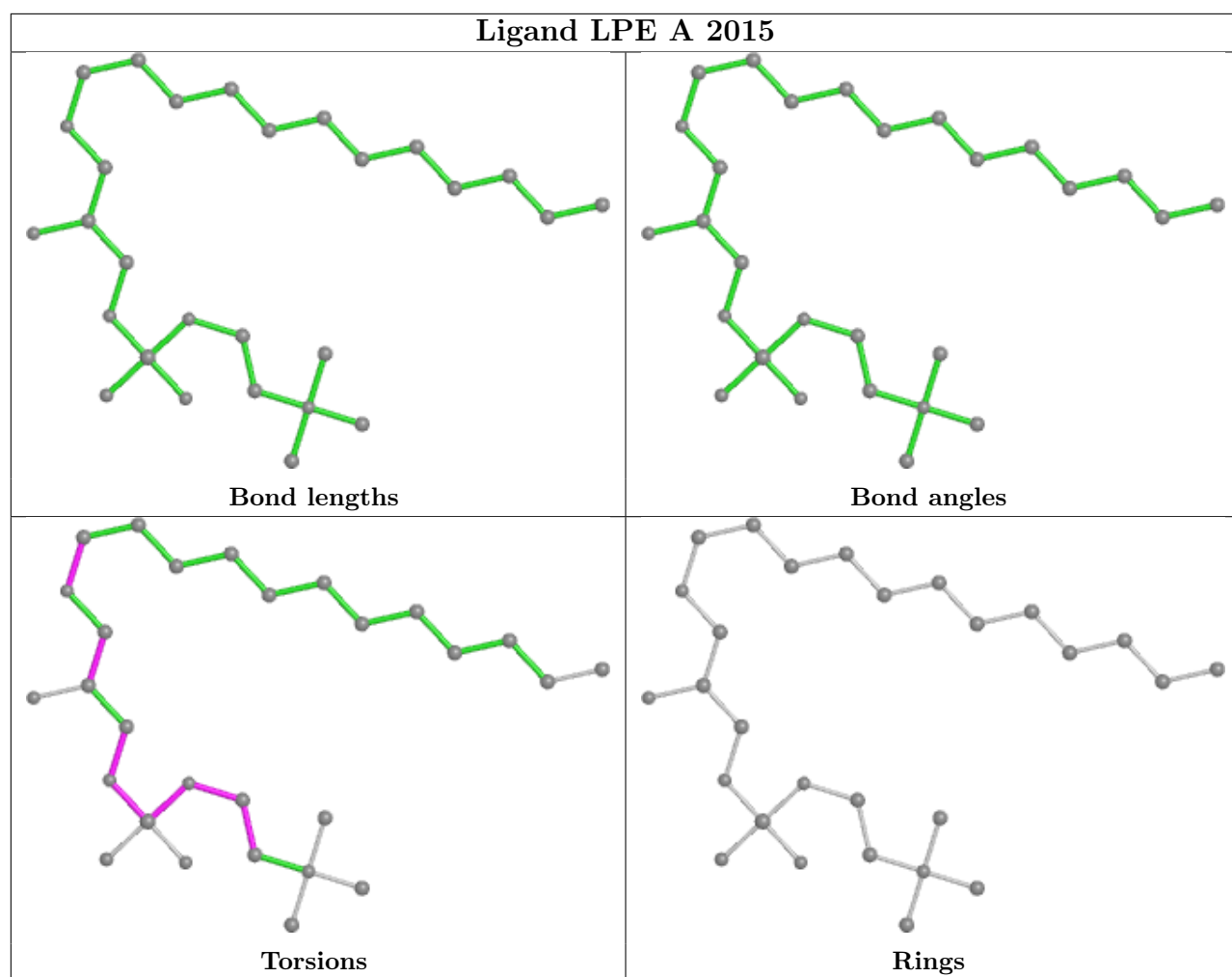
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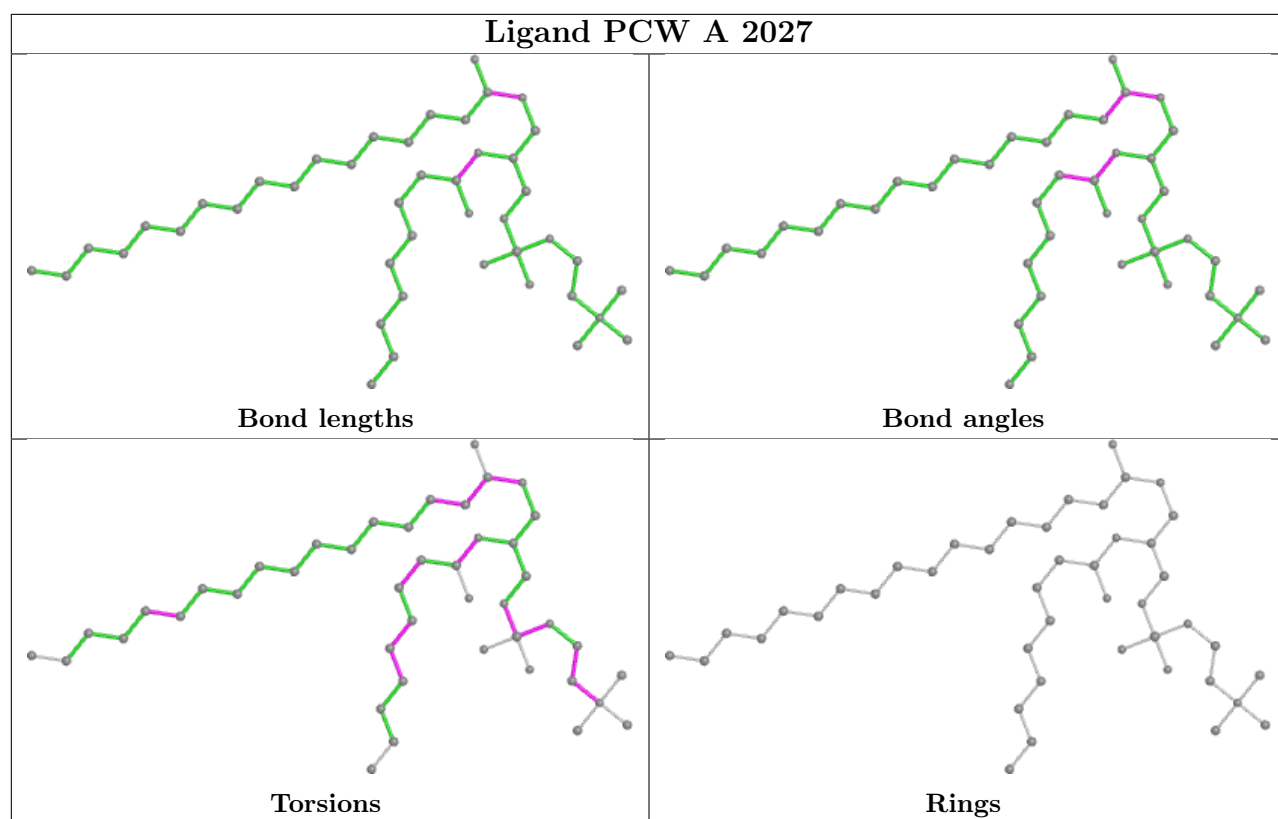
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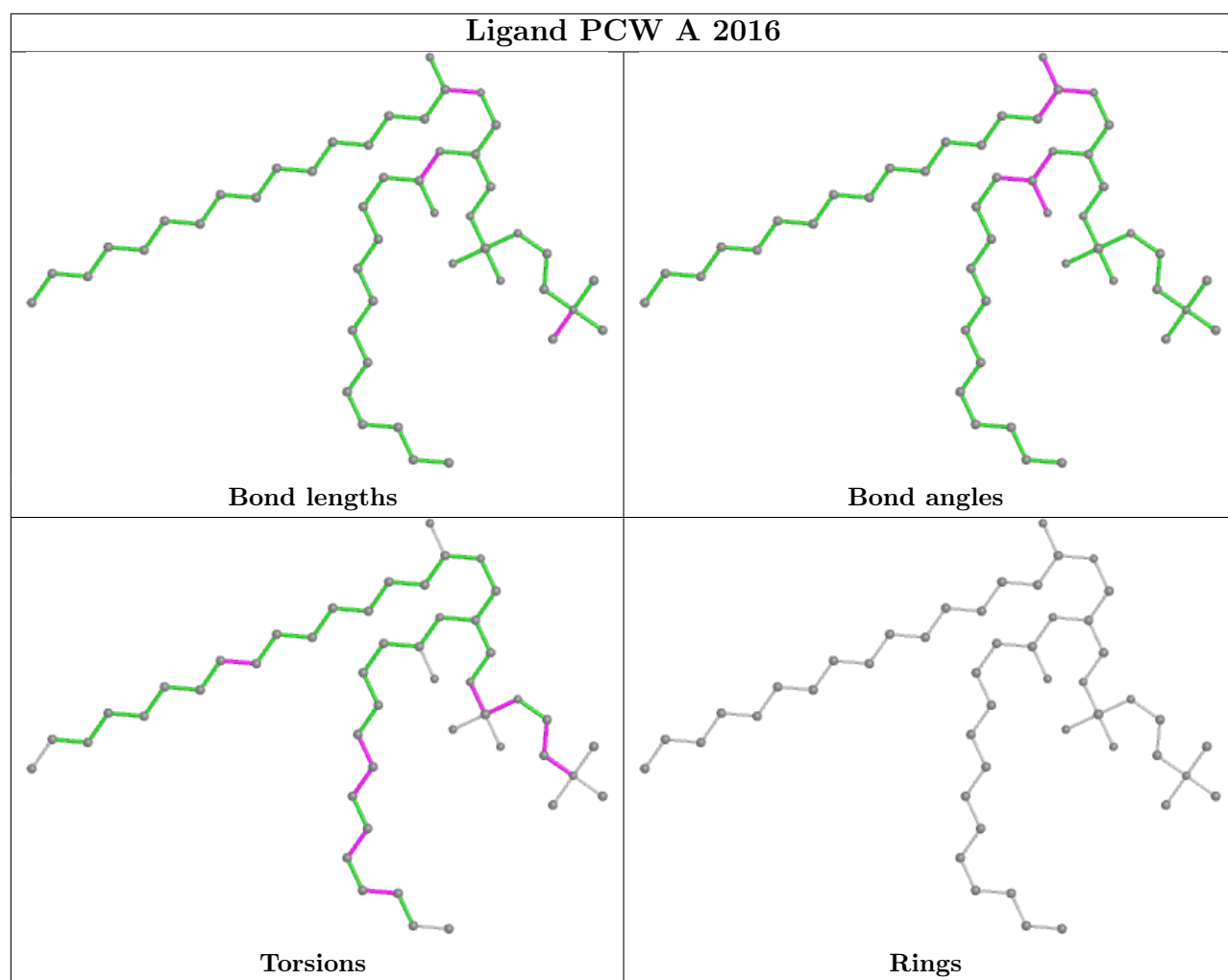
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	2013	PCW	22	0
8	A	2029	Y01	18	0
10	A	2019	LPE	8	0
10	A	2021	LPE	9	0
7	A	2003	P5S	12	0
10	A	2011	LPE	2	0
7	A	2017	P5S	9	0
8	A	2005	Y01	3	0
11	A	2018	PCW	6	0
8	A	2009	Y01	5	0
6	A	2008	NAG	9	0
10	A	2012	LPE	9	0
10	A	2026	LPE	10	0
10	B	304	LPE	10	0
8	A	2006	Y01	16	0
10	A	2023	LPE	8	0
10	A	2014	LPE	17	0

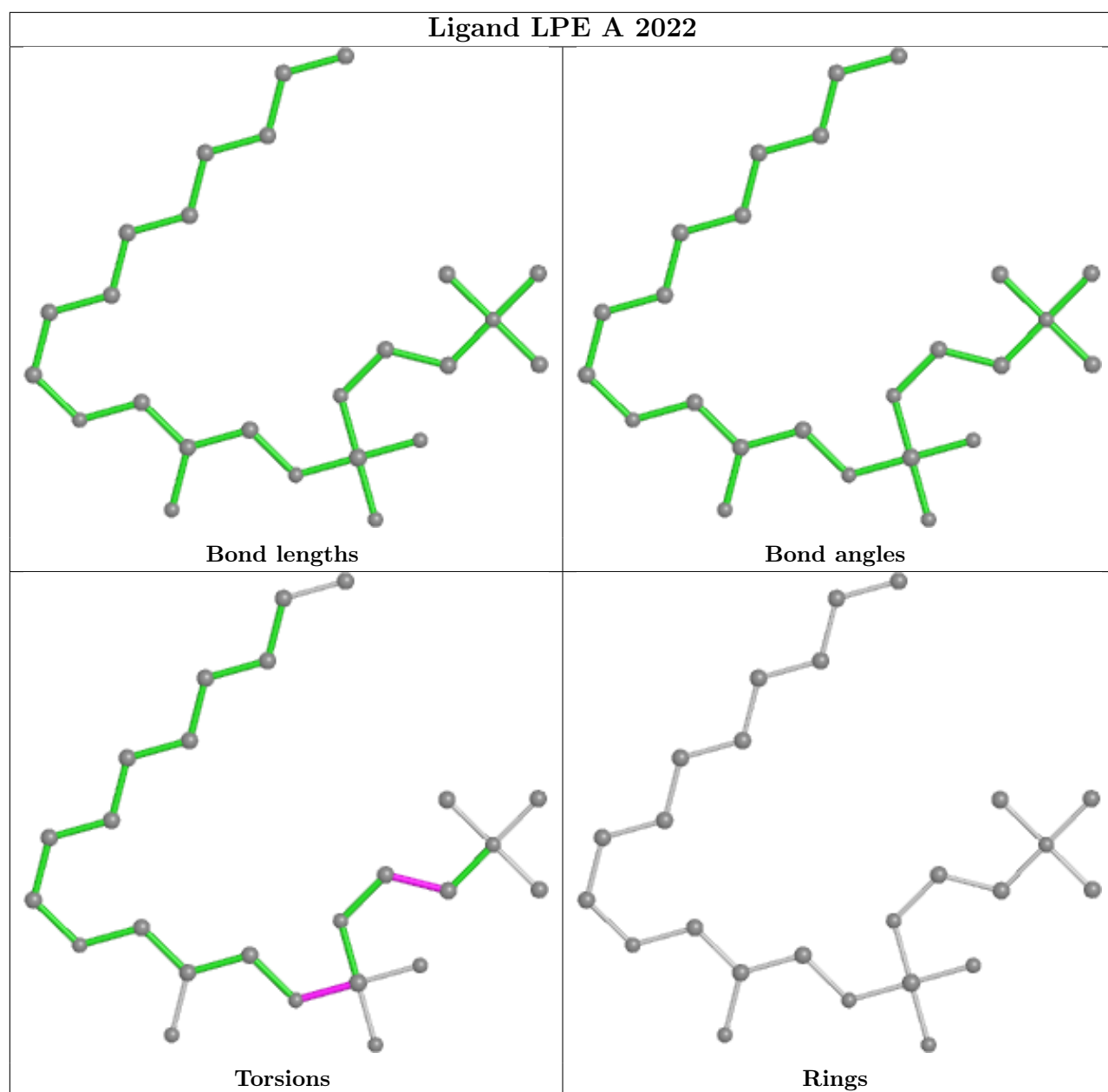
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

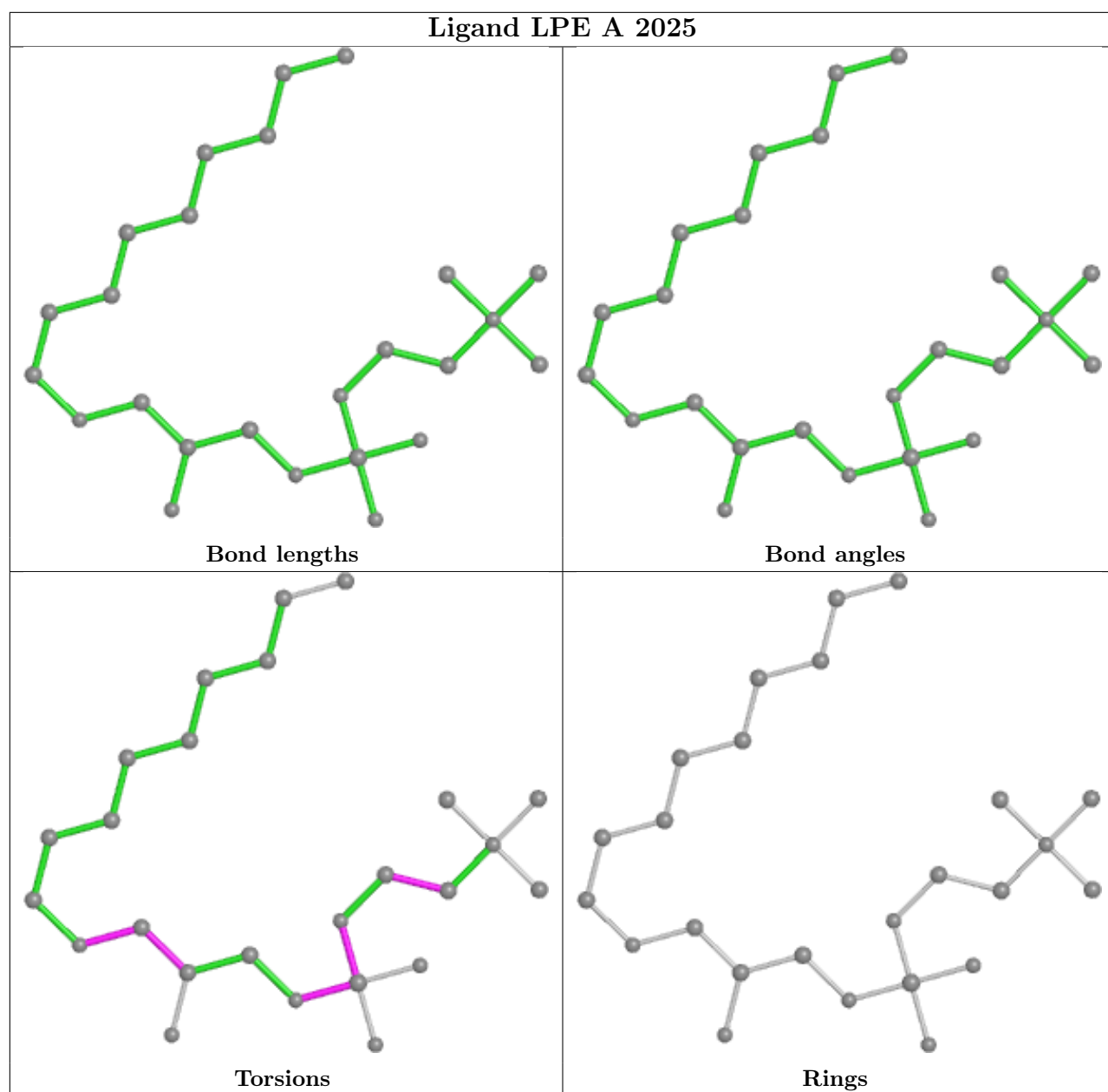


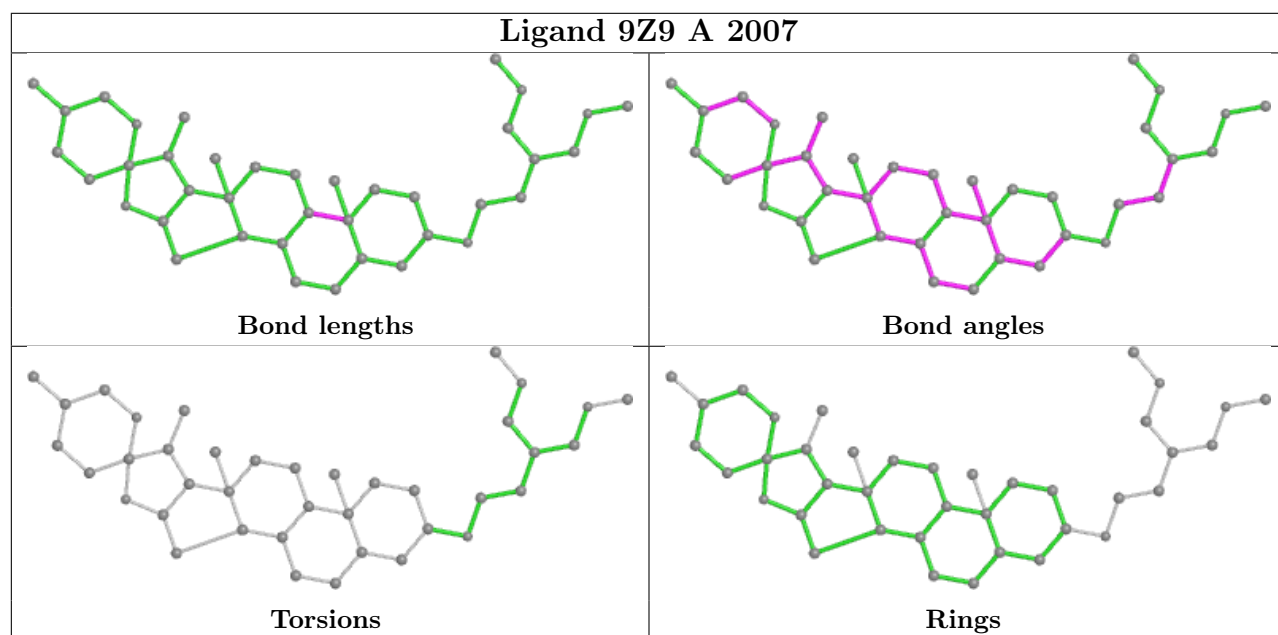
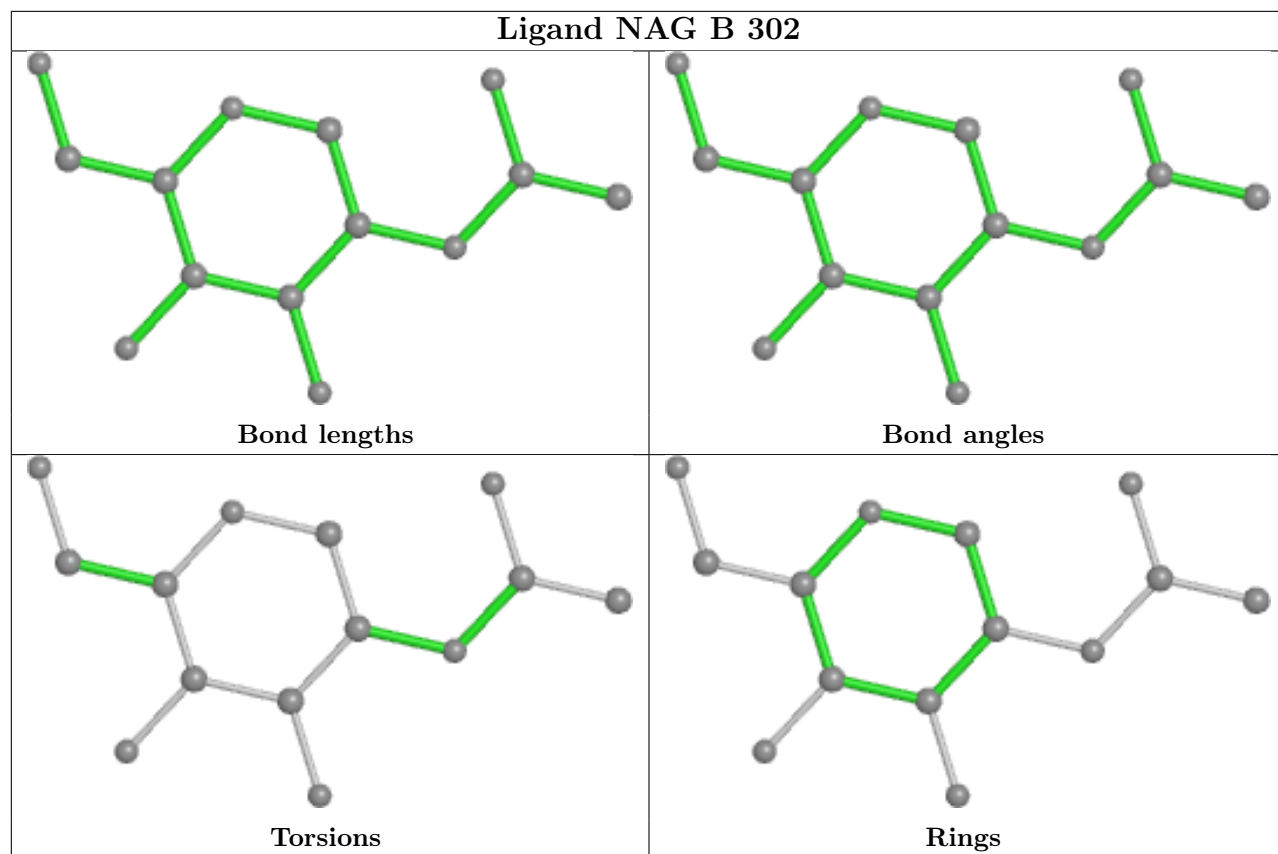


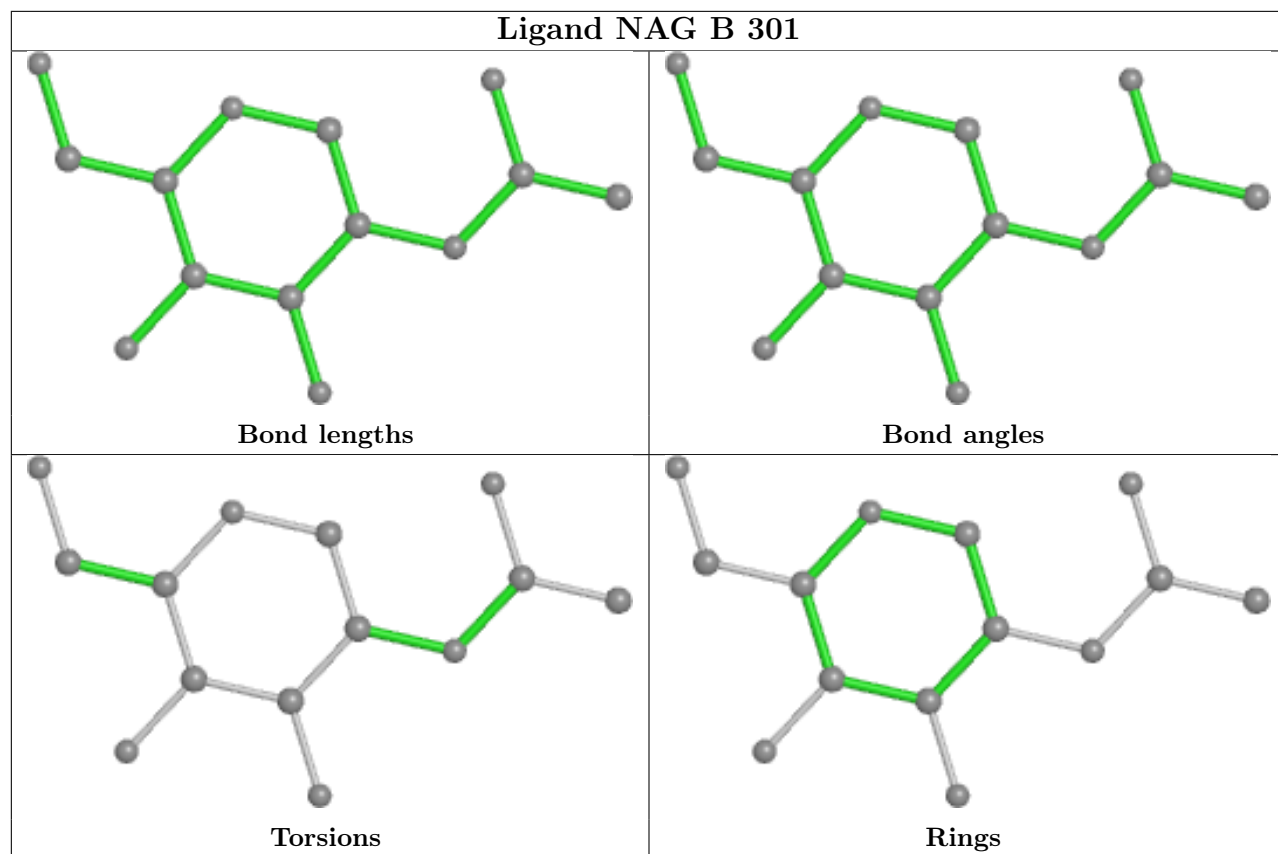


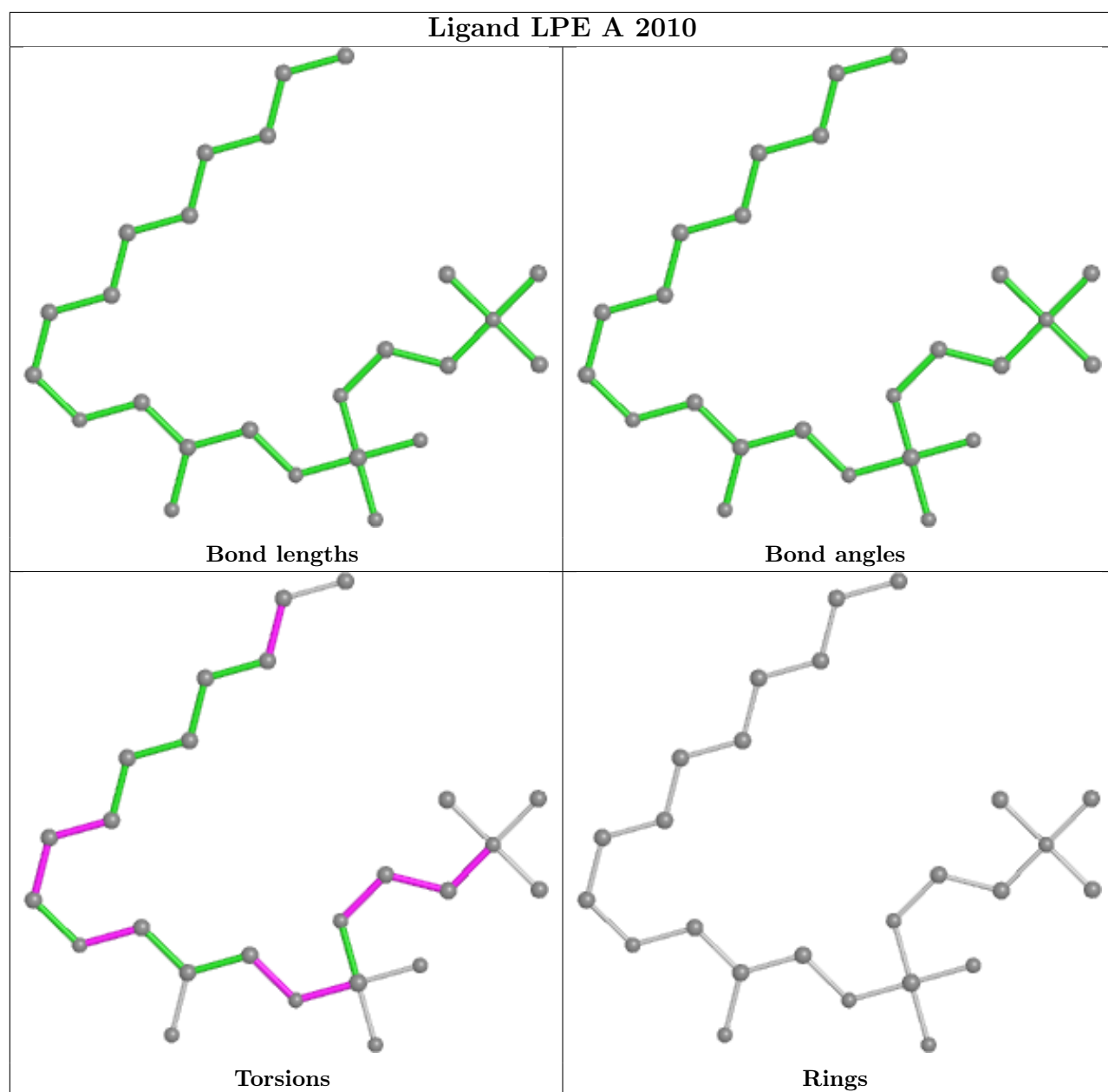


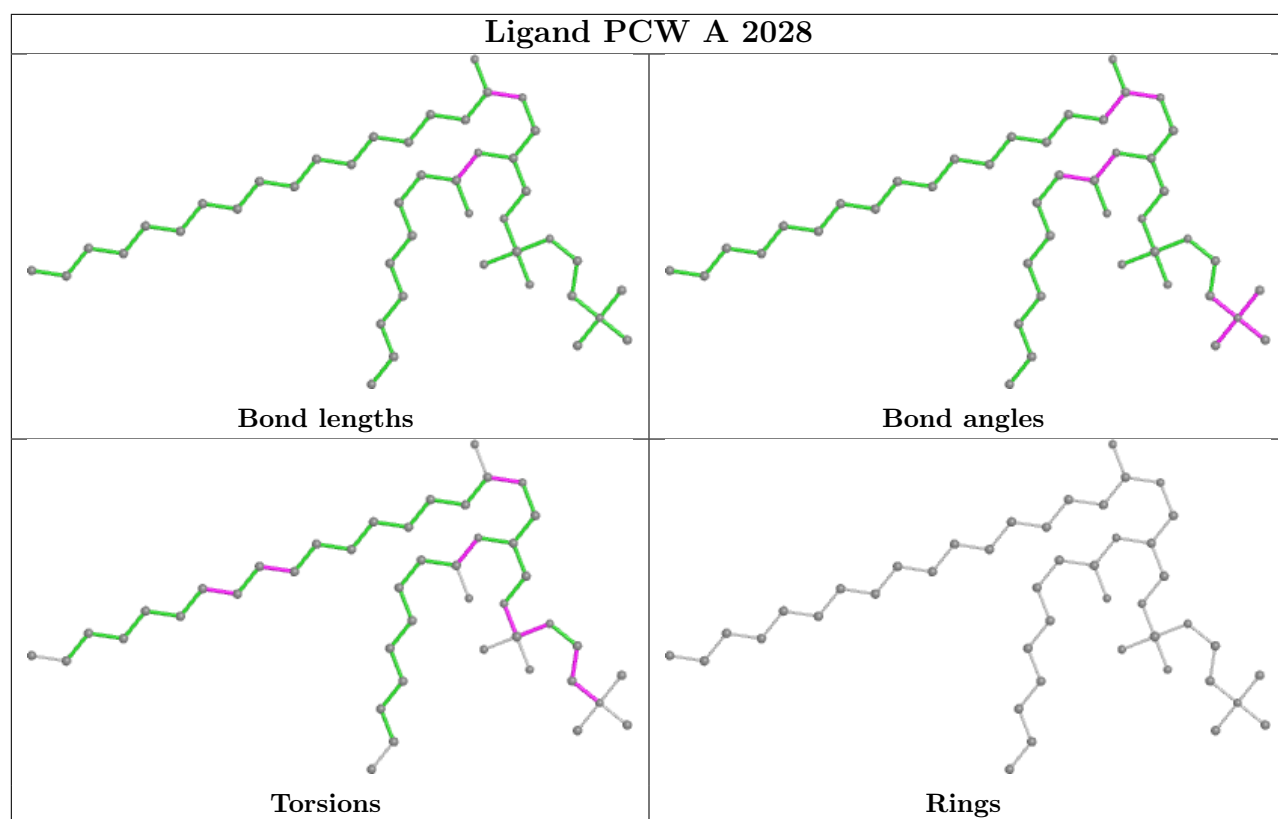


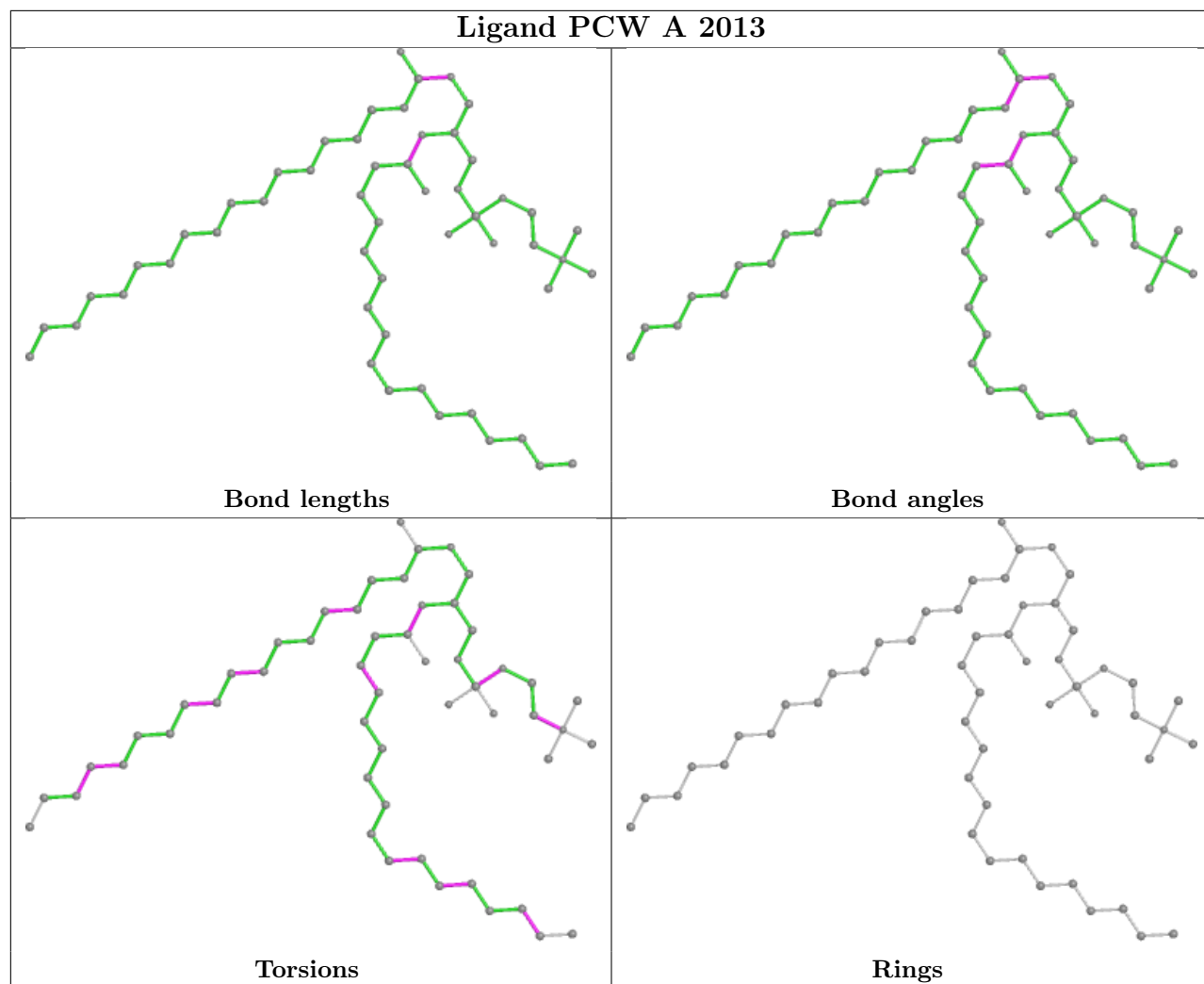


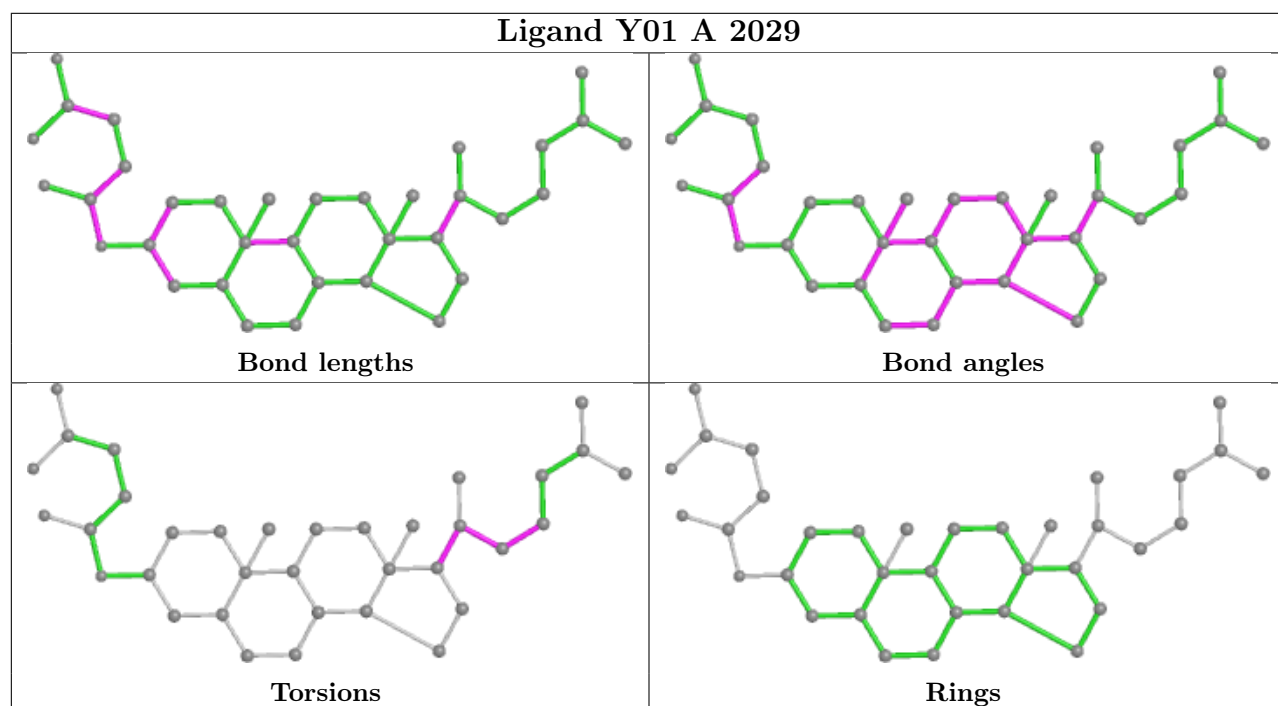
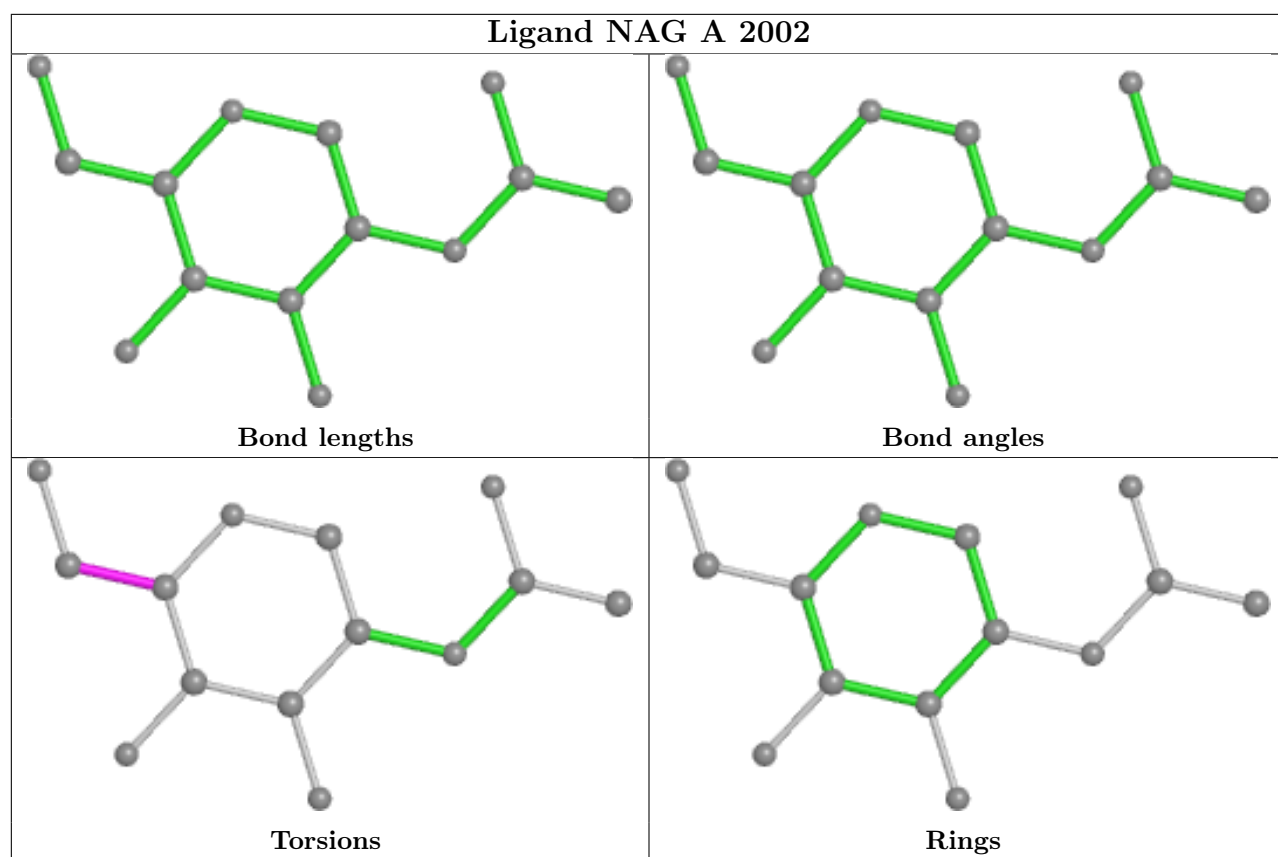


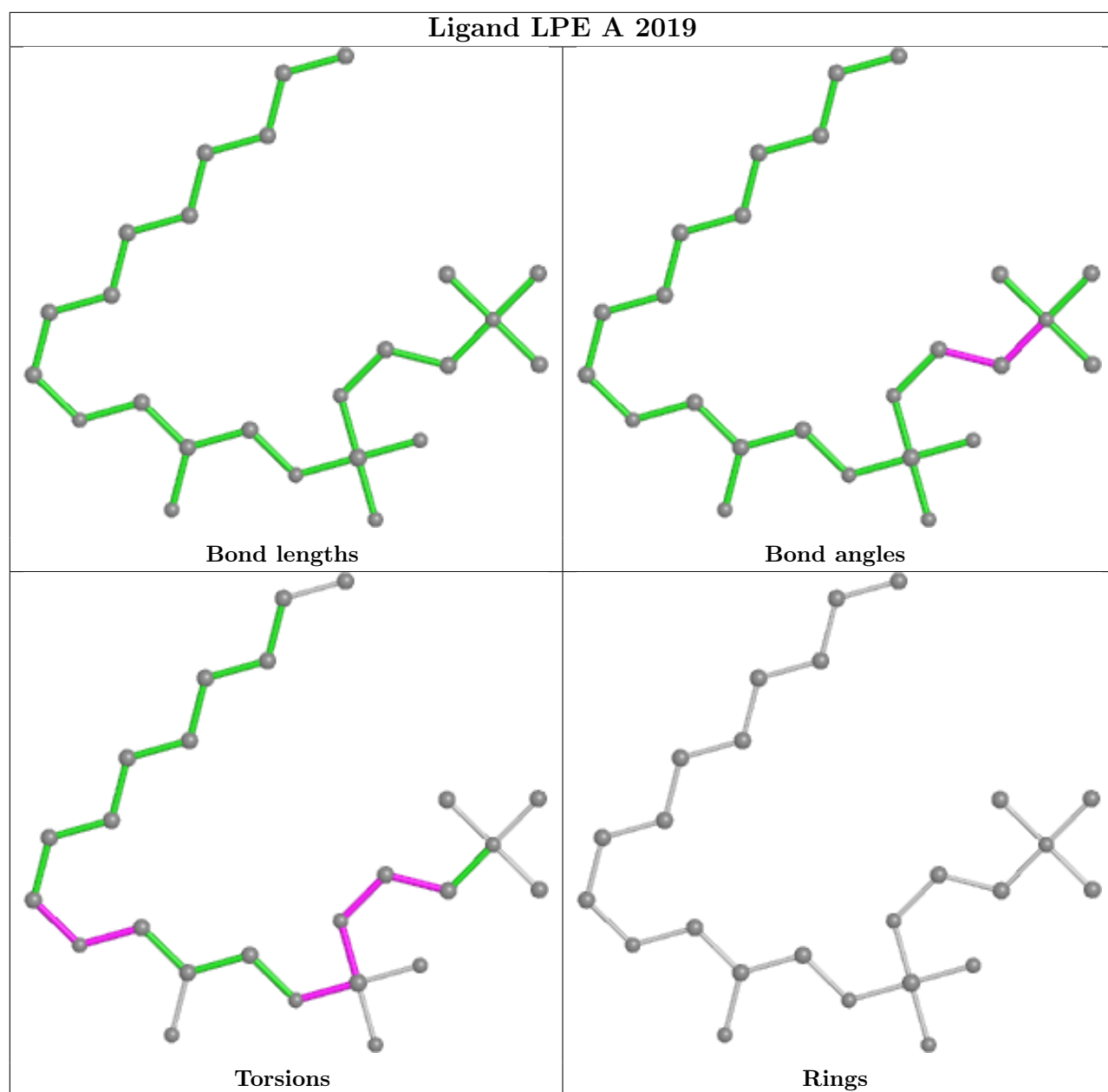


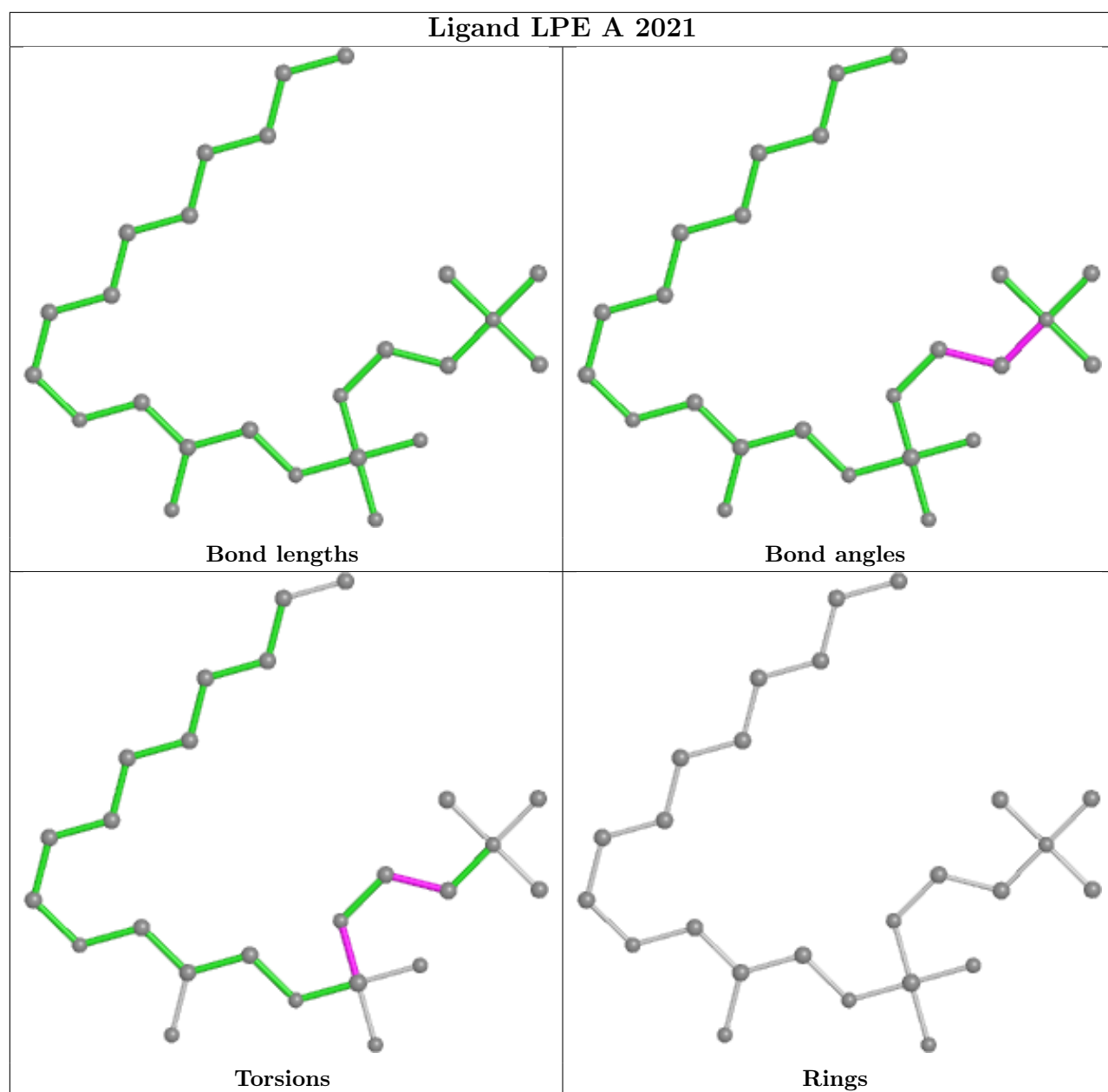


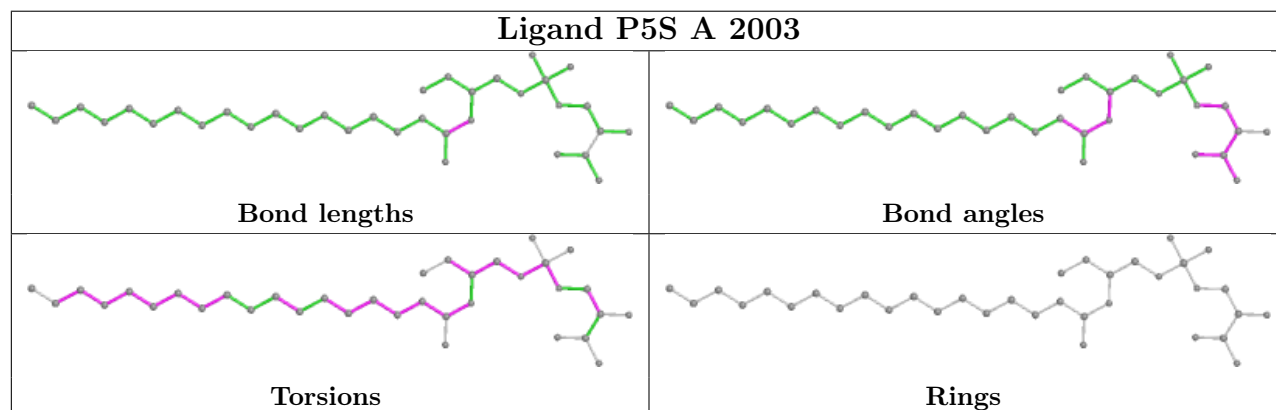
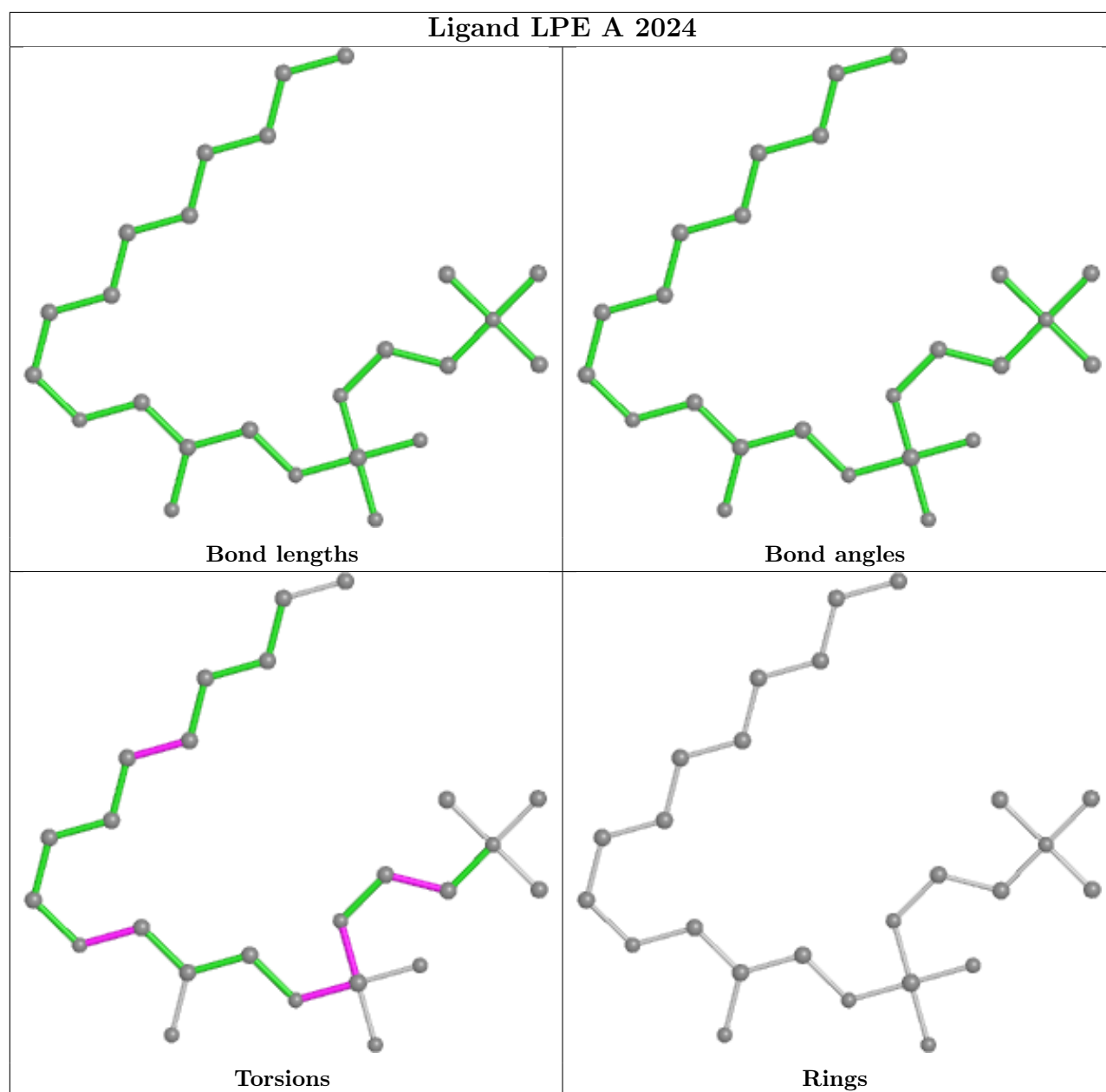


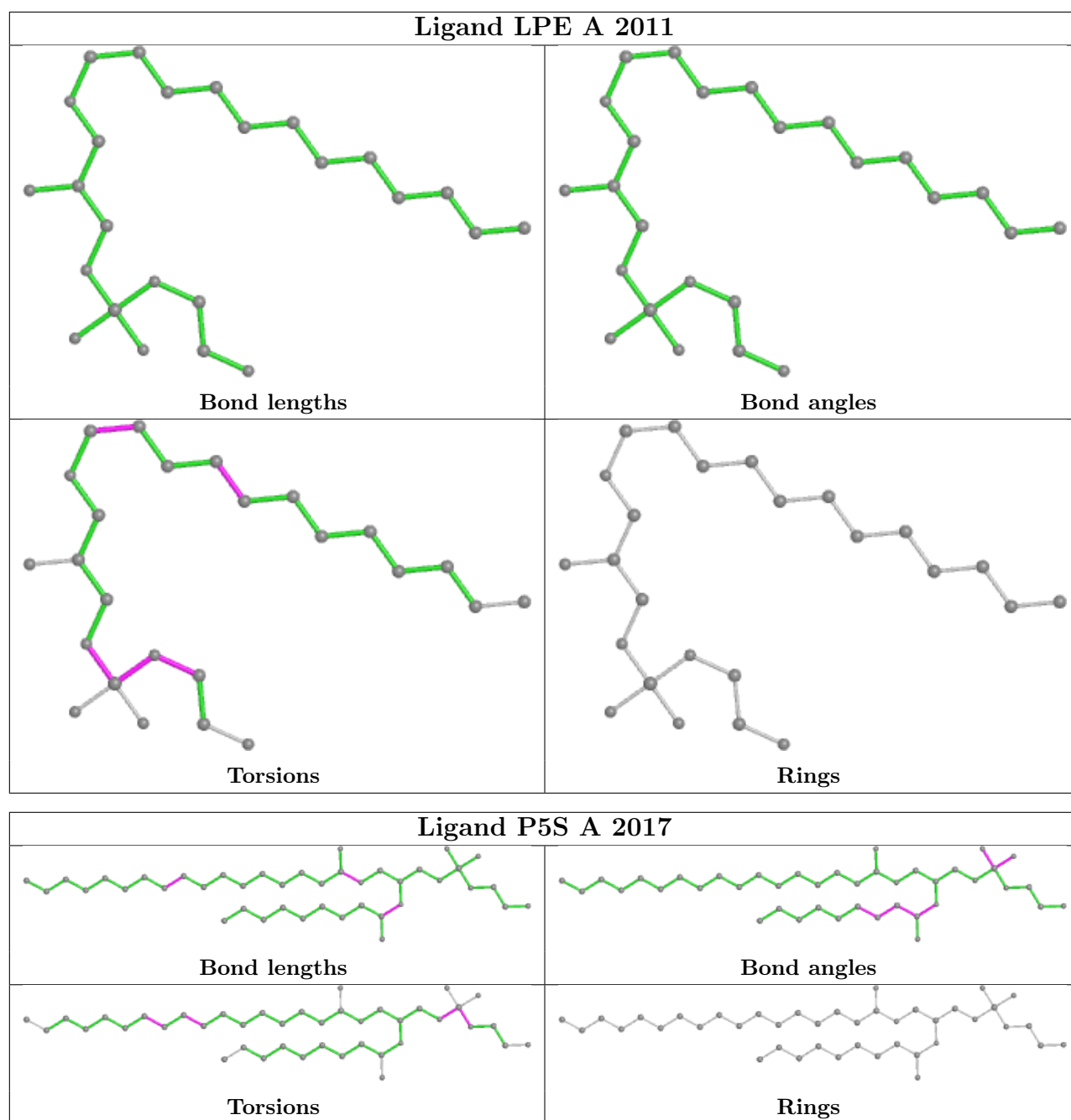


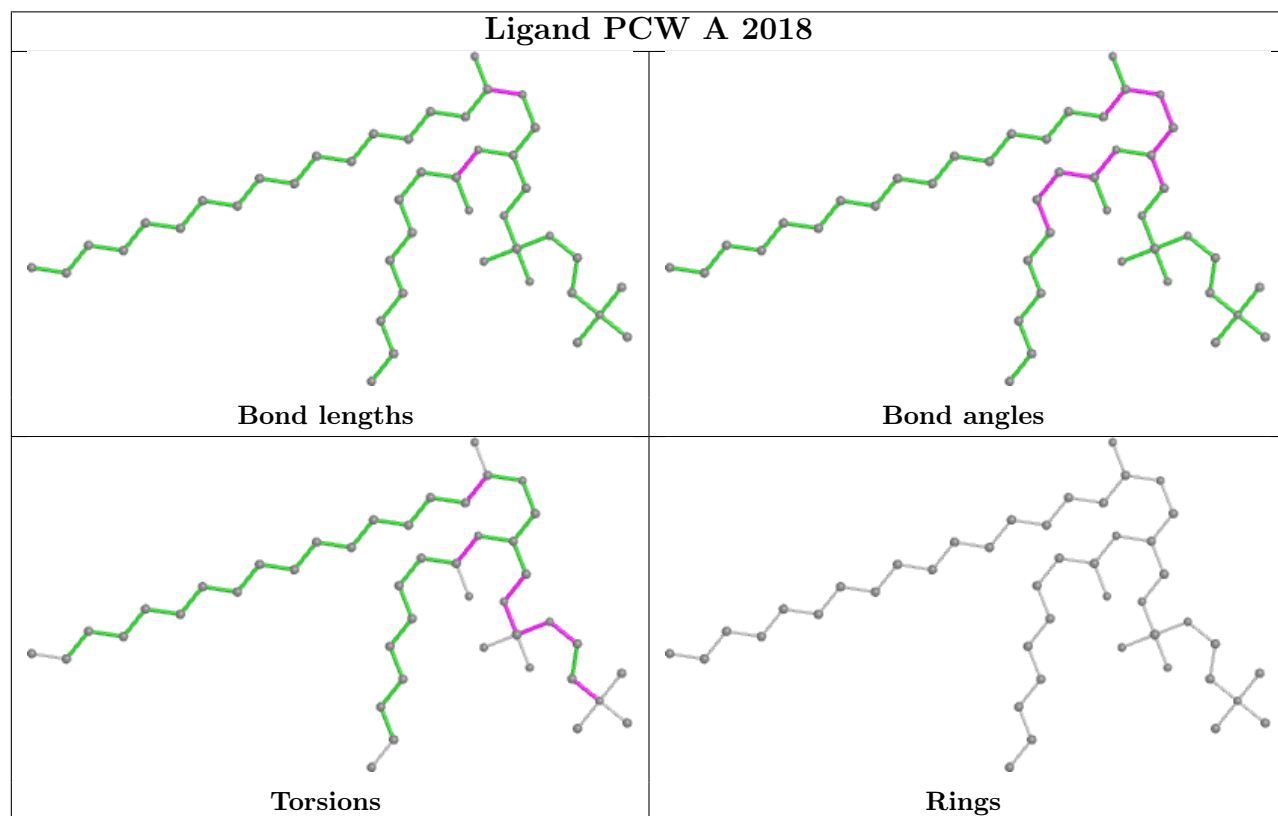
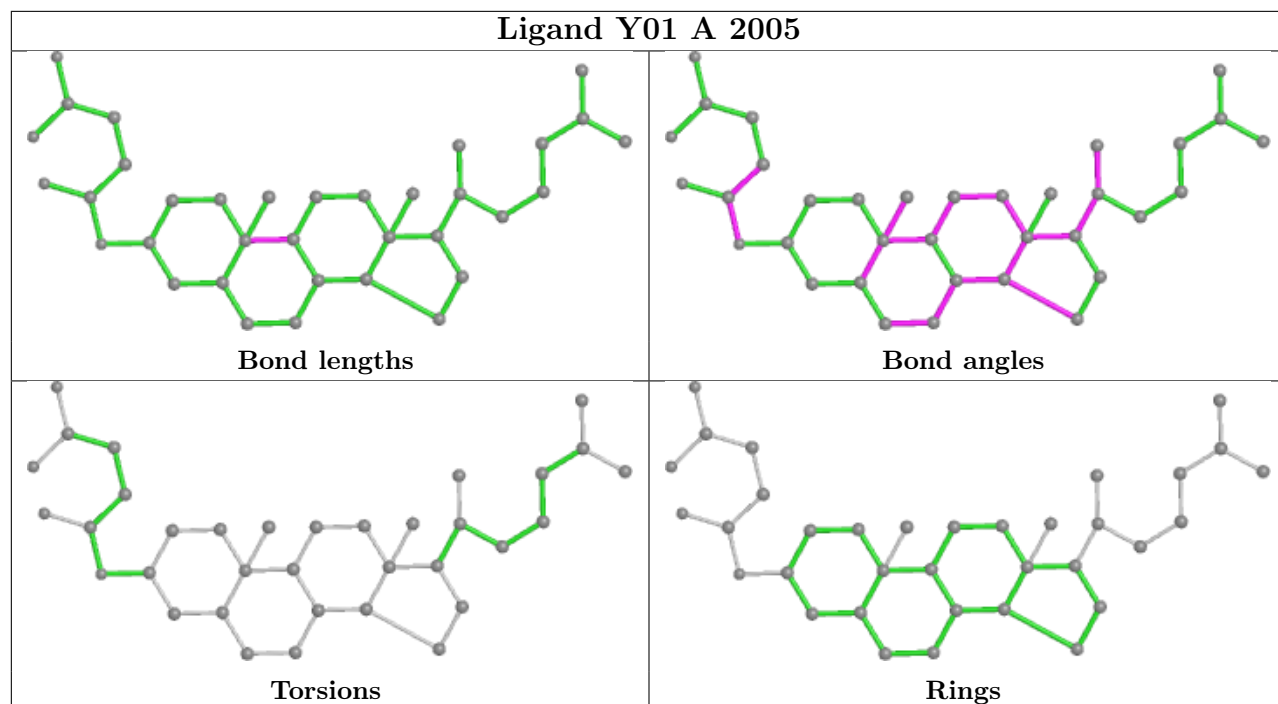


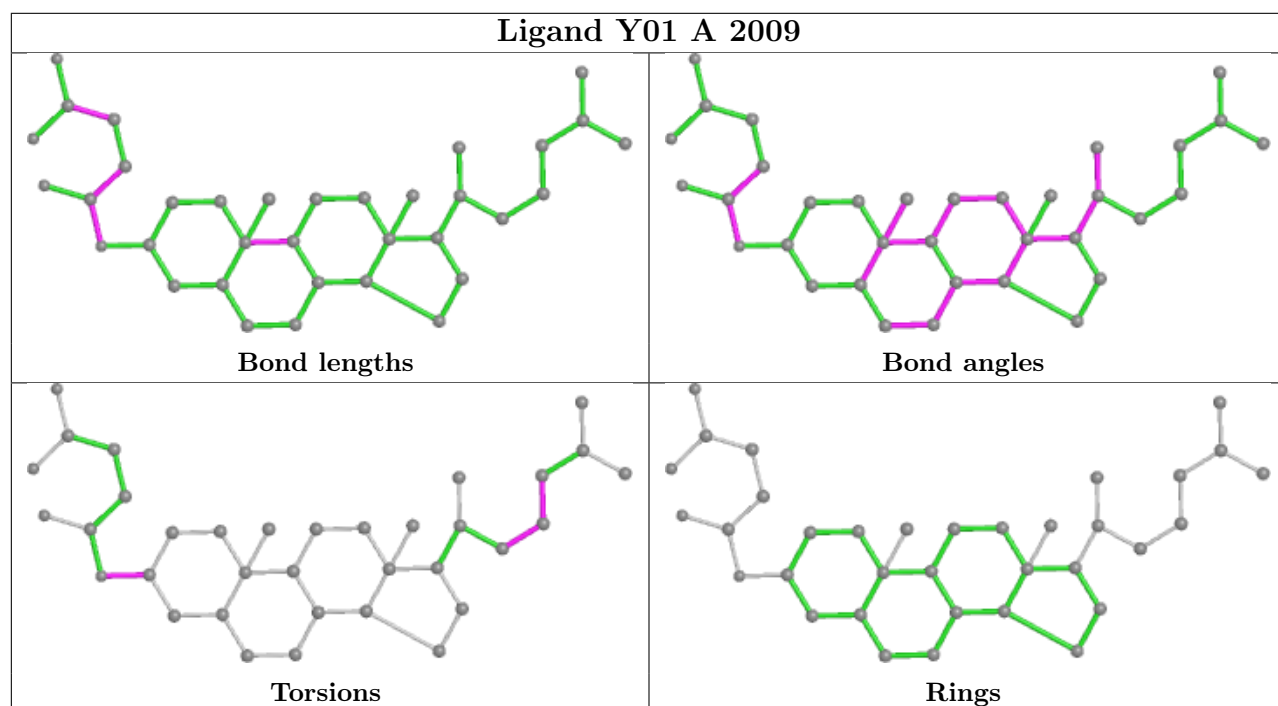
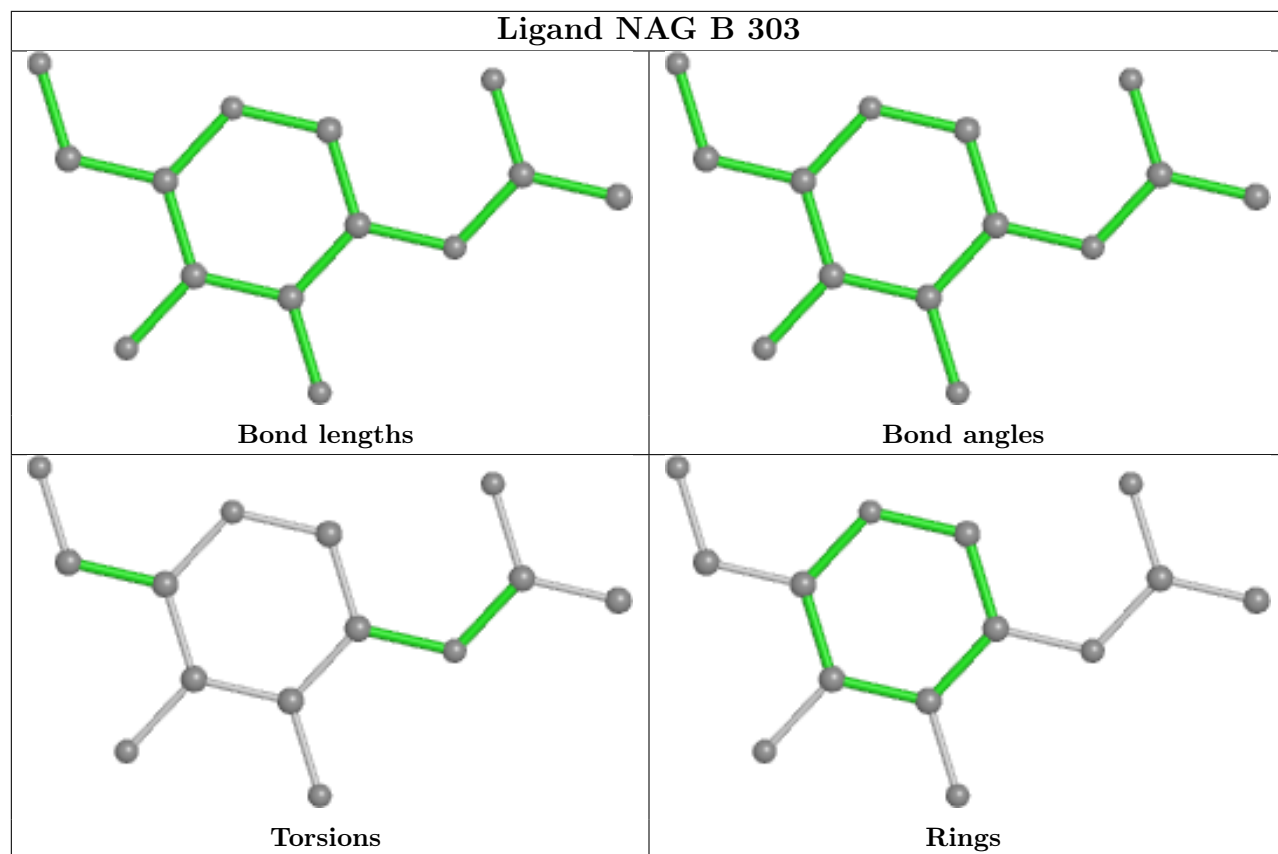


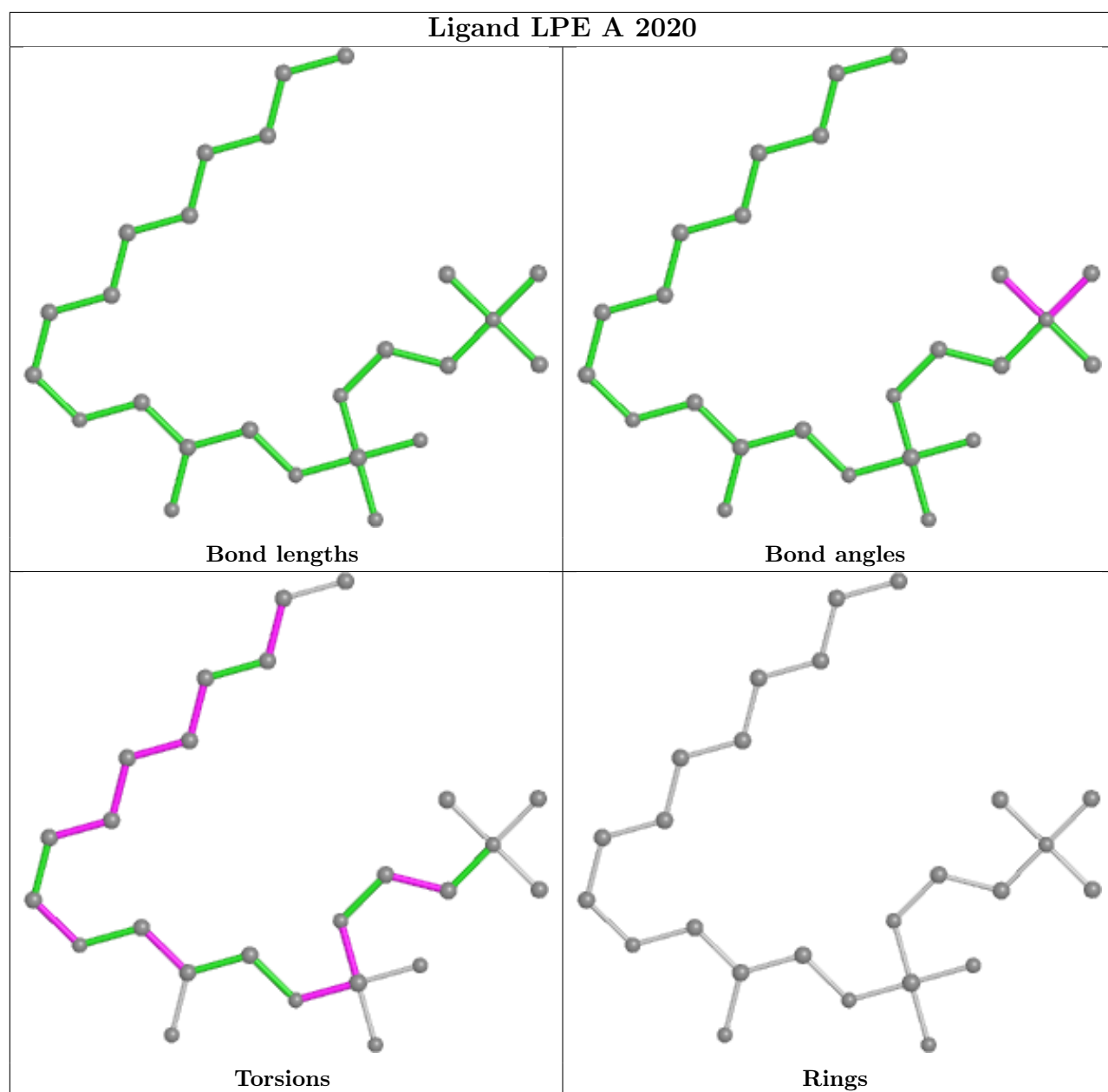


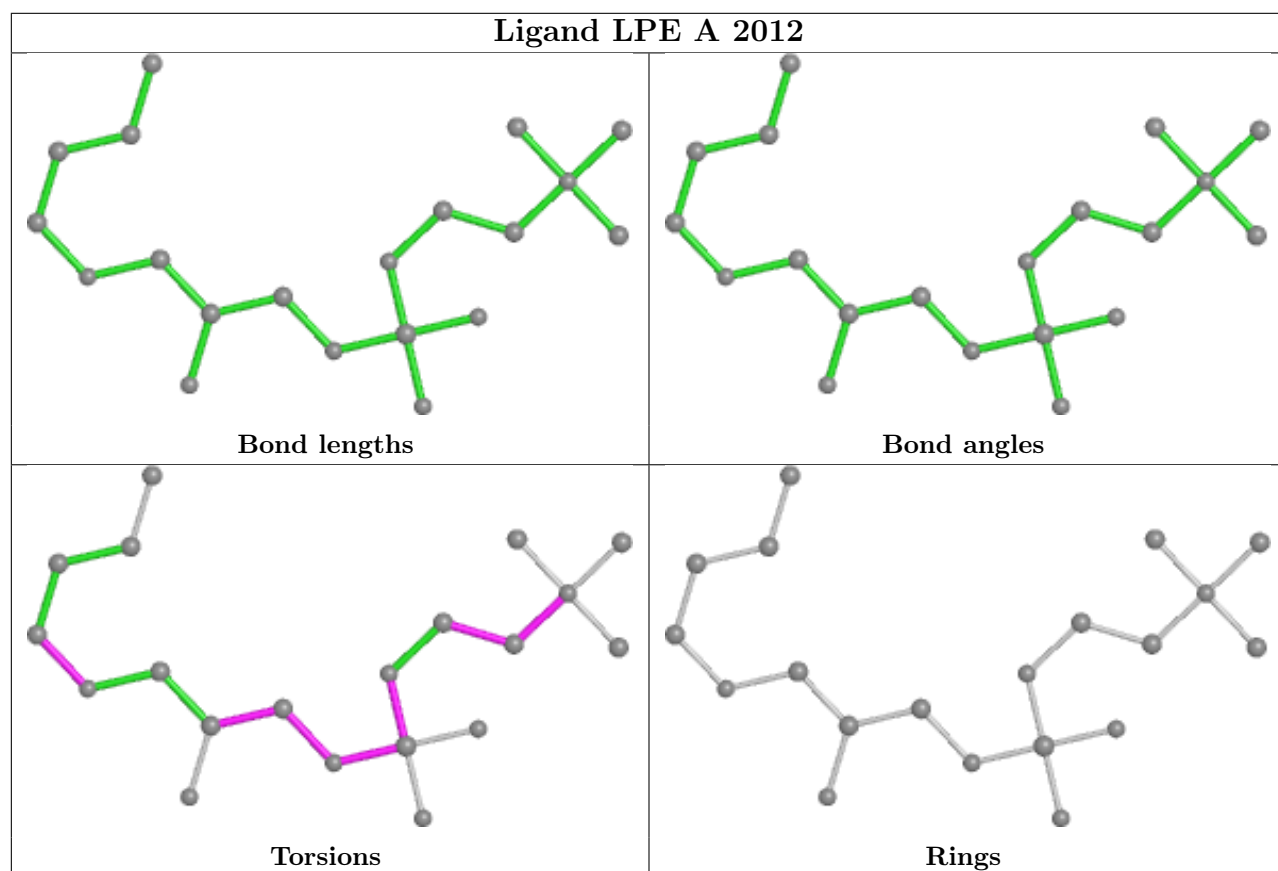
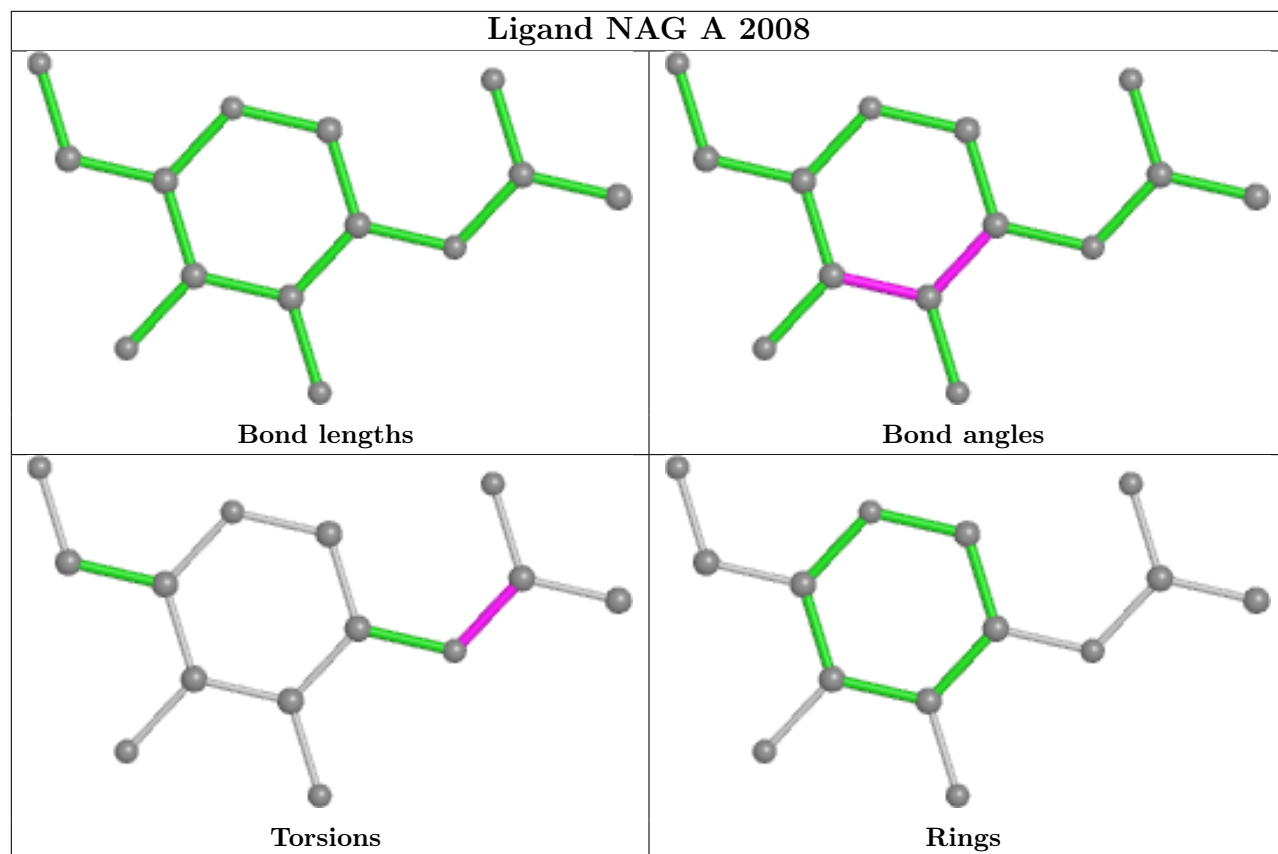


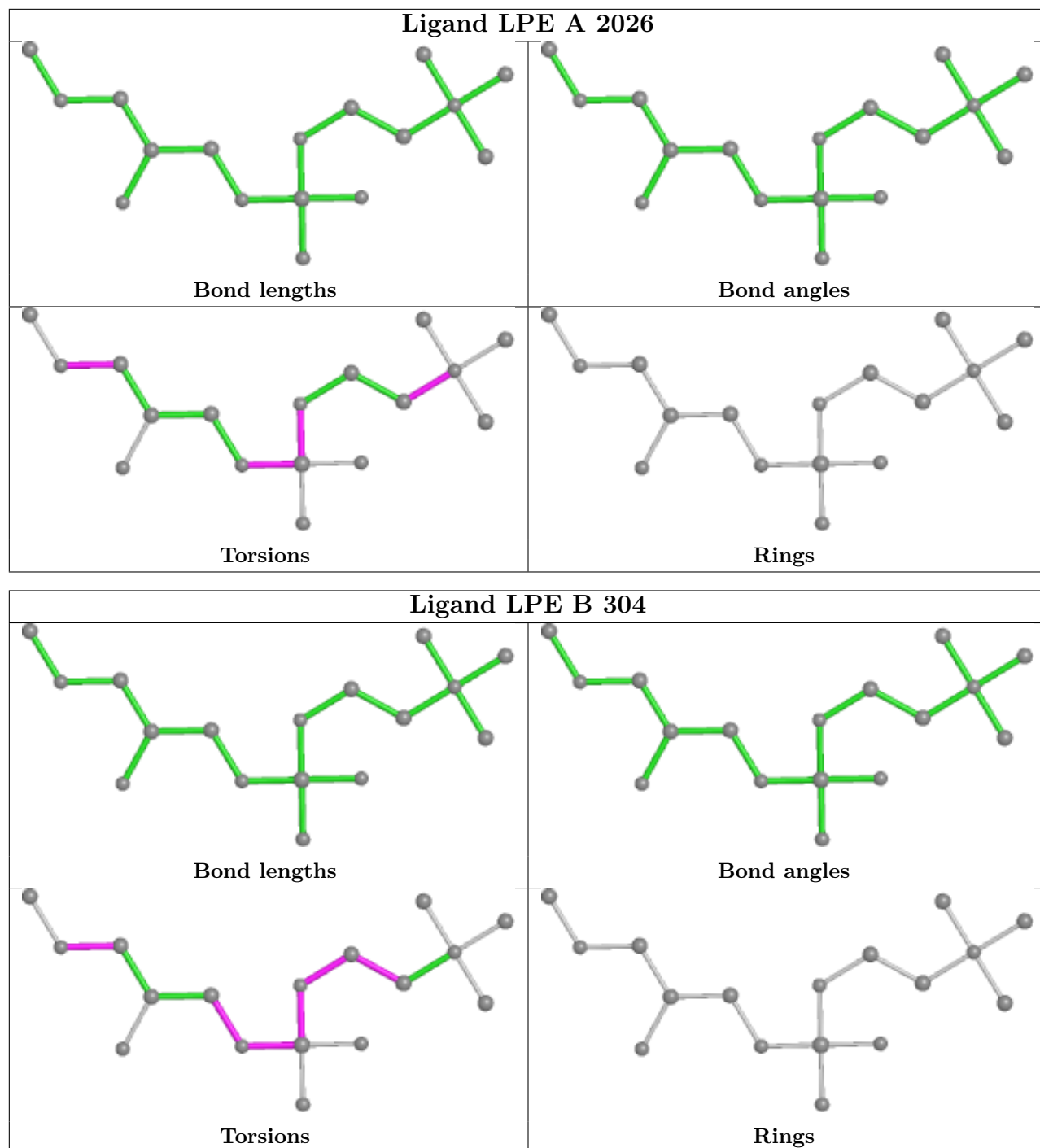


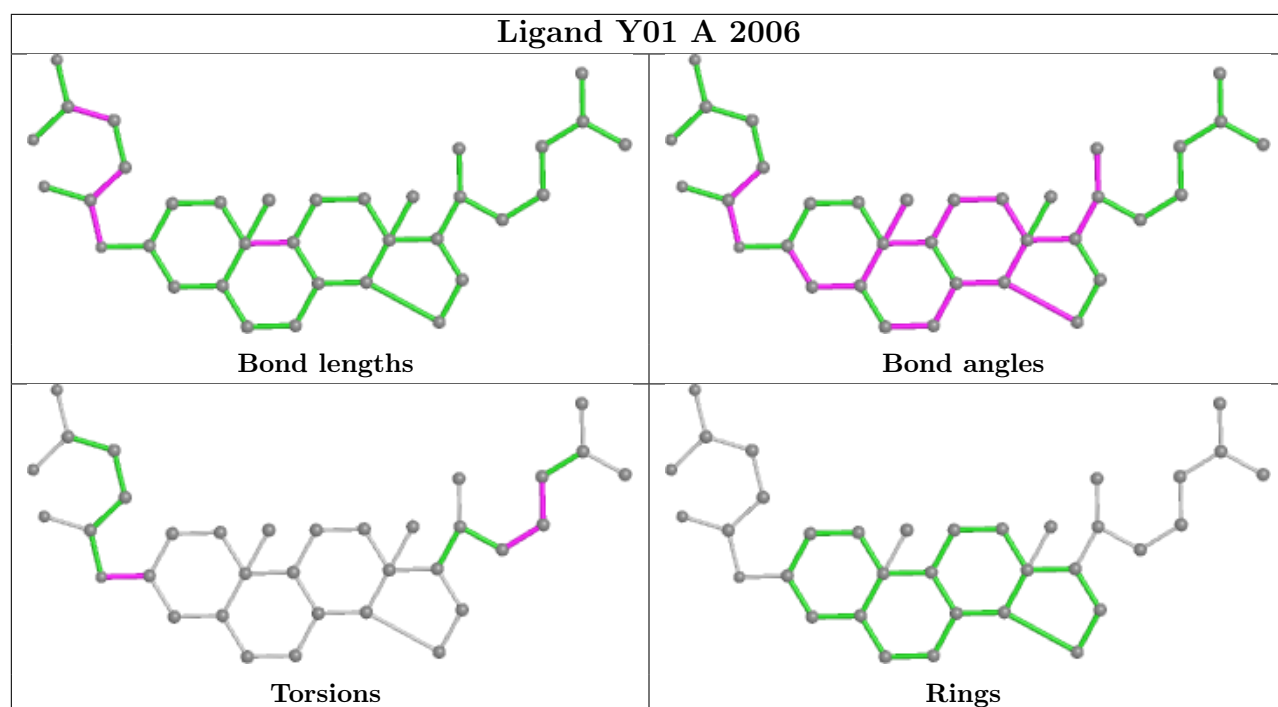


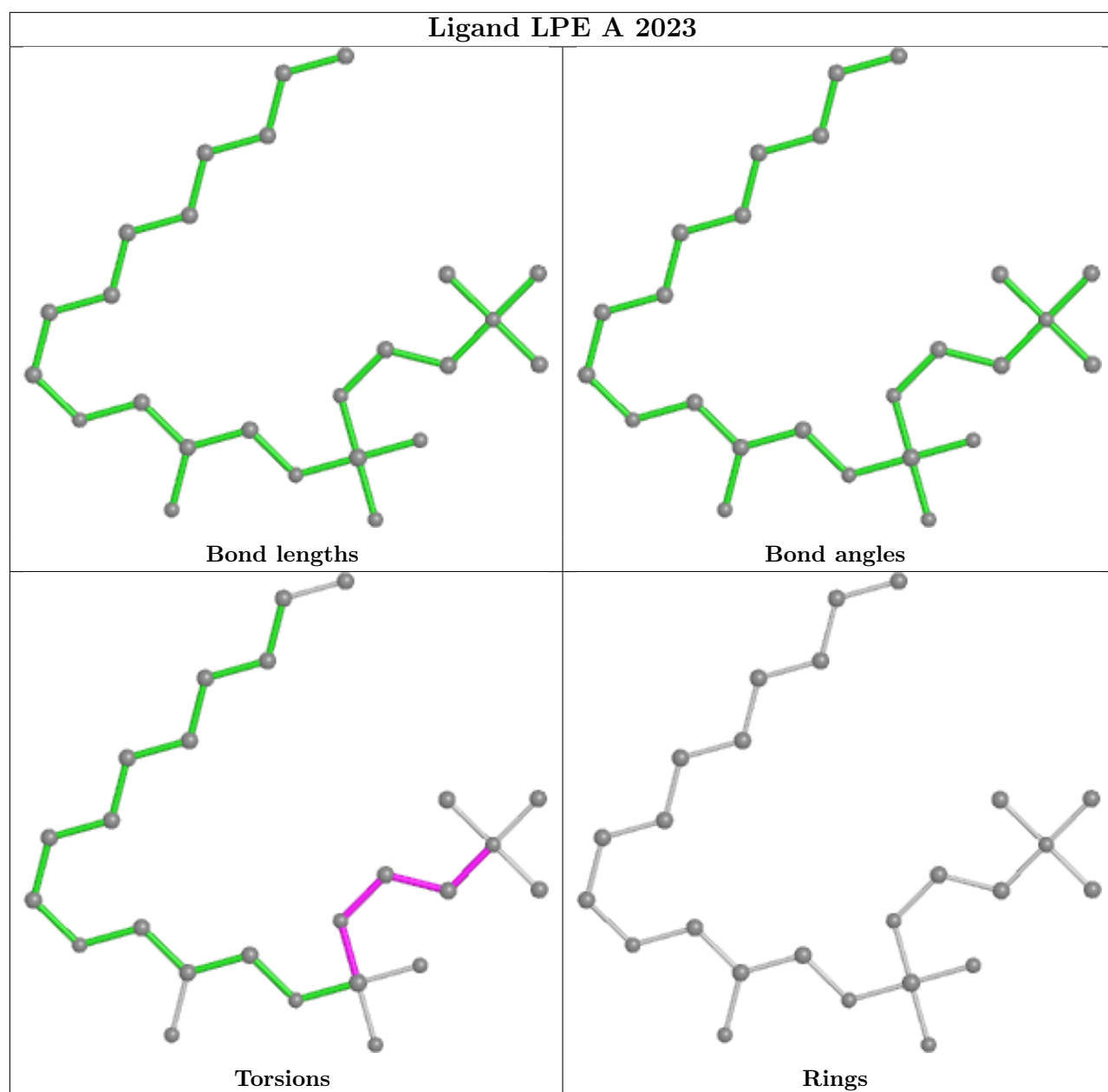


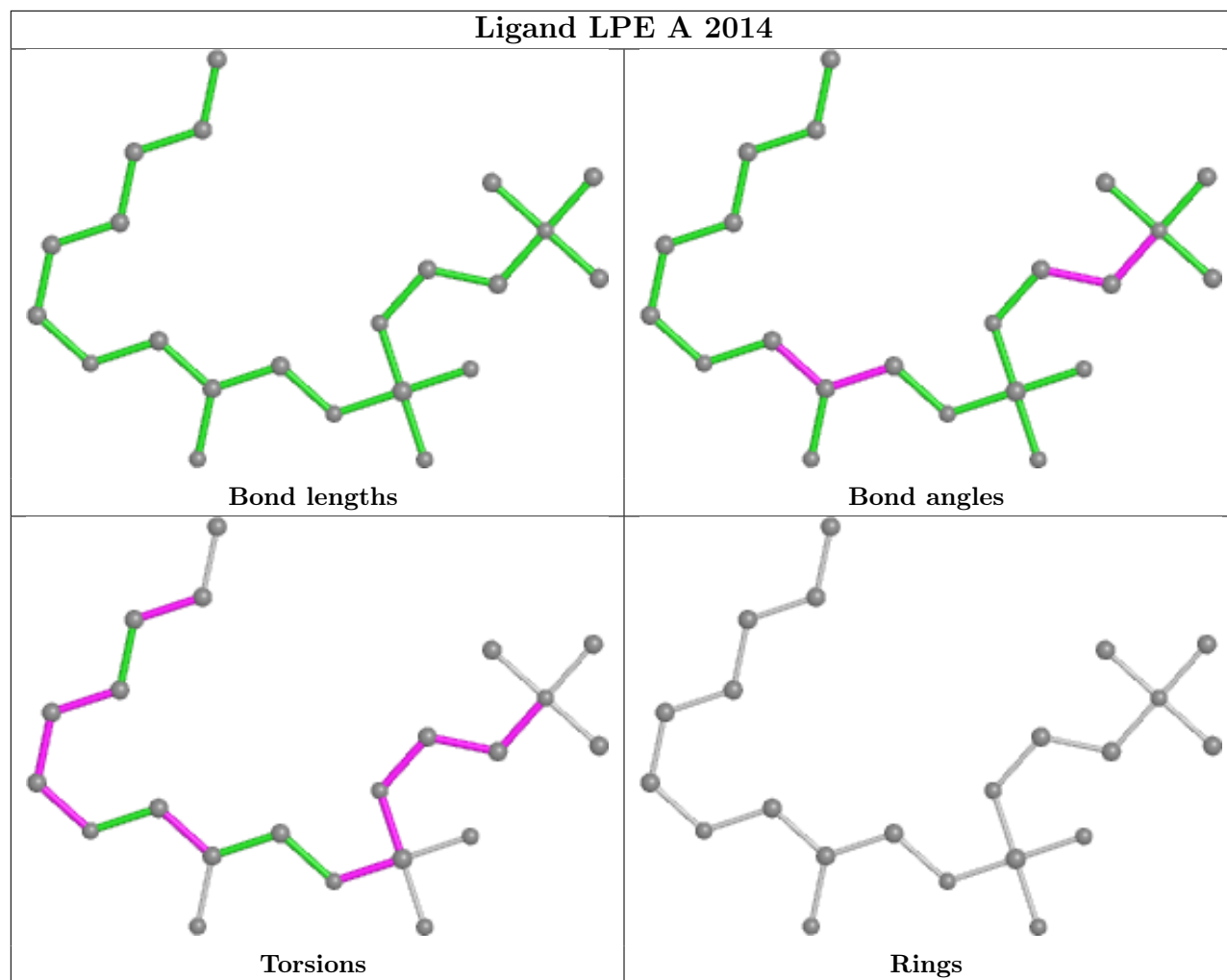












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

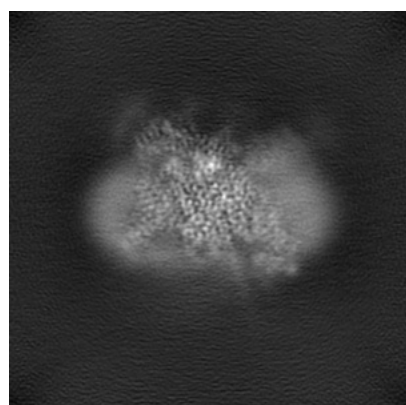
6 Map visualisation [i](#)

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

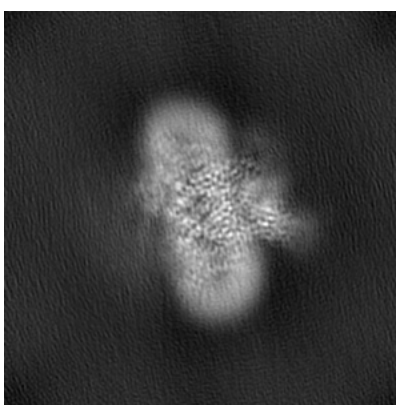
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

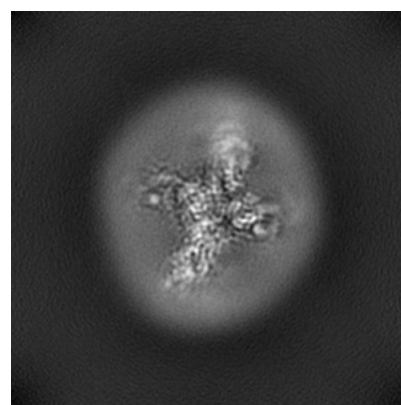
6.1.1 Primary map



X



Y

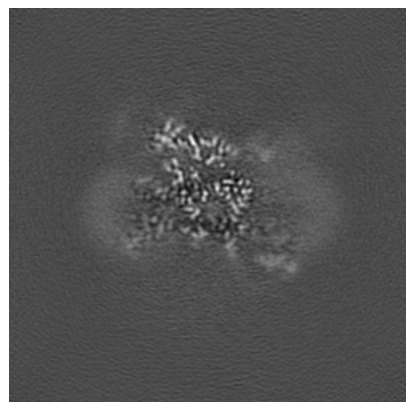


Z

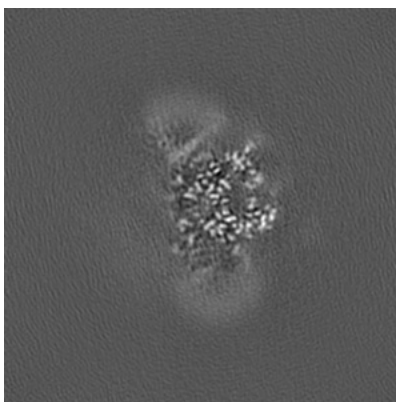
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

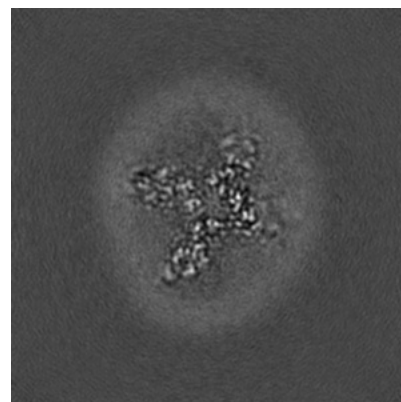
6.2.1 Primary map



X Index: 120



Y Index: 120

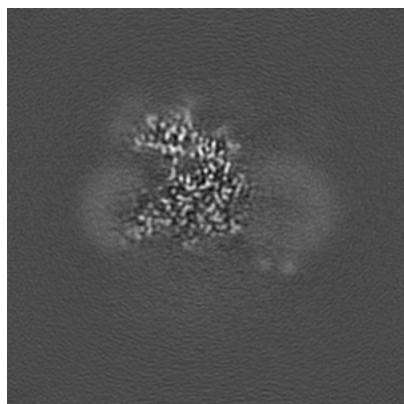


Z Index: 120

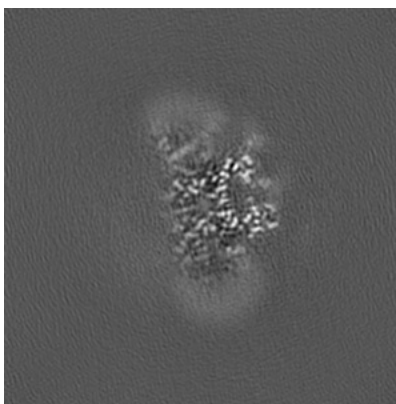
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

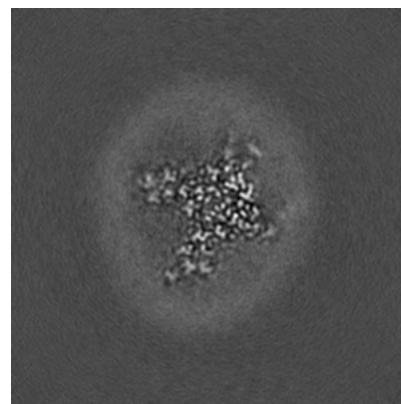
6.3.1 Primary map



X Index: 112



Y Index: 122

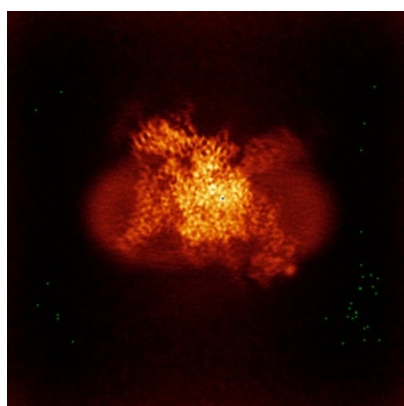


Z Index: 126

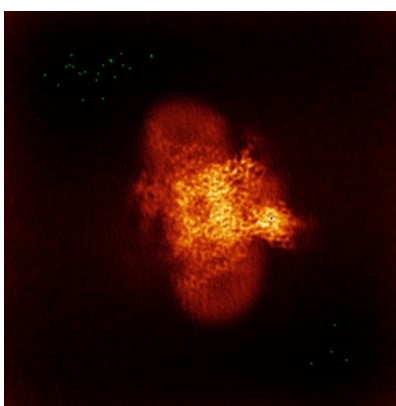
The images above show the largest variance slices of the map in three orthogonal directions.

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

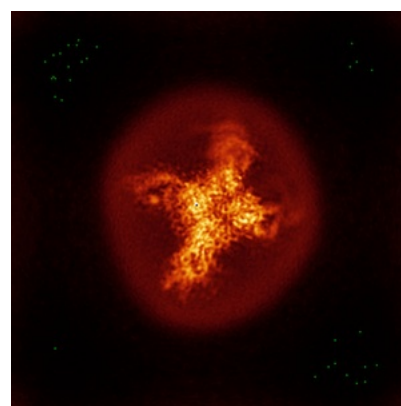
6.4.1 Primary map



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 [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.63. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

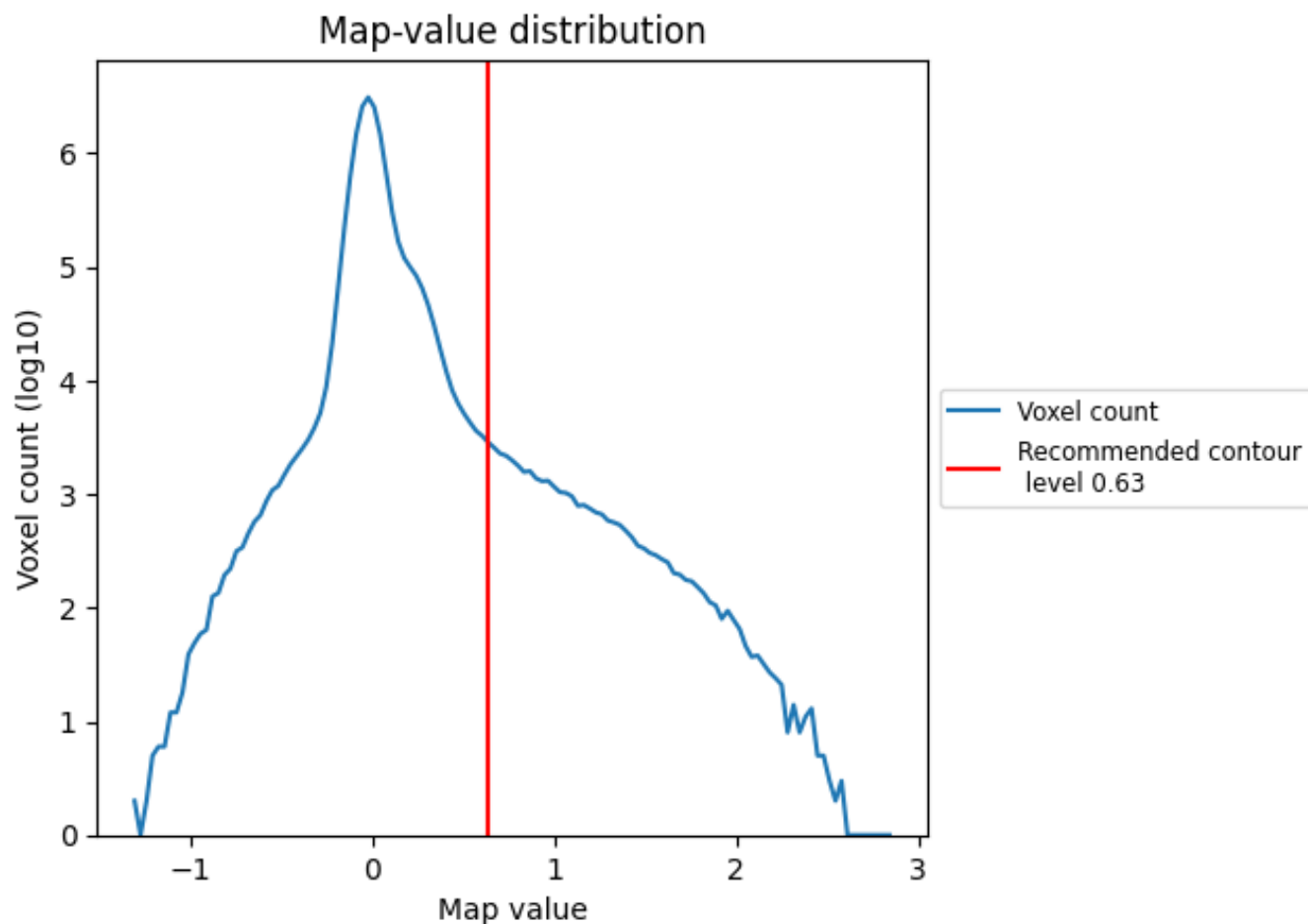
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

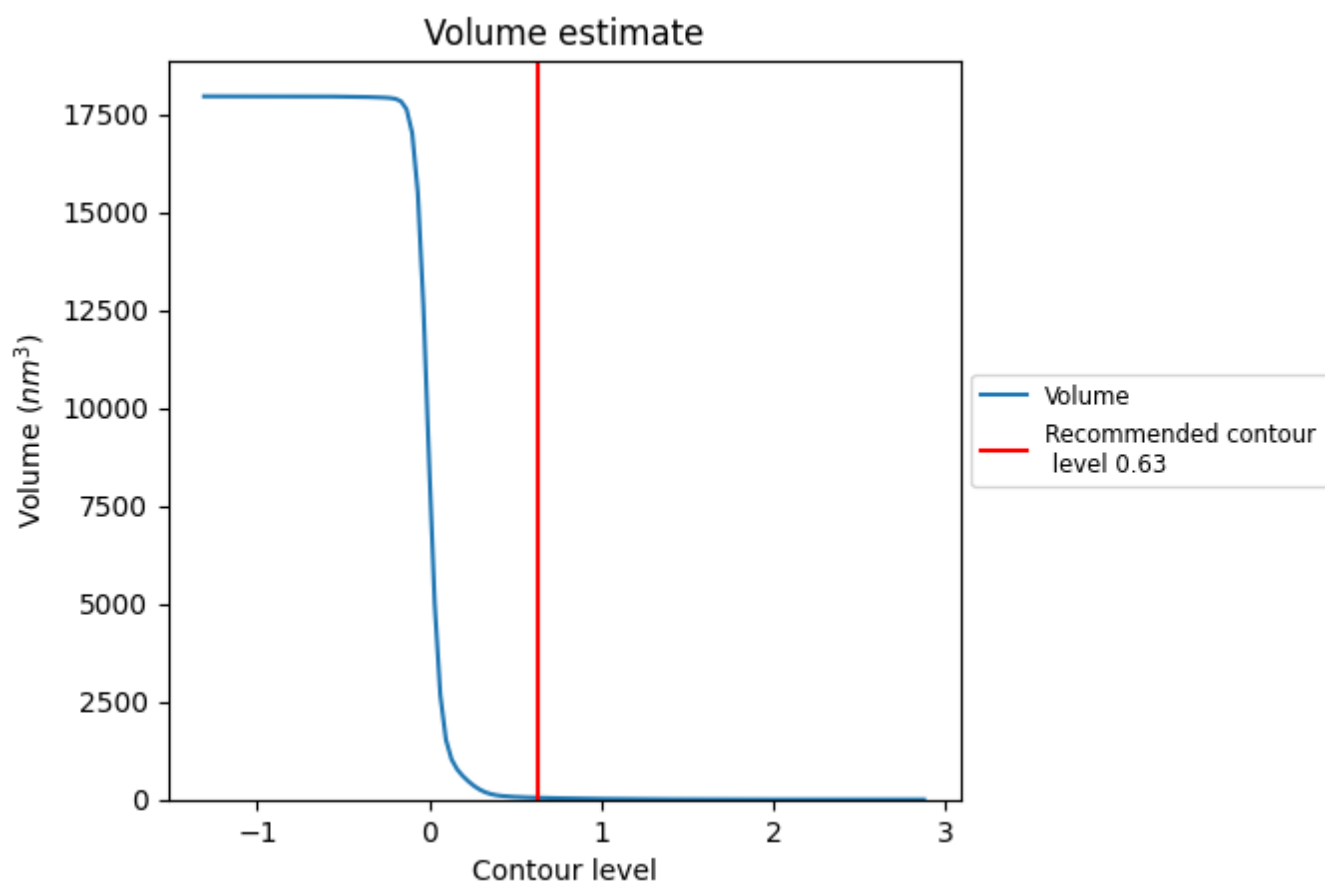
This section contains the results of statistical analysis of the map.

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.

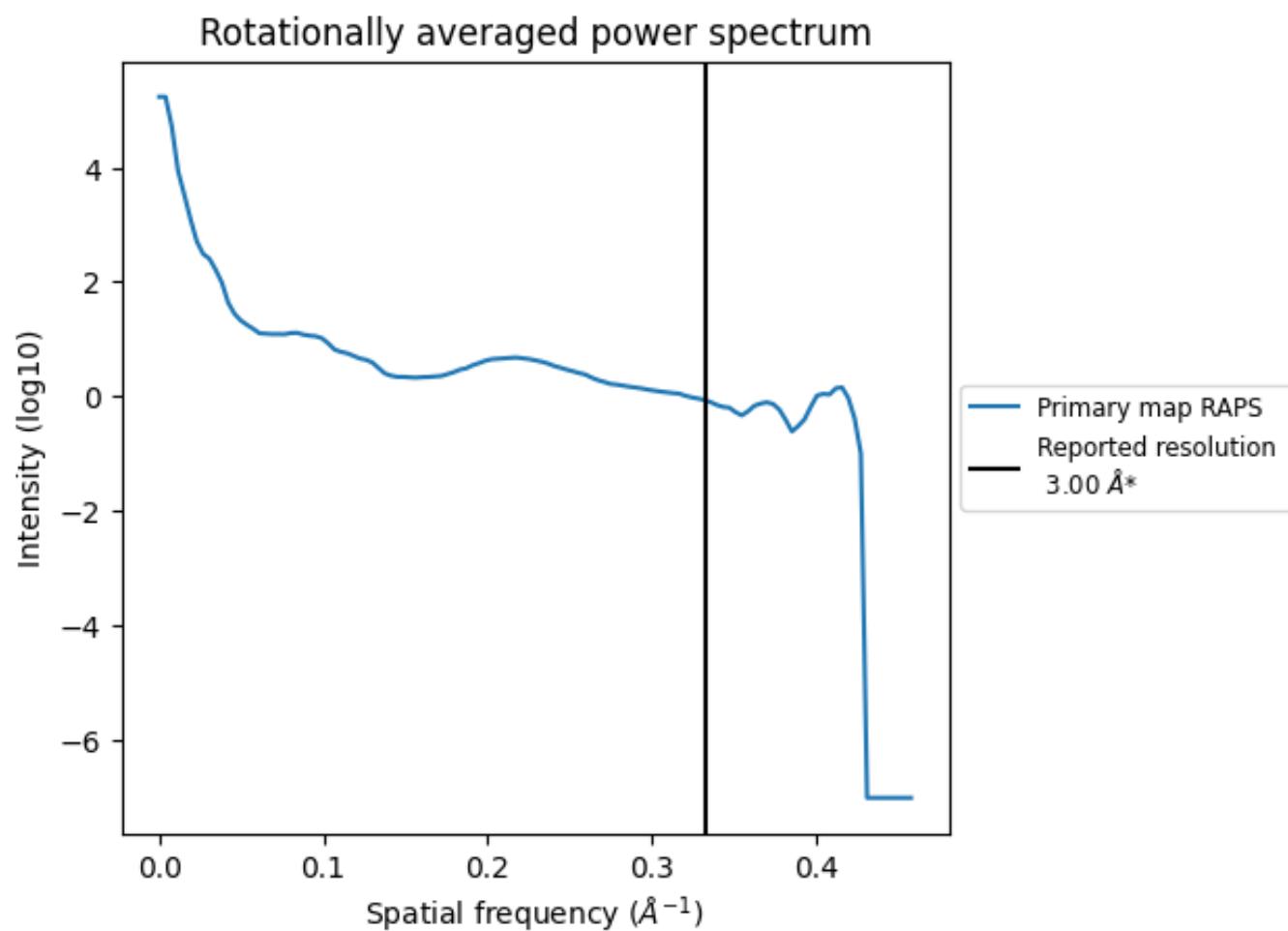
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm³; 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

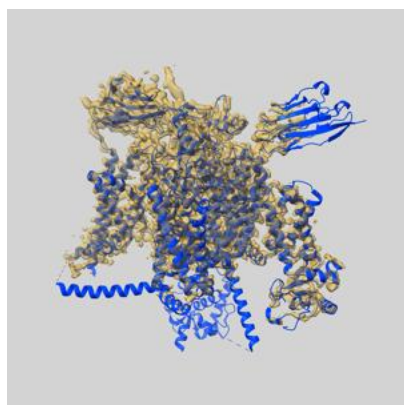
8 Fourier-Shell correlation ⓘ

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

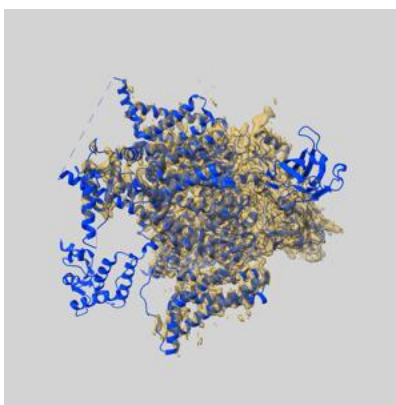
9 Map-model fit [i](#)

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](#).

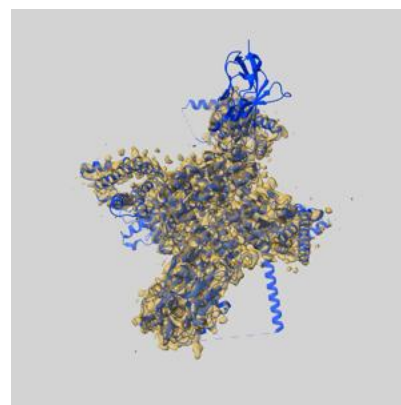
9.1 Map-model overlay [i](#)



X



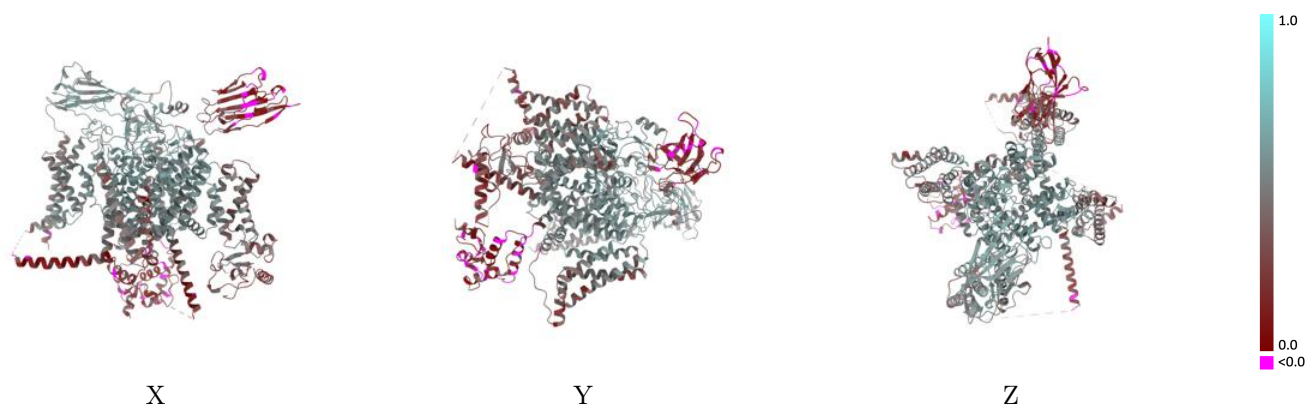
Y



Z

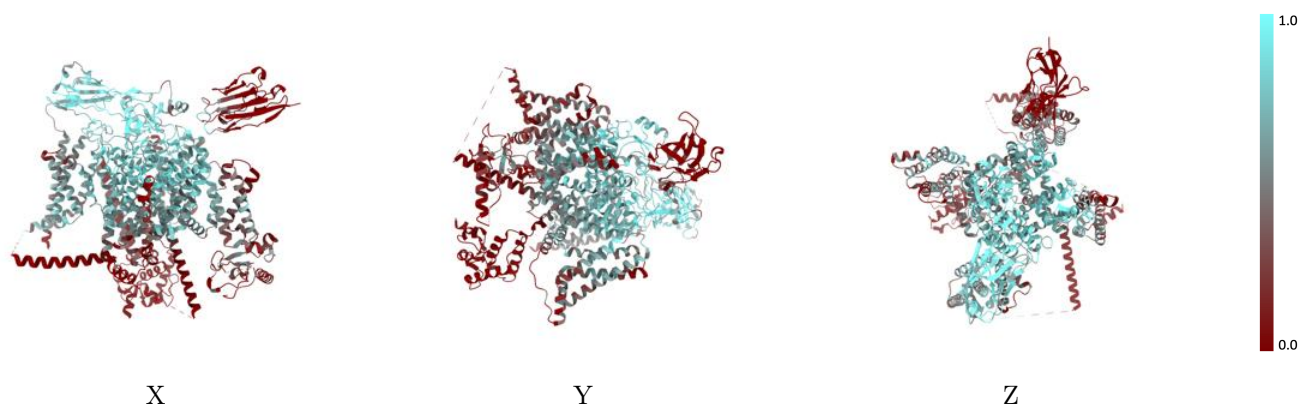
The images above show the 3D surface view of the map at the recommended contour level 0.63 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



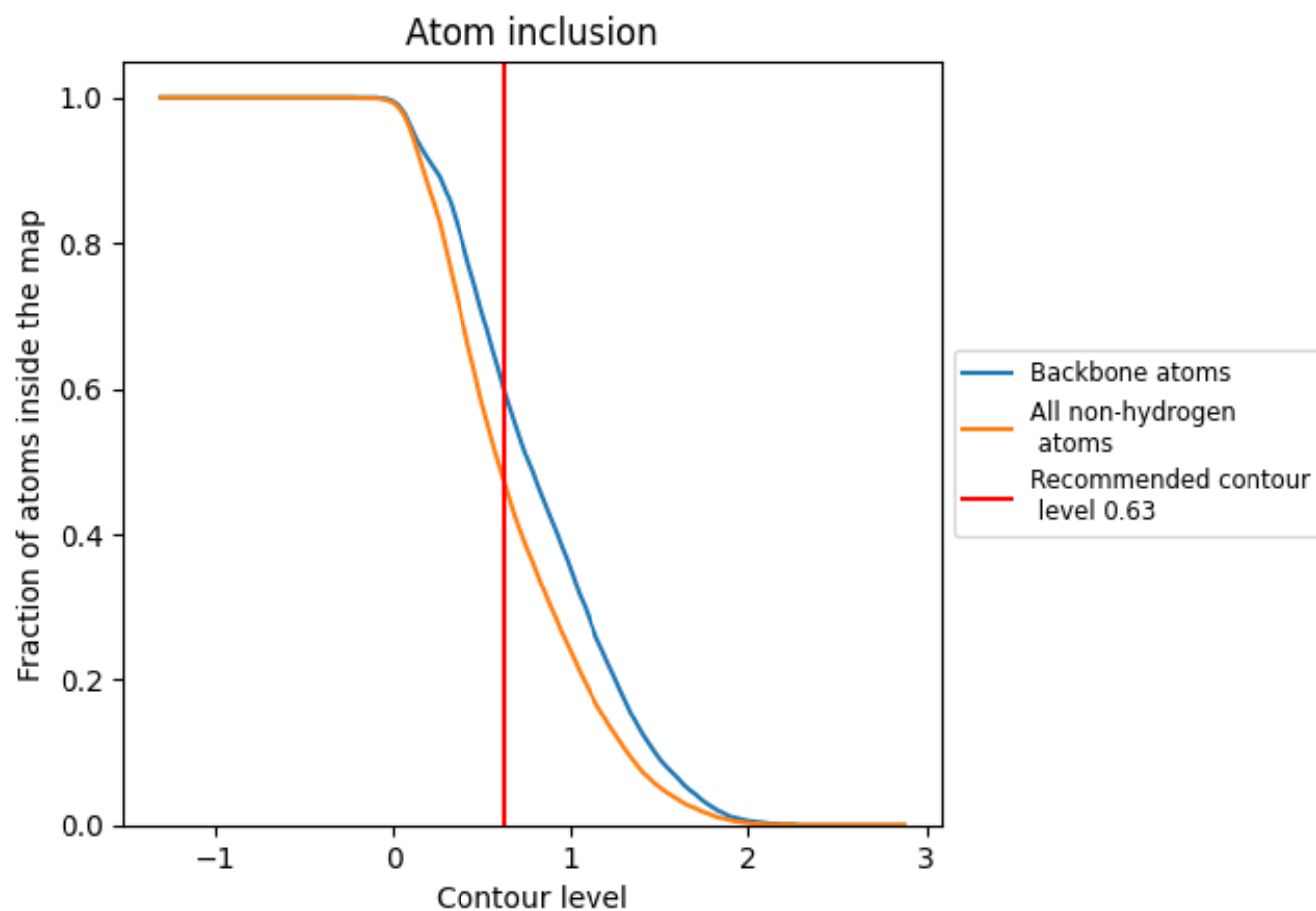
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.63).

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	<div></div> 0.4680	<div></div> 0.4310
A	<div></div> 0.4680	<div></div> 0.4410
B	<div></div> 0.6940	<div></div> 0.5070
C	<div></div> 0.1130	<div></div> 0.1840
D	<div></div> 0.4640	<div></div> 0.4680
E	<div></div> 0.5710	<div></div> 0.4350
F	<div></div> 0.6790	<div></div> 0.4410

1.0

0.0

<0.0