



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:56 AM UTC

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

This is a 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:

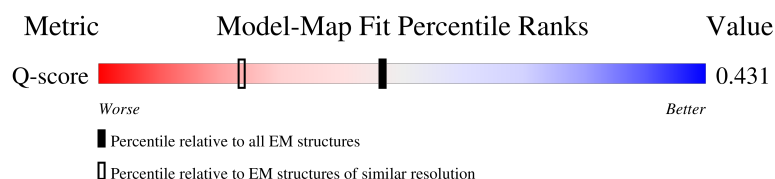
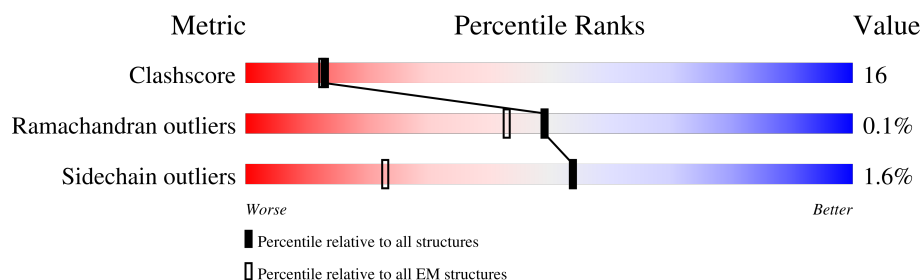
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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	2031	25% 48% 21% 30%
2	B	218	8% 56% 22% 21%
3	C	215	48% 49% 6% 45%
4	D	2	50% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	2	
4	F	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PCW	A	2013	-	-	X	-
6	NAG	A	2008	-	-	X	-

2 Entry composition [i](#)

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

Continued on next page...

Continued from previous page...

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

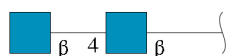
- Molecule 2 is a protein called Sodium channel subunit beta-1.

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.



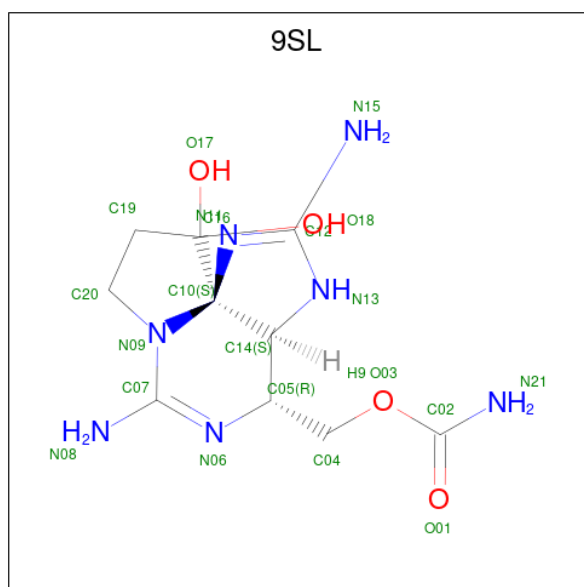
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is [(3aS,4R,10aS)-2,6-diamino-10,10-dihydroxy-3a,4,9,10-tetrahydro-3H,8H-pyrrolo[1,2-c]purin-4-yl]methyl carbamate (CCD ID: 9SL) (formula: C₁₀H₁₇N₇O₄) (labeled as "Ligand of Interest" by depositor).



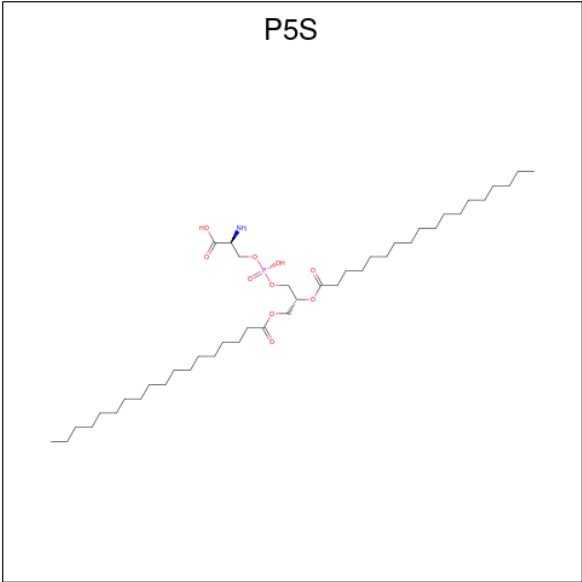
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			21	10	7	4	

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



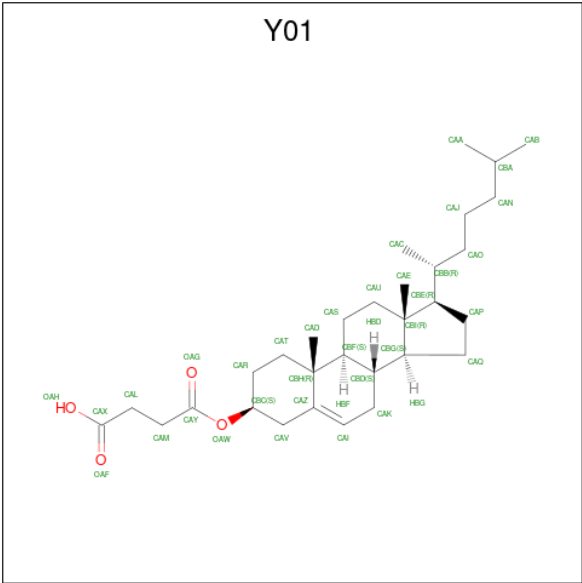
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	

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



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

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



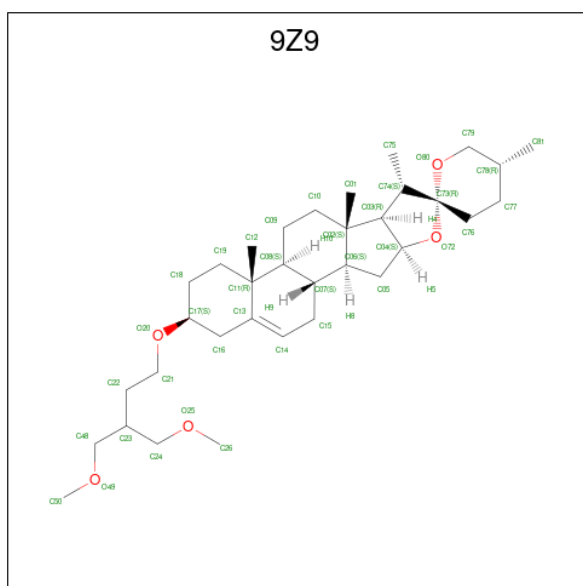
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	

Continued on next page...

Continued from previous page...

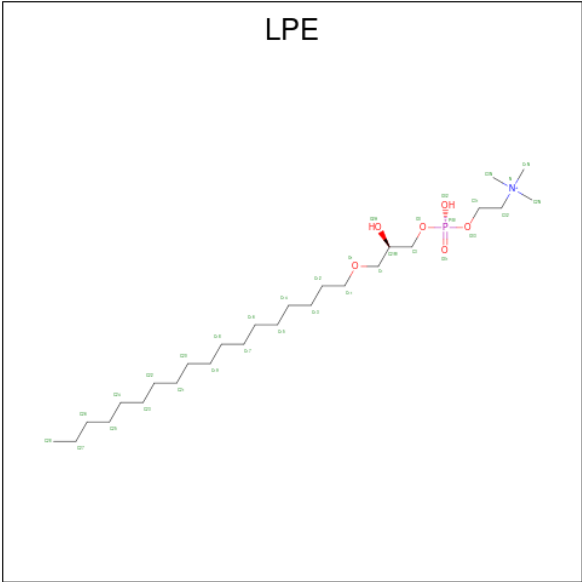
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	

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



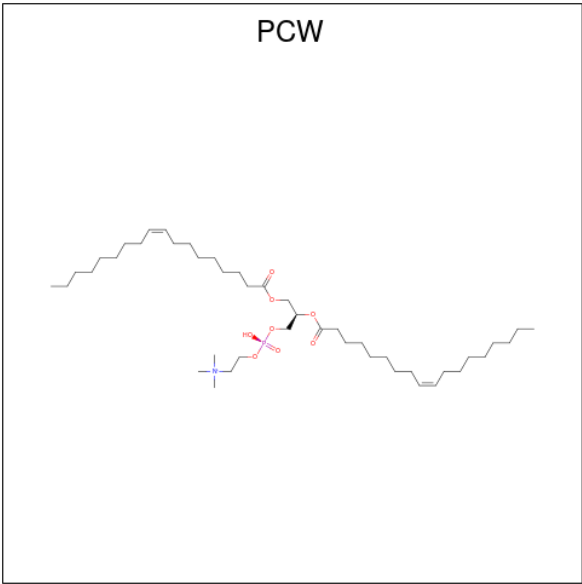
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			39	34	5	

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



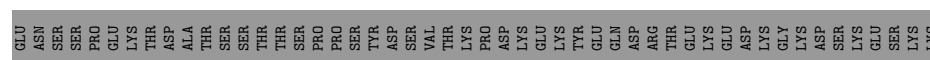
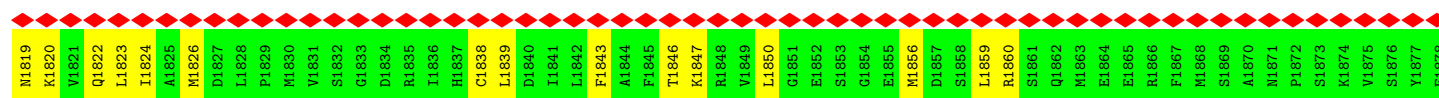
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			20	12	1	6	1	
10	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
10	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17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

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

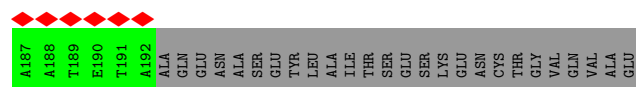
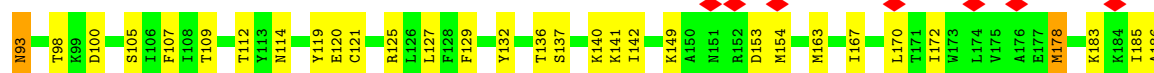
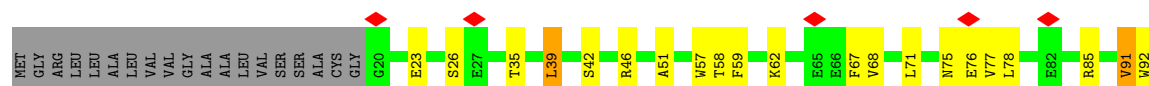


Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			53	43	1	8	1	
11	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

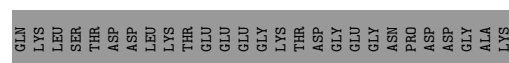
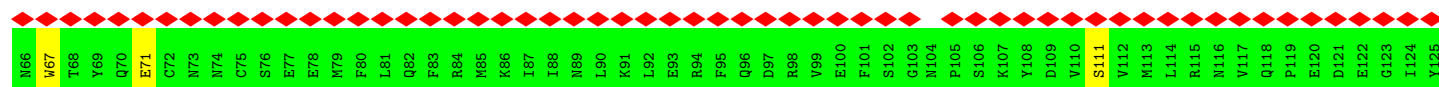
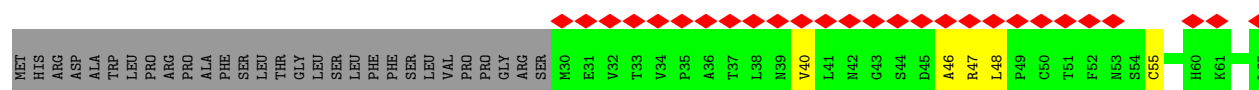




• Molecule 2: Sodium channel subunit beta-1



• Molecule 3: Sodium channel subunit beta-2



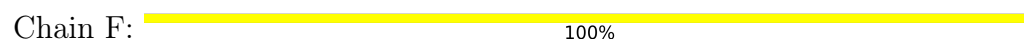
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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 ($\text{\AA}$)	261.84, 261.84, 261.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9SL, P5S, Y01, NAG, LPE, 9Z9, PCW

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	2/11693 (0.0%)	0.65	16/15834 (0.1%)
2	B	0.37	0/1442	0.48	0/1949
3	C	0.35	0/1011	0.58	0/1367
All	All	0.43	2/14146 (0.0%)	0.63	16/19150 (0.1%)

All (2) bond length outliers are listed below:

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

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1418	SER	N-CA-C	8.82	122.34	108.67
1	A	1419	VAL	N-CA-C	8.58	118.59	110.53
1	A	1769	GLU	N-CA-C	7.68	122.53	110.32
1	A	1421	VAL	N-CA-C	7.51	118.28	110.62
1	A	1249	GLY	CA-C-O	-6.21	117.94	122.23
1	A	896	VAL	N-CA-C	6.19	116.93	110.62
1	A	127	LEU	N-CA-C	-6.08	105.84	113.20
1	A	1494	GLN	N-CA-C	5.74	117.77	108.41
1	A	1771	THR	N-CA-C	5.56	117.34	111.28
1	A	1768	GLU	N-CA-C	5.37	116.81	111.07
1	A	274	LYS	CA-C-N	-5.27	115.77	122.77
1	A	274	LYS	C-N-CA	-5.27	115.77	122.77
1	A	1492	LYS	N-CA-C	5.19	121.27	109.81
1	A	1335	PHE	N-CA-C	5.08	116.90	111.36
1	A	988	LEU	N-CA-C	-5.05	105.68	111.14
1	A	1665	ASN	N-CA-C	5.05	119.49	113.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11419	0	11645	378	0
2	B	1416	0	1380	43	0
3	C	980	0	935	4	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
5	A	21	0	0	3	0
6	A	28	0	26	9	0
6	B	42	0	39	0	0
7	A	76	0	96	21	0
8	A	175	0	245	48	0
9	A	39	0	0	9	0
10	A	312	0	426	84	0
10	B	17	0	19	9	0
11	A	232	0	321	35	0
All	All	14841	0	15207	493	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (493) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1602:TYR:CE2	1:A:1603:PHE:CE1	1.76	1.65
1:A:1602:TYR:CE2	1:A:1603:PHE:HE1	1.04	1.64
1:A:1602:TYR:CD2	1:A:1603:PHE:CE1	1.92	1.53
2:B:178:MET:HE1	10:B:304:LPE:C1	1.55	1.35
1:A:1602:TYR:CD2	1:A:1603:PHE:CD1	2.18	1.28
1:A:1602:TYR:HD2	1:A:1603:PHE:CD1	1.52	1.26
2:B:178:MET:CE	10:B:304:LPE:H12	1.70	1.21
1:A:1738:PHE:CD2	10:A:2014:LPE:H1N2	1.75	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1330:ILE:CD1	8:A:2006:Y01:HAB2	1.71	1.18
1:A:1738:PHE:CE2	10:A:2014:LPE:H1N2	1.81	1.15
1:A:1330:ILE:HD12	8:A:2006:Y01:HAB2	1.34	1.09
1:A:963:PHE:CE1	9:A:2007:9Z9:C77	2.37	1.08
1:A:1257:ALA:CB	10:A:2015:LPE:H31	1.84	1.07
1:A:1330:ILE:HD12	8:A:2006:Y01:CAB	1.85	1.07
2:B:178:MET:HE1	10:B:304:LPE:H12	1.10	1.06
11:A:2013:PCW:C37	8:A:2029:Y01:HAQ1	1.89	1.02
1:A:1602:TYR:HE2	1:A:1603:PHE:CE1	1.30	1.02
1:A:1307:MET:HE1	10:A:2023:LPE:C19	1.91	1.01
1:A:1375:ASN:ND2	6:A:2008:NAG:C2	2.23	1.00
11:A:2013:PCW:H371	8:A:2029:Y01:HAQ1	1.45	0.99
1:A:1375:ASN:CG	6:A:2008:NAG:C1	2.36	0.97
2:B:178:MET:CE	10:B:304:LPE:C1	2.37	0.95
11:A:2013:PCW:C37	8:A:2029:Y01:CAQ	2.45	0.94
1:A:1307:MET:CE	10:A:2023:LPE:C19	2.46	0.93
10:A:2021:LPE:H1N3	10:A:2022:LPE:O32	1.70	0.92
1:A:1301:LEU:HD11	10:A:2014:LPE:H151	1.55	0.88
10:A:2012:LPE:H1N1	11:A:2013:PCW:C8	2.04	0.88
1:A:1738:PHE:CE2	10:A:2014:LPE:C1N	2.56	0.88
1:A:1457:ILE:HD13	9:A:2007:9Z9:C12	2.04	0.87
1:A:364:GLU:OE2	5:A:2001:9SL:N11	2.07	0.86
1:A:1624:VAL:HG21	7:A:2017:P5S:H29A	1.57	0.85
1:A:1179:TRP:CZ3	10:A:2025:LPE:H321	2.13	0.84
1:A:1324:VAL:HG21	1:A:1455:VAL:HG21	1.57	0.84
2:B:178:MET:HE1	10:B:304:LPE:O1	1.76	0.84
1:A:1653:LEU:HD23	10:A:2014:LPE:C16	2.07	0.84
1:A:1257:ALA:HB1	10:A:2015:LPE:H31	1.60	0.83
10:A:2012:LPE:H1N1	11:A:2013:PCW:H83	1.59	0.82
1:A:1735:VAL:HG23	10:A:2014:LPE:H2N1	1.62	0.82
1:A:1301:LEU:HD11	10:A:2014:LPE:C15	2.10	0.81
1:A:1457:ILE:CD1	9:A:2007:9Z9:C12	2.59	0.80
1:A:1477:GLU:HG3	10:A:2019:LPE:H1N1	1.65	0.79
1:A:1578:TRP:CH2	7:A:2017:P5S:H26	2.19	0.77
1:A:1330:ILE:CD1	8:A:2006:Y01:CAB	2.52	0.77
1:A:963:PHE:HE1	9:A:2007:9Z9:C77	1.95	0.76
1:A:1375:ASN:O	6:A:2008:NAG:H82	1.85	0.76
1:A:1738:PHE:HD2	10:A:2014:LPE:H1N2	1.43	0.75
11:A:2013:PCW:H372	8:A:2029:Y01:CAQ	2.16	0.75
1:A:1508:ILE:HA	1:A:1511:LEU:HD12	1.69	0.74
1:A:1735:VAL:CG2	10:A:2014:LPE:H2N1	2.18	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:MET:HE3	10:B:304:LPE:H12	1.67	0.73
11:A:2013:PCW:H381	8:A:2029:Y01:HAQ2	1.71	0.73
1:A:1384:ASN:OD1	1:A:1388:ASN:ND2	2.22	0.72
1:A:1781:MET:HA	1:A:1784:GLU:HG2	1.69	0.72
10:A:2021:LPE:C32	10:A:2022:LPE:H31	2.19	0.72
1:A:1477:GLU:HG3	10:A:2019:LPE:C1N	2.20	0.72
1:A:1785:VAL:HA	1:A:1788:LYS:HD2	1.72	0.72
1:A:1282:ASP:HA	1:A:1287:LYS:HG3	1.70	0.71
1:A:1738:PHE:HE2	10:A:2014:LPE:C1N	2.02	0.71
2:B:178:MET:HE2	10:B:304:LPE:O2H	1.91	0.71
1:A:1307:MET:HE3	10:A:2023:LPE:C19	2.21	0.71
11:A:2013:PCW:H381	8:A:2029:Y01:CAQ	2.21	0.71
1:A:1477:GLU:CG	10:A:2019:LPE:H1N1	2.21	0.70
1:A:1257:ALA:HB3	10:A:2015:LPE:H31	1.71	0.69
1:A:1330:ILE:HD12	8:A:2006:Y01:CAA	2.22	0.69
1:A:1366:ASN:OD1	1:A:1368:SER:OG	2.11	0.69
1:A:1578:TRP:CH2	7:A:2017:P5S:C26	2.75	0.69
11:A:2013:PCW:H372	8:A:2029:Y01:HAQ1	1.71	0.68
11:A:2013:PCW:C38	8:A:2029:Y01:CAQ	2.73	0.67
1:A:909:HIS:HD2	1:A:911:ASN:H	1.43	0.67
7:A:2003:P5S:H54A	10:A:2025:LPE:H171	1.76	0.67
10:A:2021:LPE:H321	10:A:2022:LPE:H31	1.77	0.67
1:A:1677:ASP:OD2	2:B:46:ARG:NH2	2.27	0.67
1:A:1558:PHE:O	1:A:1561:GLU:HG2	1.95	0.66
1:A:1653:LEU:CD2	10:A:2014:LPE:C16	2.74	0.66
10:A:2012:LPE:H1N1	11:A:2013:PCW:H82	1.77	0.66
1:A:9:PRO:HA	1:A:63:TYR:HA	1.78	0.66
1:A:1251:LYS:CE	10:A:2026:LPE:H312	2.26	0.65
11:A:2013:PCW:C37	8:A:2029:Y01:HAQ2	2.27	0.65
1:A:293:LEU:HD22	1:A:298:ASP:HB3	1.79	0.65
1:A:1330:ILE:HD13	8:A:2006:Y01:HAB2	1.74	0.64
1:A:64:GLY:O	1:A:95:LYS:NZ	2.30	0.64
1:A:1602:TYR:CE2	1:A:1603:PHE:CZ	2.73	0.64
1:A:1375:ASN:OD1	6:A:2008:NAG:C1	2.46	0.64
1:A:1330:ILE:HD11	8:A:2006:Y01:HAJ1	1.80	0.63
1:A:1179:TRP:CZ3	10:A:2025:LPE:C32	2.81	0.63
1:A:324:CYS:SG	1:A:328:TYR:HB2	2.38	0.63
2:B:51:ALA:HB2	2:B:127:LEU:HD13	1.80	0.63
1:A:230:GLY:O	1:A:234:ILE:HG12	1.99	0.62
1:A:1759:ILE:CD1	9:A:2007:9Z9:C03	2.78	0.62
1:A:927:GLU:OE2	5:A:2001:9SL:C04	2.48	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:LEU:CD2	10:A:2014:LPE:H151	2.30	0.62
1:A:1330:ILE:HD12	8:A:2006:Y01:HAA3	1.82	0.62
10:A:2021:LPE:H321	10:A:2022:LPE:O32	1.99	0.62
11:A:2013:PCW:C38	8:A:2029:Y01:HAQ2	2.30	0.61
1:A:1307:MET:HE1	10:A:2023:LPE:C18	2.30	0.61
1:A:1257:ALA:CB	10:A:2015:LPE:C3	2.72	0.61
1:A:1628:LYS:NZ	7:A:2017:P5S:O13	2.33	0.61
2:B:178:MET:CE	10:B:304:LPE:O2H	2.48	0.61
1:A:816:VAL:O	1:A:820:LEU:HG	2.01	0.60
1:A:388:LEU:HD11	7:A:2017:P5S:H34	1.83	0.60
1:A:99:ARG:HG2	1:A:181:PHE:CE2	2.36	0.60
8:A:2009:Y01:HAC1	8:A:2009:Y01:HAE2	1.83	0.60
1:A:1218:ARG:NH2	2:B:23:GLU:O	2.28	0.60
1:A:1485:MET:HE2	10:A:2020:LPE:H132	1.82	0.60
1:A:1578:TRP:CZ3	7:A:2017:P5S:H26	2.36	0.60
8:A:2004:Y01:HAC1	8:A:2004:Y01:HAE2	1.84	0.60
8:A:2005:Y01:HAE2	8:A:2005:Y01:HAC1	1.83	0.60
1:A:1375:ASN:ND2	6:A:2008:NAG:H2	2.16	0.60
1:A:1375:ASN:HD22	6:A:2008:NAG:C7	2.15	0.60
1:A:730:TRP:HA	1:A:733:PHE:CZ	2.36	0.59
1:A:65:ASP:OD1	1:A:66:ILE:N	2.35	0.59
1:A:151:TRP:H	1:A:151:TRP:CD1	2.20	0.59
1:A:149:PRO:HB2	1:A:151:TRP:HD1	1.67	0.59
1:A:1250:TYR:H	7:A:2003:P5S:H45	1.67	0.59
8:A:2006:Y01:HAC1	8:A:2006:Y01:HAE2	1.83	0.59
1:A:27:ILE:HA	1:A:30:ARG:HD2	1.84	0.59
2:B:129:PHE:HB2	2:B:132:TYR:HB3	1.84	0.59
1:A:183:PHE:HD2	1:A:184:LEU:HD22	1.68	0.59
1:A:1257:ALA:HB3	10:A:2015:LPE:C3	2.32	0.59
2:B:98:THR:C	2:B:100:ASP:H	2.09	0.59
1:A:1577:GLY:H	11:A:2018:PCW:H51	1.68	0.58
1:A:1673:ASP:OD1	1:A:1673:ASP:O	2.21	0.58
11:A:2013:PCW:H381	8:A:2029:Y01:CAP	2.33	0.58
11:A:2018:PCW:H19	11:A:2027:PCW:H261	1.85	0.58
2:B:136:THR:HG22	2:B:137:SER:H	1.68	0.58
2:B:91:VAL:HG23	2:B:107:PHE:HB3	1.85	0.58
1:A:1304:PHE:CE2	10:A:2023:LPE:C19	2.87	0.58
11:A:2013:PCW:H371	8:A:2029:Y01:CAQ	2.21	0.58
1:A:1513:THR:HG22	1:A:1513:THR:O	2.02	0.58
11:A:2013:PCW:H372	8:A:2029:Y01:HAQ2	1.83	0.58
1:A:1641:LEU:HB3	10:A:2019:LPE:H11	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1771:THR:HG23	1:A:1773:PRO:HD3	1.85	0.57
1:A:1850:LEU:HD23	1:A:1856:MET:HG2	1.86	0.57
1:A:86:LYS:NZ	1:A:86:LYS:H	2.01	0.57
1:A:1430:SER:HB3	1:A:1433:MET:HG2	1.86	0.57
7:A:2003:P5S:H42	10:A:2026:LPE:O32	2.05	0.57
2:B:23:GLU:OE1	2:B:140:LYS:NZ	2.37	0.57
1:A:388:LEU:O	1:A:392:TYR:HB3	2.04	0.57
7:A:2017:P5S:C35	7:A:2017:P5S:C46	2.83	0.57
1:A:179:GLY:H	1:A:182:THR:HG21	1.69	0.57
1:A:834:LEU:HD21	1:A:835:ARG:HH11	1.69	0.57
10:A:2010:LPE:O32	10:A:2012:LPE:H3N1	2.05	0.56
1:A:1331:PHE:CZ	1:A:1443:PHE:HB3	2.40	0.56
1:A:1375:ASN:ND2	6:A:2008:NAG:C7	2.68	0.56
1:A:318:SER:OG	1:A:319:THR:N	2.39	0.56
1:A:1607:THR:HA	1:A:1610:ARG:HH11	1.71	0.56
1:A:1348:TYR:CE2	1:A:1384:ASN:HB2	2.41	0.56
7:A:2003:P5S:H46	10:A:2025:LPE:H11	1.88	0.56
10:A:2011:LPE:H21	11:A:2013:PCW:H131	1.88	0.56
2:B:153:ASP:OD1	2:B:154:MET:N	2.40	0.55
1:A:1521:ILE:HD12	1:A:1561:GLU:OE2	2.05	0.55
1:A:1251:LYS:HE2	10:A:2026:LPE:C31	2.36	0.55
1:A:1304:PHE:HE2	10:A:2023:LPE:C19	2.20	0.55
1:A:1602:TYR:CE2	1:A:1603:PHE:CD1	2.62	0.55
1:A:223:LYS:O	1:A:227:VAL:HG22	2.06	0.54
1:A:1847:LYS:HA	1:A:1856:MET:HE3	1.89	0.54
2:B:57:TRP:HB2	2:B:71:LEU:HG	1.89	0.54
2:B:93:ASN:HB3	2:B:105:SER:OG	2.07	0.54
1:A:226:SER:HA	1:A:232:LYS:HE2	1.90	0.54
1:A:1824:ILE:HG21	1:A:1887:LYS:HD3	1.89	0.54
1:A:1457:ILE:HD12	9:A:2007:9Z9:C12	2.36	0.54
1:A:1184:THR:O	1:A:1188:ILE:HG12	2.08	0.53
1:A:737:ILE:HA	1:A:740:ILE:HB	1.89	0.53
1:A:1375:ASN:OD1	6:A:2008:NAG:O5	2.27	0.53
2:B:178:MET:CE	10:B:304:LPE:C2	2.87	0.53
1:A:812:ASP:OD1	1:A:844:LYS:NZ	2.31	0.53
1:A:998:GLY:O	1:A:1002:VAL:HG23	2.08	0.53
1:A:1251:LYS:HZ1	10:A:2026:LPE:H1N3	1.73	0.53
1:A:1491:LYS:NZ	11:A:2027:PCW:H72	2.22	0.53
1:A:1846:THR:HG23	1:A:1856:MET:HE1	1.90	0.53
1:A:1737:ILE:O	1:A:1741:VAL:HG12	2.07	0.53
1:A:1580:ILE:O	1:A:1584:VAL:HG23	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1491:LYS:C	1:A:1493:PRO:HD3	2.34	0.53
1:A:335:ARG:NH1	1:A:336:ASN:O	2.40	0.53
1:A:1250:TYR:OH	10:A:2025:LPE:H172	2.09	0.53
1:A:1478:GLN:HG2	10:A:2019:LPE:H311	1.90	0.53
1:A:1602:TYR:HD2	1:A:1603:PHE:CE1	1.63	0.53
10:A:2021:LPE:C3N	10:A:2022:LPE:H31	2.39	0.52
1:A:1331:PHE:HZ	1:A:1443:PHE:HB3	1.72	0.52
10:A:2012:LPE:C1N	11:A:2013:PCW:H82	2.39	0.52
7:A:2003:P5S:H42	10:A:2026:LPE:P	2.49	0.52
1:A:778:ILE:HG13	1:A:779:GLY:N	2.24	0.52
1:A:861:ASN:ND2	1:A:969:SER:OG	2.43	0.52
1:A:1567:ILE:HD12	1:A:1568:SER:N	2.25	0.52
1:A:1588:ILE:HG22	1:A:1615:ALA:HB1	1.91	0.52
1:A:1179:TRP:HZ3	10:A:2025:LPE:H321	1.68	0.52
1:A:1298:LEU:HD23	10:A:2014:LPE:C16	2.40	0.52
1:A:1577:GLY:HA2	1:A:1580:ILE:HD12	1.91	0.52
10:A:2010:LPE:O32	10:A:2012:LPE:C3N	2.58	0.52
1:A:149:PRO:HB2	1:A:151:TRP:CD1	2.44	0.52
1:A:1499:ARG:HD2	1:A:1500:PRO:HD2	1.92	0.52
1:A:1307:MET:HE1	10:A:2023:LPE:H182	1.92	0.51
1:A:804:PHE:O	1:A:810:ILE:HD11	2.10	0.51
1:A:1294:ALA:O	1:A:1657:ILE:HG23	2.10	0.51
8:A:2004:Y01:HAE2	8:A:2004:Y01:CAC	2.41	0.51
1:A:101:ASN:OD1	1:A:101:ASN:N	2.44	0.51
3:C:47:ARG:NH2	3:C:111[B]:SER:OG	2.43	0.51
1:A:376:LYS:HE3	1:A:1678:MET:HE3	1.93	0.51
1:A:729:TYR:HA	1:A:732:LYS:HD2	1.93	0.51
1:A:1838:CYS:SG	1:A:1839:LEU:N	2.84	0.51
1:A:151:TRP:O	1:A:155:VAL:HG23	2.11	0.51
1:A:1377:SER:OG	1:A:1378:GLN:N	2.44	0.51
1:A:165:PHE:O	1:A:169:VAL:HG23	2.11	0.51
1:A:1365:PRO:HD2	1:A:1369:GLU:HG3	1.92	0.51
1:A:324:CYS:SG	1:A:325:PRO:HD2	2.51	0.51
1:A:1330:ILE:CD1	8:A:2006:Y01:HAA3	2.41	0.50
1:A:1250:TYR:HD2	7:A:2003:P5S:H45A	1.77	0.50
1:A:1624:VAL:HG21	7:A:2017:P5S:C29	2.33	0.50
1:A:1570:ARG:HG3	1:A:1571:HIS:H	1.75	0.50
1:A:72:SER:OG	1:A:121:LYS:HE3	2.10	0.50
1:A:834:LEU:O	1:A:838:ARG:HG2	2.12	0.50
1:A:1301:LEU:HD11	10:A:2014:LPE:H152	1.92	0.50
1:A:1417:ASP:OD1	1:A:1427:TYR:HA	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:SER:O	1:A:215:THR:HG23	2.12	0.50
1:A:1655:MET:HE1	10:A:2021:LPE:C19	2.42	0.50
7:A:2003:P5S:H50	10:A:2025:LPE:H122	1.94	0.50
8:A:2006:Y01:HAE2	8:A:2006:Y01:CAC	2.41	0.50
10:A:2012:LPE:C1N	11:A:2013:PCW:C8	2.86	0.50
1:A:167:SER:O	1:A:171:ILE:HG13	2.12	0.49
1:A:811:PHE:CZ	1:A:815:ILE:HD11	2.47	0.49
1:A:995:ILE:O	1:A:999:ILE:HG12	2.12	0.49
1:A:1528:ASN:ND2	1:A:1532:MET:HE3	2.28	0.49
1:A:1235:TYR:HE2	2:B:170:LEU:HD11	1.77	0.49
1:A:1509:PHE:CD2	1:A:1509:PHE:C	2.90	0.49
1:A:1250:TYR:CE2	7:A:2003:P5S:H49	2.47	0.49
1:A:50:SER:N	1:A:79:ASP:OD2	2.43	0.49
1:A:86:LYS:H	1:A:86:LYS:HZ2	1.60	0.49
2:B:78:LEU:HD12	2:B:92:TRP:HB2	1.94	0.49
10:A:2021:LPE:H3N2	10:A:2022:LPE:H31	1.94	0.49
1:A:1738:PHE:HE2	10:A:2014:LPE:H1N3	1.78	0.49
1:A:221:ALA:O	1:A:224:THR:OG1	2.28	0.49
7:A:2003:P5S:H46	10:A:2025:LPE:C1	2.42	0.48
1:A:1453:ILE:HG21	9:A:2007:9Z9:C76	2.43	0.48
2:B:185:ILE:HG13	2:B:186:ALA:N	2.28	0.48
1:A:1330:ILE:HD12	8:A:2006:Y01:CBA	2.41	0.48
1:A:988:LEU:C	1:A:988:LEU:HD23	2.38	0.48
1:A:1179:TRP:CD1	1:A:1183:LYS:HE2	2.48	0.48
8:A:2029:Y01:HAE2	8:A:2029:Y01:HBB	1.60	0.48
1:A:1251:LYS:HZ1	10:A:2026:LPE:H3N2	1.76	0.48
1:A:1584:VAL:O	1:A:1588:ILE:HG13	2.13	0.48
1:A:1549:TRP:O	1:A:1553:VAL:HG23	2.12	0.48
1:A:73:GLU:H	1:A:90:VAL:HG23	1.77	0.48
1:A:812:ASP:O	1:A:816:VAL:HG23	2.13	0.48
1:A:1310:VAL:HG23	1:A:1650:LEU:HD22	1.95	0.48
1:A:1653:LEU:HD13	10:A:2023:LPE:H182	1.95	0.48
8:A:2005:Y01:HAC1	8:A:2005:Y01:HAU2	1.96	0.48
1:A:1185:CYS:SG	1:A:1246:ILE:HG21	2.54	0.48
1:A:1333:LEU:HD22	8:A:2029:Y01:HAA1	1.95	0.48
11:A:2018:PCW:C19	11:A:2027:PCW:H261	2.44	0.48
1:A:1525:ILE:HD13	1:A:1622:ARG:HB2	1.95	0.48
1:A:1752:VAL:O	1:A:1756:ILE:HG12	2.13	0.48
8:A:2004:Y01:HAC1	8:A:2004:Y01:HAU2	1.96	0.48
1:A:276:PHE:CE1	1:A:302:TYR:HB3	2.49	0.48
8:A:2009:Y01:OAG	8:A:2009:Y01:HAV2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:OE2	5:A:2001:9SL:C12	2.61	0.47
1:A:1251:LYS:CE	10:A:2026:LPE:C31	2.92	0.47
1:A:392:TYR:CZ	1:A:1637:LEU:HB2	2.50	0.47
8:A:2006:Y01:HAC1	8:A:2006:Y01:HAU2	1.96	0.47
11:A:2018:PCW:H31	11:A:2027:PCW:H31	1.95	0.47
1:A:228:ILE:HD12	1:A:231:LEU:HD22	1.95	0.47
1:A:90:VAL:HG12	1:A:100:PHE:HE2	1.79	0.47
1:A:1289:LEU:HD13	1:A:1292:LEU:HD12	1.96	0.47
8:A:2006:Y01:HAV2	8:A:2006:Y01:OAG	2.14	0.47
8:A:2009:Y01:HAC1	8:A:2009:Y01:HAU2	1.96	0.47
11:A:2018:PCW:H31	11:A:2027:PCW:C3	2.45	0.47
1:A:324:CYS:SG	1:A:328:TYR:CB	3.03	0.47
1:A:379:MET:HE2	1:A:1689:ILE:HG12	1.97	0.47
1:A:1478:GLN:HG2	10:A:2019:LPE:C31	2.45	0.47
1:A:1260:TRP:CE3	8:A:2004:Y01:CAE	2.98	0.47
1:A:1754:MET:HE1	10:A:2019:LPE:C19	2.45	0.47
1:A:320:ASP:HB3	10:A:2021:LPE:H1N2	1.97	0.47
7:A:2003:P5S:H43A	10:A:2026:LPE:H12	1.96	0.47
1:A:1392:VAL:HB	8:A:2029:Y01:HBG	1.97	0.46
1:A:747:ASP:OD1	1:A:987:ASN:HB2	2.14	0.46
1:A:1186:TYR:HA	1:A:1247:ALA:HB1	1.97	0.46
1:A:1260:TRP:CE3	8:A:2004:Y01:HAE3	2.50	0.46
1:A:1586:VAL:O	1:A:1590:ILE:HG22	2.15	0.46
1:A:817:THR:O	1:A:821:VAL:HG23	2.15	0.46
1:A:822:GLU:HG2	1:A:834:LEU:HD22	1.95	0.46
1:A:1260:TRP:CZ3	8:A:2004:Y01:HAE3	2.49	0.46
1:A:53:LEU:HD13	1:A:78:LEU:HB3	1.98	0.46
1:A:84:ASP:OD1	1:A:85:LYS:N	2.48	0.46
1:A:271:LEU:HD12	1:A:343:SER:HA	1.97	0.46
1:A:1696:THR:O	1:A:1697:SER:OG	2.33	0.46
1:A:13:VAL:HG23	1:A:76:GLU:HB2	1.97	0.46
1:A:907:ARG:HD2	1:A:1413:TYR:CD1	2.50	0.46
1:A:972:SER:O	1:A:976:LEU:HG	2.16	0.46
1:A:139:ASN:HD21	1:A:220:ARG:HD2	1.81	0.46
1:A:972:SER:HB2	1:A:975:ASN:ND2	2.31	0.46
1:A:1280:TYR:HB3	1:A:1283:LEU:CD1	2.46	0.46
1:A:125:HIS:CE1	1:A:127:LEU:HD23	2.51	0.46
1:A:128:PHE:CG	1:A:128:PHE:O	2.69	0.46
1:A:148:PRO:HB3	1:A:152:THR:HG21	1.97	0.46
1:A:839:LEU:O	1:A:842:VAL:HG23	2.16	0.46
1:A:1677:ASP:OD1	1:A:1677:ASP:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:THR:HG23	2:B:68:VAL:C	2.41	0.46
1:A:332:LYS:NZ	1:A:1537:GLU:OE2	2.41	0.46
1:A:798:MET:HG2	1:A:802:GLU:HB2	1.97	0.46
1:A:1243:LEU:HA	1:A:1243:LEU:HD23	1.77	0.46
1:A:1822:GLN:O	1:A:1826:MET:HG3	2.16	0.46
1:A:259:PHE:HZ	1:A:388:LEU:HD13	1.81	0.45
1:A:820:LEU:HA	1:A:823:LEU:HG	1.98	0.45
1:A:1275:ALA:HB1	1:A:1286:ILE:HD13	1.98	0.45
1:A:1709:ASN:O	1:A:1730:CYS:HB2	2.17	0.45
2:B:26:SER:HB2	2:B:39:LEU:H	1.80	0.45
1:A:212:ALA:O	1:A:215:THR:OG1	2.29	0.45
1:A:1179:TRP:CH2	10:A:2025:LPE:H321	2.52	0.45
1:A:1232:ILE:HG13	2:B:163:MET:HG3	1.98	0.45
1:A:1298:LEU:CD2	10:A:2014:LPE:C15	2.93	0.45
8:A:2009:Y01:HAE2	8:A:2009:Y01:CAC	2.41	0.45
2:B:98:THR:C	2:B:100:ASP:N	2.75	0.45
1:A:811:PHE:O	1:A:815:ILE:HG13	2.16	0.45
1:A:1748:PHE:O	1:A:1752:VAL:HG23	2.16	0.45
1:A:88:PHE:CE1	1:A:100:PHE:HB2	2.52	0.45
1:A:1533:MET:HE1	10:A:2024:LPE:H122	1.99	0.45
1:A:1754:MET:O	1:A:1758:VAL:HG23	2.17	0.45
1:A:374:ALA:HB1	1:A:378:TYR:CD2	2.51	0.45
1:A:963:PHE:CD1	9:A:2007:9Z9:C77	2.97	0.45
1:A:1330:ILE:HD13	8:A:2029:Y01:HAA3	1.97	0.45
1:A:1177:ILE:O	1:A:1181:ILE:HG12	2.17	0.45
1:A:1305:GLU:H	1:A:1305:GLU:CD	2.23	0.45
2:B:42:SER:O	2:B:42:SER:OG	2.33	0.45
1:A:367:TYR:OH	1:A:1689:ILE:HG23	2.17	0.45
1:A:1251:LYS:NZ	10:A:2026:LPE:H1N3	2.31	0.45
1:A:15:PHE:HA	1:A:76:GLU:HG3	1.99	0.44
1:A:1457:ILE:HG13	1:A:1458:ASP:N	2.32	0.44
10:A:2014:LPE:O32	10:A:2015:LPE:H201	2.16	0.44
1:A:168:LEU:O	1:A:172:LEU:HB2	2.17	0.44
1:A:189:ASN:HA	1:A:192:ASP:OD1	2.17	0.44
1:A:1326:LEU:HD23	1:A:1326:LEU:HA	1.79	0.44
2:B:42:SER:OG	2:B:125:ARG:NH2	2.49	0.44
1:A:14:HIS:O	1:A:16:THR:HG23	2.16	0.44
1:A:1375:ASN:O	6:A:2008:NAG:C8	2.59	0.44
2:B:121:CYS:HB3	2:B:140:LYS:HB2	1.99	0.44
1:A:1623:LEU:HD23	1:A:1623:LEU:HA	1.82	0.44
1:A:1697:SER:O	1:A:1700:TRP:HD1	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HD13	1:A:289:ILE:HA	1.81	0.44
1:A:338:ASP:HB2	1:A:342:THR:HG22	1.99	0.44
1:A:847:LYS:HD3	1:A:847:LYS:HA	1.72	0.44
11:A:2028:PCW:H322	11:A:2028:PCW:H351	1.81	0.44
8:A:2009:Y01:HAN2	8:A:2009:Y01:HAC3	2.00	0.44
1:A:774:ASN:O	1:A:778:ILE:HG23	2.18	0.44
1:A:1333:LEU:HA	1:A:1336:SER:OG	2.18	0.44
1:A:193:PHE:O	1:A:197:VAL:HG23	2.18	0.44
1:A:1268:VAL:HG13	1:A:1289:LEU:HD12	2.00	0.44
1:A:1792:ASP:N	1:A:1792:ASP:OD2	2.44	0.44
2:B:35:THR:HG22	2:B:109:THR:HA	1.99	0.44
1:A:772:PHE:O	1:A:776:LEU:HG	2.18	0.44
1:A:776:LEU:O	1:A:780:ASN:ND2	2.51	0.44
1:A:816:VAL:O	1:A:819:SER:OG	2.28	0.43
1:A:986:ASN:O	1:A:989:GLN:N	2.50	0.43
1:A:1216:ILE:HD12	1:A:1216:ILE:HA	1.89	0.43
1:A:1666:PHE:CD1	1:A:1707:ILE:HD13	2.53	0.43
11:A:2013:PCW:H63	11:A:2013:PCW:H41	1.69	0.43
2:B:119:TYR:HB2	2:B:142:ILE:HB	2.00	0.43
1:A:761:MET:HE3	1:A:761:MET:HB2	1.87	0.43
1:A:1282:ASP:HA	1:A:1287:LYS:CG	2.43	0.43
1:A:1412:MET:O	1:A:1416:VAL:HG13	2.19	0.43
10:A:2026:LPE:H312	10:A:2026:LPE:H3N2	1.72	0.43
1:A:143:MET:HE1	1:A:221:ALA:HB2	2.01	0.43
1:A:251:LEU:HB2	1:A:1630:ILE:HD12	1.99	0.43
1:A:1481:TYR:CD2	10:A:2019:LPE:H321	2.53	0.43
1:A:1528:ASN:HD21	1:A:1619:ARG:HH11	1.67	0.43
1:A:1694:ILE:HG21	1:A:1703:LEU:HD12	1.99	0.43
3:C:128:TYR:C	3:C:129:ILE:HG13	2.43	0.43
1:A:427:LEU:O	1:A:431:LYS:HG2	2.17	0.43
1:A:830:GLY:O	1:A:833:VAL:HG22	2.18	0.43
1:A:1655:MET:HE1	10:A:2021:LPE:H171	2.01	0.43
1:A:1670:LYS:HB3	1:A:1670:LYS:HE2	1.77	0.43
1:A:1759:ILE:HD13	9:A:2007:9Z9:C03	2.48	0.43
1:A:19:SER:O	1:A:23:ILE:HG13	2.17	0.43
1:A:23:ILE:HG12	1:A:26:ARG:NH2	2.33	0.43
1:A:139:ASN:ND2	1:A:220:ARG:HD2	2.33	0.43
1:A:244:LYS:HE3	1:A:244:LYS:HB3	1.84	0.43
1:A:1248:TYR:O	1:A:1252:THR:OG1	2.36	0.43
10:A:2019:LPE:H311	10:A:2019:LPE:H2N3	1.61	0.43
1:A:333:ILE:HD12	1:A:333:ILE:HA	1.78	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:TRP:HZ3	10:A:2025:LPE:O31	2.01	0.43
1:A:1517:PHE:O	1:A:1521:ILE:HG12	2.17	0.43
1:A:1707:ILE:HD12	1:A:1740:PHE:HE2	1.84	0.43
1:A:1529:MET:HG2	1:A:1533:MET:HE3	2.00	0.43
1:A:215:THR:O	1:A:218:VAL:HG12	2.19	0.43
10:A:2021:LPE:C1N	10:A:2022:LPE:O32	2.55	0.43
1:A:736:CYS:O	1:A:740:ILE:HG13	2.19	0.43
1:A:1491:LYS:HZ1	11:A:2027:PCW:H72	1.83	0.43
1:A:1798:GLU:HB3	1:A:1801:LYS:HE2	2.00	0.43
1:A:1824:ILE:HG22	1:A:1884:LEU:HD12	2.01	0.43
8:A:2005:Y01:HAE2	8:A:2005:Y01:CAC	2.41	0.43
1:A:23:ILE:HG21	1:A:86:LYS:HA	2.01	0.42
1:A:918:LEU:HD23	1:A:918:LEU:HA	1.85	0.42
2:B:58:THR:O	2:B:120:GLU:N	2.46	0.42
1:A:1250:TYR:CE2	7:A:2003:P5S:C49	3.02	0.42
1:A:1250:TYR:HD1	1:A:1254:PHE:HE2	1.67	0.42
2:B:58:THR:CG2	2:B:67:PHE:HB3	2.49	0.42
1:A:153:LYS:HE2	1:A:153:LYS:HB3	1.86	0.42
1:A:389:GLY:O	1:A:393:LEU:HB2	2.19	0.42
1:A:1250:TYR:HE2	10:A:2025:LPE:H152	1.84	0.42
2:B:172:ILE:HD13	2:B:172:ILE:HA	1.86	0.42
1:A:1602:TYR:CD2	1:A:1603:PHE:CZ	2.86	0.42
1:A:57:LYS:HE3	1:A:57:LYS:HB3	1.83	0.42
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.75	0.42
8:A:2006:Y01:HAC3	8:A:2006:Y01:HAN2	2.00	0.42
1:A:952:MET:O	1:A:956:ASN:ND2	2.31	0.42
1:A:1221:THR:O	1:A:1225:ILE:HG12	2.19	0.42
1:A:1498:PRO:HG2	1:A:1572:TYR:CZ	2.55	0.42
2:B:59:PHE:HE2	2:B:85:ARG:HH21	1.68	0.42
2:B:119:TYR:O	2:B:141:LYS:HA	2.20	0.42
1:A:743:ASP:N	1:A:744:PRO:HD2	2.35	0.42
1:A:819:SER:O	1:A:823:LEU:HG	2.17	0.42
1:A:1798:GLU:HG2	1:A:1800:SER:H	1.83	0.42
10:A:2012:LPE:H1N3	11:A:2013:PCW:O4P	2.20	0.42
1:A:1284:GLY:HA3	1:A:1285:PRO:HD3	1.92	0.41
1:A:1843:PHE:CZ	1:A:1860:ARG:HB2	2.55	0.41
1:A:1856:MET:SD	1:A:1859:LEU:HD21	2.60	0.41
7:A:2003:P5S:H56A	7:A:2003:P5S:H53	1.86	0.41
8:A:2029:Y01:HAP1	8:A:2029:Y01:HAO2	1.36	0.41
1:A:11:SER:OG	1:A:78:LEU:HD11	2.20	0.41
1:A:780:ASN:O	1:A:784:THR:OG1	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:SER:O	1:A:1340:VAL:HG23	2.20	0.41
1:A:1388:ASN:OD1	1:A:1394:LEU:HD13	2.20	0.41
1:A:1741:VAL:HG13	10:A:2011:LPE:H171	2.02	0.41
2:B:149:LYS:HD2	2:B:149:LYS:HA	1.76	0.41
1:A:171:ILE:HG12	1:A:183:PHE:CD1	2.55	0.41
1:A:799:ASP:HB3	1:A:802:GLU:HG2	2.02	0.41
1:A:1274:VAL:HA	1:A:1277:THR:HG22	2.03	0.41
1:A:1706:PRO:HA	1:A:1709:ASN:HD21	1.85	0.41
3:C:40:VAL:HG11	3:C:46:ALA:HB2	2.03	0.41
1:A:996:LYS:HA	1:A:999:ILE:HG12	2.02	0.41
1:A:1280:TYR:HB3	1:A:1283:LEU:HD12	2.02	0.41
1:A:1543:MET:HA	1:A:1546:VAL:HG22	2.02	0.41
2:B:183:LYS:HD2	2:B:183:LYS:HA	1.87	0.41
1:A:936:MET:HE2	1:A:945:LEU:HG	2.02	0.41
1:A:1587:ILE:O	1:A:1591:VAL:HG12	2.21	0.41
1:A:1597:ASP:HA	1:A:1600:GLU:OE1	2.20	0.41
11:A:2027:PCW:H42	11:A:2027:PCW:H63	1.59	0.41
2:B:112:THR:HG23	2:B:114:ASN:H	1.83	0.41
1:A:29:GLU:HB3	1:A:33:LYS:NZ	2.35	0.41
1:A:338:ASP:C	1:A:340:GLY:H	2.28	0.41
1:A:1301:LEU:HD23	1:A:1301:LEU:HA	1.89	0.41
1:A:49:PRO:HB3	1:A:82:TYR:CE2	2.55	0.41
1:A:1186:TYR:CA	1:A:1247:ALA:HB1	2.51	0.41
1:A:1740:PHE:O	1:A:1744:ILE:HG23	2.20	0.41
8:A:2006:Y01:HAS2	8:A:2006:Y01:HAE1	1.81	0.41
1:A:67:PRO:HA	1:A:68:PRO:HD3	1.92	0.41
1:A:748:LEU:HA	1:A:751:THR:HG22	2.02	0.41
1:A:1398:SER:HB3	1:A:1411:ILE:HD13	2.02	0.41
1:A:1460:PHE:HD2	1:A:1756:ILE:HG21	1.84	0.41
1:A:1820:LYS:O	1:A:1824:ILE:HG12	2.20	0.41
3:C:67:TRP:CZ2	3:C:127:CYS:HB3	2.55	0.41
1:A:104:PRO:HA	1:A:109:LEU:O	2.20	0.41
1:A:224:THR:HA	1:A:227:VAL:CG2	2.51	0.41
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.79	0.41
1:A:998:GLY:O	1:A:1001:TYR:HB3	2.21	0.41
1:A:1360:PRO:HD2	1:A:1363:GLN:HE21	1.86	0.41
1:A:1487:LYS:HE3	1:A:1487:LYS:HB2	1.82	0.41
1:A:1491:LYS:O	1:A:1493:PRO:HD3	2.20	0.41
7:A:2017:P5S:O18	11:A:2018:PCW:O2P	2.39	0.41
1:A:879:ILE:O	1:A:883:VAL:HG12	2.20	0.41
1:A:1374:MET:HE2	1:A:1381:ARG:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1527:LEU:O	1:A:1531:THR:HG23	2.21	0.41
1:A:1588:ILE:HG12	11:A:2028:PCW:H252	2.01	0.41
1:A:1639:MET:HE3	1:A:1639:MET:HB3	1.98	0.41
11:A:2027:PCW:H341	11:A:2027:PCW:H371	1.56	0.41
2:B:59:PHE:HB2	2:B:119:TYR:CD1	2.56	0.41
1:A:315:CYS:O	1:A:373:ALA:HA	2.21	0.40
1:A:429:ARG:HA	1:A:432:LYS:HE2	2.02	0.40
1:A:730:TRP:HA	1:A:733:PHE:CE2	2.56	0.40
1:A:924:LEU:HA	1:A:924:LEU:HD23	1.76	0.40
1:A:1182:ARG:HG2	1:A:1246:ILE:O	2.21	0.40
1:A:1478:GLN:HE22	1:A:1646:ASN:HD21	1.68	0.40
1:A:818:LEU:HG	1:A:837:PHE:CD2	2.55	0.40
1:A:986:ASN:C	1:A:988:LEU:N	2.79	0.40
1:A:1309:VAL:HA	1:A:1312:ASN:ND2	2.37	0.40
1:A:1701:ASP:N	1:A:1701:ASP:OD1	2.54	0.40
1:A:1737:ILE:O	1:A:1738:PHE:C	2.64	0.40
1:A:1776:GLU:O	1:A:1780:GLU:HG2	2.21	0.40
1:A:1819:ASN:O	1:A:1823:LEU:HG	2.21	0.40
10:A:2012:LPE:C1N	11:A:2013:PCW:O4P	2.69	0.40
2:B:75:ASN:O	2:B:77:VAL:N	2.54	0.40
1:A:29:GLU:O	1:A:33:LYS:HG3	2.22	0.40
1:A:171:ILE:HG12	1:A:183:PHE:CG	2.56	0.40
1:A:835:ARG:HB2	1:A:1338:MET:HE1	2.04	0.40
1:A:1545:GLU:HG2	1:A:1549:TRP:CD1	2.57	0.40
10:A:2021:LPE:H2N3	10:A:2021:LPE:H311	1.78	0.40
1:A:187:PRO:O	1:A:190:TRP:HB2	2.21	0.40
1:A:235:VAL:O	1:A:239:ILE:HG12	2.21	0.40
1:A:337:PRO:HG2	1:A:342:THR:HG23	2.04	0.40
1:A:1240:GLU:O	1:A:1244:LYS:HG3	2.22	0.40
11:A:2016:PCW:H42	11:A:2016:PCW:H83	1.62	0.40
2:B:62:LYS:HE2	2:B:62:LYS:HB3	1.89	0.40
1:A:104:PRO:HB2	1:A:107:TYR:HA	2.03	0.40
1:A:1649:LEU:HA	1:A:1649:LEU:HD23	1.79	0.40
1:A:1803:SER:O	1:A:1819:ASN:ND2	2.53	0.40

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

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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

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

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

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	151	TRP
1	A	224	THR
1	A	242	VAL
1	A	354	LEU
1	A	370	THR
1	A	741	VAL
1	A	748	LEU
1	A	778	ILE
1	A	876	ILE
1	A	992	VAL
1	A	1232	ILE
1	A	1450	ASN
1	A	1586	VAL
1	A	1595	LEU
2	B	39	LEU
2	B	91	VAL
2	B	93	ASN
2	B	167	ILE
2	B	178	MET
3	C	48	LEU
3	C	55	CYS
3	C	71	GLU
3	C	130	MET
3	C	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	GLN
1	A	278	ASN
1	A	323	GLN
1	A	365	ASN
1	A	408	GLN
1	A	409	ASN
1	A	412	ASN
1	A	425	GLN
1	A	757	ASN
1	A	780	ASN
1	A	809	ASN
1	A	861	ASN
1	A	909	HIS
1	A	911	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	941	GLN
1	A	961	ASN
1	A	975	ASN
1	A	1276	ASN
1	A	1363	GLN
1	A	1378	GLN
1	A	1459	ASN
1	A	1463	GLN
1	A	1470	GLN
1	A	1478	GLN
1	A	1494	GLN
1	A	1502	ASN
1	A	1505	GLN
1	A	1528	ASN
1	A	1539	GLN
1	A	1721	HIS
1	A	1819	ASN
1	A	1822	GLN
1	A	1871	ASN
2	B	102	GLN
2	B	115	HIS
3	C	53	ASN
3	C	82	GLN
3	C	145	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.25	0	17,19,21	0.48	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.40	0
4	NAG	E	1	1,4	14,14,15	0.17	0	17,19,21	0.48	0
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.68	0
4	NAG	F	1	4,2	14,14,15	0.56	0	17,19,21	1.18	2 (11%)
4	NAG	F	2	4	14,14,15	0.66	0	17,19,21	1.22	1 (5%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

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

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

Continued on next page...

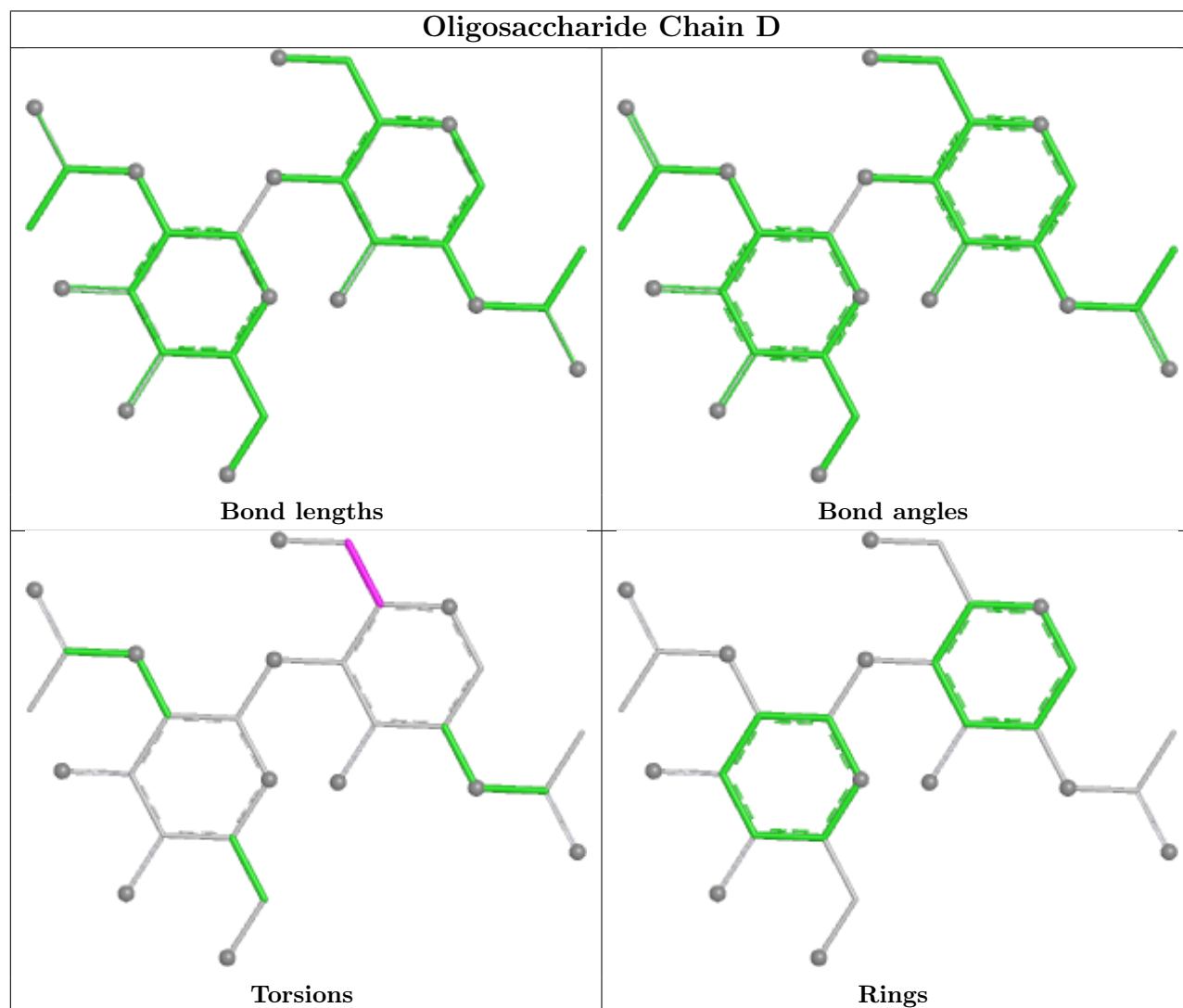
Continued from previous page...

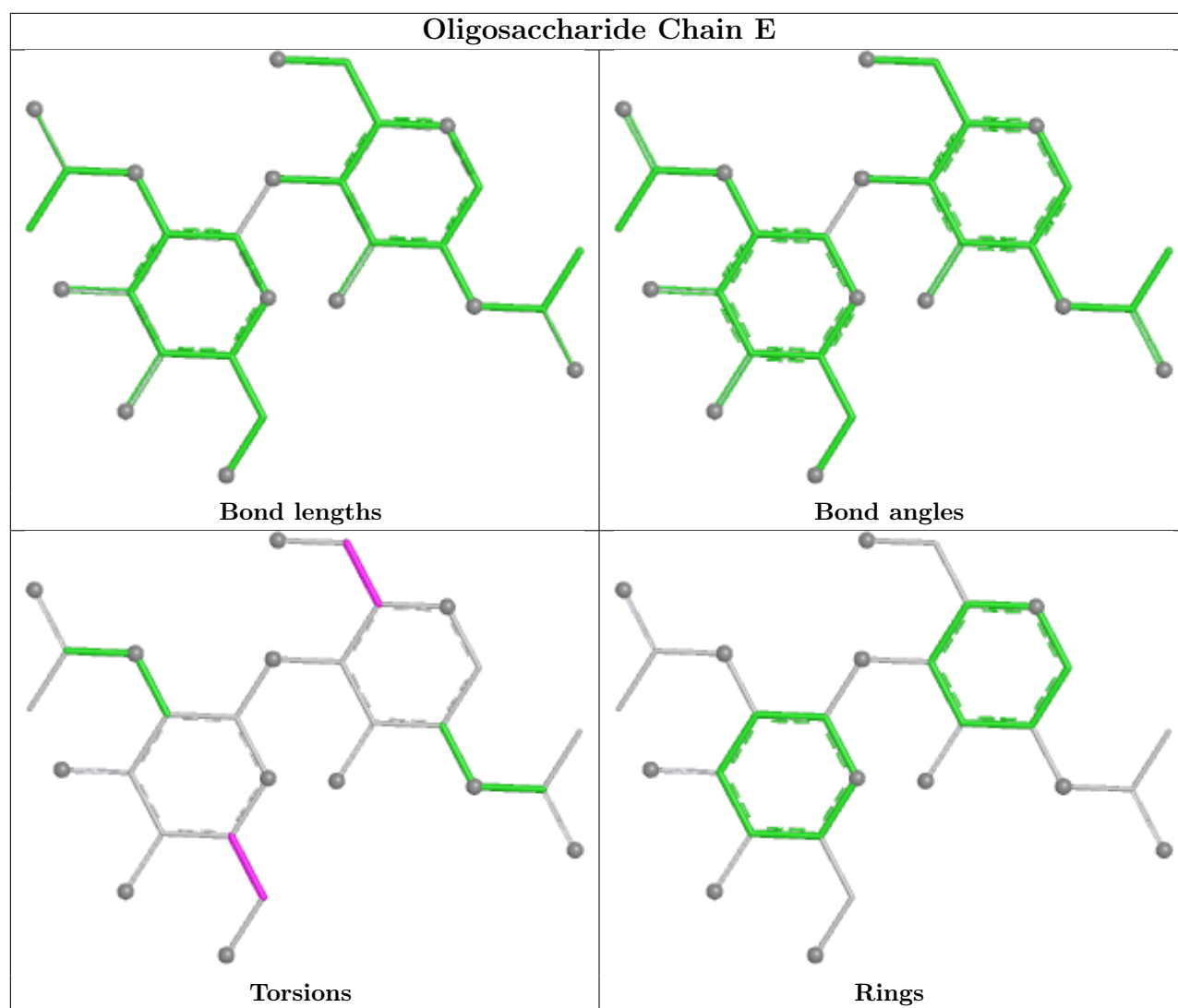
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

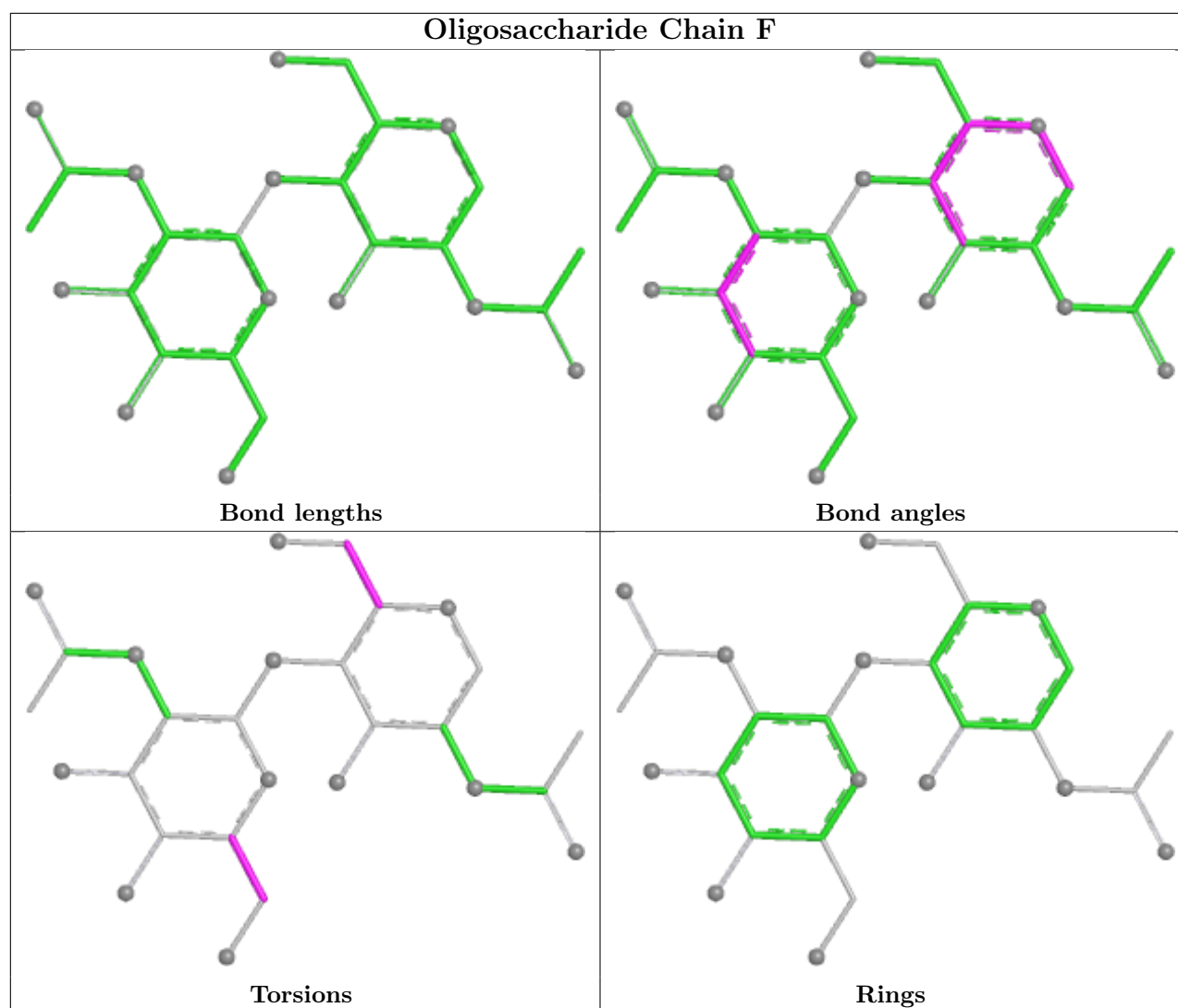
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	LPE	A	2025	-	24,24,33	0.55	0	28,30,39	0.50	0
6	NAG	B	303	2	14,14,15	0.27	0	17,19,21	0.44	0
6	NAG	B	301	2	14,14,15	0.64	0	17,19,21	0.97	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LPE	A	2025	-	-	10/25/25/34	-

Continued on next page...

Continued from previous page...

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

All (42) bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	9SL	C12-N13	8.85	1.49	1.35
5	A	2001	9SL	C07-N08	6.30	1.45	1.34
5	A	2001	9SL	C02-N21	6.16	1.44	1.33
5	A	2001	9SL	C12-N15	4.65	1.45	1.34
8	A	2029	Y01	CBB-CBE	-4.44	1.46	1.54
7	A	2017	P5S	O37-C38	4.42	1.46	1.34
11	A	2027	PCW	O3-C11	4.42	1.46	1.33
11	A	2028	PCW	O3-C11	4.29	1.45	1.33
8	A	2029	Y01	CAR-CBC	-4.22	1.40	1.51
11	A	2013	PCW	O2-C31	4.17	1.46	1.34
11	A	2013	PCW	O3-C11	4.16	1.45	1.33
5	A	2001	9SL	C05-C14	4.12	1.60	1.52
11	A	2028	PCW	O2-C31	4.11	1.45	1.34
11	A	2018	PCW	O2-C31	3.96	1.45	1.34
7	A	2017	P5S	O19-C17	3.95	1.44	1.33
11	A	2027	PCW	O2-C31	3.89	1.45	1.34
11	A	2018	PCW	O3-C11	3.88	1.44	1.33
11	A	2016	PCW	O3-C11	3.85	1.44	1.33
7	A	2017	P5S	C28-C27	-3.82	1.32	1.51
8	A	2029	Y01	OAW-CAY	3.71	1.44	1.34
11	A	2016	PCW	O2-C31	3.68	1.44	1.34
8	A	2006	Y01	OAW-CAY	3.62	1.44	1.34
8	A	2009	Y01	OAW-CAY	3.59	1.44	1.34
7	A	2003	P5S	O37-C38	3.42	1.43	1.34
8	A	2029	Y01	CAV-CBC	3.16	1.59	1.52
5	A	2001	9SL	O01-C02	-2.85	1.17	1.22
5	A	2001	9SL	O03-C02	2.83	1.39	1.35
5	A	2001	9SL	C05-N06	-2.61	1.43	1.47
8	A	2009	Y01	CAM-CAY	2.41	1.57	1.50
8	A	2006	Y01	CAM-CAY	2.41	1.57	1.50
8	A	2029	Y01	CAM-CAY	2.40	1.57	1.50
8	A	2004	Y01	CBH-CBF	-2.34	1.52	1.56
8	A	2029	Y01	CBH-CBF	-2.34	1.52	1.56
8	A	2009	Y01	CBH-CBF	-2.32	1.52	1.56
9	A	2007	9Z9	C11-C08	-2.29	1.52	1.56
8	A	2006	Y01	CBH-CBF	-2.24	1.52	1.56
8	A	2006	Y01	CAL-CAX	2.24	1.55	1.50
8	A	2005	Y01	CBH-CBF	-2.24	1.52	1.56
8	A	2009	Y01	CAL-CAX	2.23	1.55	1.50
8	A	2029	Y01	CAL-CAX	2.17	1.55	1.50
11	A	2016	PCW	C6-N	-2.16	1.43	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	9SL	C14-N13	-2.02	1.42	1.45

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2028	PCW	C8-N-C6	-11.84	77.88	108.98
11	A	2028	PCW	C8-N-C7	-11.78	78.04	108.98
11	A	2028	PCW	C8-N-C5	-8.04	77.97	109.91
5	A	2001	9SL	O03-C02-N21	7.78	120.78	111.11
7	A	2003	P5S	OG-CB-CA	7.06	114.22	108.06
8	A	2006	Y01	CBI-CBE-CBB	-6.03	110.19	119.50
8	A	2004	Y01	CBI-CBE-CBB	-6.01	110.22	119.50
8	A	2009	Y01	CBI-CBE-CBB	-6.01	110.22	119.50
8	A	2005	Y01	CBI-CBE-CBB	-5.99	110.24	119.50
7	A	2017	P5S	O37-C38-C39	5.46	123.29	111.48
8	A	2005	Y01	CBI-CBG-CBD	-5.07	107.22	114.41
8	A	2004	Y01	CBI-CBG-CBD	-5.01	107.30	114.41
8	A	2029	Y01	CBI-CBG-CBD	-4.98	107.35	114.41
8	A	2009	Y01	CBI-CBG-CBD	-4.96	107.38	114.41
8	A	2006	Y01	CBI-CBG-CBD	-4.95	107.38	114.41
11	A	2016	PCW	O2-C31-C32	4.83	121.93	111.48
9	A	2007	9Z9	C02-C06-C07	-4.59	107.90	114.41
5	A	2001	9SL	O01-C02-N21	-4.50	118.48	125.58
8	A	2029	Y01	CBI-CBE-CBB	-4.25	112.94	119.50
7	A	2003	P5S	OXT-C-O	-4.09	114.81	124.08
8	A	2005	Y01	OAW-CAY-CAM	3.97	120.08	111.48
8	A	2004	Y01	OAW-CAY-CAM	3.97	120.08	111.48
11	A	2013	PCW	O2-C31-C32	3.88	119.86	111.48
10	A	2020	LPE	C3N-N-C2N	3.84	119.07	108.98
8	A	2009	Y01	OAW-CAY-CAM	3.74	119.56	111.48
8	A	2006	Y01	OAW-CAY-CAM	3.73	119.55	111.48
9	A	2007	9Z9	C02-C03-C74	-3.71	109.52	120.50
11	A	2028	PCW	O2-C31-C32	3.69	119.47	111.48
7	A	2003	P5S	O37-C38-C39	3.67	119.41	111.48
8	A	2029	Y01	OAW-CAY-CAM	3.59	119.24	111.48
8	A	2009	Y01	CAS-CAU-CBI	-3.38	107.04	112.74
8	A	2006	Y01	CAS-CAU-CBI	-3.35	107.08	112.74
8	A	2005	Y01	CAS-CAU-CBI	-3.35	107.08	112.74
8	A	2004	Y01	CAS-CAU-CBI	-3.35	107.09	112.74
8	A	2029	Y01	CAS-CAU-CBI	-3.35	107.09	112.74
9	A	2007	9Z9	C09-C10-C02	-3.33	107.12	112.74
5	A	2001	9SL	N09-C07-N06	-3.29	120.83	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2027	PCW	O2-C31-C32	3.25	118.52	111.48
9	A	2007	9Z9	C76-C73-C74	-3.17	109.92	115.66
11	A	2016	PCW	O3-C11-C12	3.17	121.49	111.83
8	A	2004	Y01	CAD-CBH-CBF	-3.16	108.12	111.66
8	A	2005	Y01	CAD-CBH-CBF	-3.11	108.17	111.66
8	A	2009	Y01	CAD-CBH-CBF	-3.10	108.18	111.66
8	A	2006	Y01	CAD-CBH-CBF	-3.10	108.18	111.66
5	A	2001	9SL	N13-C12-N11	-3.06	107.66	115.62
8	A	2029	Y01	CAD-CBH-CBF	-3.05	108.23	111.66
9	A	2007	9Z9	C12-C11-C08	-3.00	108.29	111.66
11	A	2018	PCW	C3-C2-C1	-2.94	104.92	111.78
6	A	2008	NAG	C4-C3-C2	-2.90	106.77	111.02
11	A	2028	PCW	O3-C11-C12	2.87	120.57	111.83
10	A	2014	LPE	C3-C2-C1	-2.86	104.41	112.65
9	A	2007	9Z9	C75-C74-C73	-2.86	110.33	114.94
11	A	2018	PCW	O2-C31-C32	2.78	117.50	111.48
8	A	2029	Y01	CBG-CBI-CBE	2.77	103.28	100.10
8	A	2005	Y01	CBG-CBI-CBE	2.76	103.27	100.10
8	A	2009	Y01	CBG-CBI-CBE	2.75	103.26	100.10
8	A	2004	Y01	CBG-CBI-CBE	2.75	103.26	100.10
8	A	2006	Y01	CBG-CBI-CBE	2.74	103.25	100.10
8	A	2005	Y01	CAS-CBF-CBH	-2.70	109.75	113.08
9	A	2007	9Z9	C09-C08-C11	-2.68	109.78	113.08
10	A	2014	LPE	C31-C32-N	-2.67	107.24	115.82
8	A	2029	Y01	CAS-CBF-CBH	-2.66	109.80	113.08
8	A	2006	Y01	CAS-CBF-CBH	-2.64	109.82	113.08
8	A	2004	Y01	CAS-CBF-CBH	-2.63	109.84	113.08
8	A	2009	Y01	CAS-CBF-CBH	-2.63	109.84	113.08
11	A	2018	PCW	O3-C11-C12	2.62	119.81	111.83
11	A	2028	PCW	C7-N-C6	2.61	115.83	108.98
8	A	2009	Y01	CBD-CAK-CAI	-2.58	109.19	112.76
8	A	2004	Y01	CBD-CAK-CAI	-2.57	109.20	112.76
8	A	2005	Y01	CBD-CAK-CAI	-2.54	109.24	112.76
9	A	2007	9Z9	C07-C15-C14	-2.54	109.25	112.76
5	A	2001	9SL	O03-C02-O01	-2.54	120.74	123.08
11	A	2013	PCW	O3-C11-C12	2.53	119.54	111.83
8	A	2006	Y01	CBD-CAK-CAI	-2.53	109.26	112.76
8	A	2029	Y01	CBD-CAK-CAI	-2.53	109.26	112.76
8	A	2004	Y01	CBF-CBH-CAZ	2.51	113.33	109.65
8	A	2029	Y01	CBF-CBH-CAZ	2.51	113.33	109.65
8	A	2009	Y01	CBF-CBH-CAZ	2.50	113.31	109.65
8	A	2006	Y01	CBF-CBH-CAZ	2.49	113.29	109.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2005	Y01	CBF-CBH-CAZ	2.43	113.20	109.65
9	A	2007	9Z9	C08-C11-C13	2.41	113.18	109.65
11	A	2027	PCW	O3-C11-C12	2.40	119.14	111.83
7	A	2003	P5S	C2-O37-C38	-2.36	112.14	117.80
9	A	2007	9Z9	O80-C79-C78	-2.31	109.20	112.17
7	A	2017	P5S	C41-C40-C39	-2.29	104.70	113.13
5	A	2001	9SL	O03-C04-C05	2.29	112.95	108.46
8	A	2005	Y01	CAC-CBB-CBE	-2.29	109.45	112.88
10	A	2021	LPE	C31-C32-N	-2.27	108.53	115.82
8	A	2006	Y01	CAC-CBB-CBE	-2.25	109.51	112.88
8	A	2009	Y01	CAC-CBB-CBE	-2.24	109.53	112.88
8	A	2004	Y01	CAC-CBB-CBE	-2.23	109.54	112.88
10	A	2019	LPE	C31-C32-N	-2.23	108.68	115.82
7	A	2017	P5S	O15-P12-O13	2.19	122.65	112.44
11	A	2016	PCW	O2-C31-O31	-2.19	118.58	123.70
8	A	2004	Y01	CAQ-CBG-CBD	-2.12	115.72	119.10
5	A	2001	9SL	C14-C05-N06	2.11	116.99	111.22
8	A	2005	Y01	CAQ-CBG-CBD	-2.11	115.73	119.10
8	A	2006	Y01	CAQ-CBG-CBD	-2.11	115.73	119.10
11	A	2018	PCW	O3-C3-C2	2.10	114.44	108.40
8	A	2029	Y01	CAQ-CBG-CBD	-2.10	115.76	119.10
11	A	2018	PCW	C34-C33-C32	-2.09	105.44	113.13
9	A	2007	9Z9	C17-C16-C13	-2.09	108.37	111.45
8	A	2006	Y01	CBC-CAV-CAZ	-2.08	108.37	111.45
8	A	2009	Y01	CAQ-CBG-CBD	-2.07	115.79	119.10
11	A	2016	PCW	O3-C11-O11	-2.07	118.45	123.63
8	A	2029	Y01	CAT-CAR-CBC	2.05	113.68	110.33
8	A	2004	Y01	CBC-CAV-CAZ	-2.05	108.43	111.45
8	A	2005	Y01	CBC-CAV-CAZ	-2.05	108.43	111.45
8	A	2009	Y01	CBC-CAV-CAZ	-2.04	108.43	111.45
11	A	2018	PCW	O3-C11-O11	-2.01	118.60	123.63
8	A	2005	Y01	CAJ-CAO-CBB	-2.01	109.47	115.08
8	A	2029	Y01	CAR-CBC-CAV	2.00	113.76	110.97

There are no chirality outliers.

All (225) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2001	9SL	O01-C02-O03-C04
5	A	2001	9SL	N21-C02-O03-C04
5	A	2001	9SL	O03-C04-C05-N06
5	A	2001	9SL	O03-C04-C05-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	2003	P5S	C-CA-CB-OG
7	A	2003	P5S	N-CA-CB-OG
7	A	2003	P5S	CB-OG-P12-O13
7	A	2003	P5S	CB-OG-P12-O16
7	A	2003	P5S	C3-O16-P12-OG
7	A	2003	P5S	C3-O16-P12-O13
7	A	2003	P5S	C3-O16-P12-O15
7	A	2017	P5S	CB-OG-P12-O15
7	A	2017	P5S	C3-O16-P12-OG
7	A	2017	P5S	C3-O16-P12-O13
7	A	2017	P5S	C3-O16-P12-O15
10	A	2010	LPE	C3-O3-P-O31
10	A	2011	LPE	C3-O3-P-O31
10	A	2011	LPE	C31-O33-P-O3
10	A	2012	LPE	C3-O3-P-O32
10	A	2012	LPE	C3-O3-P-O33
10	A	2012	LPE	C31-O33-P-O31
10	A	2014	LPE	O1-C1-C2-C3
10	A	2014	LPE	C3-O3-P-O32
10	A	2014	LPE	C3-O3-P-O33
10	A	2014	LPE	C31-O33-P-O3
10	A	2014	LPE	C31-O33-P-O31
10	A	2014	LPE	C32-C31-O33-P
10	A	2014	LPE	O33-C31-C32-N
10	A	2015	LPE	C3-O3-P-O32
10	A	2015	LPE	C3-O3-P-O33
10	A	2019	LPE	C31-O33-P-O31
10	A	2019	LPE	O33-C31-C32-N
10	A	2020	LPE	C31-O33-P-O31
10	A	2021	LPE	C31-O33-P-O31
10	A	2022	LPE	C3-O3-P-O33
10	A	2023	LPE	C31-O33-P-O3
10	A	2023	LPE	C31-O33-P-O32
10	A	2024	LPE	C31-O33-P-O31
10	A	2025	LPE	O1-C1-C2-C3
10	A	2025	LPE	C3-O3-P-O32
10	A	2025	LPE	C3-O3-P-O33
10	A	2025	LPE	C31-O33-P-O3
10	A	2025	LPE	C31-O33-P-O31
10	A	2025	LPE	C31-O33-P-O32
10	A	2026	LPE	C31-O33-P-O3
10	B	304	LPE	C3-O3-P-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	B	304	LPE	C3-O3-P-O32
10	B	304	LPE	C3-O3-P-O33
10	B	304	LPE	C31-O33-P-O3
11	A	2013	PCW	C4-O4P-P-O3P
11	A	2016	PCW	O4P-C4-C5-N
11	A	2016	PCW	C4-O4P-P-O3P
11	A	2018	PCW	C32-C31-O2-C2
11	A	2018	PCW	C4-O4P-P-O3P
11	A	2027	PCW	O4P-C4-C5-N
11	A	2027	PCW	C1-O3P-P-O2P
11	A	2027	PCW	C4-O4P-P-O2P
8	A	2029	Y01	CAC-CBB-CBE-CAP
8	A	2029	Y01	CAC-CBB-CBE-CBI
11	A	2018	PCW	O31-C31-O2-C2
8	A	2029	Y01	CAJ-CAO-CBB-CAC
8	A	2029	Y01	CAO-CBB-CBE-CBI
11	A	2027	PCW	O11-C11-O3-C3
11	A	2027	PCW	C12-C11-O3-C3
6	A	2002	NAG	O5-C5-C6-O6
10	A	2025	LPE	O1-C1-C2-O2H
8	A	2029	Y01	CAO-CBB-CBE-CAP
6	A	2002	NAG	C4-C5-C6-O6
11	A	2028	PCW	C12-C11-O3-C3
8	A	2006	Y01	CAR-CBC-OAW-CAY
10	A	2023	LPE	C31-C32-N-C2N
10	A	2023	LPE	C31-C32-N-C3N
11	A	2016	PCW	C4-C5-N-C8
11	A	2018	PCW	C4-C5-N-C7
8	A	2029	Y01	CAJ-CAO-CBB-CBE
6	A	2008	NAG	C8-C7-N2-C2
8	A	2009	Y01	CAR-CBC-OAW-CAY
11	A	2028	PCW	O11-C11-O3-C3
10	A	2014	LPE	O1-C1-C2-O2H
6	A	2008	NAG	O7-C7-N2-C2
10	A	2026	LPE	C31-C32-N-C3N
11	A	2016	PCW	C4-C5-N-C7
7	A	2003	P5S	C38-C39-C40-C41
10	A	2014	LPE	O1-C11-C12-C13
10	A	2020	LPE	O1-C1-C2-O2H
8	A	2006	Y01	CAV-CBC-OAW-CAY
8	A	2009	Y01	CAV-CBC-OAW-CAY
10	A	2014	LPE	C31-C32-N-C1N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	2014	LPE	C31-C32-N-C2N
10	A	2014	LPE	C31-C32-N-C3N
11	A	2018	PCW	C4-C5-N-C6
11	A	2028	PCW	C4-C5-N-C8
10	A	2010	LPE	O1-C11-C12-C13
10	A	2020	LPE	O1-C1-C2-C3
10	A	2023	LPE	C31-C32-N-C1N
10	A	2011	LPE	O1-C11-C12-C13
7	A	2017	P5S	C25-C26-C27-C28
7	A	2003	P5S	C46-C48-C49-C50
7	A	2017	P5S	C27-C28-C29-C30
11	A	2016	PCW	C4-C5-N-C6
10	A	2020	LPE	C12-C13-C14-C15
11	A	2013	PCW	C32-C31-O2-C2
7	A	2003	P5S	C41-C42-C43-C44
11	A	2027	PCW	C33-C34-C35-C36
7	A	2003	P5S	C52-C53-C54-C55
10	A	2026	LPE	C31-C32-N-C1N
10	A	2026	LPE	C31-C32-N-C2N
11	A	2018	PCW	C4-C5-N-C8
11	A	2013	PCW	C32-C33-C34-C35
7	A	2003	P5S	C39-C38-O37-C2
11	A	2028	PCW	C32-C31-O2-C2
11	A	2027	PCW	C31-C32-C33-C34
7	A	2003	P5S	C51-C52-C53-C54
10	A	2020	LPE	C14-C15-C16-C17
11	A	2013	PCW	C24-C25-C26-C27
11	A	2013	PCW	O31-C31-O2-C2
10	A	2010	LPE	C2-C1-O1-C11
7	A	2003	P5S	C48-C49-C50-C51
10	A	2024	LPE	C13-C14-C15-C16
10	A	2011	LPE	C13-C14-C15-C16
8	A	2029	Y01	CAN-CAJ-CAO-CBB
11	A	2016	PCW	C35-C36-C37-C38
11	A	2016	PCW	C34-C35-C36-C37
10	A	2015	LPE	O1-C1-C2-O2H
10	B	304	LPE	C2-C3-O3-P
11	A	2013	PCW	C41-C42-C43-C44
7	A	2003	P5S	C1-C2-C3-O16
7	A	2003	P5S	O47-C38-O37-C2
11	A	2028	PCW	O31-C31-O2-C2
7	A	2003	P5S	C2-C3-O16-P12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	2026	LPE	C2-C1-O1-C11
10	A	2015	LPE	O1-C1-C2-C3
10	A	2020	LPE	C11-C12-C13-C14
10	A	2020	LPE	C16-C17-C18-C19
10	A	2019	LPE	C2-C1-O1-C11
10	B	304	LPE	C2-C1-O1-C11
8	A	2006	Y01	CAO-CAJ-CAN-CBA
8	A	2009	Y01	CAO-CAJ-CAN-CBA
7	A	2003	P5S	O37-C2-C3-O16
10	A	2011	LPE	C32-C31-O33-P
10	B	304	LPE	C32-C31-O33-P
11	A	2013	PCW	C4-C5-N-C7
10	A	2020	LPE	C12-C11-O1-C1
10	A	2010	LPE	O33-C31-C32-N
10	A	2012	LPE	O33-C31-C32-N
10	A	2015	LPE	O33-C31-C32-N
10	A	2020	LPE	O33-C31-C32-N
10	A	2021	LPE	O33-C31-C32-N
10	A	2022	LPE	O33-C31-C32-N
10	A	2023	LPE	O33-C31-C32-N
10	A	2024	LPE	O33-C31-C32-N
10	A	2025	LPE	O33-C31-C32-N
10	B	304	LPE	O33-C31-C32-N
11	A	2028	PCW	O4P-C4-C5-N
7	A	2003	P5S	C40-C41-C42-C43
10	A	2012	LPE	C12-C11-O1-C1
11	A	2013	PCW	C4-C5-N-C6
11	A	2027	PCW	O31-C31-O2-C2
10	A	2014	LPE	C12-C11-O1-C1
10	A	2019	LPE	C12-C11-O1-C1
11	A	2028	PCW	C19-C20-C21-C22
11	A	2027	PCW	C34-C35-C36-C37
10	A	2010	LPE	C11-C12-C13-C14
7	A	2003	P5S	CB-OG-P12-O15
7	A	2017	P5S	CB-OG-P12-O16
10	A	2011	LPE	C3-O3-P-O32
10	A	2011	LPE	C3-O3-P-O33
10	A	2011	LPE	C31-O33-P-O31
10	A	2012	LPE	C3-O3-P-O31
10	A	2015	LPE	C31-O33-P-O31
10	A	2019	LPE	C3-O3-P-O31
10	A	2020	LPE	C3-O3-P-O32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	2022	LPE	C3-O3-P-O31
10	A	2023	LPE	C31-O33-P-O31
10	A	2025	LPE	C3-O3-P-O31
10	A	2026	LPE	C31-O33-P-O31
10	B	304	LPE	C31-O33-P-O31
11	A	2013	PCW	C4-C5-N-C8
11	A	2013	PCW	C4-O4P-P-O2P
11	A	2016	PCW	C1-O3P-P-O2P
11	A	2016	PCW	C4-O4P-P-O2P
11	A	2018	PCW	C1-O3P-P-O2P
11	A	2018	PCW	C4-O4P-P-O2P
11	A	2028	PCW	C1-O3P-P-O2P
11	A	2028	PCW	C4-O4P-P-O2P
10	A	2024	LPE	C2-C1-O1-C11
10	A	2010	LPE	C2-C3-O3-P
11	A	2018	PCW	C2-C1-O3P-P
10	A	2014	LPE	C13-C14-C15-C16
7	A	2003	P5S	C50-C51-C52-C53
11	A	2016	PCW	C17-C18-C19-C20
11	A	2016	PCW	C37-C38-C39-C40
11	A	2027	PCW	C32-C31-O2-C2
10	A	2015	LPE	C12-C11-O1-C1
10	A	2012	LPE	C2-C3-O3-P
10	A	2025	LPE	C2-C1-O1-C11
11	A	2013	PCW	C23-C24-C25-C26
10	A	2014	LPE	C11-C12-C13-C14
11	A	2027	PCW	C11-C12-C13-C14
11	A	2013	PCW	C44-C45-C46-C47
7	A	2003	P5S	C43-C44-C45-C46
7	A	2003	P5S	O19-C1-C2-O37
11	A	2027	PCW	C21-C22-C23-C24
7	A	2003	P5S	C39-C40-C41-C42
11	A	2013	PCW	C17-C18-C19-C20
7	A	2003	P5S	C53-C54-C55-C56
10	A	2015	LPE	C2-C3-O3-P
11	A	2013	PCW	C13-C14-C15-C16
11	A	2016	PCW	C39-C40-C41-C42
11	A	2013	PCW	C39-C40-C41-C42
11	A	2018	PCW	O3-C11-C12-C13
11	A	2028	PCW	C17-C18-C19-C20
11	A	2013	PCW	C19-C20-C21-C22
10	A	2010	LPE	C31-C32-N-C2N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	2020	LPE	C13-C14-C15-C16
11	A	2027	PCW	C4-C5-N-C6
10	A	2010	LPE	C16-C17-C18-C19
10	A	2012	LPE	C31-C32-N-C2N
11	A	2027	PCW	C4-C5-N-C7
8	A	2006	Y01	CAN-CAJ-CAO-CBB
8	A	2009	Y01	CAN-CAJ-CAO-CBB
7	A	2003	P5S	C49-C50-C51-C52
11	A	2027	PCW	O3-C11-C12-C13
7	A	2003	P5S	O37-C38-C39-C40
7	A	2017	P5S	C39-C38-O37-C2

There are no ring outliers.

29 monomers are involved in 189 short contacts:

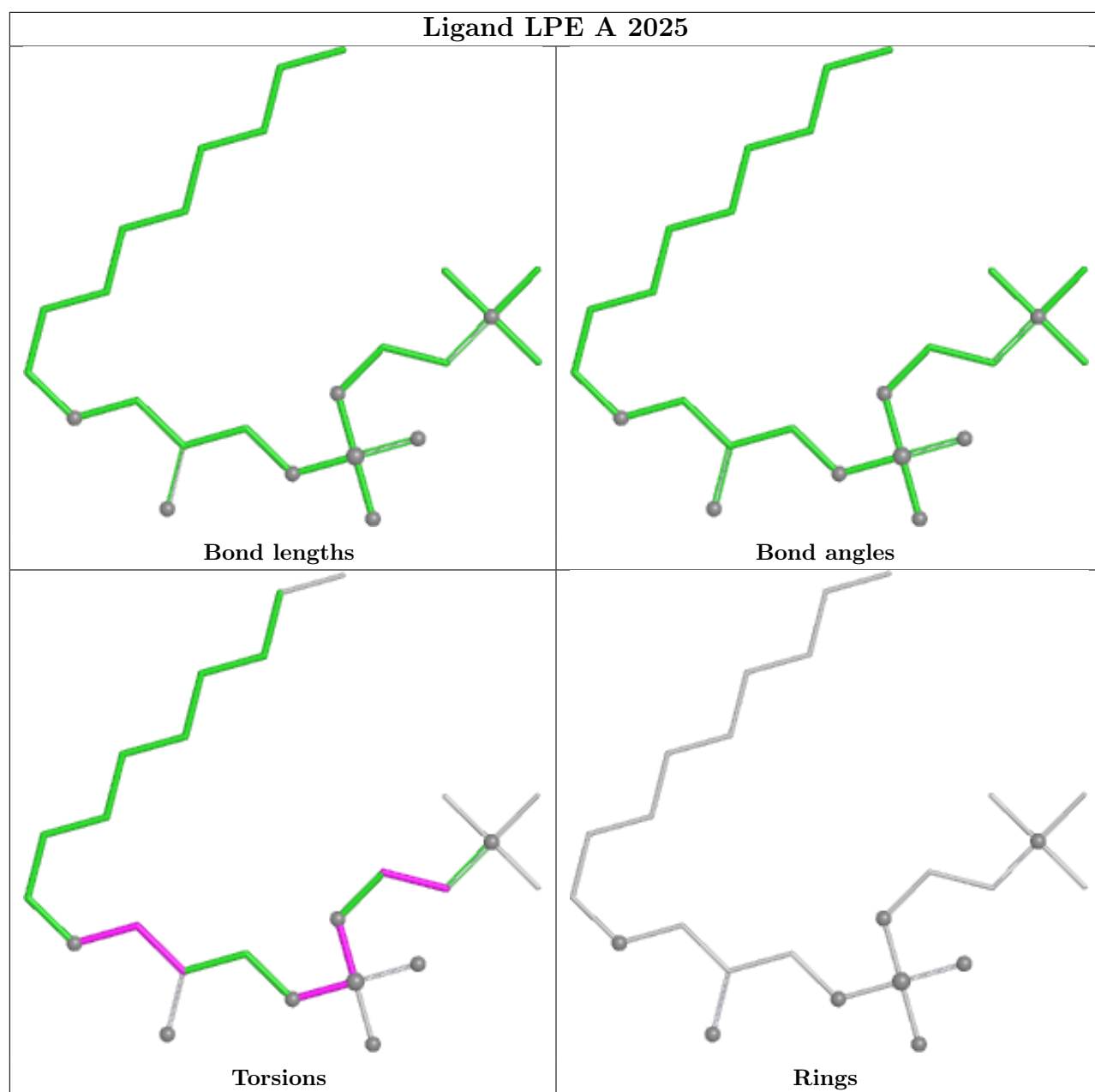
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2025	LPE	11	0
7	A	2003	P5S	12	0
10	A	2021	LPE	11	0
10	A	2011	LPE	2	0
11	A	2018	PCW	6	0
6	A	2008	NAG	9	0
10	A	2015	LPE	6	0
8	A	2005	Y01	3	0
10	A	2023	LPE	8	0
11	A	2028	PCW	2	0
10	A	2010	LPE	2	0
10	A	2012	LPE	9	0
7	A	2017	P5S	9	0
8	A	2006	Y01	16	0
8	A	2009	Y01	5	0
10	A	2024	LPE	1	0
10	B	304	LPE	9	0
8	A	2004	Y01	6	0
11	A	2016	PCW	1	0
10	A	2019	LPE	9	0
11	A	2013	PCW	22	0
8	A	2029	Y01	18	0
10	A	2022	LPE	7	0
10	A	2026	LPE	10	0
5	A	2001	9SL	3	0
10	A	2020	LPE	1	0

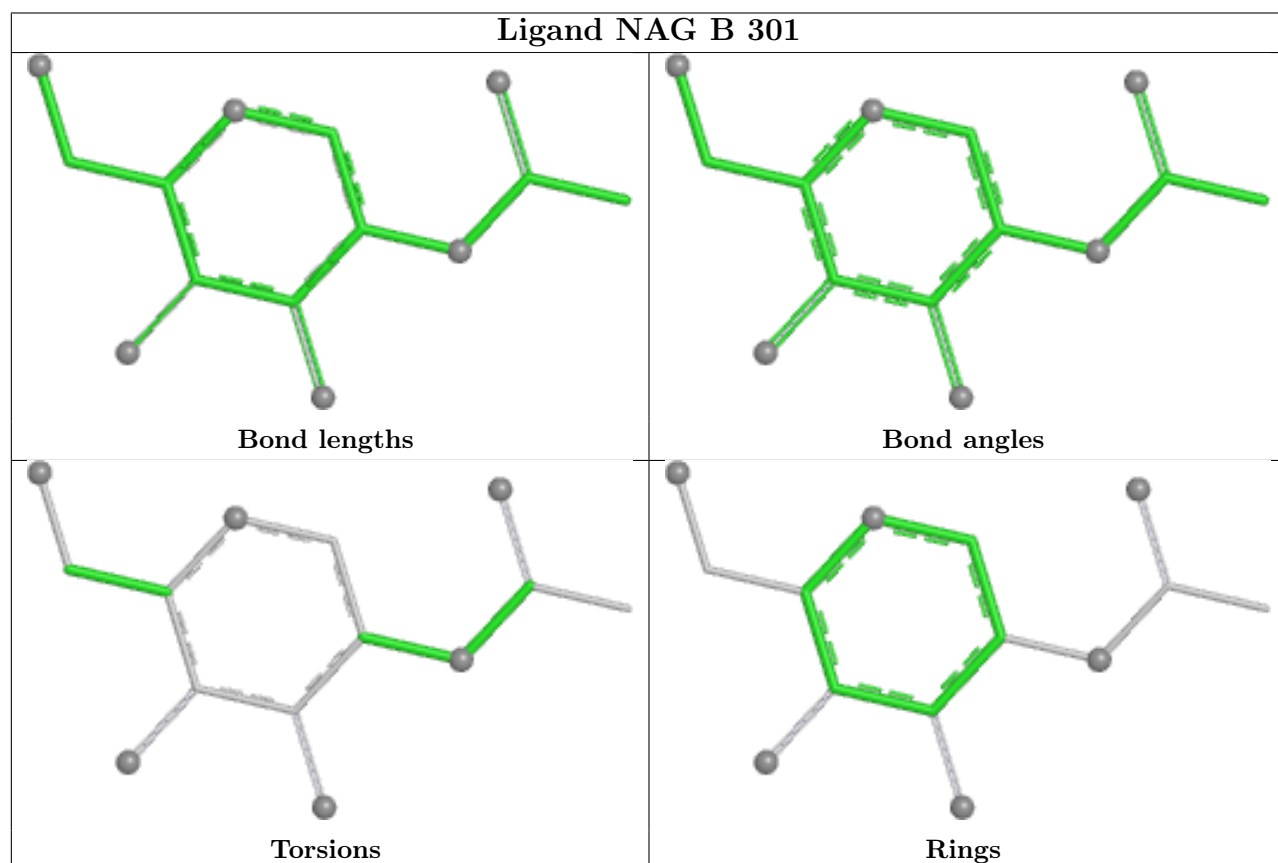
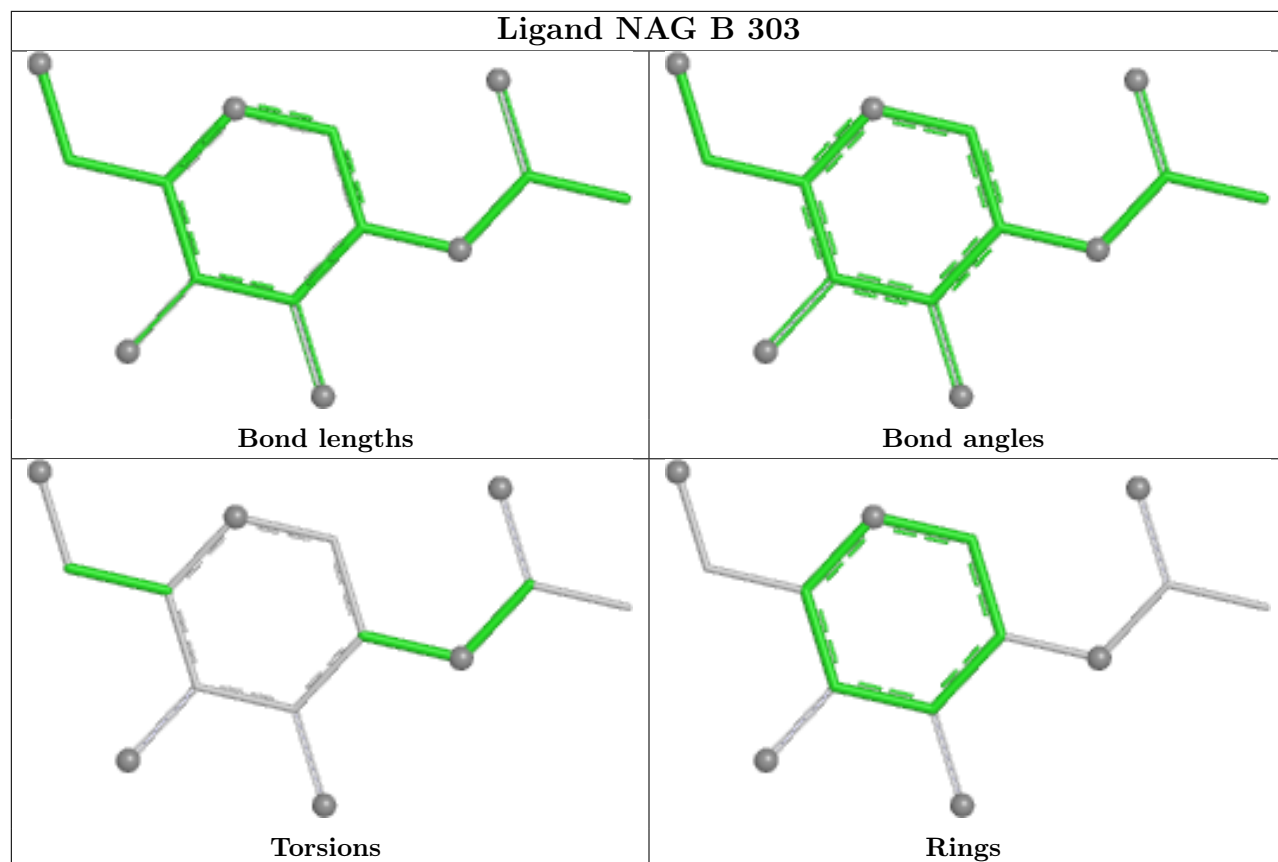
Continued on next page...

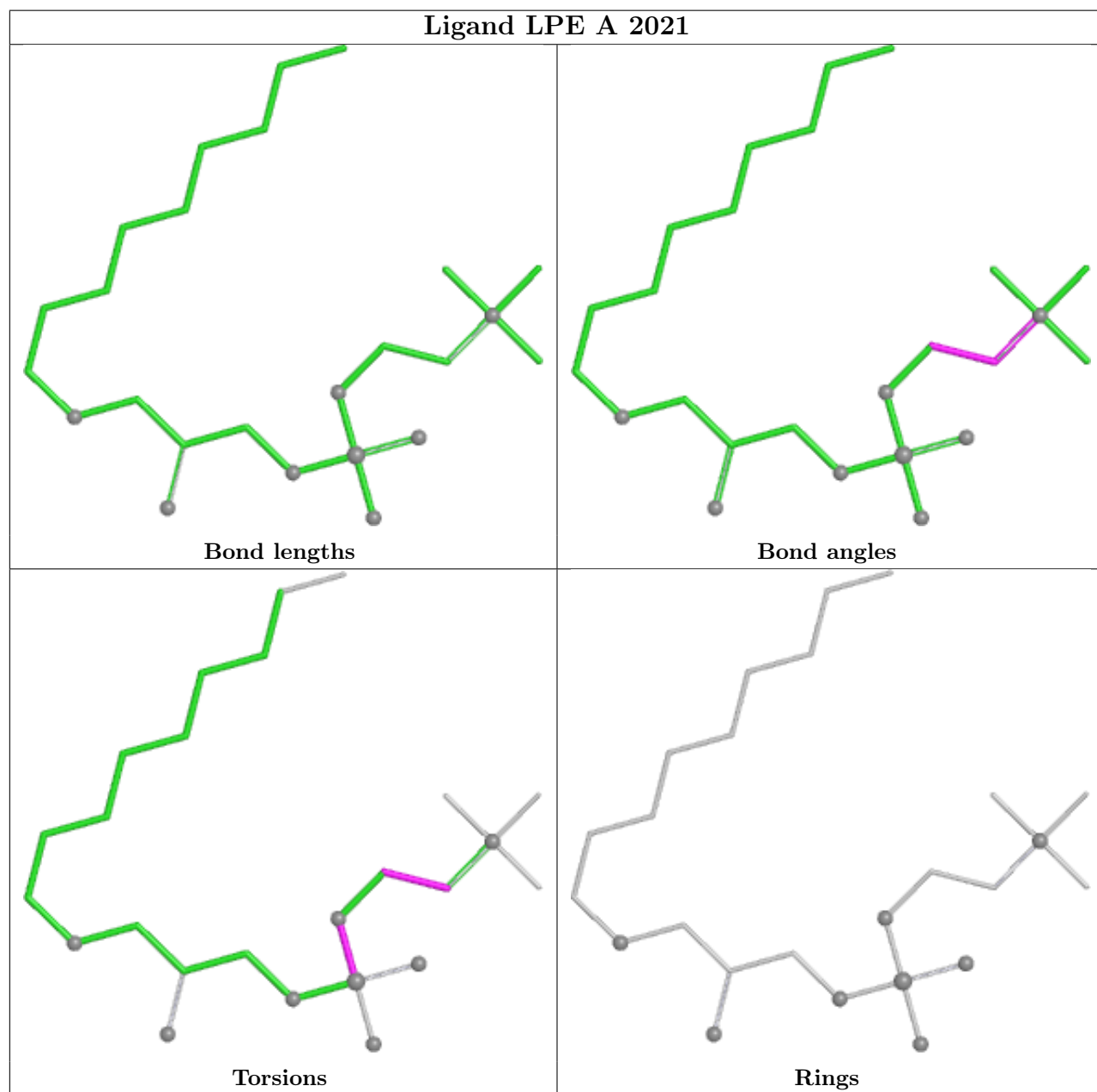
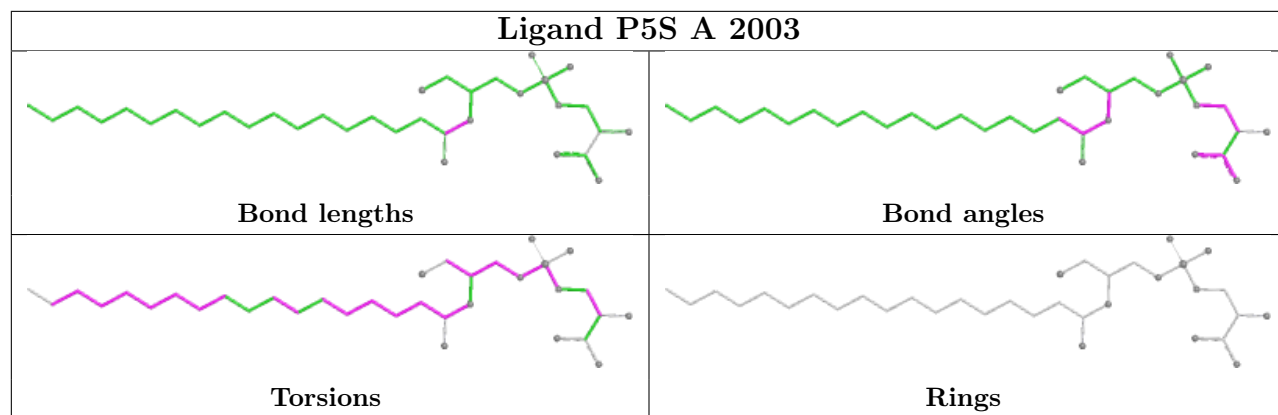
Continued from previous page...

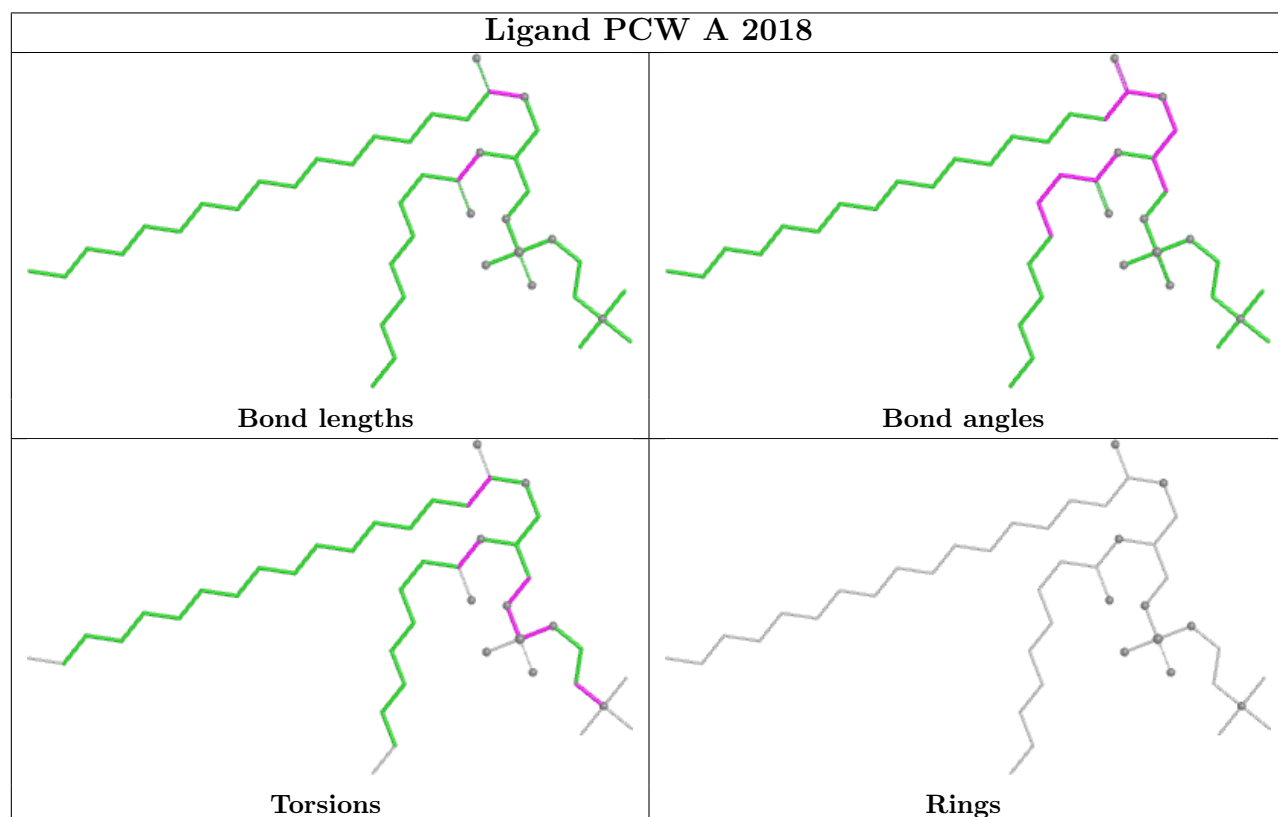
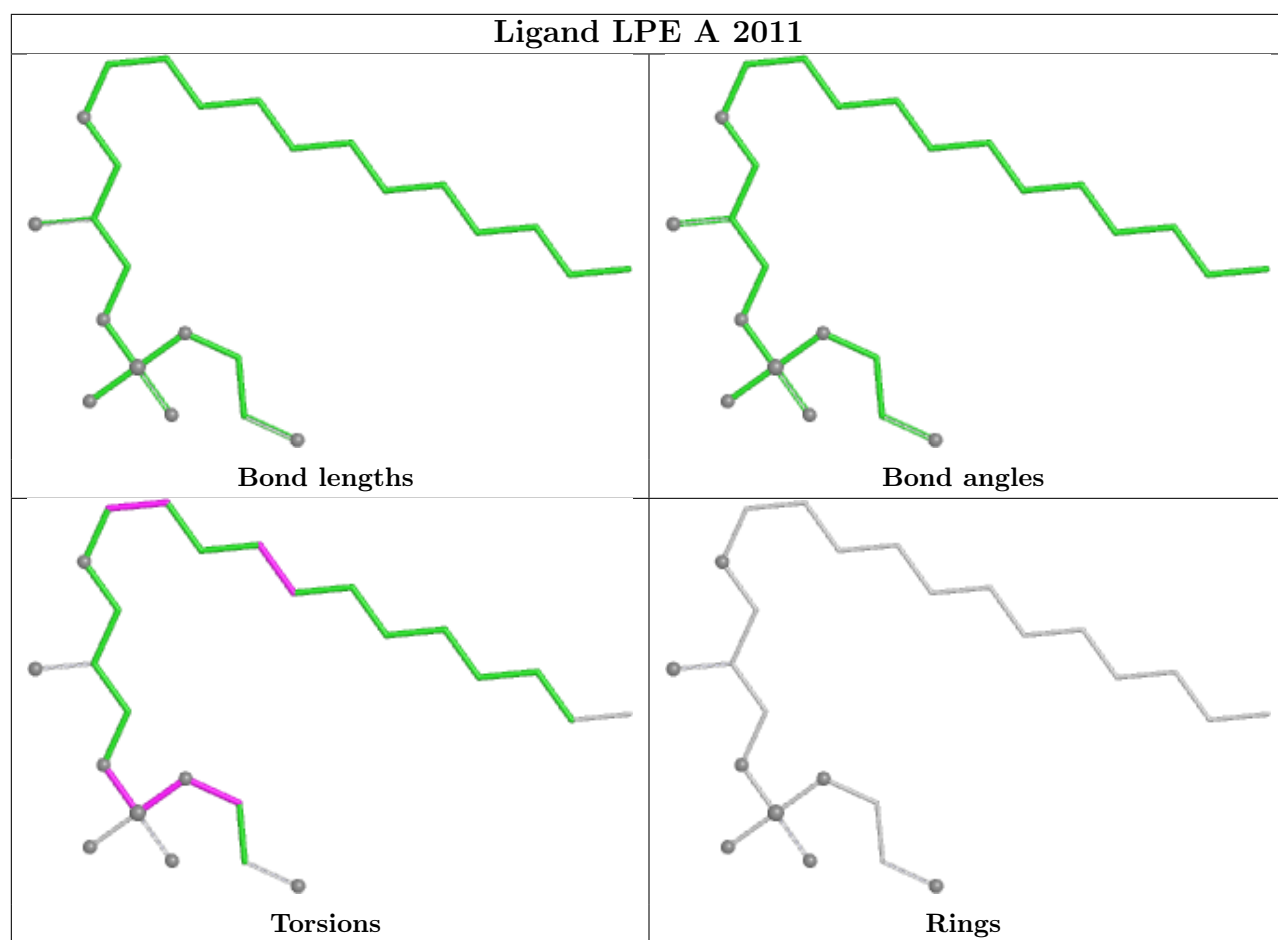
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2007	9Z9	9	0
10	A	2014	LPE	17	0
11	A	2027	PCW	8	0

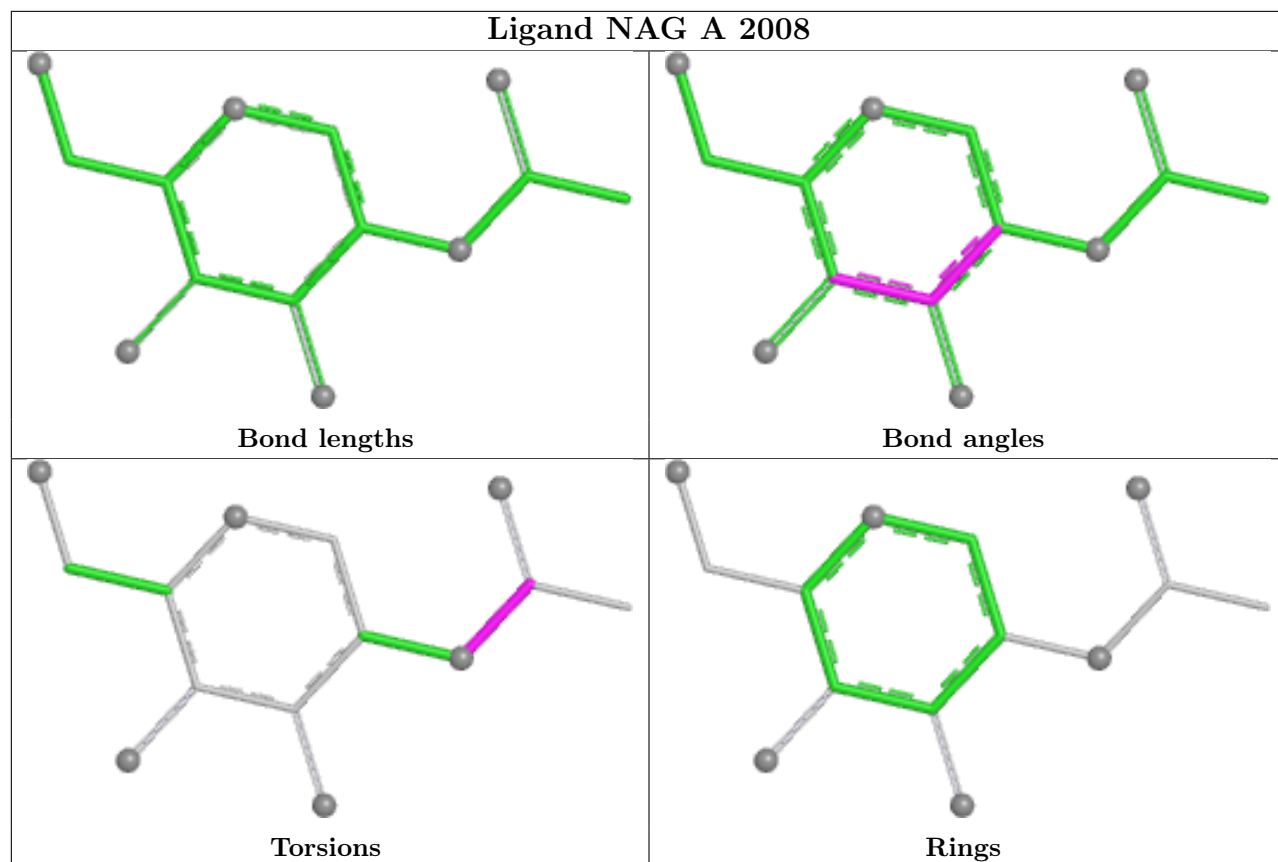
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

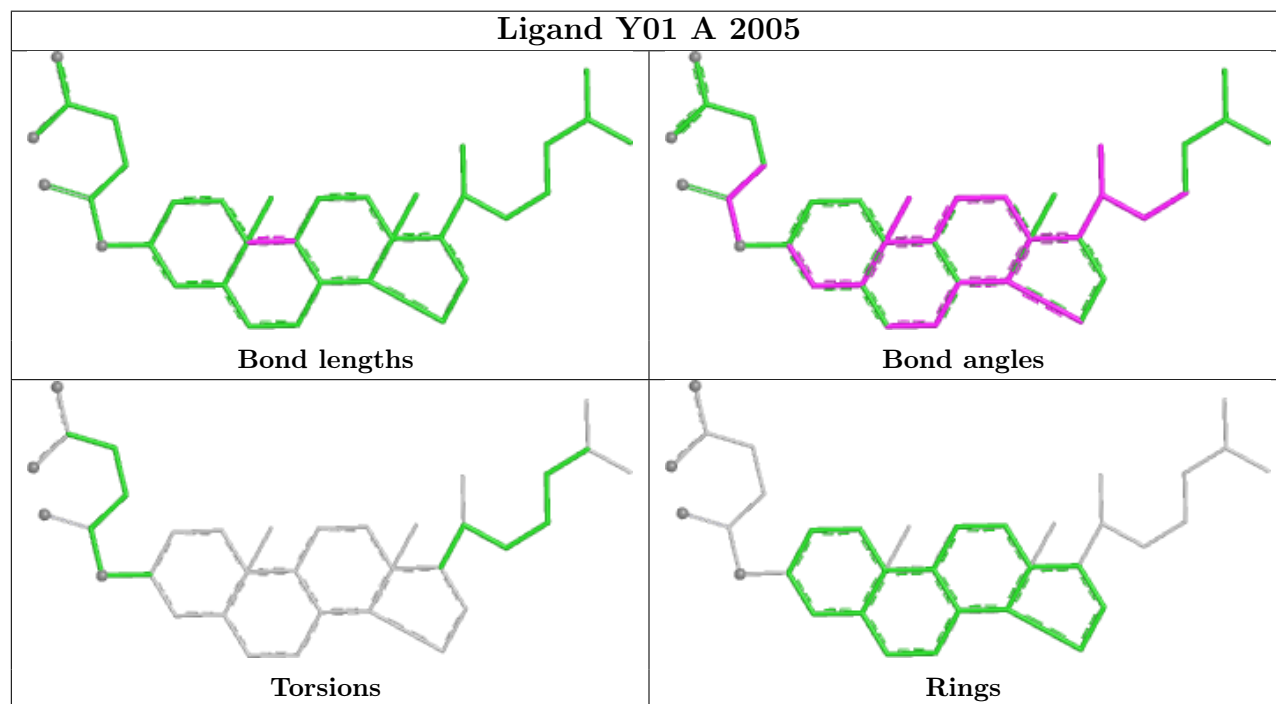
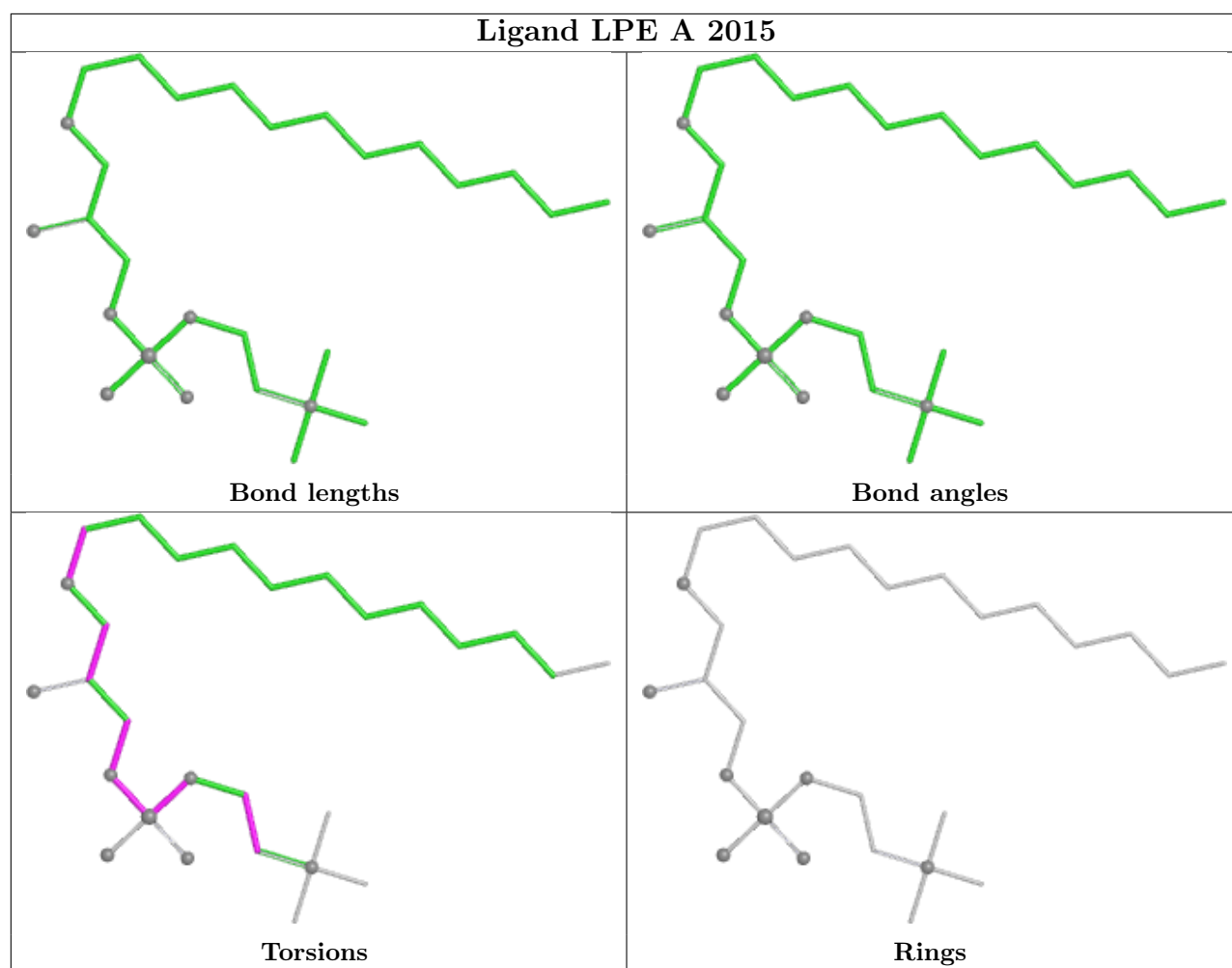


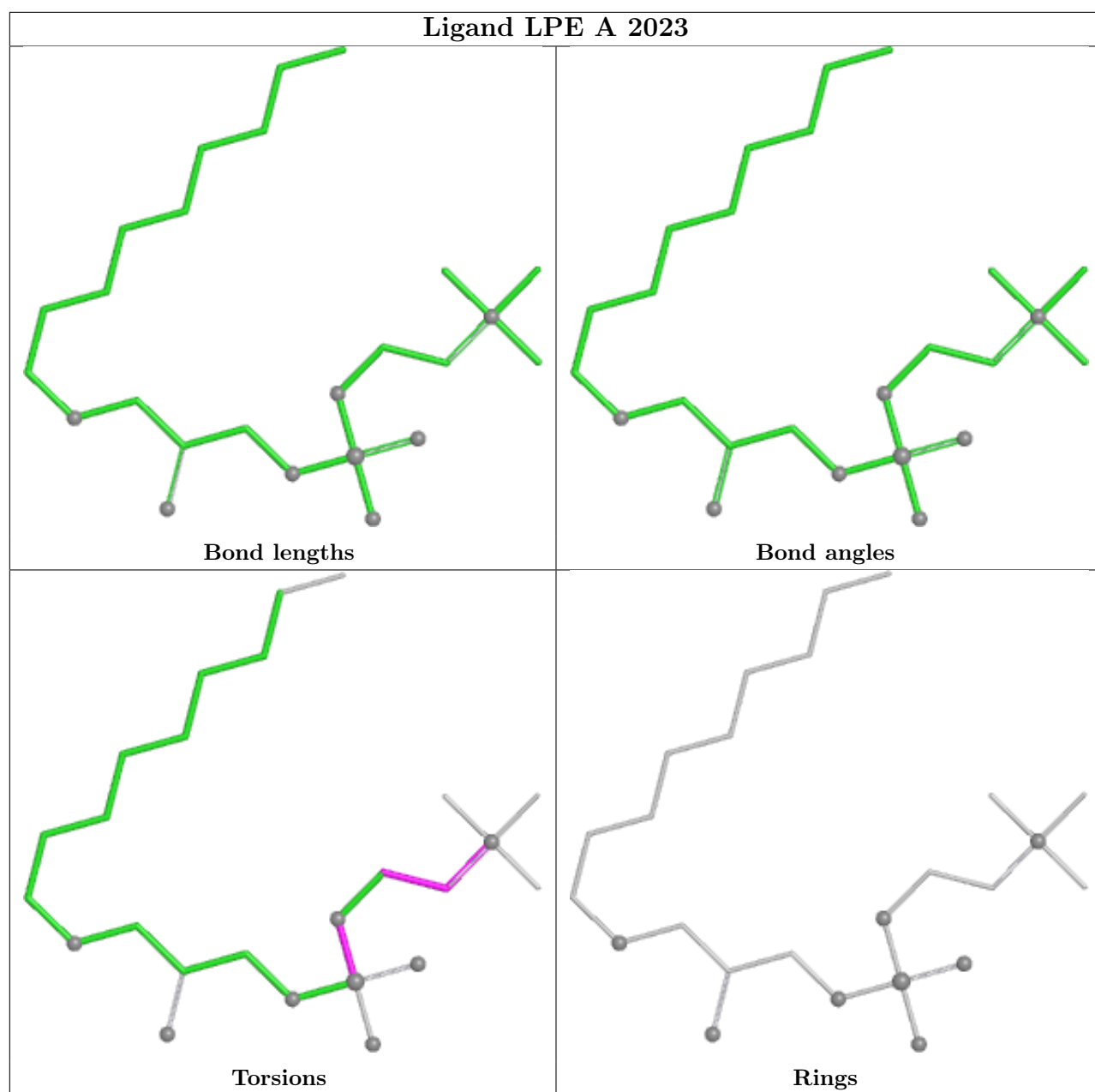


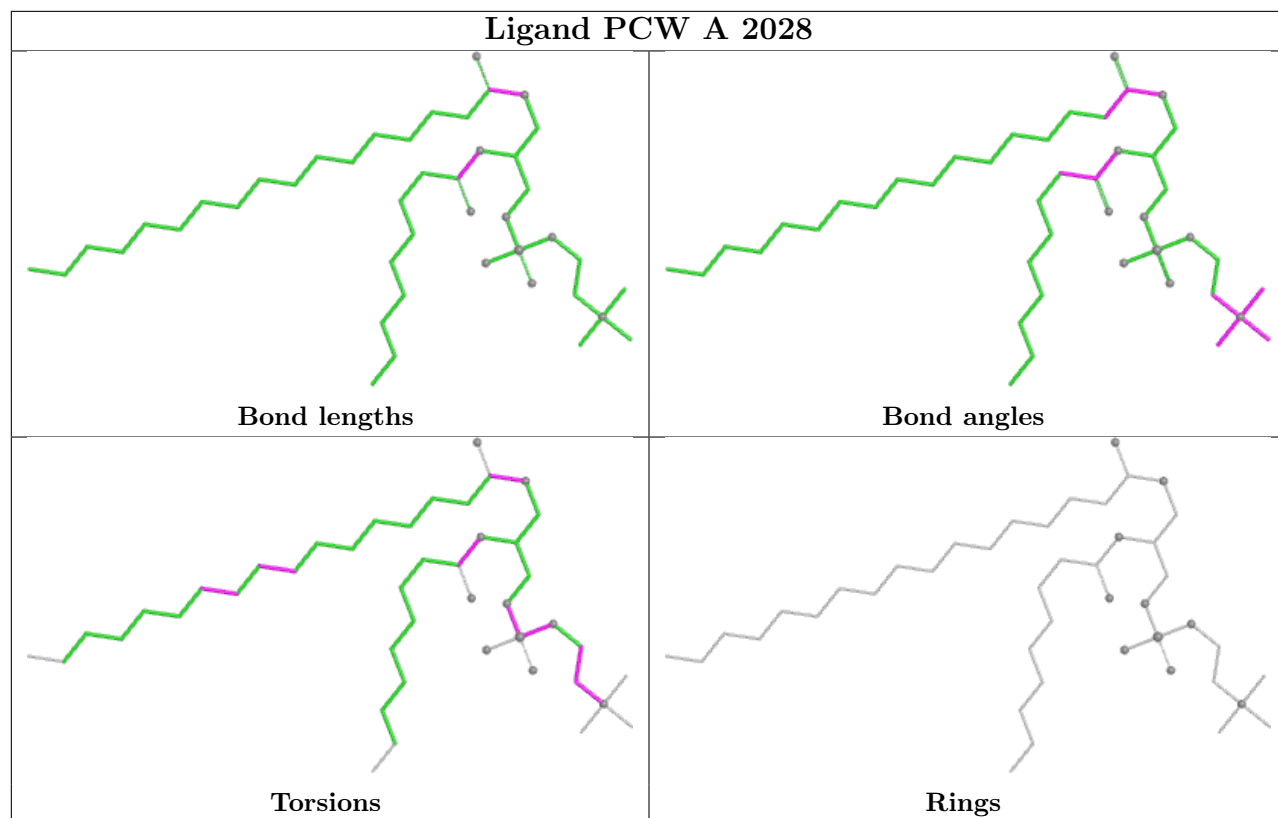


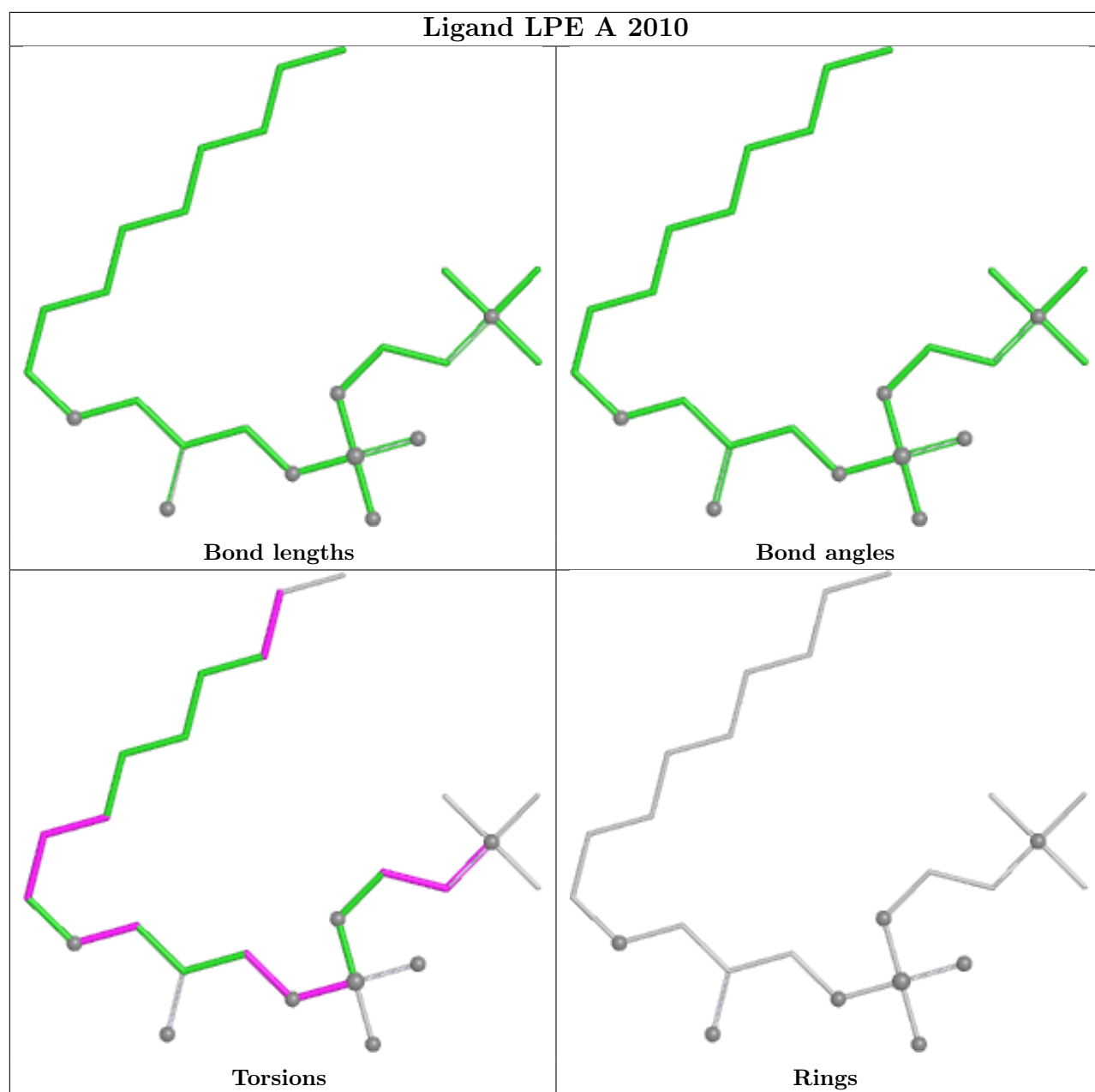


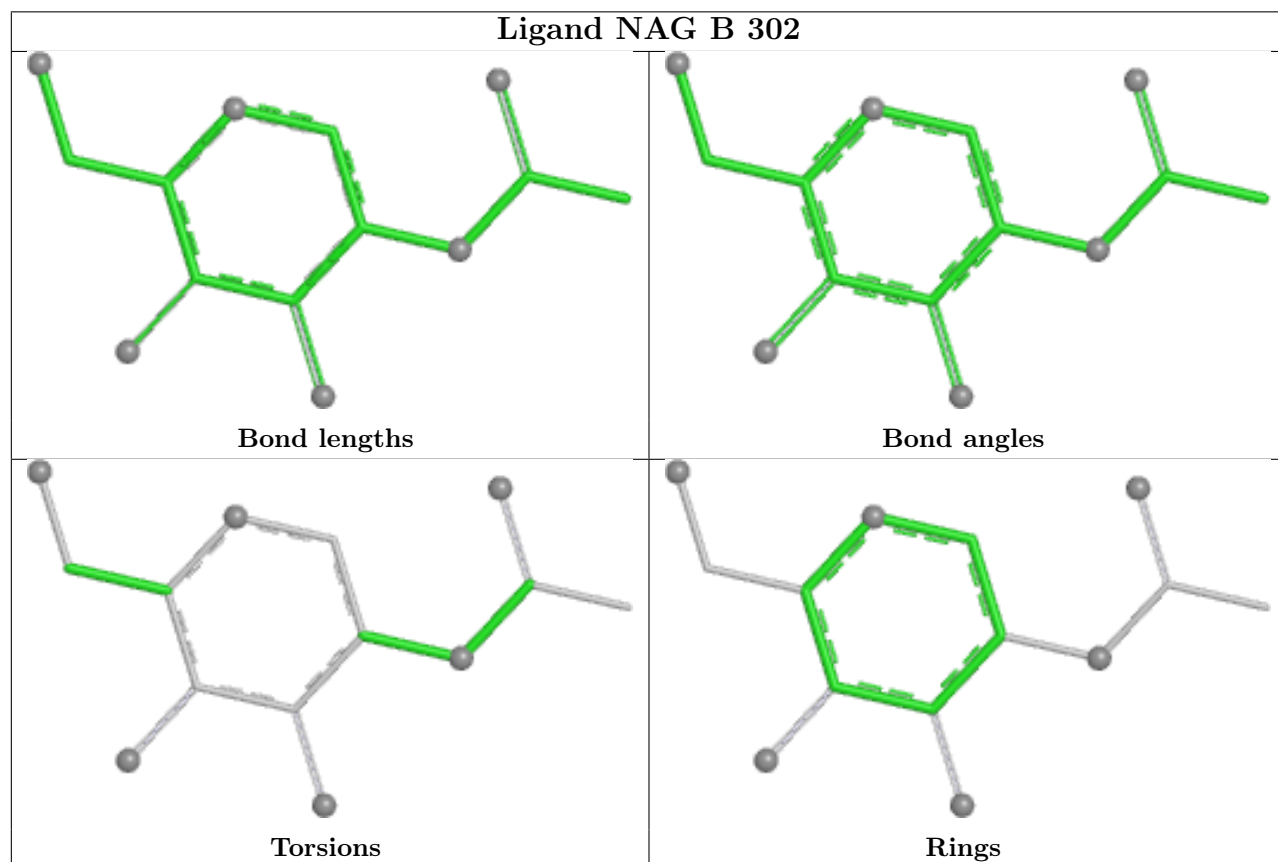
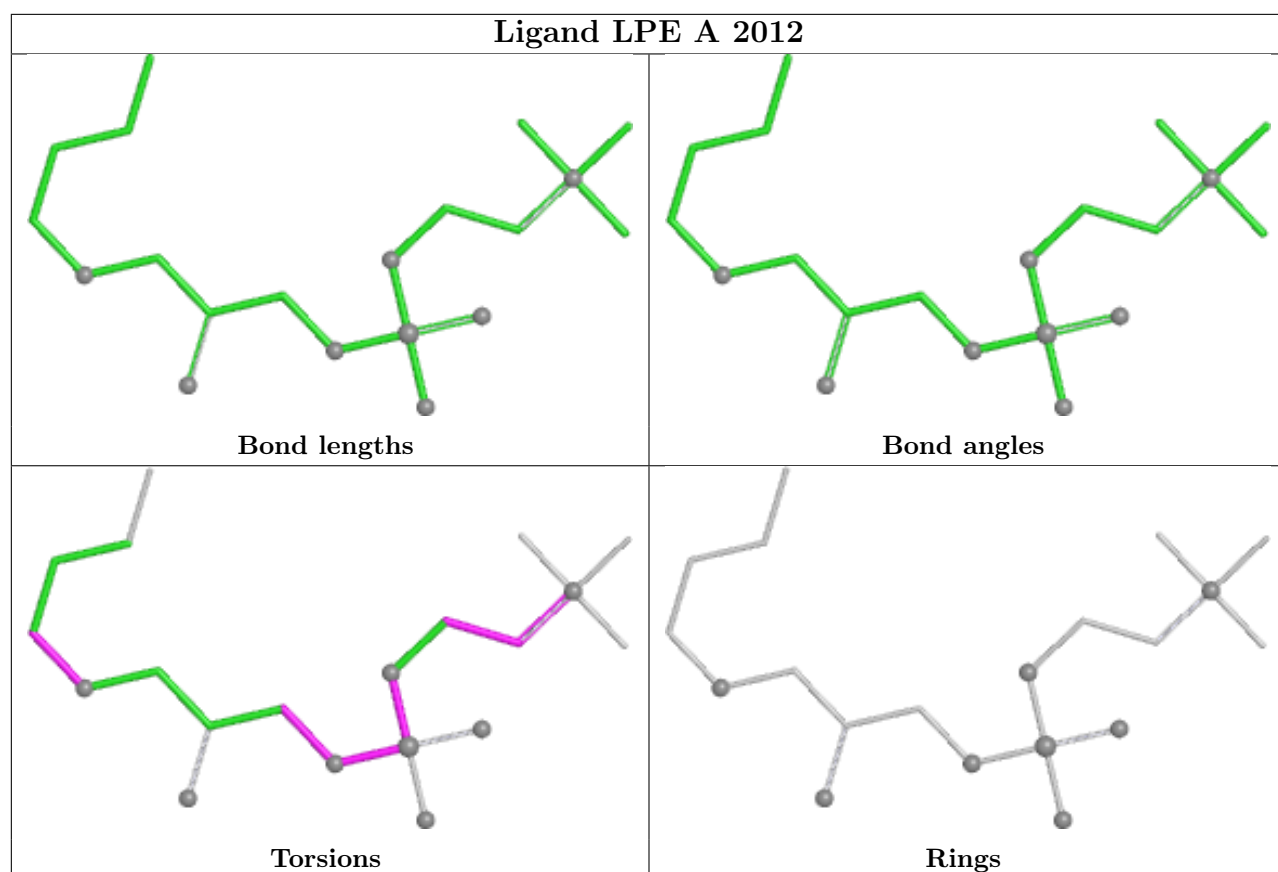


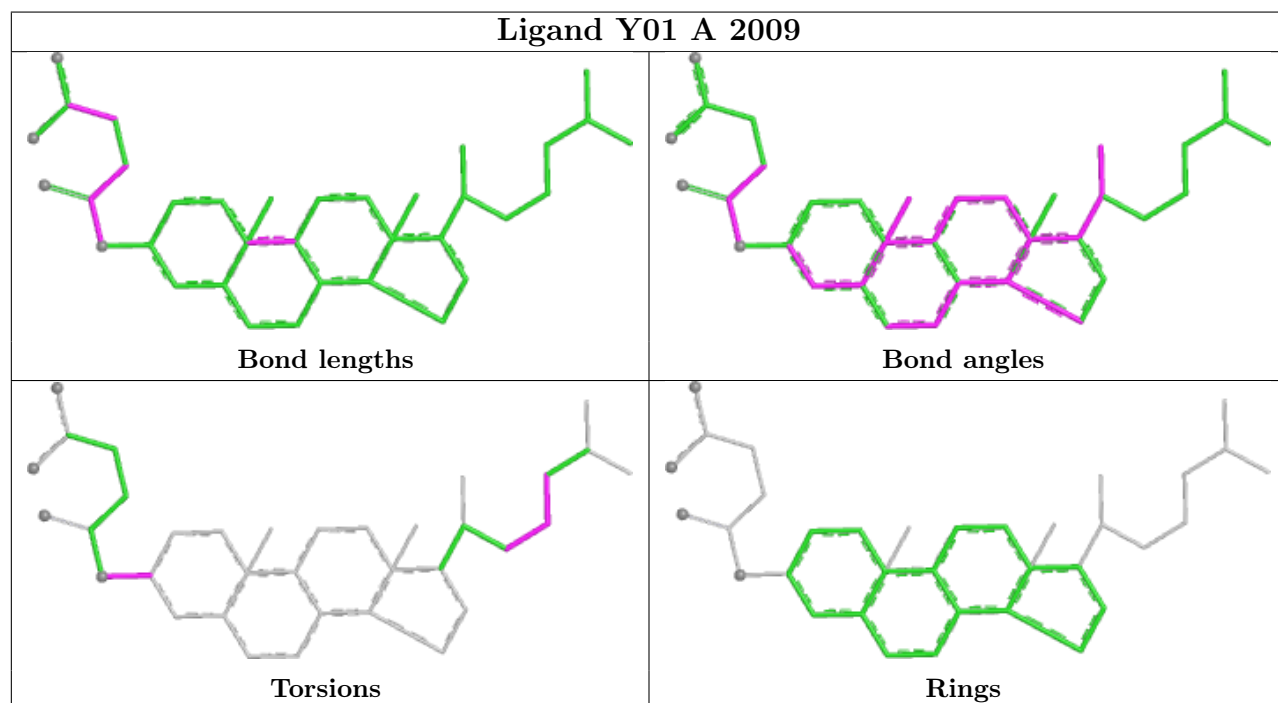
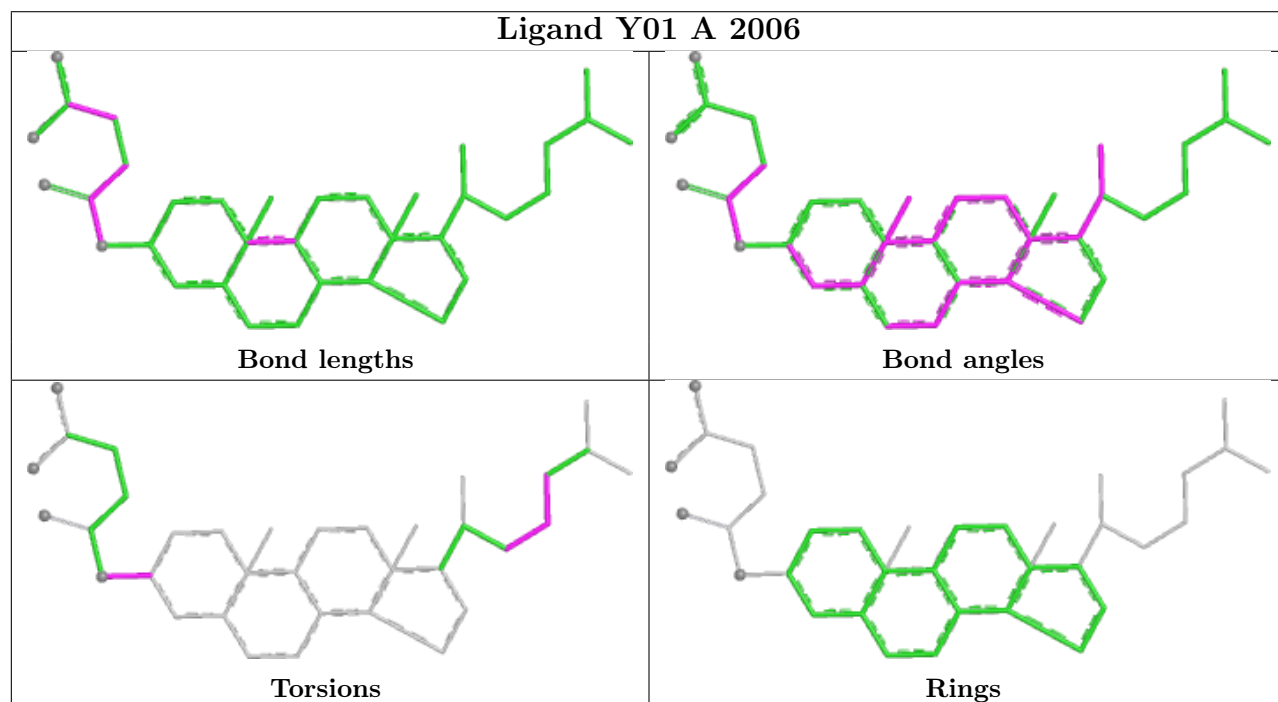
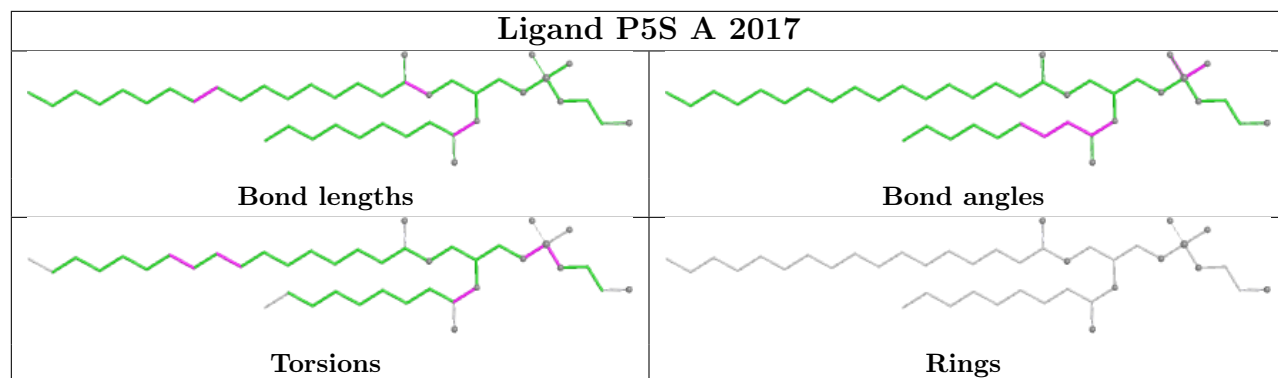


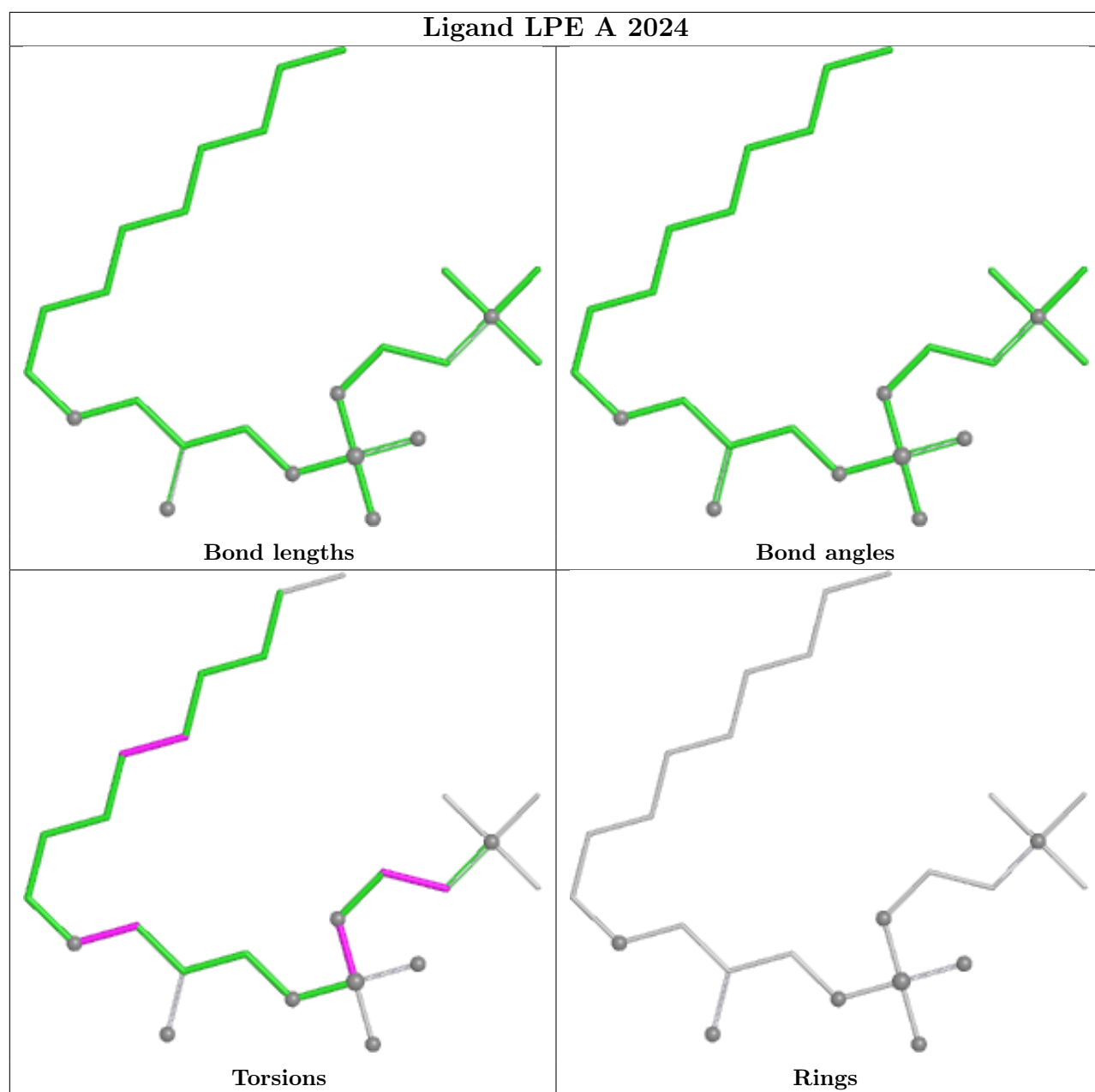


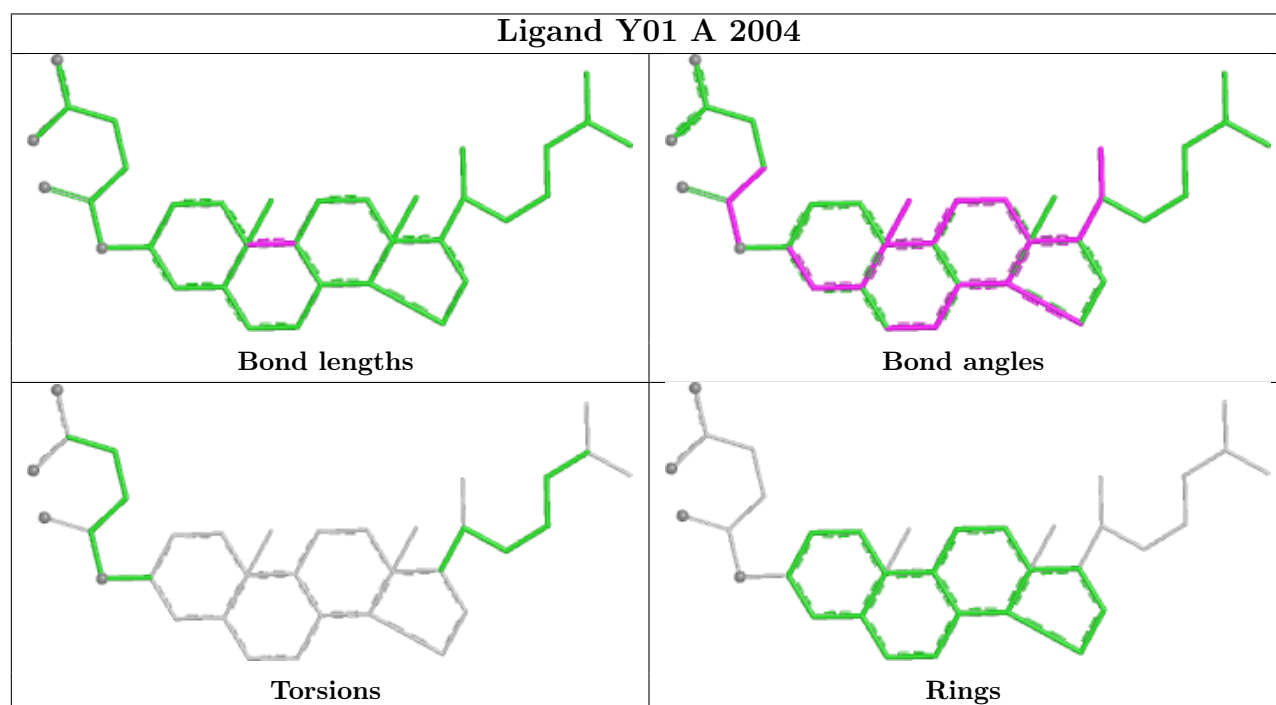
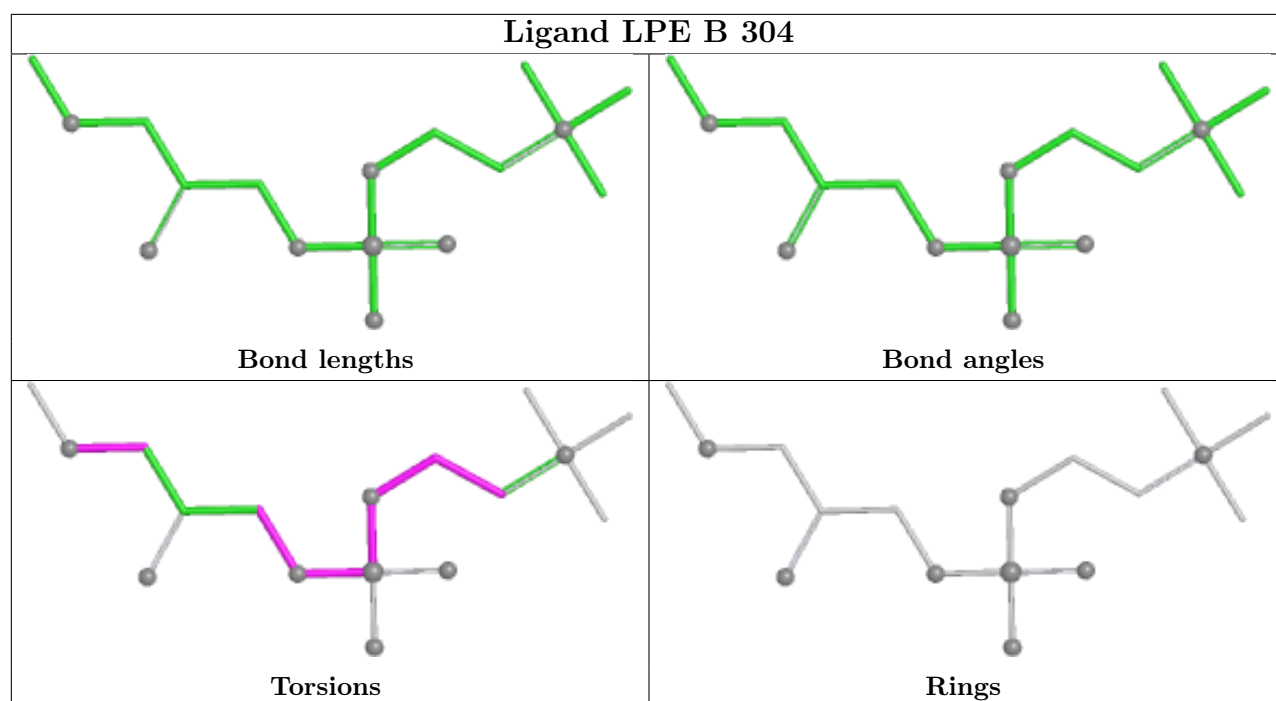


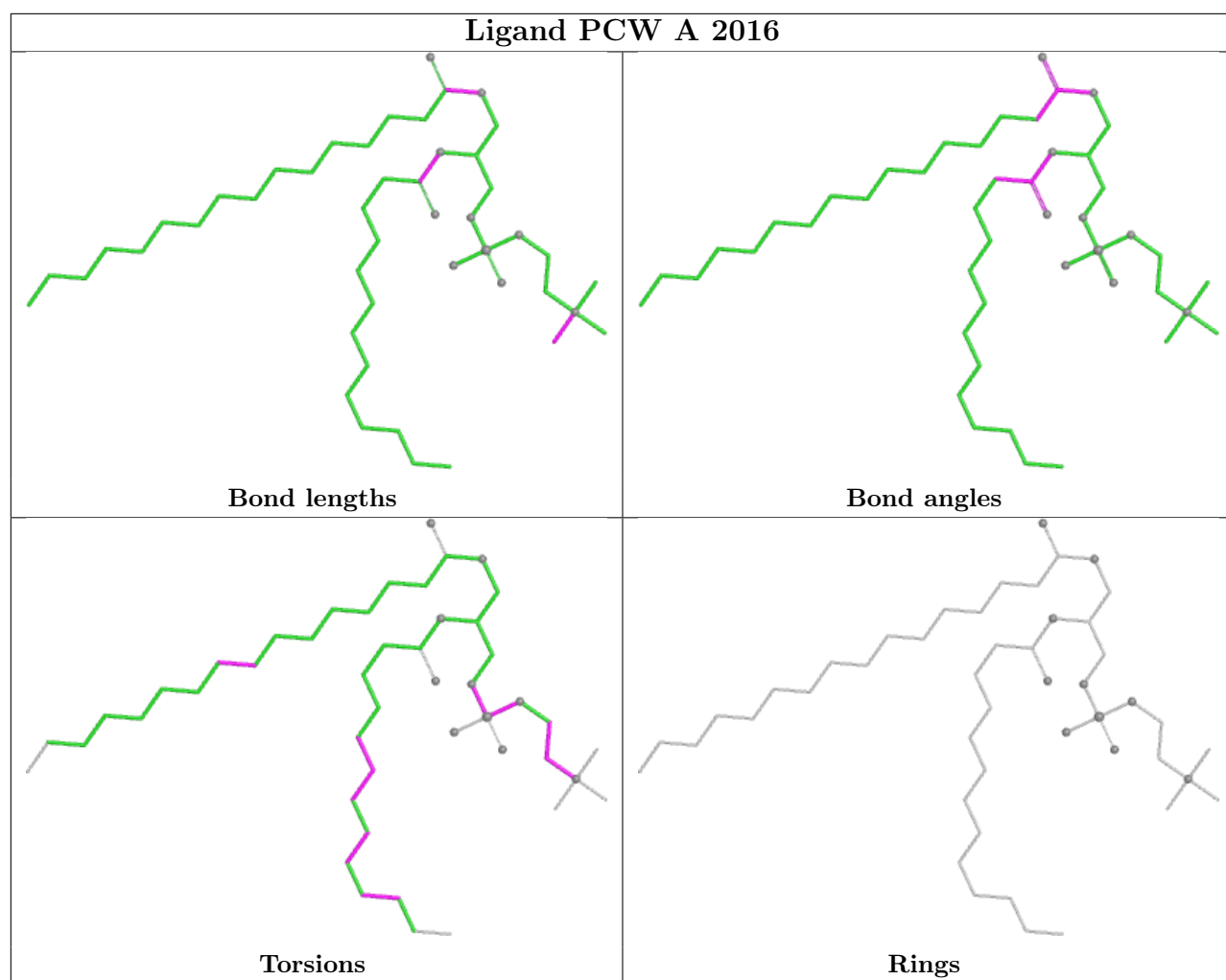


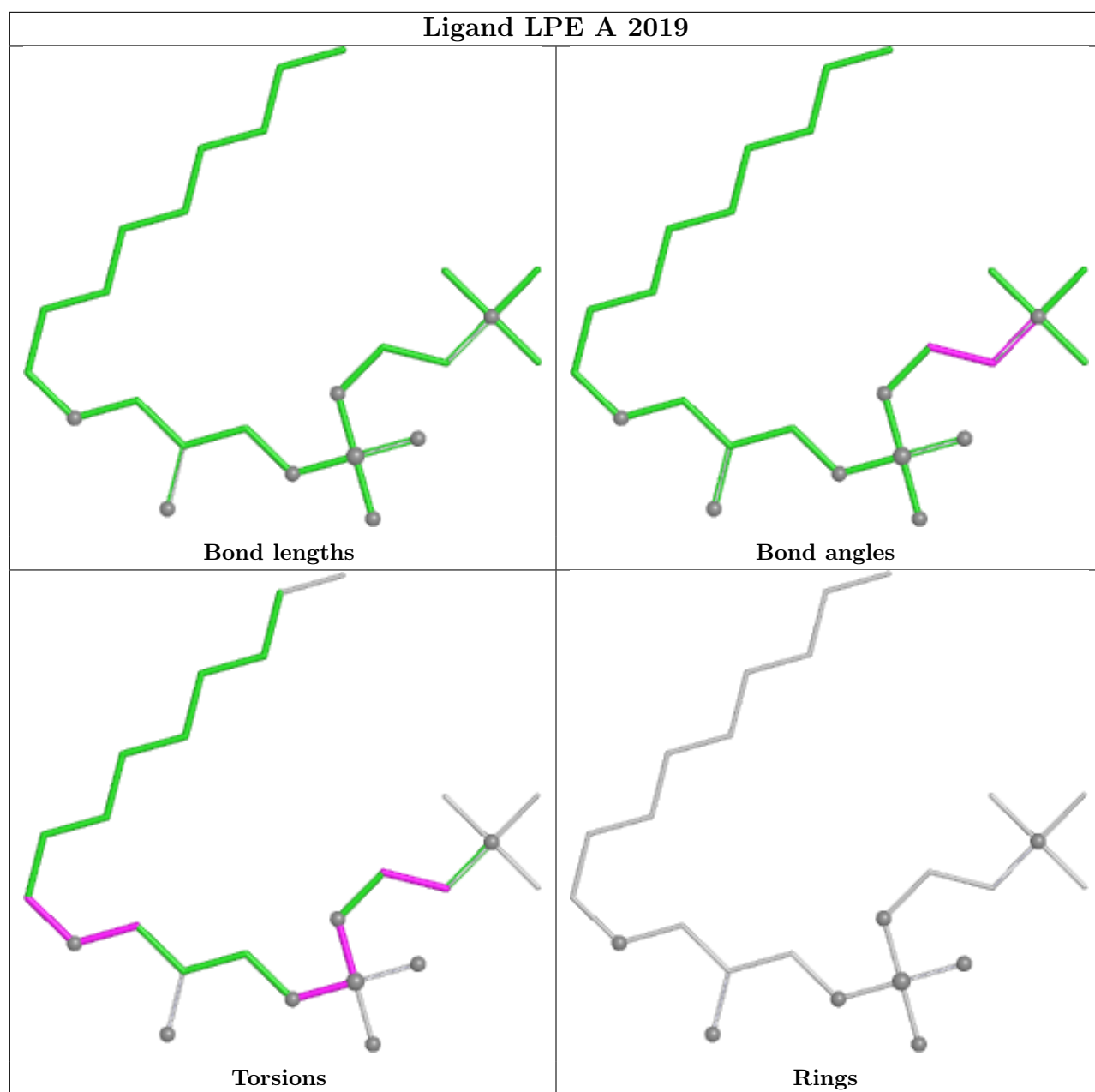




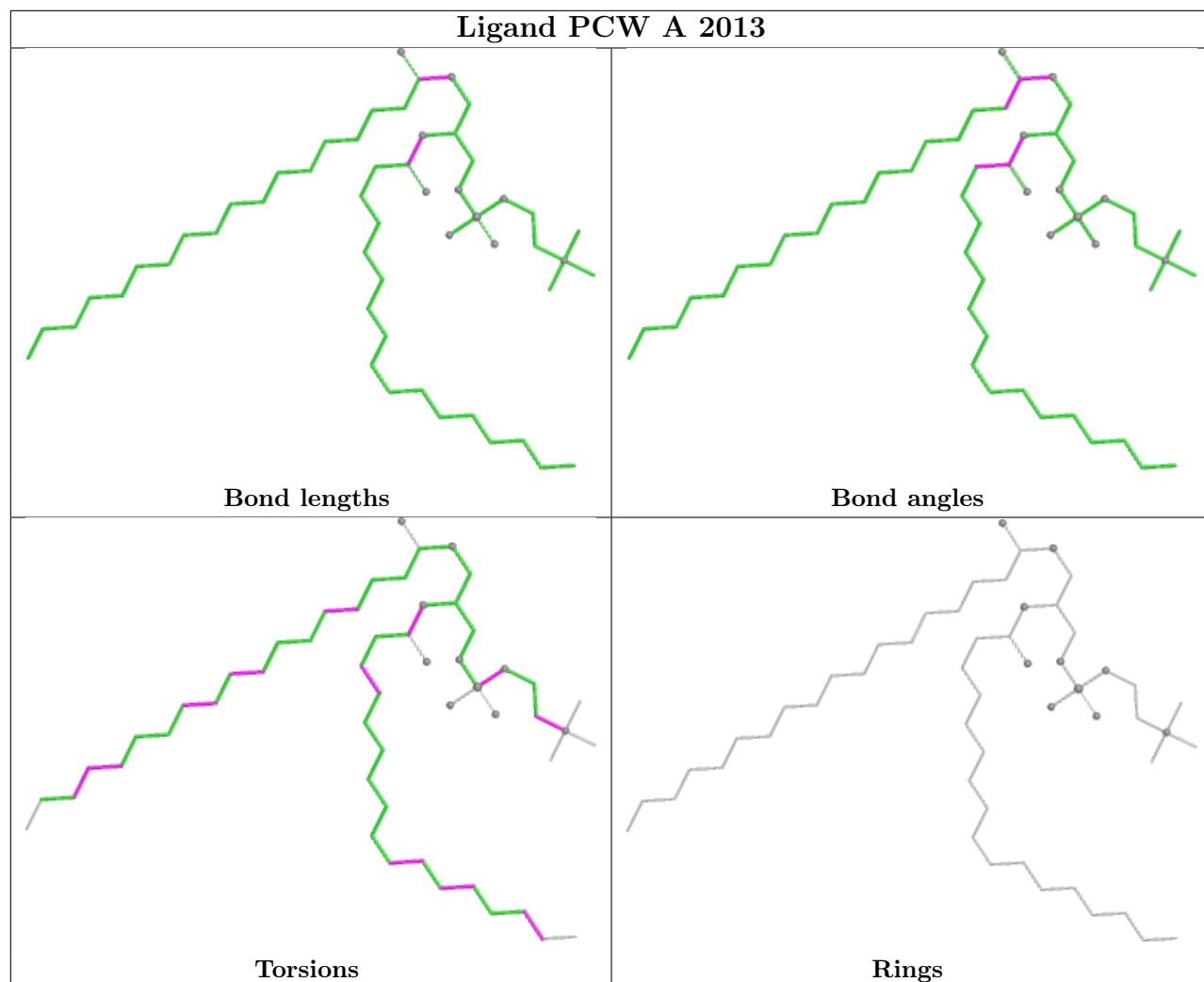




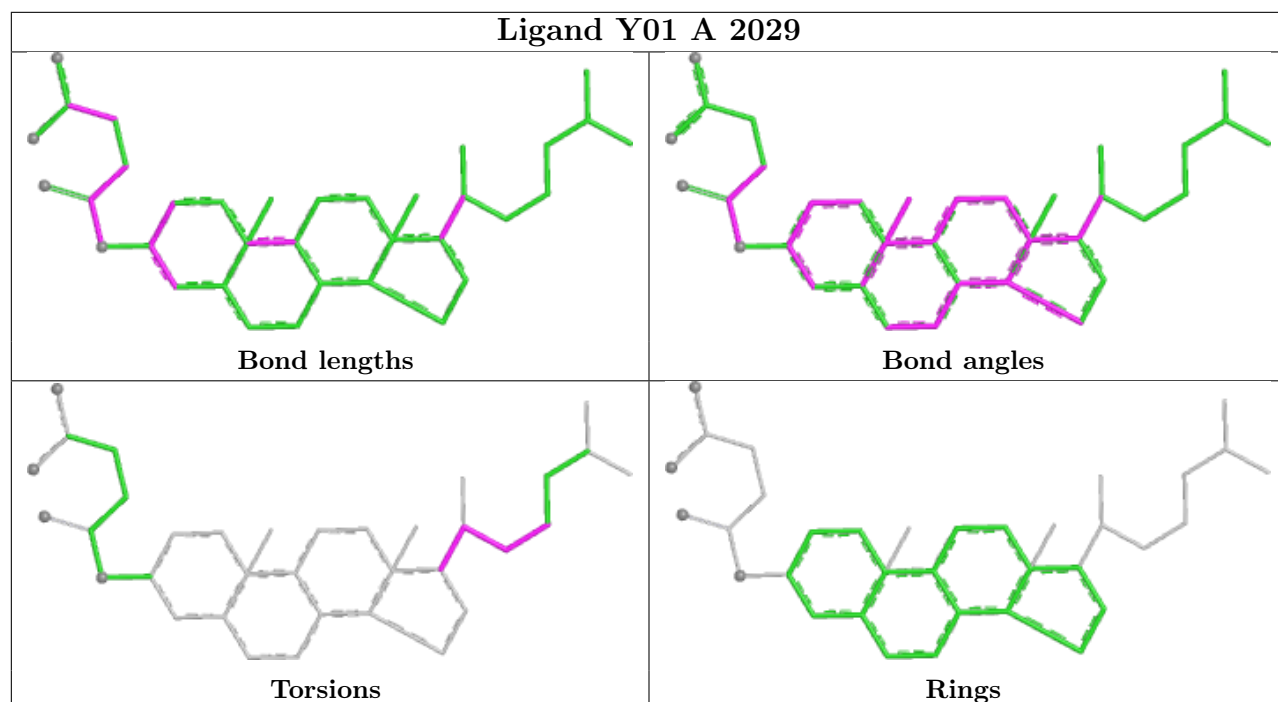


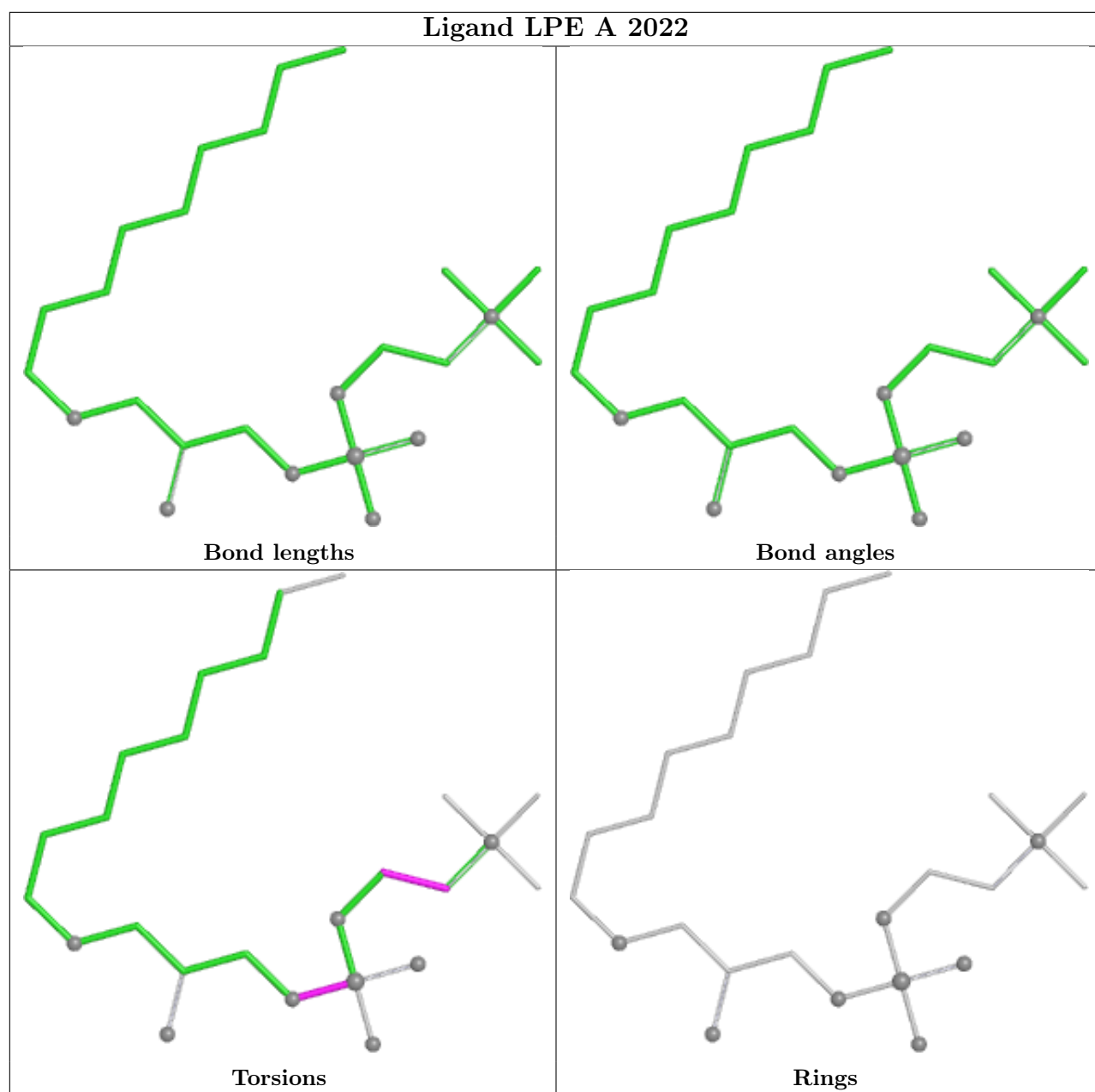


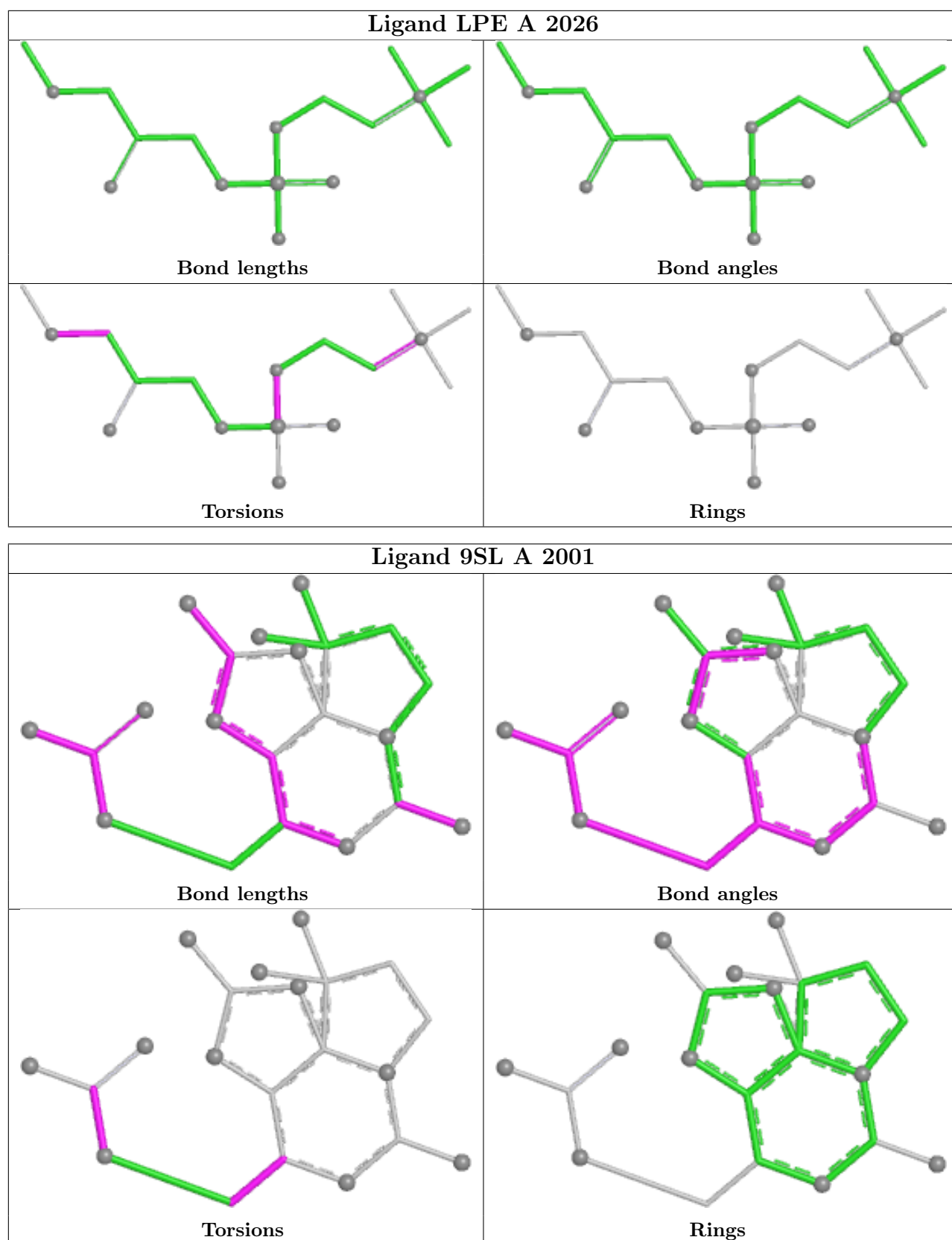
Ligand PCW A 2013

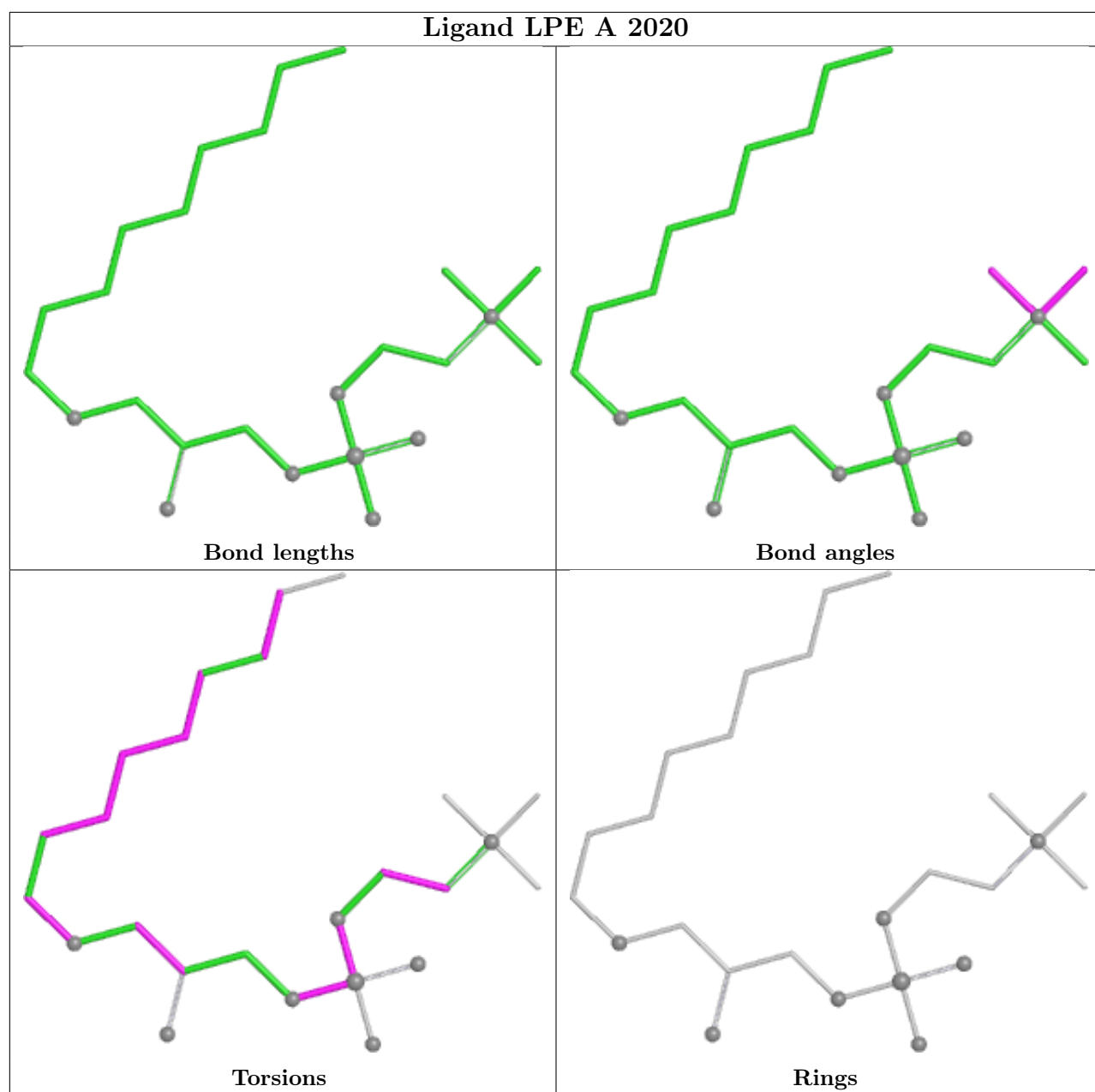


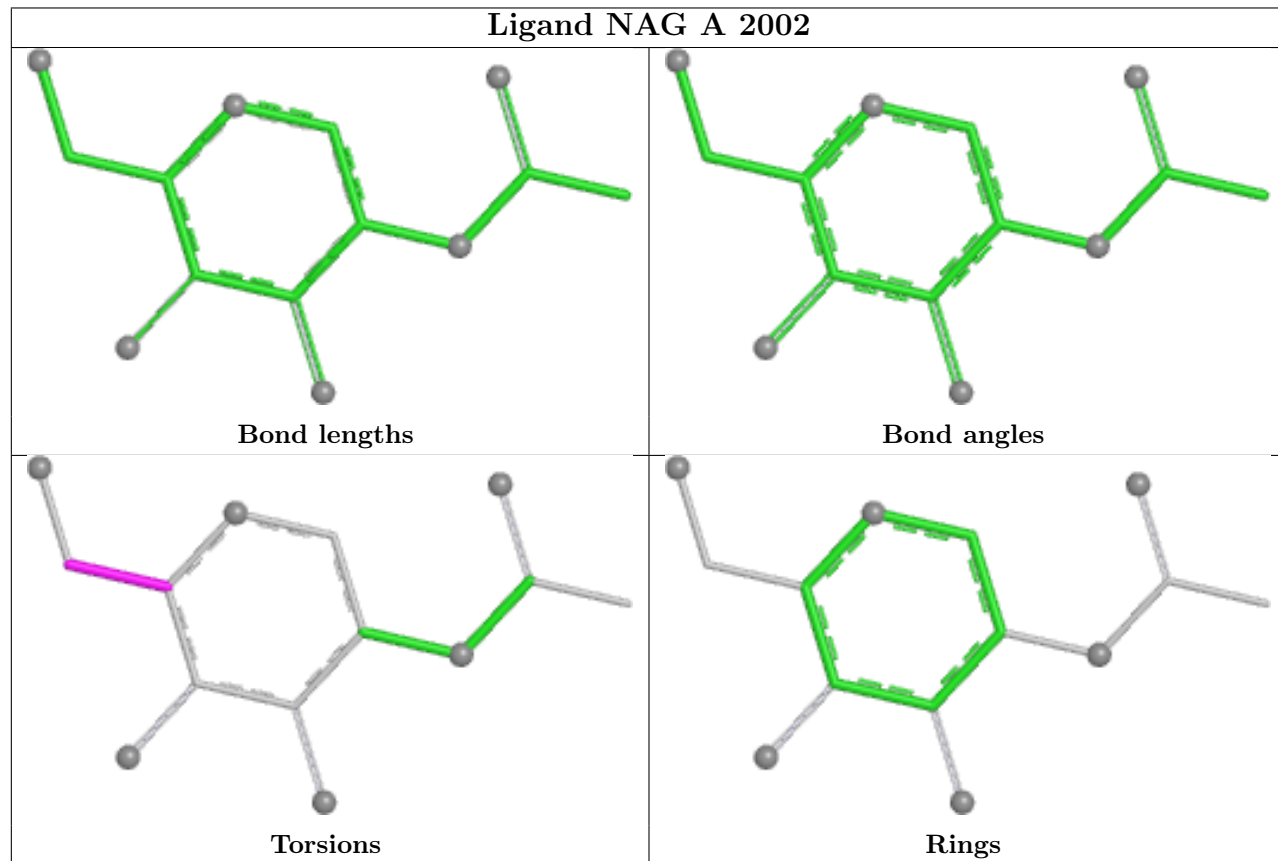
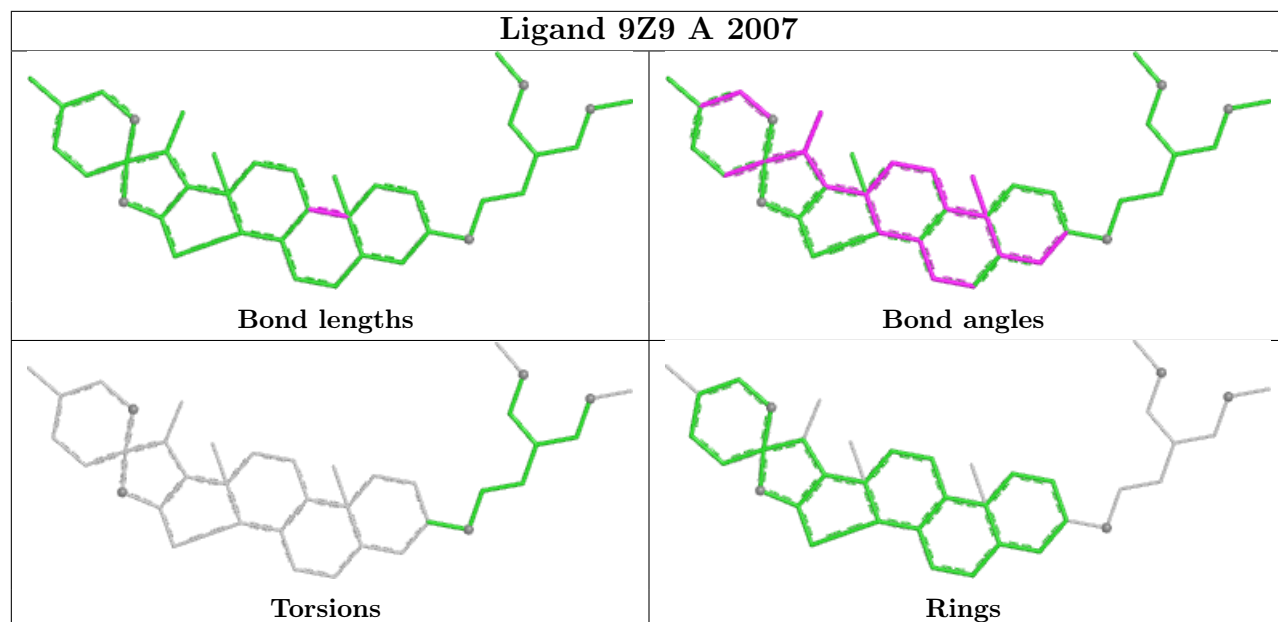
Ligand Y01 A 2029

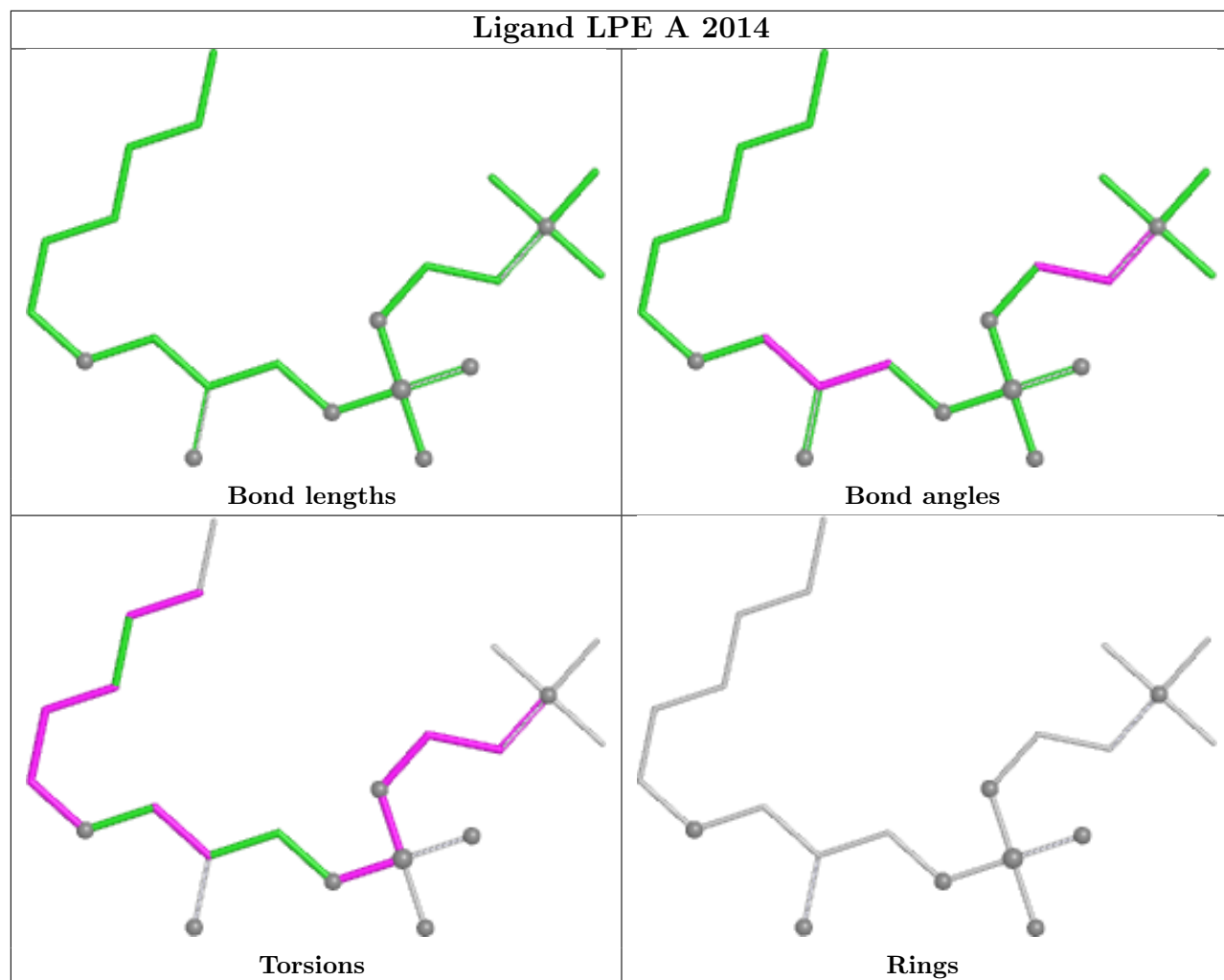


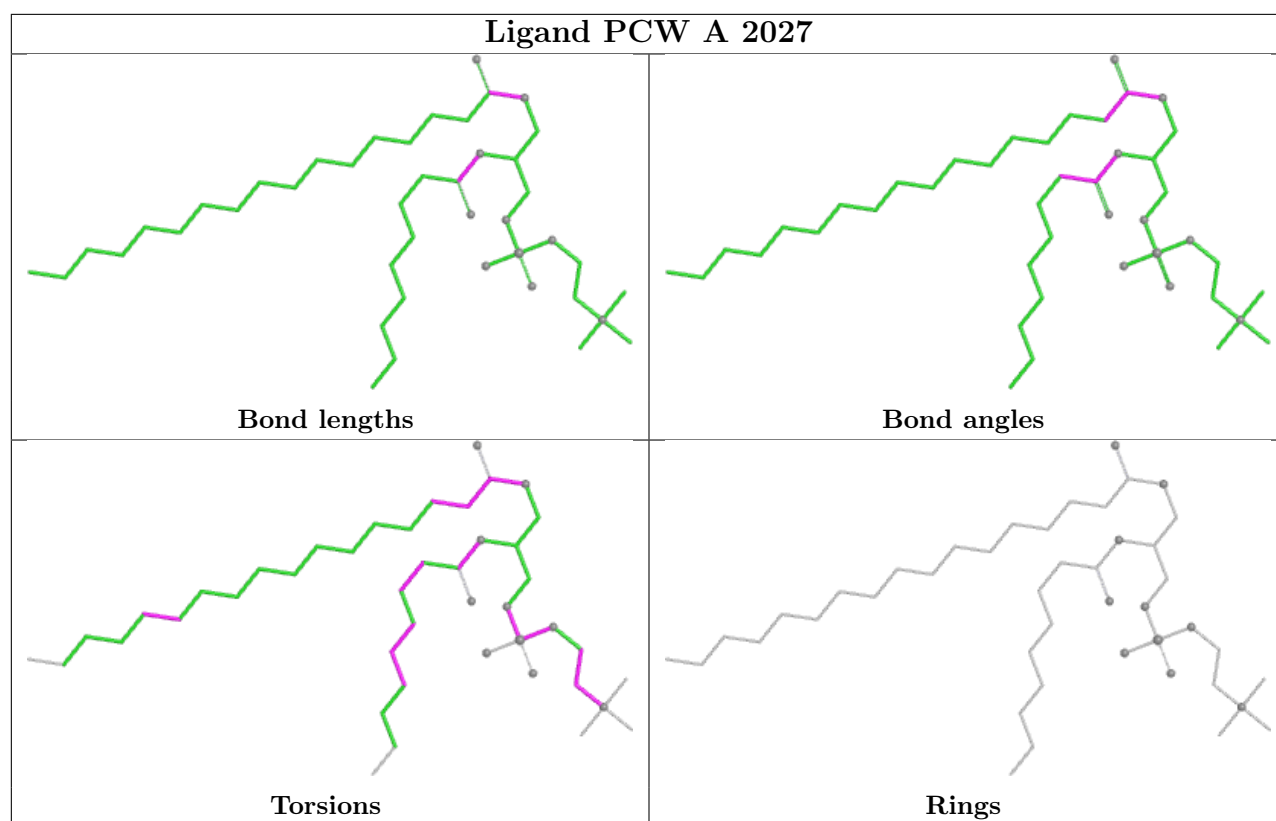












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

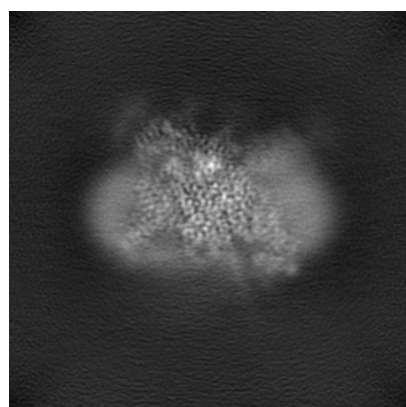
6 Map visualisation [i](#)

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

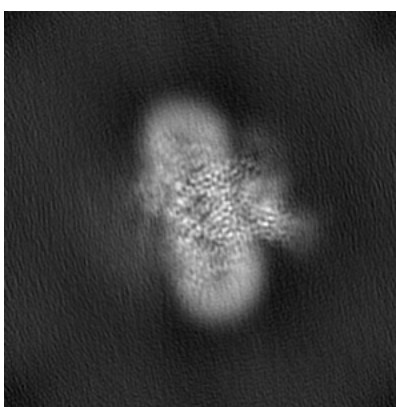
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

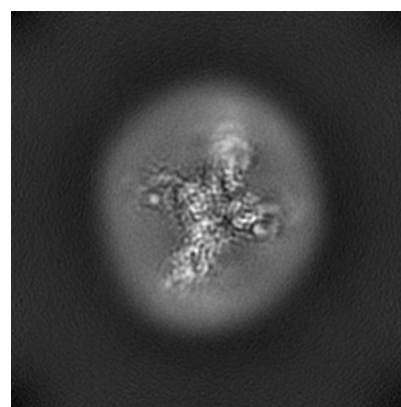
6.1.1 Primary map



X



Y

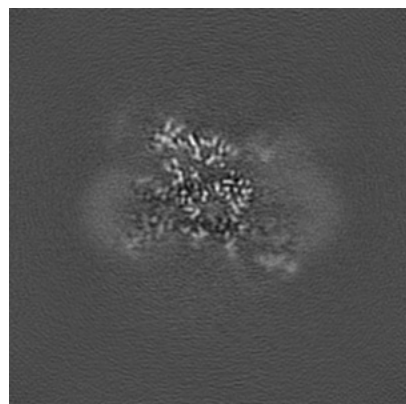


Z

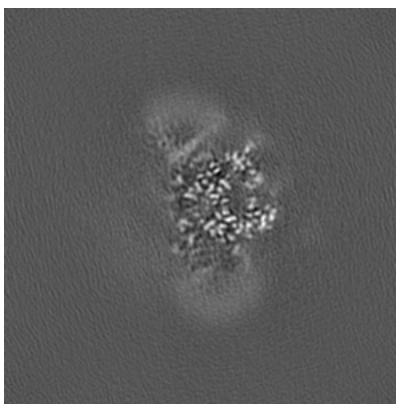
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

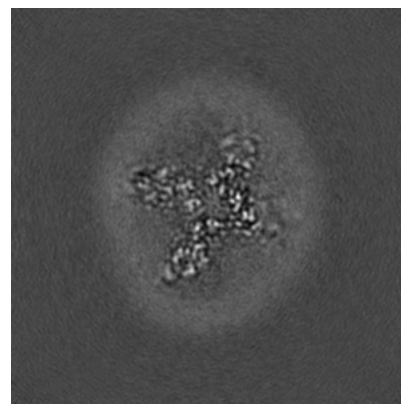
6.2.1 Primary map



X Index: 120



Y Index: 120

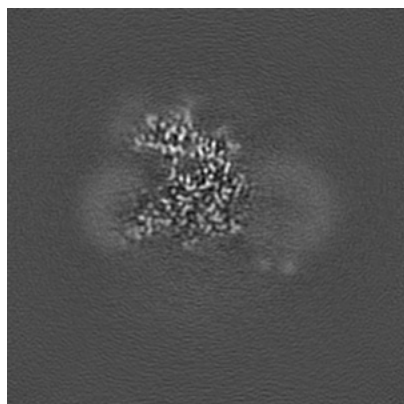


Z Index: 120

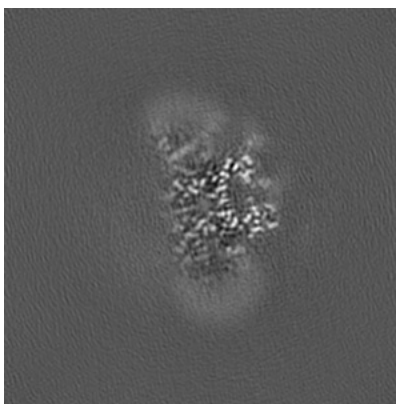
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

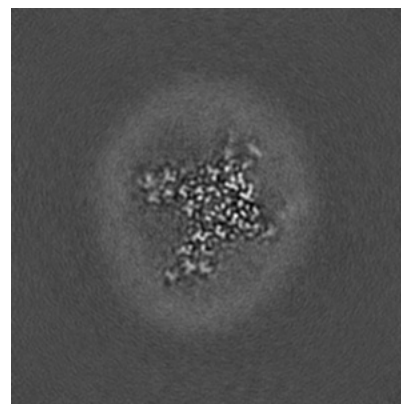
6.3.1 Primary map



X Index: 112



Y Index: 122

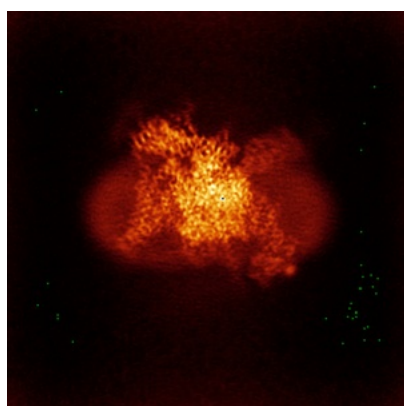


Z Index: 126

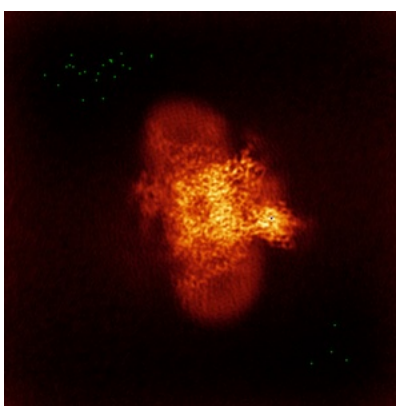
The images above show the largest variance slices of the map in three orthogonal directions.

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

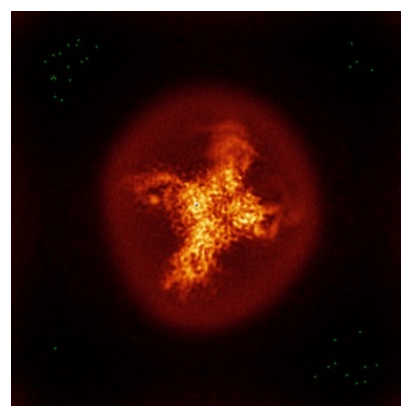
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

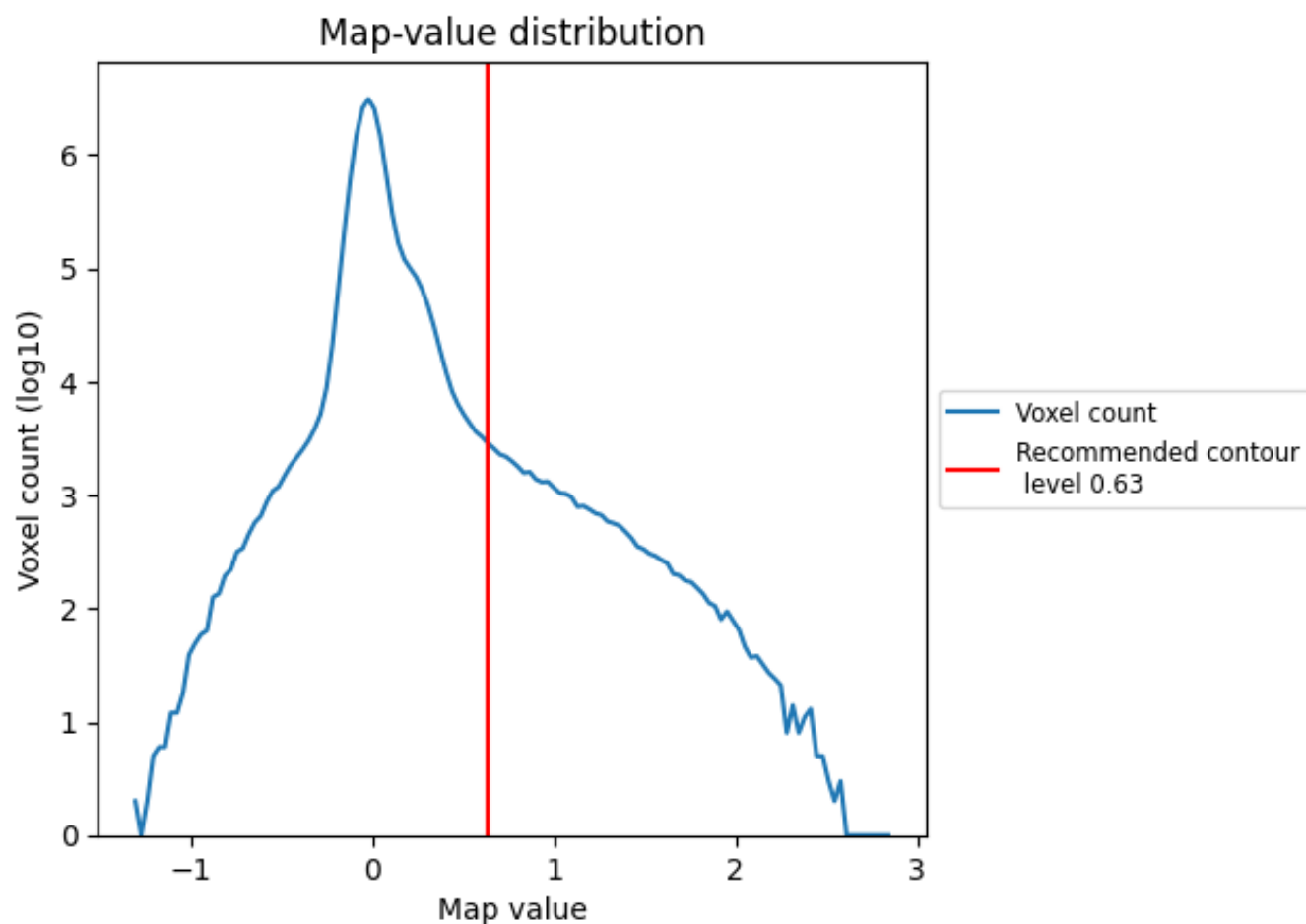
6.6 Mask visualisation

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

7 Map analysis [i](#)

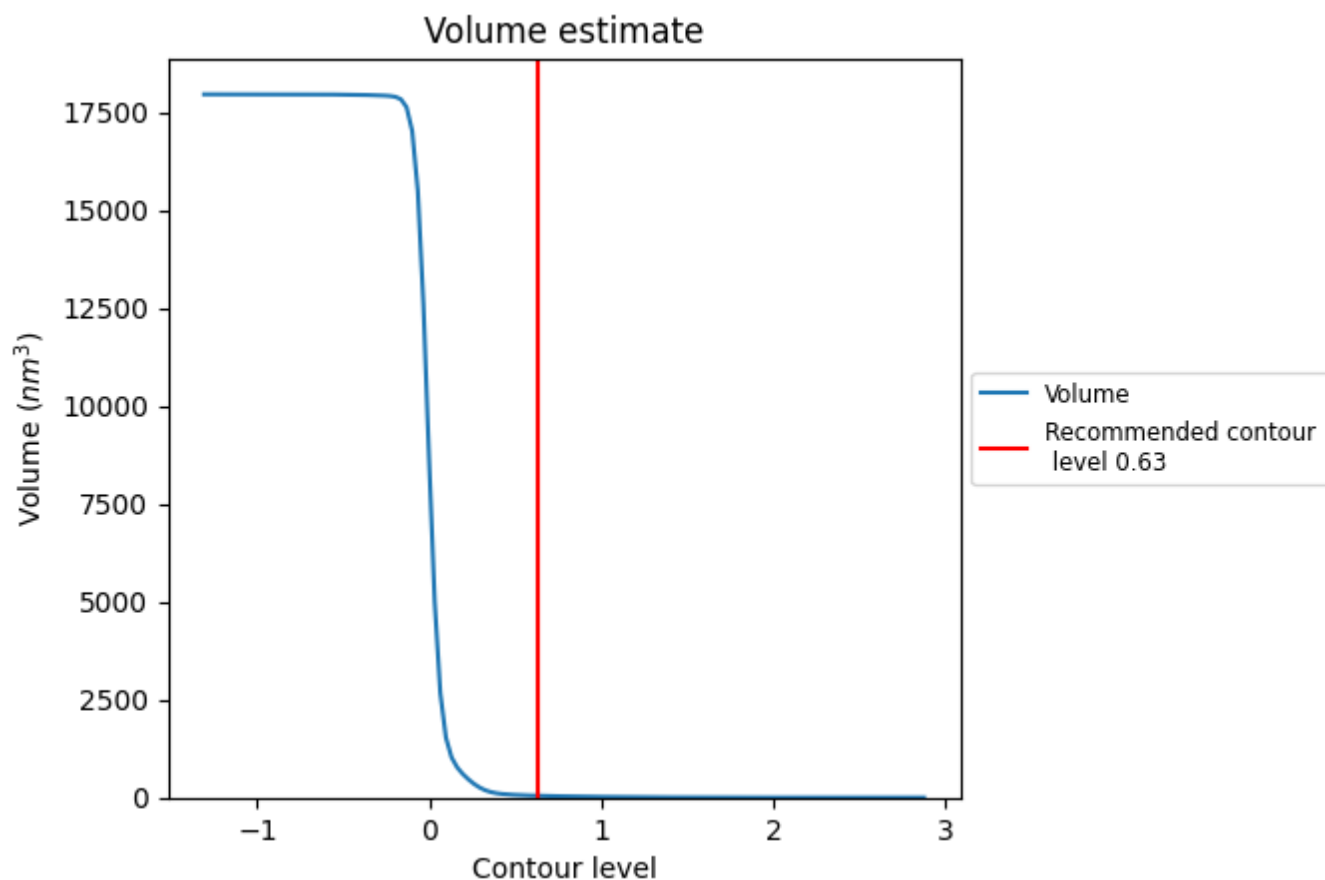
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

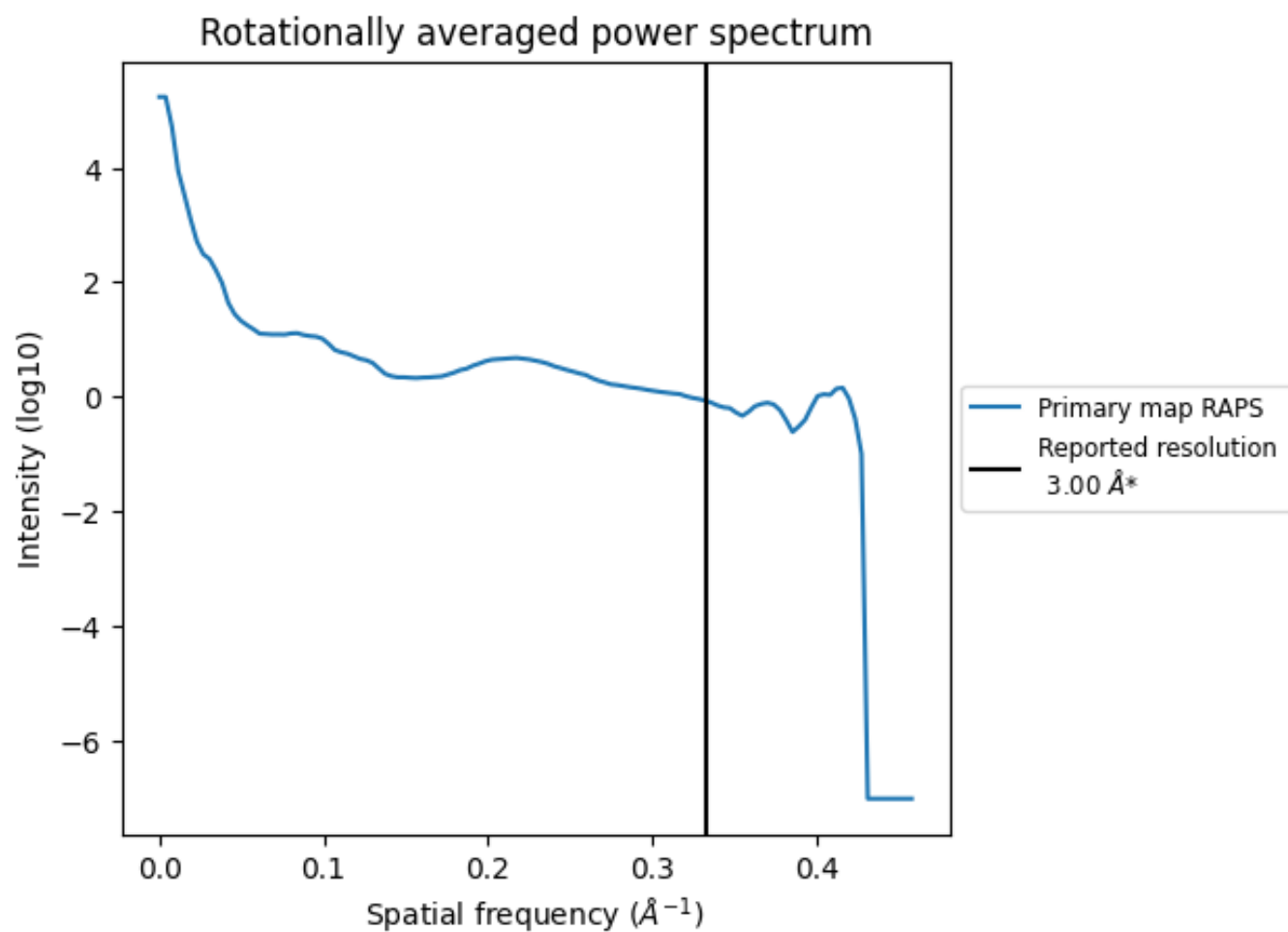
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ



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

8 Fourier-Shell correlation

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

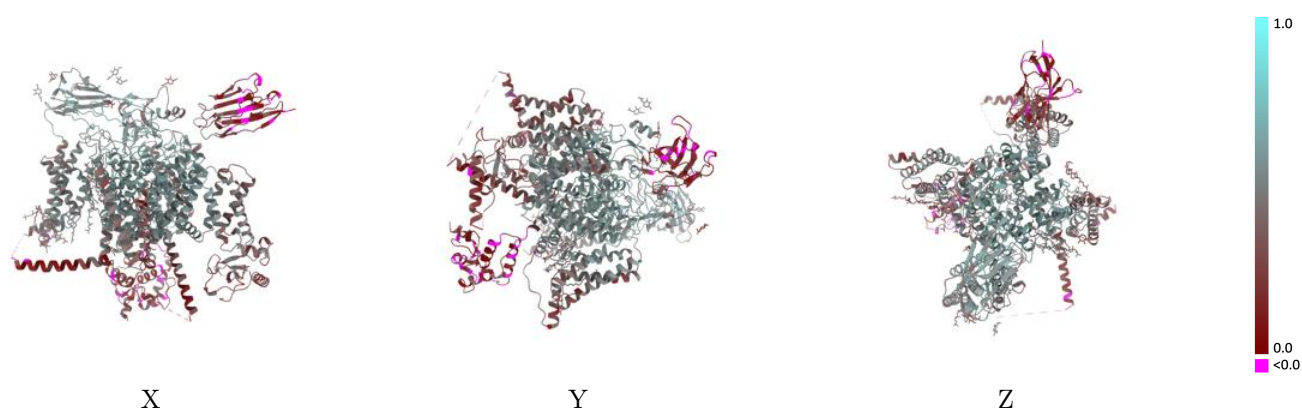
9 Map-model fit [i](#)

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

9.1 Map-model overlay [i](#)

This section was not generated.

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

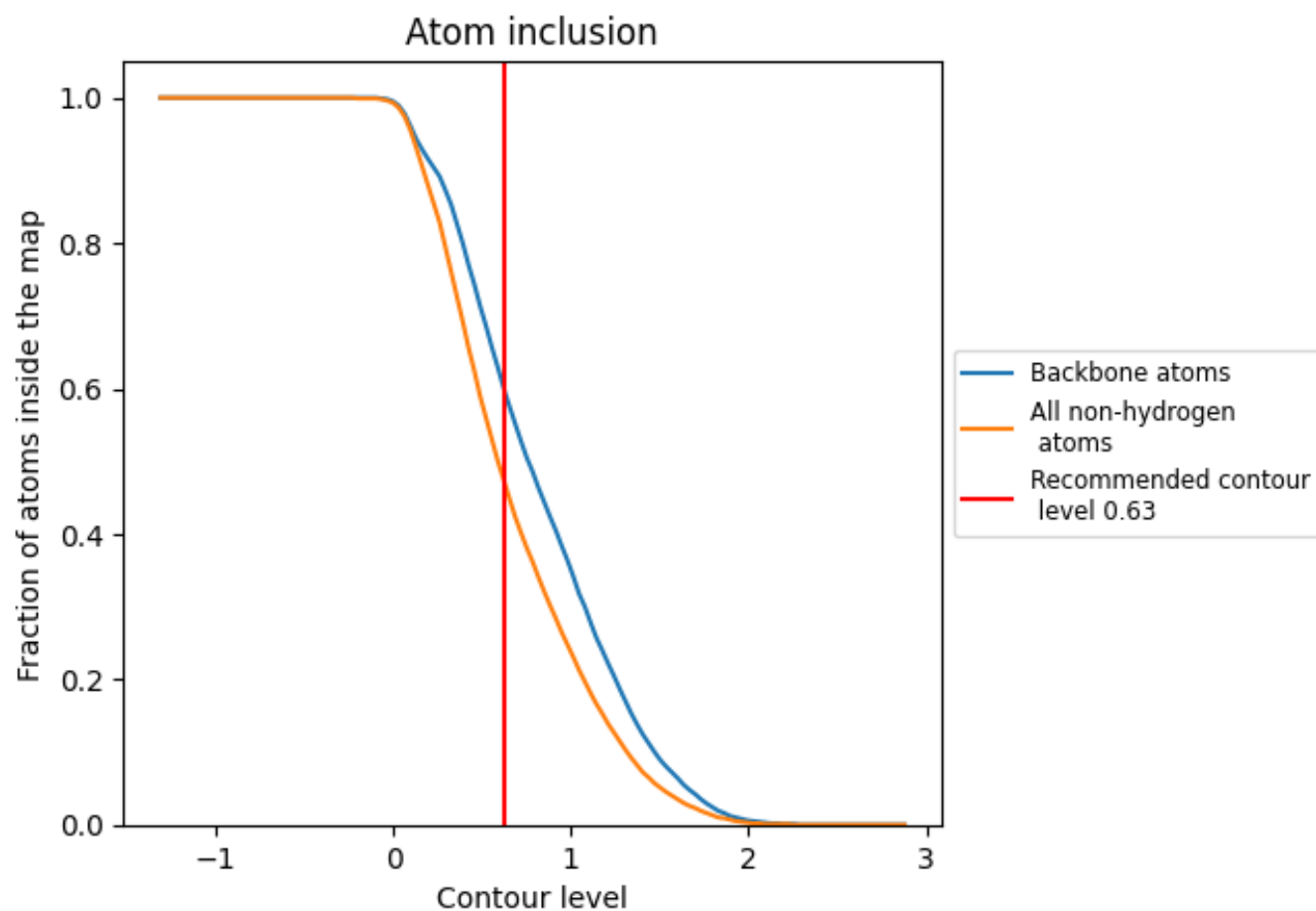


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.63) and Q-score for the entire model and for each chain.

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

1.0

0.0

<0.0