



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:26 PM UTC

PDB ID : 7PIL / pdb_00007pil
EMDB ID : EMD-13441
Title : Cryo-EM structure of the Rhodobacter sphaeroides RC-LH1-PufXY monomer complex at 2.5 Å
Authors : Qian, P.; Hunter, C.N.
Deposited on : 2021-08-20
Resolution : 2.50 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

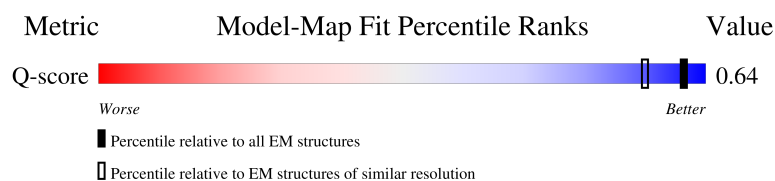
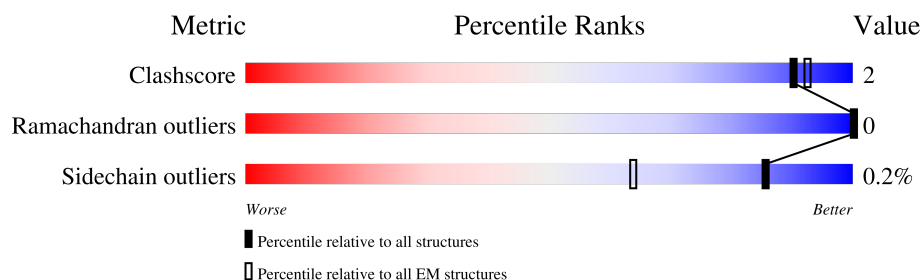
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

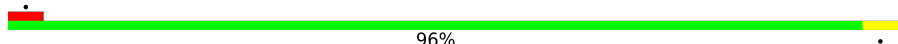
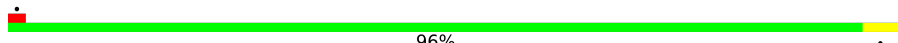
The reported resolution of this entry is 2.50 Å.

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



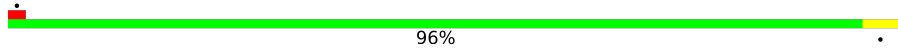
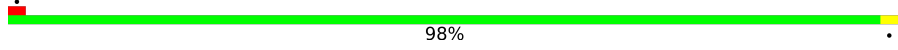
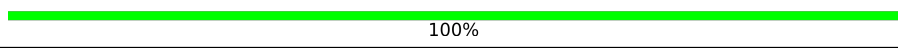
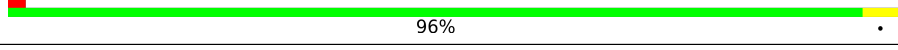
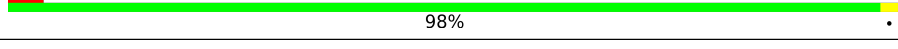
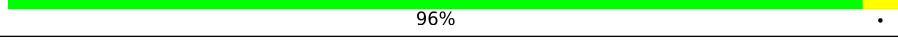
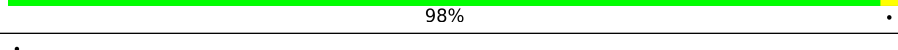
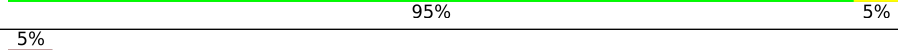
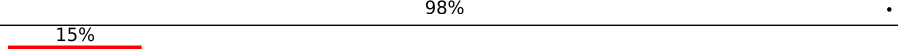
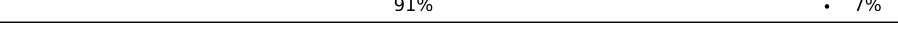
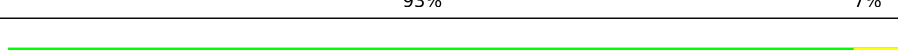
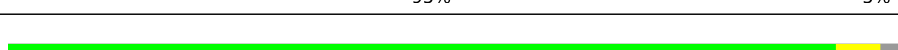
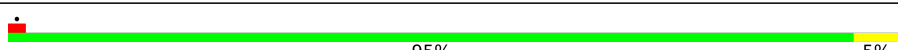
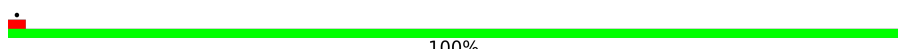
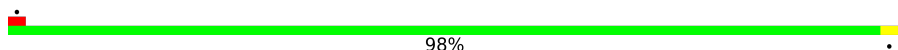
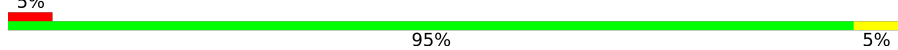
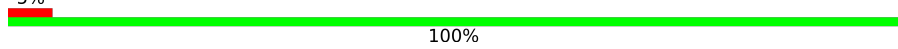
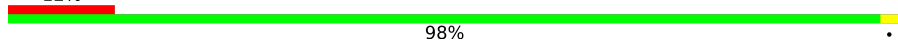
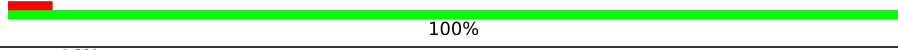
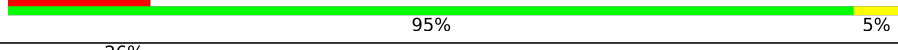
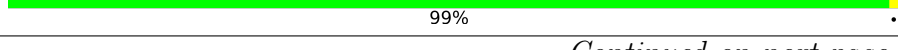
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	AA	55	
1	AB	55	
1	AC	55	
1	AD	55	

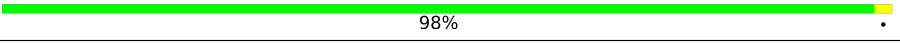
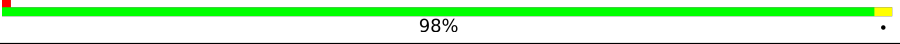
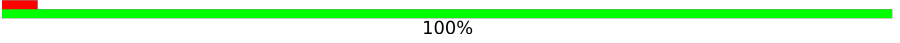
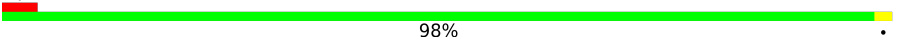
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Mol	Chain	Length	Quality of chain
1	AE	55	
1	AF	55	
1	AG	55	
1	AH	55	
1	AI	55	
1	AJ	55	
1	AK	55	
1	AL	55	
1	AM	55	
1	AN	55	
2	BA	43	
2	BB	43	
2	BC	43	
2	BD	43	
2	BE	43	
2	BF	43	
2	BG	43	
2	BH	43	
2	BI	43	
2	BJ	43	
2	BK	43	
2	BL	43	
2	BM	43	
2	BN	43	
3	H	246	

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Mol	Chain	Length	Quality of chain
4	L	281	 98%
5	M	307	 98%
6	UU	49	 100%
7	X	55	 98%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 22480 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 Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	46	Total	C	N	O	S	0	0
			392	271	60	58	3		
1	AB	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AC	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
1	AD	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AE	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AF	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AG	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AH	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AI	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AJ	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AK	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AL	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AM	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AN	51	Total	C	N	O	S	0	0
			432	296	69	65	2		

- Molecule 2 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	43	Total	C	N	O	S	0	0
			352	236	55	60	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BC	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
2	BD	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BE	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BF	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BG	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BH	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BI	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BJ	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BK	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BL	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BM	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BN	38	Total	C	N	O	S	0	0
			317	213	50	53	1		

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	246	Total	C	N	O	S	0	0
			1867	1196	316	345	10		

- Molecule 4 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		

- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	307	Total	C	N	O	S	0	0
			2445	1630	400	404	11		

- Molecule 6 is a protein called RC-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UU	49	Total	C	N	O	S	0	0
			363	247	56	57	3		

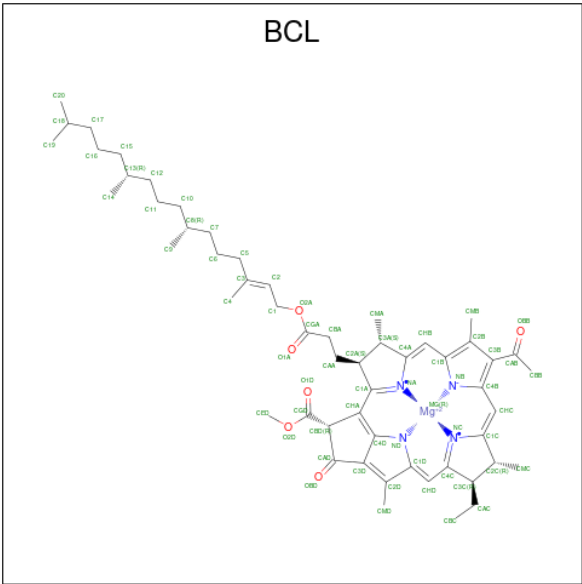
- Molecule 7 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	55	Total	C	N	O	S	0	0
			422	281	71	67	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	53	LEU	ARG	conflict	UNP P13402

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	AA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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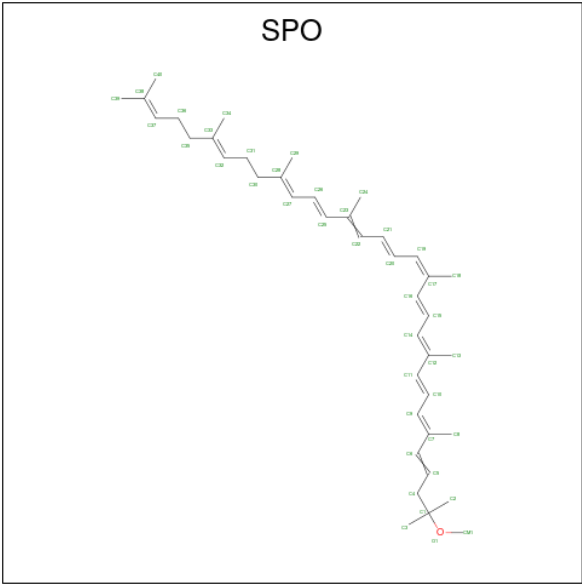
Mol	Chain	Residues	Atoms					AltConf
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8	AC	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AF	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AG	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	BA	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	BB	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	BC	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	BD	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	BF	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
8	BG	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BH	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BI	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BJ	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BN	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 9 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



Mol	Chain	Residues	Atoms			AltConf
9	AA	1	Total	C	O	0
			42	41	1	

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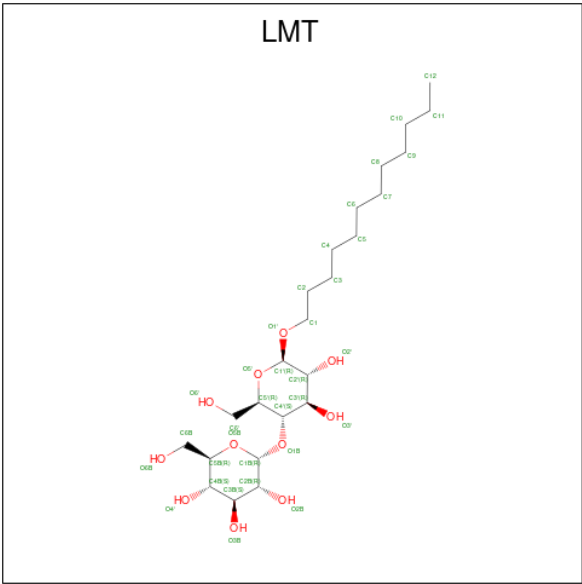
Mol	Chain	Residues	Atoms			AltConf
9	AB	1	Total	C	O	0
			42	41	1	
9	AC	1	Total	C	O	0
			42	41	1	
9	AC	1	Total	C	O	0
			42	41	1	
9	AD	1	Total	C	O	0
			42	41	1	
9	AD	1	Total	C	O	0
			42	41	1	
9	AE	1	Total	C	O	0
			42	41	1	
9	AF	1	Total	C	O	0
			42	41	1	
9	AF	1	Total	C	O	0
			42	41	1	
9	AG	1	Total	C	O	0
			42	41	1	
9	AG	1	Total	C	O	0
			42	41	1	
9	AH	1	Total	C	O	0
			42	41	1	
9	AH	1	Total	C	O	0
			42	41	1	
9	AI	1	Total	C	O	0
			42	41	1	
9	AI	1	Total	C	O	0
			42	41	1	
9	AJ	1	Total	C	O	0
			42	41	1	
9	AJ	1	Total	C	O	0
			42	41	1	
9	AK	1	Total	C	O	0
			42	41	1	
9	AK	1	Total	C	O	0
			42	41	1	
9	AL	1	Total	C	O	0
			42	41	1	
9	AM	1	Total	C	O	0
			42	41	1	
9	AM	1	Total	C	O	0
			42	41	1	

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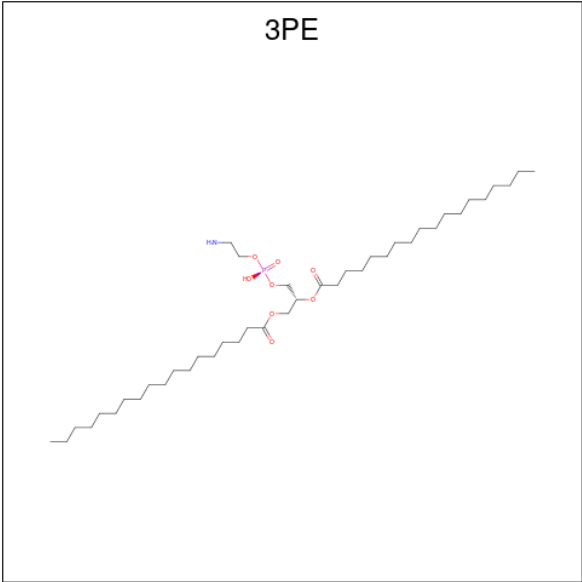
Mol	Chain	Residues	Atoms			AltConf
9	BA	1	Total	C	O	0
			42	41	1	
9	BE	1	Total	C	O	0
			42	41	1	
9	BL	1	Total	C	O	0
			42	41	1	
9	M	1	Total	C	O	0
			42	41	1	

- Molecule 10 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



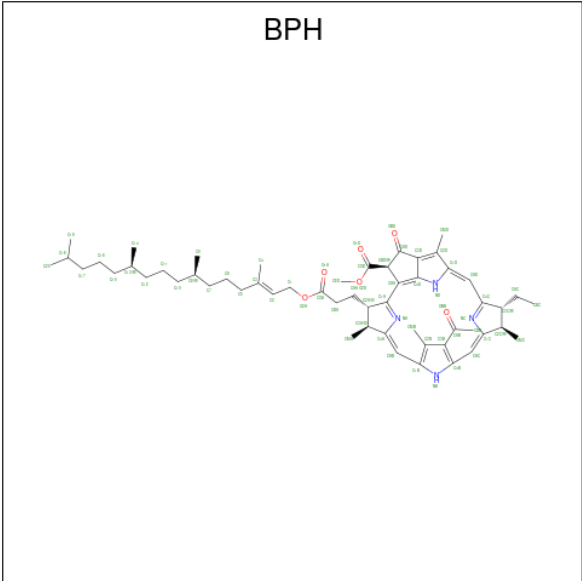
Mol	Chain	Residues	Atoms			AltConf
10	AA	1	Total	C	O	0
			35	24	11	
10	AB	1	Total	C	O	0
			35	24	11	
10	M	1	Total	C	O	0
			35	24	11	
10	X	1	Total	C	O	0
			35	24	11	

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



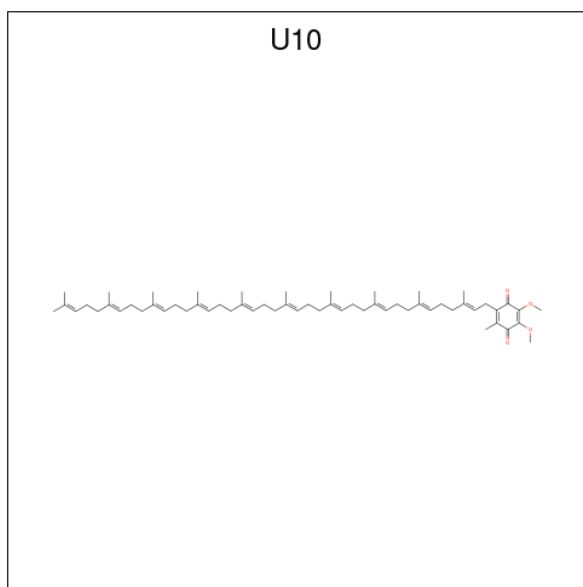
Mol	Chain	Residues	Atoms					AltConf
11	AB	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	AC	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	H	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 12 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆) (labeled as "Ligand of Interest" by depositor).



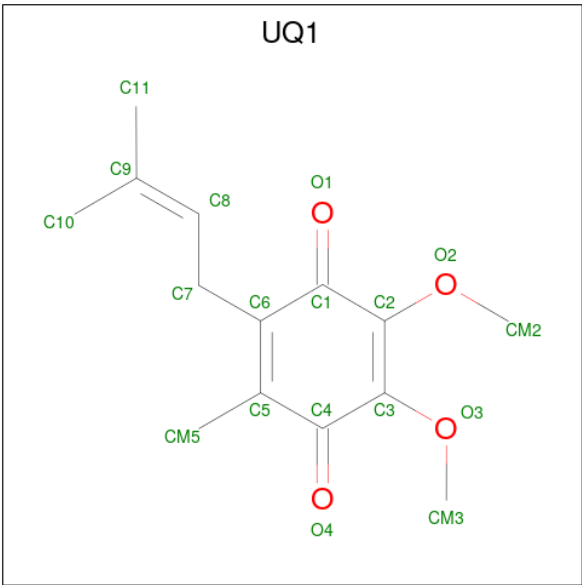
Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	N	O	0
			65	55	4	6	
12	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 13 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



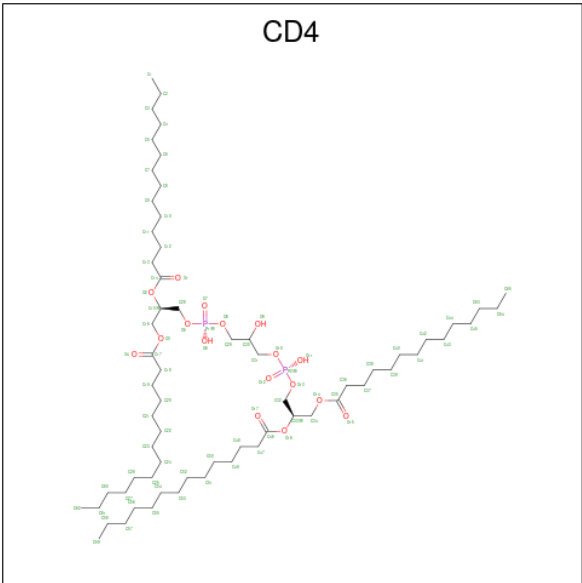
Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			63	59	4	
13	M	1	Total	C	O	0
			63	59	4	

- Molecule 14 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



Mol	Chain	Residues	Atoms			AltConf
14	L	1	Total	C	O	0
			18	14	4	

- Molecule 15 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoyloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (CCD ID: CD4) (formula: C₆₅H₁₂₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 16 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
16	M	1	Total 1	Fe 1	0

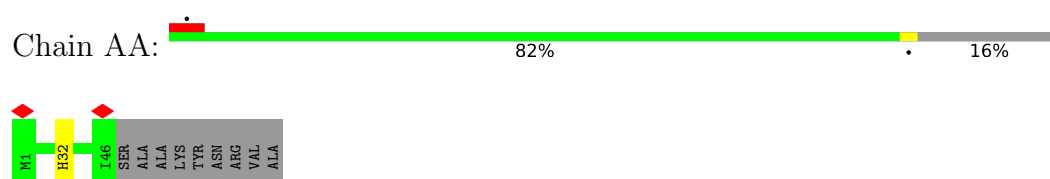
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		AltConf
17	AB	1	Total 1	O 1	0
17	H	2	Total 2	O 2	0
17	X	1	Total 1	O 1	0

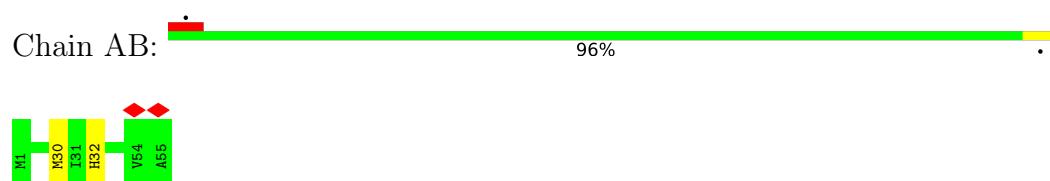
3 Residue-property plots [i](#)

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

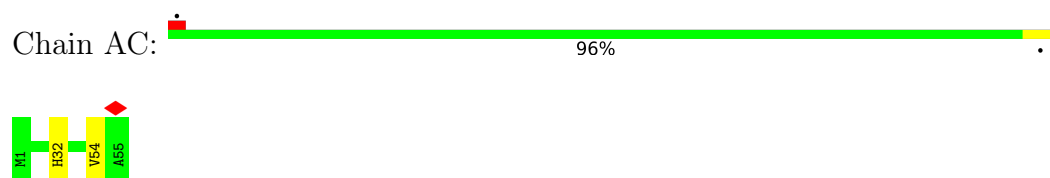
- Molecule 1: Light-harvesting protein B-875 alpha chain



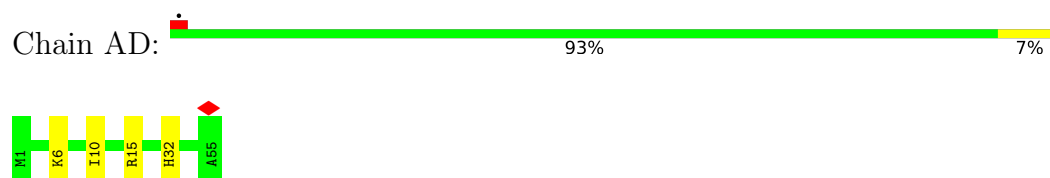
- Molecule 1: Light-harvesting protein B-875 alpha chain



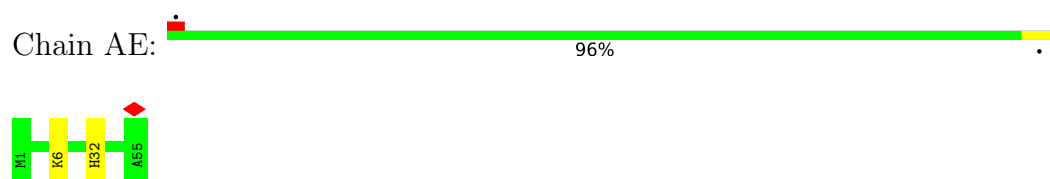
- Molecule 1: Light-harvesting protein B-875 alpha chain



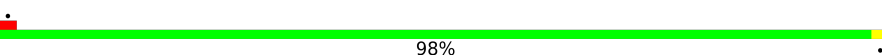
- Molecule 1: Light-harvesting protein B-875 alpha chain

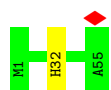


- Molecule 1: Light-harvesting protein B-875 alpha chain

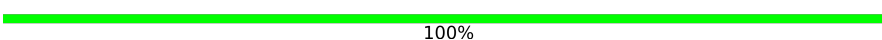


- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AF:  98%

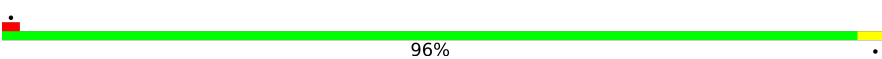


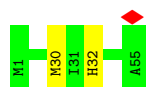
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AG:  100%

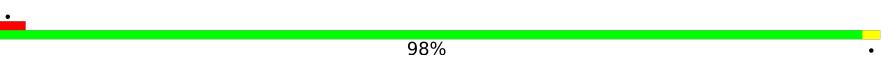
There are no outlier residues recorded for this chain.

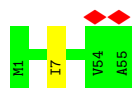
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AH:  96%

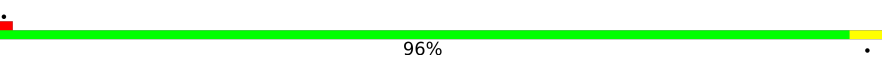


- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AI:  98%

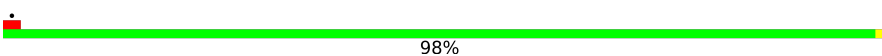


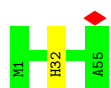
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AJ:  96%

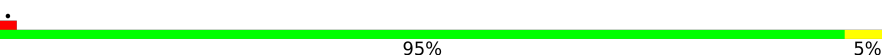


- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AK:  98%

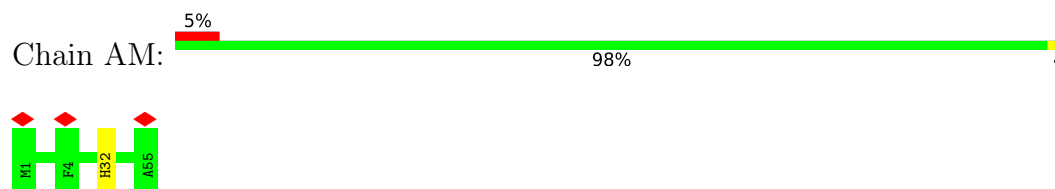


- Molecule 1: Light-harvesting protein B-875 alpha chain

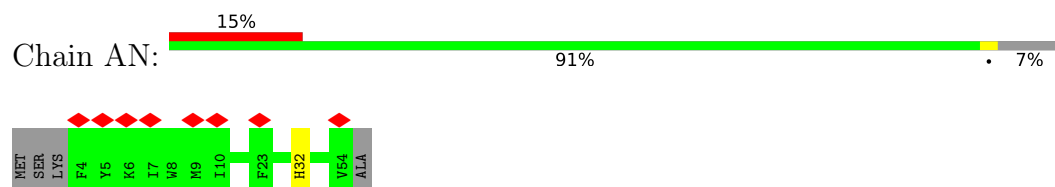
Chain AL:  95%



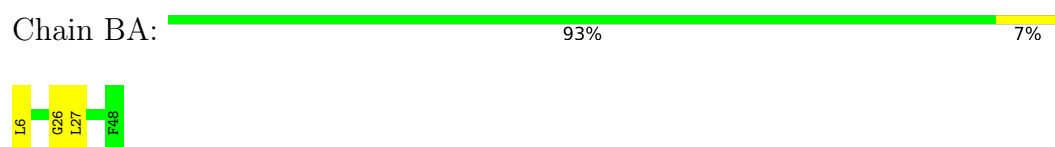
- Molecule 1: Light-harvesting protein B-875 alpha chain



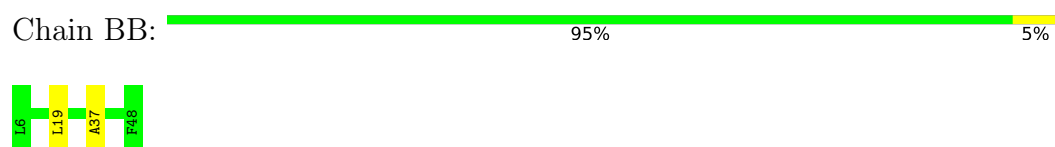
- Molecule 1: Light-harvesting protein B-875 alpha chain



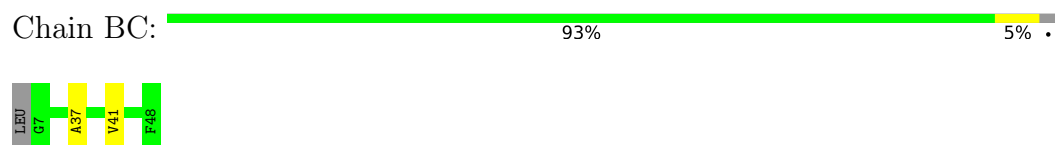
- Molecule 2: Light-harvesting protein B-875 beta chain



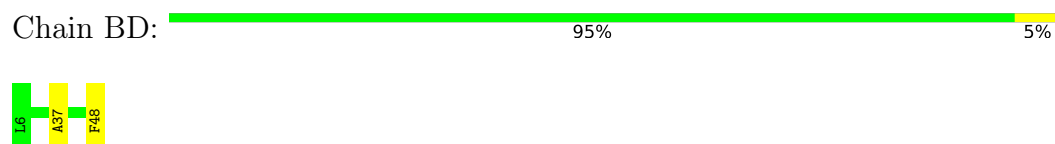
- Molecule 2: Light-harvesting protein B-875 beta chain



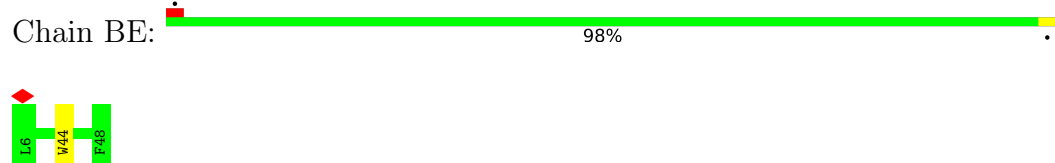
- Molecule 2: Light-harvesting protein B-875 beta chain



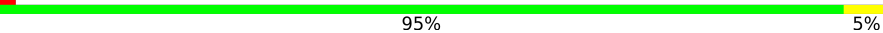
- Molecule 2: Light-harvesting protein B-875 beta chain



- Molecule 2: Light-harvesting protein B-875 beta chain

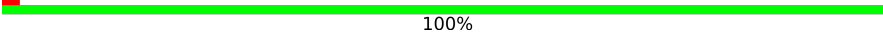


- Molecule 2: Light-harvesting protein B-875 beta chain

Chain BF:  95% 5%

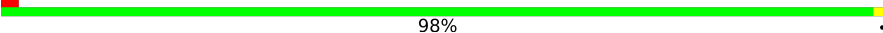


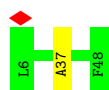
- Molecule 2: Light-harvesting protein B-875 beta chain

Chain BG:  100%

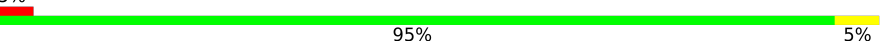


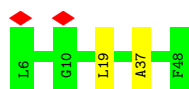
- Molecule 2: Light-harvesting protein B-875 beta chain

Chain BH:  98%



- Molecule 2: Light-harvesting protein B-875 beta chain

Chain BI:  5% 95% 5%

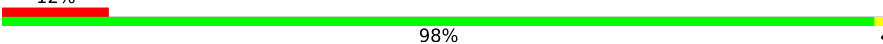


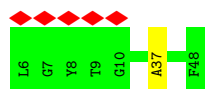
- Molecule 2: Light-harvesting protein B-875 beta chain

Chain BJ:  5% 100%

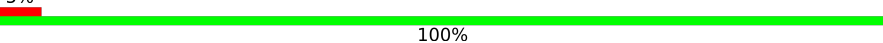


- Molecule 2: Light-harvesting protein B-875 beta chain

Chain BK:  12% 98%

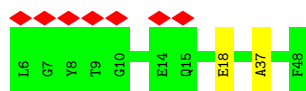


- Molecule 2: Light-harvesting protein B-875 beta chain

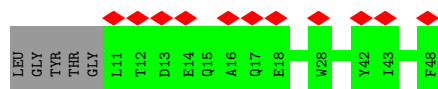
Chain BL:  5% 100%



- Molecule 2: Light-harvesting protein B-875 beta chain



- Molecule 2: Light-harvesting protein B-875 beta chain



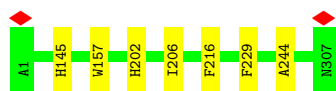
- Molecule 3: Reaction center protein H chain



- Molecule 4: Reaction center protein L chain



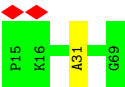
- Molecule 5: Reaction center protein M chain



- Molecule 6: RC-Y



- Molecule 7: Intrinsic membrane protein PufX



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	250613	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 ($e^-/\text{\AA}^2$)	44.94	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0187	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, CD4, U10, UQ1, BPH, 3PE, BCL, FE, SPO

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	AA	0.19	0/405	0.46	0/549
1	AB	0.19	0/475	0.49	0/642
1	AC	0.19	0/474	0.51	0/642
1	AD	0.17	0/475	0.45	0/642
1	AE	0.19	0/475	0.49	0/642
1	AF	0.19	0/475	0.49	0/642
1	AG	0.18	0/475	0.49	0/642
1	AH	0.19	0/475	0.50	0/642
1	AI	0.19	0/475	0.49	0/642
1	AJ	0.19	0/475	0.49	0/642
1	AK	0.18	0/475	0.50	0/642
1	AL	0.18	0/475	0.51	0/642
1	AM	0.20	0/475	0.50	0/642
1	AN	0.18	0/446	0.44	0/606
2	BA	0.15	0/365	0.40	0/499
2	BB	0.16	0/365	0.45	0/499
2	BC	0.15	0/357	0.41	0/488
2	BD	0.14	0/365	0.42	0/499
2	BE	0.14	0/365	0.43	0/499
2	BF	0.16	0/365	0.45	0/499
2	BG	0.14	0/365	0.44	0/499
2	BH	0.14	0/365	0.46	0/499
2	BI	0.15	0/365	0.44	0/499
2	BJ	0.14	0/365	0.44	0/499
2	BK	0.15	0/365	0.48	0/499
2	BL	0.16	0/365	0.45	0/499
2	BM	0.16	0/365	0.46	0/499
2	BN	0.17	0/329	0.43	0/450
3	H	0.17	0/1917	0.48	0/2609
4	L	0.18	0/2320	0.48	0/3175
5	M	0.17	0/2538	0.49	0/3464
6	UU	0.16	0/374	0.45	0/505

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	X	0.19	0/434	0.51	0/586
All	All	0.17	0/19199	0.47	0/26124

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AD	15	ARG	Sidechain

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	AA	392	0	412	1	0
1	AB	461	0	482	2	0
1	AC	460	0	482	3	0
1	AD	461	0	482	3	0
1	AE	461	0	482	2	0
1	AF	461	0	482	1	0
1	AG	461	0	482	0	0
1	AH	461	0	482	3	0
1	AI	461	0	482	1	0
1	AJ	461	0	482	2	0
1	AK	461	0	482	1	0
1	AL	461	0	482	4	0
1	AM	461	0	482	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AN	432	0	447	1	0
2	BA	352	0	336	3	0
2	BB	352	0	336	2	0
2	BC	344	0	325	2	0
2	BD	352	0	336	2	0
2	BE	352	0	336	1	0
2	BF	352	0	336	2	0
2	BG	352	0	336	0	0
2	BH	352	0	336	1	0
2	BI	352	0	336	2	0
2	BJ	352	0	336	0	0
2	BK	352	0	336	1	0
2	BL	352	0	336	0	0
2	BM	352	0	336	2	0
2	BN	317	0	303	0	0
3	H	1867	0	1864	2	0
4	L	2232	0	2187	4	0
5	M	2445	0	2359	4	0
6	UU	363	0	358	0	0
7	X	422	0	436	1	0
8	AA	66	0	74	1	0
8	AB	66	0	74	3	0
8	AC	66	0	74	1	0
8	AD	66	0	74	0	0
8	AE	132	0	148	2	0
8	AF	66	0	74	1	0
8	AG	66	0	74	0	0
8	AH	66	0	74	0	0
8	AI	66	0	74	1	0
8	AJ	66	0	74	3	0
8	AK	132	0	148	1	0
8	AL	66	0	74	0	0
8	AM	132	0	148	2	0
8	AN	66	0	74	0	0
8	BA	66	0	74	1	0
8	BB	66	0	74	1	0
8	BC	66	0	74	2	0
8	BD	66	0	74	1	0
8	BF	66	0	74	1	0
8	BG	66	0	74	0	0
8	BH	66	0	74	1	0
8	BI	66	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	BJ	66	0	74	1	0
8	BL	66	0	74	1	0
8	BN	66	0	74	0	0
8	L	132	0	148	0	0
8	M	132	0	148	0	0
9	AA	42	0	60	2	0
9	AB	42	0	60	3	0
9	AC	84	0	120	2	0
9	AD	84	0	120	2	0
9	AE	42	0	60	3	0
9	AF	84	0	120	5	0
9	AG	84	0	120	0	0
9	AH	84	0	120	3	0
9	AI	84	0	120	4	0
9	AJ	84	0	120	3	0
9	AK	84	0	120	2	0
9	AL	42	0	60	2	0
9	AM	84	0	120	4	0
9	BA	42	0	60	3	0
9	BE	42	0	60	2	0
9	BL	42	0	60	0	0
9	M	42	0	60	2	0
10	AA	35	0	45	0	0
10	AB	35	0	45	0	0
10	M	35	0	46	0	0
10	X	35	0	46	0	0
11	AB	51	0	82	0	0
11	AC	51	0	82	0	0
11	H	102	0	164	1	0
12	L	65	0	76	0	0
12	M	65	0	76	1	0
13	L	63	0	90	1	0
13	M	63	0	90	1	0
14	L	18	0	18	0	0
15	M	84	0	124	1	0
16	M	1	0	0	0	0
17	AB	1	0	0	0	0
17	H	2	0	0	0	0
17	X	1	0	0	0	0
All	All	22480	0	23419	77	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 2.

All (77) 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)
9:AI:102:SPO:H132	8:AJ:101:BCL:H42	1.70	0.73
2:BD:48:PHE:HB3	9:BE:1000:SPO:H343	1.72	0.72
1:AH:30:MET:HE3	9:M:407:SPO:H401	1.76	0.67
1:AC:54:VAL:O	1:AC:54:VAL:HG23	1.97	0.64
2:BE:44:TRP:CD1	9:BE:1000:SPO:H342	2.32	0.64
13:M:404:U10:H371	13:M:404:U10:H502	1.80	0.63
1:AD:6:LYS:HB3	9:AE:102:SPO:H402	1.81	0.63
1:AH:30:MET:HE2	9:AH:101:SPO:HM12	1.84	0.59
9:AH:101:SPO:H132	8:AI:101:BCL:H42	1.86	0.57
9:AB:103:SPO:H242	2:BB:37:ALA:HB1	1.87	0.57
9:AI:102:SPO:H402	2:BI:19:LEU:HA	1.87	0.56
8:AA:1001:BCL:H41	7:X:31:ALA:HB2	1.87	0.56
4:L:38:THR:HG21	4:L:100:TRP:HE3	1.71	0.55
1:AL:6:LYS:HB3	9:AM:1002:SPO:H402	1.89	0.54
9:AD:103:SPO:H242	2:BD:37:ALA:HB1	1.92	0.52
8:AB:101:BCL:H72	8:AB:101:BCL:H41	1.92	0.51
1:AA:32:HIS:CE1	8:BA:102:BCL:HMD3	2.45	0.51
8:AB:101:BCL:HED2	9:AB:103:SPO:H16	1.91	0.51
9:AH:103:SPO:H242	2:BH:37:ALA:HB1	1.92	0.51
9:AF:103:SPO:H242	2:BF:37:ALA:HB1	1.92	0.50
1:AL:32:HIS:CE1	8:BL:102:BCL:HMD3	2.48	0.49
1:AJ:25:PHE:HB2	8:AJ:101:BCL:H43	1.95	0.49
1:AK:32:HIS:CE1	8:AK:103:BCL:HMD3	2.47	0.49
9:AA:1002:SPO:H402	2:BB:19:LEU:HA	1.94	0.49
5:M:157:TRP:CE2	9:M:407:SPO:H293	2.48	0.49
1:AE:6:LYS:HD3	9:AF:101:SPO:H393	1.95	0.48
1:AC:32:HIS:CE1	8:BC:101:BCL:HMD3	2.47	0.48
9:AK:104:SPO:H242	2:BK:37:ALA:HB1	1.95	0.48
1:AB:32:HIS:CE1	8:BB:1001:BCL:HMD3	2.49	0.48
13:L:302:U10:H402	13:L:302:U10:H33	1.95	0.47
1:AD:32:HIS:CE1	8:BD:101:BCL:HMD3	2.50	0.47
5:M:229:PHE:HB2	5:M:244:ALA:HB2	1.96	0.47
9:AI:103:SPO:H242	2:BI:37:ALA:HB1	1.96	0.47
1:AF:32:HIS:CE1	8:BF:101:BCL:HMD3	2.50	0.47
2:BA:27:LEU:HD13	9:BA:101:SPO:C20	2.45	0.46
9:AJ:103:SPO:H341	9:AJ:103:SPO:C37	2.46	0.46
3:H:40:TYR:CE2	11:H:302:3PE:H112	2.51	0.46
9:AM:1004:SPO:H242	2:BM:37:ALA:HB1	1.98	0.45
5:M:202:HIS:CE1	5:M:206:ILE:HD11	2.51	0.45
1:AJ:32:HIS:CE1	8:BJ:101:BCL:HMD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:173:HIS:CE1	4:L:177:ILE:HD11	2.51	0.45
1:AM:32:HIS:CE1	8:AM:1003:BCL:HMD3	2.53	0.44
1:AE:32:HIS:CE1	8:AE:103:BCL:HMD3	2.54	0.43
9:BA:101:SPO:H291	9:BA:101:SPO:H311	1.66	0.43
5:M:145:HIS:CD2	15:M:405:CD4:H30	2.53	0.43
9:AC:103:SPO:H26	9:AC:103:SPO:H241	1.90	0.43
9:AD:103:SPO:H341	9:AD:103:SPO:C37	2.48	0.43
9:AA:1002:SPO:H393	2:BA:6:LEU:HD23	2.00	0.43
9:AF:103:SPO:H26	9:AF:103:SPO:H241	1.90	0.43
9:AF:101:SPO:H26	9:AF:101:SPO:H241	1.89	0.43
1:AI:7:ILE:HB	9:AJ:102:SPO:H343	2.01	0.42
1:AH:32:HIS:CE1	8:BH:101:BCL:HMD3	2.54	0.42
1:AC:54:VAL:O	1:AC:54:VAL:CG2	2.67	0.42
9:AC:103:SPO:H242	2:BC:37:ALA:HB1	2.00	0.42
9:AE:102:SPO:H6	8:AF:102:BCL:HMB2	2.02	0.42
2:BA:26:GLY:HA3	9:BA:101:SPO:C27	2.50	0.42
1:AL:6:LYS:NZ	2:BM:18:GLU:OE2	2.40	0.42
9:AL:1002:SPO:H26	9:AL:1002:SPO:H241	1.93	0.42
2:BC:41:VAL:HG11	8:BC:101:BCL:HBC1	2.02	0.42
8:AB:101:BCL:OBB	8:AB:101:BCL:HHC	2.19	0.41
9:AI:102:SPO:H341	9:AI:102:SPO:H361	1.83	0.41
1:AL:20:GLN:HE21	9:AL:1002:SPO:C20	2.33	0.41
1:AB:30:MET:HE1	4:L:48:LEU:HD23	2.03	0.41
8:AC:102:BCL:OBB	8:AC:102:BCL:HHC	2.21	0.41
1:AD:10:ILE:HD11	9:AE:102:SPO:H403	2.03	0.41
9:AJ:102:SPO:H241	9:AJ:102:SPO:H26	1.84	0.41
9:AM:1002:SPO:H41	1:AN:32:HIS:CG	2.56	0.41
8:AJ:101:BCL:H61	8:AJ:101:BCL:H41	1.93	0.41
12:M:402:BPH:HHD	12:M:402:BPH:HBC3	2.03	0.41
9:AM:1004:SPO:H26	9:AM:1004:SPO:H241	1.90	0.41
3:H:157:ASP:OD1	3:H:157:ASP:N	2.54	0.41
9:AF:101:SPO:H403	2:BF:19:LEU:HD12	2.02	0.40
9:AB:103:SPO:H26	9:AB:103:SPO:H241	1.86	0.40
9:AK:104:SPO:H26	9:AK:104:SPO:H241	1.84	0.40
8:AM:1001:BCL:HHC	8:AM:1001:BCL:OBB	2.21	0.40
8:AE:101:BCL:OBB	8:AE:101:BCL:HHC	2.22	0.40
4:L:210:ASP:OD1	4:L:210:ASP:N	2.54	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	AA	44/55 (80%)	43 (98%)	1 (2%)	0	100	100
1	AB	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AC	53/55 (96%)	53 (100%)	0	0	100	100
1	AD	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AE	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AF	53/55 (96%)	53 (100%)	0	0	100	100
1	AG	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AH	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AI	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
1	AJ	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AK	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
1	AL	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AM	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AN	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	BA	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
2	BB	41/43 (95%)	41 (100%)	0	0	100	100
2	BC	40/43 (93%)	40 (100%)	0	0	100	100
2	BD	41/43 (95%)	41 (100%)	0	0	100	100
2	BE	41/43 (95%)	41 (100%)	0	0	100	100
2	BF	41/43 (95%)	41 (100%)	0	0	100	100
2	BG	41/43 (95%)	41 (100%)	0	0	100	100
2	BH	41/43 (95%)	41 (100%)	0	0	100	100
2	BI	41/43 (95%)	41 (100%)	0	0	100	100
2	BJ	41/43 (95%)	41 (100%)	0	0	100	100
2	BK	41/43 (95%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BL	41/43 (95%)	41 (100%)	0	0	100	100
2	BM	41/43 (95%)	41 (100%)	0	0	100	100
2	BN	36/43 (84%)	35 (97%)	1 (3%)	0	100	100
3	H	244/246 (99%)	240 (98%)	4 (2%)	0	100	100
4	L	279/281 (99%)	273 (98%)	6 (2%)	0	100	100
5	M	305/307 (99%)	297 (97%)	8 (3%)	0	100	100
6	UU	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
7	X	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
All	All	2225/2310 (96%)	2188 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AA	43/49 (88%)	43 (100%)	0	100	100
1	AB	49/49 (100%)	49 (100%)	0	100	100
1	AC	49/49 (100%)	49 (100%)	0	100	100
1	AD	49/49 (100%)	49 (100%)	0	100	100
1	AE	49/49 (100%)	49 (100%)	0	100	100
1	AF	49/49 (100%)	49 (100%)	0	100	100
1	AG	49/49 (100%)	49 (100%)	0	100	100
1	AH	49/49 (100%)	49 (100%)	0	100	100
1	AI	49/49 (100%)	49 (100%)	0	100	100
1	AJ	49/49 (100%)	49 (100%)	0	100	100
1	AK	49/49 (100%)	49 (100%)	0	100	100
1	AL	49/49 (100%)	49 (100%)	0	100	100
1	AM	49/49 (100%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AN	46/49 (94%)	46 (100%)	0	100	100
2	BA	35/35 (100%)	35 (100%)	0	100	100
2	BB	35/35 (100%)	35 (100%)	0	100	100
2	BC	34/35 (97%)	34 (100%)	0	100	100
2	BD	35/35 (100%)	35 (100%)	0	100	100
2	BE	35/35 (100%)	35 (100%)	0	100	100
2	BF	35/35 (100%)	35 (100%)	0	100	100
2	BG	35/35 (100%)	35 (100%)	0	100	100
2	BH	35/35 (100%)	35 (100%)	0	100	100
2	BI	35/35 (100%)	35 (100%)	0	100	100
2	BJ	35/35 (100%)	35 (100%)	0	100	100
2	BK	35/35 (100%)	35 (100%)	0	100	100
2	BL	35/35 (100%)	35 (100%)	0	100	100
2	BM	35/35 (100%)	35 (100%)	0	100	100
2	BN	32/35 (91%)	32 (100%)	0	100	100
3	H	198/198 (100%)	197 (100%)	1 (0%)	81	92
4	L	220/220 (100%)	218 (99%)	2 (1%)	70	87
5	M	240/240 (100%)	239 (100%)	1 (0%)	84	93
6	UU	33/33 (100%)	33 (100%)	0	100	100
7	X	42/42 (100%)	42 (100%)	0	100	100
All	All	1896/1909 (99%)	1892 (100%)	4 (0%)	85	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	231	ASP
4	L	210	ASP
4	L	247	CYS
5	M	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	20	GLN

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Mol	Chain	Res	Type
1	AI	20	GLN
1	AL	20	GLN
2	BJ	17	GLN
5	M	138	GLN
5	M	259	ASN
5	M	299	GLN
5	M	300	ASN
5	M	307	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 73 ligands modelled in this entry, 1 is monoatomic - leaving 72 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	BCL	AL	1001	-	69,74,74	1.18	5 (7%)	79,115,115	1.42	12 (15%)
9	SPO	AK	104	-	41,41,41	0.18	0	47,50,50	0.37	0
8	BCL	L	304	-	69,74,74	1.17	5 (7%)	79,115,115	1.25	9 (11%)
10	LMT	AA	1003	-	36,36,36	1.05	4 (11%)	47,47,47	0.95	2 (4%)
8	BCL	AK	103	-	69,74,74	1.16	5 (7%)	79,115,115	1.30	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	LMT	M	401	-	36,36,36	1.02	4 (11%)	47,47,47	0.98	2 (4%)
13	U10	M	404	-	63,63,63	2.72	17 (26%)	78,79,79	1.66	17 (21%)
8	BCL	AG	102	-	69,74,74	1.16	4 (5%)	79,115,115	1.32	9 (11%)
8	BCL	AH	102	-	69,74,74	1.19	5 (7%)	79,115,115	1.35	10 (12%)
11	3PE	AC	104	-	50,50,50	0.53	0	53,55,55	0.58	1 (1%)
9	SPO	AJ	103	-	41,41,41	0.27	0	47,50,50	0.62	1 (2%)
9	SPO	AL	1002	-	41,41,41	0.28	0	47,50,50	0.60	1 (2%)
8	BCL	AK	101	-	69,74,74	1.20	4 (5%)	79,115,115	1.39	11 (13%)
8	BCL	BF	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.26	9 (11%)
9	SPO	AB	103	-	41,41,41	0.30	0	47,50,50	0.67	2 (4%)
8	BCL	BH	101	-	69,74,74	1.17	5 (7%)	79,115,115	1.32	9 (11%)
9	SPO	AC	103	-	41,41,41	0.19	0	47,50,50	0.24	0
9	SPO	AI	102	-	41,41,41	0.27	0	47,50,50	0.67	1 (2%)
9	SPO	BE	1000	-	41,41,41	0.26	0	47,50,50	0.46	0
13	U10	L	302	-	63,63,63	2.75	17 (26%)	78,79,79	1.57	19 (24%)
8	BCL	AI	101	-	69,74,74	1.20	4 (5%)	79,115,115	1.35	10 (12%)
8	BCL	AJ	101	-	69,74,74	1.19	5 (7%)	79,115,115	1.50	10 (12%)
14	UQ1	L	303	-	18,18,18	0.78	0	24,25,25	1.83	6 (25%)
9	SPO	AJ	102	-	41,41,41	0.22	0	47,50,50	0.51	0
8	BCL	AB	101	-	69,74,74	1.21	6 (8%)	79,115,115	1.43	11 (13%)
8	BCL	AC	102	-	69,74,74	1.16	4 (5%)	79,115,115	1.31	9 (11%)
8	BCL	BC	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.30	9 (11%)
8	BCL	M	406	-	69,74,74	1.13	5 (7%)	79,115,115	1.37	11 (13%)
12	BPH	M	402	-	59,70,70	1.12	4 (6%)	59,101,101	1.89	10 (16%)
11	3PE	H	302	-	50,50,50	0.51	0	53,55,55	0.67	2 (3%)
9	SPO	AG	103	-	41,41,41	0.22	0	47,50,50	0.45	0
10	LMT	X	101	-	36,36,36	1.07	4 (11%)	47,47,47	0.91	2 (4%)
8	BCL	AM	1003	-	69,74,74	1.16	4 (5%)	79,115,115	1.31	9 (11%)
8	BCL	AA	1001	-	69,74,74	1.23	5 (7%)	79,115,115	1.28	8 (10%)
9	SPO	AF	103	-	41,41,41	0.25	0	47,50,50	0.35	0
9	SPO	AM	1002	-	41,41,41	0.21	0	47,50,50	0.39	0
9	SPO	AF	101	-	41,41,41	0.27	0	47,50,50	0.52	1 (2%)
9	SPO	AM	1004	-	41,41,41	0.27	0	47,50,50	0.38	0
12	BPH	L	301	-	59,70,70	1.08	3 (5%)	59,101,101	1.88	10 (16%)
11	3PE	AB	102	-	50,50,50	0.53	0	53,55,55	0.55	1 (1%)
9	SPO	AD	101	-	41,41,41	0.17	0	47,50,50	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SPO	AK	102	-	41,41,41	0.20	0	47,50,50	0.36	0
9	SPO	AE	102	-	41,41,41	0.23	0	47,50,50	0.45	0
9	SPO	AH	103	-	41,41,41	0.21	0	47,50,50	0.47	0
11	3PE	H	301	-	50,50,50	0.53	0	53,55,55	0.52	1 (1%)
8	BCL	AD	102	-	69,74,74	1.17	4 (5%)	79,115,115	1.49	10 (12%)
9	SPO	AH	101	-	41,41,41	0.16	0	47,50,50	0.41	0
8	BCL	AE	103	-	69,74,74	1.16	5 (7%)	79,115,115	1.36	10 (12%)
15	CD4	M	405	-	83,83,83	0.50	0	89,95,95	0.98	4 (4%)
8	BCL	AN	101	-	69,74,74	1.18	6 (8%)	79,115,115	1.29	9 (11%)
9	SPO	AA	1002	-	41,41,41	0.21	0	47,50,50	0.57	1 (2%)
9	SPO	AI	103	-	41,41,41	0.30	0	47,50,50	0.86	2 (4%)
8	BCL	AE	101	-	69,74,74	1.16	4 (5%)	79,115,115	1.34	9 (11%)
8	BCL	BI	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.32	11 (13%)
9	SPO	AC	101	-	41,41,41	0.18	0	47,50,50	0.40	0
9	SPO	M	407	-	41,41,41	0.20	0	47,50,50	0.44	0
8	BCL	M	403	-	69,74,74	1.20	6 (8%)	79,115,115	1.33	9 (11%)
9	SPO	AG	101	-	41,41,41	0.22	0	47,50,50	0.37	0
8	BCL	AM	1001	-	69,74,74	1.18	4 (5%)	79,115,115	1.40	11 (13%)
8	BCL	BG	101	-	69,74,74	1.17	5 (7%)	79,115,115	1.32	10 (12%)
8	BCL	BD	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.35	12 (15%)
8	BCL	L	305	-	69,74,74	1.14	5 (7%)	79,115,115	1.33	10 (12%)
8	BCL	BA	102	-	69,74,74	1.16	5 (7%)	79,115,115	1.36	12 (15%)
8	BCL	AF	102	-	69,74,74	1.19	5 (7%)	79,115,115	1.38	9 (11%)
8	BCL	BB	1001	-	69,74,74	1.14	5 (7%)	79,115,115	1.32	10 (12%)
9	SPO	BL	101	-	41,41,41	0.25	0	47,50,50	0.37	0
8	BCL	BL	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.30	11 (13%)
9	SPO	BA	101	-	41,41,41	0.19	0	47,50,50	0.60	1 (2%)
9	SPO	AD	103	-	41,41,41	0.20	0	47,50,50	0.41	0
10	LMT	AB	104	-	36,36,36	1.08	4 (11%)	47,47,47	0.84	0
8	BCL	BN	101	-	69,74,74	1.19	4 (5%)	79,115,115	1.38	10 (12%)
8	BCL	BJ	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.30	9 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	AL	1001	-	-	5/41/137/137	-
9	SPO	AK	104	-	-	8/47/47/47	-
8	BCL	L	304	-	-	0/41/137/137	-
10	LMT	AA	1003	-	-	3/21/61/61	0/2/2/2
8	BCL	AK	103	-	-	5/41/137/137	-
10	LMT	M	401	-	-	4/21/61/61	0/2/2/2
13	U10	M	404	-	-	7/63/87/87	0/1/1/1
8	BCL	AG	102	-	-	0/41/137/137	-
8	BCL	AH	102	-	-	0/41/137/137	-
11	3PE	AC	104	-	-	12/54/54/54	-
9	SPO	AJ	103	-	-	4/47/47/47	-
9	SPO	AL	1002	-	-	3/47/47/47	-
8	BCL	AK	101	-	-	5/41/137/137	-
8	BCL	BF	101	-	-	8/41/137/137	-
9	SPO	AB	103	-	-	8/47/47/47	-
8	BCL	BH	101	-	-	6/41/137/137	-
9	SPO	AC	103	-	-	3/47/47/47	-
9	SPO	AI	102	-	-	5/47/47/47	-
9	SPO	BE	1000	-	-	7/47/47/47	-
13	U10	L	302	-	-	13/63/87/87	0/1/1/1
8	BCL	AI	101	-	-	10/41/137/137	-
8	BCL	AJ	101	-	-	6/41/137/137	-
14	UQ1	L	303	-	-	4/9/33/33	0/1/1/1
9	SPO	AJ	102	-	-	6/47/47/47	-
8	BCL	AB	101	-	-	5/41/137/137	-
8	BCL	AC	102	-	-	10/41/137/137	-
8	BCL	BC	101	-	-	7/41/137/137	-
8	BCL	M	406	-	-	5/41/137/137	-
12	BPH	M	402	-	-	4/37/105/105	0/5/6/6
11	3PE	H	302	-	-	14/54/54/54	-
9	SPO	AG	103	-	-	2/47/47/47	-
10	LMT	X	101	-	-	1/21/61/61	0/2/2/2
8	BCL	AM	1003	-	-	6/41/137/137	-
8	BCL	AA	1001	-	-	5/41/137/137	-
9	SPO	AF	103	-	-	2/47/47/47	-
9	SPO	AM	1002	-	-	2/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SPO	AF	101	-	-	4/47/47/47	-
9	SPO	AM	1004	-	-	3/47/47/47	-
12	BPH	L	301	-	-	4/37/105/105	0/5/6/6
11	3PE	AB	102	-	-	9/54/54/54	-
9	SPO	AD	101	-	-	5/47/47/47	-
9	SPO	AK	102	-	-	4/47/47/47	-
9	SPO	AE	102	-	-	3/47/47/47	-
9	SPO	AH	103	-	-	3/47/47/47	-
11	3PE	H	301	-	-	16/54/54/54	-
8	BCL	AD	102	-	-	4/41/137/137	-
9	SPO	AH	101	-	-	2/47/47/47	-
8	BCL	AE	103	-	-	5/41/137/137	-
15	CD4	M	405	-	-	12/94/94/94	-
8	BCL	AN	101	-	-	4/41/137/137	-
9	SPO	AA	1002	-	-	8/47/47/47	-
9	SPO	AI	103	-	-	3/47/47/47	-
8	BCL	AE	101	-	-	3/41/137/137	-
8	BCL	BI	101	-	-	3/41/137/137	-
9	SPO	AC	101	-	-	2/47/47/47	-
9	SPO	M	407	-	-	3/47/47/47	-
8	BCL	M	403	-	-	1/41/137/137	-
9	SPO	AG	101	-	-	2/47/47/47	-
8	BCL	AM	1001	-	-	3/41/137/137	-
8	BCL	BG	101	-	-	4/41/137/137	-
8	BCL	BD	101	-	-	2/41/137/137	-
8	BCL	L	305	-	-	3/41/137/137	-
8	BCL	BA	102	-	-	4/41/137/137	-
8	BCL	AF	102	-	-	3/41/137/137	-
8	BCL	BB	1001	-	-	7/41/137/137	-
9	SPO	BL	101	-	-	5/47/47/47	-
8	BCL	BL	102	-	-	10/41/137/137	-
9	SPO	BA	101	-	-	3/47/47/47	-
9	SPO	AD	103	-	-	4/47/47/47	-
10	LMT	AB	104	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	BN	101	-	-	5/41/137/137	-
8	BCL	BJ	101	-	-	7/41/137/137	-

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	302	U10	C43-C44	6.36	1.47	1.33
13	M	404	U10	C43-C44	6.34	1.47	1.33
13	L	302	U10	C48-C49	6.33	1.47	1.33
13	L	302	U10	C18-C19	6.32	1.47	1.33
13	M	404	U10	C18-C19	6.30	1.47	1.33
13	L	302	U10	C23-C24	6.29	1.47	1.33
13	M	404	U10	C28-C29	6.28	1.47	1.33
13	L	302	U10	C38-C39	6.28	1.47	1.33
13	M	404	U10	C8-C9	6.27	1.47	1.33
13	M	404	U10	C48-C49	6.26	1.47	1.33
13	L	302	U10	C8-C9	6.25	1.47	1.33
13	M	404	U10	C33-C34	6.25	1.47	1.33
13	L	302	U10	C33-C34	6.24	1.47	1.33
13	L	302	U10	C28-C29	6.23	1.47	1.33
13	M	404	U10	C38-C39	6.22	1.47	1.33
13	L	302	U10	C13-C14	6.21	1.47	1.33
13	M	404	U10	C13-C14	6.18	1.47	1.33
13	M	404	U10	C23-C24	6.18	1.47	1.33
8	AA	1001	BCL	MG-NA	5.63	2.19	2.06
8	M	403	BCL	MG-NA	5.56	2.19	2.06
8	AB	101	BCL	MG-NA	5.45	2.19	2.06
8	AL	1001	BCL	MG-NA	5.43	2.19	2.06
13	L	302	U10	O4-C4	-5.43	1.23	1.36
8	AM	1001	BCL	MG-NA	5.42	2.19	2.06
8	BN	101	BCL	MG-NA	5.41	2.19	2.06
8	AJ	101	BCL	MG-NA	5.38	2.19	2.06
8	AF	102	BCL	MG-NA	5.37	2.19	2.06
8	AH	102	BCL	MG-NA	5.34	2.19	2.06
8	AD	102	BCL	MG-NA	5.32	2.18	2.06
8	AI	101	BCL	MG-NA	5.31	2.18	2.06
8	AC	102	BCL	MG-NA	5.27	2.18	2.06
8	AN	101	BCL	MG-NA	5.26	2.18	2.06
8	AK	101	BCL	MG-NA	5.25	2.18	2.06
8	BH	101	BCL	MG-NA	5.23	2.18	2.06
13	M	404	U10	C53-C54	5.19	1.48	1.32
8	AE	103	BCL	MG-NA	5.16	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AG	102	BCL	MG-NA	5.16	2.18	2.06
8	AE	101	BCL	MG-NA	5.14	2.18	2.06
13	L	302	U10	C53-C54	5.09	1.47	1.32
8	AM	1003	BCL	MG-NA	5.07	2.18	2.06
8	BI	101	BCL	MG-NA	5.06	2.18	2.06
8	BD	101	BCL	MG-NA	5.06	2.18	2.06
8	BC	101	BCL	MG-NA	5.05	2.18	2.06
8	BJ	101	BCL	MG-NA	5.05	2.18	2.06
8	L	304	BCL	MG-NA	5.05	2.18	2.06
8	BL	102	BCL	MG-NA	5.04	2.18	2.06
8	BF	101	BCL	MG-NA	5.02	2.18	2.06
8	BB	1001	BCL	MG-NA	5.02	2.18	2.06
8	BG	101	BCL	MG-NA	5.02	2.18	2.06
8	BA	102	BCL	MG-NA	5.01	2.18	2.06
8	AK	103	BCL	MG-NA	4.97	2.18	2.06
8	L	305	BCL	MG-NA	4.95	2.18	2.06
8	M	406	BCL	MG-NA	4.94	2.18	2.06
13	L	302	U10	O3-C3	-4.87	1.25	1.36
13	M	404	U10	O3-C3	-4.82	1.25	1.36
13	M	404	U10	O4-C4	-4.76	1.25	1.36
8	AA	1001	BCL	MG-NC	4.16	2.16	2.06
12	L	301	BPH	CBD-CGD	-4.12	1.47	1.52
12	M	402	BPH	CBD-CGD	-4.11	1.47	1.52
8	AI	101	BCL	MG-NC	3.93	2.15	2.06
8	AJ	101	BCL	MG-NC	3.93	2.15	2.06
8	BF	101	BCL	MG-NC	3.91	2.15	2.06
8	BJ	101	BCL	MG-NC	3.91	2.15	2.06
8	AB	101	BCL	MG-NC	3.91	2.15	2.06
8	BH	101	BCL	MG-NC	3.90	2.15	2.06
8	AH	102	BCL	MG-NC	3.87	2.15	2.06
8	AD	102	BCL	MG-NC	3.86	2.15	2.06
8	AL	1001	BCL	MG-NC	3.85	2.15	2.06
8	L	304	BCL	MG-NC	3.85	2.15	2.06
8	AM	1001	BCL	MG-NC	3.82	2.15	2.06
8	AF	102	BCL	MG-NC	3.80	2.15	2.06
8	AK	101	BCL	MG-NC	3.79	2.15	2.06
8	BG	101	BCL	MG-NC	3.79	2.15	2.06
8	AN	101	BCL	MG-NC	3.77	2.15	2.06
8	AE	103	BCL	MG-NC	3.77	2.15	2.06
8	AC	102	BCL	MG-NC	3.77	2.15	2.06
8	AM	1003	BCL	MG-NC	3.76	2.15	2.06
8	BB	1001	BCL	MG-NC	3.74	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	BD	101	BCL	MG-NC	3.74	2.15	2.06
8	BA	102	BCL	MG-NC	3.73	2.15	2.06
8	BI	101	BCL	MG-NC	3.72	2.15	2.06
8	BL	102	BCL	MG-NC	3.72	2.15	2.06
8	BC	101	BCL	MG-NC	3.71	2.15	2.06
8	BN	101	BCL	MG-NC	3.70	2.15	2.06
8	AG	102	BCL	MG-NC	3.69	2.15	2.06
8	AK	103	BCL	MG-NC	3.69	2.15	2.06
8	AE	101	BCL	MG-NC	3.62	2.14	2.06
8	M	403	BCL	MG-NC	3.61	2.14	2.06
8	M	406	BCL	MG-NC	3.55	2.14	2.06
8	L	305	BCL	MG-NC	3.43	2.14	2.06
12	M	402	BPH	C3D-CAD	-3.22	1.41	1.47
12	L	301	BPH	C3D-CAD	-3.18	1.41	1.47
13	L	302	U10	C4-C5	-3.17	1.39	1.48
13	M	404	U10	C4-C5	-3.14	1.39	1.48
12	L	301	BPH	C3B-C4B	3.02	1.46	1.41
12	M	402	BPH	C3B-C4B	2.99	1.46	1.41
8	AA	1001	BCL	C3B-C4B	2.99	1.47	1.41
8	AK	101	BCL	C3B-C4B	2.97	1.47	1.41
8	AG	102	BCL	C3B-C4B	2.96	1.47	1.41
8	BN	101	BCL	C3B-C4B	2.94	1.46	1.41
8	AD	102	BCL	C3B-C4B	2.94	1.46	1.41
8	AE	101	BCL	C3B-C4B	2.93	1.46	1.41
8	AH	102	BCL	C3B-C4B	2.92	1.46	1.41
8	AN	101	BCL	C3B-C4B	2.92	1.46	1.41
8	AK	103	BCL	C3B-C4B	2.92	1.46	1.41
8	AJ	101	BCL	C3B-C4B	2.90	1.46	1.41
8	AM	1003	BCL	C3B-C4B	2.90	1.46	1.41
8	AL	1001	BCL	C3B-C4B	2.89	1.46	1.41
8	AM	1001	BCL	C3B-C4B	2.88	1.46	1.41
8	AF	102	BCL	C3B-C4B	2.87	1.46	1.41
8	AI	101	BCL	C3B-C4B	2.86	1.46	1.41
8	BH	101	BCL	C3B-C4B	2.86	1.46	1.41
8	BB	1001	BCL	C3B-C4B	2.85	1.46	1.41
8	M	403	BCL	C3B-C4B	2.85	1.46	1.41
8	AC	102	BCL	C3B-C4B	2.82	1.46	1.41
8	BC	101	BCL	C3B-C4B	2.82	1.46	1.41
8	AE	103	BCL	C3B-C4B	2.82	1.46	1.41
8	BD	101	BCL	C3B-C4B	2.79	1.46	1.41
8	L	304	BCL	C3B-C4B	2.78	1.46	1.41
8	BI	101	BCL	C3B-C4B	2.76	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AB	101	BCL	C3B-C4B	2.76	1.46	1.41
8	BL	102	BCL	C3B-C4B	2.76	1.46	1.41
8	BJ	101	BCL	C3B-C4B	2.75	1.46	1.41
8	M	406	BCL	C3B-C4B	2.72	1.46	1.41
8	BG	101	BCL	C3B-C4B	2.71	1.46	1.41
8	BA	102	BCL	C3B-C4B	2.69	1.46	1.41
13	L	302	U10	C3-C2	-2.64	1.41	1.48
13	M	404	U10	C6-C5	-2.64	1.39	1.46
13	L	302	U10	C6-C5	-2.61	1.39	1.46
8	M	406	BCL	CHD-C1D	2.56	1.43	1.38
8	BF	101	BCL	C3B-C4B	2.53	1.46	1.41
8	AB	101	BCL	CHD-C1D	2.53	1.43	1.38
10	AA	1003	LMT	O3'-C3'	-2.53	1.36	1.43
8	L	305	BCL	C3B-C4B	2.50	1.46	1.41
10	AB	104	LMT	O3'-C3'	-2.49	1.36	1.43
10	AB	104	LMT	O2'-C2'	-2.43	1.36	1.43
8	AK	101	BCL	CHD-C1D	2.43	1.43	1.38
10	M	401	LMT	O3'-C3'	-2.43	1.36	1.43
10	X	101	LMT	O3'-C3'	-2.42	1.37	1.43
13	L	302	U10	C6-C1	2.42	1.39	1.35
13	M	404	U10	C3-C2	-2.39	1.42	1.48
8	BH	101	BCL	CHD-C1D	2.38	1.43	1.38
13	M	404	U10	C6-C1	2.37	1.39	1.35
8	L	305	BCL	CHD-C1D	2.37	1.43	1.38
8	M	403	BCL	CHD-C1D	2.37	1.43	1.38
8	BN	101	BCL	CHD-C1D	2.36	1.43	1.38
8	BG	101	BCL	CHD-C1D	2.31	1.42	1.38
8	BD	101	BCL	CHD-C1D	2.29	1.42	1.38
8	BJ	101	BCL	CHD-C1D	2.28	1.42	1.38
8	AD	102	BCL	CHD-C1D	2.28	1.42	1.38
8	BA	102	BCL	CHD-C1D	2.27	1.42	1.38
8	AK	103	BCL	CHD-C1D	2.26	1.42	1.38
10	AA	1003	LMT	O2B-C2B	-2.25	1.37	1.43
8	AJ	101	BCL	CHD-C1D	2.24	1.42	1.38
8	AG	102	BCL	CHD-C1D	2.24	1.42	1.38
13	M	404	U10	C1-C2	-2.23	1.39	1.47
8	AL	1001	BCL	CHD-C1D	2.23	1.42	1.38
8	BF	101	BCL	CHD-C1D	2.22	1.42	1.38
8	AM	1003	BCL	CHD-C1D	2.22	1.42	1.38
8	AN	101	BCL	CHD-C1D	2.22	1.42	1.38
8	AA	1001	BCL	CHD-C1D	2.22	1.42	1.38
8	AI	101	BCL	CHD-C1D	2.21	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	BI	101	BCL	CHD-C1D	2.21	1.42	1.38
13	L	302	U10	C1-C2	-2.21	1.39	1.47
8	AM	1001	BCL	CHD-C1D	2.20	1.42	1.38
8	AH	102	BCL	CHD-C1D	2.20	1.42	1.38
8	AE	101	BCL	CHD-C1D	2.17	1.42	1.38
8	AF	102	BCL	CHD-C1D	2.16	1.42	1.38
8	AE	103	BCL	CHD-C1D	2.16	1.42	1.38
10	M	401	LMT	O3B-C3B	-2.16	1.37	1.43
10	AA	1003	LMT	O3B-C3B	-2.15	1.37	1.43
8	BC	101	BCL	CHD-C1D	2.15	1.42	1.38
8	BL	102	BCL	CHD-C1D	2.15	1.42	1.38
10	X	101	LMT	O3B-C3B	-2.15	1.37	1.43
8	AC	102	BCL	CHD-C1D	2.15	1.42	1.38
8	BC	101	BCL	C3D-C4D	-2.14	1.39	1.44
10	X	101	LMT	O2B-C2B	-2.14	1.37	1.43
10	AA	1003	LMT	O2'-C2'	-2.13	1.37	1.43
8	BI	101	BCL	C3D-C4D	-2.12	1.39	1.44
8	BA	102	BCL	C3D-C4D	-2.12	1.39	1.44
8	AB	101	BCL	C1D-ND	2.12	1.40	1.37
10	AB	104	LMT	O2B-C2B	-2.12	1.37	1.43
8	M	403	BCL	C3D-C4D	-2.11	1.39	1.44
8	L	304	BCL	C3D-C4D	-2.11	1.39	1.44
10	M	401	LMT	O2'-C2'	-2.10	1.37	1.43
8	BD	101	BCL	C3D-C4D	-2.10	1.39	1.44
8	BJ	101	BCL	C3D-C4D	-2.09	1.39	1.44
8	L	305	BCL	C3D-C4D	-2.09	1.39	1.44
8	AK	103	BCL	C3D-C4D	-2.08	1.39	1.44
8	BL	102	BCL	C3D-C4D	-2.08	1.39	1.44
8	AE	103	BCL	C3D-C4D	-2.08	1.39	1.44
10	M	401	LMT	O2B-C2B	-2.08	1.37	1.43
8	BB	1001	BCL	CHD-C1D	2.08	1.42	1.38
8	L	304	BCL	CHD-C1D	2.07	1.42	1.38
8	BB	1001	BCL	C3D-C4D	-2.07	1.39	1.44
8	BG	101	BCL	C3D-C4D	-2.07	1.39	1.44
8	AJ	101	BCL	C1D-ND	2.07	1.40	1.37
10	AB	104	LMT	O3B-C3B	-2.06	1.37	1.43
8	BH	101	BCL	C3D-C4D	-2.06	1.39	1.44
8	AF	102	BCL	C3D-C4D	-2.05	1.39	1.44
10	X	101	LMT	O2'-C2'	-2.05	1.37	1.43
8	AN	101	BCL	C1D-ND	2.05	1.40	1.37
8	AN	101	BCL	C3D-C4D	-2.04	1.39	1.44
8	M	403	BCL	CBD-CGD	-2.03	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AB	101	BCL	C3D-C4D	-2.03	1.39	1.44
8	BF	101	BCL	C3D-C4D	-2.02	1.39	1.44
8	M	406	BCL	C3D-C4D	-2.02	1.39	1.44
8	AH	102	BCL	C3D-C4D	-2.01	1.39	1.44
12	M	402	BPH	C1D-C2D	2.01	1.41	1.39
8	AA	1001	BCL	C3D-C4D	-2.01	1.39	1.44
8	AL	1001	BCL	C3D-C4D	-2.00	1.39	1.44

All (405) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	402	BPH	C4D-CHA-CBD	-10.27	103.53	108.45
12	L	301	BPH	C4D-CHA-CBD	-10.21	103.56	108.45
8	AD	102	BCL	C1-C2-C3	5.34	134.95	126.20
8	M	403	BCL	C4D-CHA-C1A	5.31	127.58	121.24
8	BG	101	BCL	C4D-CHA-C1A	5.31	127.58	121.24
8	AK	101	BCL	C4D-CHA-C1A	5.31	127.58	121.24
8	AJ	101	BCL	C1-C2-C3	5.30	134.88	126.20
8	AC	102	BCL	C4D-CHA-C1A	5.30	127.56	121.24
8	AE	103	BCL	C4D-CHA-C1A	5.27	127.53	121.24
8	AI	101	BCL	C4D-CHA-C1A	5.27	127.53	121.24
8	AG	102	BCL	C4D-CHA-C1A	5.21	127.46	121.24
8	AM	1003	BCL	C4D-CHA-C1A	5.21	127.46	121.24
8	AL	1001	BCL	C4D-CHA-C1A	5.21	127.46	121.24
8	AH	102	BCL	C4D-CHA-C1A	5.18	127.42	121.24
8	AD	102	BCL	C4D-CHA-C1A	5.15	127.38	121.24
8	BL	102	BCL	C4D-CHA-C1A	5.15	127.38	121.24
8	M	406	BCL	C4D-CHA-C1A	5.13	127.36	121.24
8	BC	101	BCL	C4D-CHA-C1A	5.12	127.35	121.24
8	BJ	101	BCL	C4D-CHA-C1A	5.10	127.33	121.24
8	AM	1001	BCL	C4D-CHA-C1A	5.10	127.33	121.24
8	AB	101	BCL	C4D-CHA-C1A	5.10	127.33	121.24
8	BI	101	BCL	C4D-CHA-C1A	5.08	127.31	121.24
8	AE	101	BCL	C4D-CHA-C1A	5.07	127.29	121.24
8	AK	103	BCL	C4D-CHA-C1A	5.07	127.29	121.24
8	BF	101	BCL	C4D-CHA-C1A	5.07	127.29	121.24
8	L	305	BCL	C4D-CHA-C1A	5.06	127.28	121.24
8	AJ	101	BCL	C4D-CHA-C1A	5.05	127.27	121.24
8	BD	101	BCL	C4D-CHA-C1A	5.03	127.25	121.24
8	BA	102	BCL	C4D-CHA-C1A	4.98	127.19	121.24
8	BN	101	BCL	C4D-CHA-C1A	4.97	127.17	121.24
8	BH	101	BCL	C4D-CHA-C1A	4.96	127.16	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	BB	1001	BCL	C4D-CHA-C1A	4.93	127.13	121.24
14	L	303	UQ1	C6-C5-C4	4.89	123.03	119.17
8	AF	102	BCL	C4D-CHA-C1A	4.85	127.03	121.24
8	AA	1001	BCL	C4D-CHA-C1A	4.83	127.00	121.24
8	L	304	BCL	C4D-CHA-C1A	4.62	126.75	121.24
8	AN	101	BCL	C4D-CHA-C1A	4.61	126.75	121.24
8	M	406	BCL	CHD-C1D-ND	-4.23	118.86	124.80
8	L	305	BCL	C1D-ND-C4D	-4.10	103.43	106.31
12	M	402	BPH	C4D-ND-C1D	-4.04	104.03	108.87
12	L	301	BPH	C4D-ND-C1D	-3.98	104.11	108.87
13	M	404	U10	C4M-O4-C4	3.95	130.35	116.47
14	L	303	UQ1	C8-C7-C6	3.90	121.69	112.08
13	M	404	U10	C3M-O3-C3	3.90	130.17	116.47
8	AL	1001	BCL	C1-C2-C3	3.85	132.51	126.20
8	AB	101	BCL	C1-C2-C3	3.85	132.50	126.20
14	L	303	UQ1	CM3-O3-C3	3.80	129.84	116.47
8	L	305	BCL	CHD-C1D-ND	-3.77	119.50	124.80
8	AG	102	BCL	C4A-NA-C1A	3.68	108.36	106.68
8	AF	102	BCL	C4A-NA-C1A	3.68	108.36	106.68
8	AM	1001	BCL	C1D-ND-C4D	-3.68	103.73	106.31
8	AI	101	BCL	CHD-C1D-ND	-3.68	119.62	124.80
8	AK	101	BCL	C1D-ND-C4D	-3.64	103.75	106.31
8	AD	102	BCL	C1D-ND-C4D	-3.64	103.76	106.31
8	AK	101	BCL	CHD-C1D-ND	-3.64	119.68	124.80
8	AL	1001	BCL	C1D-ND-C4D	-3.63	103.76	106.31
8	AE	101	BCL	C4A-NA-C1A	3.61	108.33	106.68
8	AC	102	BCL	CHD-C1D-ND	-3.60	119.73	124.80
8	AE	101	BCL	C1D-ND-C4D	-3.60	103.79	106.31
8	AM	1001	BCL	C4A-NA-C1A	3.59	108.32	106.68
13	L	302	U10	C25-C24-C26	3.59	121.45	115.23
8	AC	102	BCL	C1D-ND-C4D	-3.58	103.80	106.31
8	AG	102	BCL	CHD-C1D-ND	-3.57	119.78	124.80
8	L	304	BCL	CHD-C1D-ND	-3.56	119.79	124.80
8	AM	1001	BCL	CHD-C1D-ND	-3.54	119.82	124.80
8	AH	102	BCL	CHD-C1D-ND	-3.54	119.82	124.80
8	AE	101	BCL	CHD-C1D-ND	-3.54	119.82	124.80
8	AD	102	BCL	CHD-C1D-ND	-3.54	119.83	124.80
8	AJ	101	BCL	CHD-C1D-ND	-3.53	119.84	124.80
8	AN	101	BCL	CHD-C1D-ND	-3.52	119.84	124.80
8	M	403	BCL	C1D-ND-C4D	-3.52	103.84	106.31
8	AH	102	BCL	C1D-ND-C4D	-3.52	103.84	106.31
8	AA	1001	BCL	C1D-ND-C4D	-3.51	103.85	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AF	102	BCL	C1D-ND-C4D	-3.50	103.86	106.31
8	AA	1001	BCL	CHD-C1D-ND	-3.50	119.88	124.80
8	AN	101	BCL	C1D-ND-C4D	-3.50	103.86	106.31
8	L	304	BCL	C1D-ND-C4D	-3.50	103.86	106.31
8	AB	101	BCL	C1D-ND-C4D	-3.49	103.86	106.31
8	AB	101	BCL	CHD-C1D-ND	-3.48	119.90	124.80
8	AL	1001	BCL	CHD-C1D-ND	-3.48	119.90	124.80
8	AB	101	BCL	C4A-NA-C1A	3.48	108.27	106.68
8	AM	1003	BCL	CHD-C1D-ND	-3.47	119.92	124.80
8	BN	101	BCL	CHD-C1D-ND	-3.46	119.93	124.80
8	BF	101	BCL	CHD-C1D-ND	-3.46	119.93	124.80
8	AJ	101	BCL	C1D-ND-C4D	-3.45	103.89	106.31
8	BG	101	BCL	CHD-C1D-ND	-3.45	119.95	124.80
8	AF	102	BCL	CHD-C1D-ND	-3.43	119.97	124.80
8	AG	102	BCL	C1D-ND-C4D	-3.42	103.91	106.31
8	M	403	BCL	CHA-C1A-NA	-3.42	118.65	126.39
8	BJ	101	BCL	CHD-C1D-ND	-3.42	119.99	124.80
8	AA	1001	BCL	C4A-NA-C1A	3.41	108.24	106.68
8	BC	101	BCL	C1D-ND-C4D	-3.41	103.92	106.31
8	AM	1003	BCL	C1D-ND-C4D	-3.41	103.92	106.31
8	BN	101	BCL	C4A-NA-C1A	3.41	108.23	106.68
8	M	403	BCL	CHD-C1D-ND	-3.39	120.03	124.80
8	AD	102	BCL	C4A-NA-C1A	3.39	108.23	106.68
8	AE	103	BCL	CHD-C1D-ND	-3.39	120.03	124.80
8	M	406	BCL	C1D-ND-C4D	-3.39	103.94	106.31
8	BI	101	BCL	CHD-C1D-ND	-3.38	120.04	124.80
8	AJ	101	BCL	C4A-NA-C1A	3.38	108.22	106.68
12	M	402	BPH	C3D-C4D-ND	3.36	112.01	107.71
8	BB	1001	BCL	CHD-C1D-ND	-3.35	120.08	124.80
8	BL	102	BCL	CHD-C1D-ND	-3.35	120.08	124.80
8	AL	1001	BCL	C4A-NA-C1A	3.35	108.21	106.68
8	BC	101	BCL	CHD-C1D-ND	-3.34	120.10	124.80
8	BN	101	BCL	C1D-ND-C4D	-3.34	103.97	106.31
8	M	403	BCL	C4A-NA-C1A	3.34	108.20	106.68
8	AK	103	BCL	CHD-C1D-ND	-3.32	120.12	124.80
8	BH	101	BCL	CHD-C1D-ND	-3.32	120.13	124.80
12	L	301	BPH	C3D-C4D-ND	3.32	111.96	107.71
8	AE	103	BCL	C1D-ND-C4D	-3.31	103.99	106.31
8	AN	101	BCL	C4A-NA-C1A	3.31	108.19	106.68
8	AH	102	BCL	C4A-NA-C1A	3.31	108.19	106.68
8	AI	101	BCL	C1D-ND-C4D	-3.30	104.00	106.31
8	BD	101	BCL	C1D-ND-C4D	-3.30	104.00	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	405	CD4	O2-C14-C13	3.29	118.60	111.48
8	BJ	101	BCL	C1D-ND-C4D	-3.29	104.00	106.31
8	AK	101	BCL	C4A-NA-C1A	3.28	108.18	106.68
8	BA	102	BCL	CHD-C1D-ND	-3.28	120.19	124.80
8	AF	102	BCL	C1-C2-C3	-3.27	120.84	126.20
8	BB	1001	BCL	C1D-ND-C4D	-3.27	104.02	106.31
8	BF	101	BCL	C1D-ND-C4D	-3.25	104.03	106.31
8	BD	101	BCL	CHD-C1D-ND	-3.24	120.24	124.80
8	BL	102	BCL	C1D-ND-C4D	-3.24	104.04	106.31
8	AI	101	BCL	CHA-C1A-NA	-3.22	119.09	126.39
8	BA	102	BCL	C1D-ND-C4D	-3.22	104.05	106.31
8	BI	101	BCL	C1D-ND-C4D	-3.22	104.05	106.31
8	AE	103	BCL	C4A-NA-C1A	3.21	108.14	106.68
8	BA	102	BCL	C4A-NA-C1A	3.21	108.14	106.68
8	BG	101	BCL	C1D-ND-C4D	-3.20	104.06	106.31
8	BH	101	BCL	C1D-ND-C4D	-3.20	104.07	106.31
13	L	302	U10	C12-C13-C14	-3.19	120.32	127.62
11	H	302	3PE	C2-O21-C21	3.19	125.42	117.80
12	M	402	BPH	OBD-CAD-CBD	-3.17	121.17	125.82
8	AK	103	BCL	C1D-ND-C4D	-3.17	104.09	106.31
13	M	404	U10	C17-C18-C19	-3.17	120.38	127.62
8	BF	101	BCL	CHA-C1A-NA	-3.16	119.25	126.39
8	AC	102	BCL	CHA-C1A-NA	-3.13	119.30	126.39
12	L	301	BPH	OBD-CAD-CBD	-3.12	121.24	125.82
8	AB	101	BCL	CHA-C1A-NA	-3.11	119.34	126.39
8	BL	102	BCL	CHA-C1A-NA	-3.10	119.36	126.39
8	AE	103	BCL	CHA-C1A-NA	-3.09	119.39	126.39
8	BH	101	BCL	CHA-C1A-NA	-3.09	119.40	126.39
8	BD	101	BCL	CHA-C1A-NA	-3.08	119.41	126.39
8	BH	101	BCL	C4A-NA-C1A	3.07	108.08	106.68
8	BI	101	BCL	CHA-C1A-NA	-3.07	119.43	126.39
8	AJ	101	BCL	CHA-C1A-NA	-3.07	119.44	126.39
8	AH	102	BCL	CHA-C1A-NA	-3.05	119.49	126.39
8	BB	1001	BCL	CHA-C1A-NA	-3.05	119.50	126.39
8	BN	101	BCL	CHA-C1A-NA	-3.04	119.50	126.39
8	AN	101	BCL	CHA-C1A-NA	-3.04	119.50	126.39
8	AK	103	BCL	CHA-C1A-NA	-3.04	119.52	126.39
8	M	406	BCL	C4A-NA-C1A	3.03	108.06	106.68
8	AM	1003	BCL	CHA-C1A-NA	-3.02	119.54	126.39
8	BC	101	BCL	CHA-C1A-NA	-3.02	119.55	126.39
8	BJ	101	BCL	CHA-C1A-NA	-3.02	119.55	126.39
8	BA	102	BCL	CHA-C1A-NA	-3.02	119.56	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AF	102	BCL	CHA-C1A-NA	-3.01	119.58	126.39
13	M	404	U10	C35-C34-C36	3.01	120.45	115.23
8	AE	101	BCL	CHA-C1A-NA	-2.99	119.62	126.39
8	AM	1003	BCL	C4A-NA-C1A	2.99	108.04	106.68
8	AK	101	BCL	CHA-C1A-NA	-2.98	119.63	126.39
8	BD	101	BCL	C4A-NA-C1A	2.98	108.04	106.68
8	L	305	BCL	CHA-C1A-NA	-2.98	119.64	126.39
8	AC	102	BCL	C4A-NA-C1A	2.98	108.04	106.68
8	AG	102	BCL	CHA-C1A-NA	-2.97	119.66	126.39
8	BG	101	BCL	CHA-C1A-NA	-2.97	119.66	126.39
13	L	302	U10	C30-C29-C31	2.97	120.39	115.23
13	M	404	U10	C40-C39-C41	2.96	120.37	115.23
8	AA	1001	BCL	CHA-C1A-NA	-2.96	119.69	126.39
8	AM	1001	BCL	CHA-C1A-NA	-2.95	119.70	126.39
8	M	406	BCL	CHA-C1A-NA	-2.94	119.72	126.39
13	M	404	U10	C25-C24-C26	2.94	120.34	115.23
9	AI	103	SPO	C20-C21-C22	2.94	129.53	123.52
13	M	404	U10	C50-C49-C51	2.94	120.33	115.23
8	AD	102	BCL	CHA-C1A-NA	-2.93	119.75	126.39
15	M	405	CD4	O3-C17-C18	2.93	120.76	111.83
8	L	305	BCL	C2A-C1A-CHA	2.90	128.90	123.87
9	AB	103	SPO	C1-C4-C5	2.90	120.51	112.98
8	AL	1001	BCL	CHA-C1A-NA	-2.90	119.83	126.39
8	BC	101	BCL	C4A-NA-C1A	2.89	108.00	106.68
8	BB	1001	BCL	C4A-NA-C1A	2.87	107.99	106.68
13	L	302	U10	C3M-O3-C3	2.86	126.54	116.47
8	BB	1001	BCL	C1-O2A-CGA	2.86	123.58	116.65
13	L	302	U10	C47-C48-C49	-2.86	121.09	127.62
9	AI	102	SPO	C1-C4-C5	2.83	120.34	112.98
13	L	302	U10	C7-C6-C1	-2.80	120.08	124.89
8	BG	101	BCL	C4A-NA-C1A	2.80	107.95	106.68
8	L	304	BCL	CHA-C1A-NA	-2.79	120.07	126.39
13	L	302	U10	C45-C44-C46	2.79	120.07	115.23
13	L	302	U10	C32-C33-C34	-2.78	121.25	127.62
8	AE	103	BCL	CBA-CAA-C2A	2.78	122.07	113.79
13	M	404	U10	C10-C9-C11	2.78	120.06	115.23
10	AA	1003	LMT	C3'-C4'-C5'	-2.78	104.78	110.93
10	M	401	LMT	C3'-C4'-C5'	-2.77	104.78	110.93
8	BG	101	BCL	C1-C2-C3	-2.74	121.71	126.20
8	BD	101	BCL	C2A-C1A-CHA	2.72	128.59	123.87
12	L	301	BPH	CMB-C2B-C3B	2.72	130.12	124.68
8	BI	101	BCL	C1-C2-C3	-2.71	121.76	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	404	U10	C22-C23-C24	-2.71	121.43	127.62
8	BL	102	BCL	C1-O2A-CGA	2.70	123.19	116.65
13	M	404	U10	C30-C29-C31	2.70	119.91	115.23
10	M	401	LMT	C1-O1'-C1'	2.69	118.27	113.68
8	BA	102	BCL	CBA-CAA-C2A	2.69	121.79	113.79
8	BH	101	BCL	C2A-C1A-CHA	2.69	128.53	123.87
8	AJ	101	BCL	C2A-C1A-CHA	2.69	128.53	123.87
13	M	404	U10	C20-C19-C21	2.68	119.88	115.23
13	L	302	U10	C1M-C1-C6	-2.67	120.06	124.45
9	AL	1002	SPO	C1-C4-C5	2.67	119.91	112.98
13	M	404	U10	C15-C14-C16	2.66	119.85	115.23
8	M	403	BCL	C2A-C1A-CHA	2.65	128.47	123.87
13	L	302	U10	C7-C8-C9	-2.65	122.27	126.83
13	M	404	U10	C47-C48-C49	-2.65	121.57	127.62
8	M	406	BCL	C2A-C1A-CHA	2.64	128.44	123.87
13	M	404	U10	C45-C44-C46	2.64	119.81	115.23
8	BD	101	BCL	C1-O2A-CGA	2.62	123.00	116.65
8	AK	103	BCL	C1-C2-C3	-2.61	121.91	126.20
12	M	402	BPH	CMB-C2B-C3B	2.61	129.90	124.68
8	AF	102	BCL	C2A-C1A-CHA	2.61	128.40	123.87
8	AK	103	BCL	C4A-NA-C1A	2.59	107.86	106.68
8	AK	101	BCL	C1-C2-C3	2.59	130.44	126.20
8	BI	101	BCL	C4A-NA-C1A	2.57	107.85	106.68
13	M	404	U10	C12-C13-C14	-2.57	121.74	127.62
8	AD	102	BCL	C6-C5-C3	2.57	119.73	113.47
13	L	302	U10	C10-C9-C11	2.56	119.68	115.23
8	L	304	BCL	C4A-NA-C1A	2.56	107.85	106.68
9	AA	1002	SPO	C1-C4-C5	2.56	119.62	112.98
13	L	302	U10	C40-C39-C41	2.55	119.65	115.23
8	AI	101	BCL	C2A-C1A-CHA	2.53	128.26	123.87
8	AE	101	BCL	C2A-C1A-CHA	2.53	128.26	123.87
12	M	402	BPH	C2D-C1D-ND	2.53	111.26	109.43
8	BJ	101	BCL	C1-C2-C3	-2.53	122.05	126.20
8	AM	1001	BCL	C1-C2-C3	2.51	130.31	126.20
8	L	304	BCL	C2A-C1A-CHA	2.51	128.22	123.87
12	L	301	BPH	C2D-C1D-ND	2.51	111.24	109.43
8	BJ	101	BCL	C4A-NA-C1A	2.51	107.82	106.68
15	M	405	CD4	O14-C35-C36	2.49	119.43	111.83
8	AG	102	BCL	CMB-C2B-C1B	-2.47	121.65	125.42
8	L	305	BCL	C4A-NA-C1A	2.47	107.80	106.68
8	AH	102	BCL	C2A-C1A-CHA	2.46	128.14	123.87
8	AH	102	BCL	C1-C2-C3	-2.46	122.17	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	406	BCL	C1-O2A-CGA	2.46	122.60	116.65
8	AE	103	BCL	CMB-C2B-C1B	-2.45	121.68	125.42
8	L	305	BCL	C1-O2A-CGA	2.45	122.59	116.65
15	M	405	CD4	O16-C46-C47	2.45	116.78	111.48
8	AB	101	BCL	C2A-C1A-CHA	2.44	128.10	123.87
8	AK	101	BCL	C2A-C1A-CHA	2.43	128.09	123.87
8	BF	101	BCL	C2A-C1A-CHA	2.43	128.08	123.87
14	L	303	UQ1	O4-C4-C3	2.42	126.16	121.03
8	BA	102	BCL	C1-O2A-CGA	2.42	122.50	116.65
8	BB	1001	BCL	C2A-C1A-CHA	2.41	128.06	123.87
8	AM	1003	BCL	C2A-C1A-CHA	2.41	128.05	123.87
8	AD	102	BCL	CMB-C2B-C1B	-2.40	121.76	125.42
8	AM	1001	BCL	CMB-C2B-C1B	-2.40	121.76	125.42
8	BN	101	BCL	C1-O2A-CGA	2.40	122.45	116.65
12	L	301	BPH	OBB-CAB-CBB	-2.39	115.09	120.19
8	AF	102	BCL	CMB-C2B-C1B	-2.39	121.78	125.42
8	AK	101	BCL	OBB-CAB-CBB	-2.38	114.44	119.77
8	BA	102	BCL	C2A-C1A-CHA	2.38	127.99	123.87
8	M	406	BCL	C1C-NC-C4C	2.37	107.76	106.68
8	AK	103	BCL	CMB-C2B-C1B	-2.37	121.81	125.42
8	AE	101	BCL	OBB-CAB-CBB	-2.37	114.47	119.77
8	AM	1001	BCL	OBB-CAB-CBB	-2.36	114.47	119.77
8	AD	102	BCL	OBB-CAB-CBB	-2.36	114.47	119.77
12	M	402	BPH	OBB-CAB-CBB	-2.36	115.15	120.19
11	AB	102	3PE	O12-P-O14	2.36	123.41	112.44
11	H	302	3PE	O12-P-O14	2.36	123.41	112.44
8	AN	101	BCL	CMB-C2B-C1B	-2.35	121.84	125.42
8	AL	1001	BCL	OBB-CAB-CBB	-2.35	114.50	119.77
8	AI	101	BCL	CMB-C2B-C1B	-2.35	121.84	125.42
8	M	403	BCL	OBB-CAB-CBB	-2.35	114.51	119.77
8	L	304	BCL	CMB-C2B-C1B	-2.35	121.84	125.42
8	AJ	101	BCL	CMB-C2B-C1B	-2.35	121.84	125.42
12	L	301	BPH	C1-C2-C3	-2.35	122.35	126.20
8	AM	1001	BCL	C6-C5-C3	2.35	119.19	113.47
8	AI	101	BCL	OBB-CAB-CBB	-2.34	114.53	119.77
8	AF	102	BCL	OBB-CAB-CBB	-2.34	114.53	119.77
8	AK	101	BCL	C6-C5-C3	2.34	119.16	113.47
8	BC	101	BCL	C2A-C1A-CHA	2.34	127.92	123.87
8	BA	102	BCL	OBB-CAB-CBB	-2.33	114.54	119.77
8	AI	101	BCL	CAA-CBA-CGA	2.33	119.83	113.21
12	M	402	BPH	O2D-CGD-CBD	2.33	113.51	110.95
8	AK	101	BCL	CMB-C2B-C1B	-2.33	121.87	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	BN	101	BCL	CMB-C2B-C1B	-2.33	121.87	125.42
8	AC	102	BCL	OBB-CAB-CBB	-2.33	114.56	119.77
8	AJ	101	BCL	OBB-CAB-CBB	-2.33	114.56	119.77
8	BN	101	BCL	OBB-CAB-CBB	-2.32	114.57	119.77
8	AH	102	BCL	OBB-CAB-CBB	-2.32	114.58	119.77
9	AB	103	SPO	C31-C30-C28	2.32	120.86	113.19
8	M	403	BCL	CMB-C2B-C1B	-2.32	121.89	125.42
8	AE	103	BCL	OBB-CAB-CBB	-2.31	114.59	119.77
8	AB	101	BCL	OBB-CAB-CBB	-2.31	114.60	119.77
10	X	101	LMT	O1'-C1'-C2'	2.31	111.78	108.27
8	BL	102	BCL	CMB-C2B-C1B	-2.31	121.91	125.42
8	AA	1001	BCL	CMB-C2B-C1B	-2.30	121.91	125.42
8	AN	101	BCL	OBB-CAB-CBB	-2.30	114.61	119.77
8	BL	102	BCL	OBB-CAB-CBB	-2.30	114.61	119.77
8	BD	101	BCL	CMB-C2B-C1B	-2.30	121.91	125.42
8	BN	101	BCL	C2A-C1A-CHA	2.30	127.86	123.87
10	X	101	LMT	C1'-O5'-C5'	-2.30	109.23	113.72
8	M	406	BCL	OBB-CAB-CBB	-2.30	114.63	119.77
8	AM	1003	BCL	CMB-C2B-C1B	-2.29	121.93	125.42
8	BH	101	BCL	CMB-C2B-C1B	-2.29	121.94	125.42
11	H	301	3PE	O12-P-O14	2.29	123.09	112.44
8	BL	102	BCL	C2A-C1A-CHA	2.28	127.83	123.87
8	AG	102	BCL	OBB-CAB-CBB	-2.28	114.67	119.77
8	BD	101	BCL	OBB-CAB-CBB	-2.28	114.67	119.77
8	AA	1001	BCL	C2A-C1A-CHA	2.28	127.82	123.87
8	AL	1001	BCL	CMB-C2B-C1B	-2.27	121.95	125.42
8	BI	101	BCL	CMB-C2B-C1B	-2.27	121.96	125.42
8	L	304	BCL	OBB-CAB-CBB	-2.27	114.68	119.77
8	BC	101	BCL	CMB-C2B-C1B	-2.27	121.96	125.42
9	AI	103	SPO	C25-C23-C22	2.27	122.58	119.01
8	BB	1001	BCL	OBB-CAB-CBB	-2.27	114.69	119.77
8	AH	102	BCL	CMB-C2B-C1B	-2.27	121.97	125.42
9	AF	101	SPO	C36-C35-C33	-2.26	105.69	113.19
8	BJ	101	BCL	CMB-C2B-C1B	-2.26	121.98	125.42
8	AE	101	BCL	CMB-C2B-C1B	-2.26	121.98	125.42
8	AK	103	BCL	OBB-CAB-CBB	-2.25	114.73	119.77
8	BH	101	BCL	C1-O2A-CGA	2.25	122.09	116.65
8	AM	1003	BCL	OBB-CAB-CBB	-2.25	114.73	119.77
8	BL	102	BCL	C4A-NA-C1A	2.24	107.70	106.68
8	BA	102	BCL	CMB-C2B-C1B	-2.23	122.03	125.42
9	AJ	103	SPO	C1-C4-C5	2.23	118.77	112.98
8	AB	101	BCL	CMB-C2B-C1B	-2.22	122.03	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	BD	101	BCL	CAA-CBA-CGA	2.22	119.51	113.21
8	BH	101	BCL	OBB-CAB-CBB	-2.22	114.81	119.77
8	AC	102	BCL	C2A-C1A-CHA	2.22	127.71	123.87
8	AG	102	BCL	C2A-C1A-CHA	2.21	127.71	123.87
8	AN	101	BCL	C2A-C1A-CHA	2.21	127.71	123.87
8	BG	101	BCL	CMB-C2B-C1B	-2.21	122.06	125.42
8	BI	101	BCL	OBB-CAB-CBB	-2.21	114.82	119.77
8	BI	101	BCL	C2A-C1A-CHA	2.21	127.70	123.87
8	AC	102	BCL	CMB-C2B-C1B	-2.21	122.06	125.42
12	M	402	BPH	C1-O2A-CGA	2.20	121.97	116.65
8	BC	101	BCL	OBB-CAB-CBB	-2.20	114.85	119.77
8	AA	1001	BCL	OBB-CAB-CBB	-2.20	114.85	119.77
8	BL	102	BCL	CAB-C3B-C2B	2.20	132.31	127.74
9	BA	101	SPO	C36-C35-C33	-2.19	105.92	113.19
8	AL	1001	BCL	C1-O2A-CGA	2.19	121.95	116.65
11	AC	104	3PE	O12-P-O14	2.19	122.63	112.44
8	AD	102	BCL	C2A-C1A-CHA	2.19	127.66	123.87
8	BJ	101	BCL	OBB-CAB-CBB	-2.18	114.88	119.77
8	BF	101	BCL	CMB-C2B-C1B	-2.18	122.09	125.42
8	BB	1001	BCL	CMB-C2B-C1B	-2.18	122.10	125.42
8	AE	103	BCL	C2A-C1A-CHA	2.18	127.64	123.87
8	AL	1001	BCL	CAB-C3B-C2B	2.18	132.26	127.74
14	L	303	UQ1	C7-C6-C1	-2.17	115.99	118.52
8	BG	101	BCL	C1-O2A-CGA	2.17	121.91	116.65
8	AL	1001	BCL	C6-C5-C3	2.17	118.76	113.47
12	L	301	BPH	CMD-C2D-C3D	2.17	129.02	124.68
8	AE	103	BCL	CAB-C3B-C2B	2.17	132.25	127.74
8	M	406	BCL	CMB-C2B-C1B	-2.17	122.12	125.42
8	AB	101	BCL	CAB-C3B-C2B	2.16	132.24	127.74
13	L	302	U10	C6-C1-C2	2.16	120.88	119.17
8	M	406	BCL	CAB-C3B-C2B	2.16	132.23	127.74
8	AI	101	BCL	C4A-NA-C1A	2.16	107.66	106.68
8	BN	101	BCL	CAB-C3B-C2B	2.16	132.22	127.74
8	AK	103	BCL	C2A-C1A-CHA	2.15	127.59	123.87
13	L	302	U10	O3-C3-C2	2.15	123.88	116.64
12	M	402	BPH	CMD-C2D-C3D	2.14	128.97	124.68
8	AI	101	BCL	CAB-C3B-C2B	2.14	132.19	127.74
8	L	305	BCL	OBB-CAB-CBB	-2.14	114.98	119.77
13	M	404	U10	O2-C2-C1	-2.14	114.75	120.73
8	BG	101	BCL	C2A-C1A-CHA	2.13	127.57	123.87
8	AJ	101	BCL	C6-C5-C3	2.13	118.66	113.47
8	BA	102	BCL	CAB-C3B-C2B	2.13	132.16	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	BL	102	BCL	CAA-CBA-CGA	2.13	119.25	113.21
8	L	305	BCL	CAB-C3B-C2B	2.12	132.16	127.74
8	BF	101	BCL	OBb-CAB-CBB	-2.12	115.02	119.77
8	AM	1001	BCL	CAB-C3B-C2B	2.12	132.15	127.74
8	AN	101	BCL	CAB-C3B-C2B	2.12	132.14	127.74
8	BI	101	BCL	CAB-C3B-C2B	2.11	132.13	127.74
13	L	302	U10	C20-C19-C21	2.11	118.89	115.23
13	L	302	U10	C56-C54-C55	2.11	119.45	114.59
8	AM	1001	BCL	C2A-C1A-CHA	2.11	127.53	123.87
8	BD	101	BCL	CAB-C3B-C2B	2.10	132.11	127.74
8	BG	101	BCL	OBb-CAB-CBB	-2.09	115.08	119.77
8	L	305	BCL	CMB-C2B-C1B	-2.09	122.24	125.42
8	BF	101	BCL	CAB-C3B-C2B	2.09	132.08	127.74
8	BA	102	BCL	C1-C2-C3	-2.09	122.78	126.20
8	AK	101	BCL	CAB-C3B-C2B	2.08	132.07	127.74
8	AH	102	BCL	CAB-C3B-C2B	2.08	132.07	127.74
13	L	302	U10	O3-C3-C4	-2.08	115.76	123.64
12	L	301	BPH	O2D-CGD-CBD	2.07	113.23	110.95
8	AK	103	BCL	CAB-C3B-C2B	2.07	132.05	127.74
14	L	303	UQ1	CM2-O2-C2	2.07	123.75	116.47
8	BB	1001	BCL	CAB-C3B-C2B	2.06	132.02	127.74
10	AA	1003	LMT	O5B-C5B-C4B	2.06	113.41	109.70
8	BJ	101	BCL	CAB-C3B-C2B	2.06	132.01	127.74
8	M	403	BCL	CAB-C3B-C2B	2.05	132.01	127.74
13	M	404	U10	C4-C3-C2	-2.05	116.93	120.69
8	BF	101	BCL	C4A-NA-C1A	2.05	107.61	106.68
8	AB	101	BCL	O2A-CGA-O1A	-2.05	118.50	123.63
8	BI	101	BCL	C1C-NC-C4C	2.05	107.61	106.68
13	L	302	U10	C50-C49-C51	2.04	118.77	115.23
8	AE	101	BCL	CAB-C3B-C2B	2.04	131.98	127.74
13	L	302	U10	C15-C14-C16	2.04	118.77	115.23
8	L	304	BCL	CAB-C3B-C2B	2.04	131.97	127.74
8	AC	102	BCL	CAB-C3B-C2B	2.03	131.96	127.74
8	BD	101	BCL	C1C-NC-C4C	2.03	107.60	106.68
8	BC	101	BCL	CAB-C3B-C2B	2.02	131.95	127.74
8	AL	1001	BCL	C2A-C1A-CHA	2.01	127.36	123.87
8	AG	102	BCL	CAB-C3B-C2B	2.01	131.92	127.74
8	AM	1003	BCL	CAB-C3B-C2B	2.00	131.90	127.74

There are no chirality outliers.

All (363) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	AN	101	BCL	C4-C3-C5-C6
8	BA	102	BCL	C3A-C2A-CAA-CBA
8	BB	1001	BCL	C1A-C2A-CAA-CBA
8	BC	101	BCL	C1A-C2A-CAA-CBA
8	BF	101	BCL	C3A-C2A-CAA-CBA
8	BI	101	BCL	C1A-C2A-CAA-CBA
8	BJ	101	BCL	C1A-C2A-CAA-CBA
8	BL	102	BCL	C1A-C2A-CAA-CBA
9	AB	103	SPO	O1-C1-C4-C5
9	AB	103	SPO	C2-C1-C4-C5
9	AI	103	SPO	C1-C4-C5-C6
9	BE	1000	SPO	O1-C1-C4-C5
9	BE	1000	SPO	C2-C1-C4-C5
9	BE	1000	SPO	C3-C1-C4-C5
11	AB	102	3PE	C1-O11-P-O12
11	AB	102	3PE	C1-O11-P-O13
11	AB	102	3PE	C1-O11-P-O14
11	AB	102	3PE	C11-O13-P-O12
11	AB	102	3PE	C2-C1-O11-P
11	AC	104	3PE	C1-O11-P-O12
11	AC	104	3PE	C1-O11-P-O13
11	AC	104	3PE	C11-O13-P-O14
11	AC	104	3PE	C12-C11-O13-P
11	H	302	3PE	C1-O11-P-O12
11	H	302	3PE	C1-O11-P-O13
11	H	302	3PE	C11-O13-P-O11
11	H	302	3PE	C11-O13-P-O14
15	M	405	CD4	C32-O13-P2-O10
15	M	405	CD4	C32-O13-P2-O11
15	M	405	CD4	O16-C33-C34-O14
8	AK	101	BCL	C4-C3-C5-C6
9	BL	101	SPO	C29-C28-C30-C31
8	AK	101	BCL	C2-C3-C5-C6
9	BL	101	SPO	C27-C28-C30-C31
10	AB	104	LMT	O5'-C5'-C6'-O6'
10	AB	104	LMT	C4'-C5'-C6'-O6'
8	AI	101	BCL	C4-C3-C5-C6
8	AI	101	BCL	C2-C3-C5-C6
8	AN	101	BCL	C2-C3-C5-C6
9	AC	103	SPO	C28-C30-C31-C32
9	AJ	102	SPO	C28-C30-C31-C32
9	AJ	103	SPO	C28-C30-C31-C32
9	BA	101	SPO	C28-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
8	AI	101	BCL	C11-C10-C8-C9
8	AM	1003	BCL	C11-C10-C8-C9
9	AI	103	SPO	C24-C23-C25-C26
9	AI	103	SPO	C22-C23-C25-C26
8	BH	101	BCL	C3-C5-C6-C7
8	AD	102	BCL	C3-C5-C6-C7
9	AD	103	SPO	C28-C30-C31-C32
9	AI	102	SPO	C33-C35-C36-C37
13	L	302	U10	C29-C31-C32-C33
13	L	302	U10	C4-C3-O3-C3M
13	M	404	U10	C4-C3-O3-C3M
14	L	303	UQ1	C2-C3-O3-CM3
8	BA	102	BCL	C2A-CAA-CBA-CGA
10	X	101	LMT	O5'-C5'-C6'-O6'
9	AD	101	SPO	C34-C33-C35-C36
10	AA	1003	LMT	C2'-C1'-O1'-C1
9	AJ	102	SPO	C33-C35-C36-C37
13	L	302	U10	C24-C26-C27-C28
9	AF	103	SPO	C15-C16-C17-C18
9	AG	103	SPO	C15-C16-C17-C18
9	AJ	103	SPO	C5-C6-C7-C8
9	AK	104	SPO	C10-C11-C12-C13
9	AK	104	SPO	C15-C16-C17-C18
9	AM	1004	SPO	C15-C16-C17-C18
9	BE	1000	SPO	C15-C16-C17-C18
9	M	407	SPO	C15-C16-C17-C18
8	AE	103	BCL	C2A-CAA-CBA-CGA
8	BC	101	BCL	C5-C6-C7-C8
8	BB	1001	BCL	C5-C6-C7-C8
8	BN	101	BCL	C13-C15-C16-C17
10	AA	1003	LMT	O5'-C1'-O1'-C1
8	BB	1001	BCL	C2-C1-O2A-CGA
8	BJ	101	BCL	C5-C6-C7-C8
8	AF	102	BCL	C15-C16-C17-C18
11	H	301	3PE	C21-C22-C23-C24
8	AK	103	BCL	C13-C15-C16-C17
11	H	302	3PE	C26-C27-C28-C29
8	AC	102	BCL	C3A-C2A-CAA-CBA
8	AI	101	BCL	C3A-C2A-CAA-CBA
8	AK	103	BCL	C3A-C2A-CAA-CBA
8	BB	1001	BCL	C3A-C2A-CAA-CBA
8	BC	101	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	BI	101	BCL	C3A-C2A-CAA-CBA
8	BJ	101	BCL	C3A-C2A-CAA-CBA
8	BL	102	BCL	C3A-C2A-CAA-CBA
9	AI	102	SPO	C34-C33-C35-C36
11	H	301	3PE	C22-C23-C24-C25
11	H	302	3PE	C34-C35-C36-C37
11	H	301	3PE	C39-C3A-C3B-C3C
9	AA	1002	SPO	C34-C33-C35-C36
14	L	303	UQ1	C6-C7-C8-C9
11	AB	102	3PE	C23-C24-C25-C26
8	BH	101	BCL	C10-C11-C12-C13
9	AI	102	SPO	C32-C33-C35-C36
8	AB	101	BCL	C3-C5-C6-C7
8	BB	1001	BCL	C8-C10-C11-C12
8	BL	102	BCL	C5-C6-C7-C8
8	BL	102	BCL	C2-C1-O2A-CGA
8	AK	103	BCL	C3-C5-C6-C7
8	AC	102	BCL	C2A-CAA-CBA-CGA
8	AM	1003	BCL	C5-C6-C7-C8
8	AC	102	BCL	C1A-C2A-CAA-CBA
8	AI	101	BCL	C1A-C2A-CAA-CBA
8	AK	103	BCL	C1A-C2A-CAA-CBA
8	BA	102	BCL	C1A-C2A-CAA-CBA
8	BF	101	BCL	C1A-C2A-CAA-CBA
8	BD	101	BCL	C8-C10-C11-C12
8	AF	102	BCL	C6-C7-C8-C10
8	AK	101	BCL	C11-C10-C8-C7
8	BC	101	BCL	C12-C13-C15-C16
12	M	402	BPH	C12-C13-C15-C16
9	AA	1002	SPO	C3-C1-C4-C5
9	AB	103	SPO	C3-C1-C4-C5
9	AL	1002	SPO	C2-C1-C4-C5
9	AL	1002	SPO	C3-C1-C4-C5
9	AA	1002	SPO	C32-C33-C35-C36
8	AI	101	BCL	C2A-CAA-CBA-CGA
8	BN	101	BCL	C6-C7-C8-C9
12	M	402	BPH	C14-C13-C15-C16
15	M	405	CD4	C32-C33-C34-O14
8	BN	101	BCL	C4-C3-C5-C6
9	AB	103	SPO	C29-C28-C30-C31
9	AB	103	SPO	C27-C28-C30-C31
9	AD	101	SPO	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
8	BH	101	BCL	C5-C6-C7-C8
8	AB	101	BCL	C10-C11-C12-C13
11	AC	104	3PE	C38-C39-C3A-C3B
8	AA	1001	BCL	C16-C17-C18-C19
8	AA	1001	BCL	C16-C17-C18-C20
8	BD	101	BCL	C2A-CAA-CBA-CGA
9	AA	1002	SPO	C33-C35-C36-C37
8	AE	103	BCL	C4-C3-C5-C6
13	L	302	U10	C15-C14-C16-C17
8	BN	101	BCL	C2-C3-C5-C6
13	L	302	U10	C48-C49-C51-C52
10	AA	1003	LMT	O5B-C5B-C6B-O6B
8	AF	102	BCL	C6-C7-C8-C9
8	AK	101	BCL	C11-C10-C8-C9
8	AN	101	BCL	C11-C10-C8-C9
8	BC	101	BCL	C14-C13-C15-C16
15	M	405	CD4	C27-C60-C61-C62
11	H	301	3PE	O11-C1-C2-C3
8	AL	1001	BCL	C11-C12-C13-C15
8	L	305	BCL	C12-C13-C15-C16
8	AM	1001	BCL	C13-C15-C16-C17
11	H	302	3PE	C2C-C2D-C2E-C2F
8	AE	103	BCL	C3A-C2A-CAA-CBA
9	AC	103	SPO	C29-C28-C30-C31
9	AF	101	SPO	C29-C28-C30-C31
9	AF	101	SPO	C27-C28-C30-C31
8	BA	102	BCL	C3-C5-C6-C7
8	AI	101	BCL	C5-C6-C7-C8
11	AC	104	3PE	C1-C2-C3-O31
13	L	302	U10	C50-C49-C51-C52
11	H	302	3PE	C31-C32-C33-C34
8	AE	103	BCL	C2-C3-C5-C6
13	L	302	U10	C33-C34-C36-C37
8	AC	102	BCL	C15-C16-C17-C18
9	AB	103	SPO	C34-C33-C35-C36
12	L	301	BPH	C4-C3-C5-C6
13	L	302	U10	C35-C34-C36-C37
9	AC	103	SPO	C27-C28-C30-C31
13	L	302	U10	C13-C14-C16-C17
10	M	401	LMT	O5B-C5B-C6B-O6B
11	H	301	3PE	C2A-C2B-C2C-C2D
8	AL	1001	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	AB	101	BCL	C4C-C3C-CAC-CBC
8	BC	101	BCL	C4C-C3C-CAC-CBC
12	L	301	BPH	C2-C3-C5-C6
11	AC	104	3PE	O11-C1-C2-C3
9	AH	103	SPO	C15-C16-C17-C18
9	AK	102	SPO	C5-C6-C7-C8
11	H	301	3PE	C2-C1-O11-P
10	AB	104	LMT	C4B-C5B-C6B-O6B
8	AE	101	BCL	C11-C10-C8-C7
8	AL	1001	BCL	C6-C7-C8-C10
9	BL	101	SPO	C1-C4-C5-C6
9	AG	103	SPO	C15-C16-C17-C19
9	AK	104	SPO	C10-C11-C12-C14
9	AK	104	SPO	C15-C16-C17-C19
8	BL	102	BCL	C4-C3-C5-C6
9	BA	101	SPO	C29-C28-C30-C31
11	H	301	3PE	O11-C1-C2-O21
15	M	405	CD4	C28-C15-C16-O3
11	AB	102	3PE	C12-C11-O13-P
8	AB	101	BCL	C11-C12-C13-C14
8	AI	101	BCL	C11-C12-C13-C14
9	AA	1002	SPO	O1-C1-C4-C5
9	AF	101	SPO	O1-C1-C4-C5
9	AJ	102	SPO	O1-C1-C4-C5
9	AL	1002	SPO	O1-C1-C4-C5
8	L	305	BCL	C15-C16-C17-C18
11	H	302	3PE	C28-C29-C2A-C2B
8	AD	102	BCL	C4-C3-C5-C6
8	AC	102	BCL	C16-C17-C18-C20
10	M	401	LMT	C2-C1-O1'-C1'
14	L	303	UQ1	C4-C3-O3-CM3
8	AC	102	BCL	C16-C17-C18-C19
8	AC	102	BCL	C11-C12-C13-C15
8	AI	101	BCL	C11-C12-C13-C15
8	AJ	101	BCL	C11-C10-C8-C7
8	AM	1001	BCL	C6-C7-C8-C10
8	BL	102	BCL	C11-C12-C13-C15
15	M	405	CD4	C41-C42-C43-C44
11	AC	104	3PE	C2-C1-O11-P
11	AC	104	3PE	O11-C1-C2-O21
8	AE	101	BCL	C11-C10-C8-C9
8	AL	1001	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
8	AM	1001	BCL	C6-C7-C8-C9
8	L	305	BCL	C14-C13-C15-C16
11	AC	104	3PE	O21-C2-C3-O31
8	BH	101	BCL	C4-C3-C5-C6
11	H	301	3PE	C29-C2A-C2B-C2C
11	AC	104	3PE	C11-O13-P-O11
8	BL	102	BCL	C2-C3-C5-C6
9	AB	103	SPO	C32-C33-C35-C36
15	M	405	CD4	O3-C17-C18-C19
11	H	302	3PE	C1-C2-O21-C21
8	AC	102	BCL	C11-C12-C13-C14
8	AD	102	BCL	C11-C12-C13-C14
15	M	405	CD4	C39-C40-C41-C42
8	BL	102	BCL	C2A-CAA-CBA-CGA
13	M	404	U10	C35-C34-C36-C37
13	L	302	U10	C5-C4-O4-C4M
15	M	405	CD4	O2-C15-C16-O3
8	BJ	101	BCL	C2-C1-O2A-CGA
9	AC	101	SPO	C29-C28-C30-C31
13	M	404	U10	C44-C46-C47-C48
8	AA	1001	BCL	C15-C16-C17-C18
9	AA	1002	SPO	C29-C28-C30-C31
9	AG	101	SPO	C29-C28-C30-C31
9	AH	101	SPO	C29-C28-C30-C31
9	AM	1002	SPO	C29-C28-C30-C31
13	L	302	U10	C12-C11-C9-C10
8	BJ	101	BCL	C14-C13-C15-C16
8	BG	101	BCL	C2A-CAA-CBA-CGA
8	AD	102	BCL	C2-C3-C5-C6
8	BH	101	BCL	C2-C3-C5-C6
9	AA	1002	SPO	C27-C28-C30-C31
9	AH	101	SPO	C27-C28-C30-C31
13	L	302	U10	C12-C11-C9-C8
9	AK	102	SPO	C29-C28-C30-C31
9	AC	101	SPO	C27-C28-C30-C31
13	M	404	U10	C33-C34-C36-C37
10	M	401	LMT	C9-C10-C11-C12
8	BB	1001	BCL	C15-C16-C17-C18
12	L	301	BPH	C8-C10-C11-C12
15	M	405	CD4	C33-C32-O13-P2
11	H	301	3PE	C2B-C2C-C2D-C2E
9	BE	1000	SPO	C15-C16-C17-C19

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Mol	Chain	Res	Type	Atoms
9	AE	102	SPO	C29-C28-C30-C31
9	AM	1002	SPO	C27-C28-C30-C31
9	AD	101	SPO	C33-C35-C36-C37
8	AA	1001	BCL	C11-C12-C13-C14
11	H	301	3PE	C2D-C2E-C2F-C2G
15	M	405	CD4	C43-C44-C45-C63
9	AJ	102	SPO	C29-C28-C30-C31
9	AE	102	SPO	C27-C28-C30-C31
9	AG	101	SPO	C27-C28-C30-C31
9	AK	102	SPO	C27-C28-C30-C31
8	BI	101	BCL	C2A-CAA-CBA-CGA
8	AE	103	BCL	C1A-C2A-CAA-CBA
8	BG	101	BCL	C1A-C2A-CAA-CBA
11	H	301	3PE	C26-C27-C28-C29
9	AD	101	SPO	C29-C28-C30-C31
9	BE	1000	SPO	C34-C33-C35-C36
9	AJ	103	SPO	C35-C36-C37-C38
8	BJ	101	BCL	C12-C13-C15-C16
8	AM	1003	BCL	C2A-CAA-CBA-CGA
11	H	301	3PE	C32-C33-C34-C35
11	H	302	3PE	C2A-C2B-C2C-C2D
8	AB	101	BCL	C2C-C3C-CAC-CBC
9	AI	102	SPO	C3-C1-C4-C5
8	AL	1001	BCL	C10-C11-C12-C13
9	AB	103	SPO	C15-C16-C17-C18
8	M	406	BCL	C4-C3-C5-C6
9	AM	1004	SPO	C29-C28-C30-C31
9	AD	101	SPO	C27-C28-C30-C31
9	AJ	102	SPO	C27-C28-C30-C31
13	M	404	U10	C48-C49-C51-C52
9	AH	103	SPO	C11-C10-C9-C7
8	BF	101	BCL	C4-C3-C5-C6
9	AJ	102	SPO	C34-C33-C35-C36
13	M	404	U10	C50-C49-C51-C52
8	M	406	BCL	C2-C3-C5-C6
9	BA	101	SPO	C27-C28-C30-C31
11	H	301	3PE	C37-C38-C39-C3A
11	AB	102	3PE	C29-C2A-C2B-C2C
8	AJ	101	BCL	C4C-C3C-CAC-CBC
10	M	401	LMT	C5'-C4'-O1B-C1B
11	H	302	3PE	C2E-C2F-C2G-C2H
11	H	302	3PE	C3B-C3C-C3D-C3E

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Mol	Chain	Res	Type	Atoms
9	AF	101	SPO	C33-C35-C36-C37
8	BF	101	BCL	C14-C13-C15-C16
8	BL	102	BCL	C11-C12-C13-C14
12	M	402	BPH	C6-C7-C8-C9
8	M	406	BCL	C8-C10-C11-C12
9	AK	104	SPO	C29-C28-C30-C31
9	BE	1000	SPO	C32-C33-C35-C36
8	BF	101	BCL	O2A-C1-C2-C3
8	BN	101	BCL	O2A-C1-C2-C3
12	L	301	BPH	O2A-C1-C2-C3
13	M	404	U10	C5-C4-O4-C4M
14	L	303	UQ1	C1-C2-O2-CM2
10	AB	104	LMT	O5B-C5B-C6B-O6B
8	AN	101	BCL	C5-C6-C7-C8
11	AC	104	3PE	C3A-C3B-C3C-C3D
8	AC	102	BCL	CAA-CBA-CGA-O2A
9	AF	103	SPO	C15-C16-C17-C19
9	AM	1004	SPO	C15-C16-C17-C19
9	AI	102	SPO	O1-C1-C4-C5
13	L	302	U10	C3-C4-O4-C4M
8	AI	101	BCL	C11-C10-C8-C7
8	AM	1003	BCL	C11-C10-C8-C7
8	BF	101	BCL	C12-C13-C15-C16
8	M	406	BCL	C11-C10-C8-C7
8	AM	1003	BCL	C2-C1-O2A-CGA
11	AB	102	3PE	C27-C28-C29-C2A
11	H	301	3PE	O31-C31-C32-C33
9	AK	104	SPO	C34-C33-C35-C36
9	AK	104	SPO	C32-C33-C35-C36
9	AD	103	SPO	C30-C31-C32-C33
8	AJ	101	BCL	C2-C3-C5-C6
9	BL	101	SPO	C32-C33-C35-C36
11	H	302	3PE	C27-C28-C29-C2A
9	AD	103	SPO	C15-C16-C17-C18
8	BG	101	BCL	CAA-CBA-CGA-O2A
8	AM	1003	BCL	C1A-C2A-CAA-CBA
8	AJ	101	BCL	C4-C3-C5-C6
9	BL	101	SPO	C34-C33-C35-C36
8	BL	102	BCL	CAA-CBA-CGA-O2A
8	M	403	BCL	CAA-CBA-CGA-O2A
9	AH	103	SPO	C15-C16-C17-C19
9	AJ	103	SPO	C5-C6-C7-C9

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Mol	Chain	Res	Type	Atoms
9	AK	102	SPO	C5-C6-C7-C9
9	M	407	SPO	C15-C16-C17-C19
11	H	301	3PE	C3D-C3E-C3F-C3G
8	BB	1001	BCL	C2A-CAA-CBA-CGA
8	BC	101	BCL	C2A-CAA-CBA-CGA
8	AE	101	BCL	C8-C10-C11-C12
8	BH	101	BCL	C12-C13-C15-C16
12	M	402	BPH	C6-C7-C8-C10
8	BF	101	BCL	CAA-CBA-CGA-O2A
9	AA	1002	SPO	C2-C1-C4-C5
9	AK	104	SPO	C3-C1-C4-C5
8	AK	103	BCL	C2A-CAA-CBA-CGA
9	AD	103	SPO	C33-C35-C36-C37
9	AE	102	SPO	C28-C30-C31-C32
8	BF	101	BCL	C13-C15-C16-C17
8	BG	101	BCL	C3A-C2A-CAA-CBA
8	M	406	BCL	C3-C5-C6-C7
8	AJ	101	BCL	C11-C10-C8-C9
8	AK	101	BCL	C15-C16-C17-C18
9	M	407	SPO	C1-C4-C5-C6
11	H	301	3PE	O32-C31-C32-C33
8	AC	102	BCL	CAA-CBA-CGA-O1A
8	AJ	101	BCL	C8-C10-C11-C12
8	AA	1001	BCL	C8-C10-C11-C12
8	BJ	101	BCL	CAD-CBD-CGD-O2D
10	AB	104	LMT	C6-C7-C8-C9

There are no ring outliers.

44 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AK	104	SPO	2	0
8	AK	103	BCL	1	0
13	M	404	U10	1	0
9	AJ	103	SPO	1	0
9	AL	1002	SPO	2	0
8	BF	101	BCL	1	0
9	AB	103	SPO	3	0
8	BH	101	BCL	1	0
9	AC	103	SPO	2	0
9	AI	102	SPO	3	0
9	BE	1000	SPO	2	0

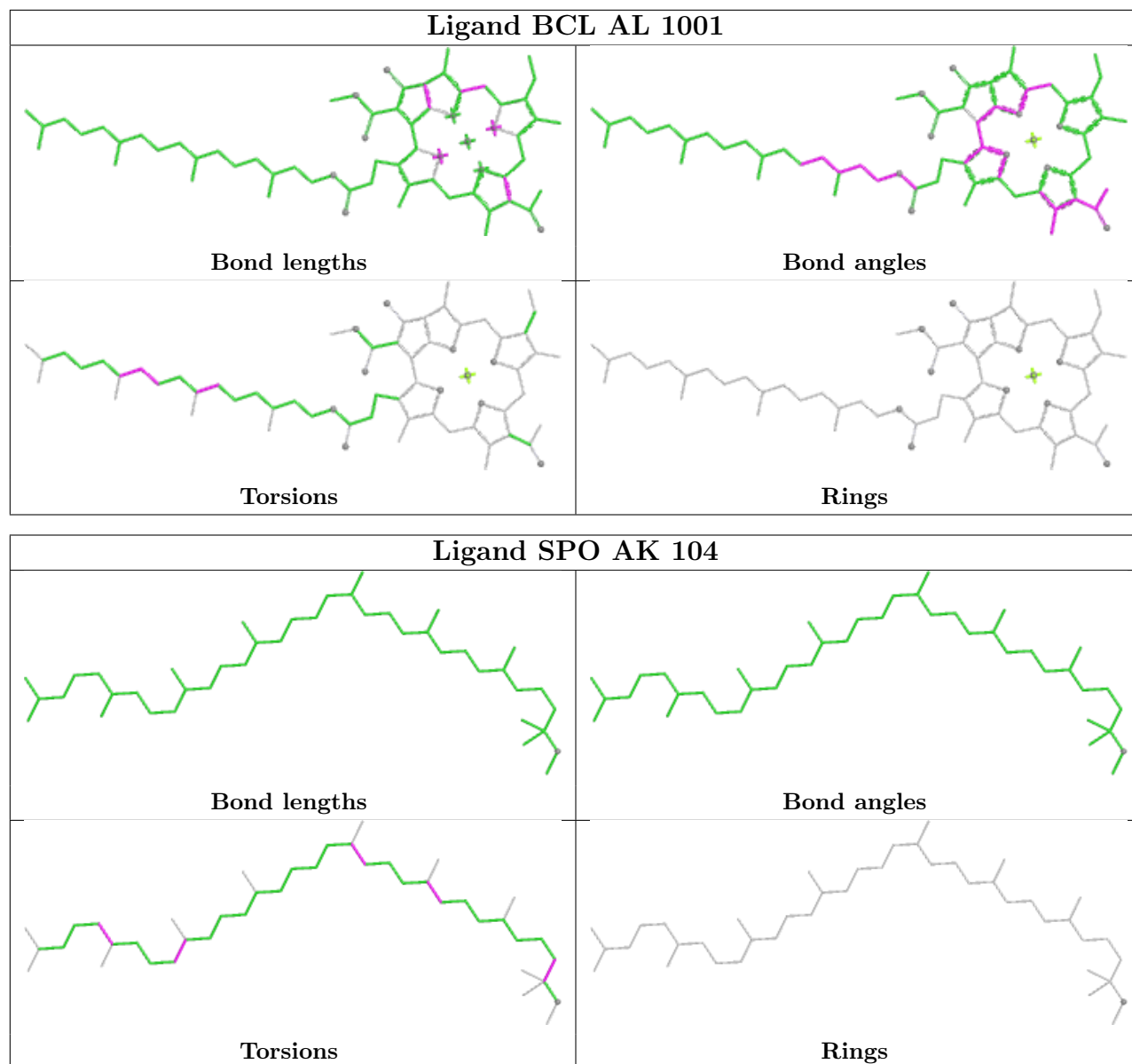
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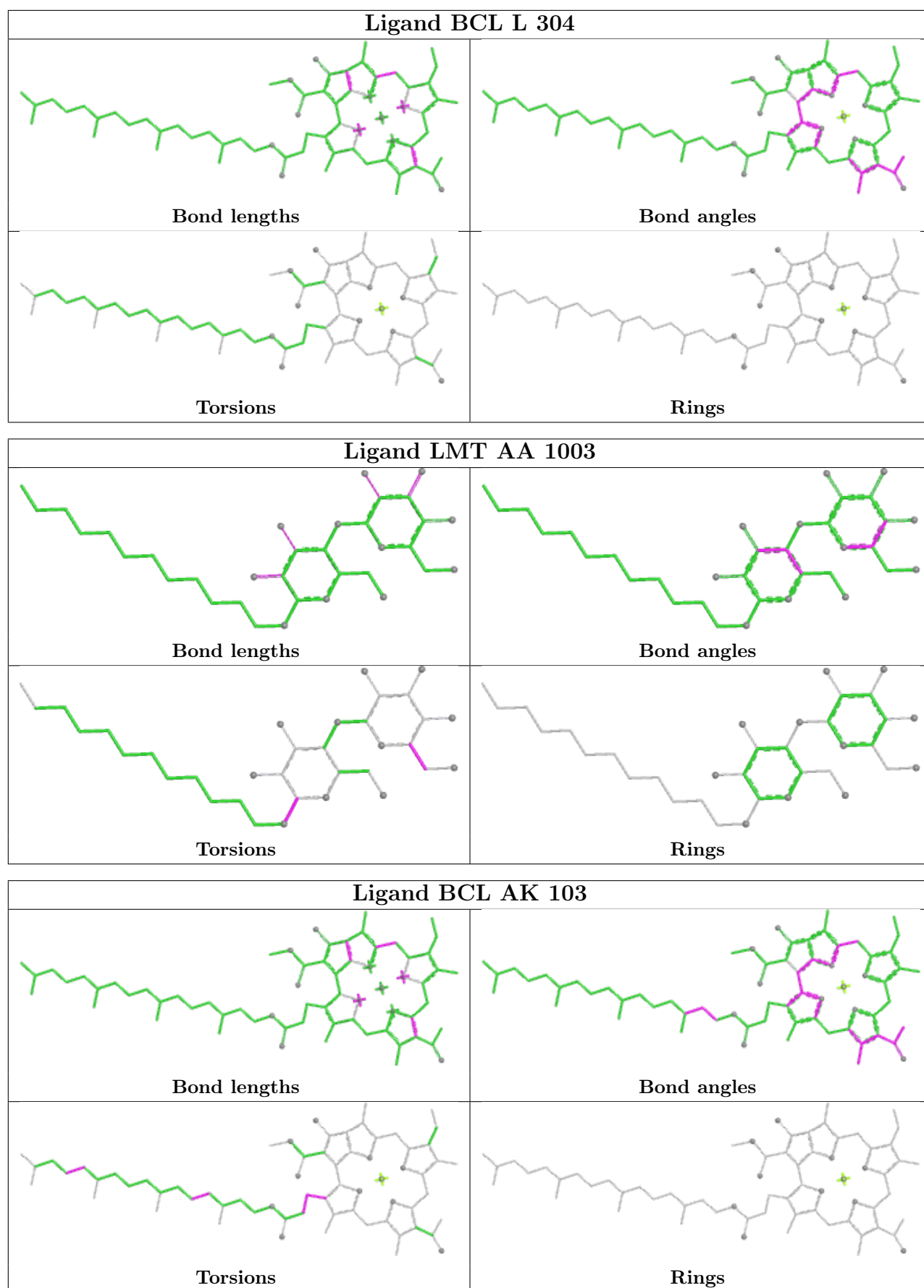
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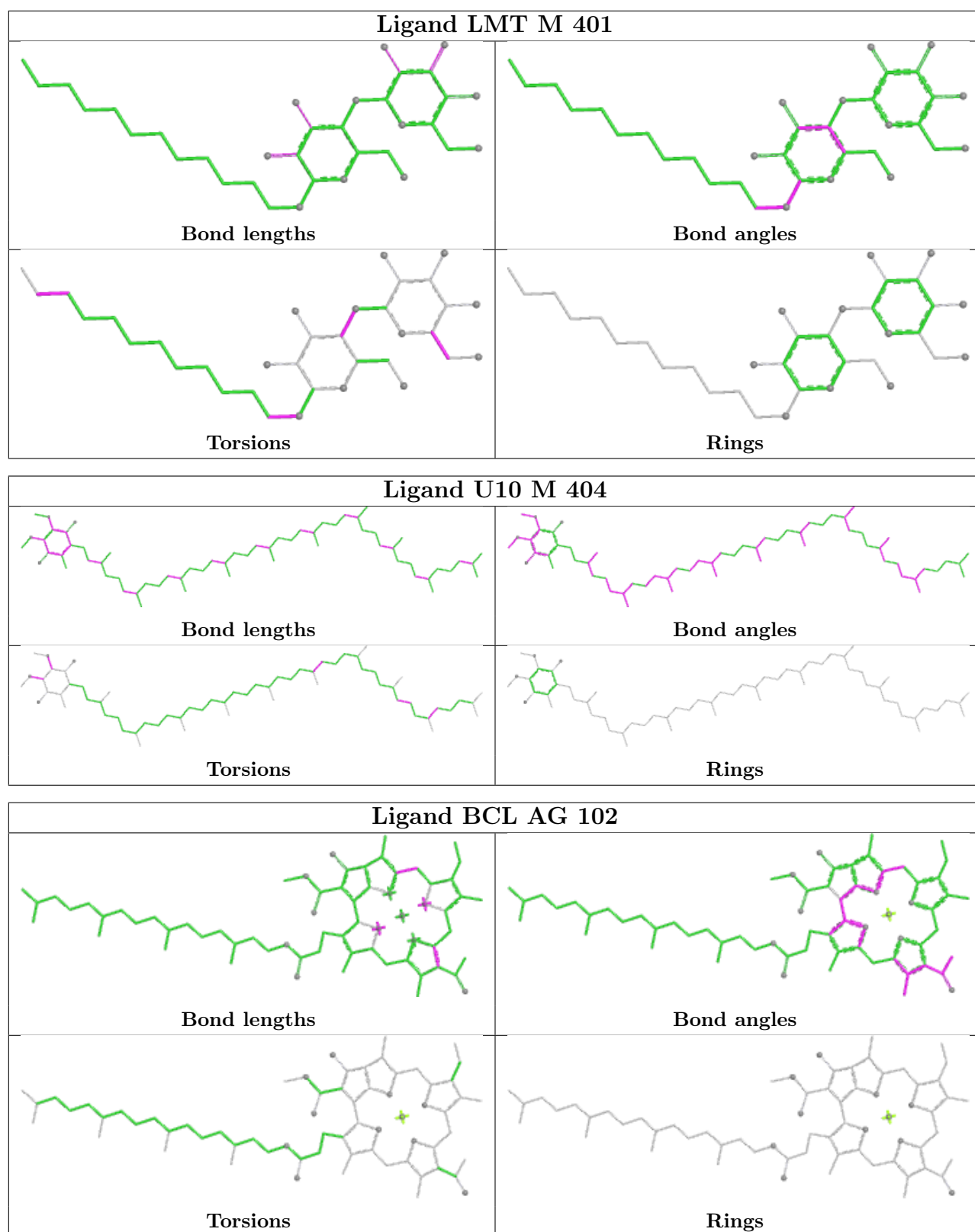
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	302	U10	1	0
8	AI	101	BCL	1	0
8	AJ	101	BCL	3	0
9	AJ	102	SPO	2	0
8	AB	101	BCL	3	0
8	AC	102	BCL	1	0
8	BC	101	BCL	2	0
12	M	402	BPH	1	0
11	H	302	3PE	1	0
8	AM	1003	BCL	1	0
8	AA	1001	BCL	1	0
9	AF	103	SPO	2	0
9	AM	1002	SPO	2	0
9	AF	101	SPO	3	0
9	AM	1004	SPO	2	0
9	AE	102	SPO	3	0
9	AH	103	SPO	1	0
9	AH	101	SPO	2	0
8	AE	103	BCL	1	0
15	M	405	CD4	1	0
9	AA	1002	SPO	2	0
9	AI	103	SPO	1	0
8	AE	101	BCL	1	0
9	M	407	SPO	2	0
8	AM	1001	BCL	1	0
8	BD	101	BCL	1	0
8	BA	102	BCL	1	0
8	AF	102	BCL	1	0
8	BB	1001	BCL	1	0
8	BL	102	BCL	1	0
9	BA	101	SPO	3	0
9	AD	103	SPO	2	0
8	BJ	101	BCL	1	0

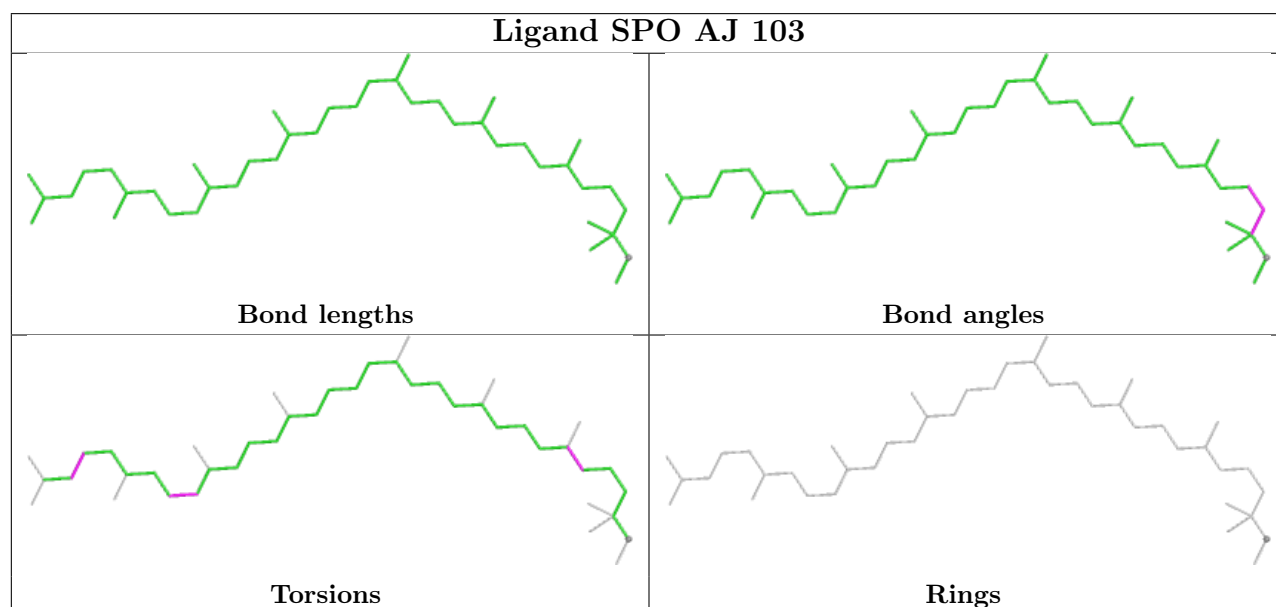
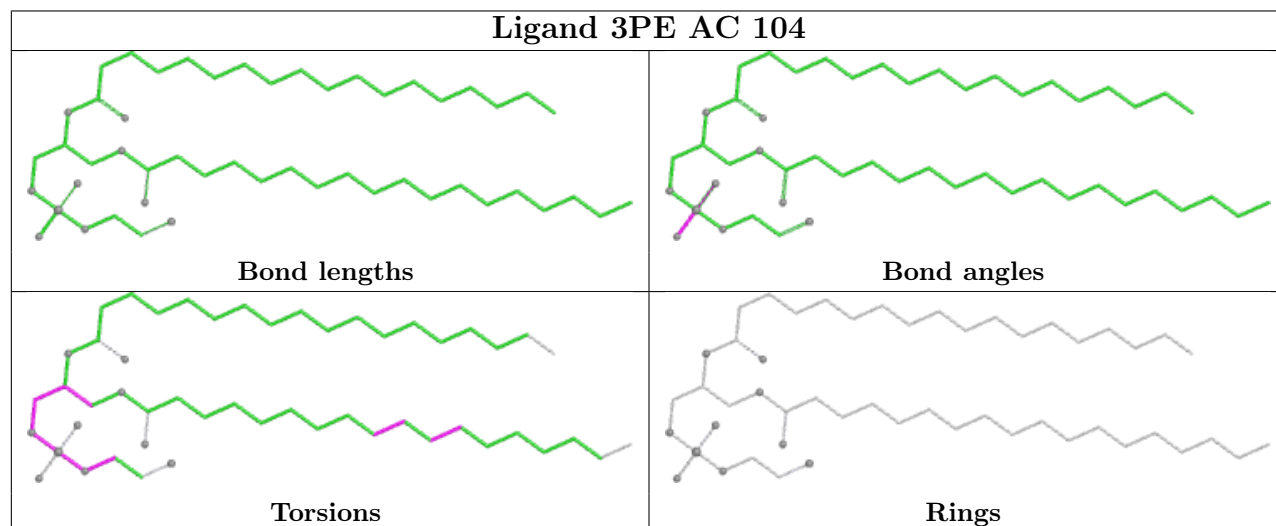
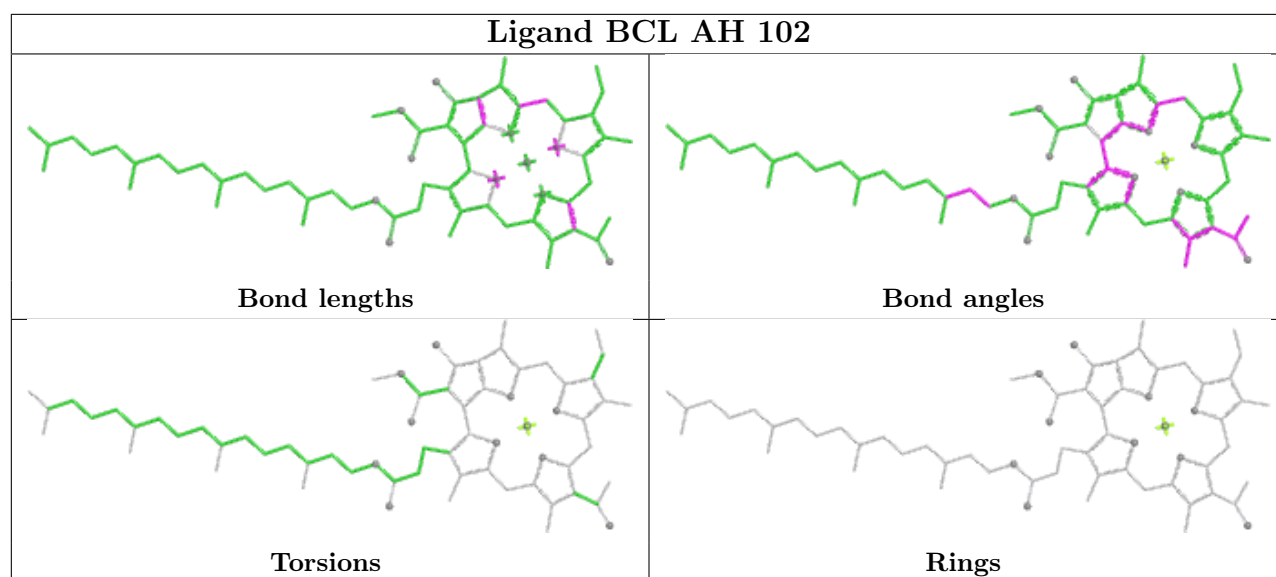
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

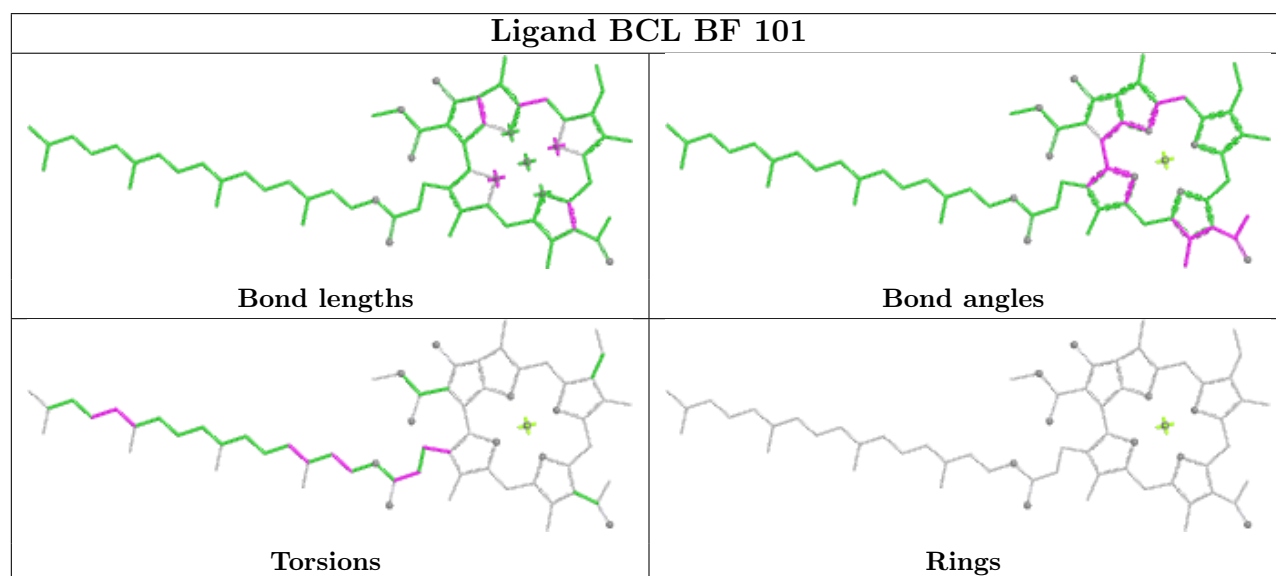
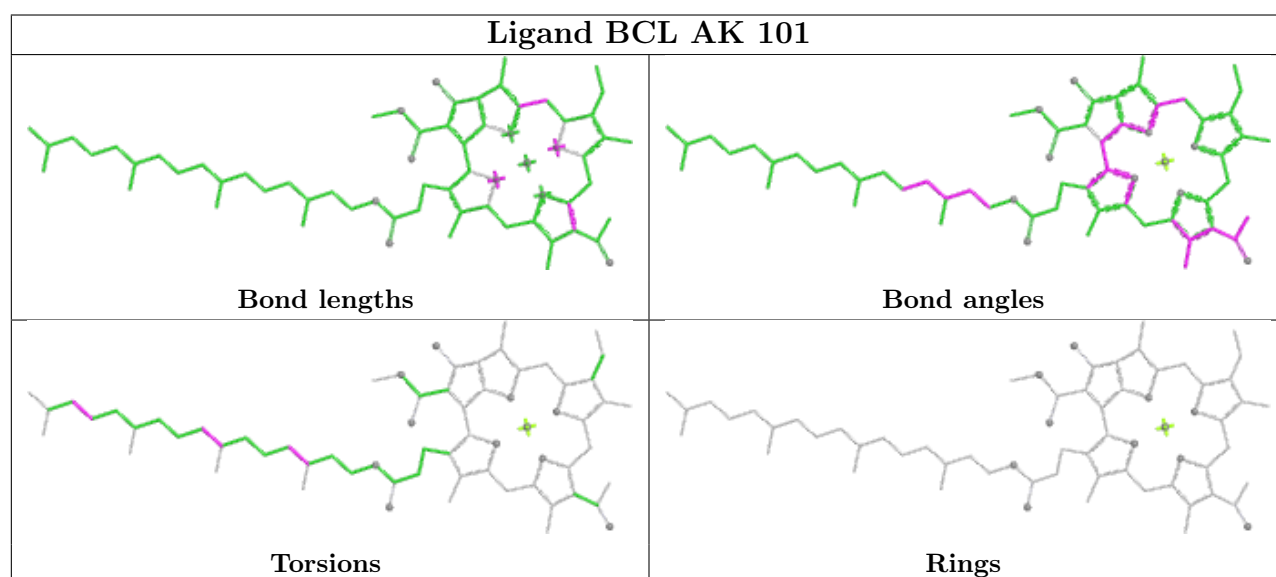
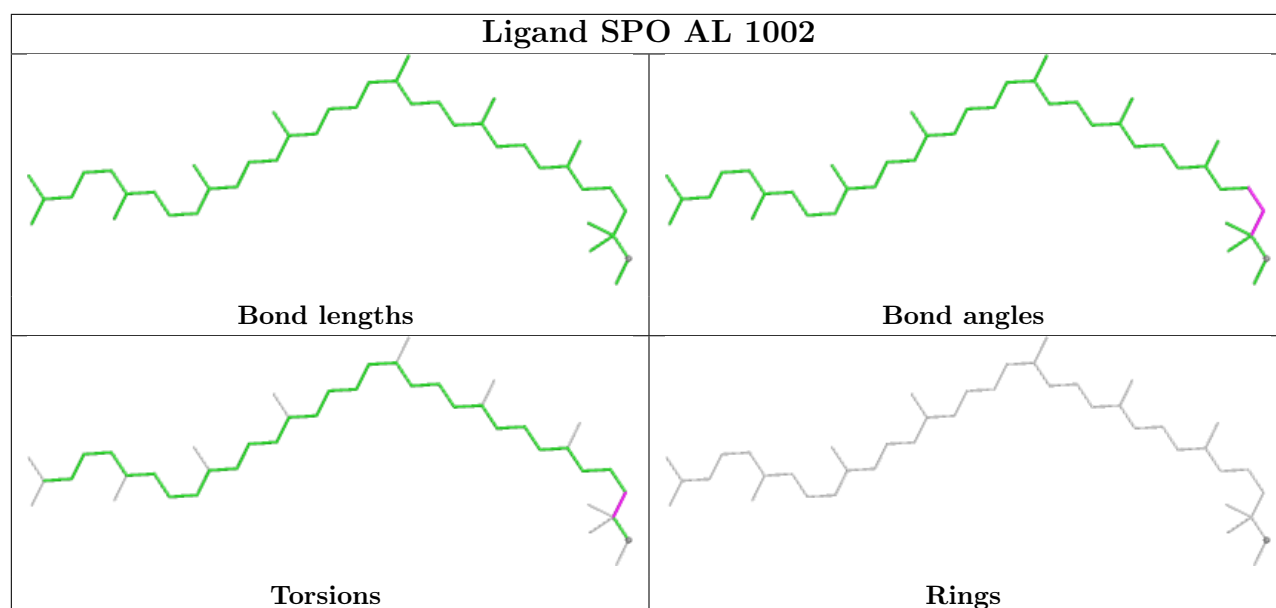
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

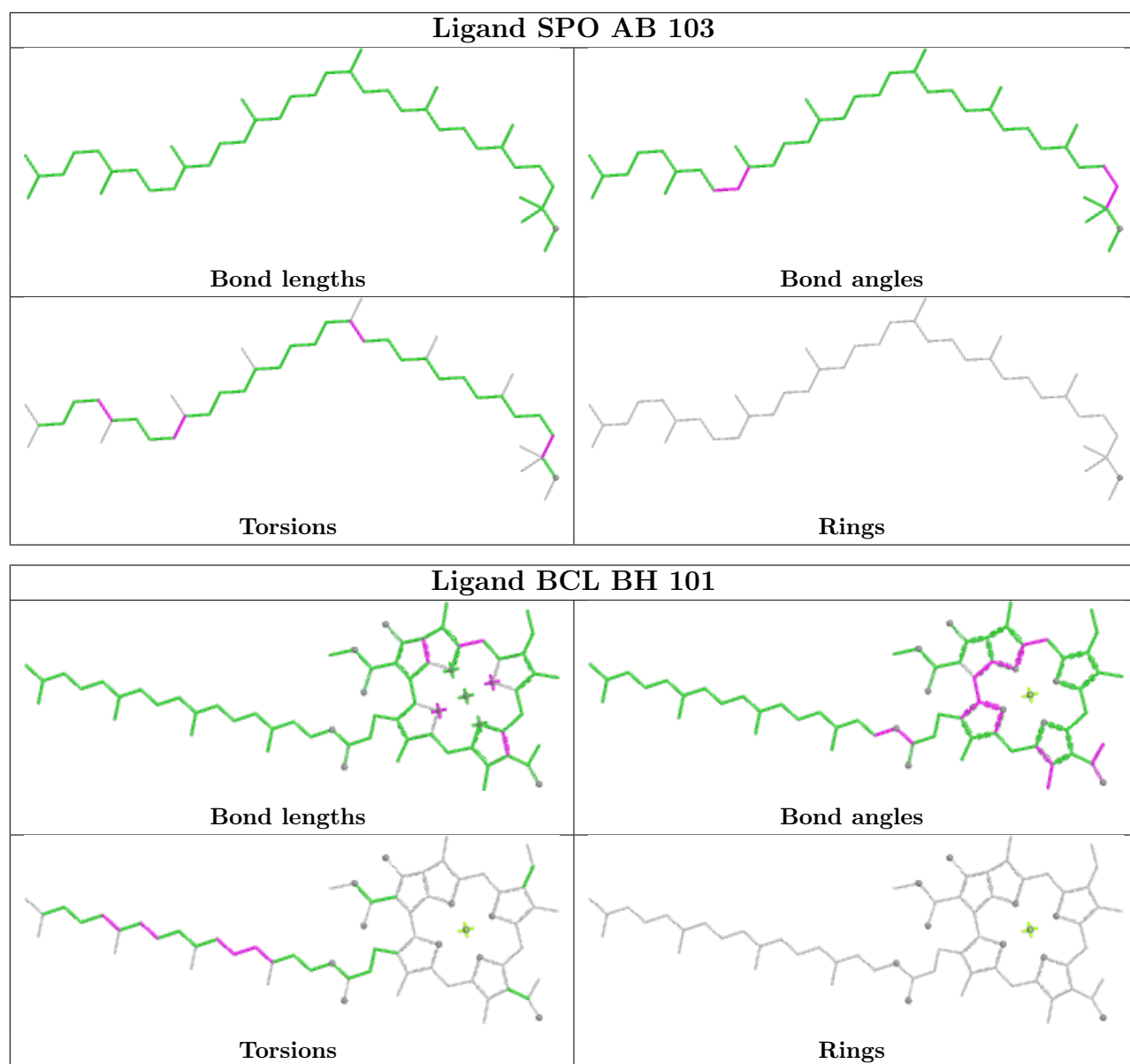


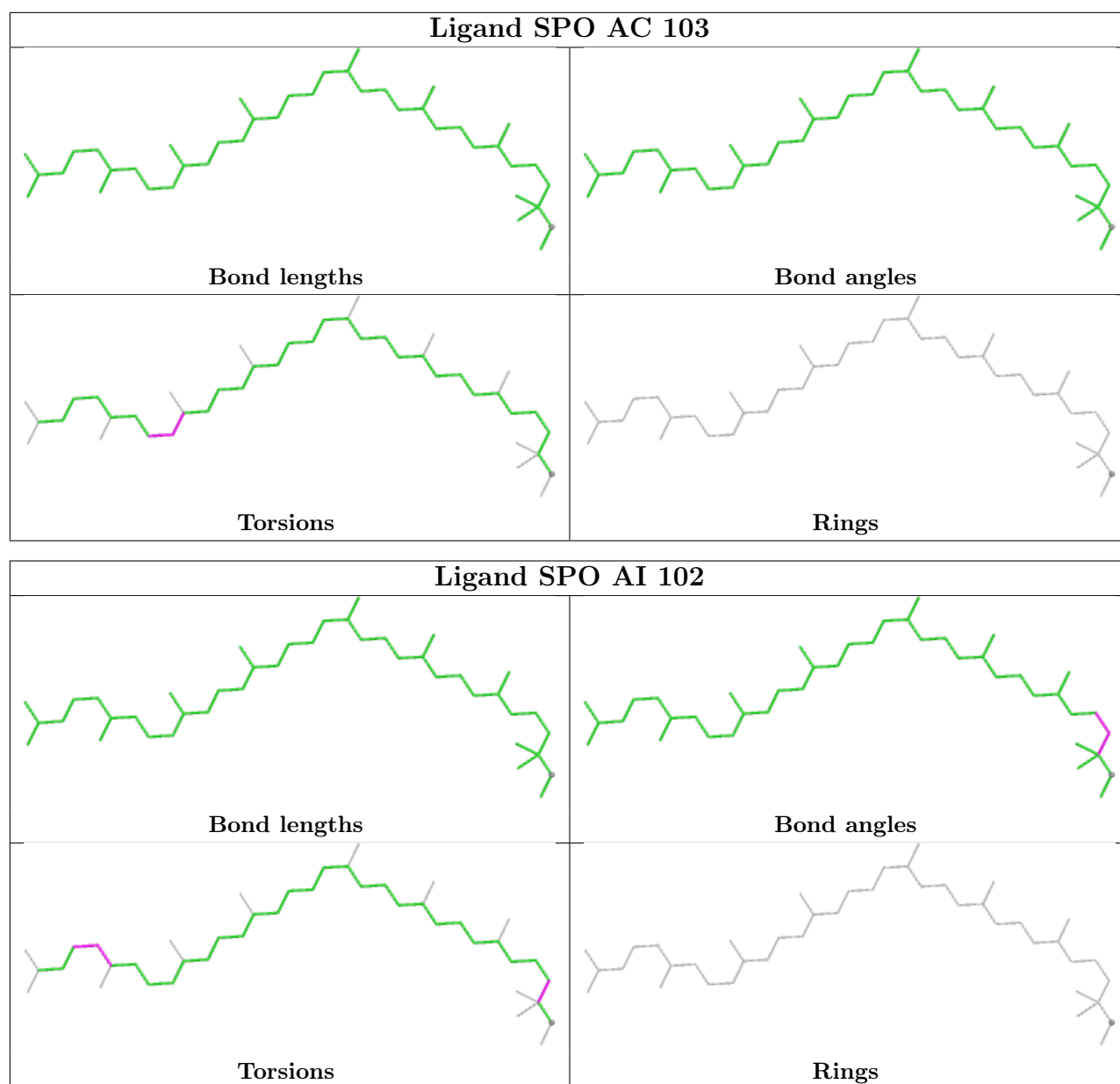


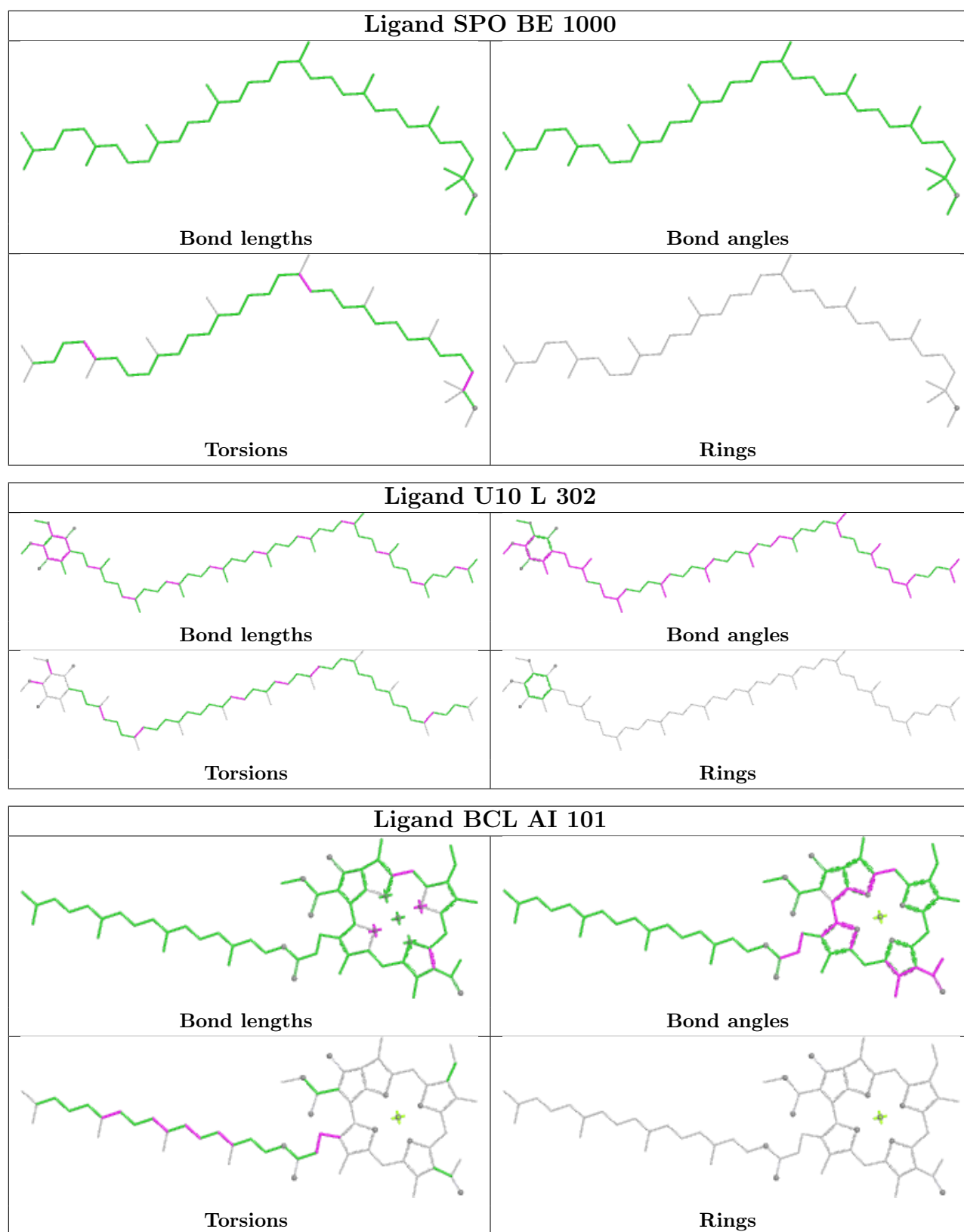


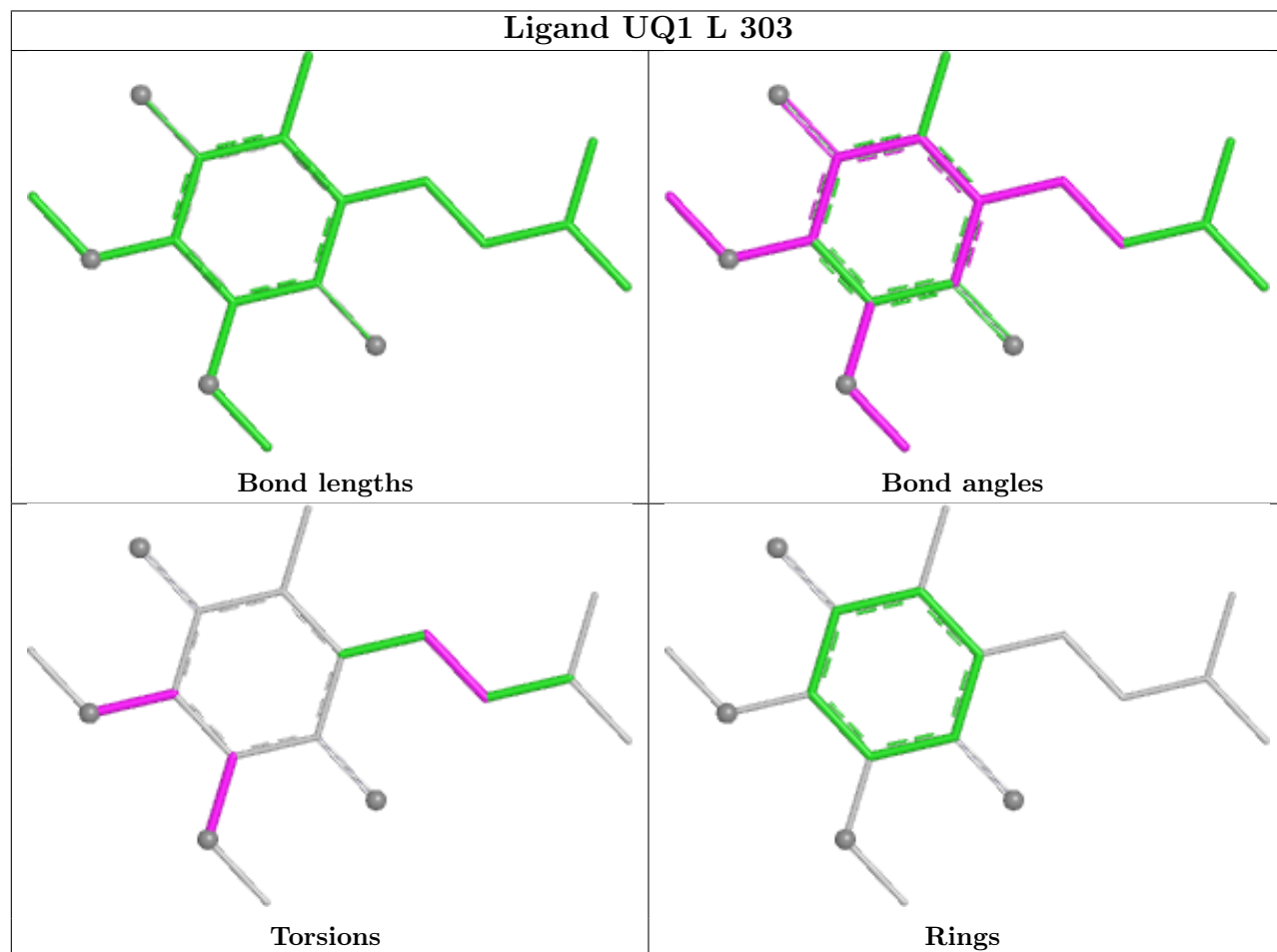
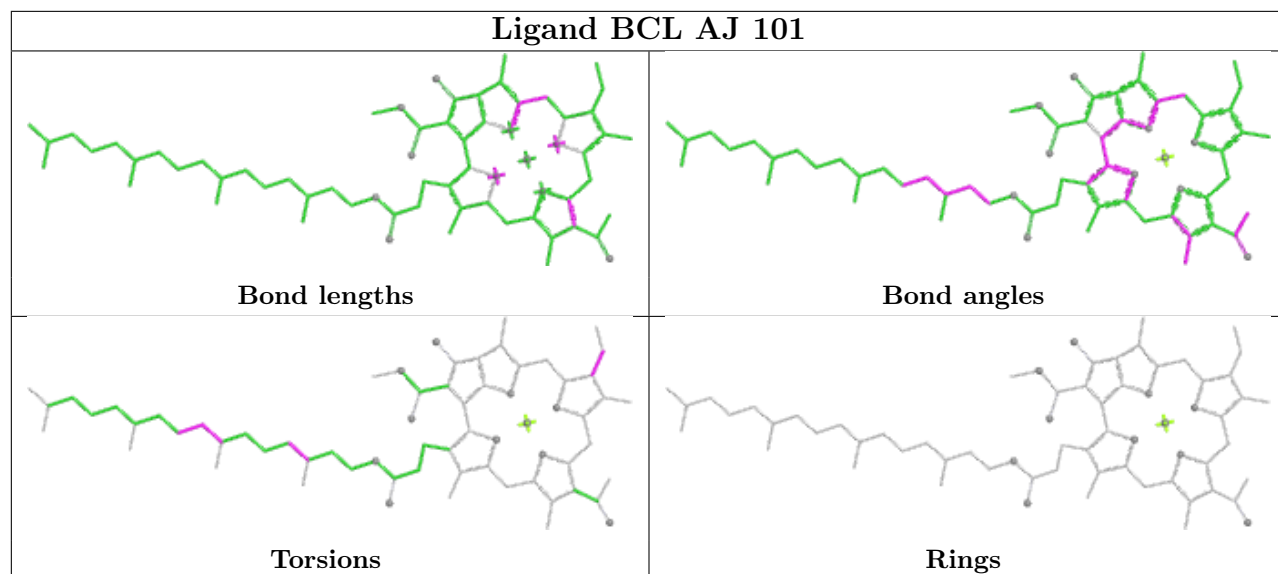


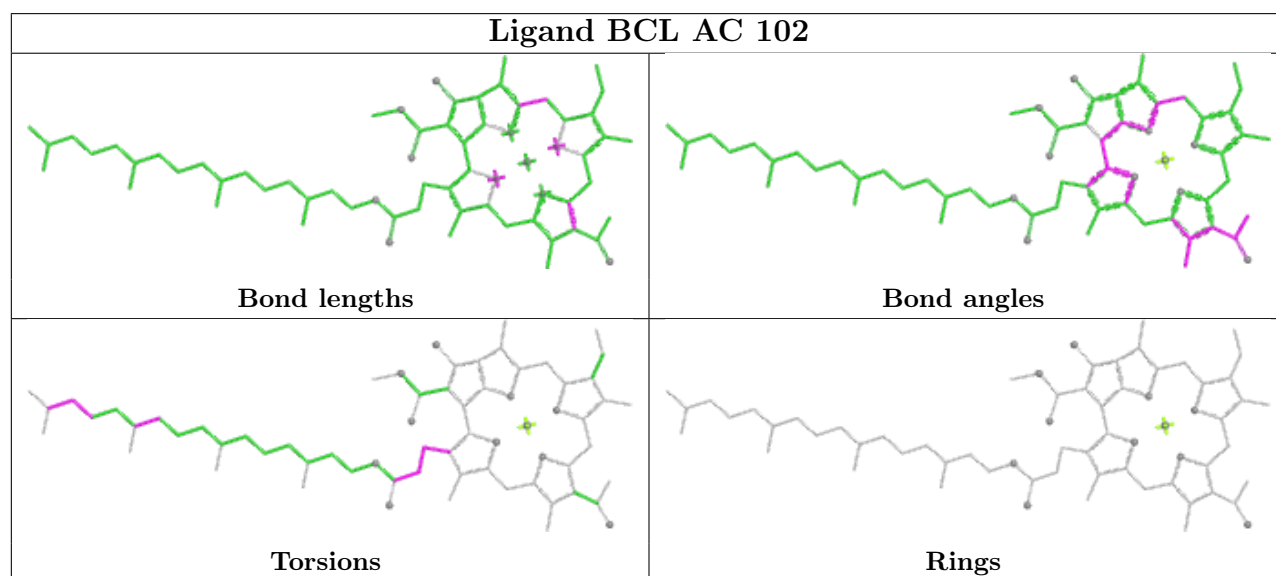
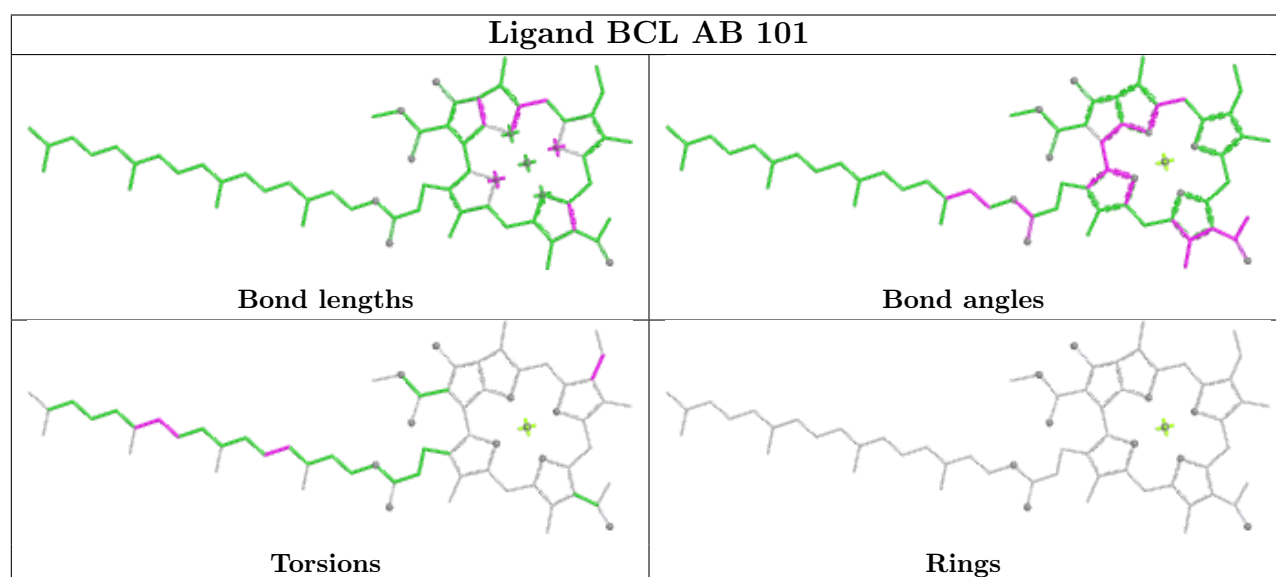
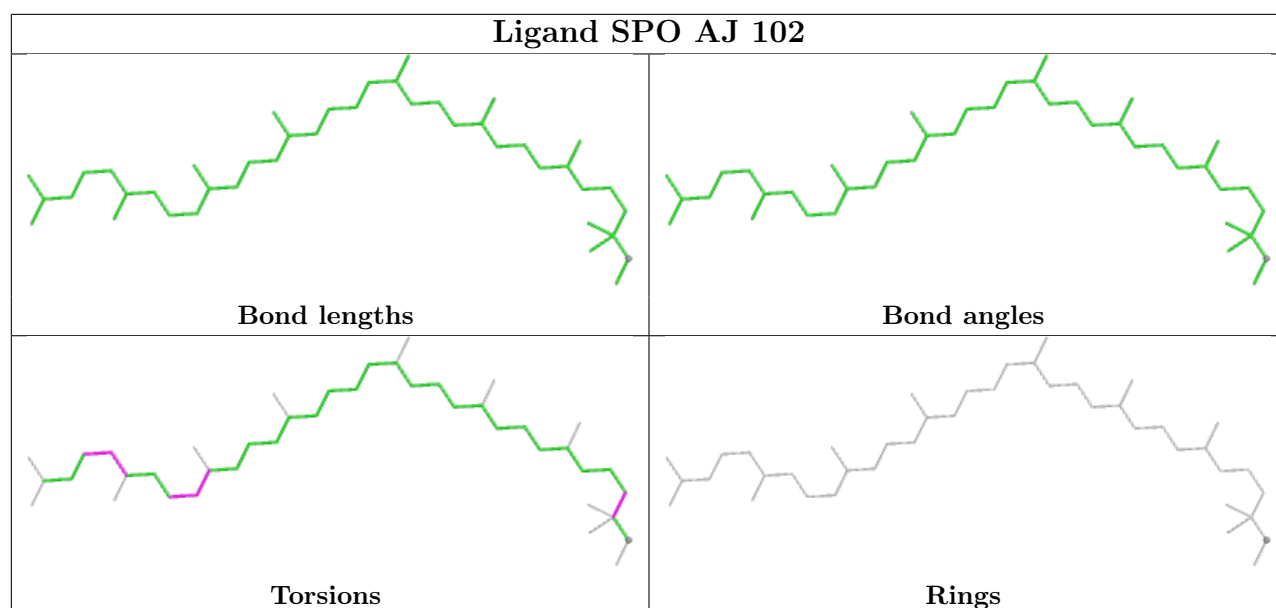


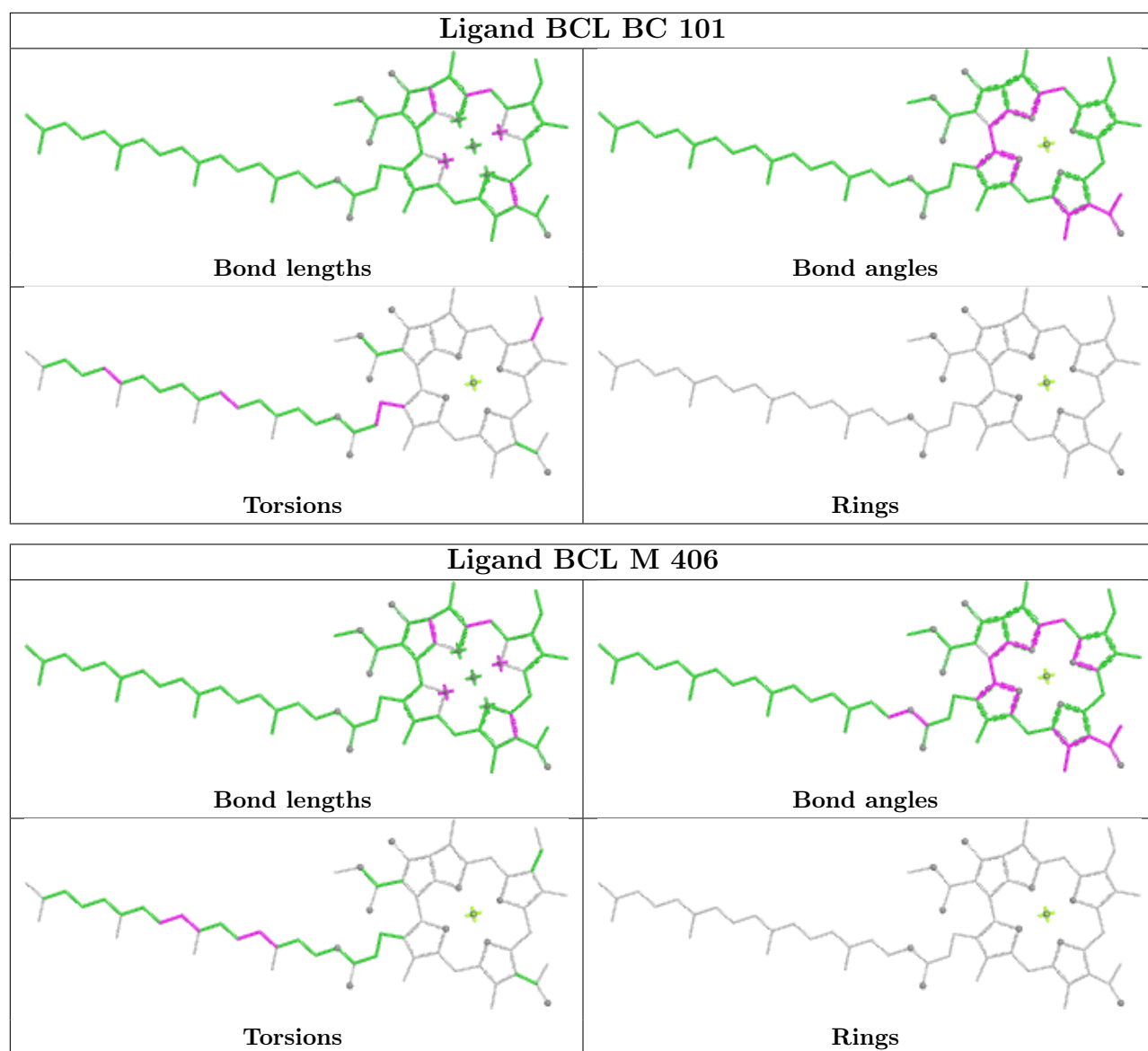


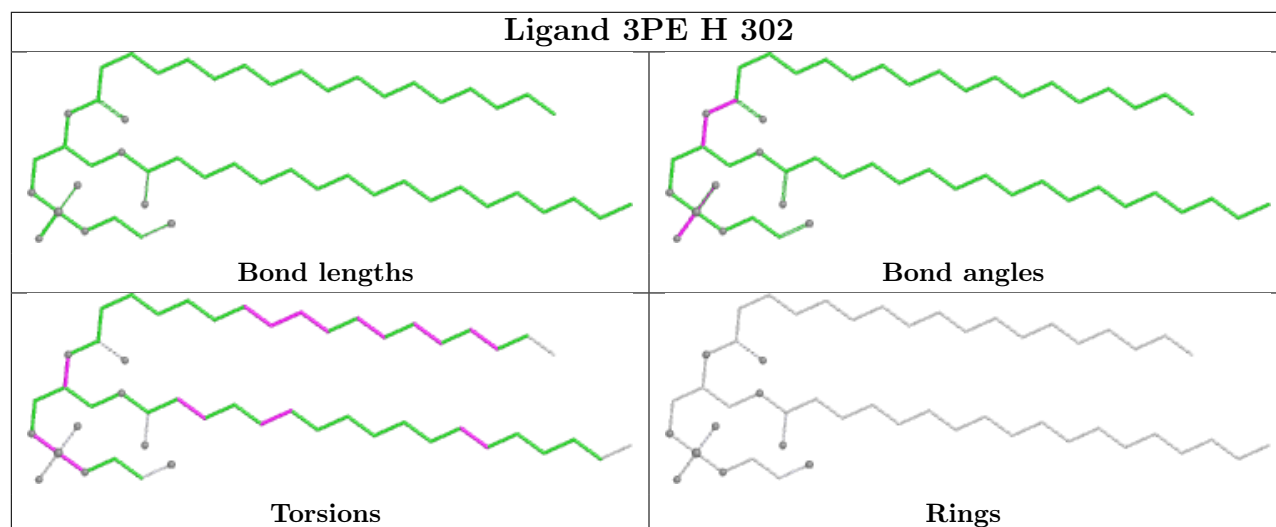
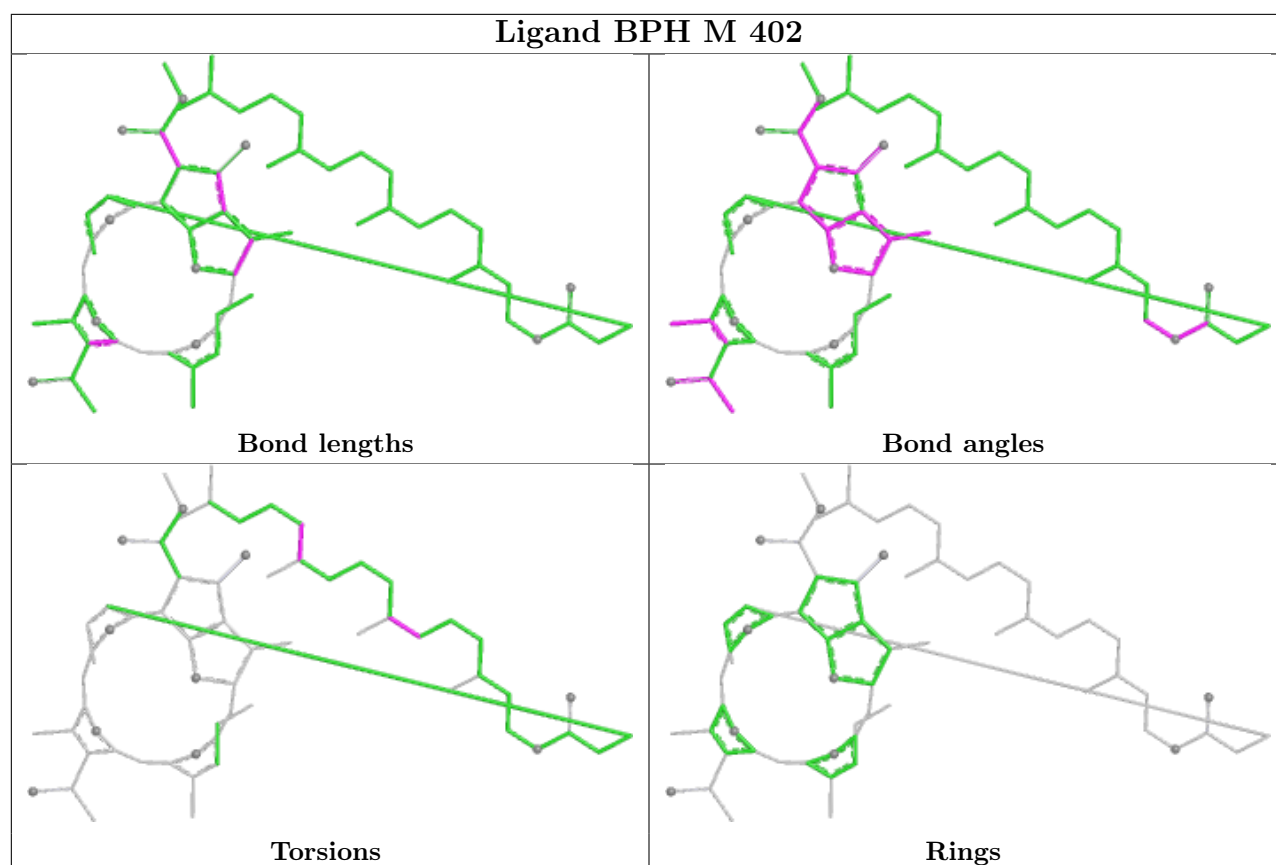


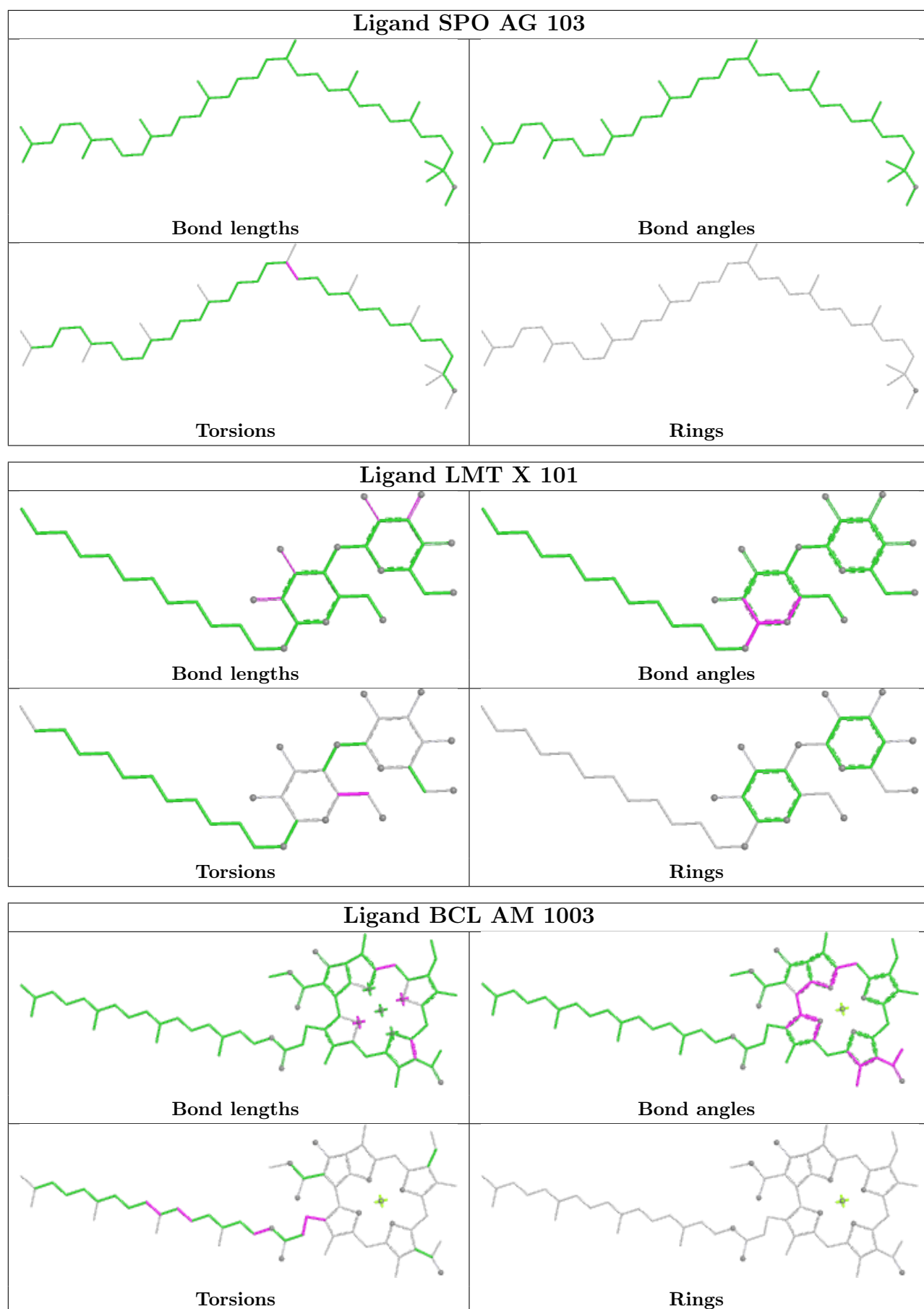


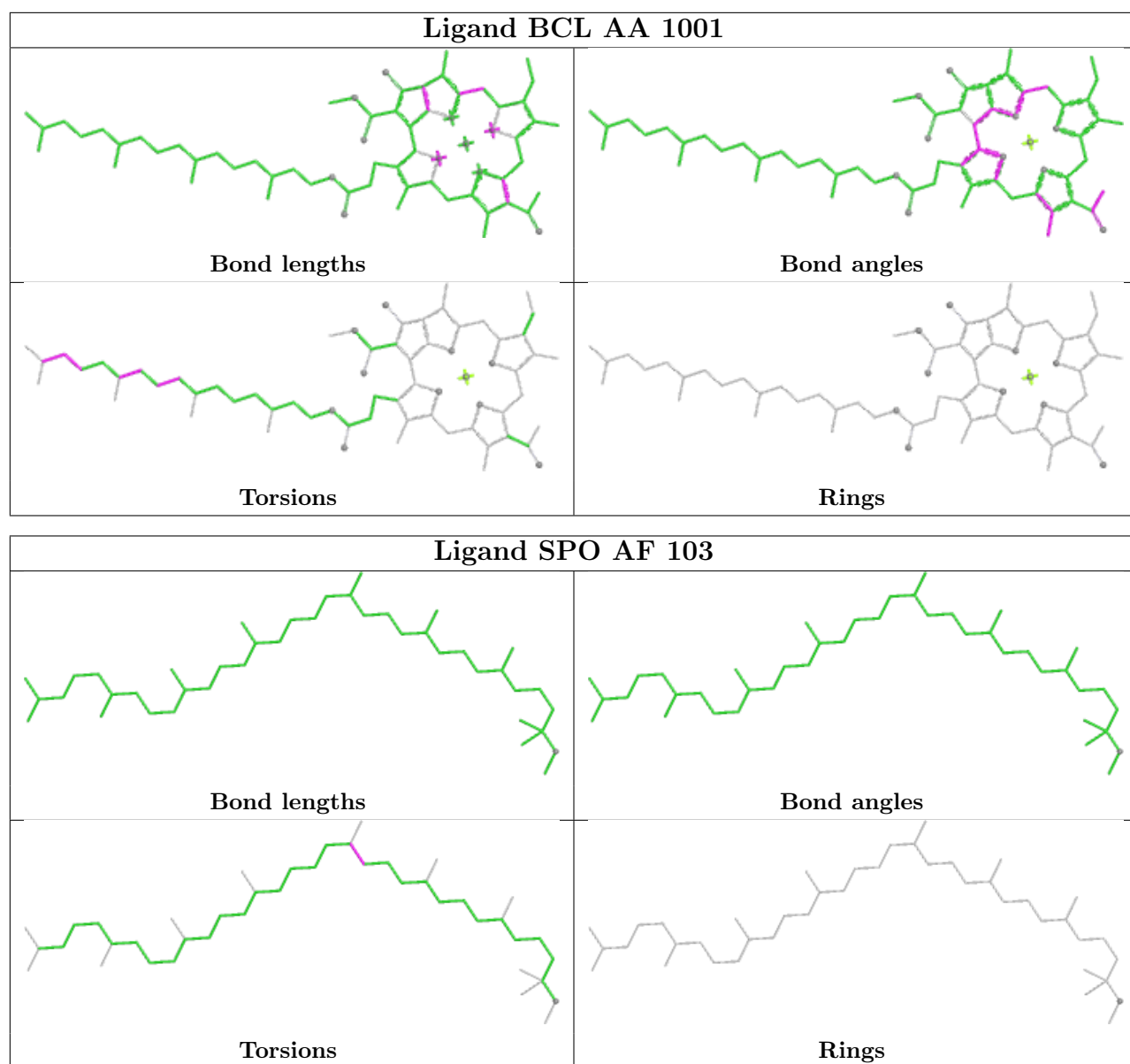


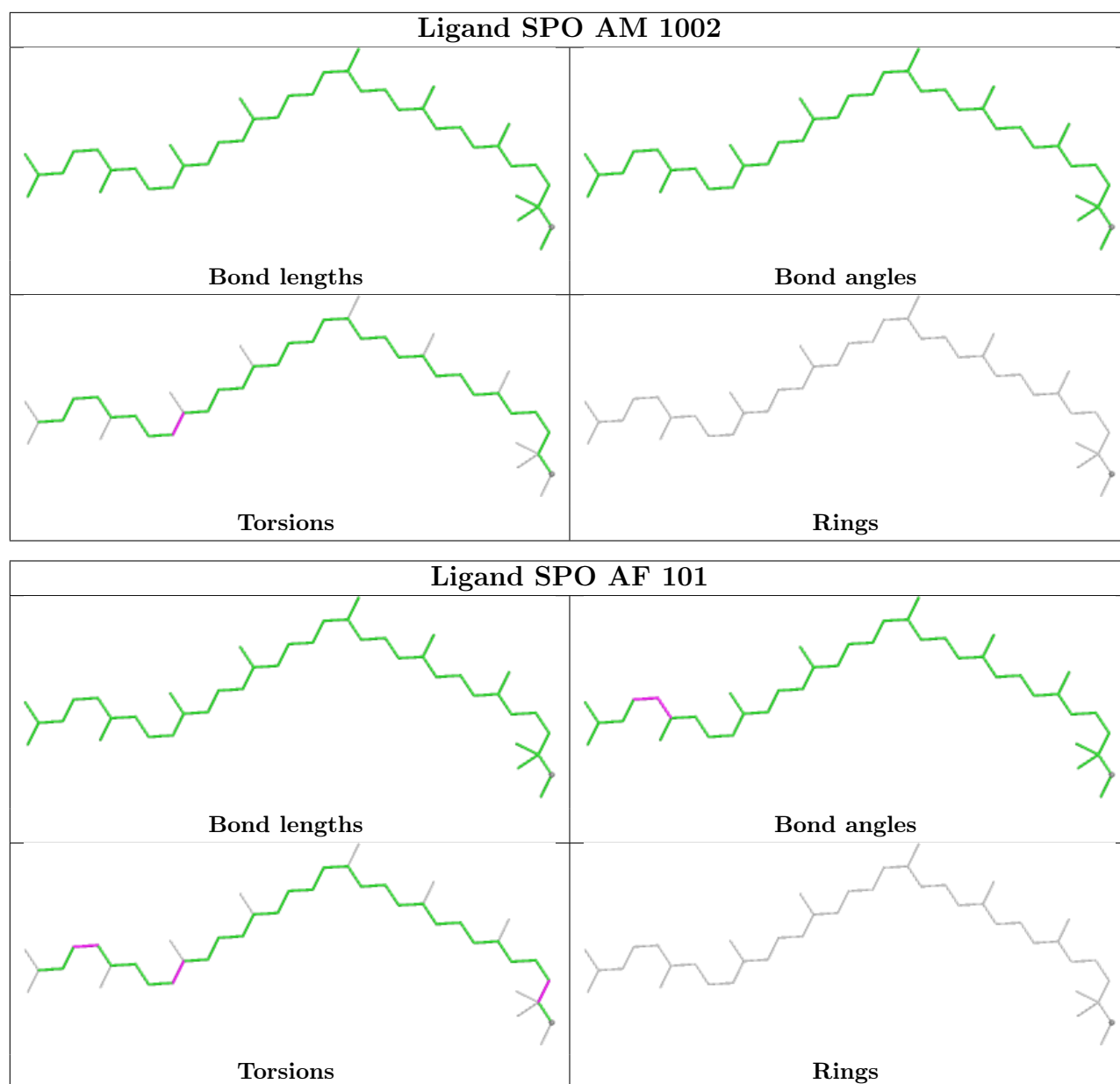


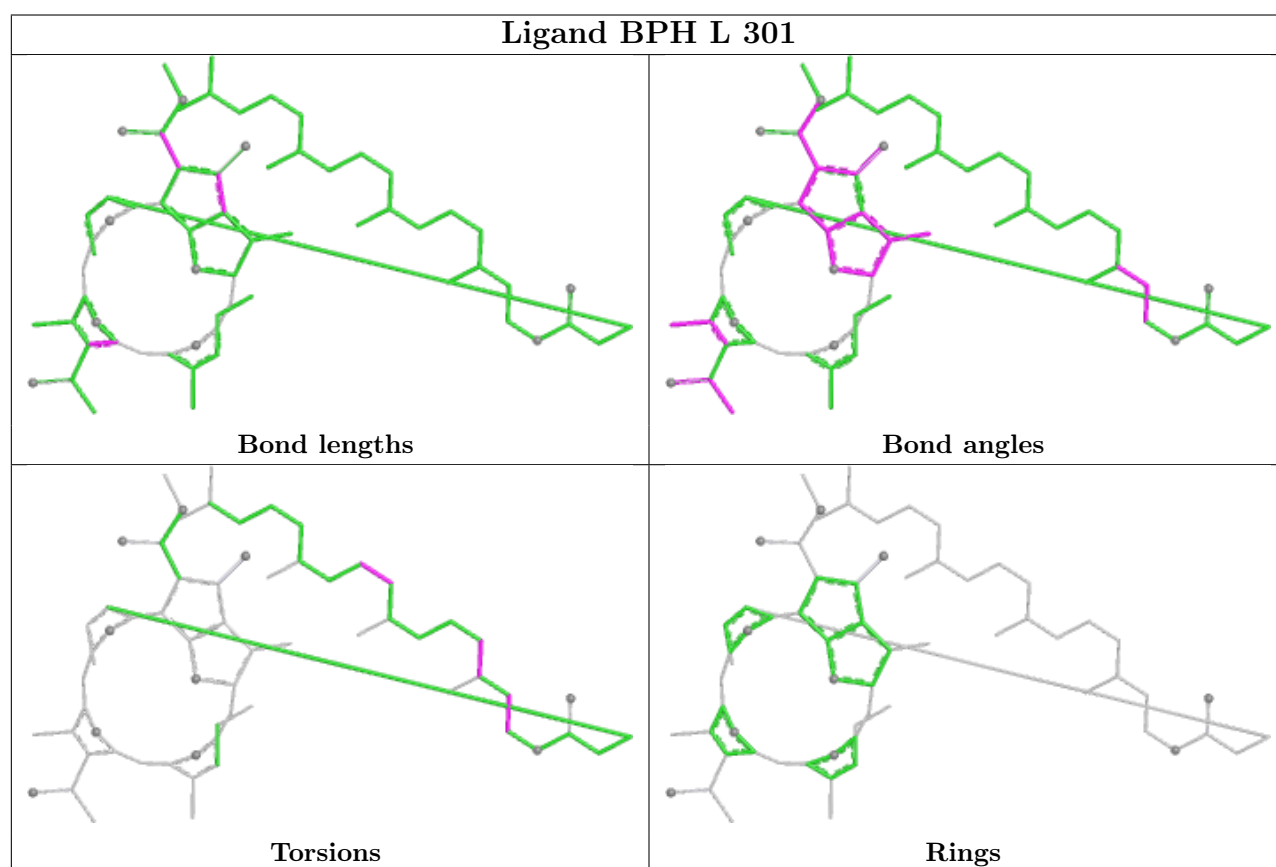
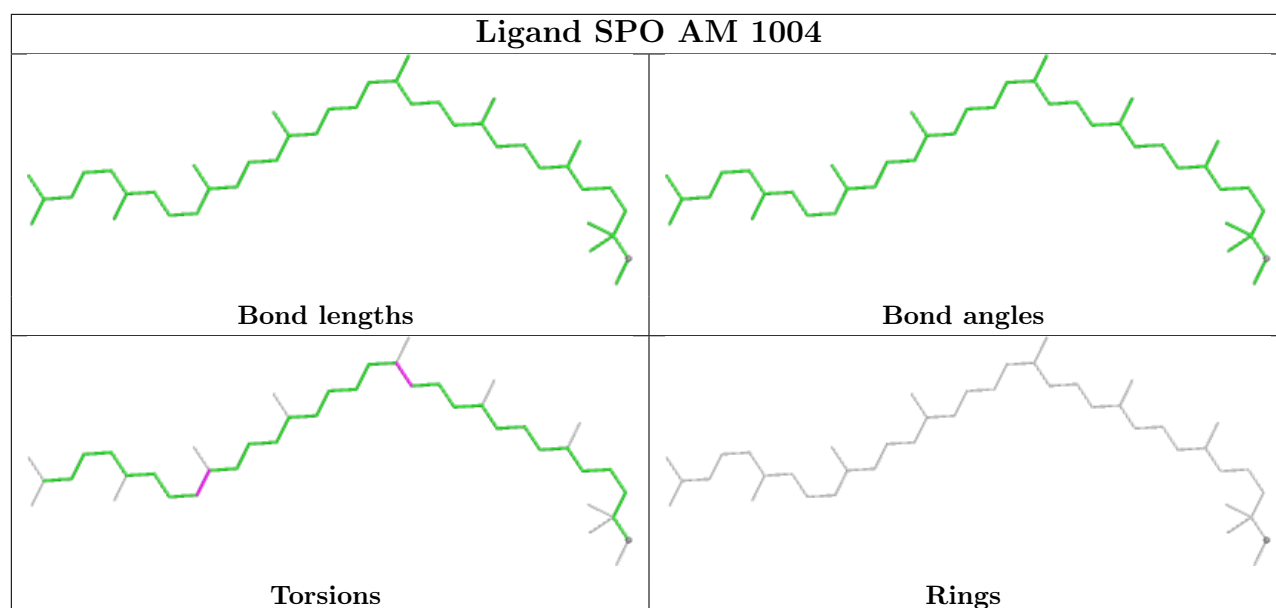


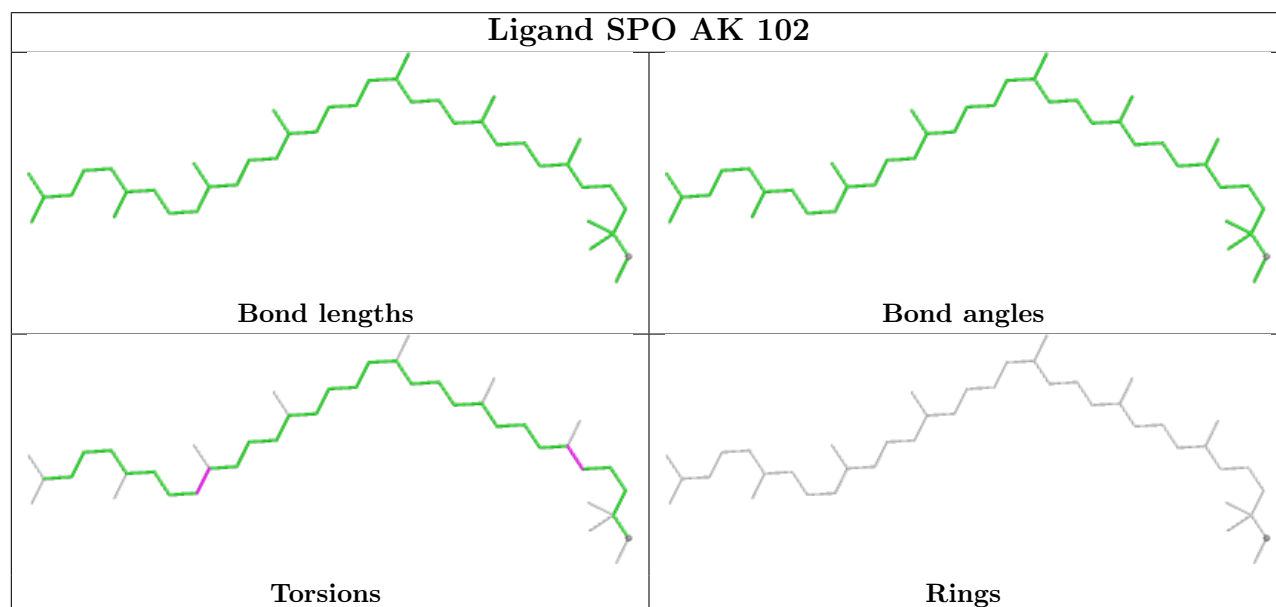
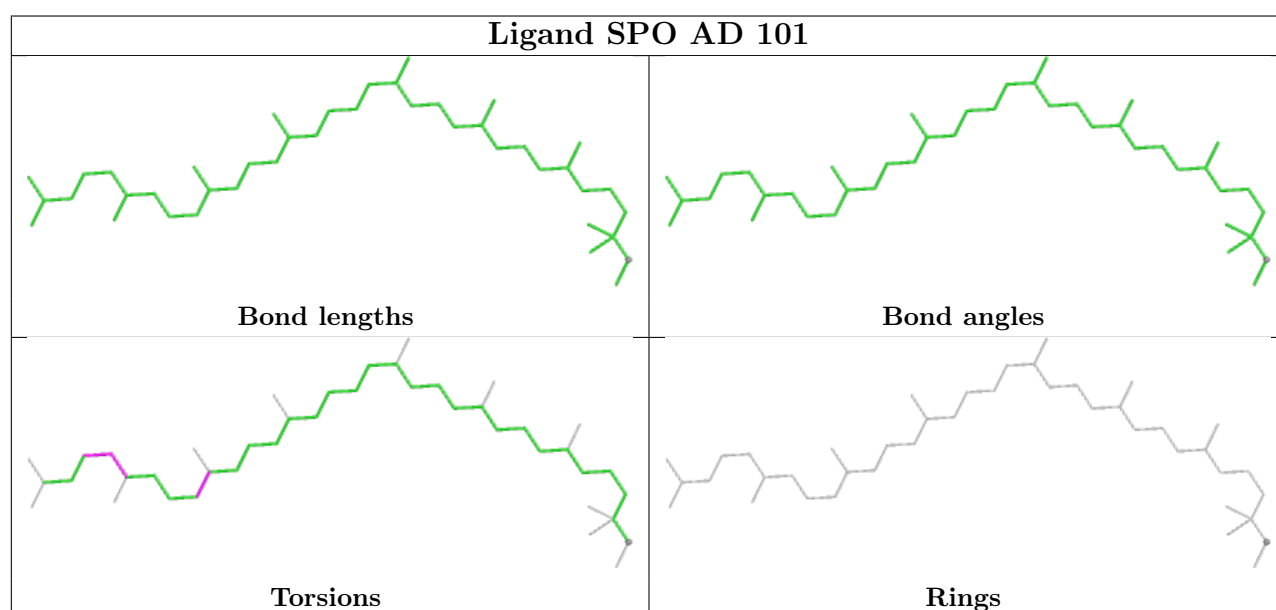
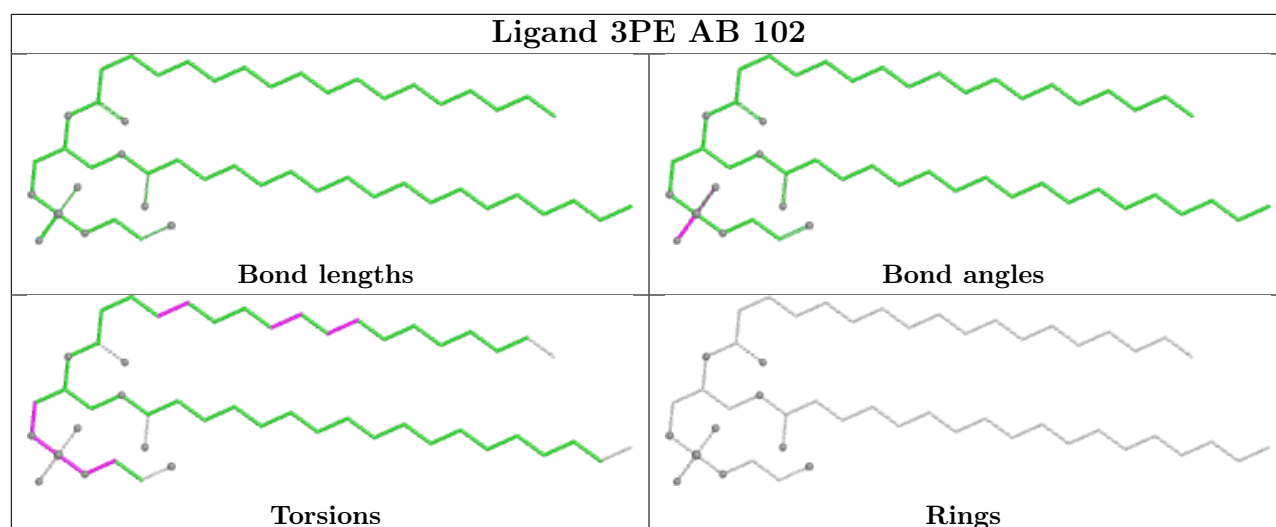


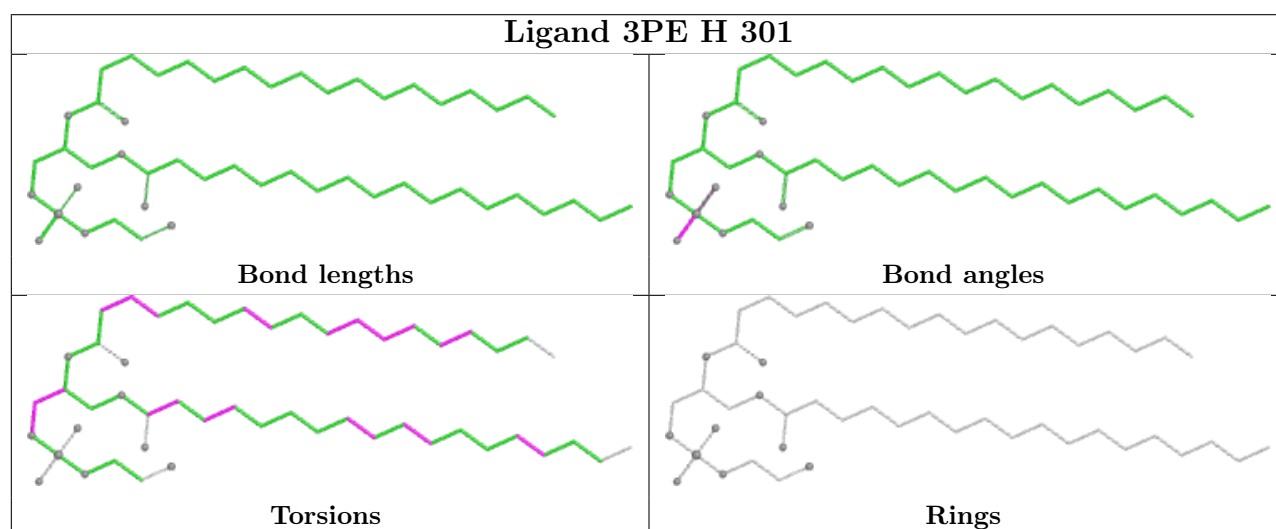
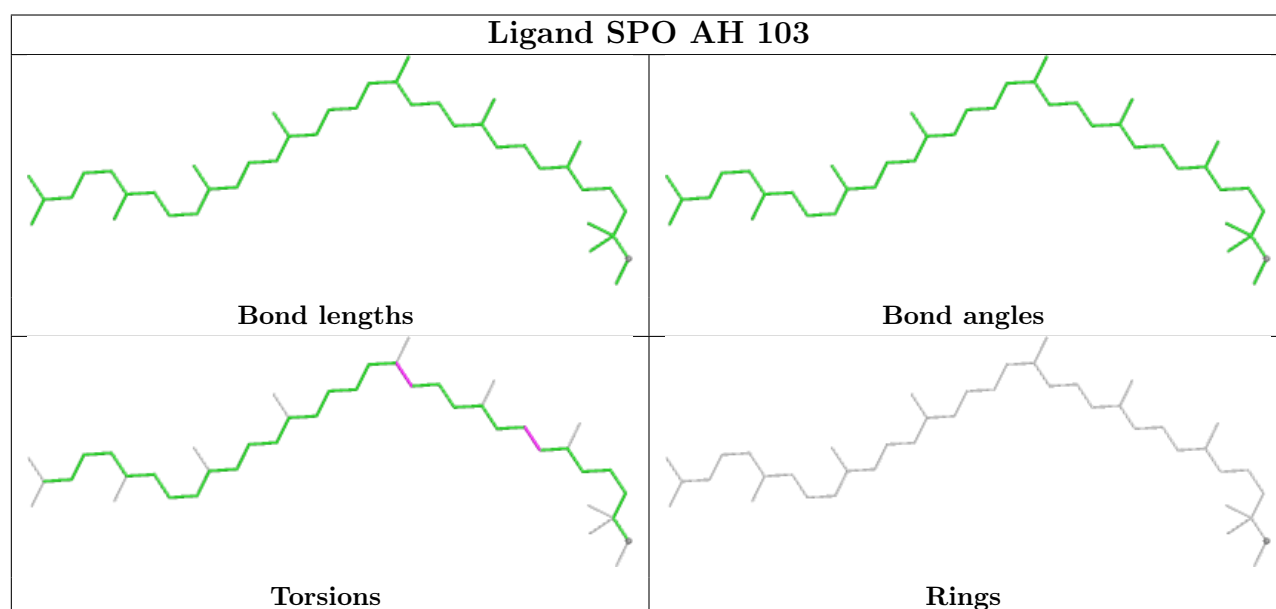
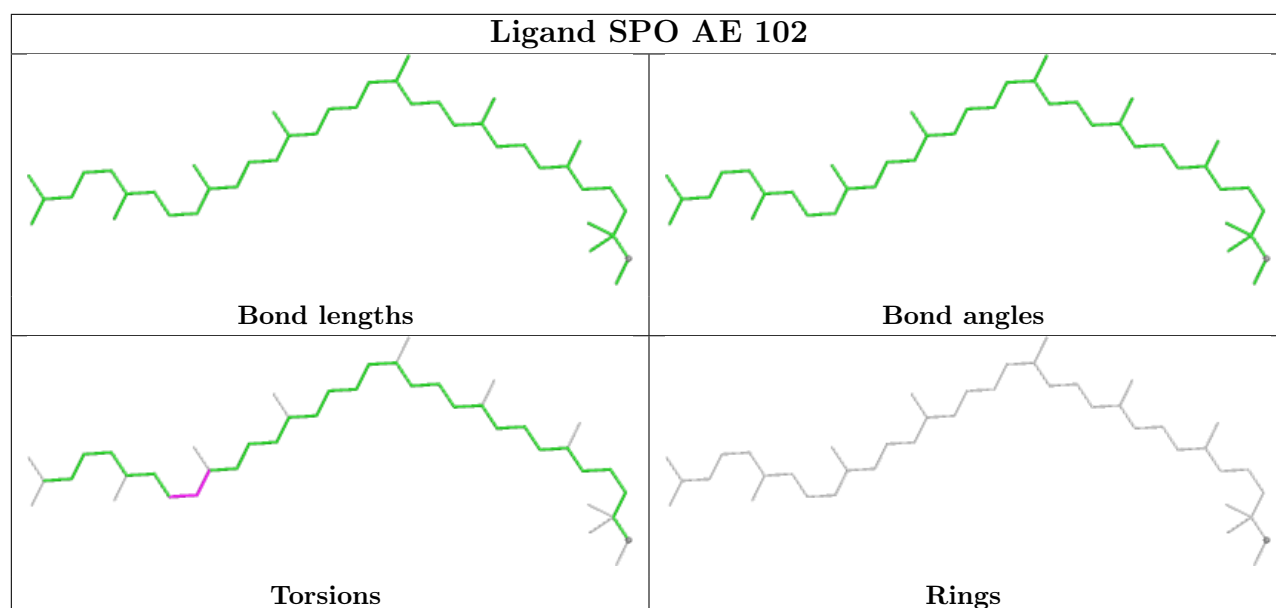


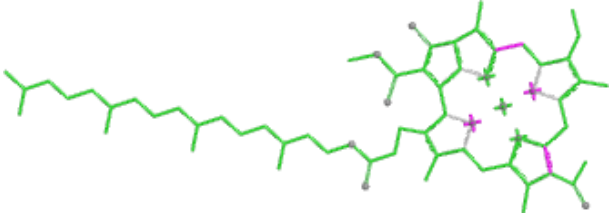
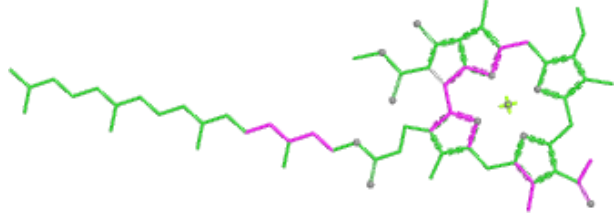
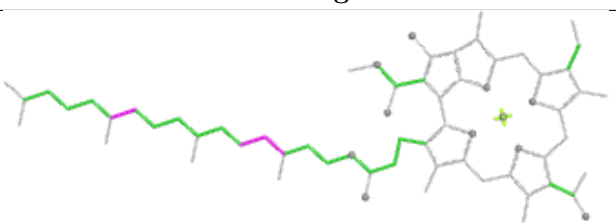
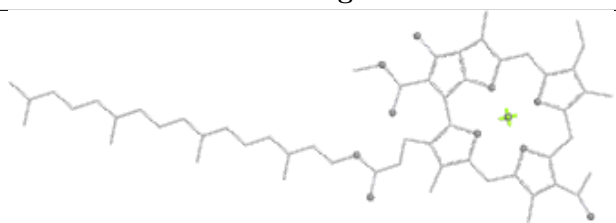
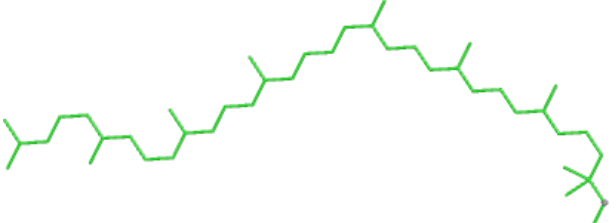
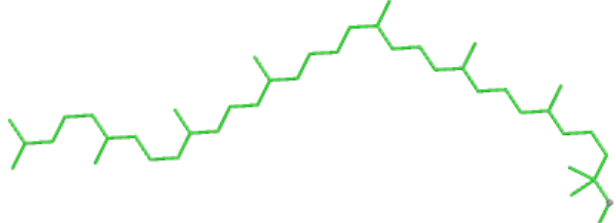
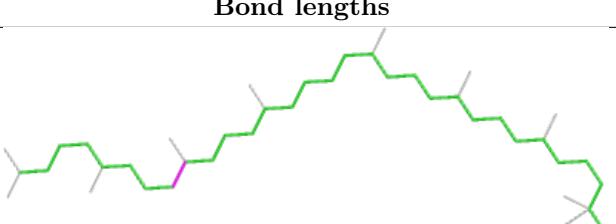
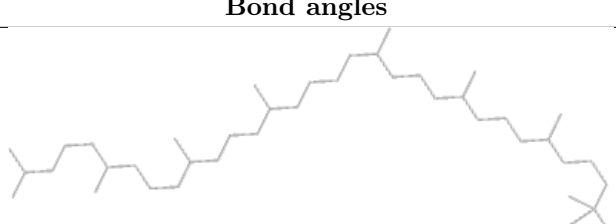
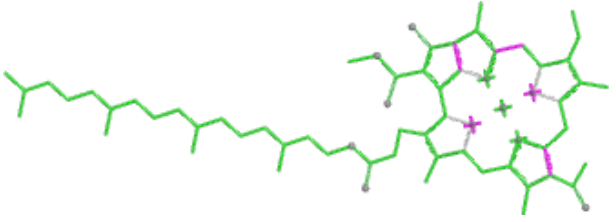
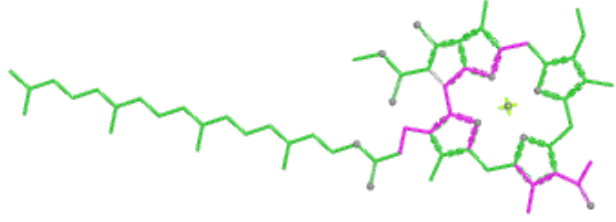
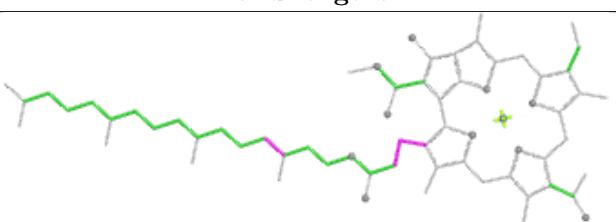
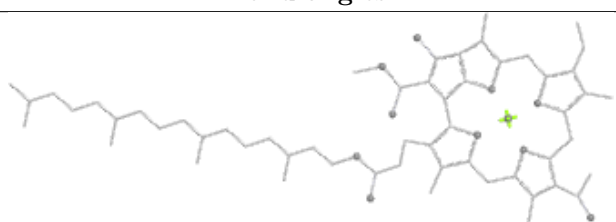


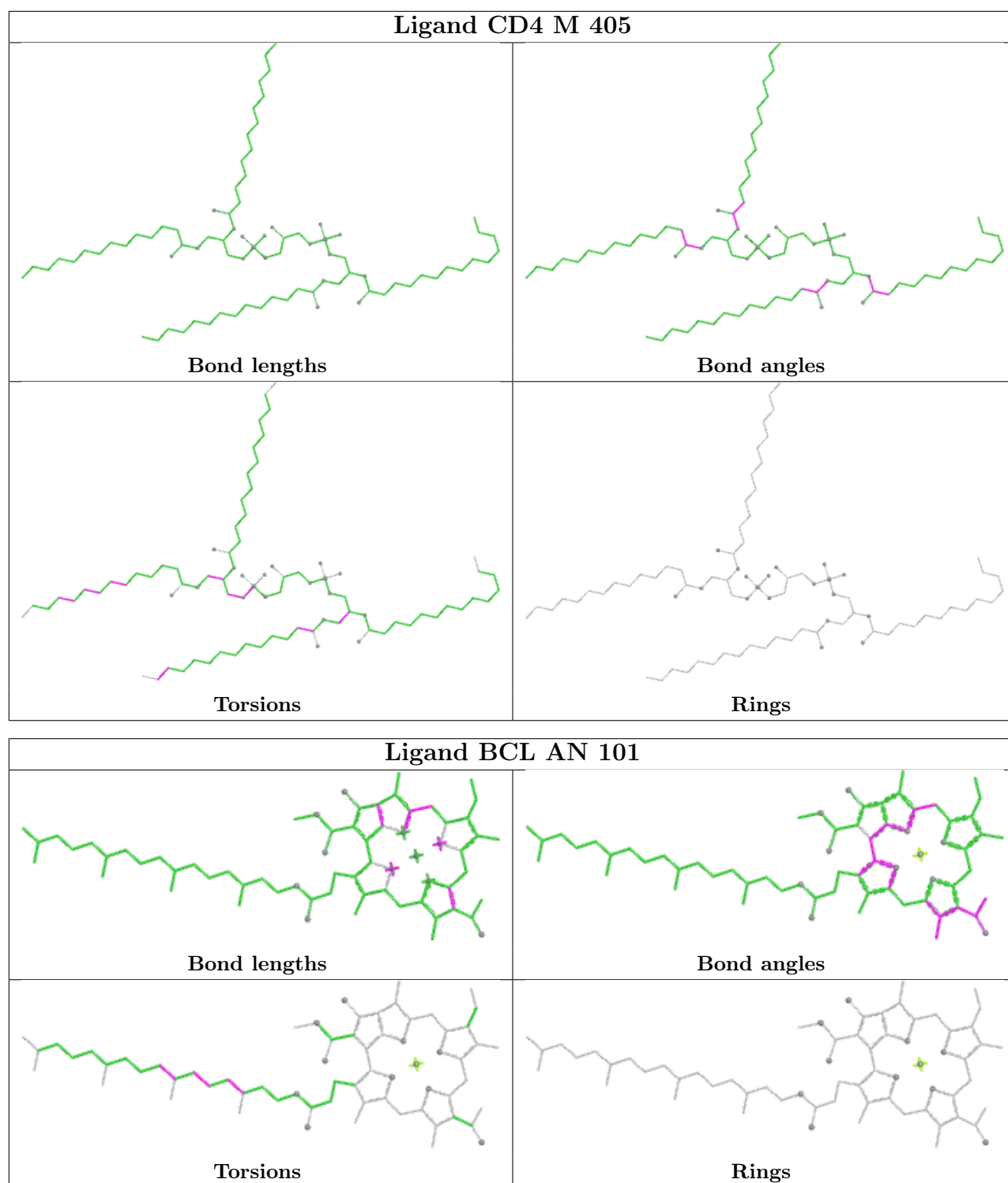


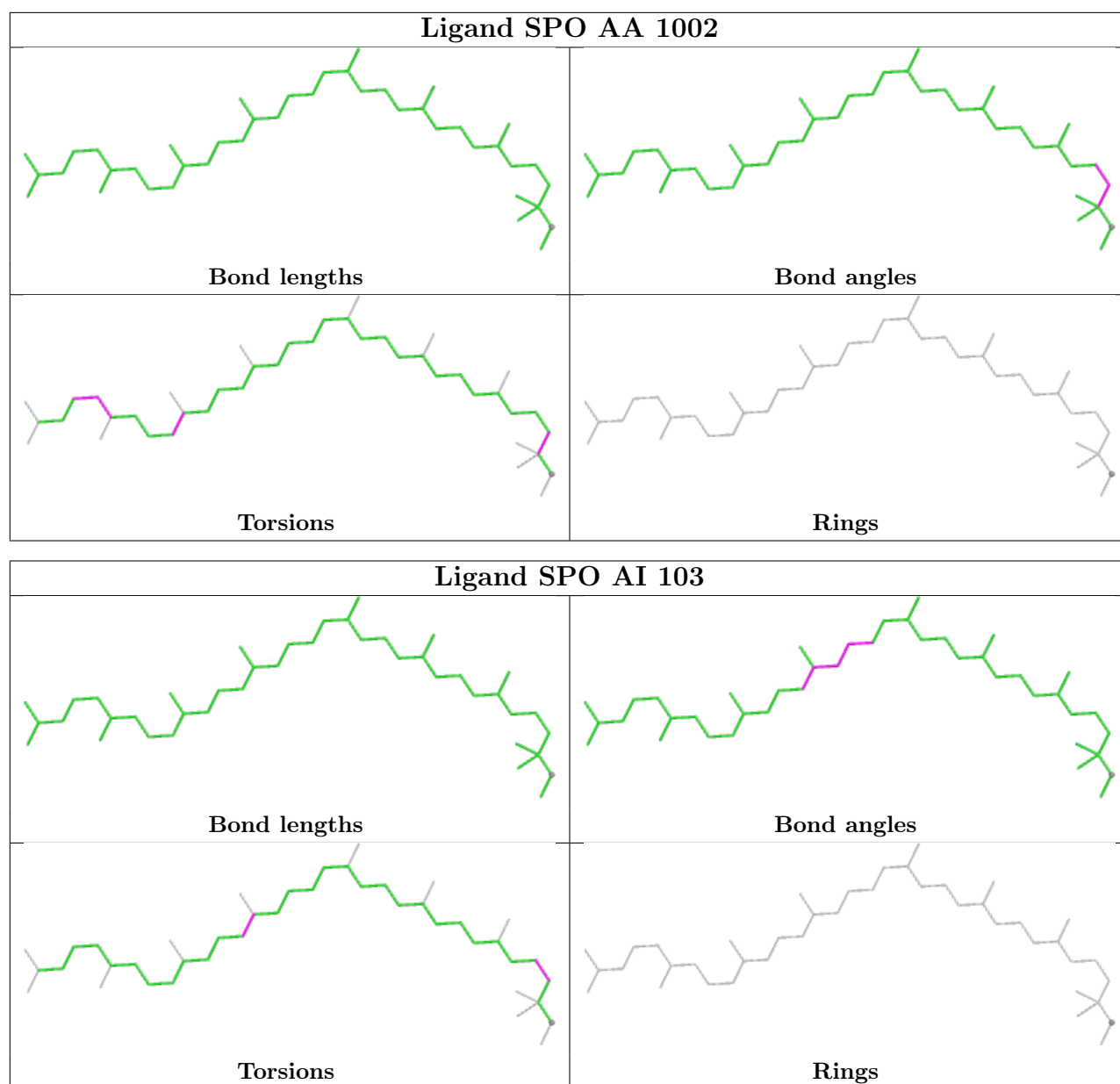


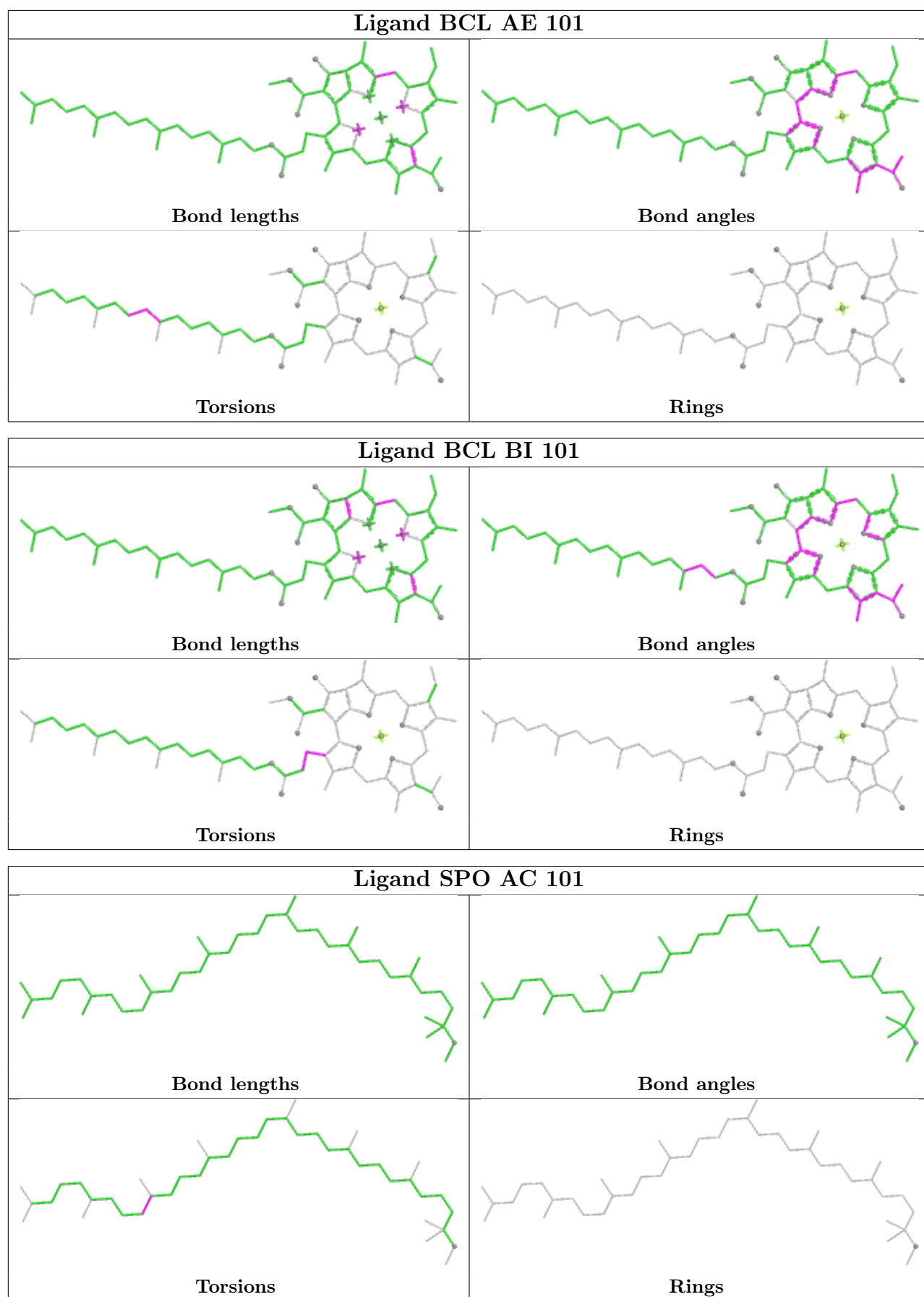


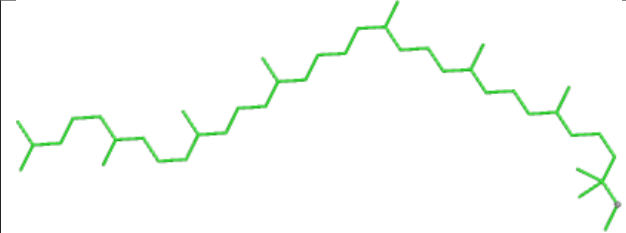
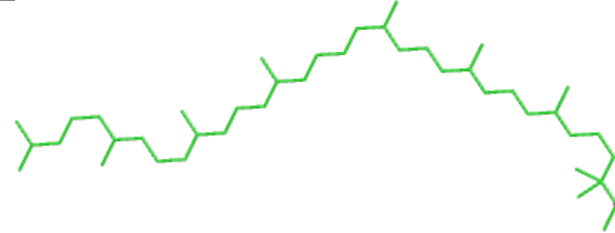
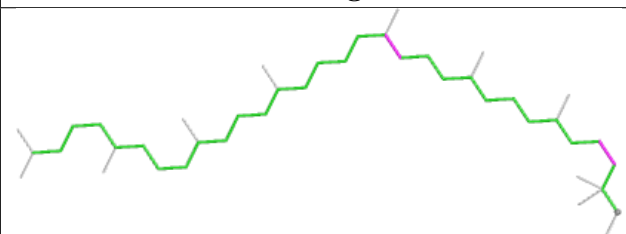
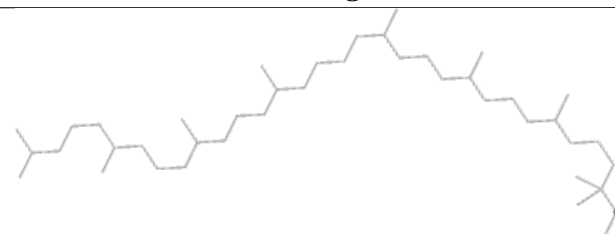
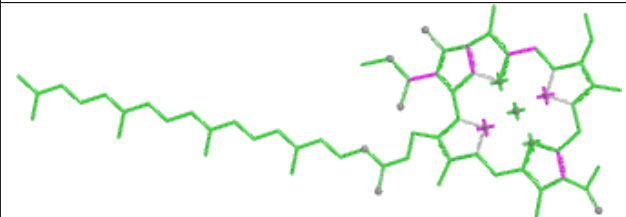
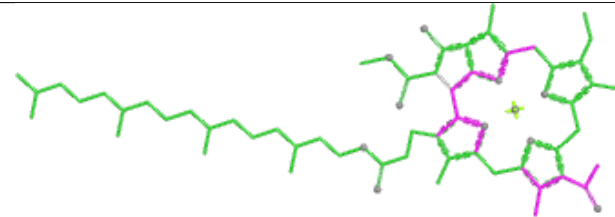
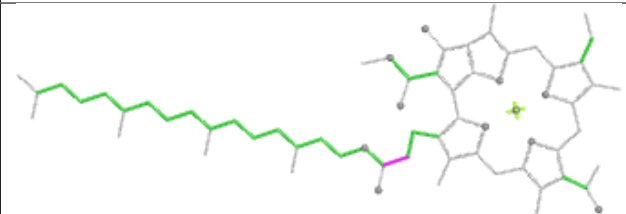
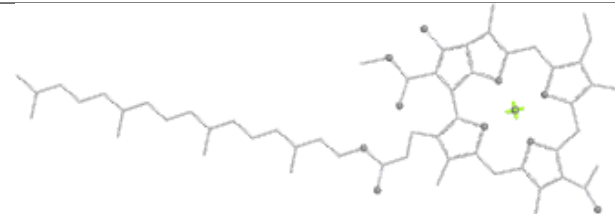


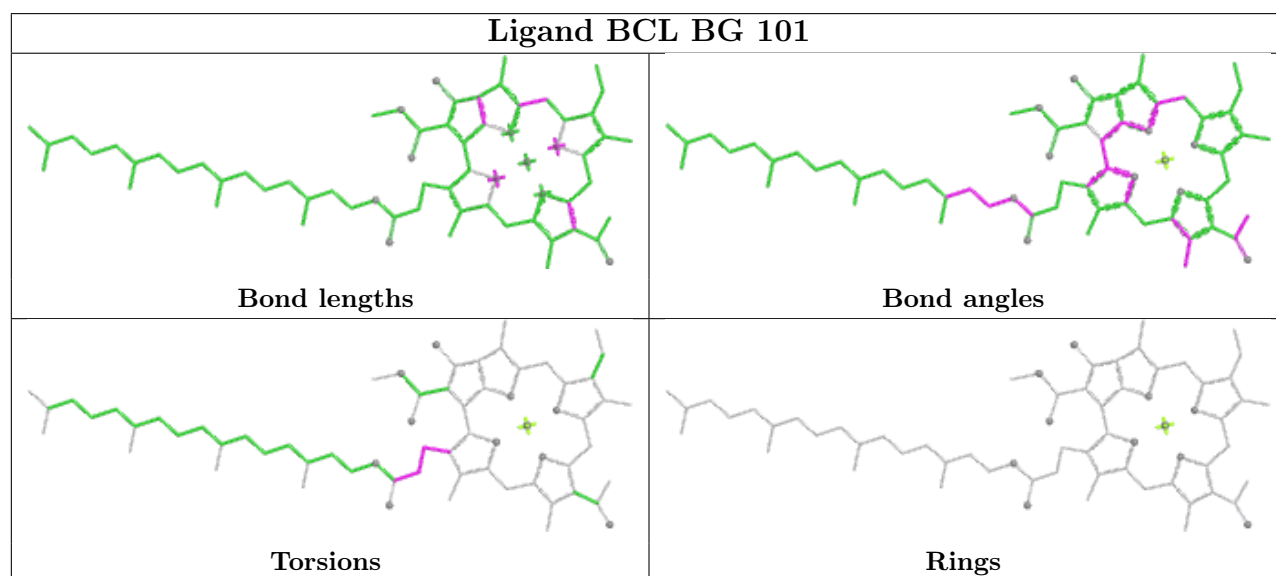
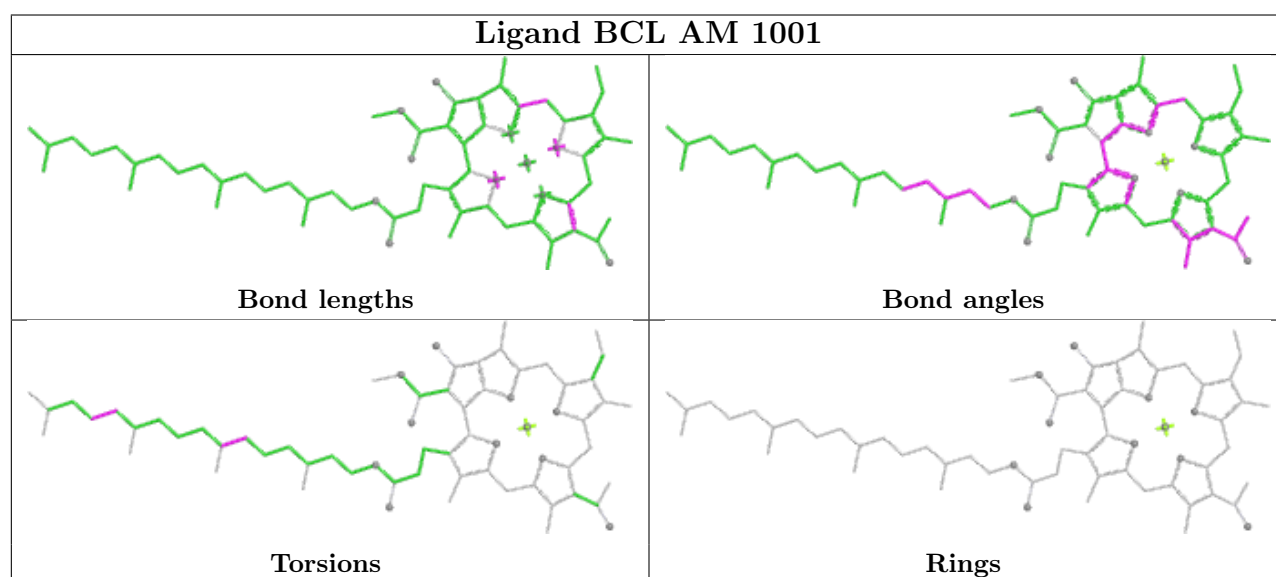
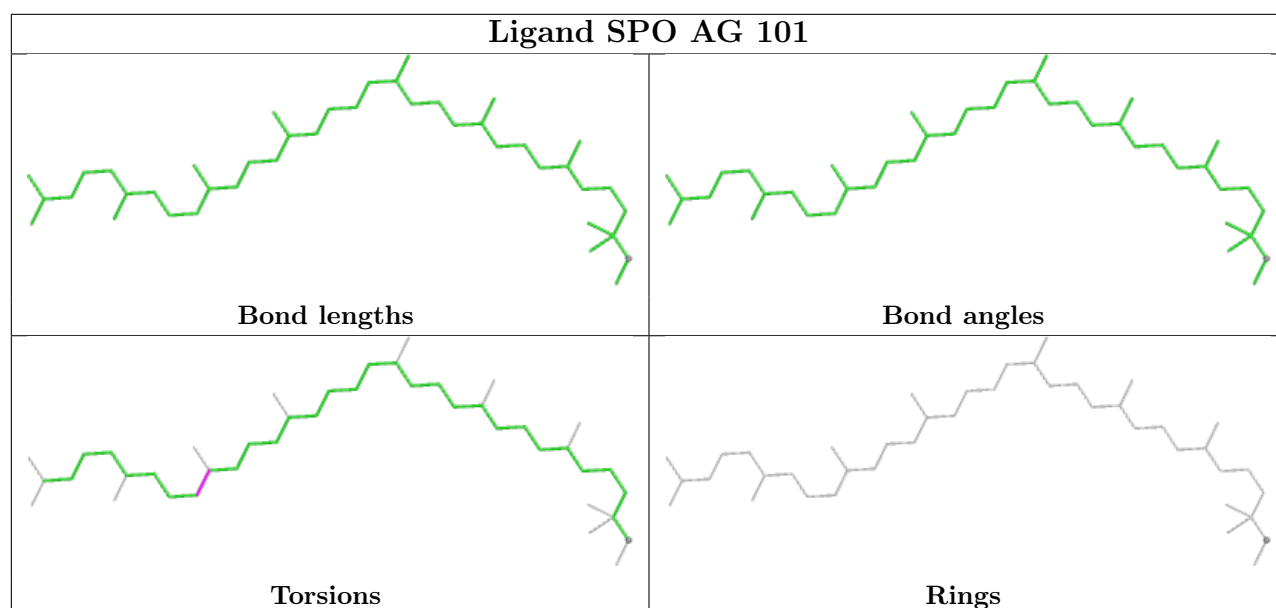
Ligand BCL AD 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO AH 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL AE 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

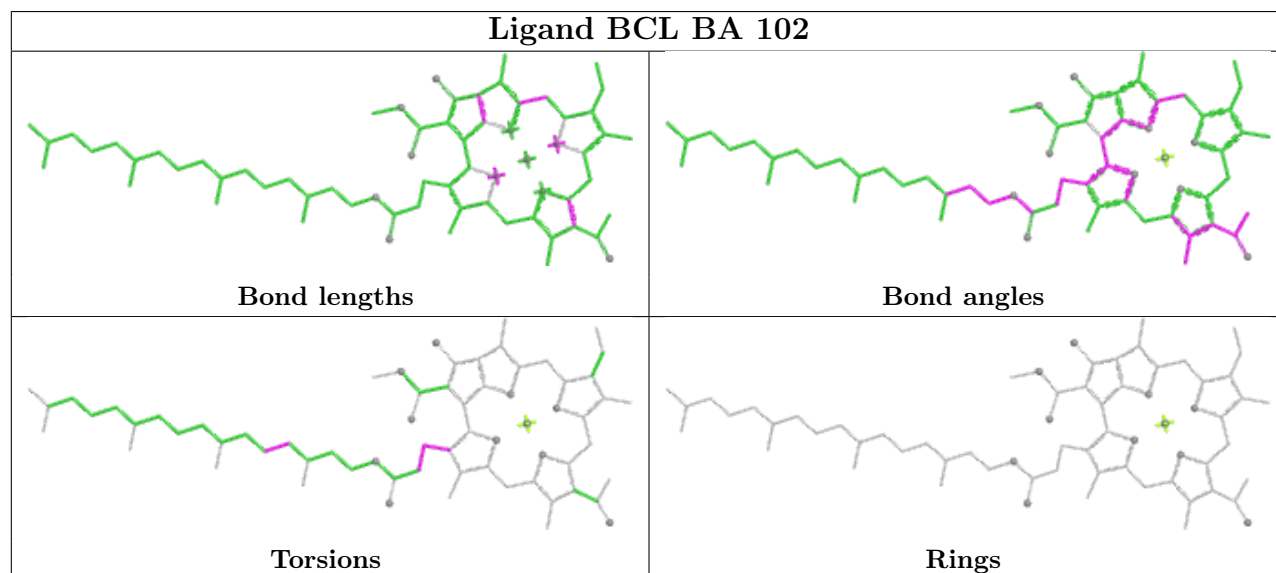
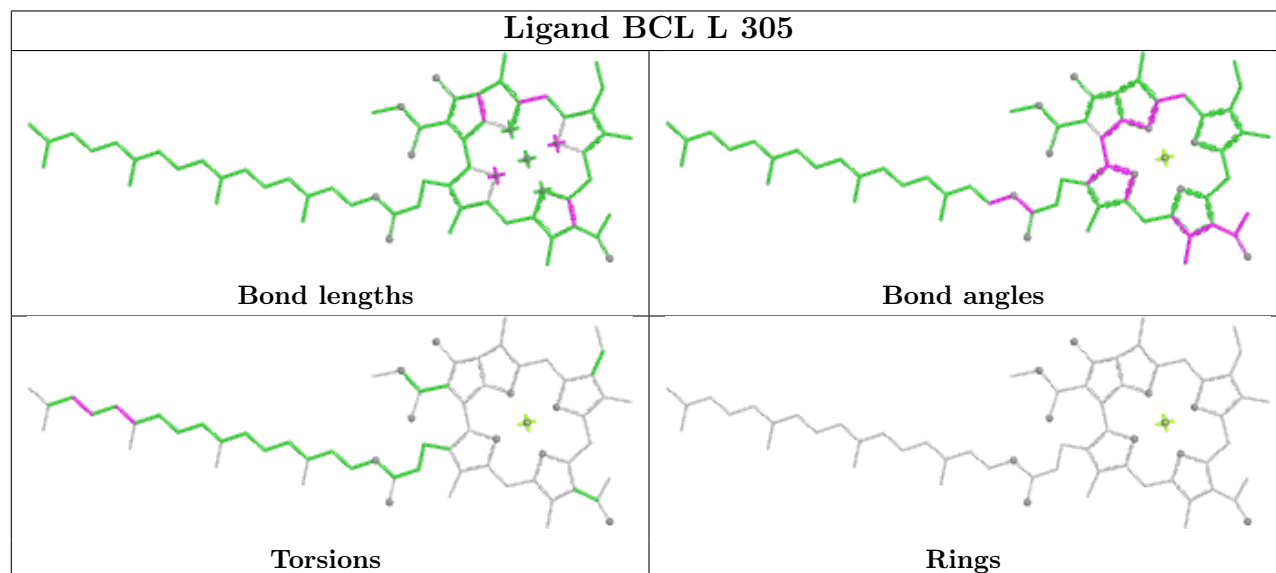
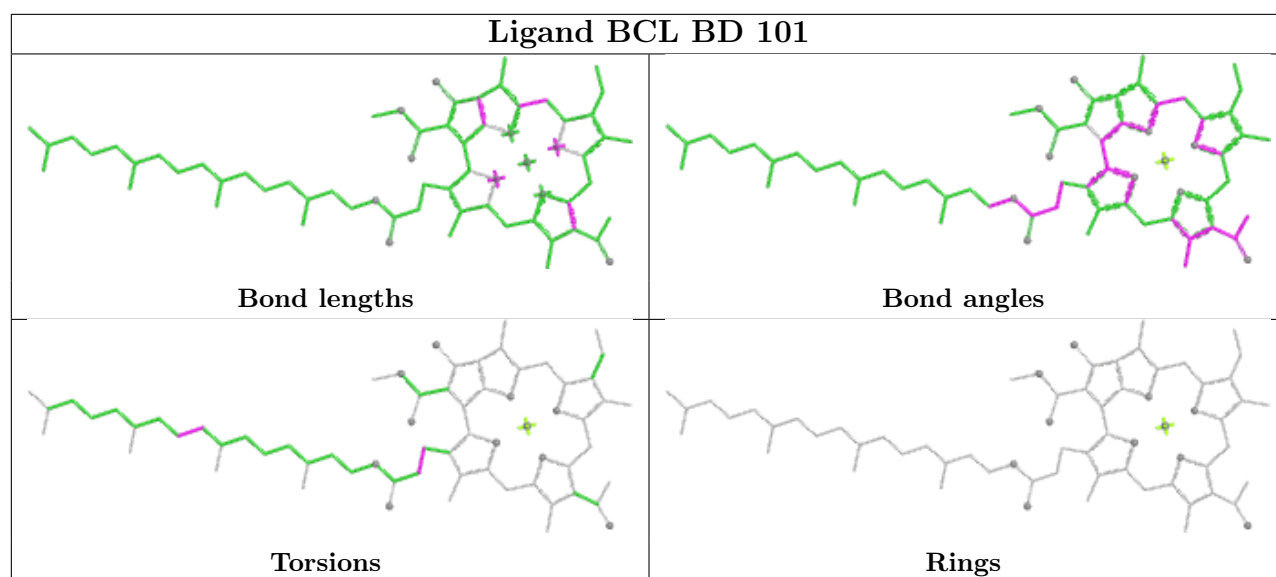


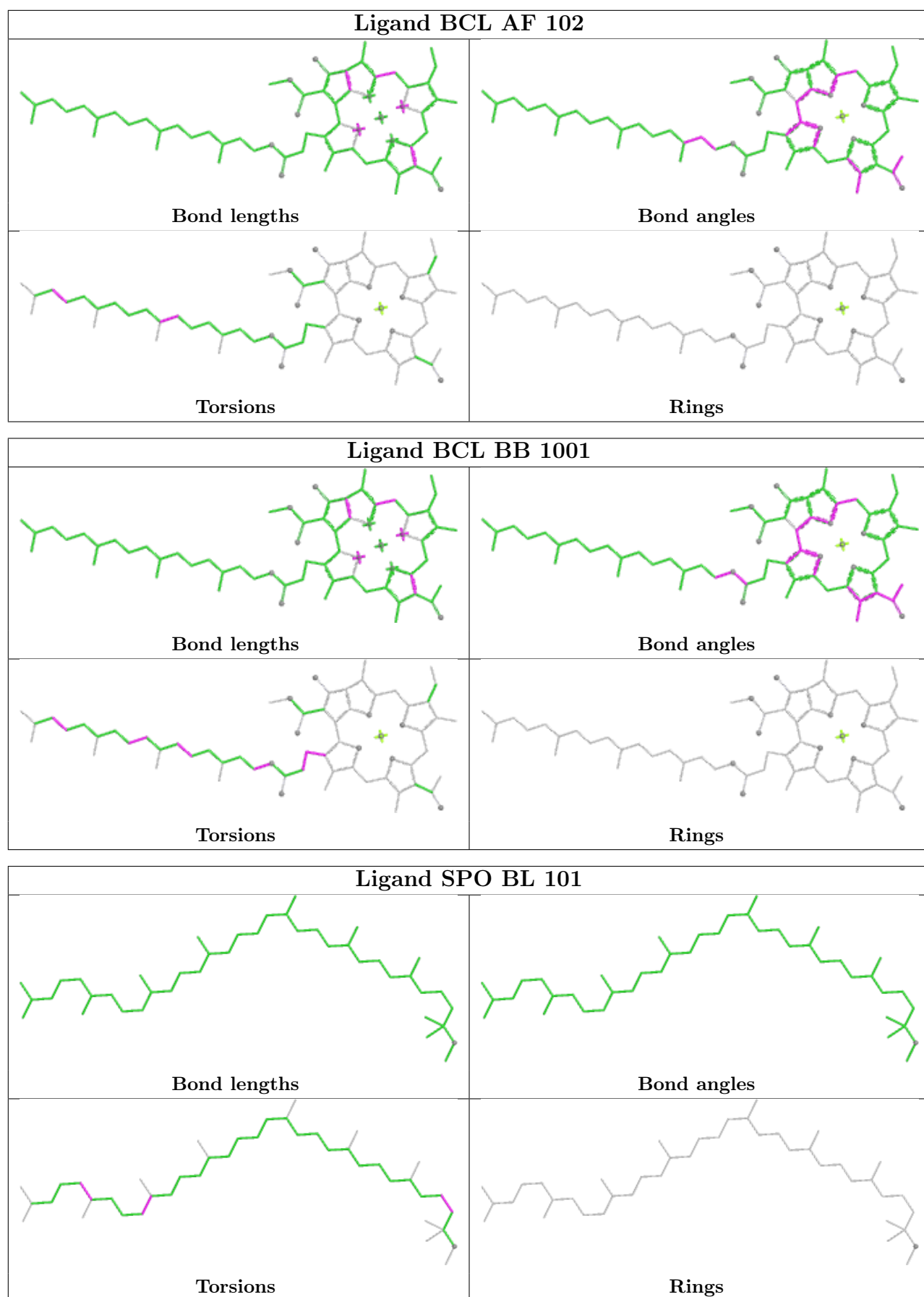


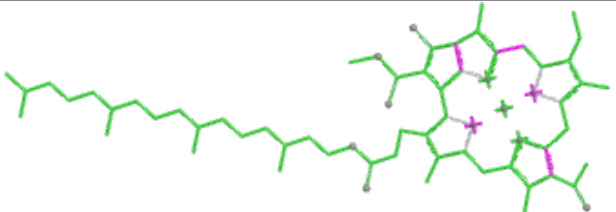
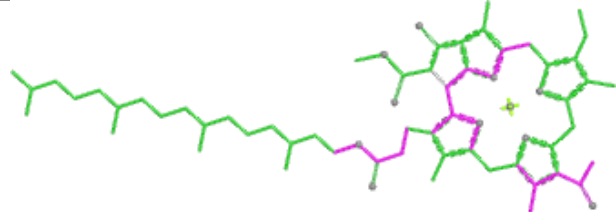
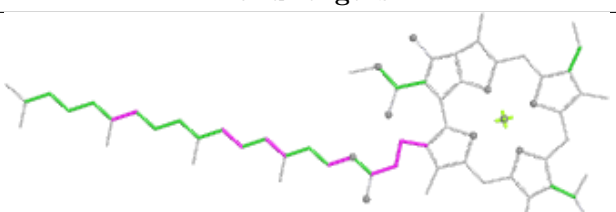
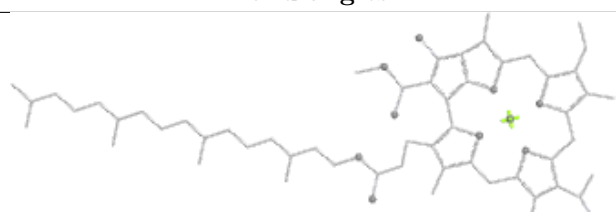


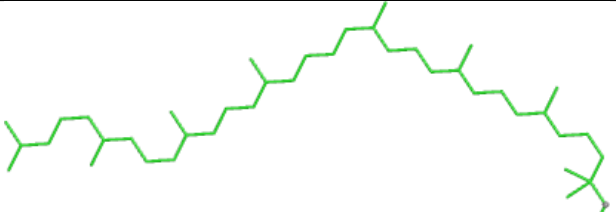
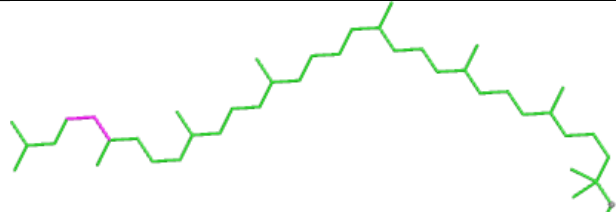
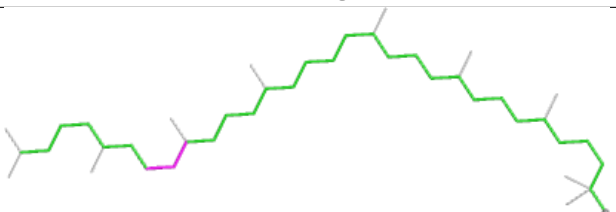
Ligand SPO M 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL M 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

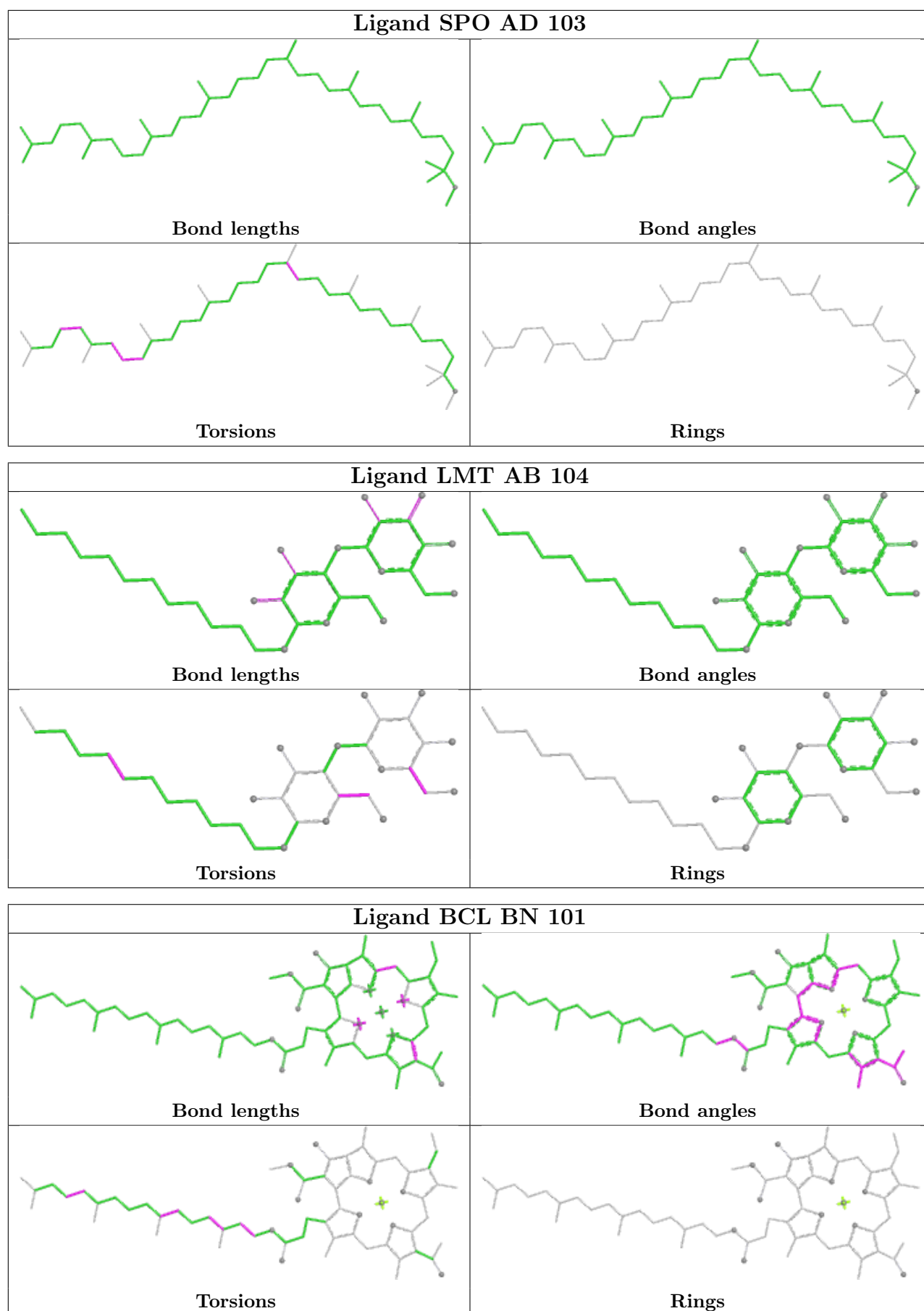


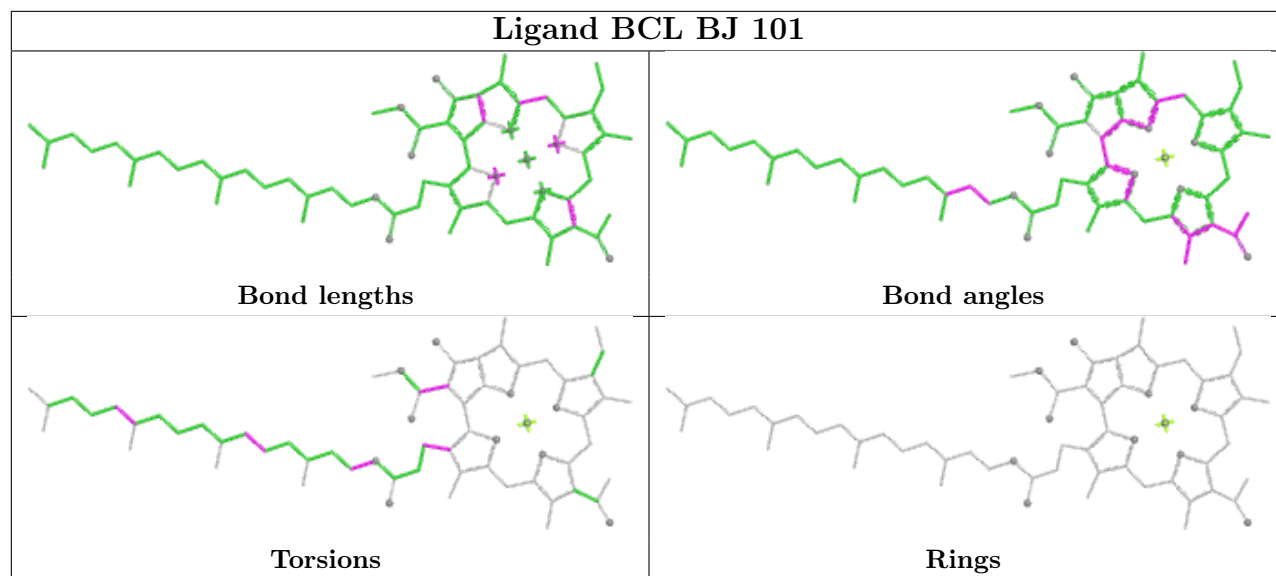




Ligand BCL BL 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SPO BA 101	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

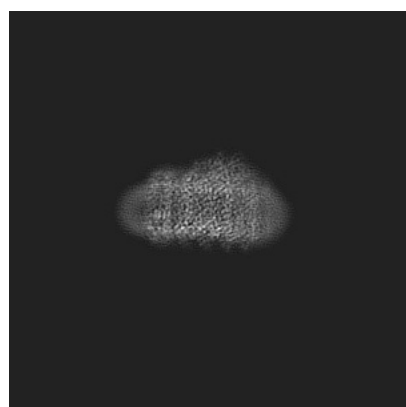
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13441. These allow visual inspection of the internal detail of the map and identification of artifacts.

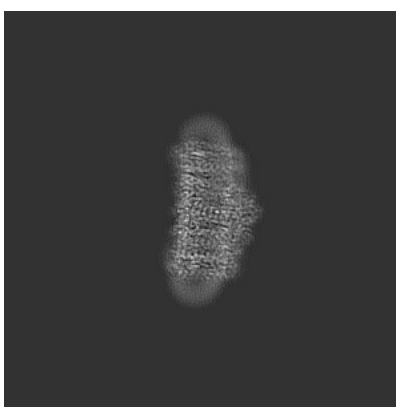
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

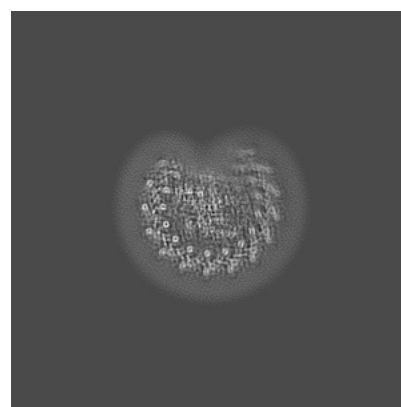
6.1.1 Primary map



X



Y

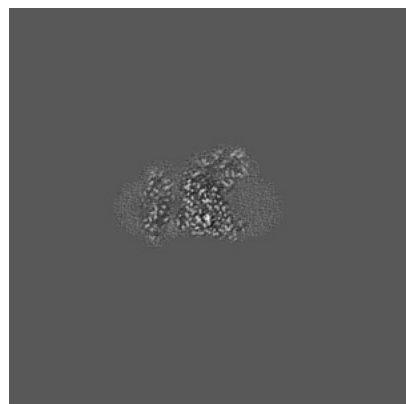


Z

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

6.2 Central slices [i](#)

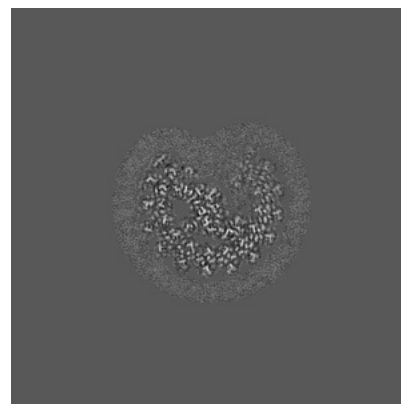
6.2.1 Primary map



X Index: 256



Y Index: 256

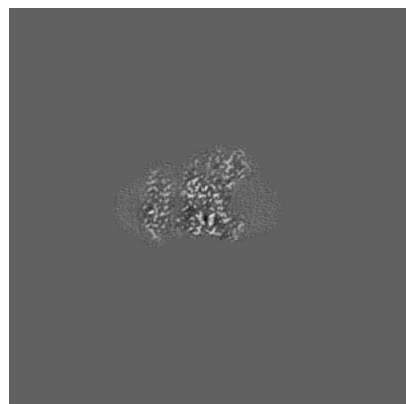


Z Index: 256

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

6.3 Largest variance slices [i](#)

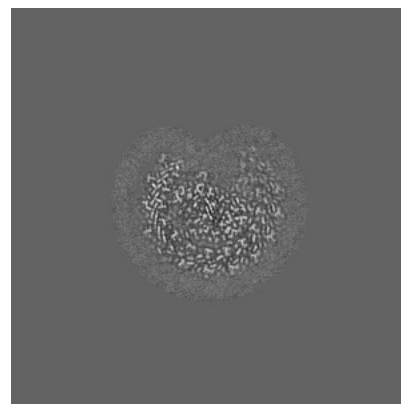
6.3.1 Primary map



X Index: 254



Y Index: 279

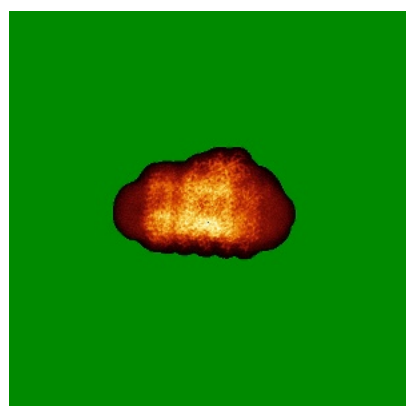


Z Index: 240

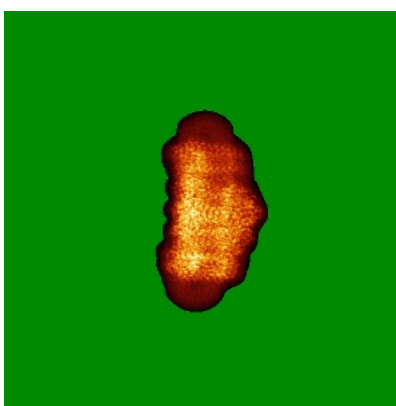
The images above show the largest variance slices of the map in three orthogonal directions.

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

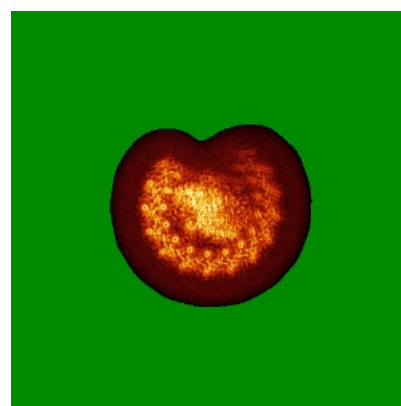
6.4.1 Primary map



X



Y

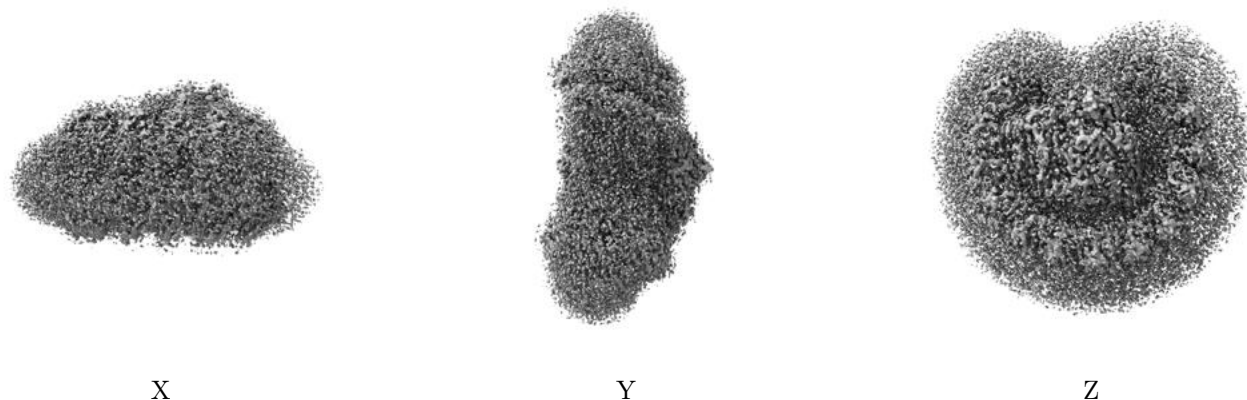


Z

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 0.0187. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

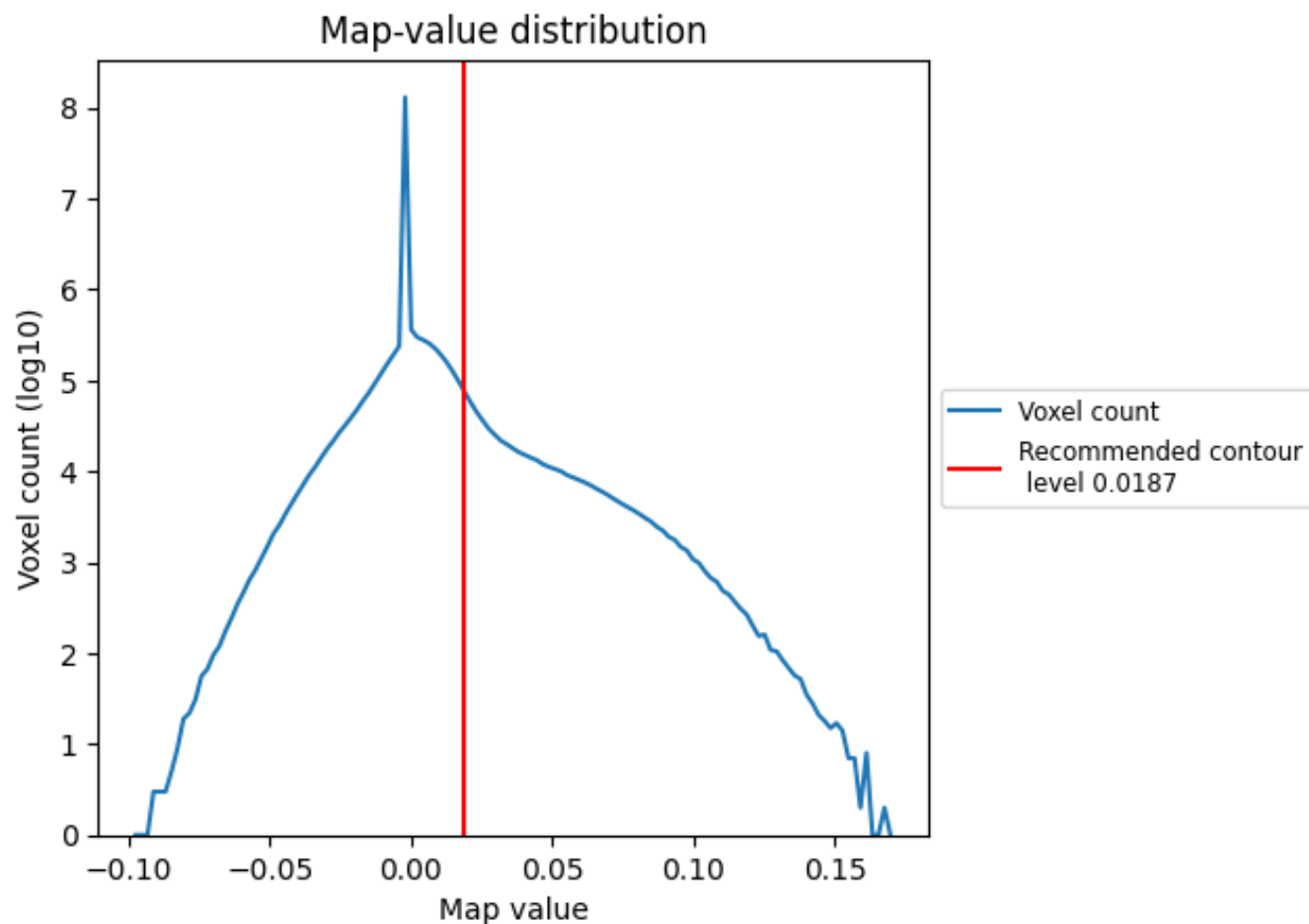
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

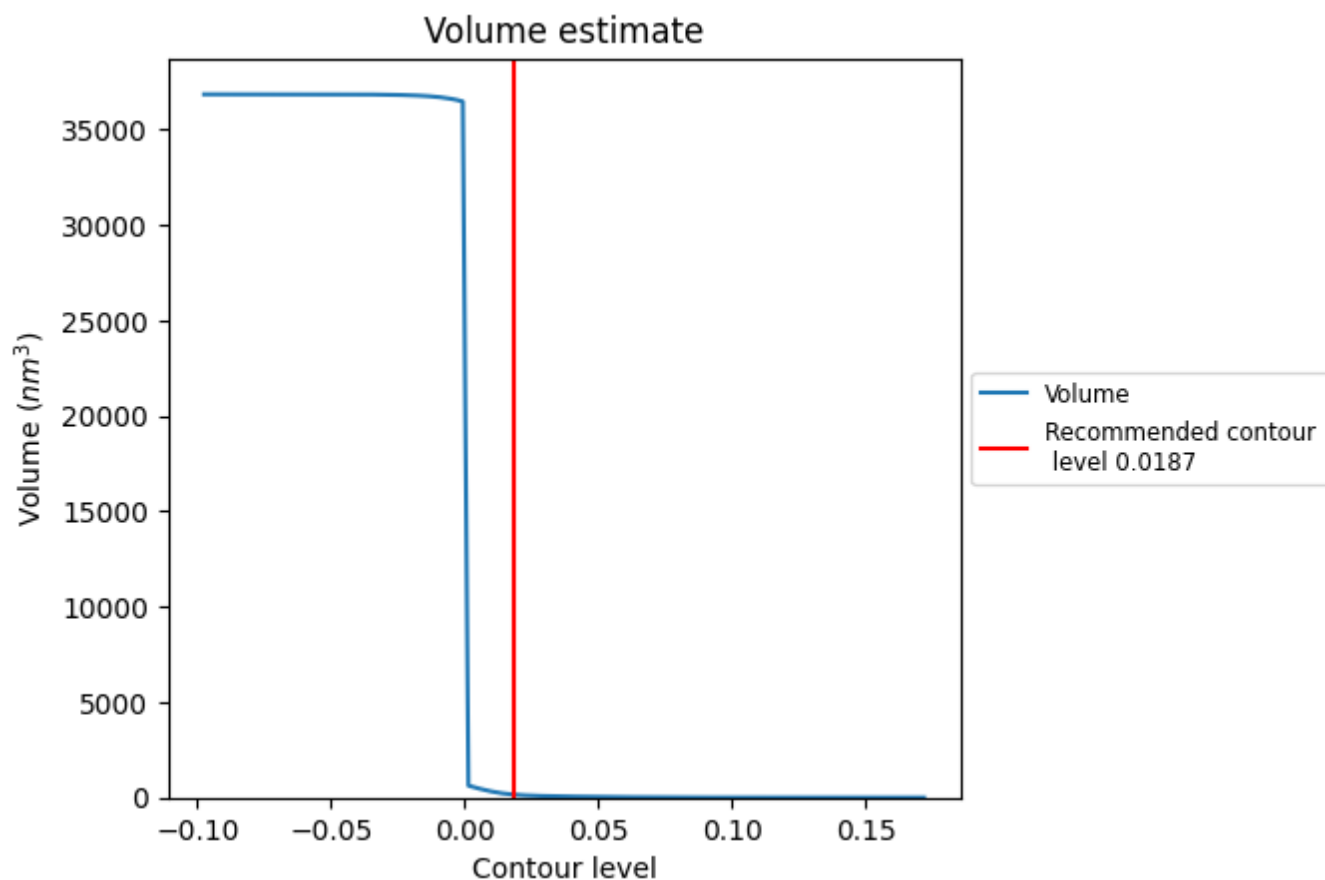
This section contains the results of statistical analysis of the map.

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.

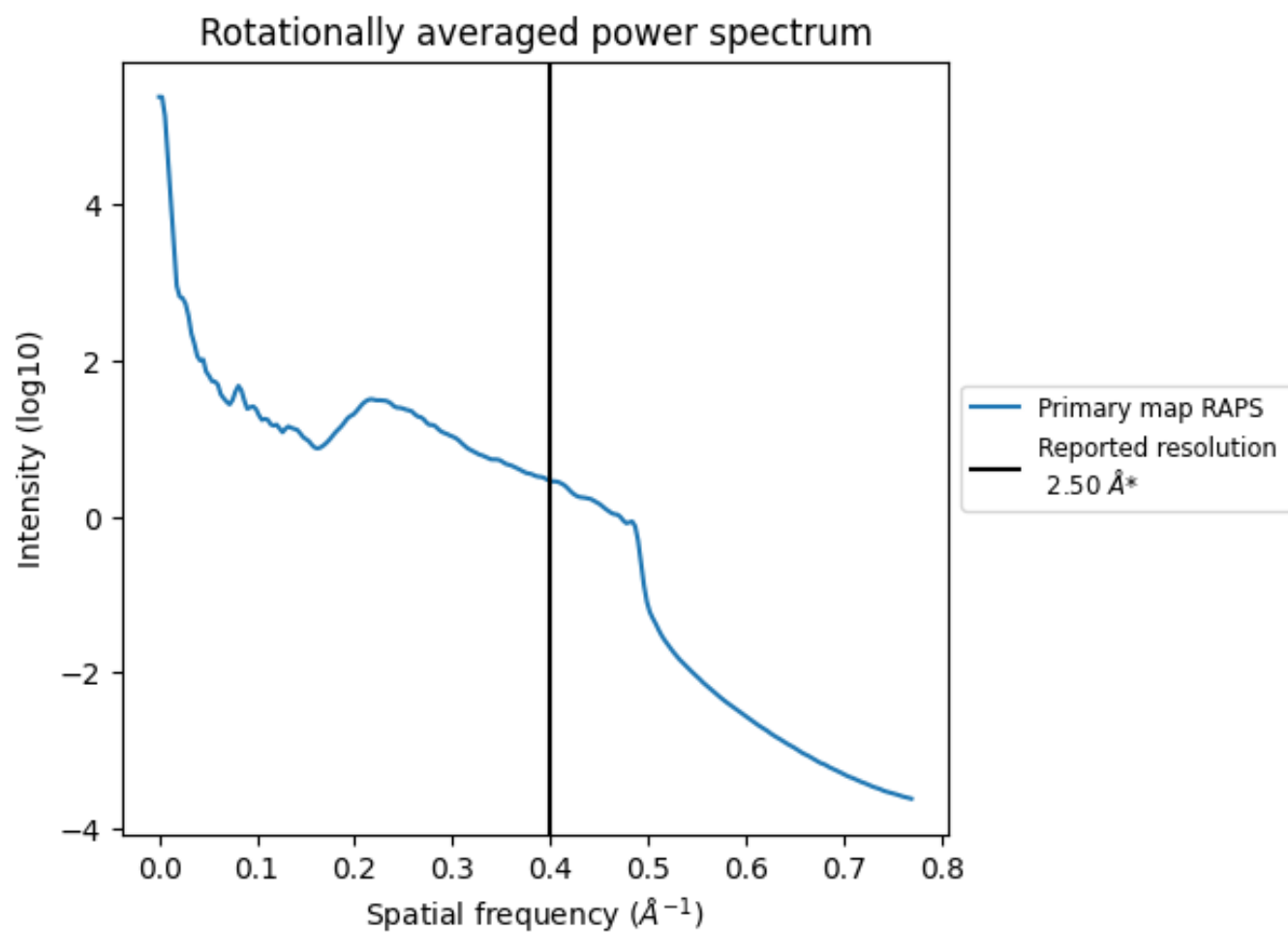
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 151 nm³; this corresponds to an approximate mass of 136 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 ⓘ

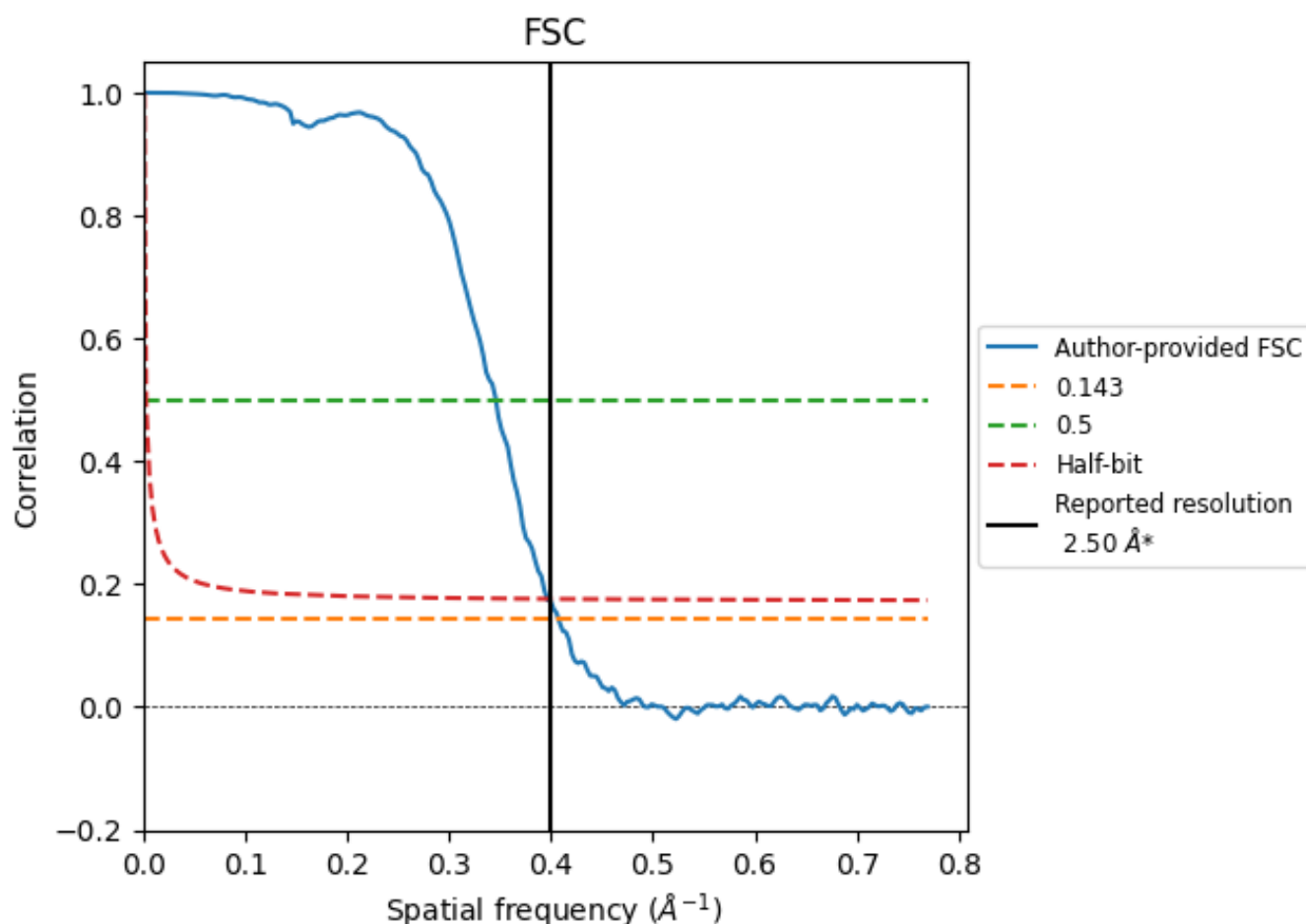


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

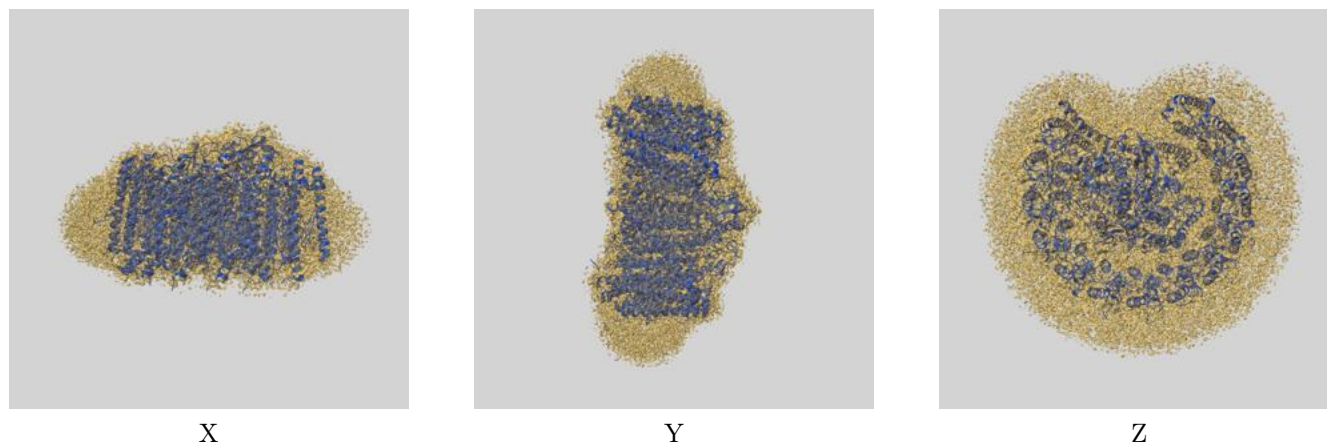
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.45	2.89	2.52
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

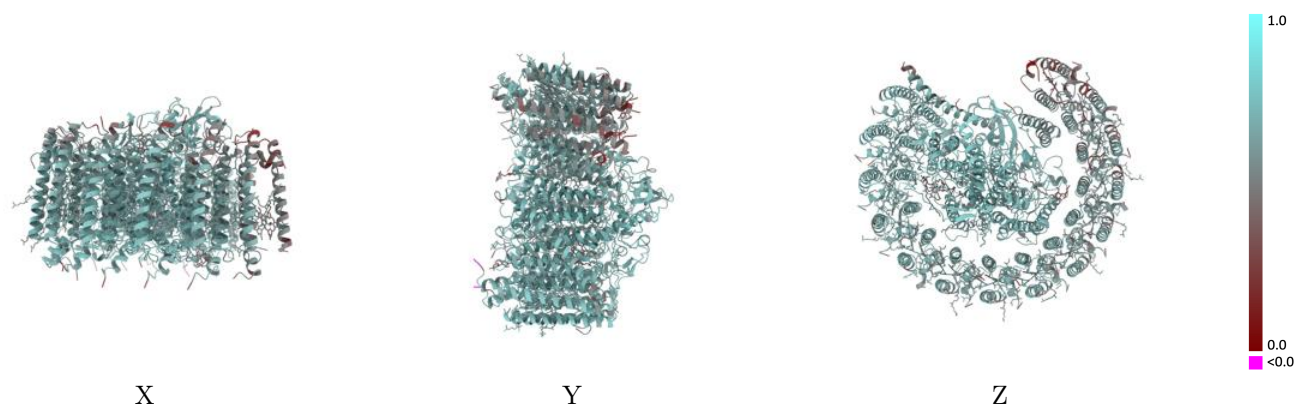
This section contains information regarding the fit between EMDB map EMD-13441 and PDB model 7PIL. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



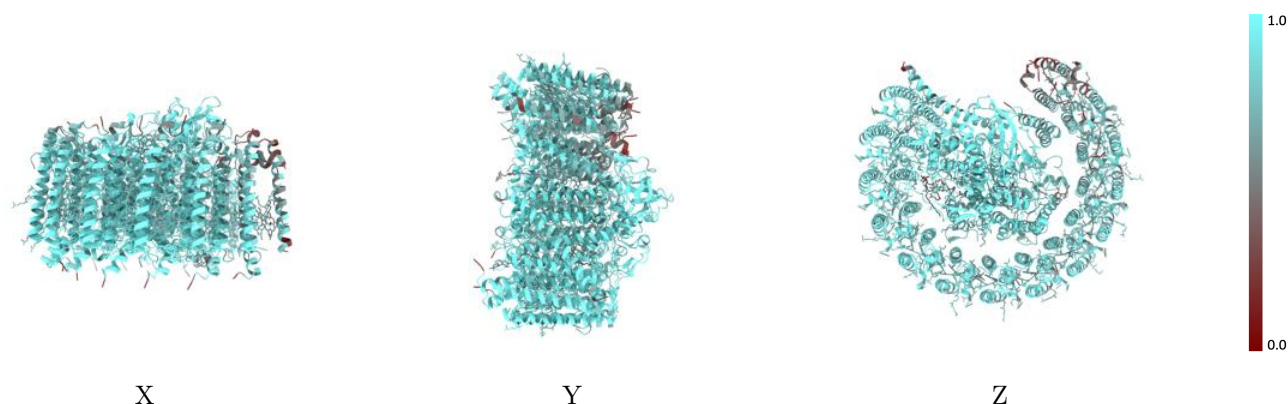
The images above show the 3D surface view of the map at the recommended contour level 0.0187 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



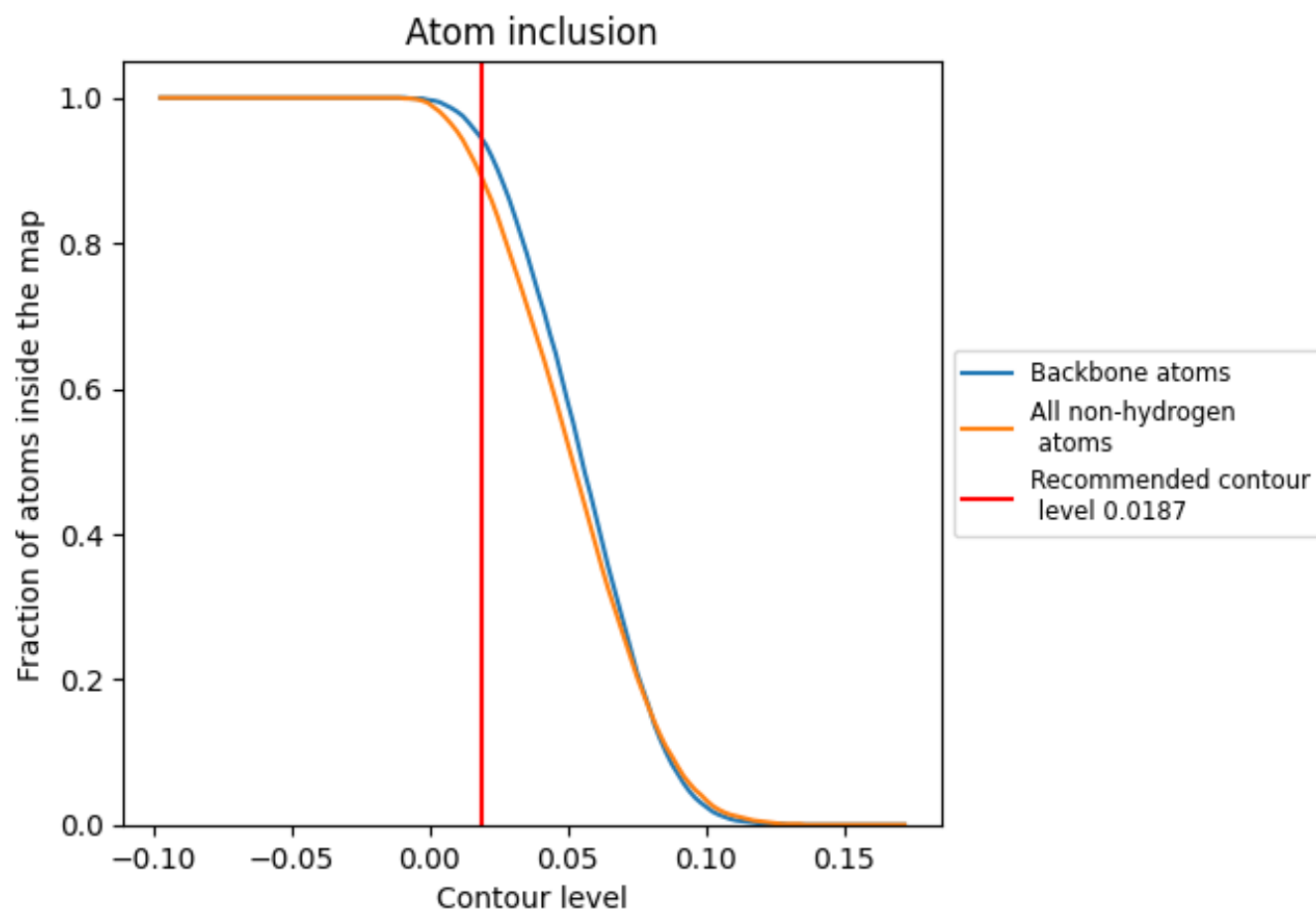
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0187).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.0187) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.6400
AA	 0.9020	 0.6480
AB	 0.8900	 0.6350
AC	 0.8960	 0.6520
AD	 0.9310	 0.6620
AE	 0.9350	 0.6610
AF	 0.9230	 0.6490
AG	 0.9110	 0.6440
AH	 0.9040	 0.6410
AI	 0.8710	 0.6270
AJ	 0.8930	 0.6250
AK	 0.8680	 0.6100
AL	 0.8480	 0.5940
AM	 0.7610	 0.5700
AN	 0.6710	 0.4990
BA	 0.8970	 0.6450
BB	 0.9260	 0.6680
BC	 0.9200	 0.6660
BD	 0.9140	 0.6490
BE	 0.9330	 0.6400
BF	 0.8770	 0.6160
BG	 0.8920	 0.6240
BH	 0.8790	 0.6230
BI	 0.8620	 0.5950
BJ	 0.8450	 0.5890
BK	 0.8340	 0.5740
BL	 0.7810	 0.5550
BM	 0.7040	 0.4850
BN	 0.5460	 0.4280
H	 0.9390	 0.6620
L	 0.9760	 0.7140
M	 0.9530	 0.6990
UU	 0.8440	 0.5950
X	 0.8470	 0.6020

