



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:11 AM UTC

PDB ID : 7WFR / pdb_00007wfr
EMDB ID : EMD-32475
Title : Human Nav1.8 with A-803467, class III
Authors : Yan, N.; Pan, X.J.; Huang, X.S.; Huang, G.X.
Deposited on : 2021-12-27
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

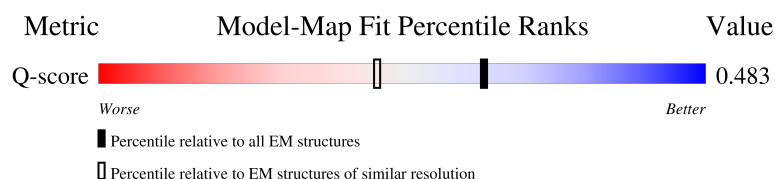
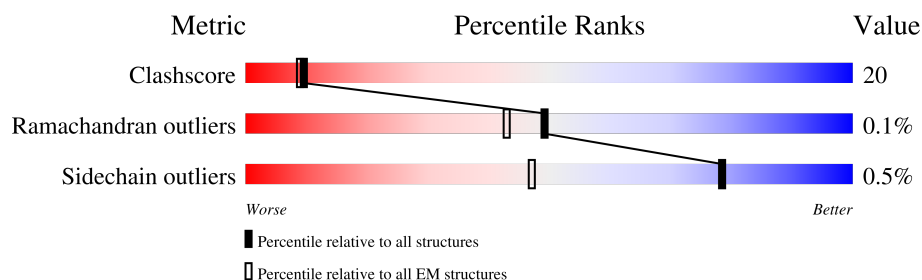
1 Overall quality at a glance

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	1956	
2	B	2	
2	C	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	95T	A	2004	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9748 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.

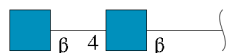
- Molecule 1 is a protein called Sodium channel protein type 10 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1100	8861	5886	1413	1500	62	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	894	PHE	SER	conflict	UNP Q9Y5Y9

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



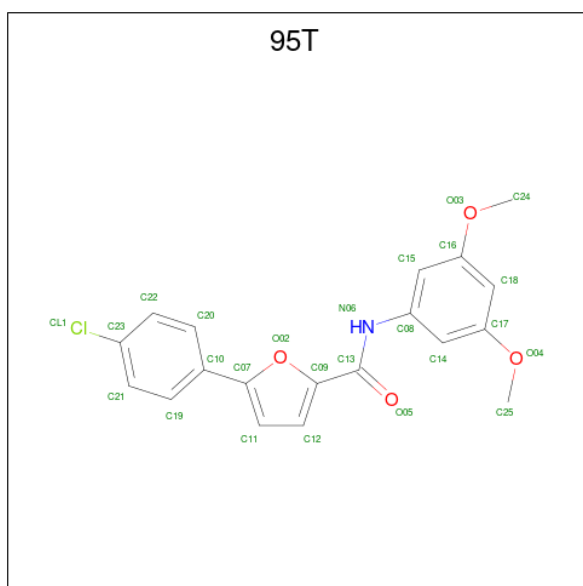
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	2	28	16	2	10	0	0
2	C	2	28	16	2	10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



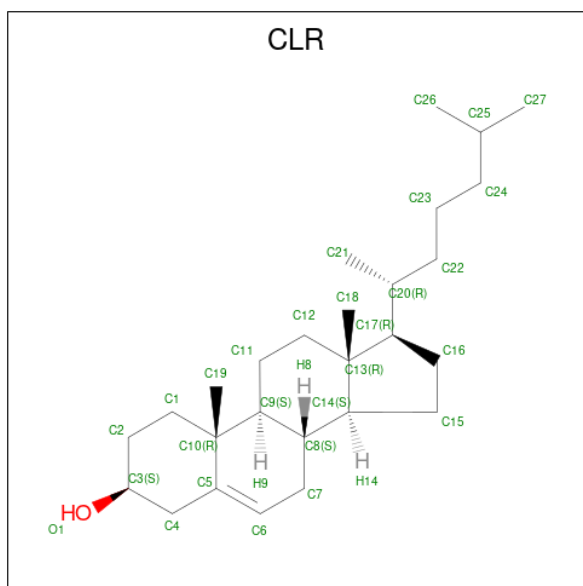
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is 5-(4-chlorophenyl)- {N}-(3,5-dimethoxyphenyl)furan-2-carboxamide (CCD ID: 95T) (formula: C₁₉H₁₆ClNO₄) (labeled as "Ligand of Interest" by depositor).



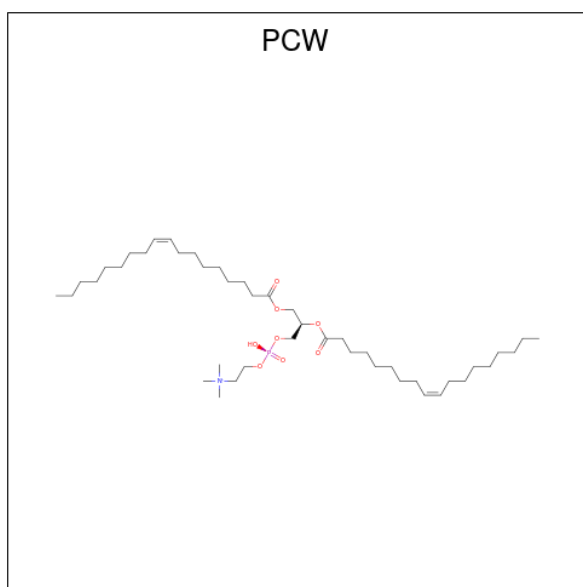
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Cl	N	O	0
			25	19	1	1	4	

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: $\text{C}_{27}\text{H}_{46}\text{O}$).



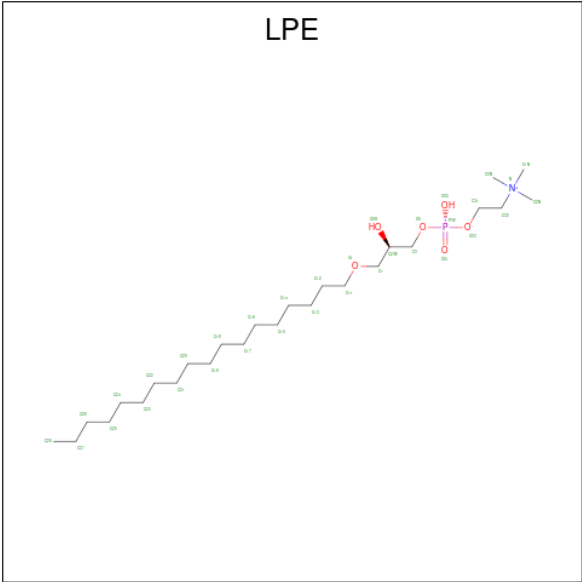
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total 28	C 27	O 1	0
5	A	1	Total 28	C 27	O 1	0
5	A	1	Total 28	C 27	O 1	0
5	A	1	Total 28	C 27	O 1	0
5	A	1	Total 28	C 27	O 1	0

- Molecule 6 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



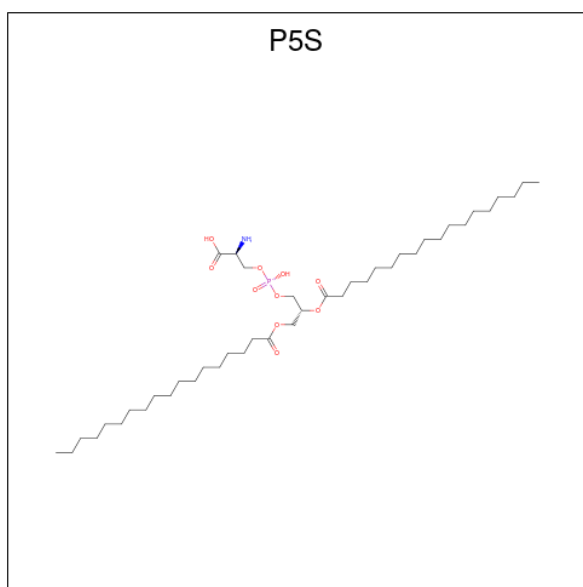
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
6	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
6	A	1	Total	C	O	P		0
			37	28	8	1		
6	A	1	Total	C	O	P		0
			41	32	8	1		
6	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
6	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	A	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 7 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: LPE) (formula: $C_{26}H_{57}NO_6P$).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
7	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
7	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
7	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
7	A	1	Total	C	O	P		0
			16	9	6	1		
7	A	1	Total	C	N	O	P	0
			23	15	1	6	1	
7	A	1	Total	C	N	O	P	0
			23	15	1	6	1	
7	A	1	Total	C	N	O	P	0
			34	26	1	6	1	
7	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
7	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
7	A	1	Total	C	N	O	P	0
			21	13	1	6	1	
7	A	1	Total	C	N	O	P	0
			34	26	1	6	1	

- Molecule 8 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	A	1	45	33	1	10	1	0



SER
SER
SER
ILE
GLN
ASN
GLU
ASP
GLU
ALA
THR
SER
MET
GLU
LEU
ILE
ALA
PRO
GLY
PRO

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



MAG1
MAG2

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



MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	274882	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	0.088	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0217	Depositor
Map size (Å)	259.8, 259.8, 259.8	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	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: LPE, 95T, CLR, P5S, PCW, NAG

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	0.27	0/9083	0.61	8/12318 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ALA	N-CA-C	11.48	123.54	111.14
1	A	1632	VAL	N-CA-C	10.50	121.50	110.05
1	A	1685	SER	N-CA-C	7.61	121.54	110.28
1	A	1210	PHE	N-CA-C	6.89	119.38	111.11
1	A	1628	SER	N-CA-C	6.13	118.04	111.36
1	A	652	VAL	N-CA-C	5.44	116.17	110.62
1	A	1332	CYS	N-CA-C	-5.10	105.84	111.71
1	A	151	ASP	N-CA-C	5.06	117.06	110.43

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	8861	0	9051	323	0
2	B	28	0	25	3	0
2	C	28	0	25	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	42	0	39	5	0
4	A	25	0	0	11	0
5	A	140	0	230	39	0
6	A	296	0	396	63	0
7	A	283	0	391	35	0
8	A	45	0	56	5	0
All	All	9748	0	10213	397	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 20.

All (397) 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)
4:A:2004:95T:C11	6:A:2013:PCW:H141	1.80	1.11
1:A:382:PHE:HE2	6:A:2006:PCW:H221	1.03	1.11
7:A:2011:LPE:H151	7:A:2012:LPE:H131	1.30	1.10
6:A:2016:PCW:H331	6:A:2016:PCW:H2	1.37	1.06
1:A:1418:ILE:CD1	5:A:2028:CLR:H17	1.87	1.03
1:A:382:PHE:CE2	6:A:2006:PCW:H221	1.96	1.01
1:A:382:PHE:CD2	6:A:2006:PCW:H242	2.02	0.94
1:A:1713:MET:HE1	4:A:2004:95T:O02	1.68	0.92
1:A:393:LEU:HD23	5:A:2028:CLR:H191	1.50	0.91
1:A:1410:LEU:HD21	6:A:2013:PCW:H20	1.54	0.89
1:A:371:LYS:HE2	1:A:1641:MET:CG	2.03	0.88
6:A:2016:PCW:H2	6:A:2016:PCW:C33	2.05	0.87
1:A:696:MET:HE1	7:A:2025:LPE:H31	1.55	0.87
1:A:1418:ILE:HD11	5:A:2028:CLR:H17	1.57	0.86
1:A:371:LYS:HE2	1:A:1641:MET:HG3	1.56	0.84
3:A:2001:NAG:O7	3:A:2001:NAG:O3	1.95	0.84
1:A:1418:ILE:HD11	5:A:2028:CLR:H122	1.59	0.82
1:A:371:LYS:CE	1:A:1641:MET:HG3	2.10	0.81
1:A:200:ALA:O	1:A:204:THR:HG23	1.80	0.81
7:A:2009:LPE:O31	7:A:2009:LPE:H3N3	1.80	0.80
1:A:1435:MET:HE2	1:A:1605:PRO:HB2	1.63	0.80
1:A:1716:MET:SD	4:A:2004:95T:C24	2.70	0.79
1:A:1306:LYS:HG2	1:A:1380:ARG:O	1.82	0.79
1:A:748:LYS:HB2	1:A:751:SER:HB3	1.65	0.78
1:A:1497:THR:HG21	5:A:2027:CLR:H12	1.65	0.78
1:A:1678:CYS:SG	1:A:1692:CYS:N	2.57	0.78
7:A:2011:LPE:H151	7:A:2012:LPE:C13	2.11	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2019:PCW:O4P	6:A:2019:PCW:H32	1.82	0.78
6:A:2019:PCW:H19	6:A:2019:PCW:H40	1.67	0.77
1:A:1238:LEU:HD12	1:A:1239:GLU:H	1.50	0.77
1:A:1284:VAL:HG11	1:A:1416:VAL:HG21	1.67	0.77
1:A:1418:ILE:HD13	5:A:2028:CLR:H17	1.66	0.76
1:A:1713:MET:CE	4:A:2004:95T:C19	2.65	0.74
7:A:2023:LPE:H322	8:A:2029:P5S:C	2.18	0.74
1:A:1501:SER:HB3	6:A:2026:PCW:O1P	1.87	0.74
1:A:1410:LEU:HD11	6:A:2013:PCW:H221	1.69	0.73
1:A:1713:MET:HE1	4:A:2004:95T:C19	2.17	0.73
7:A:2023:LPE:H322	8:A:2029:P5S:O	1.87	0.73
1:A:761:LEU:HD11	5:A:2017:CLR:H231	1.70	0.72
1:A:1700:ILE:O	1:A:1704:THR:HG23	1.89	0.72
7:A:2010:LPE:C3	7:A:2011:LPE:H321	2.19	0.71
4:A:2004:95T:C12	6:A:2013:PCW:H141	2.20	0.71
1:A:1721:ILE:CD1	5:A:2028:CLR:H183	2.21	0.71
1:A:382:PHE:CE2	6:A:2006:PCW:H242	2.25	0.71
6:A:2016:PCW:C47	5:A:2017:CLR:H262	2.21	0.71
1:A:1413:PHE:O	1:A:1417:ILE:HG12	1.91	0.70
5:A:2017:CLR:O1	5:A:2017:CLR:H192	1.92	0.69
1:A:1678:CYS:SG	1:A:1679:ASP:N	2.65	0.69
7:A:2009:LPE:H3N3	7:A:2009:LPE:P	2.33	0.69
1:A:331:ASN:HB2	1:A:335:ASN:HA	1.75	0.68
1:A:1255:LEU:HG	1:A:1258:LEU:HD12	1.75	0.68
1:A:393:LEU:CD2	5:A:2028:CLR:H191	2.24	0.68
1:A:1594:ARG:HD2	6:A:2006:PCW:O2P	1.93	0.68
7:A:2010:LPE:H32	7:A:2011:LPE:H3N2	1.73	0.68
1:A:391:LEU:HD13	1:A:1596:LEU:HD13	1.76	0.68
7:A:2010:LPE:O32	7:A:2011:LPE:H3N2	1.94	0.68
1:A:1398:PHE:O	1:A:1402:ILE:HG13	1.94	0.67
1:A:857:CYS:HA	1:A:860:VAL:HG12	1.77	0.67
1:A:775:THR:HA	1:A:778:LYS:HD3	1.75	0.67
1:A:784:VAL:CG1	7:A:2014:LPE:H162	2.24	0.67
1:A:371:LYS:HE2	1:A:1641:MET:HG2	1.77	0.67
1:A:1243:VAL:HG22	1:A:1245:PRO:HD2	1.76	0.66
1:A:1721:ILE:HD12	5:A:2028:CLR:H183	1.77	0.66
1:A:382:PHE:HD2	6:A:2006:PCW:H242	1.58	0.66
1:A:1326:VAL:HG23	1:A:1327:ASN:H	1.61	0.66
1:A:1721:ILE:CD1	5:A:2028:CLR:C18	2.74	0.66
1:A:1503:GLU:OE2	1:A:1503:GLU:N	2.27	0.66
6:A:2019:PCW:C2	6:A:2019:PCW:H332	2.25	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1571:LEU:O	1:A:1575:ILE:HG12	1.96	0.65
1:A:1158:ILE:O	1:A:1162:ILE:HG13	1.97	0.64
1:A:888:LEU:HB3	1:A:1411:ASN:HD21	1.62	0.64
1:A:1393:TYR:OH	6:A:2018:PCW:H73	1.98	0.64
1:A:352:LEU:HD23	1:A:358:TRP:HB2	1.79	0.64
1:A:749:LYS:HE3	1:A:749:LYS:HA	1.77	0.64
1:A:328:THR:HG22	1:A:329:SER:H	1.61	0.64
1:A:1696:ALA:HB3	6:A:2019:PCW:O3P	1.98	0.64
5:A:2017:CLR:H221	5:A:2017:CLR:H263	1.80	0.62
1:A:1601:MET:HB2	6:A:2006:PCW:H151	1.80	0.62
1:A:1713:MET:HE3	4:A:2004:95T:C19	2.29	0.62
1:A:1488:LEU:O	1:A:1492:THR:HG23	2.00	0.62
1:A:1410:LEU:HD21	6:A:2013:PCW:C20	2.28	0.62
1:A:175:ARG:HD2	1:A:175:ARG:O	2.00	0.62
1:A:1507:ILE:O	1:A:1511:ILE:HG13	1.99	0.61
1:A:1137:VAL:HA	1:A:1140:GLN:HE21	1.64	0.61
1:A:1230:LEU:O	1:A:1234:THR:HG23	2.01	0.61
6:A:2019:PCW:H19	6:A:2019:PCW:C40	2.30	0.61
1:A:679:THR:OG1	5:A:2005:CLR:H271	2.01	0.60
1:A:1664:ASP:OD2	1:A:1665:GLY:N	2.34	0.60
1:A:275:LYS:HE2	1:A:328:THR:HG21	1.84	0.60
1:A:1418:ILE:HD11	5:A:2028:CLR:C12	2.31	0.60
3:A:2001:NAG:HO3	3:A:2001:NAG:C7	2.08	0.60
6:A:2019:PCW:H332	6:A:2019:PCW:C3	2.31	0.60
1:A:1140:GLN:O	1:A:1144:THR:HG23	2.00	0.60
1:A:1310:CYS:H	1:A:1385:GLN:HE22	1.50	0.60
1:A:1572:PHE:O	1:A:1576:ARG:HG3	2.00	0.60
1:A:371:LYS:HD3	1:A:1652:LEU:HD11	1.84	0.59
1:A:865:ILE:HD12	1:A:865:ILE:H	1.67	0.59
1:A:1598:PHE:CD2	6:A:2006:PCW:H72	2.38	0.59
1:A:1541:VAL:O	1:A:1545:ILE:HG13	2.03	0.59
1:A:844:ARG:HG2	1:A:849:GLU:HB2	1.85	0.59
7:A:2010:LPE:O32	7:A:2011:LPE:C3N	2.50	0.59
1:A:1495:VAL:HA	5:A:2027:CLR:H122	1.84	0.58
1:A:1285:LEU:O	1:A:1289:LEU:HG	2.03	0.58
1:A:1227:ASN:O	1:A:1231:ILE:HG13	2.04	0.58
6:A:2013:PCW:O4P	7:A:2014:LPE:H1N1	2.04	0.58
6:A:2016:PCW:H411	5:A:2017:CLR:H212	1.85	0.58
6:A:2019:PCW:H332	6:A:2019:PCW:O3	2.03	0.58
1:A:1224:LEU:O	1:A:1228:ILE:HG13	2.04	0.58
7:A:2010:LPE:H32	7:A:2011:LPE:H321	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:ARG:HH21	1:A:1256:ARG:HH12	1.51	0.57
1:A:1288:CYS:SG	1:A:1409:THR:HG23	2.44	0.57
1:A:1313:TYR:HD2	1:A:1318:PHE:HB3	1.69	0.57
1:A:675:ILE:O	1:A:679:THR:HG23	2.04	0.57
1:A:1699:ILE:O	1:A:1703:THR:HG23	2.03	0.57
1:A:1704:THR:O	1:A:1708:ILE:HG13	2.04	0.57
1:A:1547:VAL:O	1:A:1551:ILE:HG12	2.04	0.57
1:A:1200:GLU:OE1	1:A:1204:LYS:HE3	2.05	0.56
1:A:1381:GLU:HB2	1:A:1384:MET:HE2	1.85	0.56
1:A:159:VAL:O	1:A:162:VAL:HG22	2.06	0.56
1:A:161:THR:O	1:A:165:THR:HG23	2.05	0.56
1:A:1717:TYR:O	1:A:1721:ILE:HG13	2.06	0.56
1:A:1238:LEU:CD1	1:A:1239:GLU:H	2.18	0.56
1:A:187:ASP:HB3	1:A:190:ASN:HB2	1.87	0.56
1:A:735:ILE:CD1	5:A:2017:CLR:H151	2.36	0.56
1:A:361:LEU:O	1:A:365:THR:HG23	2.06	0.56
7:A:2011:LPE:H131	7:A:2012:LPE:H141	1.88	0.55
1:A:247:ALA:HB1	7:A:2011:LPE:H311	1.88	0.55
1:A:1700:ILE:HD13	6:A:2019:PCW:H371	1.88	0.55
1:A:1144:THR:O	1:A:1148:ILE:HG13	2.07	0.55
1:A:1363:VAL:HA	1:A:1369:TRP:HB3	1.89	0.54
1:A:1442:TYR:CE2	7:A:2009:LPE:H312	2.41	0.54
6:A:2016:PCW:H331	6:A:2016:PCW:C2	2.23	0.54
1:A:1330:SER:O	1:A:1334:ILE:HD12	2.06	0.54
1:A:1721:ILE:HD13	5:A:2028:CLR:C18	2.37	0.54
1:A:1696:ALA:CB	6:A:2019:PCW:O3P	2.56	0.54
1:A:328:THR:HG22	1:A:329:SER:N	2.23	0.54
1:A:393:LEU:HD12	1:A:882:LEU:HD11	1.90	0.54
1:A:771:PRO:O	1:A:775:THR:HG23	2.08	0.54
1:A:1296:SER:O	1:A:1300:VAL:HG23	2.08	0.54
1:A:1313:TYR:CD2	1:A:1318:PHE:HB3	2.43	0.54
1:A:1394:MET:HE2	1:A:1394:MET:HA	1.89	0.54
5:A:2028:CLR:H121	5:A:2028:CLR:H212	1.89	0.54
1:A:224:LYS:O	1:A:228:VAL:HG23	2.07	0.54
6:A:2026:PCW:H371	6:A:2026:PCW:H141	1.90	0.53
1:A:665:PRO:O	1:A:668:GLU:HG2	2.08	0.53
8:A:2029:P5S:H44	8:A:2029:P5S:H22	1.91	0.53
1:A:813:TYR:HA	1:A:860:VAL:HG21	1.91	0.53
1:A:1190:ASP:OD2	1:A:1191:ARG:N	2.42	0.53
1:A:1443:TYR:HE2	1:A:1723:GLU:OE1	1.92	0.53
1:A:1538:GLY:HA3	6:A:2007:PCW:O31	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1503:GLU:O	1:A:1507:ILE:HG13	2.09	0.53
1:A:219:VAL:HG21	1:A:804:VAL:HG22	1.91	0.52
1:A:1404:PHE:HA	1:A:1408:PHE:HD2	1.72	0.52
7:A:2010:LPE:H31	7:A:2011:LPE:H321	1.89	0.52
2:B:1:NAG:H5	2:B:2:NAG:O5	2.08	0.52
1:A:1594:ARG:HG2	6:A:2006:PCW:H12	1.92	0.52
1:A:226:VAL:HA	1:A:232:LEU:HD22	1.91	0.52
1:A:1500:GLN:O	6:A:2026:PCW:C6	2.57	0.52
1:A:1356:GLY:O	1:A:1360:LEU:HG	2.10	0.52
1:A:1395:TYR:O	1:A:1399:VAL:HG23	2.10	0.52
1:A:1261:LEU:HD12	1:A:1261:LEU:H	1.74	0.52
1:A:1291:PHE:HE1	1:A:1295:PHE:HE1	1.57	0.52
1:A:1721:ILE:HD13	5:A:2028:CLR:H183	1.92	0.52
1:A:869:LEU:O	1:A:873:VAL:HG23	2.09	0.51
1:A:891:ASN:OD1	1:A:892:SER:N	2.43	0.51
1:A:1418:ILE:HD11	5:A:2028:CLR:C17	2.36	0.51
1:A:216:THR:O	1:A:219:VAL:HG22	2.10	0.51
6:A:2019:PCW:H171	6:A:2019:PCW:H39	1.93	0.51
1:A:1360:LEU:HB3	1:A:1401:PHE:CZ	2.46	0.51
4:A:2004:95T:C12	6:A:2013:PCW:H122	2.41	0.51
1:A:1479:ASP:OD2	1:A:1588:ARG:NH2	2.43	0.51
5:A:2005:CLR:H121	5:A:2005:CLR:H212	1.93	0.51
1:A:1345:ASN:OD1	1:A:1346:VAL:N	2.43	0.51
1:A:1568:SER:OG	7:A:2015:LPE:H2N2	2.10	0.50
1:A:788:GLY:O	1:A:792:ILE:HG13	2.11	0.50
5:A:2017:CLR:H212	5:A:2017:CLR:H121	1.92	0.50
1:A:1369:TRP:O	1:A:1373:MET:HG3	2.12	0.50
1:A:214:LEU:HA	1:A:217:PHE:CE2	2.47	0.50
1:A:789:ASN:O	1:A:793:ILE:HG23	2.10	0.50
1:A:889:LEU:HD12	5:A:2028:CLR:H151	1.93	0.50
1:A:1171:PHE:CE1	7:A:2022:LPE:C2N	2.95	0.50
1:A:801:PHE:CZ	1:A:872:THR:HG22	2.48	0.49
1:A:1522:GLU:O	1:A:1526:LYS:HG2	2.13	0.49
1:A:1542:PHE:O	1:A:1546:VAL:HG23	2.12	0.49
1:A:1561:LYS:HG2	1:A:1563:LEU:HD12	1.93	0.49
1:A:683:ALA:HB2	1:A:1297:ILE:HD11	1.94	0.49
1:A:759:ARG:O	1:A:762:ARG:HG2	2.12	0.49
1:A:216:THR:HA	1:A:219:VAL:HG22	1.94	0.49
1:A:792:ILE:O	1:A:796:ILE:HG12	2.12	0.49
6:A:2016:PCW:H2	6:A:2016:PCW:C34	2.42	0.49
1:A:851:ILE:HG12	1:A:855:TRP:CE2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:LEU:HD12	1:A:1239:GLU:N	2.25	0.49
1:A:198:THR:O	1:A:202:VAL:HG23	2.12	0.49
1:A:1659:THR:O	1:A:1660:SER:OG	2.29	0.49
1:A:1710:PHE:O	1:A:1714:VAL:HG23	2.13	0.49
1:A:1710:PHE:HB2	4:A:2004:95T:C21	2.43	0.49
1:A:732:PHE:O	1:A:736:ILE:HG12	2.12	0.49
1:A:1606:ALA:O	1:A:1610:ILE:HG13	2.12	0.48
1:A:1288:CYS:SG	1:A:1409:THR:CG2	3.01	0.48
1:A:205:ALA:C	1:A:206:ILE:HD12	2.39	0.48
1:A:698:GLN:O	1:A:702:ILE:HG23	2.13	0.48
1:A:1594:ARG:HG2	6:A:2006:PCW:H31	1.94	0.48
1:A:215:ARG:O	1:A:219:VAL:HG13	2.13	0.48
1:A:754:VAL:HG21	6:A:2018:PCW:H141	1.94	0.48
1:A:1604:LEU:HD21	6:A:2006:PCW:H20	1.93	0.48
1:A:1253:ARG:HH21	1:A:1256:ARG:NH1	2.11	0.48
1:A:1330:SER:O	1:A:1333:LYS:HB3	2.14	0.48
1:A:1641:MET:HE3	1:A:1641:MET:HB2	1.72	0.48
1:A:328:THR:CG2	1:A:329:SER:H	2.27	0.48
1:A:800:VAL:O	1:A:804:VAL:HG23	2.13	0.48
1:A:735:ILE:HD12	5:A:2017:CLR:H151	1.94	0.48
1:A:1501:SER:O	1:A:1505:THR:HG23	2.14	0.48
6:A:2019:PCW:C2	6:A:2019:PCW:C33	2.89	0.47
1:A:273:LYS:NZ	1:A:1498:ASP:OD2	2.47	0.47
1:A:1310:CYS:SG	1:A:1343:TRP:HE3	2.36	0.47
1:A:1582:ARG:HA	1:A:1585:ARG:HG3	1.96	0.47
1:A:350:PHE:CZ	1:A:874:MET:HE1	2.50	0.47
1:A:355:GLN:HE21	1:A:385:SER:HB3	1.78	0.47
1:A:382:PHE:O	1:A:386:PHE:HB3	2.14	0.47
1:A:829:ARG:HD3	1:A:1374:TYR:CZ	2.49	0.47
1:A:1199:PHE:O	1:A:1203:LEU:HD23	2.14	0.47
1:A:1598:PHE:CD2	6:A:2006:PCW:C7	2.98	0.47
1:A:1713:MET:HE1	4:A:2004:95T:C07	2.42	0.47
1:A:1373:MET:HE2	1:A:1395:TYR:HD2	1.79	0.47
1:A:695:ALA:O	1:A:699:ILE:HG12	2.15	0.47
1:A:713:VAL:HA	1:A:716:ILE:HG12	1.97	0.47
7:A:2023:LPE:H322	8:A:2029:P5S:OXT	2.14	0.47
1:A:893:PHE:HZ	1:A:1412:LEU:HD12	1.79	0.47
1:A:1407:PHE:HD1	7:A:2014:LPE:H2N2	1.80	0.47
6:A:2019:PCW:C33	6:A:2019:PCW:H2	2.43	0.47
1:A:1480:ILE:O	1:A:1484:VAL:HG23	2.15	0.47
1:A:1469:VAL:HA	1:A:1472:ILE:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LYS:HB2	1:A:297:ILE:HG13	1.96	0.47
1:A:761:LEU:HD22	1:A:764:PHE:HE1	1.80	0.47
1:A:1455:GLN:HE22	1:A:1457:PRO:HA	1.79	0.47
1:A:1437:GLU:CD	1:A:1437:GLU:H	2.23	0.46
1:A:1635:GLU:OE1	1:A:1672:ASN:ND2	2.48	0.46
1:A:669:LEU:O	1:A:673:LEU:HD23	2.15	0.46
1:A:1561:LYS:HG3	1:A:1562:SER:H	1.80	0.46
1:A:147:MET:SD	1:A:219:VAL:HG12	2.56	0.46
1:A:1460:ARG:HH22	1:A:1467:GLY:CA	2.28	0.46
1:A:281:MET:N	1:A:281:MET:HE2	2.30	0.46
1:A:851:ILE:HG12	1:A:855:TRP:CZ2	2.51	0.46
1:A:1255:LEU:O	1:A:1258:LEU:HB2	2.16	0.46
7:A:2023:LPE:H151	7:A:2023:LPE:H122	1.71	0.46
1:A:722:TYR:O	1:A:726:GLN:HG3	2.15	0.46
6:A:2013:PCW:H222	6:A:2013:PCW:H252	1.69	0.46
7:A:2015:LPE:H2N3	7:A:2015:LPE:H312	1.76	0.46
1:A:1377:VAL:HG11	1:A:1395:TYR:CE1	2.51	0.46
1:A:693:PHE:O	1:A:697:LEU:HD23	2.16	0.46
1:A:774:ASN:O	1:A:778:LYS:HG3	2.16	0.46
1:A:309:LEU:HB2	1:A:367:ARG:HD3	1.98	0.46
1:A:1161:MET:HA	1:A:1161:MET:HE2	1.97	0.46
1:A:1311:ILE:HB	1:A:1318:PHE:HB2	1.98	0.46
1:A:1368:GLY:N	1:A:1664:ASP:OD1	2.48	0.46
1:A:1519:PHE:O	1:A:1522:GLU:HG2	2.16	0.46
6:A:2016:PCW:C33	6:A:2016:PCW:C2	2.86	0.46
1:A:1414:VAL:O	1:A:1418:ILE:HG13	2.16	0.46
1:A:330:ASP:OD1	1:A:330:ASP:N	2.46	0.45
1:A:829:ARG:HD3	1:A:1374:TYR:CE1	2.51	0.45
7:A:2011:LPE:C15	7:A:2012:LPE:H131	2.21	0.45
6:A:2006:PCW:H421	6:A:2007:PCW:C21	2.47	0.45
5:A:2021:CLR:H222	5:A:2021:CLR:H162	1.68	0.45
1:A:757:SER:HA	1:A:760:LEU:HD23	1.98	0.45
1:A:1576:ARG:HH21	1:A:1579:ARG:NH2	2.14	0.45
7:A:2008:LPE:H312	7:A:2008:LPE:H3N3	1.63	0.45
1:A:1435:MET:HE1	1:A:1443:TYR:HD2	1.81	0.45
6:A:2016:PCW:H2	6:A:2016:PCW:H342	1.99	0.45
1:A:147:MET:HE1	1:A:215:ARG:HH11	1.81	0.45
1:A:1446:MET:HE1	1:A:1601:MET:HG2	1.98	0.45
6:A:2016:PCW:C11	6:A:2016:PCW:C1	2.94	0.45
6:A:2016:PCW:H31	5:A:2017:CLR:O1	2.16	0.45
6:A:2019:PCW:H32	6:A:2019:PCW:P	2.57	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LYS:HG3	1:A:1573:ARG:NH2	2.32	0.45
8:A:2029:P5S:H20	8:A:2029:P5S:H42	1.98	0.45
1:A:269:LYS:HG3	1:A:1573:ARG:HH21	1.80	0.45
1:A:1258:LEU:HD23	1:A:1261:LEU:HD11	1.97	0.45
1:A:1700:ILE:O	1:A:1704:THR:CG2	2.62	0.45
1:A:382:PHE:CD2	6:A:2006:PCW:H271	2.52	0.45
1:A:1500:GLN:O	6:A:2026:PCW:H63	2.17	0.45
1:A:1490:MET:HB2	1:A:1583:ILE:HD12	1.99	0.45
1:A:763:VAL:HB	1:A:1294:ILE:HD11	1.99	0.44
1:A:1291:PHE:HE1	1:A:1295:PHE:CE1	2.35	0.44
1:A:1453:LYS:HD3	1:A:1453:LYS:N	2.32	0.44
1:A:138:VAL:O	1:A:142:VAL:HG22	2.18	0.44
1:A:242:SER:O	1:A:246:LEU:HG	2.17	0.44
1:A:1460:ARG:HH22	1:A:1467:GLY:HA3	1.82	0.44
1:A:1495:VAL:HG21	6:A:2026:PCW:H142	1.99	0.44
1:A:192:LEU:O	1:A:196:VAL:HG23	2.18	0.44
1:A:290:SER:H	1:A:293:ARG:HH11	1.64	0.44
1:A:796:ILE:O	1:A:800:VAL:HG23	2.17	0.44
1:A:1253:ARG:NH2	1:A:1256:ARG:HH12	2.14	0.44
1:A:735:ILE:O	1:A:739:VAL:HG23	2.18	0.44
1:A:1452:LYS:HE3	1:A:1454:PRO:O	2.18	0.44
1:A:1490:MET:HG2	1:A:1494:MET:HE3	2.00	0.44
7:A:2011:LPE:H2N3	7:A:2011:LPE:H312	1.73	0.44
5:A:2027:CLR:H221	5:A:2027:CLR:H162	1.79	0.44
1:A:359:GLU:O	1:A:363:GLN:HG3	2.17	0.44
1:A:849:GLU:OE1	1:A:1369:TRP:NE1	2.46	0.44
1:A:1250:ARG:NH2	1:A:1250:ARG:HB3	2.32	0.44
1:A:1463:ASN:HB3	1:A:1466:GLN:HB3	2.00	0.44
7:A:2010:LPE:H11	7:A:2011:LPE:H1N3	2.00	0.44
6:A:2006:PCW:H341	6:A:2006:PCW:H371	1.60	0.43
7:A:2010:LPE:H2N3	7:A:2010:LPE:H311	1.80	0.43
1:A:702:ILE:HA	1:A:705:THR:HG22	2.00	0.43
1:A:1255:LEU:HD21	7:A:2020:LPE:H222	2.00	0.43
1:A:1413:PHE:O	1:A:1416:VAL:HG22	2.19	0.43
1:A:1666:LEU:O	1:A:1669:PRO:HD2	2.17	0.43
1:A:1718:ILE:O	1:A:1722:LEU:HD23	2.18	0.43
1:A:661:LEU:HA	1:A:718:ALA:HB1	2.01	0.43
1:A:1189:THR:O	1:A:1192:VAL:HG22	2.17	0.43
1:A:1341:PHE:HZ	3:A:2003:NAG:H82	1.83	0.43
1:A:1404:PHE:HA	1:A:1408:PHE:CD2	2.51	0.43
1:A:1613:LEU:O	1:A:1617:VAL:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:NAG:HO6	2:B:2:NAG:C1	2.31	0.43
1:A:1220:TRP:CE2	5:A:2021:CLR:H122	2.53	0.43
1:A:1341:PHE:CZ	3:A:2003:NAG:H82	2.54	0.43
1:A:1482:ILE:HD12	1:A:1522:GLU:OE2	2.17	0.43
1:A:367:ARG:NH1	1:A:1641:MET:HE3	2.34	0.43
1:A:1688:THR:O	1:A:1688:THR:HG22	2.19	0.43
1:A:1688:THR:O	1:A:1689:ARG:HB2	2.19	0.43
1:A:191:TRP:HA	1:A:194:PHE:HD2	1.83	0.43
1:A:1500:GLN:O	6:A:2026:PCW:H62	2.17	0.43
1:A:1509:GLY:O	1:A:1513:GLN:HG3	2.18	0.43
1:A:1502:GLU:OE2	1:A:1502:GLU:HA	2.19	0.42
6:A:2018:PCW:H351	6:A:2018:PCW:H322	1.65	0.42
6:A:2006:PCW:H72	6:A:2006:PCW:H42	1.52	0.42
1:A:272:LEU:HD12	1:A:338:SER:HA	2.00	0.42
1:A:371:LYS:CE	1:A:1641:MET:CG	2.80	0.42
1:A:1290:ILE:HD11	5:A:2005:CLR:C23	2.49	0.42
1:A:1721:ILE:HG22	1:A:1725:PHE:HE2	1.84	0.42
1:A:1721:ILE:CD1	5:A:2028:CLR:H182	2.48	0.42
1:A:651:TRP:CZ2	1:A:653:LYS:HE3	2.54	0.42
1:A:664:ASP:HB2	1:A:665:PRO:HD2	2.01	0.42
1:A:1660:SER:O	1:A:1663:TRP:HD1	2.02	0.42
1:A:1719:ALA:O	1:A:1723:GLU:HG2	2.20	0.42
1:A:664:ASP:OD1	1:A:667:ALA:HB2	2.20	0.42
1:A:758:PHE:CE2	5:A:2017:CLR:H25	2.55	0.42
1:A:1342:PHE:CE1	2:C:1:NAG:H3	2.53	0.42
1:A:665:PRO:C	1:A:667:ALA:H	2.28	0.42
1:A:705:THR:HB	1:A:759:ARG:NH1	2.35	0.42
1:A:889:LEU:CD1	5:A:2028:CLR:H151	2.49	0.42
1:A:1186:LEU:HA	1:A:1189:THR:OG1	2.20	0.42
1:A:1308:TRP:CD2	1:A:1345:ASN:HB2	2.55	0.42
1:A:1448:LYS:HA	1:A:1448:LYS:HD3	1.80	0.42
1:A:1485:LEU:HD13	1:A:1518:VAL:HG11	2.02	0.42
6:A:2007:PCW:H63	6:A:2007:PCW:H41	1.63	0.42
1:A:1537:ASN:HB3	1:A:1540:ASN:OD1	2.19	0.41
5:A:2027:CLR:H183	5:A:2027:CLR:H20	1.79	0.41
1:A:268:PHE:HA	1:A:271:ASN:ND2	2.35	0.41
1:A:1326:VAL:HG23	1:A:1327:ASN:N	2.33	0.41
1:A:1552:ALA:O	1:A:1556:PHE:HB2	2.21	0.41
7:A:2011:LPE:H142	7:A:2011:LPE:H112	1.67	0.41
1:A:355:GLN:NE2	4:A:2004:95T:O05	2.41	0.41
1:A:359:GLU:HG2	1:A:360:ARG:N	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:TYR:CD1	1:A:1600:LEU:HD13	2.55	0.41
1:A:1199:PHE:CZ	1:A:1203:LEU:HD21	2.56	0.41
1:A:1563:LEU:HD12	1:A:1563:LEU:H	1.85	0.41
1:A:146:CYS:HB2	1:A:160:PHE:CZ	2.55	0.41
1:A:299:ILE:HB	1:A:323:TYR:CE2	2.56	0.41
1:A:728:LYS:HE3	6:A:2016:PCW:C3	2.51	0.41
1:A:1330:SER:OG	2:B:1:NAG:H82	2.20	0.41
1:A:1600:LEU:HD23	6:A:2006:PCW:H161	2.01	0.41
1:A:136:ILE:O	1:A:140:ILE:HG23	2.21	0.41
1:A:665:PRO:C	1:A:667:ALA:N	2.78	0.41
1:A:172:ILE:HG23	1:A:173:LEU:HD23	2.03	0.41
1:A:219:VAL:HG23	1:A:220:LEU:HD22	2.03	0.41
1:A:859:GLU:O	3:A:2001:NAG:H82	2.21	0.41
6:A:2016:PCW:H411	5:A:2017:CLR:C21	2.51	0.41
5:A:2027:CLR:H193	5:A:2027:CLR:H111	1.83	0.41
5:A:2028:CLR:H183	5:A:2028:CLR:H212	2.02	0.41
1:A:194:PHE:O	1:A:197:ILE:HG22	2.21	0.41
1:A:1145:CYS:O	1:A:1149:VAL:HG13	2.21	0.41
1:A:1172:GLU:HA	1:A:1176:LEU:HD22	2.02	0.41
1:A:1308:TRP:CE3	1:A:1345:ASN:HB2	2.56	0.41
7:A:2011:LPE:H151	7:A:2012:LPE:C14	2.50	0.41
1:A:1694:SER:OG	6:A:2019:PCW:H12	2.21	0.41
1:A:147:MET:HE3	1:A:147:MET:HA	2.02	0.40
1:A:247:ALA:O	1:A:251:ILE:HG13	2.21	0.40
1:A:653:LYS:O	1:A:657:ILE:HG13	2.20	0.40
1:A:820:ILE:HD13	1:A:860:VAL:HB	2.02	0.40
7:A:2009:LPE:P	7:A:2009:LPE:C3N	3.08	0.40
7:A:2025:LPE:H311	7:A:2025:LPE:H3N3	1.81	0.40
1:A:271:ASN:O	1:A:274:ASN:ND2	2.55	0.40
1:A:379:LEU:HD23	1:A:379:LEU:HA	1.96	0.40
1:A:784:VAL:HG11	7:A:2014:LPE:H162	2.00	0.40
1:A:1320:LEU:HD12	1:A:1320:LEU:HA	1.87	0.40
1:A:1396:LEU:O	1:A:1400:ILE:HG12	2.22	0.40
1:A:1493:MET:CE	1:A:1583:ILE:HD11	2.51	0.40
1:A:1511:ILE:HG22	1:A:1515:PHE:CE2	2.57	0.40
1:A:216:THR:O	1:A:220:LEU:HD23	2.22	0.40
1:A:1136:ASP:OD1	1:A:1137:VAL:N	2.48	0.40
1:A:713:VAL:O	1:A:717:ILE:HG23	2.22	0.40
1:A:1335:GLN:N	1:A:1335:GLN:OE1	2.54	0.40
1:A:1500:GLN:HE21	1:A:1505:THR:HG22	1.86	0.40
1:A:1592:GLY:O	1:A:1596:LEU:HG	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2019:PCW:H381	6:A:2019:PCW:H411	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1091/1956 (56%)	1031 (94%)	59 (5%)	1 (0%)	48 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	666	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	971/1727 (56%)	966 (100%)	5 (0%)	81 89

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

Mol	Chain	Res	Type
1	A	206	ILE
1	A	654	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	741	LEU
1	A	752	LEU
1	A	1428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	A	271	ASN
1	A	274	ASN
1	A	364	GLN
1	A	1140	GLN
1	A	1283	ASN
1	A	1385	GLN
1	A	1423	GLN
1	A	1424	GLN
1	A	1439	GLN
1	A	1455	GLN
1	A	1512	ASN

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 ⓘ

4 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
2	NAG	B	1	1,2	14,14,15	0.31	0	17,19,21	0.57	0
2	NAG	B	2	2	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	C	1	1,2	14,14,15	0.29	0	17,19,21	0.57	0
2	NAG	C	2	2	14,14,15	0.29	0	17,19,21	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

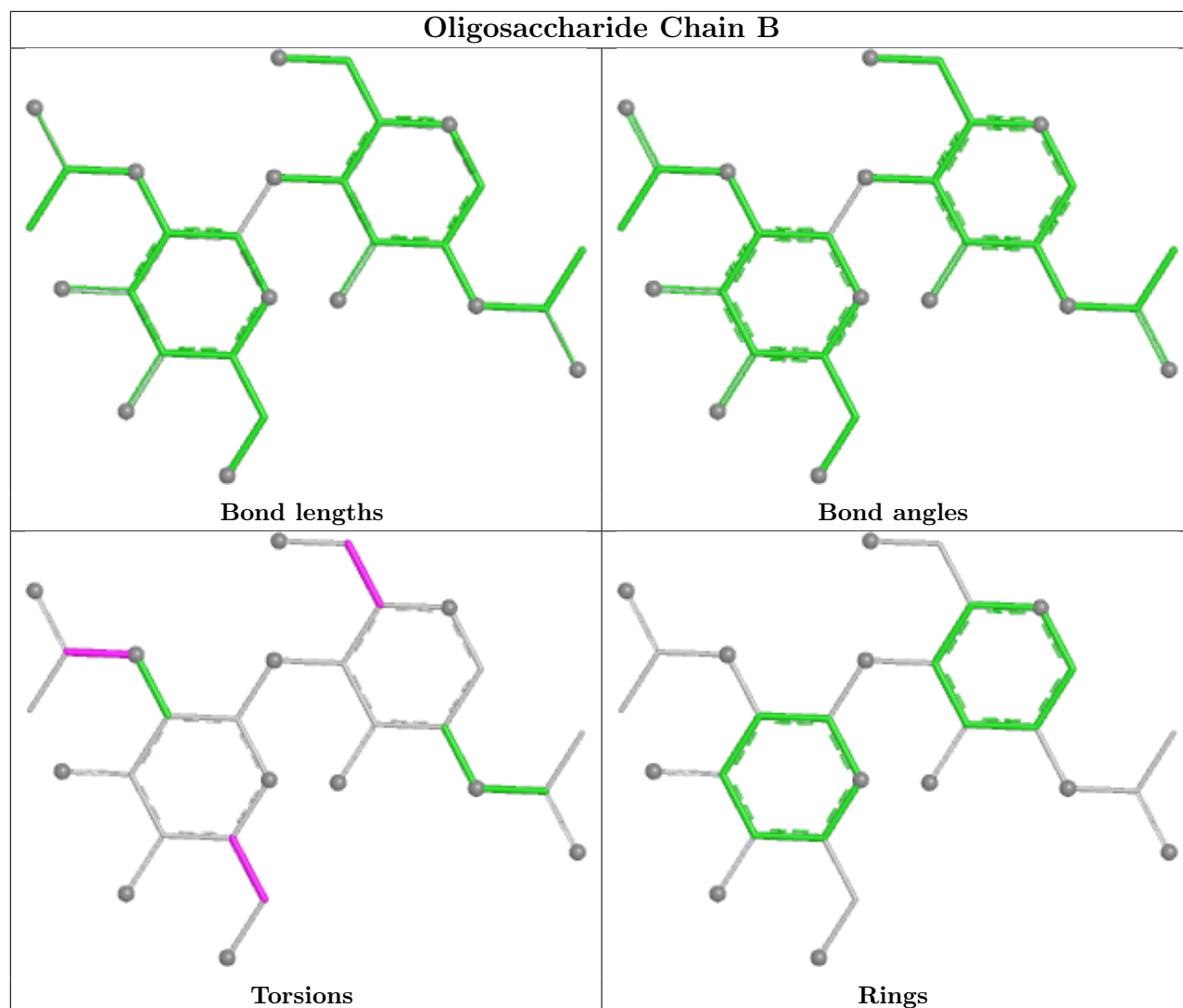
There are no ring outliers.

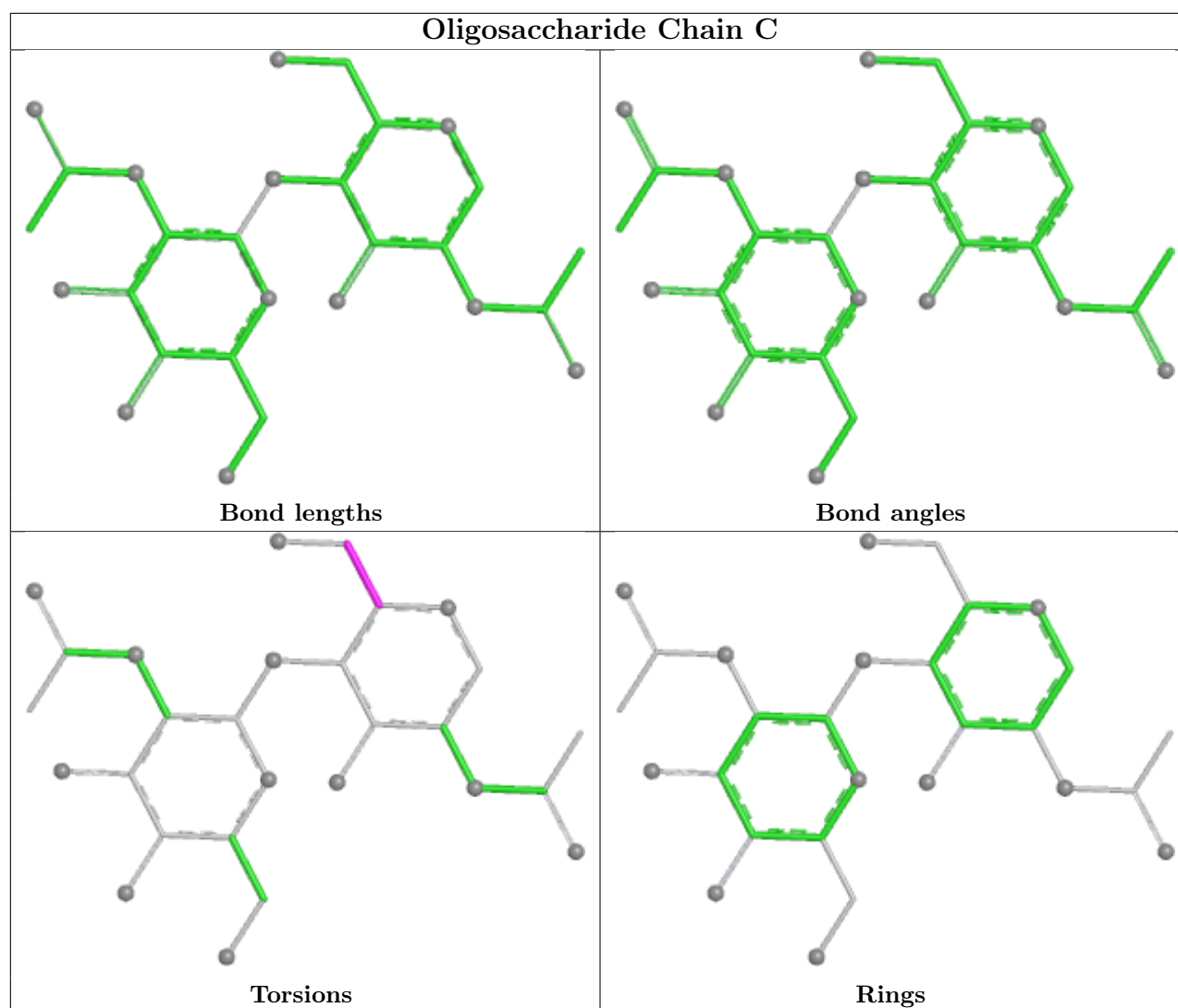
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	2	0
2	C	1	NAG	1	0
2	B	1	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

29 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	$\# Z > 2$
7	LPE	A	2010	-	21,21,33	0.58	0	25,27,39	0.59	0
7	LPE	A	2015	-	22,22,33	0.62	0	26,28,39	0.72	0
7	LPE	A	2008	-	21,21,33	0.58	0	25,27,39	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	P5S	A	2029	-	43,44,53	0.95	3 (6%)	45,51,60	1.48	8 (17%)
5	CLR	A	2028	-	31,31,31	0.74	0	48,48,48	1.30	6 (12%)
7	LPE	A	2009	-	21,21,33	0.58	0	25,27,39	0.60	0
6	PCW	A	2016	-	40,40,53	1.06	2 (5%)	43,45,61	1.20	4 (9%)
5	CLR	A	2005	-	31,31,31	0.74	0	48,48,48	1.22	5 (10%)
3	NAG	A	2002	1	14,14,15	0.29	0	17,19,21	0.57	0
5	CLR	A	2017	-	31,31,31	0.74	0	48,48,48	1.41	9 (18%)
7	LPE	A	2024	-	20,20,33	0.59	0	24,26,39	0.62	0
3	NAG	A	2003	1	14,14,15	0.28	0	17,19,21	0.56	0
7	LPE	A	2022	-	21,21,33	0.68	0	25,27,39	0.80	1 (4%)
6	PCW	A	2018	-	38,38,53	1.09	2 (5%)	44,46,61	1.09	3 (6%)
7	LPE	A	2023	-	21,21,33	0.58	0	25,27,39	0.72	0
4	95T	A	2004	-	27,27,27	0.35	0	37,37,37	0.43	0
7	LPE	A	2025	-	33,33,33	0.48	0	37,39,39	0.61	0
6	PCW	A	2013	-	36,36,53	1.12	2 (5%)	39,41,61	1.16	3 (7%)
6	PCW	A	2007	-	46,46,53	1.02	2 (4%)	52,54,61	1.19	3 (5%)
6	PCW	A	2019	-	39,39,53	1.08	2 (5%)	45,47,61	2.43	9 (20%)
3	NAG	A	2001	1	14,14,15	0.31	0	17,19,21	0.84	1 (5%)
7	LPE	A	2020	-	33,33,33	0.47	0	37,39,39	0.73	0
7	LPE	A	2012	-	15,15,33	0.60	0	16,18,39	0.85	1 (6%)
7	LPE	A	2011	-	21,21,33	0.63	0	25,27,39	0.72	0
6	PCW	A	2006	-	53,53,53	0.93	2 (3%)	59,61,61	1.11	4 (6%)
6	PCW	A	2026	-	37,37,53	1.12	2 (5%)	43,45,61	1.12	2 (4%)
5	CLR	A	2027	-	31,31,31	0.72	0	48,48,48	1.34	7 (14%)
7	LPE	A	2014	-	22,22,33	0.60	0	26,28,39	0.59	0
5	CLR	A	2021	-	31,31,31	0.86	1 (3%)	48,48,48	1.47	10 (20%)

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
7	LPE	A	2010	-	-	13/22/22/34	-
7	LPE	A	2015	-	-	8/23/23/34	-
7	LPE	A	2008	-	-	13/22/22/34	-
8	P5S	A	2029	-	-	12/50/50/59	-
5	CLR	A	2028	-	-	2/10/68/68	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LPE	A	2009	-	-	8/22/22/34	-
6	PCW	A	2016	-	-	22/42/42/57	-
5	CLR	A	2005	-	-	3/10/68/68	0/4/4/4
3	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
5	CLR	A	2017	-	-	5/10/68/68	0/4/4/4
7	LPE	A	2024	-	-	5/21/21/34	-
3	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
7	LPE	A	2022	-	-	10/22/22/34	-
6	PCW	A	2018	-	-	12/42/42/57	-
7	LPE	A	2023	-	-	4/22/22/34	-
4	95T	A	2004	-	-	12/16/16/16	0/3/3/3
7	LPE	A	2025	-	-	18/34/34/34	-
6	PCW	A	2013	-	-	25/38/38/57	-
6	PCW	A	2007	-	-	15/50/50/57	-
6	PCW	A	2019	-	-	24/43/43/57	-
3	NAG	A	2001	1	-	1/6/23/26	0/1/1/1
7	LPE	A	2020	-	-	3/34/34/34	-
7	LPE	A	2012	-	-	7/14/14/34	-
7	LPE	A	2011	-	-	7/22/22/34	-
6	PCW	A	2006	-	-	24/57/57/57	-
6	PCW	A	2026	-	-	17/41/41/57	-
5	CLR	A	2027	-	-	7/10/68/68	0/4/4/4
7	LPE	A	2014	-	-	10/23/23/34	-
5	CLR	A	2021	-	-	4/10/68/68	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2007	PCW	O3-C11	4.45	1.46	1.33
6	A	2019	PCW	O3-C11	4.28	1.45	1.33
6	A	2013	PCW	O3-C11	4.27	1.45	1.33
6	A	2016	PCW	O3-C11	4.27	1.45	1.33
6	A	2007	PCW	O2-C31	4.21	1.46	1.34
6	A	2026	PCW	O2-C31	4.18	1.46	1.34
6	A	2013	PCW	O2-C31	4.16	1.46	1.34
6	A	2006	PCW	O2-C31	4.15	1.46	1.34
6	A	2018	PCW	O3-C11	4.15	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2018	PCW	O2-C31	4.13	1.46	1.34
6	A	2016	PCW	O2-C31	4.13	1.46	1.34
6	A	2026	PCW	O3-C11	4.13	1.45	1.33
6	A	2019	PCW	O2-C31	4.10	1.45	1.34
6	A	2006	PCW	O3-C11	3.85	1.44	1.33
8	A	2029	P5S	O19-C17	3.75	1.44	1.33
8	A	2029	P5S	O37-C38	3.64	1.44	1.34
5	A	2021	CLR	C10-C9	-2.43	1.52	1.56
8	A	2029	P5S	O37-C2	-2.16	1.41	1.46

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2019	PCW	C8-N-C6	-8.57	86.48	108.98
6	A	2019	PCW	C8-N-C7	-8.55	86.51	108.98
6	A	2019	PCW	C8-N-C5	-5.89	86.50	109.91
8	A	2029	P5S	OG-CB-CA	5.06	112.47	108.06
6	A	2007	PCW	O2-C31-C32	4.86	121.99	111.48
6	A	2026	PCW	O2-C31-C32	4.36	120.91	111.48
6	A	2016	PCW	O2-C31-C32	4.11	120.38	111.48
5	A	2027	CLR	C13-C17-C20	-4.05	113.25	119.50
6	A	2019	PCW	C7-N-C6	4.05	119.60	108.98
6	A	2019	PCW	O2-C31-C32	4.02	120.17	111.48
8	A	2029	P5S	O37-C38-C39	3.96	120.05	111.48
6	A	2013	PCW	O2-C31-C32	3.81	119.72	111.48
5	A	2021	CLR	C7-C6-C5	-3.74	118.70	125.02
6	A	2006	PCW	O2-C31-C32	3.68	119.45	111.48
5	A	2017	CLR	C1-C2-C3	3.68	115.36	110.48
5	A	2005	CLR	C13-C17-C20	-3.55	114.02	119.50
5	A	2028	CLR	C4-C5-C10	3.46	120.86	116.42
6	A	2018	PCW	O2-C31-C32	3.41	118.86	111.48
5	A	2017	CLR	C13-C17-C20	-3.36	114.31	119.50
6	A	2007	PCW	O3-C11-C12	3.36	122.08	111.83
8	A	2029	P5S	O19-C17-C20	3.31	121.92	111.83
6	A	2006	PCW	O3-C11-C12	3.29	121.87	111.83
5	A	2021	CLR	C1-C10-C9	3.23	113.01	108.74
5	A	2028	CLR	C13-C17-C20	-3.21	114.54	119.50
5	A	2017	CLR	C4-C5-C10	2.95	120.20	116.42
6	A	2013	PCW	O3-C11-C12	2.77	120.28	111.83
5	A	2028	CLR	C8-C7-C6	-2.75	108.95	112.76
6	A	2018	PCW	O3-C11-C12	2.74	120.18	111.83
6	A	2019	PCW	O3-C11-C12	2.73	120.17	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2021	CLR	C8-C7-C6	-2.73	108.98	112.76
5	A	2027	CLR	C13-C14-C8	-2.70	110.59	114.41
5	A	2017	CLR	C13-C14-C8	-2.64	110.66	114.41
6	A	2016	PCW	O3-C11-C12	2.64	119.88	111.83
6	A	2026	PCW	O3-C11-C12	2.63	119.85	111.83
3	A	2001	NAG	C1-O5-C5	2.61	115.68	112.19
5	A	2028	CLR	C13-C14-C8	-2.60	110.72	114.41
8	A	2029	P5S	OXT-C-O	-2.60	118.19	124.08
5	A	2005	CLR	C13-C14-C8	-2.56	110.78	114.41
6	A	2007	PCW	O3-C3-C2	2.53	115.70	108.40
5	A	2017	CLR	C11-C12-C13	-2.52	108.48	112.74
6	A	2006	PCW	C3-C2-C1	-2.52	105.91	111.78
6	A	2019	PCW	C2-O2-C31	-2.51	111.79	117.80
5	A	2005	CLR	C11-C12-C13	-2.48	108.55	112.74
6	A	2018	PCW	C3-C2-C1	-2.48	106.01	111.78
5	A	2027	CLR	C11-C12-C13	-2.47	108.57	112.74
5	A	2005	CLR	C4-C5-C10	2.46	119.58	116.42
6	A	2019	PCW	C6-N-C5	2.46	119.69	109.91
5	A	2027	CLR	C16-C17-C20	2.45	115.89	112.18
6	A	2019	PCW	C7-N-C5	2.44	119.59	109.91
5	A	2021	CLR	C7-C8-C9	2.41	112.51	109.72
5	A	2027	CLR	C17-C13-C14	2.40	102.85	100.10
6	A	2006	PCW	O3-C11-O11	-2.39	117.65	123.63
5	A	2021	CLR	C1-C2-C3	2.38	113.63	110.48
6	A	2016	PCW	O1P-P-O2P	2.36	120.01	110.83
5	A	2028	CLR	C4-C5-C6	-2.35	117.38	120.57
7	A	2022	LPE	C3-C2-C1	-2.34	105.92	112.65
5	A	2017	CLR	C8-C7-C6	-2.34	109.52	112.76
7	A	2012	LPE	O32-P-O31	2.34	119.94	110.83
5	A	2027	CLR	C4-C5-C10	2.33	119.41	116.42
5	A	2017	CLR	C3-C4-C5	-2.32	108.35	112.05
8	A	2029	P5S	O37-C38-O47	-2.32	118.28	123.70
6	A	2013	PCW	O1P-P-O2P	2.32	119.87	110.83
5	A	2021	CLR	C13-C14-C8	-2.29	111.16	114.41
5	A	2027	CLR	C22-C20-C17	2.26	115.02	110.33
5	A	2017	CLR	C7-C6-C5	-2.26	121.21	125.02
6	A	2016	PCW	C2-O2-C31	-2.25	112.41	117.80
5	A	2021	CLR	C4-C5-C10	2.24	119.29	116.42
8	A	2029	P5S	C2-O37-C38	-2.24	112.44	117.80
5	A	2028	CLR	C11-C12-C13	-2.23	108.97	112.74
5	A	2005	CLR	C17-C13-C14	2.22	102.65	100.10
5	A	2017	CLR	C17-C13-C14	2.20	102.63	100.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2021	CLR	C19-C10-C9	-2.12	109.28	111.66
5	A	2021	CLR	C10-C9-C8	-2.11	109.64	112.71
8	A	2029	P5S	O19-C17-O18	-2.10	118.37	123.63
5	A	2021	CLR	C10-C5-C6	-2.08	119.89	122.93
8	A	2029	P5S	C40-C39-C38	-2.00	106.36	113.69

There are no chirality outliers.

All (295) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2004	95T	C09-C13-N06-C08
4	A	2004	95T	O02-C09-C13-O05
4	A	2004	95T	C12-C09-C13-O05
4	A	2004	95T	O02-C09-C13-N06
4	A	2004	95T	C12-C09-C13-N06
5	A	2027	CLR	C13-C17-C20-C21
5	A	2027	CLR	C16-C17-C20-C22
6	A	2006	PCW	O4P-C4-C5-N
6	A	2006	PCW	C4-O4P-P-O2P
6	A	2007	PCW	C1-O3P-P-O1P
6	A	2007	PCW	C1-O3P-P-O4P
6	A	2013	PCW	C1-O3P-P-O1P
6	A	2013	PCW	C1-O3P-P-O4P
6	A	2016	PCW	C2-C3-O3-C11
6	A	2016	PCW	C32-C31-O2-C2
6	A	2016	PCW	O31-C31-O2-C2
6	A	2018	PCW	C1-O3P-P-O1P
6	A	2018	PCW	C1-O3P-P-O2P
6	A	2018	PCW	C1-O3P-P-O4P
6	A	2019	PCW	C32-C31-O2-C2
6	A	2019	PCW	O31-C31-O2-C2
6	A	2019	PCW	C4-O4P-P-O3P
6	A	2026	PCW	C39-C40-C41-C42
6	A	2026	PCW	C1-O3P-P-O2P
6	A	2026	PCW	C1-O3P-P-O4P
6	A	2026	PCW	C4-O4P-P-O2P
6	A	2026	PCW	C4-O4P-P-O3P
7	A	2008	LPE	C3-O3-P-O32
7	A	2008	LPE	C3-O3-P-O33
7	A	2008	LPE	C31-O33-P-O3
7	A	2008	LPE	C31-O33-P-O31
7	A	2008	LPE	C31-O33-P-O32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	2009	LPE	O1-C1-C2-O2H
7	A	2009	LPE	O1-C1-C2-C3
7	A	2009	LPE	C3-O3-P-O31
7	A	2009	LPE	C31-O33-P-O3
7	A	2009	LPE	C31-O33-P-O31
7	A	2009	LPE	C31-O33-P-O32
7	A	2010	LPE	C1-C2-C3-O3
7	A	2010	LPE	C3-O3-P-O31
7	A	2010	LPE	C3-O3-P-O32
7	A	2010	LPE	C3-O3-P-O33
7	A	2010	LPE	C31-O33-P-O3
7	A	2010	LPE	C31-O33-P-O32
7	A	2010	LPE	O33-C31-C32-N
7	A	2011	LPE	C2-C3-O3-P
7	A	2011	LPE	C3-O3-P-O32
7	A	2011	LPE	C3-O3-P-O33
7	A	2011	LPE	C31-O33-P-O31
7	A	2014	LPE	C31-O33-P-O3
7	A	2014	LPE	C31-O33-P-O31
7	A	2014	LPE	C31-O33-P-O32
7	A	2015	LPE	O2H-C2-C3-O3
7	A	2015	LPE	C3-O3-P-O32
7	A	2015	LPE	C3-O3-P-O33
7	A	2015	LPE	C31-O33-P-O3
7	A	2015	LPE	C31-O33-P-O32
7	A	2022	LPE	C3-O3-P-O32
7	A	2022	LPE	C3-O3-P-O33
7	A	2022	LPE	C31-O33-P-O3
7	A	2022	LPE	C31-O33-P-O32
7	A	2023	LPE	C31-O33-P-O3
7	A	2023	LPE	O33-C31-C32-N
7	A	2024	LPE	C31-O33-P-O3
7	A	2025	LPE	O1-C1-C2-O2H
7	A	2025	LPE	O1-C1-C2-C3
7	A	2025	LPE	C3-O3-P-O31
7	A	2025	LPE	C3-O3-P-O33
7	A	2025	LPE	C31-O33-P-O3
7	A	2025	LPE	C32-C31-O33-P
7	A	2025	LPE	O33-C31-C32-N
8	A	2029	P5S	O-C-CA-N
8	A	2029	P5S	O47-C38-O37-C2
5	A	2027	CLR	C16-C17-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	2027	CLR	C13-C17-C20-C22
4	A	2004	95T	C18-C16-O03-C24
4	A	2004	95T	C15-C16-O03-C24
6	A	2007	PCW	O31-C31-O2-C2
8	A	2029	P5S	C39-C38-O37-C2
3	A	2002	NAG	O5-C5-C6-O6
6	A	2006	PCW	C12-C11-O3-C3
6	A	2026	PCW	O11-C11-O3-C3
7	A	2010	LPE	O2H-C2-C3-O3
6	A	2026	PCW	C12-C11-O3-C3
6	A	2007	PCW	C32-C31-O2-C2
3	A	2002	NAG	C4-C5-C6-O6
6	A	2006	PCW	O11-C11-O3-C3
5	A	2017	CLR	C17-C20-C22-C23
4	A	2004	95T	O05-C13-N06-C08
8	A	2029	P5S	OXT-C-CA-N
7	A	2015	LPE	C1-C2-C3-O3
6	A	2016	PCW	C12-C11-O3-C3
5	A	2017	CLR	C21-C20-C22-C23
6	A	2016	PCW	O11-C11-O3-C3
3	A	2003	NAG	O5-C5-C6-O6
3	A	2003	NAG	C4-C5-C6-O6
6	A	2006	PCW	C4-C5-N-C7
5	A	2017	CLR	C20-C22-C23-C24
7	A	2012	LPE	O2H-C2-C3-O3
4	A	2004	95T	C14-C17-O04-C25
4	A	2004	95T	C18-C17-O04-C25
7	A	2012	LPE	C1-C2-C3-O3
6	A	2026	PCW	C4-C5-N-C8
7	A	2014	LPE	C31-C32-N-C1N
5	A	2005	CLR	C22-C23-C24-C25
7	A	2025	LPE	O1-C11-C12-C13
5	A	2005	CLR	C20-C22-C23-C24
6	A	2026	PCW	C32-C31-O2-C2
6	A	2026	PCW	O31-C31-O2-C2
5	A	2027	CLR	C22-C23-C24-C25
6	A	2019	PCW	C31-C32-C33-C34
7	A	2022	LPE	C2-C3-O3-P
6	A	2019	PCW	C4-C5-N-C8
6	A	2026	PCW	C4-C5-N-C6
7	A	2014	LPE	C31-C32-N-C2N
7	A	2014	LPE	C31-C32-N-C3N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	2019	PCW	C12-C13-C14-C15
6	A	2006	PCW	C35-C36-C37-C38
6	A	2013	PCW	C13-C14-C15-C16
6	A	2013	PCW	C15-C16-C17-C18
6	A	2006	PCW	C4-C5-N-C6
6	A	2006	PCW	C4-C5-N-C8
6	A	2019	PCW	C4-C5-N-C7
6	A	2016	PCW	C31-C32-C33-C34
6	A	2013	PCW	C20-C21-C22-C23
6	A	2013	PCW	C12-C11-O3-C3
7	A	2012	LPE	O1-C11-C12-C13
6	A	2013	PCW	C32-C33-C34-C35
6	A	2006	PCW	C22-C23-C24-C25
6	A	2019	PCW	C13-C14-C15-C16
6	A	2016	PCW	C15-C16-C17-C18
6	A	2016	PCW	C19-C20-C21-C22
6	A	2007	PCW	C12-C13-C14-C15
7	A	2009	LPE	C12-C13-C14-C15
6	A	2013	PCW	C14-C15-C16-C17
6	A	2026	PCW	C31-C32-C33-C34
5	A	2028	CLR	C23-C24-C25-C26
5	A	2028	CLR	C23-C24-C25-C27
6	A	2026	PCW	C4-C5-N-C7
6	A	2016	PCW	O3P-C1-C2-O2
7	A	2012	LPE	C2-C1-O1-C11
6	A	2019	PCW	C16-C17-C18-C19
6	A	2016	PCW	C33-C34-C35-C36
6	A	2013	PCW	O11-C11-O3-C3
7	A	2025	LPE	C12-C13-C14-C15
6	A	2013	PCW	C16-C17-C18-C19
6	A	2006	PCW	C15-C16-C17-C18
6	A	2006	PCW	C34-C35-C36-C37
6	A	2013	PCW	C1-C2-C3-O3
3	A	2001	NAG	C3-C2-N2-C7
6	A	2016	PCW	C41-C42-C43-C44
5	A	2021	CLR	C13-C17-C20-C22
7	A	2025	LPE	C24-C25-C26-C27
5	A	2021	CLR	C16-C17-C20-C21
5	A	2021	CLR	C13-C17-C20-C21
6	A	2016	PCW	C34-C35-C36-C37
6	A	2016	PCW	C12-C13-C14-C15
6	A	2006	PCW	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	2019	PCW	C14-C15-C16-C17
6	A	2016	PCW	C35-C36-C37-C38
7	A	2008	LPE	C2-C1-O1-C11
7	A	2014	LPE	C2-C1-O1-C11
7	A	2025	LPE	C13-C14-C15-C16
7	A	2025	LPE	C22-C23-C24-C25
5	A	2017	CLR	C23-C24-C25-C27
6	A	2019	PCW	C33-C34-C35-C36
7	A	2010	LPE	C13-C14-C15-C16
6	A	2016	PCW	C44-C45-C46-C47
6	A	2013	PCW	C21-C22-C23-C24
5	A	2027	CLR	C17-C20-C22-C23
7	A	2010	LPE	C12-C13-C14-C15
6	A	2016	PCW	O3P-C1-C2-C3
6	A	2013	PCW	C23-C24-C25-C26
6	A	2018	PCW	C33-C34-C35-C36
6	A	2019	PCW	C35-C36-C37-C38
6	A	2019	PCW	C1-C2-C3-O3
6	A	2013	PCW	C36-C37-C38-C39
7	A	2025	LPE	C2-C1-O1-C11
8	A	2029	P5S	O37-C2-C3-O16
7	A	2025	LPE	C21-C22-C23-C24
6	A	2013	PCW	O2-C2-C3-O3
6	A	2019	PCW	O2-C2-C3-O3
6	A	2013	PCW	C22-C23-C24-C25
6	A	2026	PCW	C35-C36-C37-C38
5	A	2017	CLR	C23-C24-C25-C26
8	A	2029	P5S	C28-C29-C30-C31
5	A	2021	CLR	C16-C17-C20-C22
8	A	2029	P5S	C1-C2-C3-O16
6	A	2016	PCW	C1-O3P-P-O1P
6	A	2007	PCW	C3-C2-O2-C31
6	A	2006	PCW	O3P-C1-C2-O2
7	A	2014	LPE	C12-C11-O1-C1
6	A	2019	PCW	C5-C4-O4P-P
7	A	2024	LPE	C32-C31-O33-P
4	A	2004	95T	C15-C08-N06-C13
7	A	2009	LPE	O1-C11-C12-C13
6	A	2019	PCW	C32-C33-C34-C35
7	A	2025	LPE	C11-C12-C13-C14
6	A	2016	PCW	C32-C33-C34-C35
7	A	2012	LPE	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	2025	LPE	C16-C17-C18-C19
6	A	2018	PCW	O4P-C4-C5-N
6	A	2019	PCW	O4P-C4-C5-N
7	A	2015	LPE	O33-C31-C32-N
7	A	2020	LPE	O33-C31-C32-N
7	A	2022	LPE	O33-C31-C32-N
7	A	2024	LPE	O33-C31-C32-N
8	A	2029	P5S	N-CA-CB-OG
7	A	2010	LPE	C2-C1-O1-C11
6	A	2006	PCW	C16-C17-C18-C19
6	A	2006	PCW	C32-C33-C34-C35
4	A	2004	95T	C14-C08-N06-C13
7	A	2011	LPE	C12-C11-O1-C1
6	A	2026	PCW	C33-C34-C35-C36
6	A	2006	PCW	C4-O4P-P-O1P
6	A	2006	PCW	C4-O4P-P-O3P
6	A	2007	PCW	C4-O4P-P-O2P
6	A	2019	PCW	C4-O4P-P-O2P
6	A	2026	PCW	C1-O3P-P-O1P
6	A	2026	PCW	C4-O4P-P-O1P
7	A	2010	LPE	C31-O33-P-O31
7	A	2014	LPE	C3-O3-P-O31
7	A	2020	LPE	C31-O33-P-O31
7	A	2023	LPE	C31-O33-P-O31
7	A	2024	LPE	C3-O3-P-O31
7	A	2024	LPE	C31-O33-P-O31
7	A	2025	LPE	C31-O33-P-O31
7	A	2023	LPE	C2-C1-O1-C11
6	A	2018	PCW	C2-C1-O3P-P
6	A	2006	PCW	C21-C22-C23-C24
6	A	2006	PCW	C19-C20-C21-C22
7	A	2008	LPE	O2H-C2-C3-O3
7	A	2020	LPE	C12-C11-O1-C1
7	A	2008	LPE	O1-C1-C2-C3
7	A	2008	LPE	C1-C2-C3-O3
6	A	2013	PCW	C33-C34-C35-C36
6	A	2013	PCW	O31-C31-O2-C2
6	A	2006	PCW	O2-C2-C3-O3
6	A	2018	PCW	C39-C40-C41-C42
6	A	2013	PCW	C32-C31-O2-C2
6	A	2016	PCW	C40-C41-C42-C43
7	A	2011	LPE	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	2019	PCW	C36-C37-C38-C39
7	A	2022	LPE	O1-C1-C2-C3
6	A	2007	PCW	C39-C40-C41-C42
7	A	2012	LPE	C12-C11-O1-C1
6	A	2018	PCW	C31-C32-C33-C34
8	A	2029	P5S	C45-C46-C48-C49
7	A	2025	LPE	C25-C26-C27-C28
7	A	2022	LPE	C11-C12-C13-C14
6	A	2019	PCW	C2-C1-O3P-P
7	A	2010	LPE	C11-C12-C13-C14
6	A	2019	PCW	C17-C18-C19-C20
7	A	2008	LPE	O1-C1-C2-O2H
6	A	2006	PCW	C24-C25-C26-C27
6	A	2007	PCW	C31-C32-C33-C34
6	A	2006	PCW	C39-C40-C41-C42
6	A	2013	PCW	C17-C18-C19-C20
7	A	2022	LPE	C12-C13-C14-C15
6	A	2007	PCW	C4-C5-N-C6
6	A	2006	PCW	O3P-C1-C2-C3
6	A	2007	PCW	O2-C2-C3-O3
7	A	2008	LPE	C31-C32-N-C3N
7	A	2011	LPE	O1-C1-C2-O2H
6	A	2013	PCW	C19-C20-C21-C22
5	A	2005	CLR	C13-C17-C20-C21
6	A	2006	PCW	C17-C18-C19-C20
6	A	2016	PCW	C17-C18-C19-C20
6	A	2007	PCW	C4-C5-N-C8
6	A	2018	PCW	C37-C38-C39-C40
7	A	2012	LPE	C2-C3-O3-P
7	A	2008	LPE	C31-C32-N-C1N
7	A	2015	LPE	C31-C32-N-C2N
6	A	2018	PCW	O3P-C1-C2-O2
8	A	2029	P5S	O37-C38-C39-C40
6	A	2007	PCW	C4-C5-N-C7
6	A	2016	PCW	O3-C11-C12-C13
8	A	2029	P5S	C39-C40-C41-C42
6	A	2019	PCW	C34-C35-C36-C37
6	A	2013	PCW	O3-C11-C12-C13
6	A	2007	PCW	O3-C11-C12-C13
7	A	2014	LPE	C12-C13-C14-C15
7	A	2022	LPE	C31-C32-N-C2N
5	A	2027	CLR	C23-C24-C25-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	2013	PCW	O2-C31-C32-C33
6	A	2019	PCW	O2-C31-C32-C33
6	A	2016	PCW	O11-C11-C12-C13
6	A	2018	PCW	O2-C31-C32-C33
8	A	2029	P5S	O47-C38-C39-C40
6	A	2007	PCW	O11-C11-C12-C13
6	A	2013	PCW	C31-C32-C33-C34
7	A	2008	LPE	C31-C32-N-C2N
6	A	2019	PCW	O3-C11-C12-C13
6	A	2013	PCW	O11-C11-C12-C13
6	A	2018	PCW	O31-C31-C32-C33

There are no ring outliers.

27 monomers are involved in 147 short contacts:

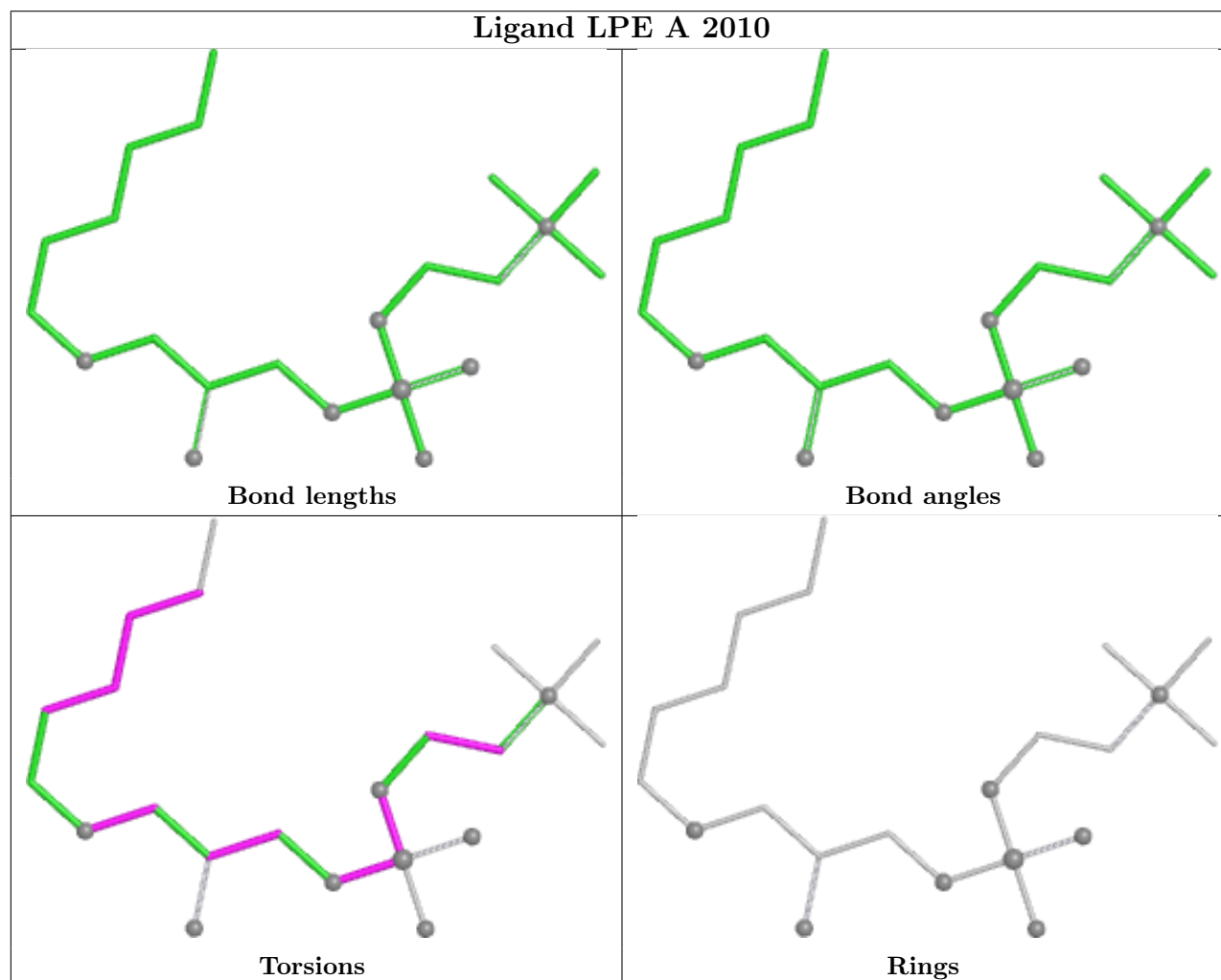
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2010	LPE	8	0
7	A	2015	LPE	2	0
7	A	2008	LPE	1	0
8	A	2029	P5S	5	0
5	A	2028	CLR	18	0
7	A	2009	LPE	4	0
6	A	2016	PCW	12	0
5	A	2005	CLR	3	0
5	A	2017	CLR	11	0
3	A	2003	NAG	2	0
7	A	2022	LPE	1	0
6	A	2018	PCW	3	0
7	A	2023	LPE	4	0
4	A	2004	95T	11	0
7	A	2025	LPE	2	0
6	A	2013	PCW	8	0
6	A	2007	PCW	3	0
6	A	2019	PCW	15	0
3	A	2001	NAG	3	0
7	A	2020	LPE	1	0
7	A	2012	LPE	5	0
7	A	2011	LPE	15	0
6	A	2006	PCW	17	0
6	A	2026	PCW	6	0
5	A	2027	CLR	5	0
7	A	2014	LPE	4	0

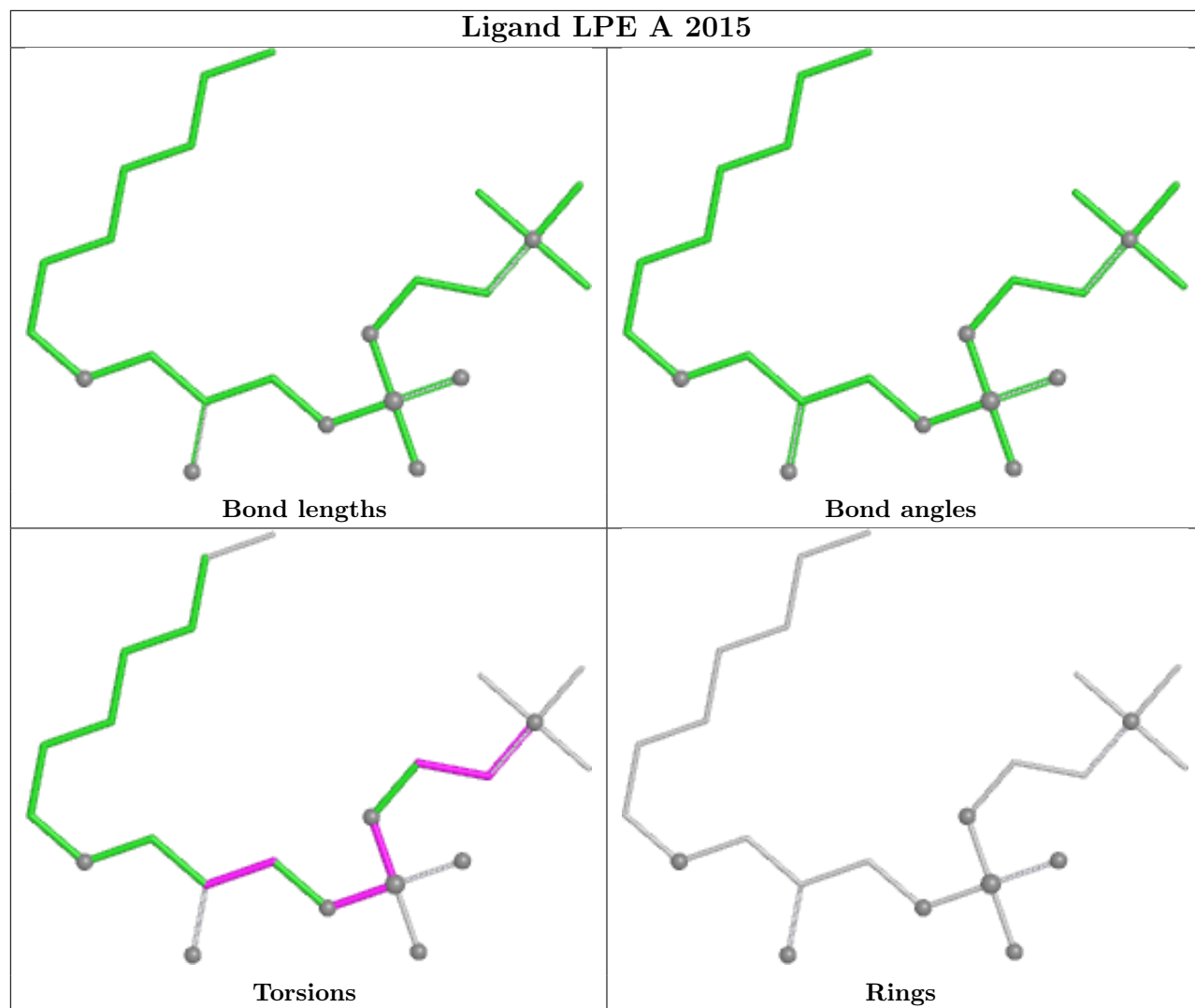
Continued on next page...

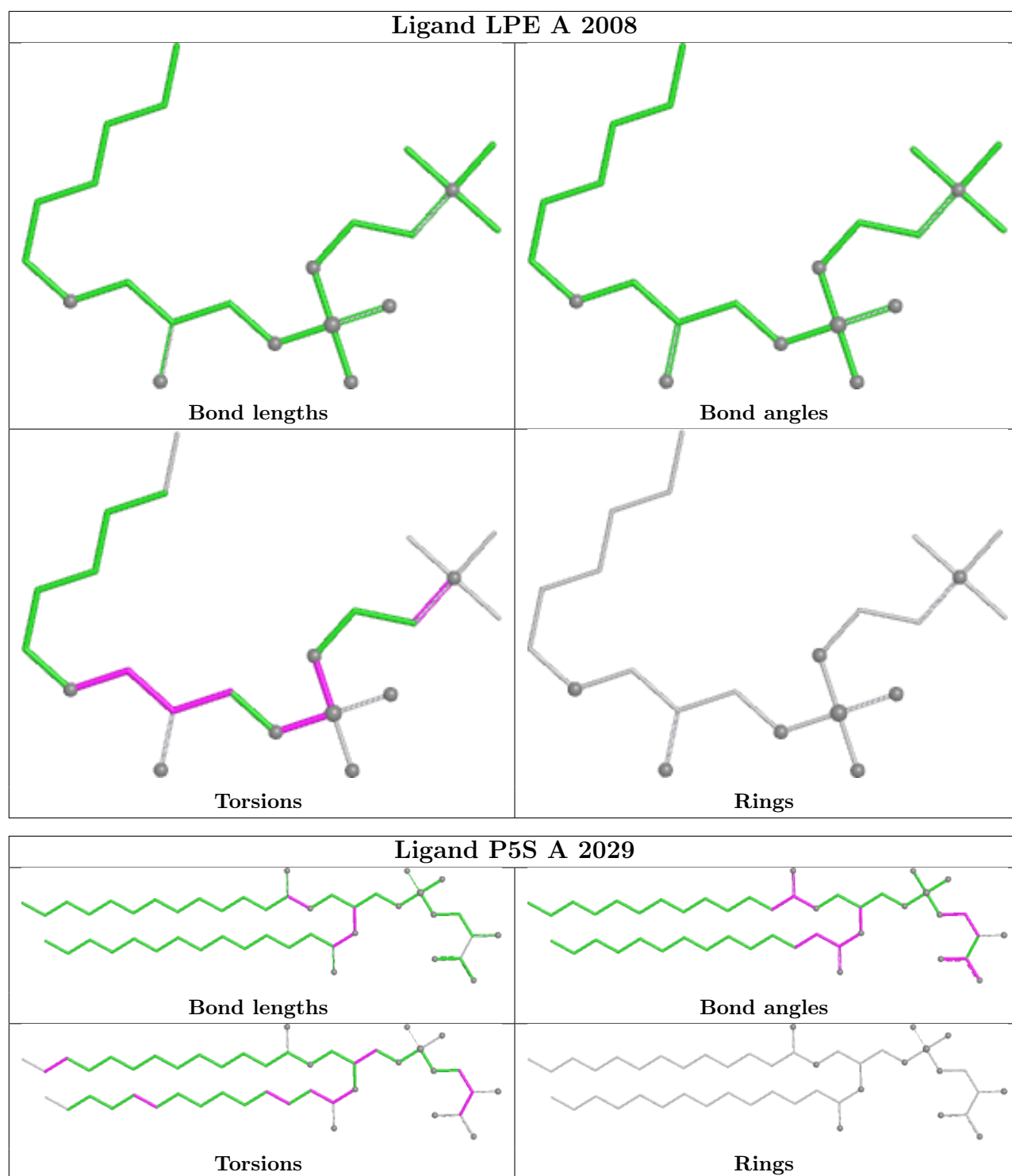
Continued from previous page...

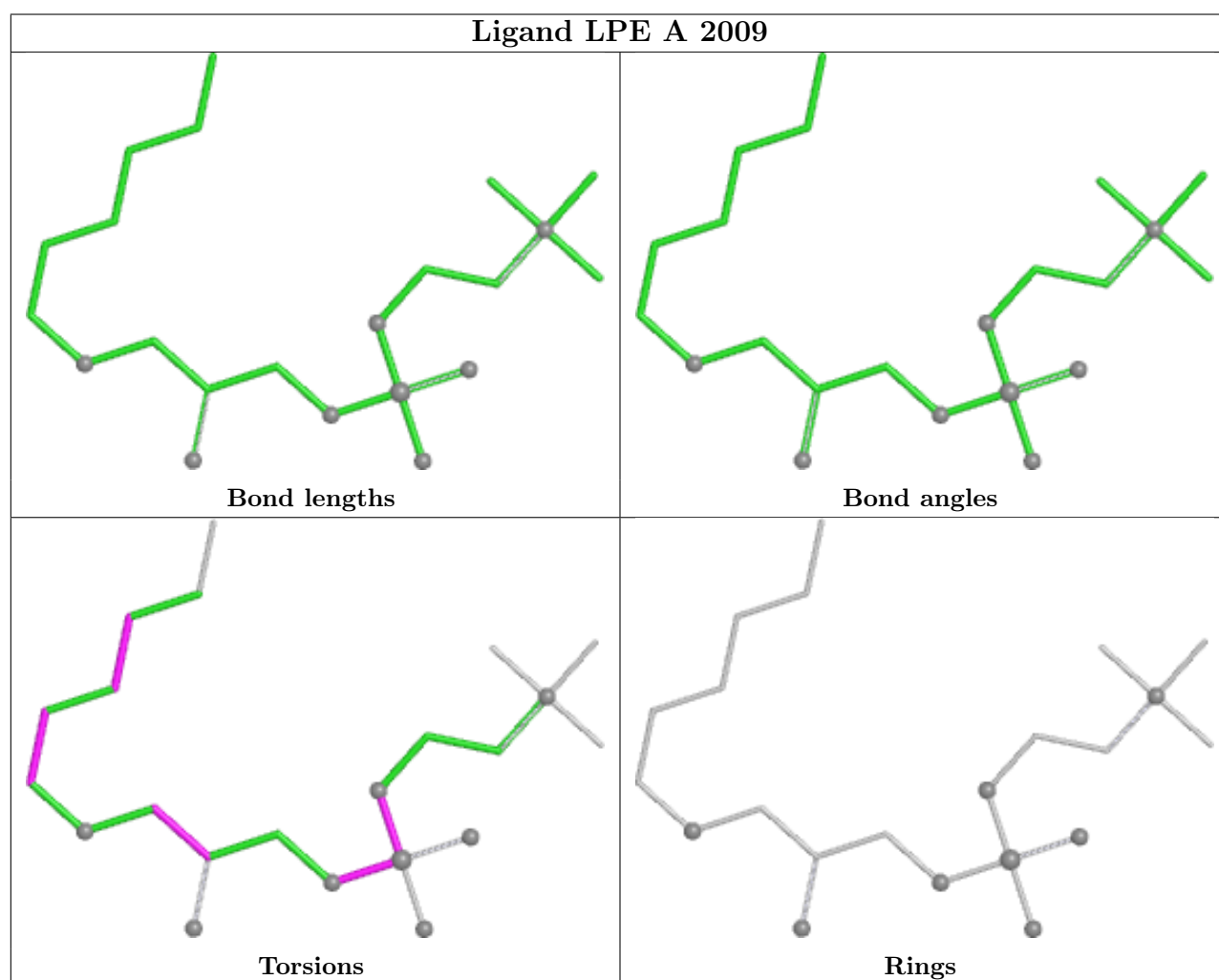
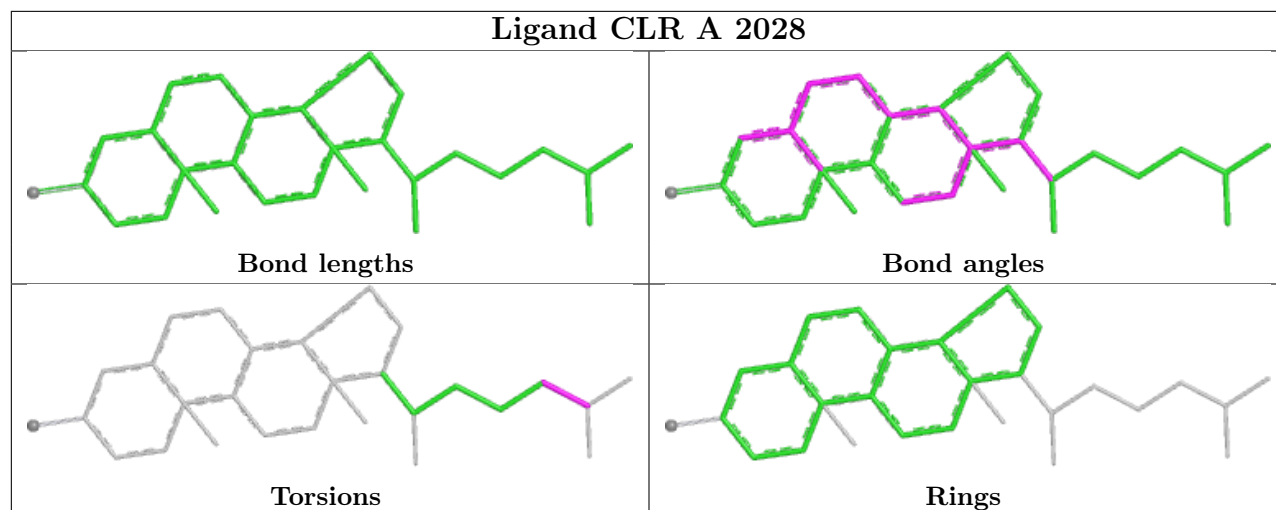
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2021	CLR	2	0

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.

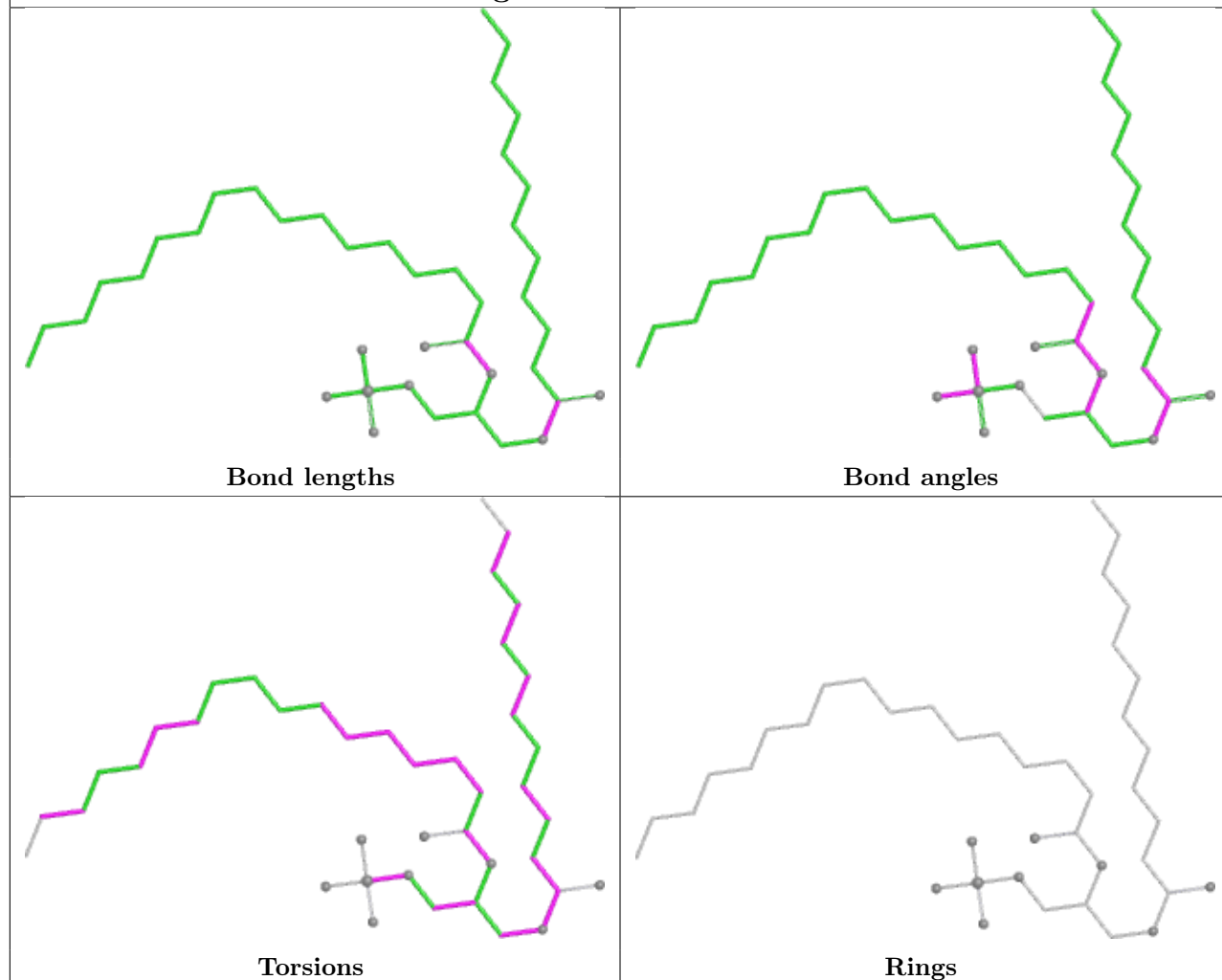




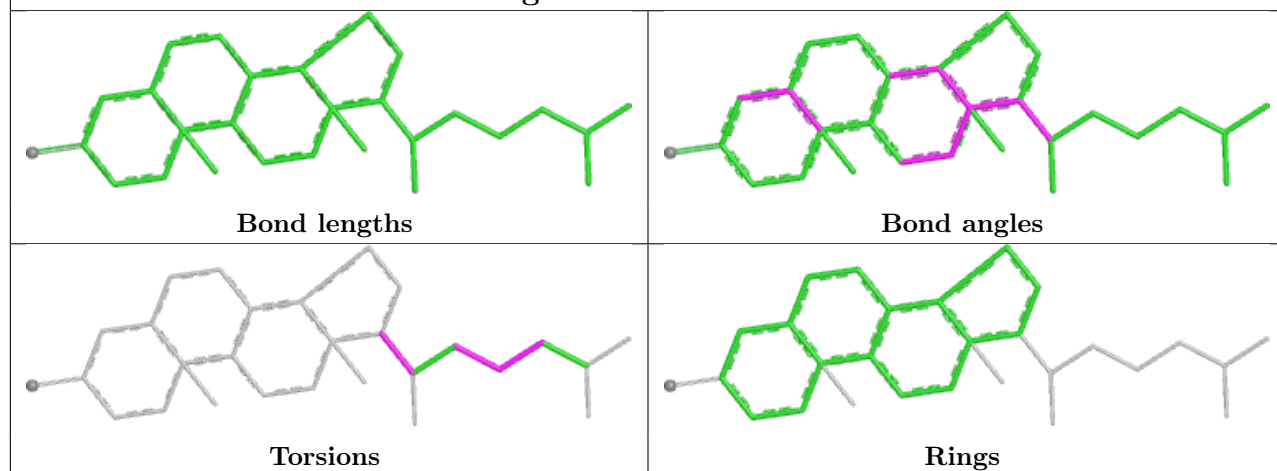


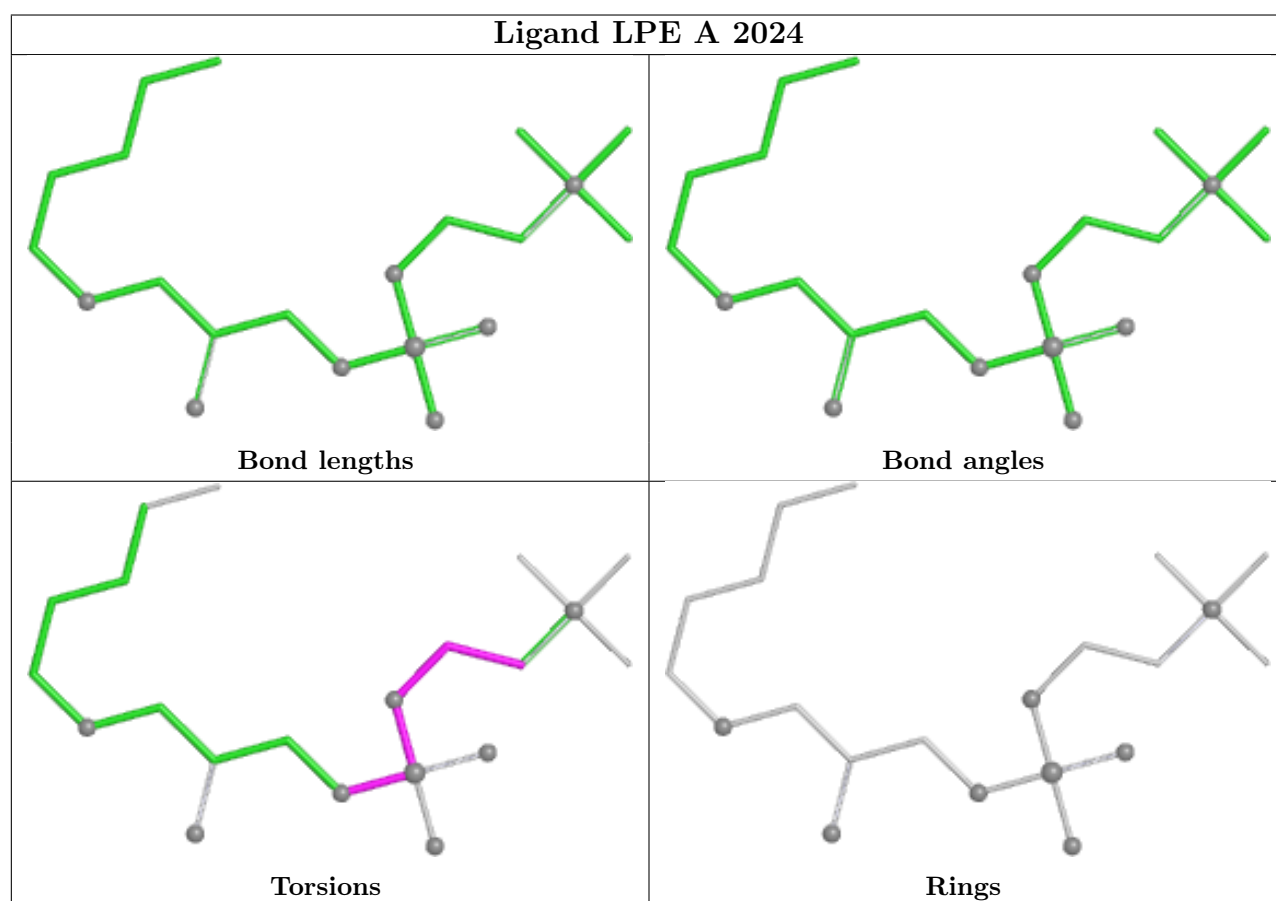
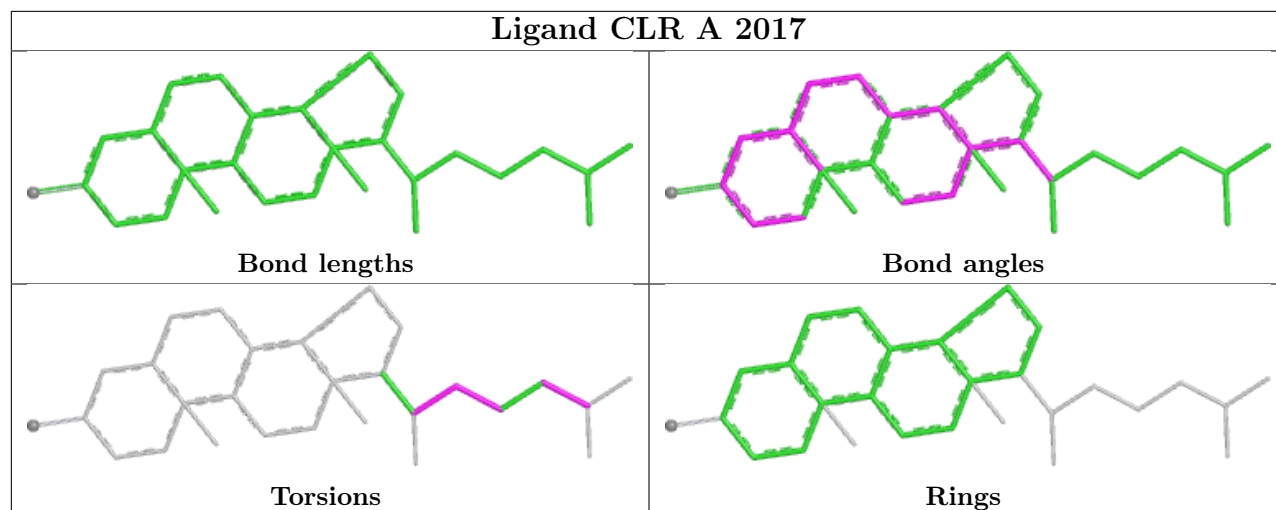


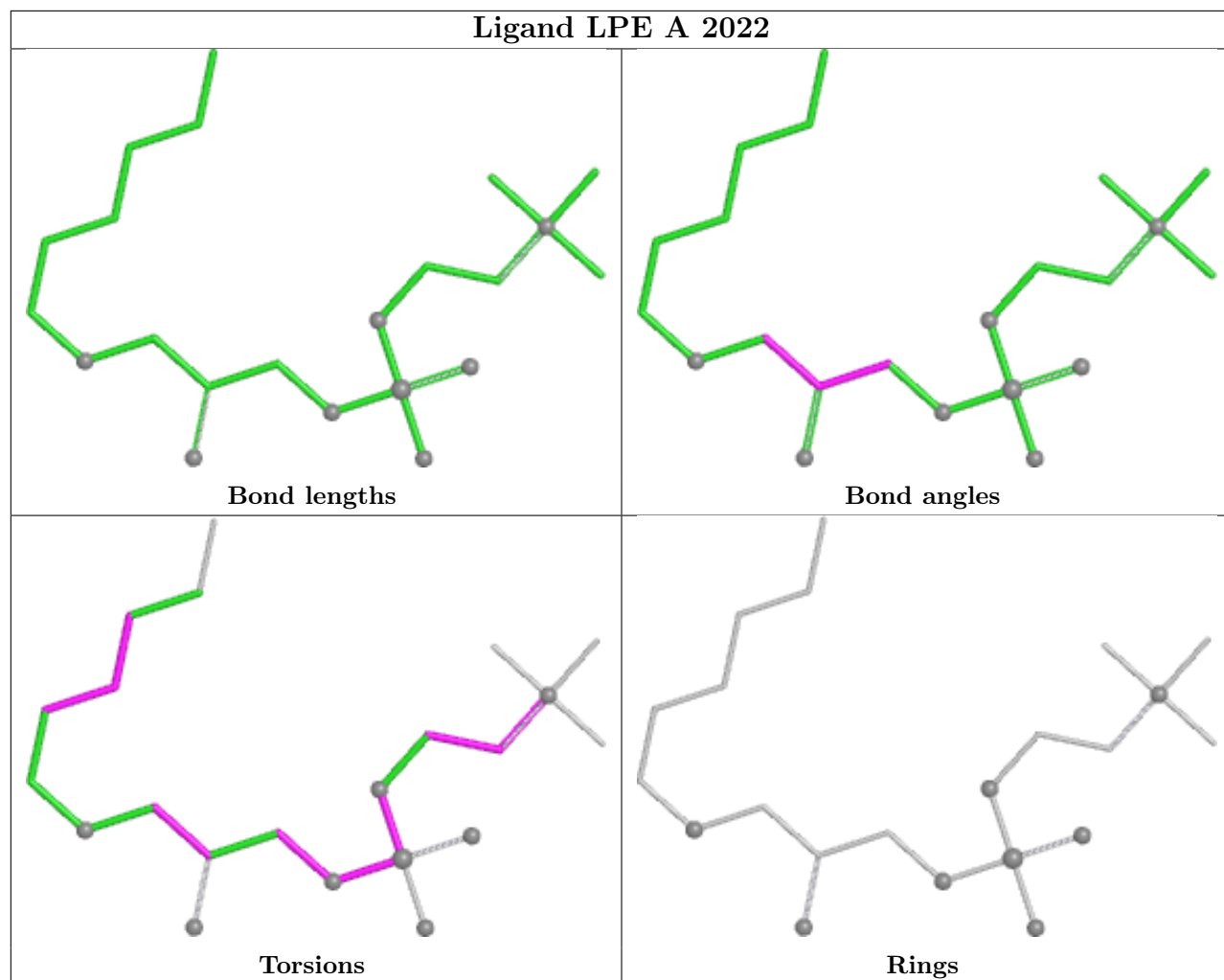
Ligand PCW A 2016

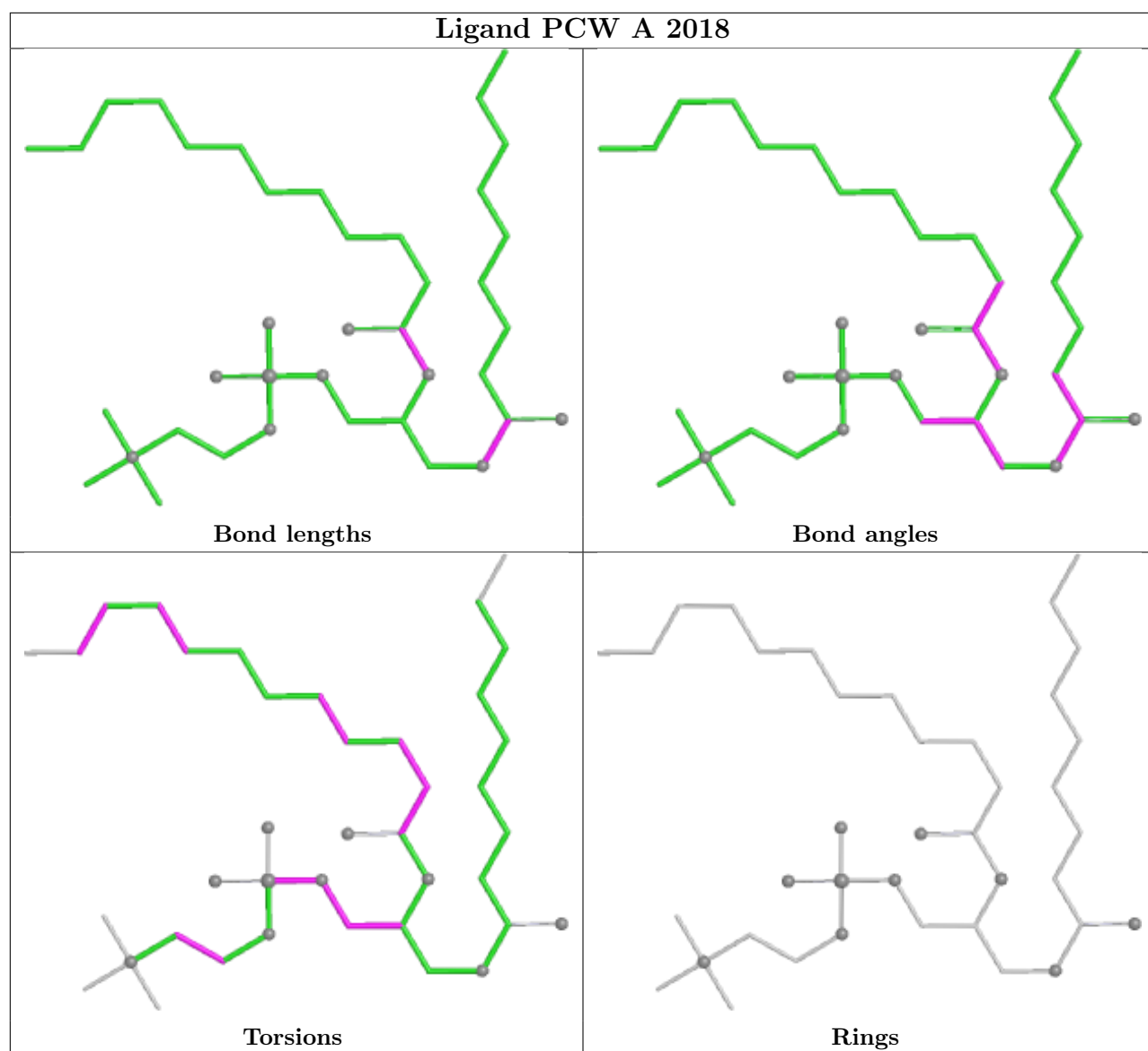


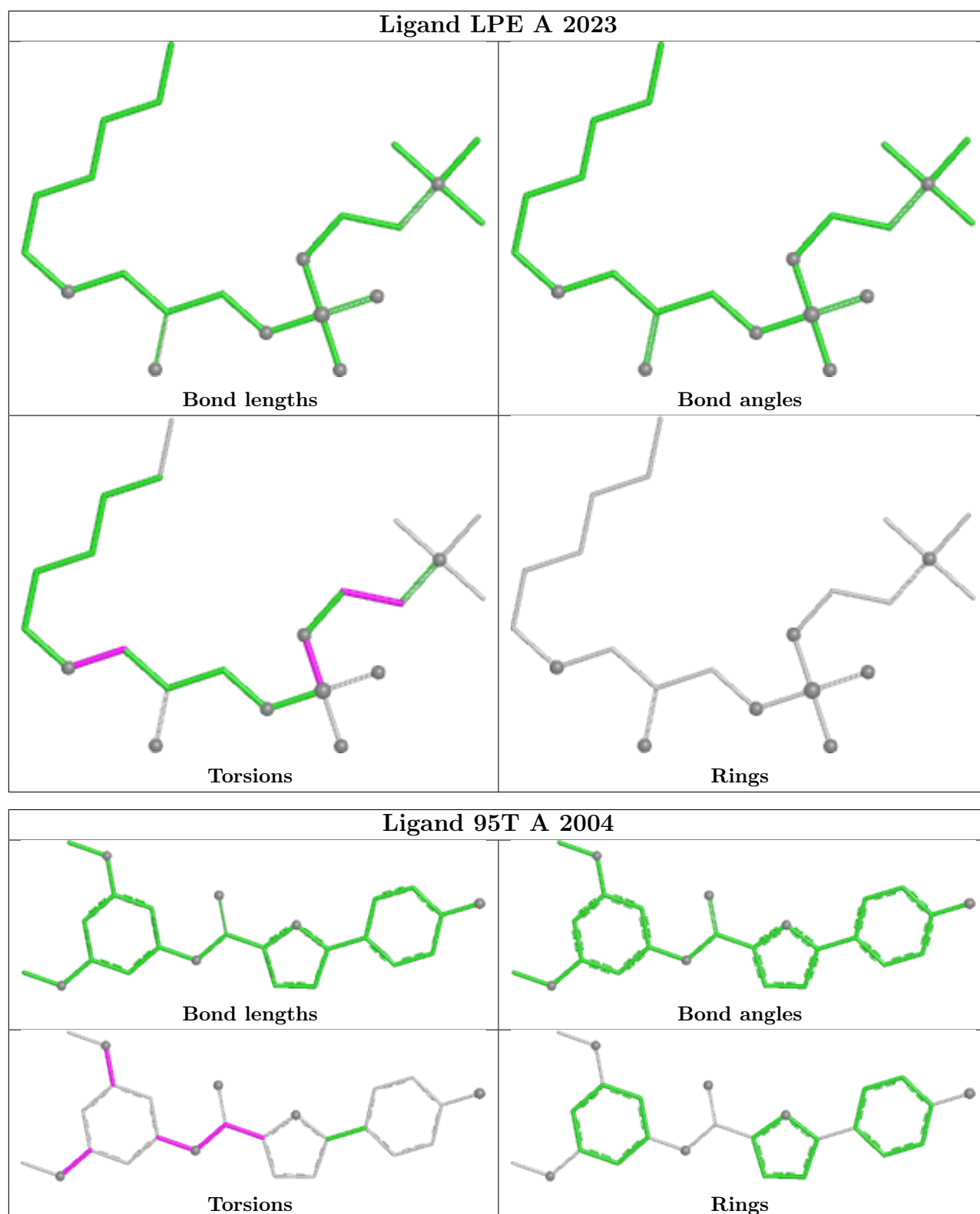
Ligand CLR A 2005

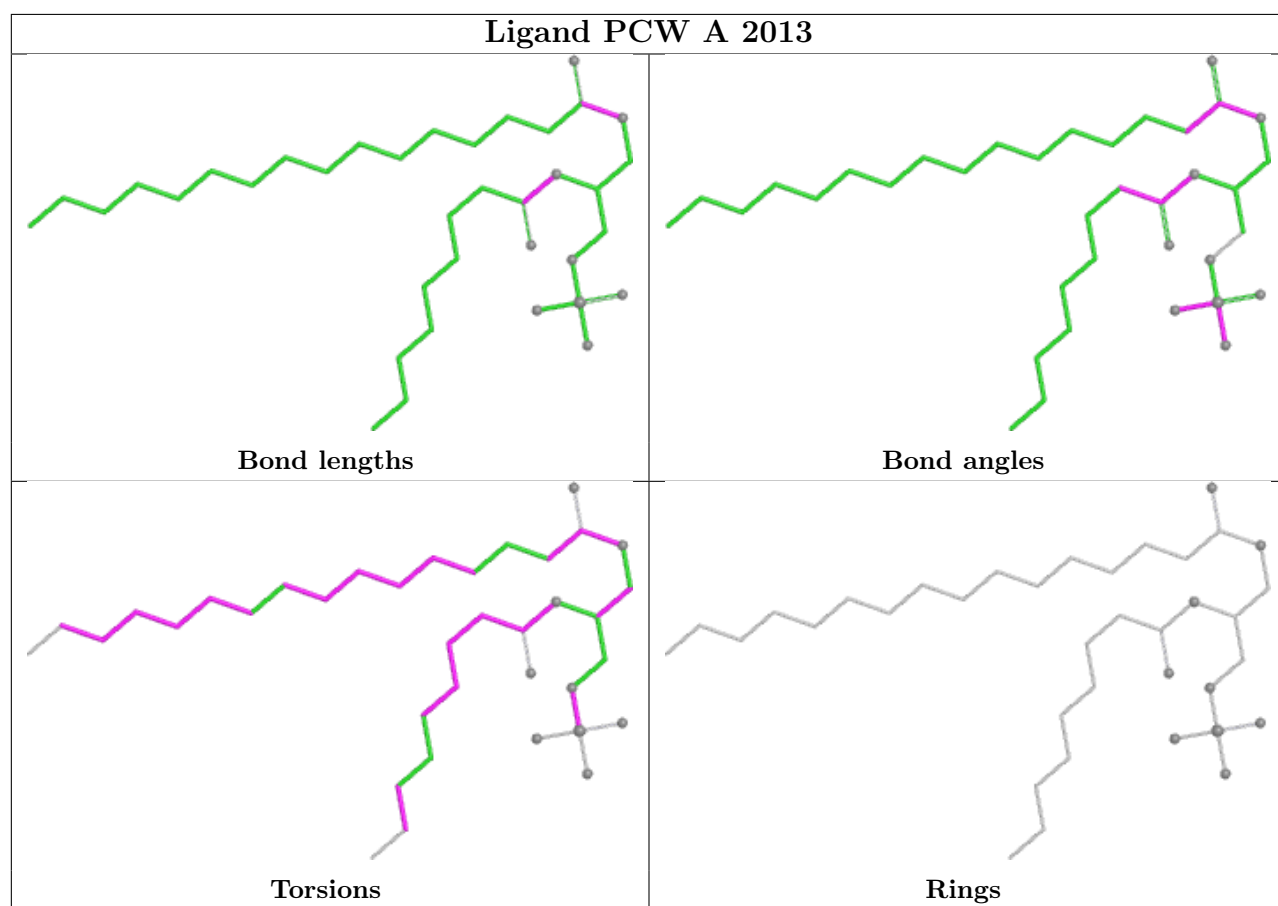
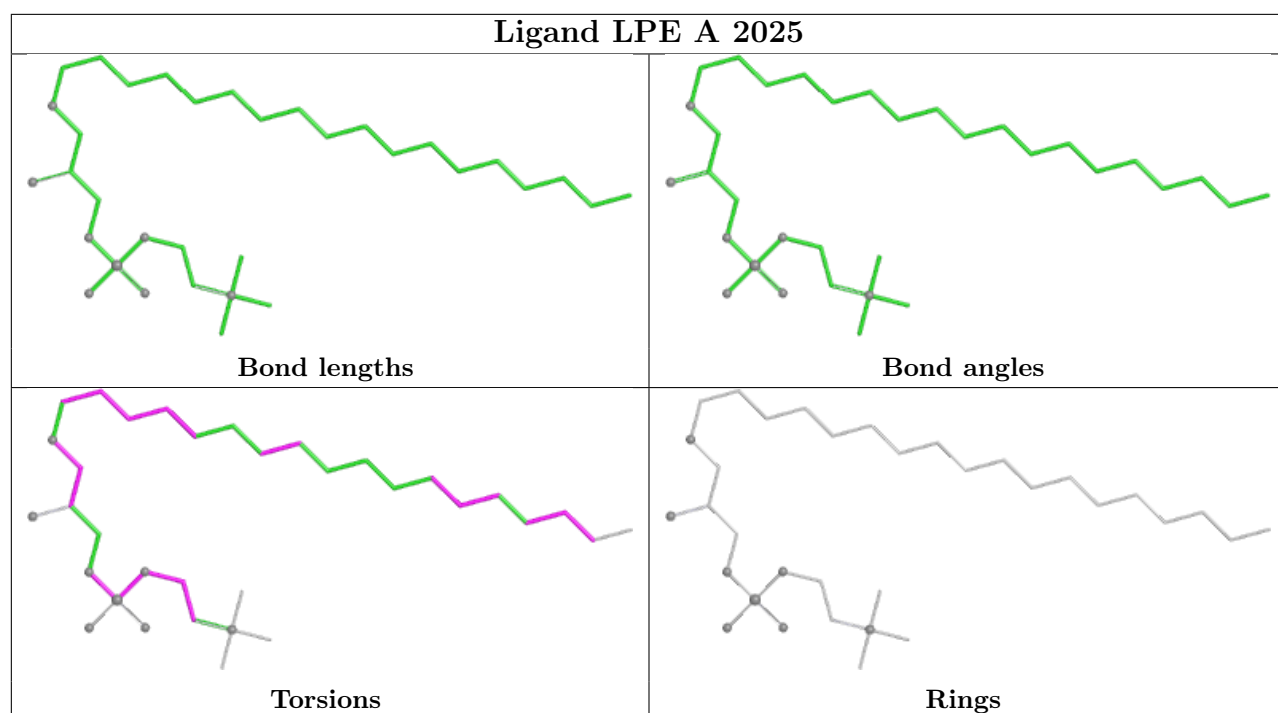


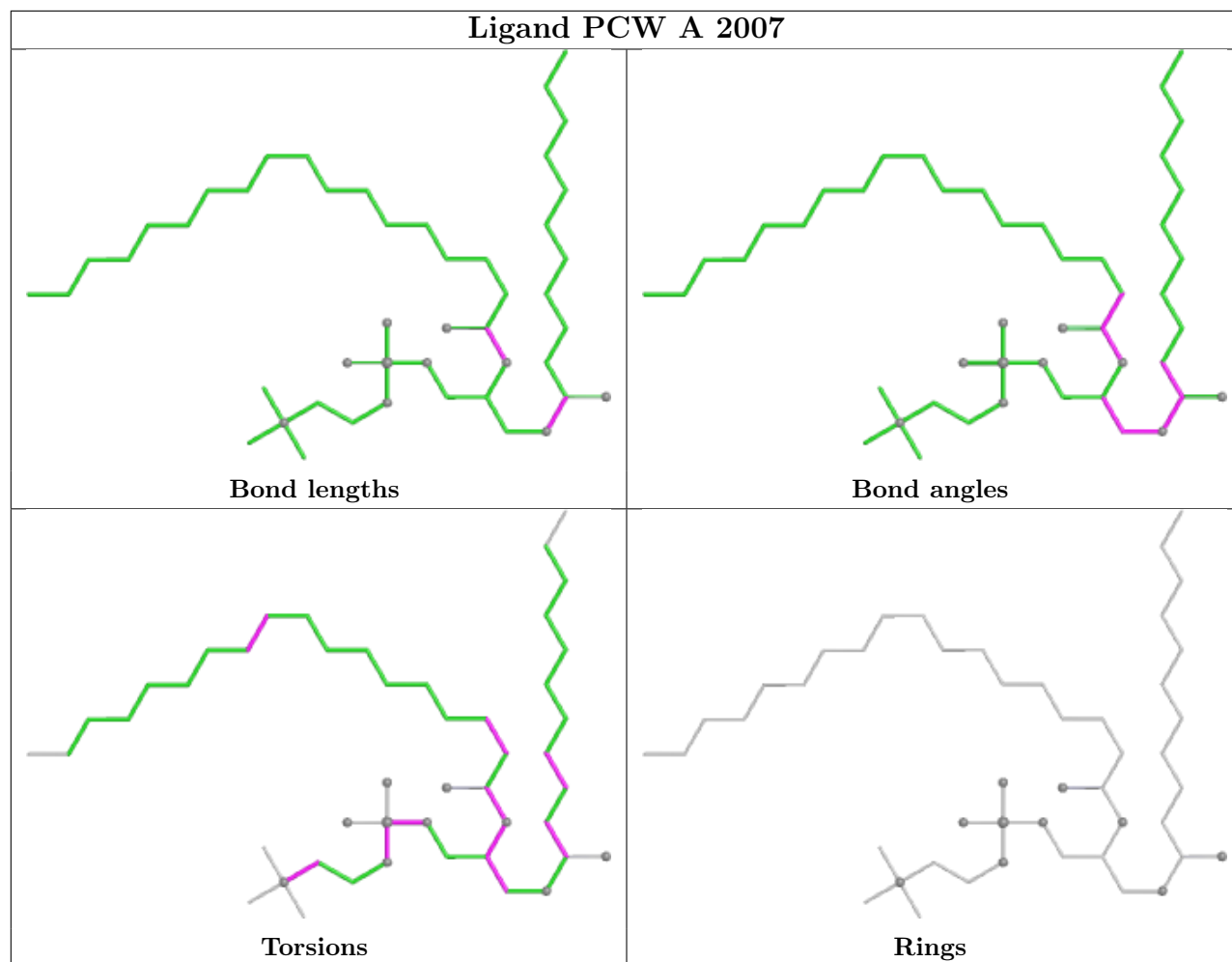


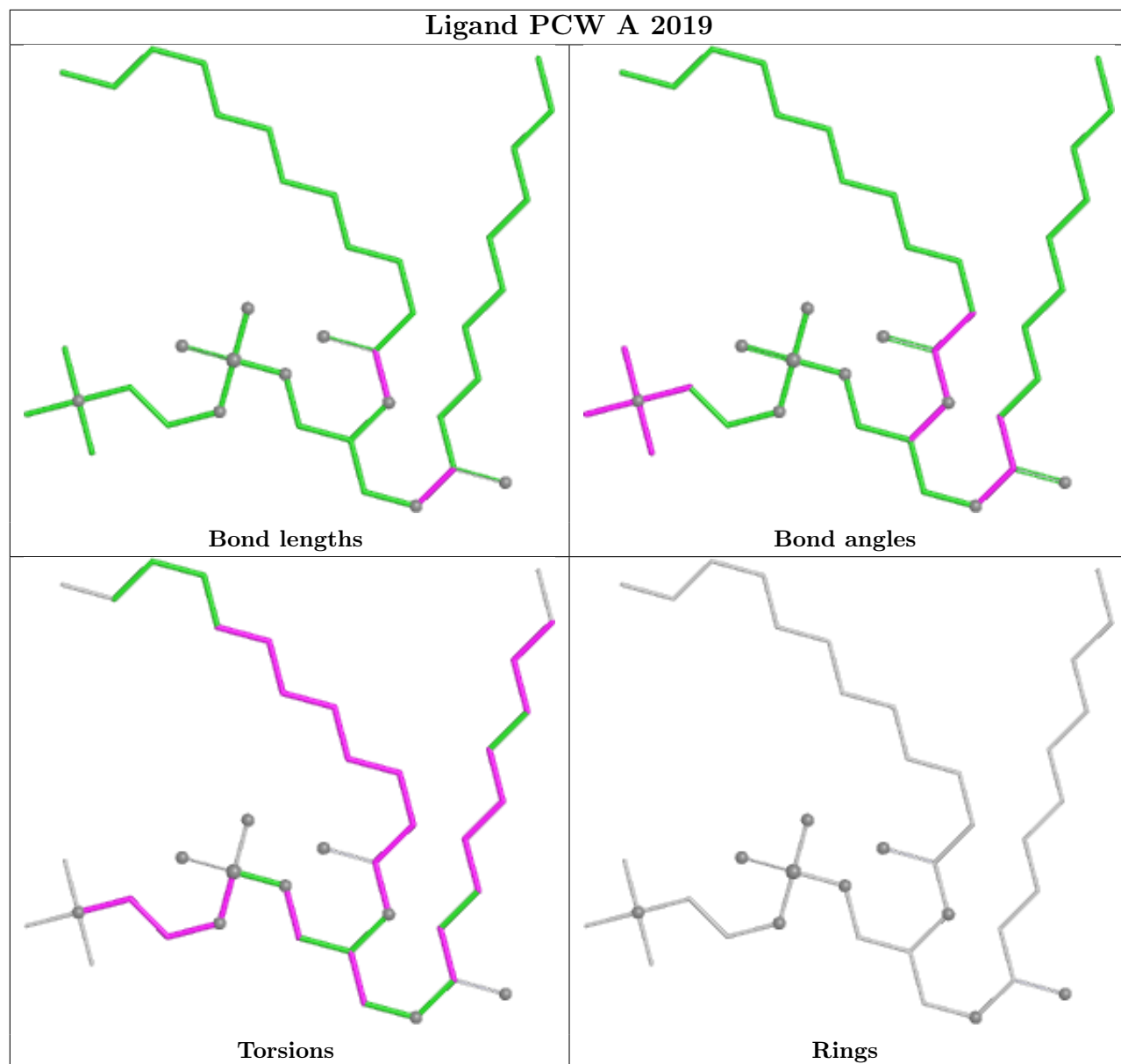


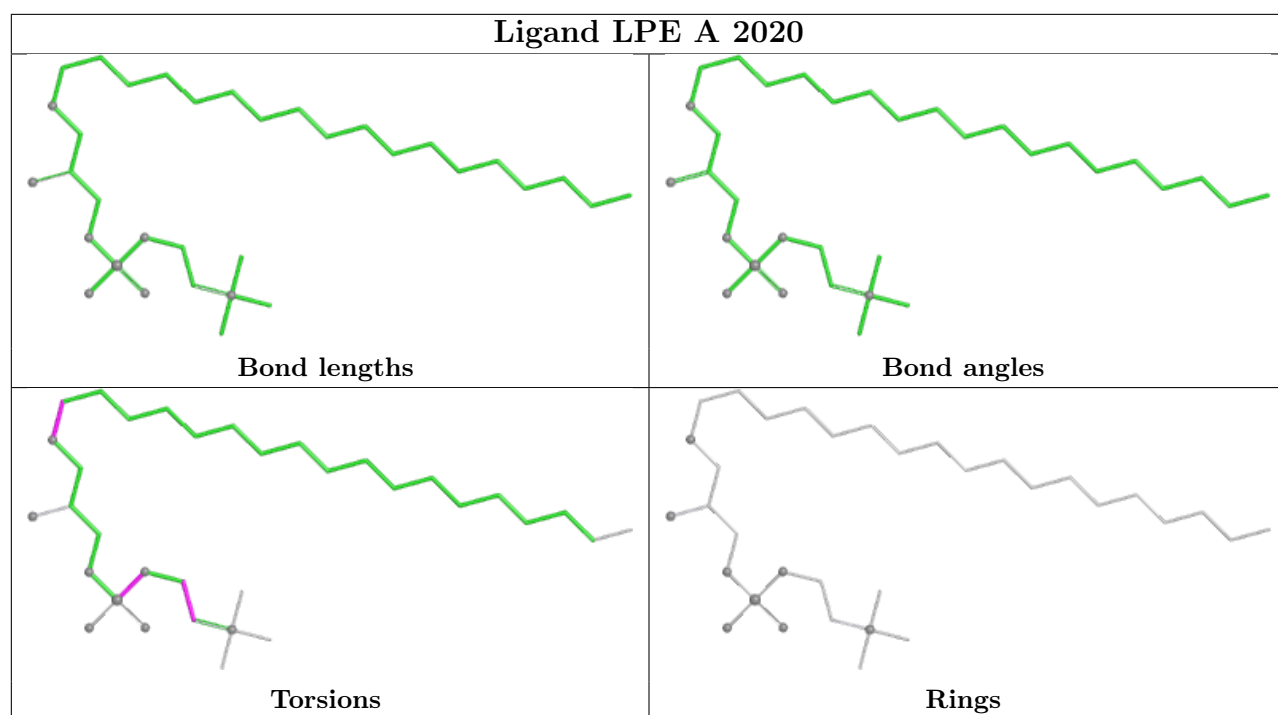


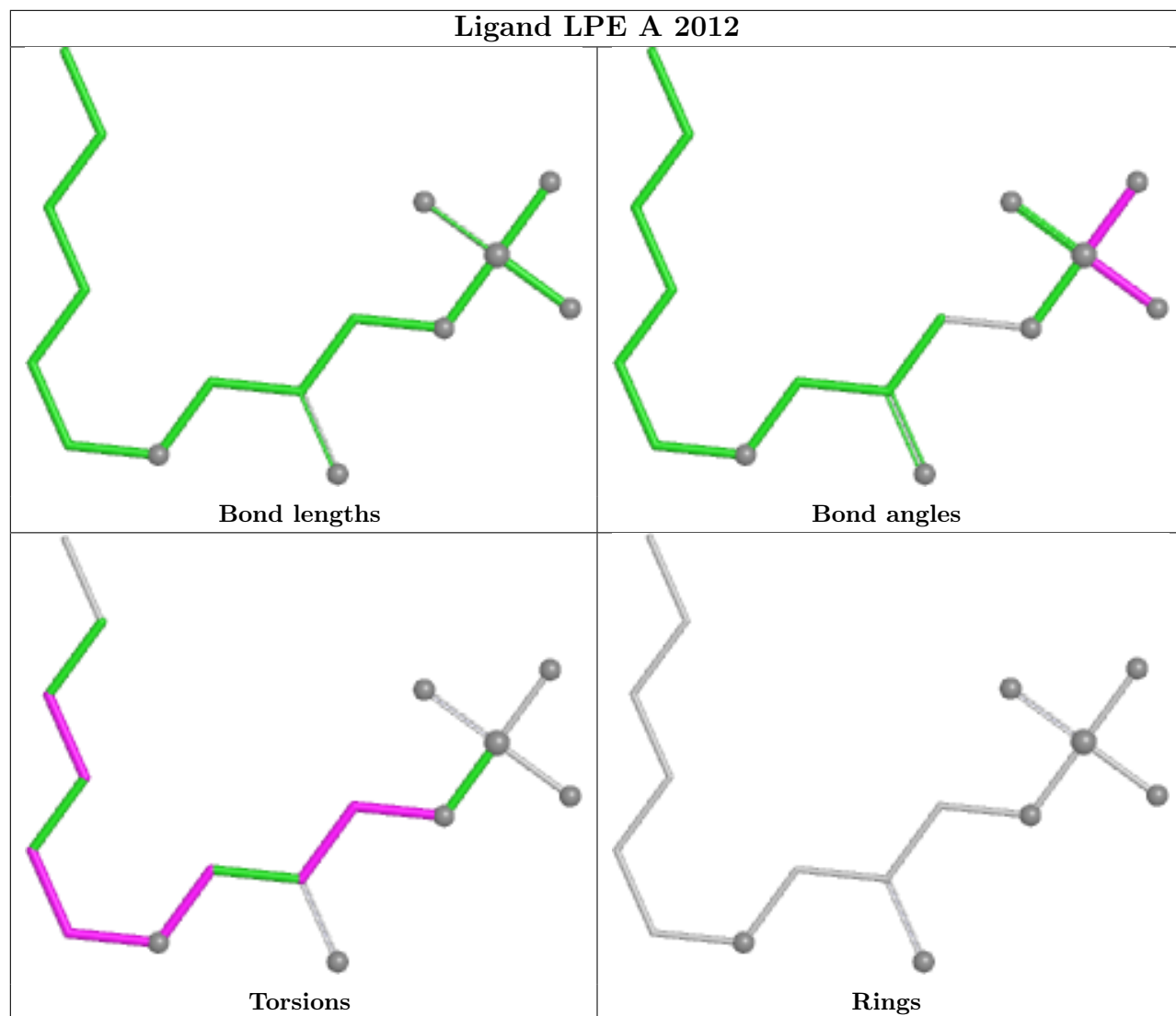


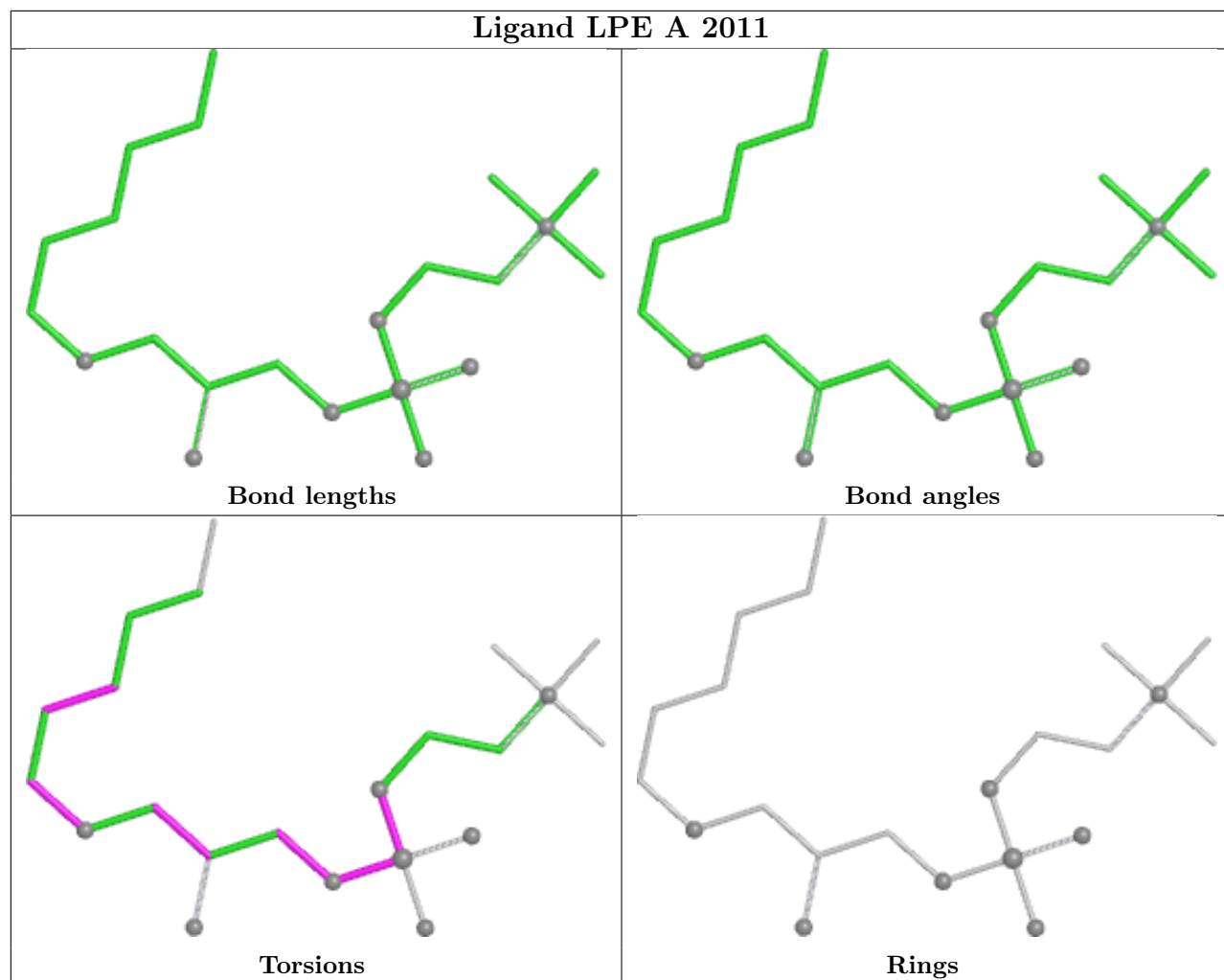


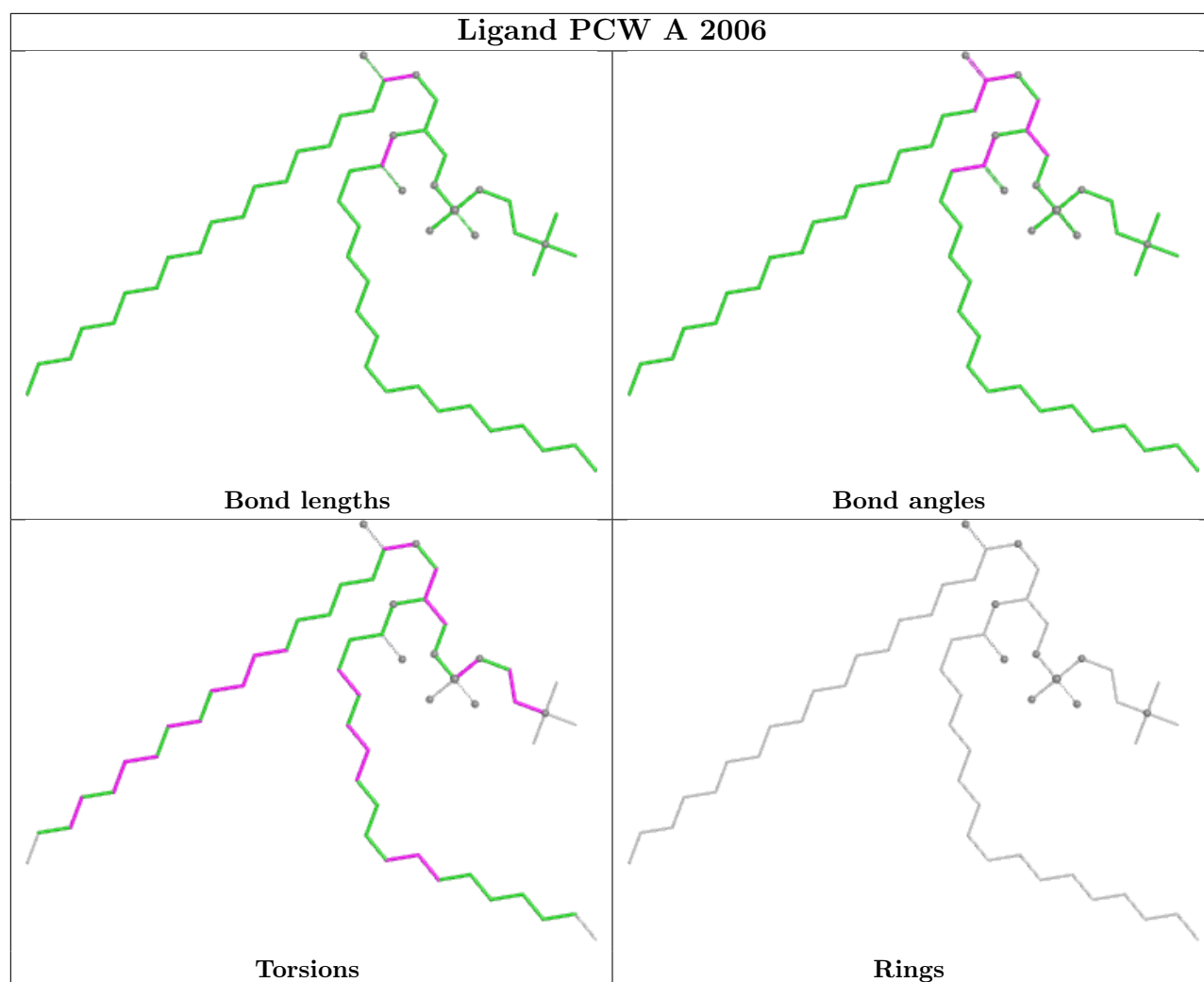




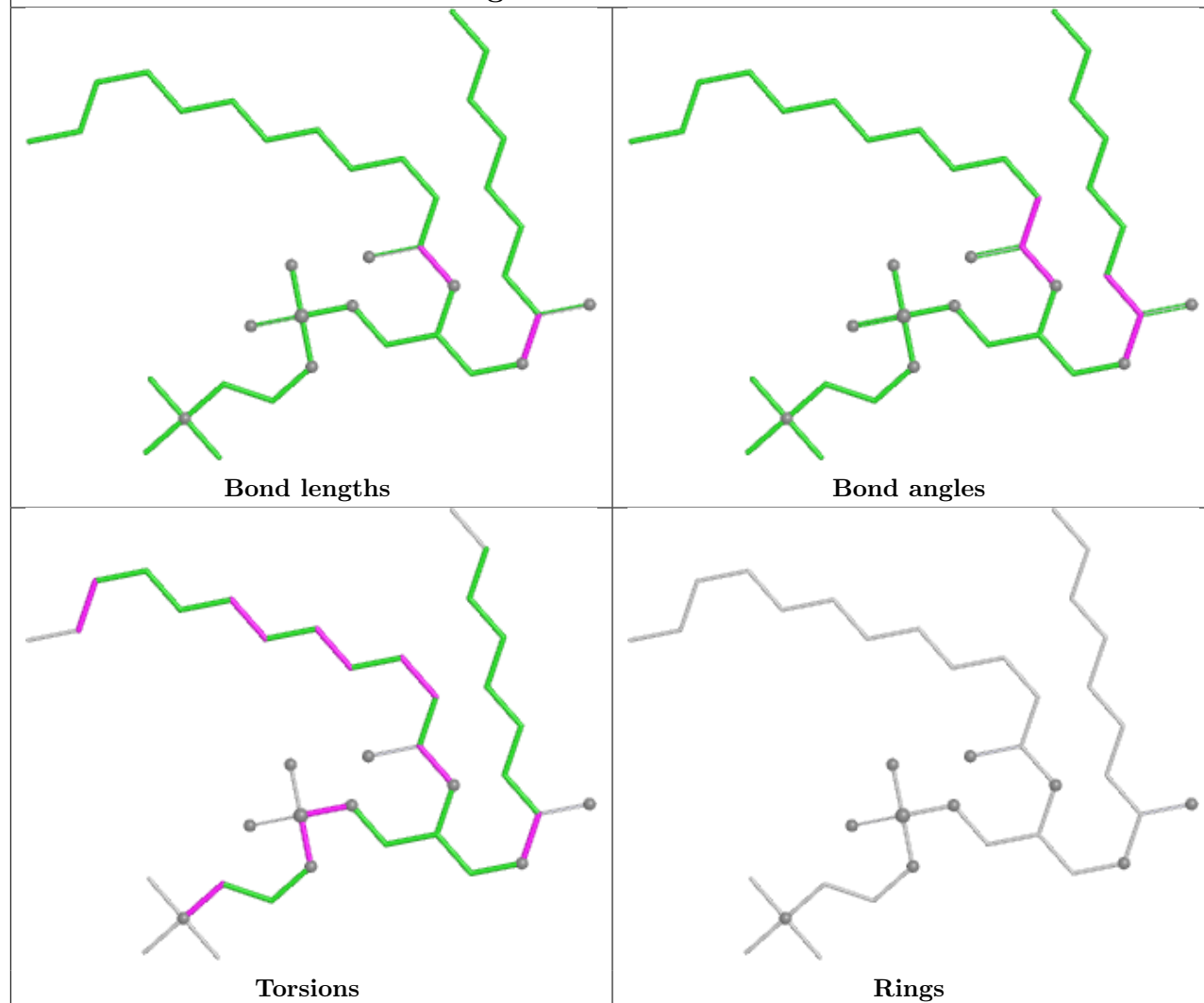




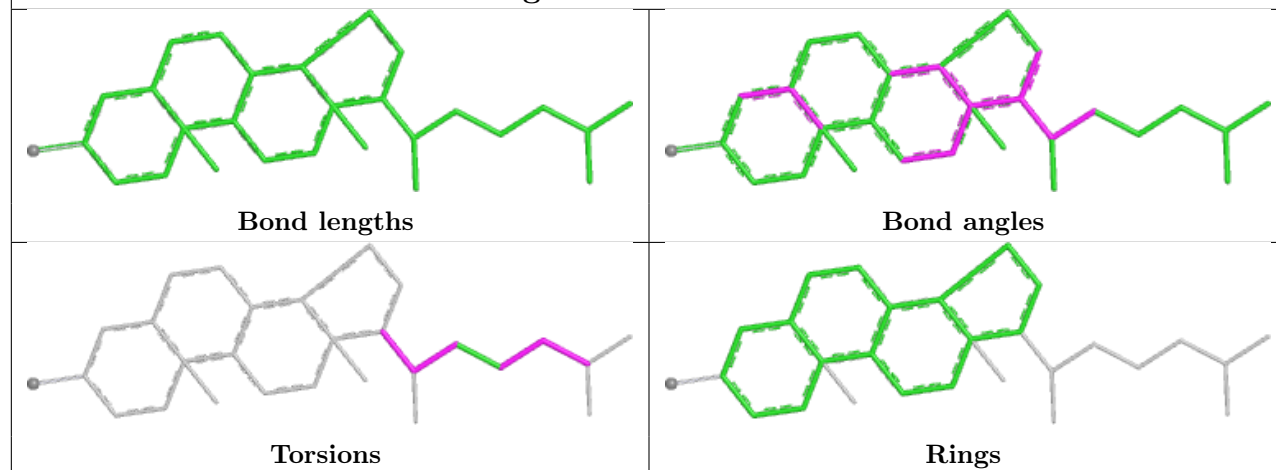


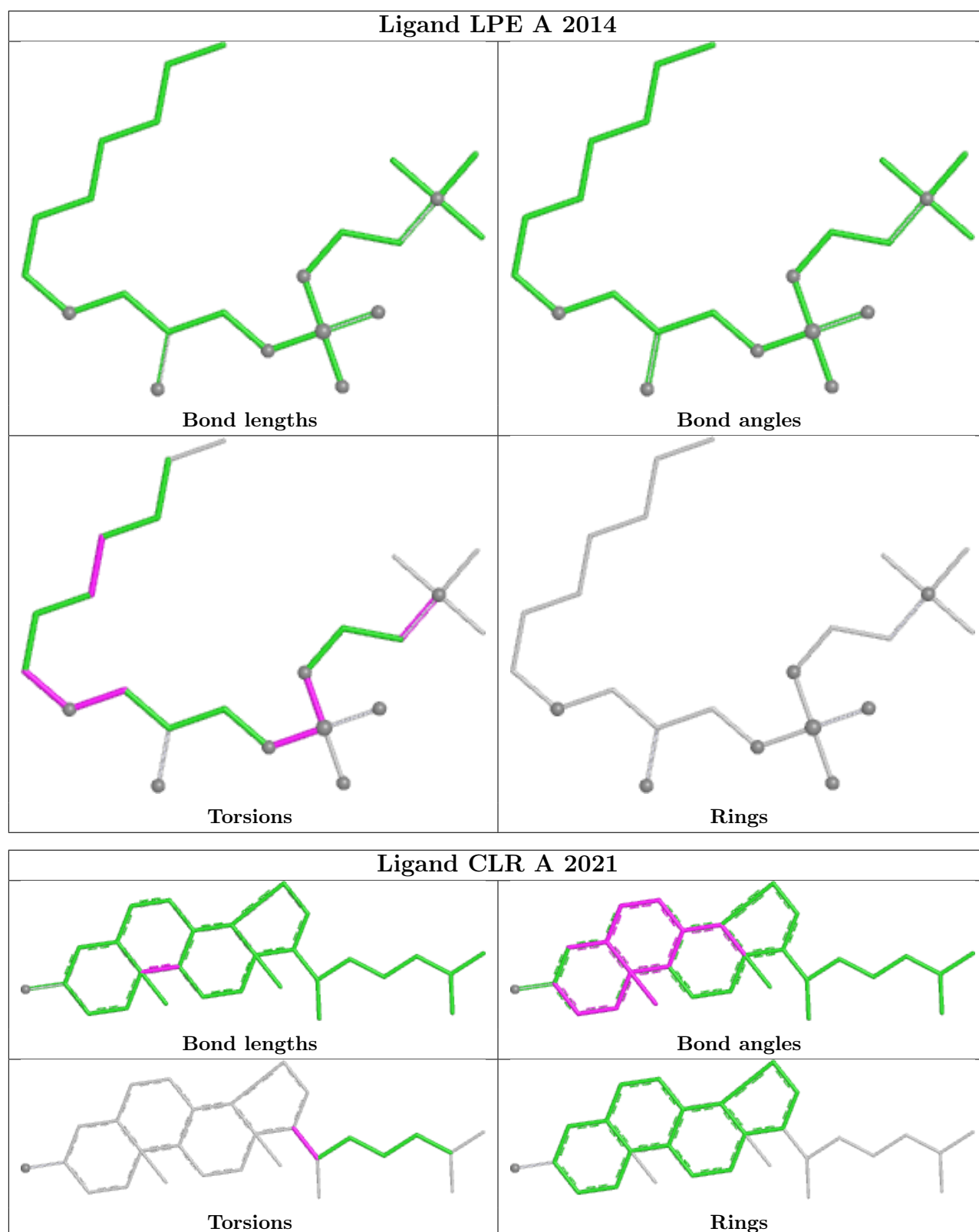


Ligand PCW A 2026



Ligand CLR A 2027





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

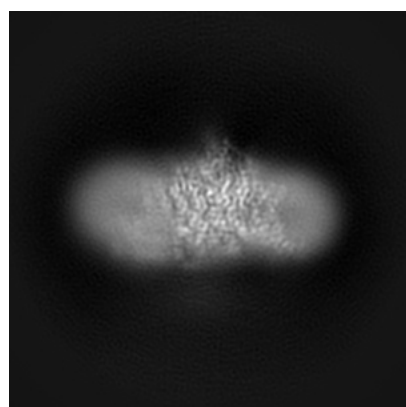
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32475. These allow visual inspection of the internal detail of the map and identification of artifacts.

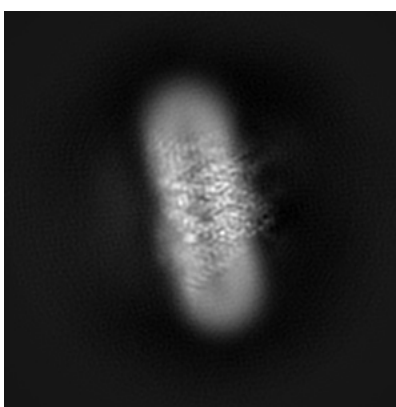
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

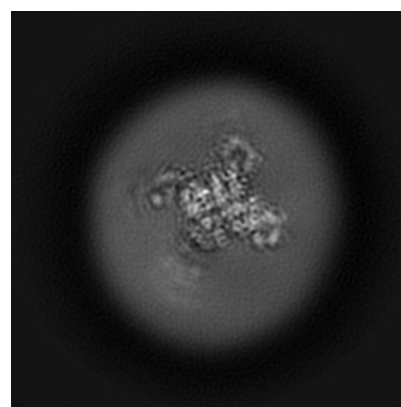
6.1.1 Primary map



X



Y

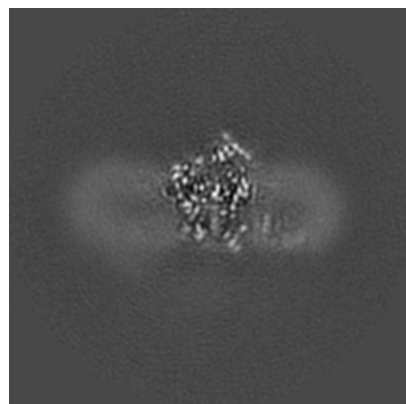


Z

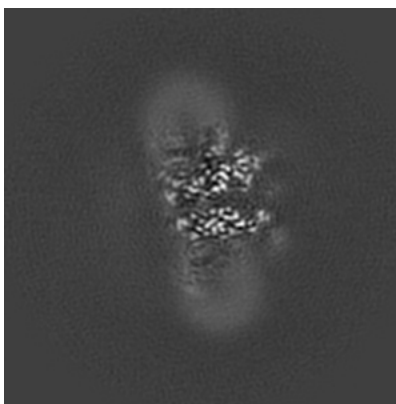
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

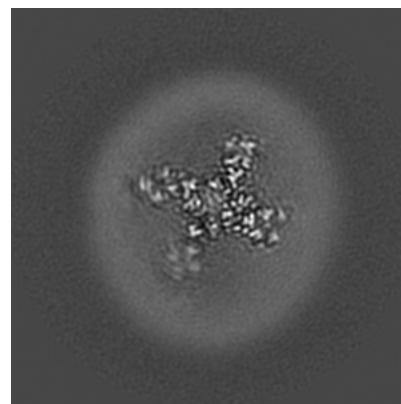
6.2.1 Primary map



X Index: 120



Y Index: 120

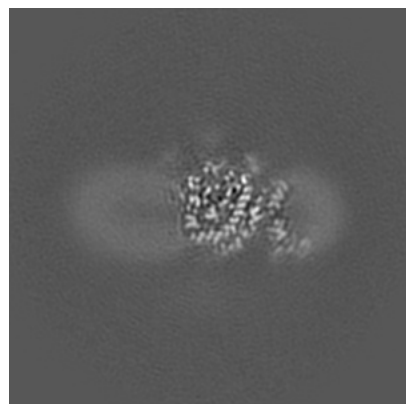


Z Index: 120

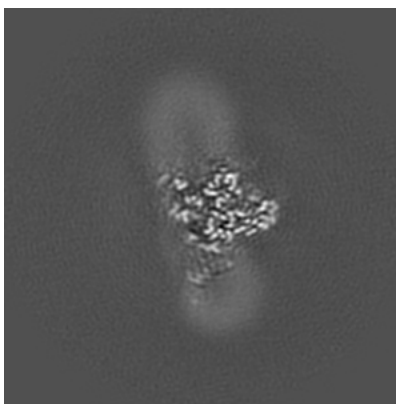
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

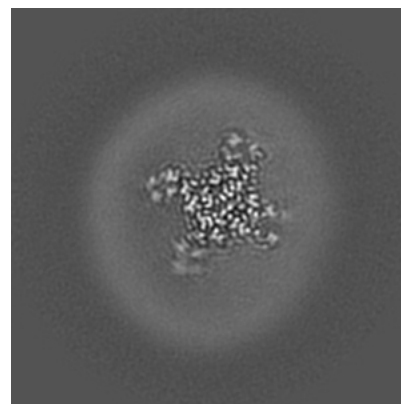
6.3.1 Primary map



X Index: 134



Y Index: 130

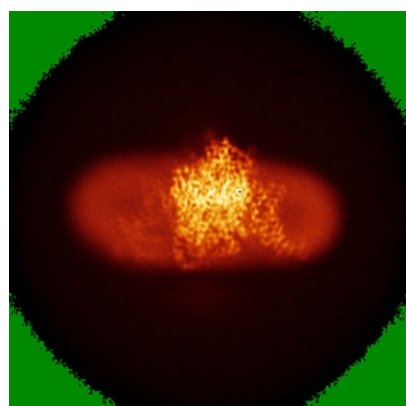


Z Index: 126

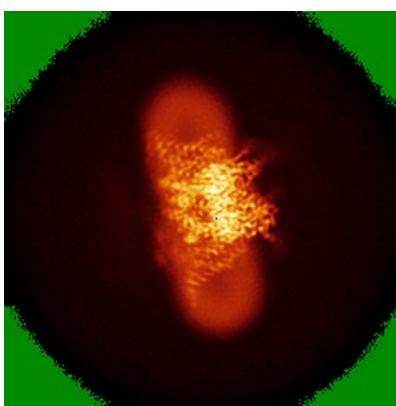
The images above show the largest variance slices of the map in three orthogonal directions.

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

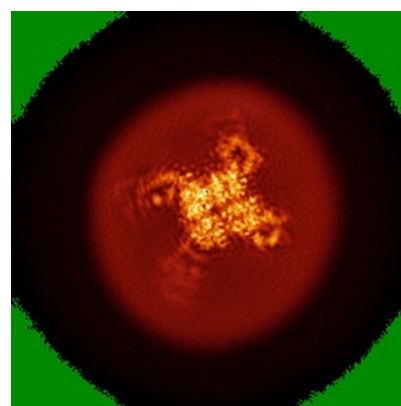
6.4.1 Primary map



X



Y

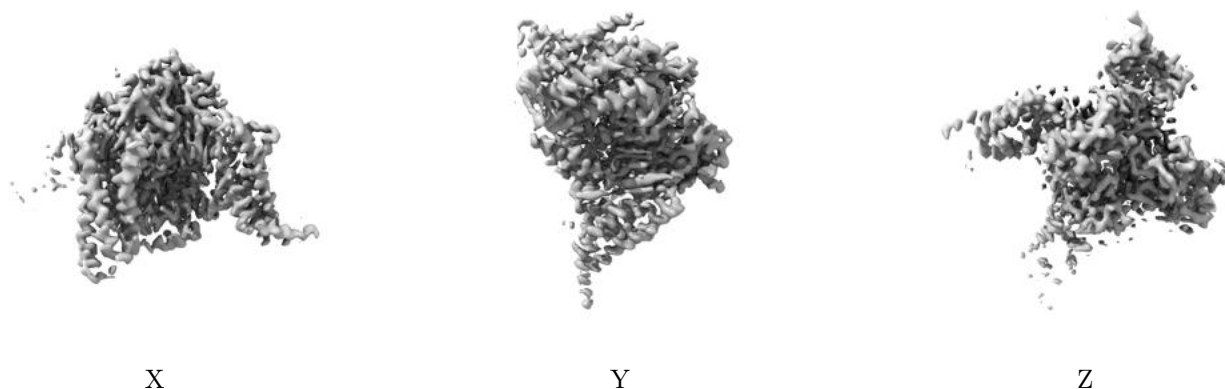


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0217. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

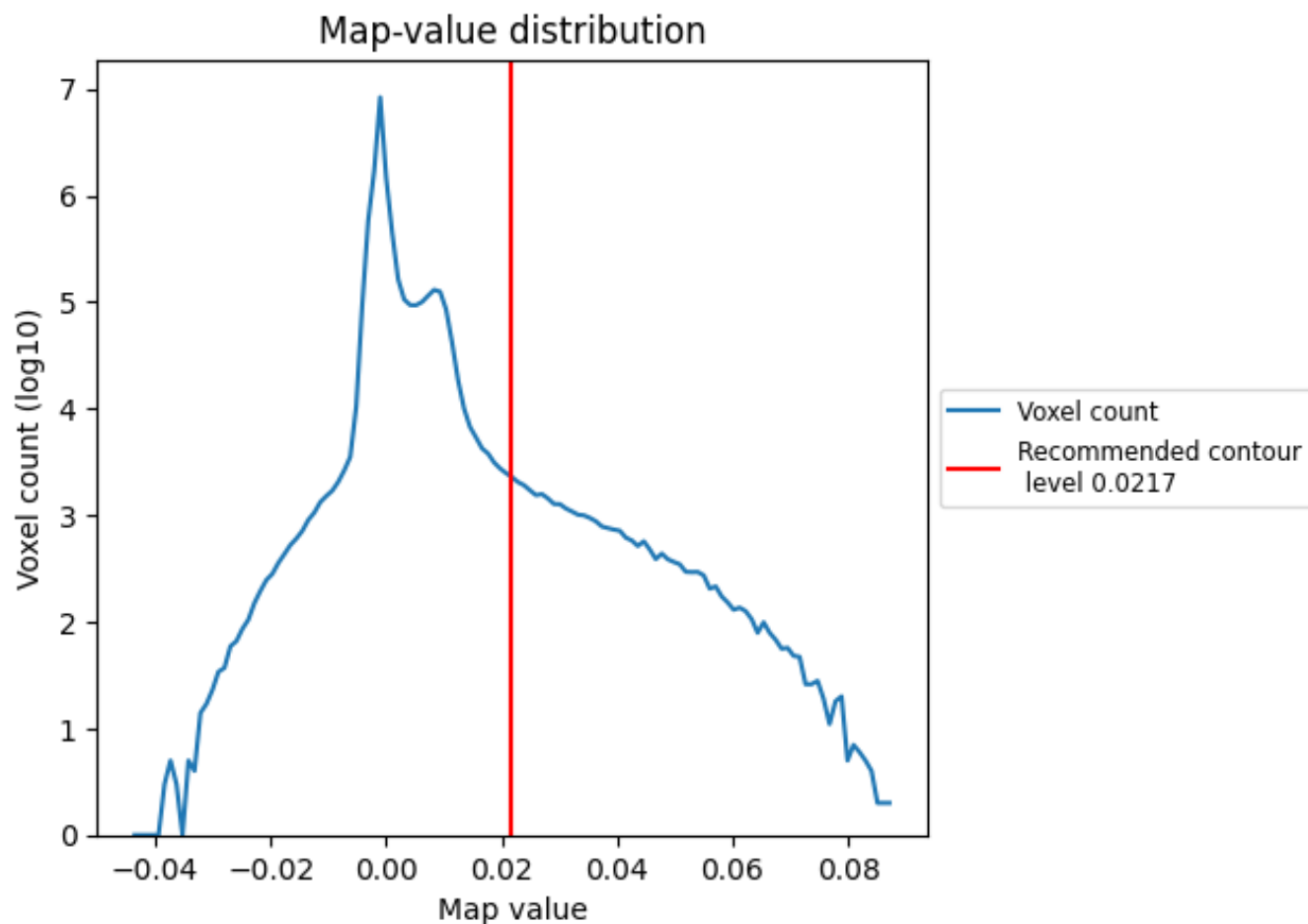
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

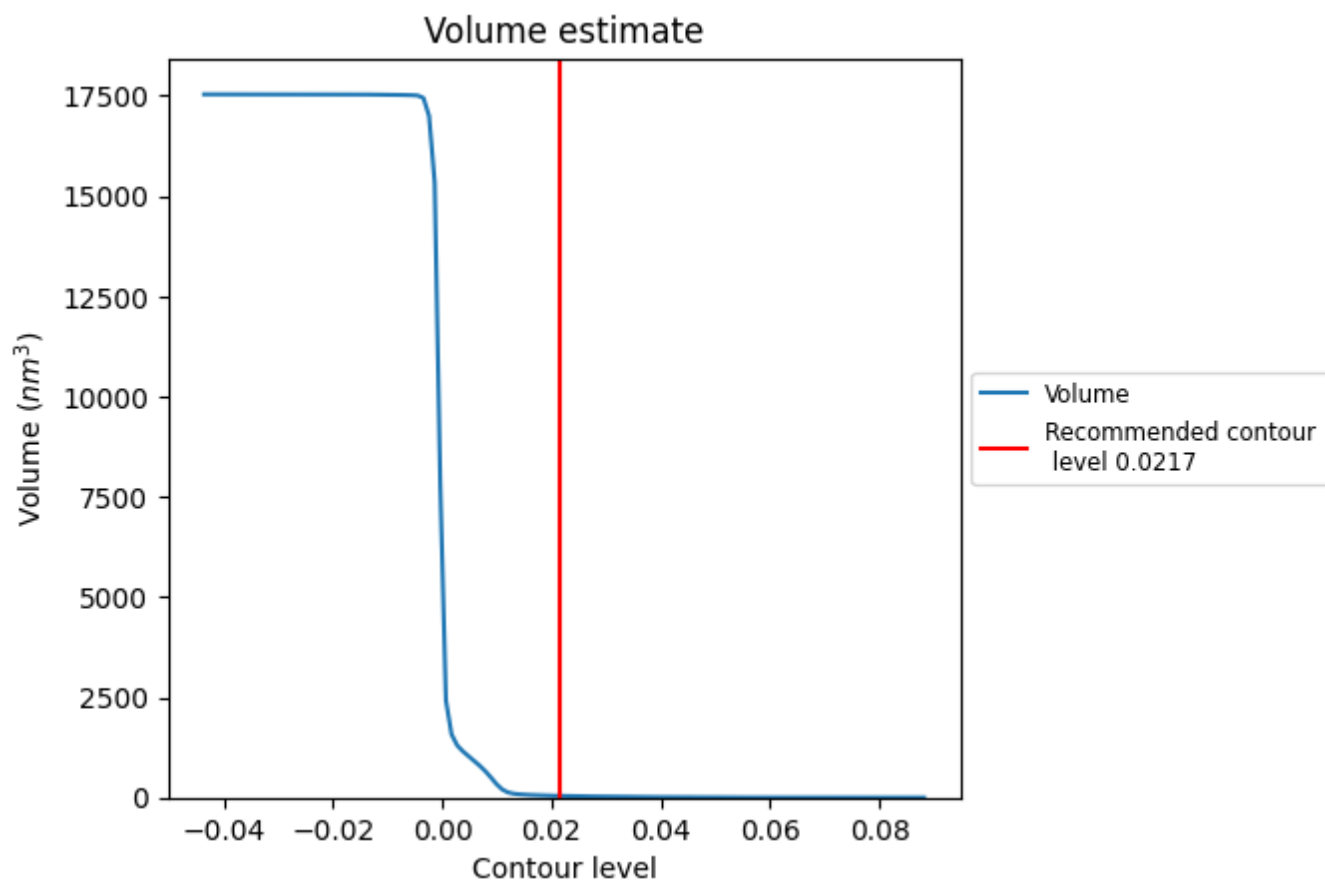
This section contains the results of statistical analysis of the map.

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.

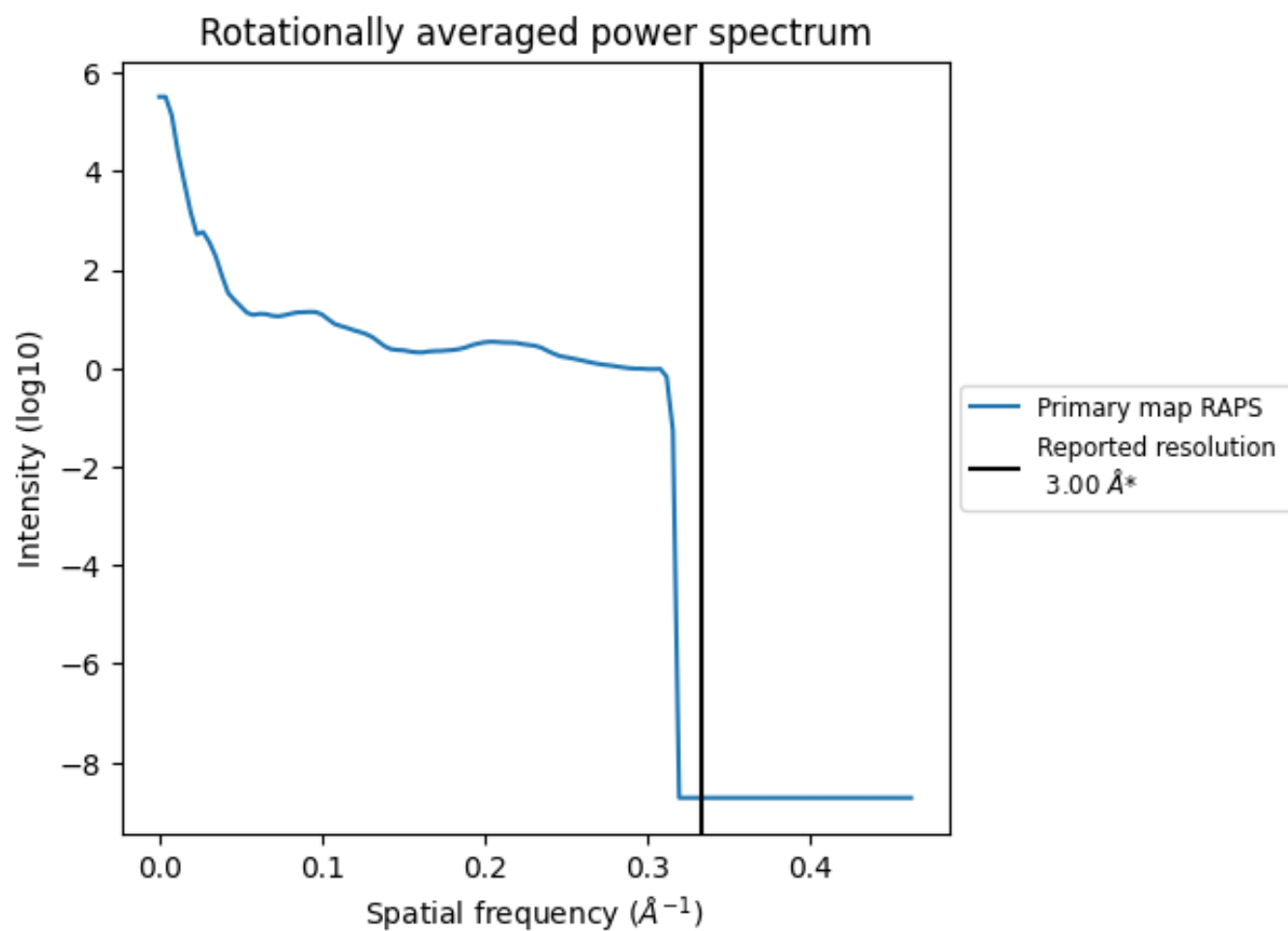
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 41 nm³; this corresponds to an approximate mass of 37 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

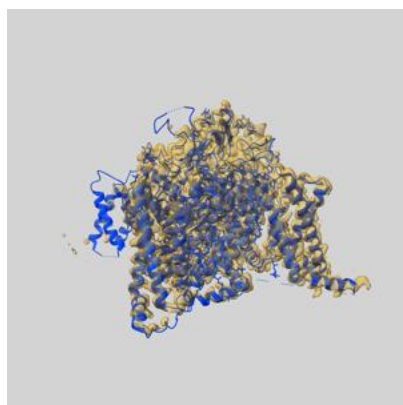
8 Fourier-Shell correlation

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

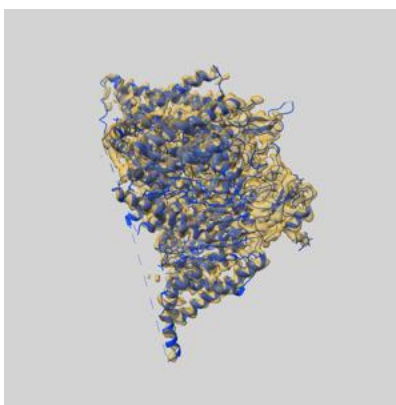
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32475 and PDB model 7WFR. Per-residue inclusion information can be found in section [3](#) on page [10](#).

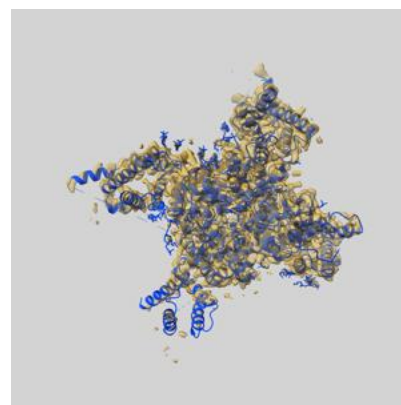
9.1 Map-model overlay [i](#)



X



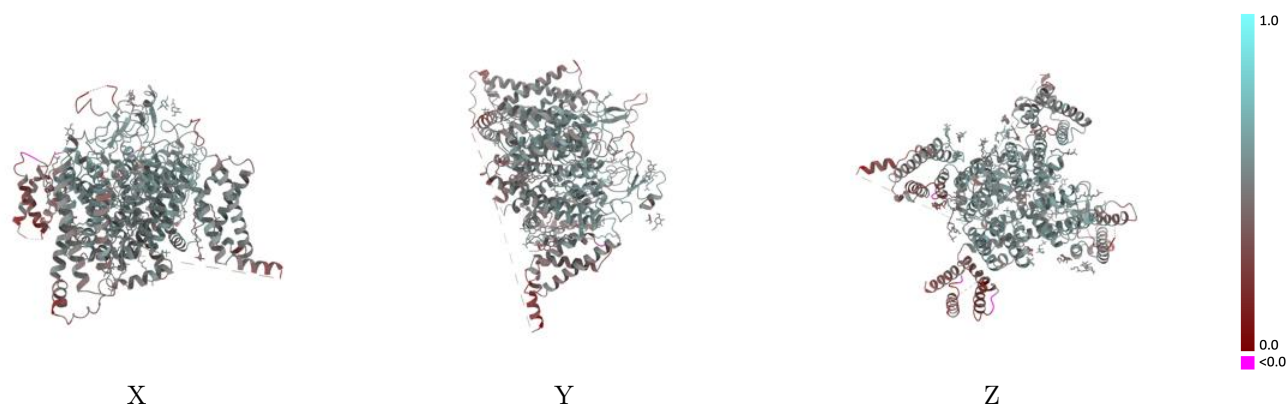
Y



Z

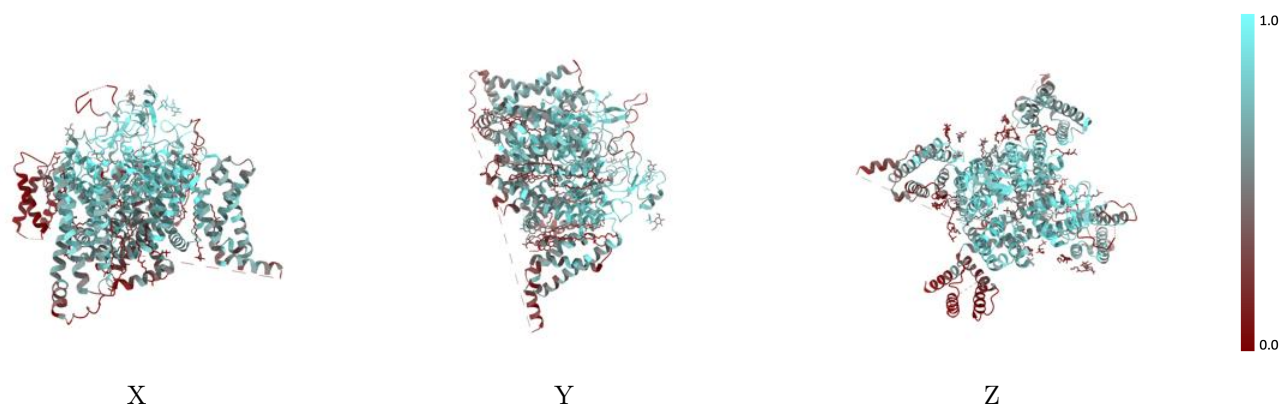
The images above show the 3D surface view of the map at the recommended contour level 0.0217 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



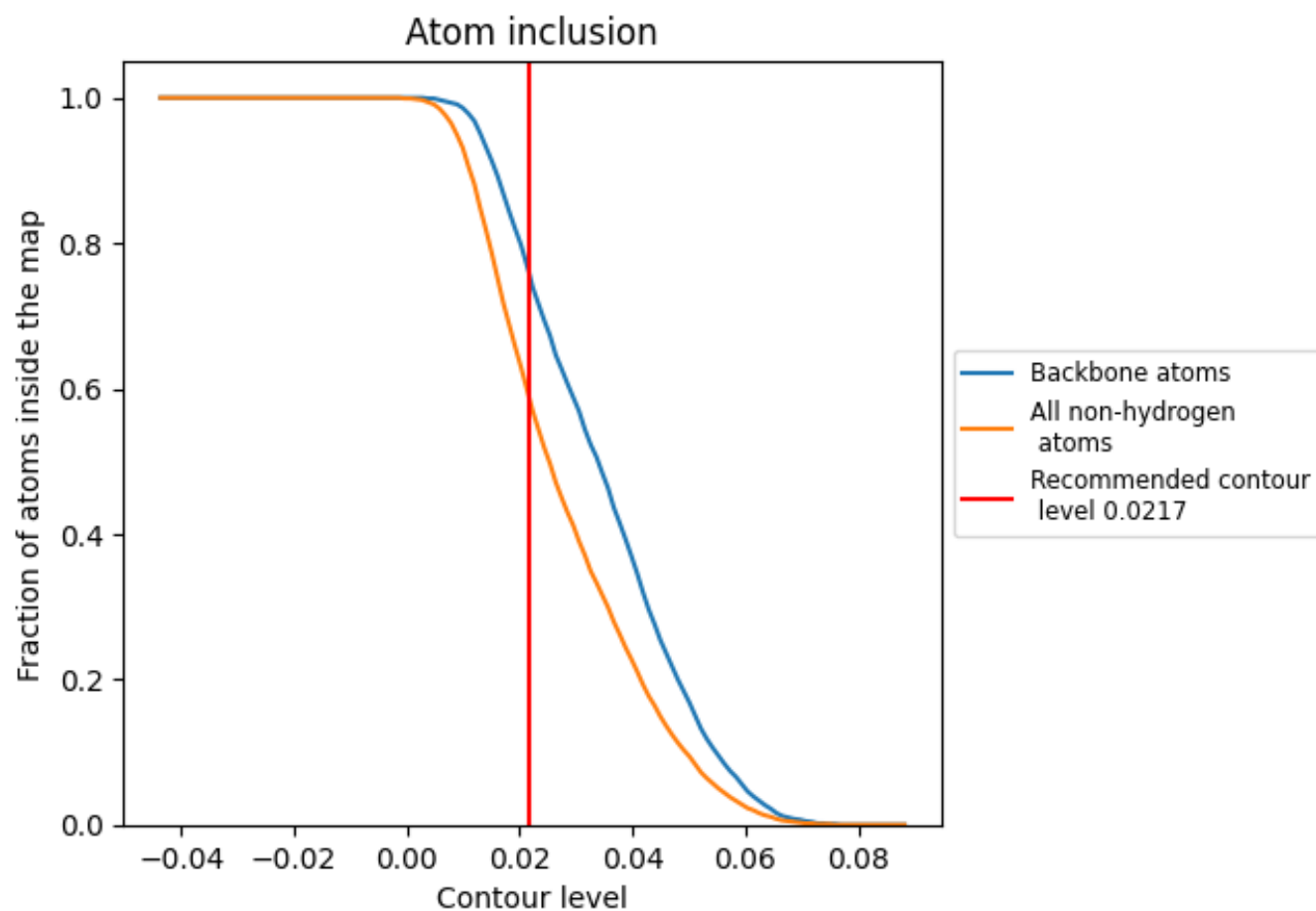
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0217).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 59% 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 (0.0217) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5880	0.4830
A	0.5870	0.4830
B	0.5710	0.4310
C	0.7500	0.5480

