



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 06:43 AM JST

PDB ID : 7E0J / pdb_00007e0j
EMDB ID : EMD-30934
Title : LHCII-1 in the state transition supercomplex PSI-LHCI-LHCII from the double phosphatase mutant pph1;pbcp of *Chlamydomonas reinhardtii*.
Authors : Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.
Deposited on : 2021-01-28
Resolution : 3.13 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

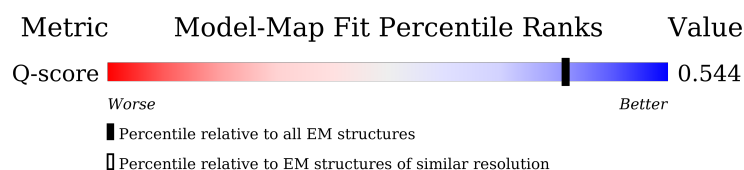
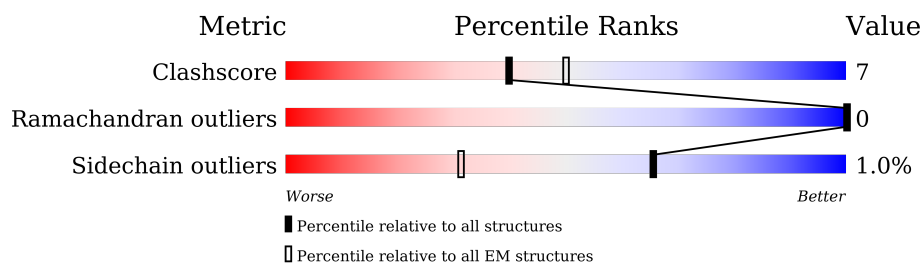
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 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	14478 (2.63 - 3.63)

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	X	249	
2	Y	257	
3	Z	256	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8140 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	220	Total	C	N	O	S	0	0
			1675	1088	273	309	5		

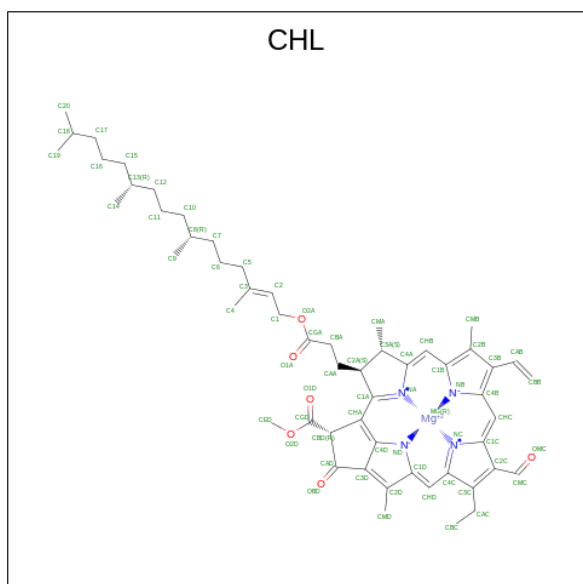
- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	220	Total	C	N	O	S	0	0
			1679	1086	273	315	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

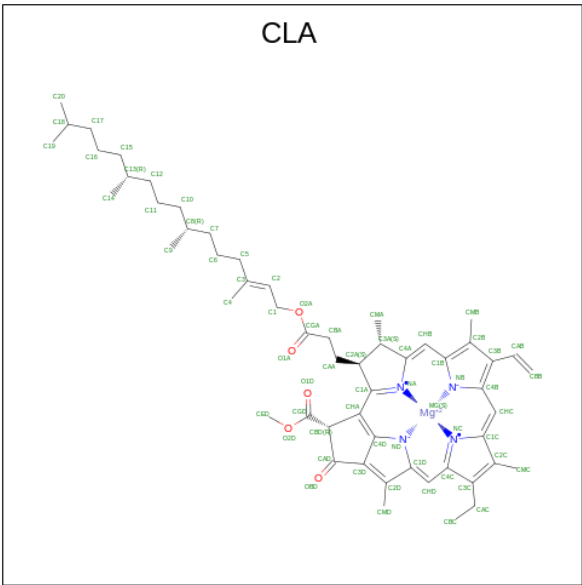
Mol	Chain	Residues	Atoms					AltConf	Trace	
3	Z	232	Total	C	N	O	P	S	0	0
			1780	1154	291	329	1	5		

- Molecule 4 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
4	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Y	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
4	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Z	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
4	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Z	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
4	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 5 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



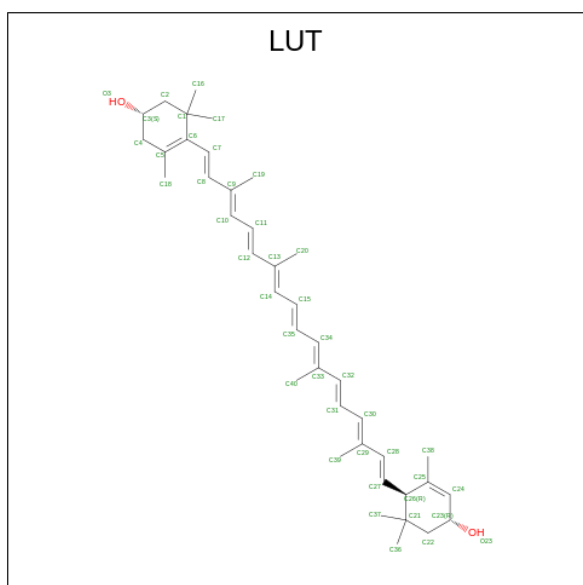
Mol	Chain	Residues	Atoms					AltConf
5	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	X	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
5	X	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
5	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	X	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
5	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
5	Y	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
5	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
5	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Y	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
5	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
5	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

- Molecule 6 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



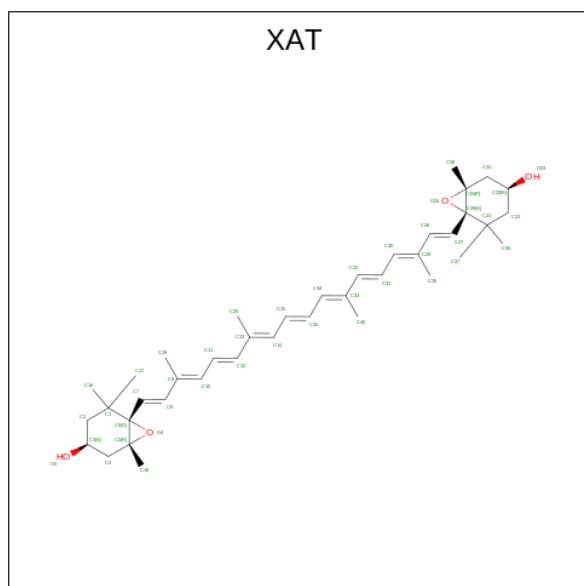
Mol	Chain	Residues	Atoms			AltConf
6	X	1	Total	C	O	0
			42	40	2	

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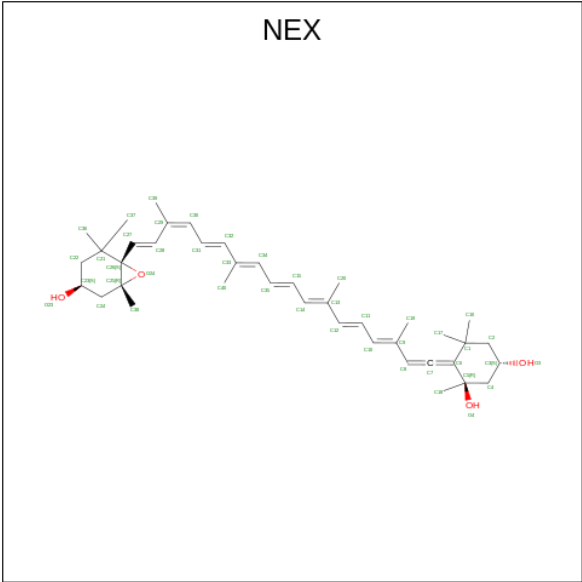
Mol	Chain	Residues	Atoms			AltConf
6	X	1	Total	C	O	0
			42	40	2	
6	Y	1	Total	C	O	0
			42	40	2	
6	Y	1	Total	C	O	0
			42	40	2	
6	Z	1	Total	C	O	0
			42	40	2	
6	Z	1	Total	C	O	0
			42	40	2	

- Molecule 7 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



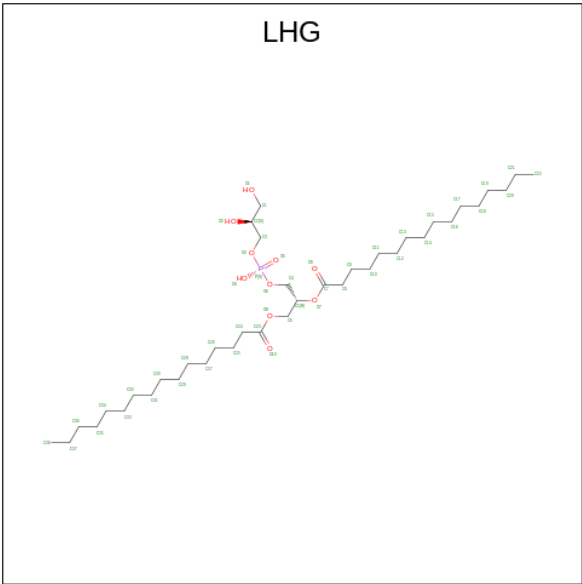
Mol	Chain	Residues	Atoms			AltConf
7	X	1	Total	C	O	0
			44	40	4	
7	Y	1	Total	C	O	0
			44	40	4	
7	Z	1	Total	C	O	0
			44	40	4	

- Molecule 8 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
8	X	1	Total	C	O	0
			44	40	4	
8	Y	1	Total	C	O	0
			43	40	3	
8	Z	1	Total	C	O	0
			44	40	4	

- Molecule 9 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).

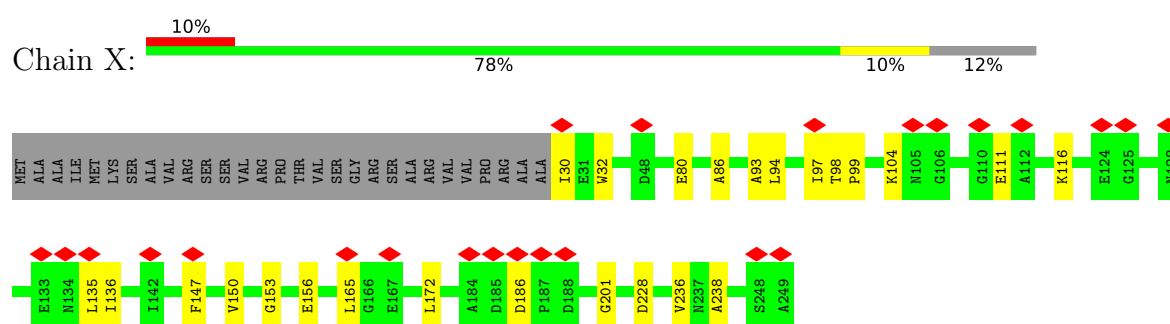


Mol	Chain	Residues	Atoms				AltConf
9	X	1	Total 49	C 38	O 10	P 1	0
9	Y	1	Total 49	C 38	O 10	P 1	0
9	Z	1	Total 49	C 38	O 10	P 1	0

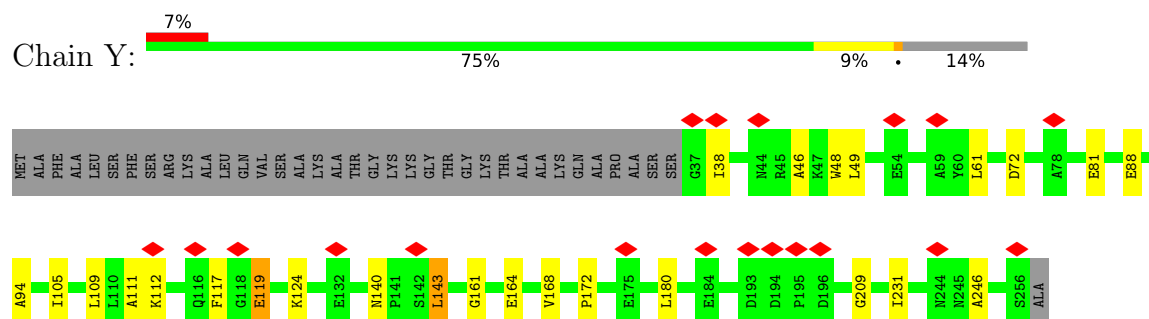
3 Residue-property plots

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.

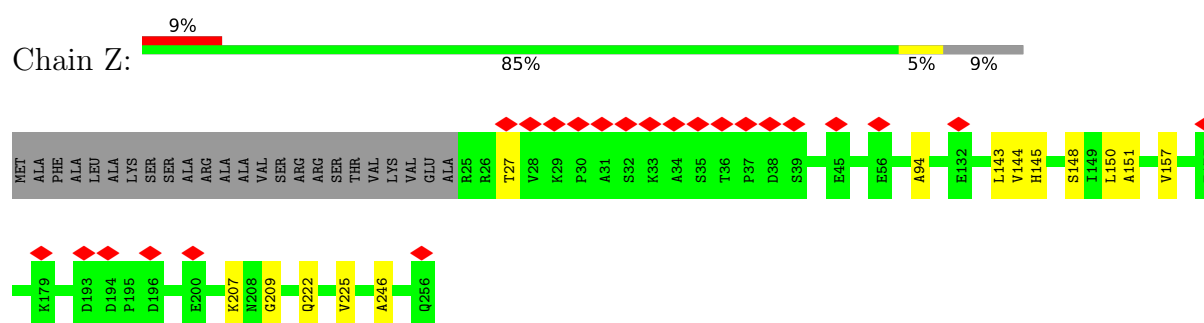
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5625	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, CLA, XAT, NEX, TPO, CHL, LUT

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	X	0.23	0/1725	0.47	0/2348
2	Y	0.29	0/1727	0.48	0/2350
3	Z	0.13	0/1822	0.31	0/2474
All	All	0.22	0/5274	0.43	0/7172

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	1675	0	1617	26	0
2	Y	1679	0	1620	30	0
3	Z	1780	0	1723	11	0
4	X	310	0	311	13	0
4	Y	335	0	302	15	0
4	Z	338	0	309	14	0
5	X	436	0	415	6	0
5	Y	429	0	389	5	0
5	Z	496	0	520	2	0
6	X	84	0	112	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Y	84	0	112	3	0
6	Z	84	0	112	5	0
7	X	44	0	56	3	0
7	Y	44	0	56	3	0
7	Z	44	0	56	4	0
8	X	44	0	56	2	0
8	Y	43	0	55	2	0
8	Z	44	0	56	2	0
9	X	49	0	74	1	0
9	Y	49	0	74	1	0
9	Z	49	0	74	3	0
All	All	8140	0	8099	115	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 7.

The worst 5 of 115 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)
2:Y:140:ASN:HD22	2:Y:143:LEU:HD13	1.20	1.03
2:Y:140:ASN:HD22	2:Y:143:LEU:CD1	1.72	1.01
1:X:135:LEU:CD2	1:X:136:ILE:HG12	1.91	1.00
1:X:135:LEU:HD23	1:X:136:ILE:HG12	1.54	0.86
1:X:135:LEU:HD22	1:X:136:ILE:HG12	1.59	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	X	218/249 (88%)	207 (95%)	11 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y	218/257 (85%)	202 (93%)	16 (7%)	0	100	100
3	Z	229/256 (90%)	223 (97%)	6 (3%)	0	100	100
All	All	665/762 (87%)	632 (95%)	33 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	165/187 (88%)	163 (99%)	2 (1%)	63	74
2	Y	170/194 (88%)	167 (98%)	3 (2%)	51	69
3	Z	178/195 (91%)	178 (100%)	0	100	100
All	All	513/576 (89%)	508 (99%)	5 (1%)	65	76

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

Mol	Chain	Res	Type
1	X	104	LYS
1	X	186	ASP
2	Y	81	GLU
2	Y	119	GLU
2	Y	143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	Z	131	GLN
3	Z	169	ASN
1	X	148	GLN
2	Y	140	ASN
2	Y	145	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TPO	Z	27	3	8,10,11	1.09	0	10,14,16	1.63	1 (10%)

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
3	TPO	Z	27	3	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	27	TPO	P-OG1-CB	-4.56	109.43	123.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

56 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CLA	Z	613	3	69,73,73	1.26	6 (8%)	83,113,113	1.14	6 (7%)
4	CHL	X	609	1	70,74,74	1.92	18 (25%)	80,114,114	2.78	25 (31%)
5	CLA	Z	603	3	69,73,73	1.24	6 (8%)	83,113,113	1.24	4 (4%)
6	LUT	X	1620	-	42,43,43	0.80	0	51,60,60	1.93	10 (19%)
4	CHL	Z	607	-	70,74,74	1.89	19 (27%)	80,114,114	2.99	26 (32%)
5	CLA	Y	613	2	69,73,73	1.27	9 (13%)	83,113,113	1.16	8 (9%)
5	CLA	Y	610	2	69,73,73	1.28	8 (11%)	83,113,113	1.14	8 (9%)
4	CHL	Y	607	-	70,74,74	1.90	20 (28%)	80,114,114	2.90	27 (33%)
5	CLA	X	603	1	66,70,73	1.29	8 (12%)	79,109,113	1.21	6 (7%)
5	CLA	Y	614	2	52,56,73	1.47	7 (13%)	62,92,113	1.24	6 (9%)
4	CHL	X	605	1	50,54,74	2.30	19 (38%)	56,90,114	2.84	27 (48%)
4	CHL	X	608	-	70,74,74	1.88	18 (25%)	80,114,114	2.87	24 (30%)
5	CLA	X	613	1	69,73,73	1.27	8 (11%)	83,113,113	1.17	8 (9%)
5	CLA	X	604	-	53,57,73	1.43	8 (15%)	62,93,113	1.20	6 (9%)
4	CHL	Y	606	-	50,54,74	2.30	18 (36%)	56,90,114	2.81	25 (44%)
9	LHG	Y	2630	5	48,48,48	0.96	2 (4%)	51,54,54	0.97	2 (3%)
6	LUT	Z	1621	-	42,43,43	0.76	1 (2%)	51,60,60	1.77	13 (25%)
6	LUT	Z	1620	-	42,43,43	0.75	1 (2%)	51,60,60	1.77	12 (23%)
6	LUT	Y	1621	-	42,43,43	0.77	0	51,60,60	1.75	13 (25%)
8	NEX	Z	1623	-	38,46,46	1.14	2 (5%)	50,70,70	2.33	15 (30%)
5	CLA	X	611	9	49,53,73	1.49	6 (12%)	59,89,113	1.33	7 (11%)
5	CLA	X	612	1	47,51,73	1.50	7 (14%)	56,86,113	1.30	6 (10%)
7	XAT	Z	1622	-	39,47,47	0.93	2 (5%)	54,74,74	4.35	23 (42%)
8	NEX	X	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.44	16 (32%)
6	LUT	Y	1620	-	42,43,43	0.80	1 (2%)	51,60,60	1.94	11 (21%)
4	CHL	X	607	-	70,74,74	1.90	20 (28%)	80,114,114	2.90	27 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CHL	X	601	1	70,74,74	1.88	18 (25%)	80,114,114	2.90	26 (32%)
4	CHL	Y	601	2	70,74,74	1.89	18 (25%)	80,114,114	2.90	26 (32%)
6	LUT	X	1621	-	42,43,43	0.79	1 (2%)	51,60,60	1.75	13 (25%)
4	CHL	Z	605	3	48,52,74	2.27	18 (37%)	53,87,114	2.80	27 (50%)
5	CLA	Z	614	3	58,62,73	1.38	7 (12%)	69,99,113	1.18	6 (8%)
5	CLA	Y	603	2	59,63,73	1.37	7 (11%)	71,101,113	1.26	6 (8%)
7	XAT	X	1622	-	39,47,47	0.95	2 (5%)	54,74,74	4.40	24 (44%)
8	NEX	Y	1623	-	40,45,46	1.03	2 (5%)	50,67,70	2.47	16 (32%)
9	LHG	Z	2630	5	48,48,48	0.94	2 (4%)	51,54,54	0.85	2 (3%)
5	CLA	Z	602	3	64,68,73	1.32	7 (10%)	77,107,113	1.14	6 (7%)
4	CHL	Z	608	-	54,58,74	2.21	17 (31%)	59,94,114	2.70	26 (44%)
4	CHL	Y	605	2	46,50,74	2.39	18 (39%)	51,85,114	2.96	27 (52%)
5	CLA	Z	612	3	69,73,73	1.27	5 (7%)	83,113,113	1.14	4 (4%)
5	CLA	Y	602	2	62,66,73	1.34	7 (11%)	74,104,113	1.16	5 (6%)
5	CLA	Y	612	2	49,53,73	1.50	7 (14%)	59,89,113	1.31	6 (10%)
4	CHL	Z	606	-	50,54,74	2.33	19 (38%)	56,90,114	2.82	26 (46%)
5	CLA	Y	611	9	47,51,73	1.51	7 (14%)	56,86,113	1.30	5 (8%)
4	CHL	Z	609	3	70,74,74	1.98	18 (25%)	80,114,114	2.70	23 (28%)
5	CLA	X	610	1	69,73,73	1.28	7 (10%)	83,113,113	1.13	8 (9%)
4	CHL	Z	601	3	70,74,74	1.90	18 (25%)	80,114,114	2.88	28 (35%)
5	CLA	X	614	1	46,50,73	1.51	7 (15%)	55,85,113	1.27	5 (9%)
4	CHL	Y	609	2	70,74,74	1.92	18 (25%)	80,114,114	2.77	25 (31%)
5	CLA	X	602	1	69,73,73	1.27	8 (11%)	83,113,113	1.12	5 (6%)
5	CLA	Z	610	3	69,73,73	1.25	7 (10%)	83,113,113	1.17	8 (9%)
4	CHL	Y	608	-	53,57,74	2.26	19 (35%)	59,93,114	2.73	27 (45%)
5	CLA	Z	604	-	61,65,73	1.35	6 (9%)	73,103,113	1.21	7 (9%)
9	LHG	X	2630	5	48,48,48	0.96	2 (4%)	51,54,54	0.96	2 (3%)
7	XAT	Y	1622	-	39,47,47	0.96	2 (5%)	54,74,74	4.40	24 (44%)
5	CLA	Z	611	9	69,73,73	1.24	5 (7%)	83,113,113	1.15	5 (6%)
5	CLA	Y	604	-	54,58,73	1.43	8 (14%)	65,95,113	1.20	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	Z	613	3	-	16/39/115/115	-
4	CHL	X	609	1	-	16/41/117/117	-
5	CLA	Z	603	3	-	21/39/115/115	-
6	LUT	X	1620	-	-	2/29/67/67	0/2/2/2
4	CHL	Z	607	-	-	17/41/117/117	-
5	CLA	Y	613	2	-	18/39/115/115	-
5	CLA	Y	610	2	-	9/39/115/115	-
4	CHL	Y	607	-	-	23/41/117/117	-
5	CLA	X	603	1	-	9/36/112/115	-
5	CLA	Y	614	2	-	9/19/95/115	-
4	CHL	X	605	1	-	3/17/93/117	-
4	CHL	X	608	-	-	24/41/117/117	-
5	CLA	X	613	1	-	18/39/115/115	-
5	CLA	X	604	-	-	7/20/96/115	-
4	CHL	Y	606	-	-	2/17/93/117	-
9	LHG	Y	2630	5	-	11/53/53/53	-
6	LUT	Z	1621	-	-	2/29/67/67	0/2/2/2
6	LUT	Z	1620	-	-	0/29/67/67	0/2/2/2
6	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
8	NEX	Z	1623	-	-	3/27/83/83	0/3/3/3
5	CLA	X	611	9	-	10/15/91/115	-
5	CLA	X	612	1	-	4/13/89/115	-
7	XAT	Z	1622	-	-	4/31/93/93	0/4/4/4
8	NEX	X	1623	-	-	3/27/83/83	0/3/3/3
6	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
4	CHL	X	607	-	-	23/41/117/117	-
4	CHL	X	601	1	-	23/41/117/117	-
4	CHL	Y	601	2	-	23/41/117/117	-
6	LUT	X	1621	-	-	1/29/67/67	0/2/2/2
4	CHL	Z	605	3	-	1/15/91/117	-
5	CLA	Z	614	3	-	9/26/102/115	-
5	CLA	Y	603	2	-	9/27/103/115	-
7	XAT	X	1622	-	-	4/31/93/93	0/4/4/4
8	NEX	Y	1623	-	-	3/27/80/83	0/3/3/3
9	LHG	Z	2630	5	-	17/53/53/53	-
5	CLA	Z	602	3	-	4/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHL	Z	608	-	-	6/22/98/117	-
4	CHL	Y	605	2	-	2/12/88/117	-
5	CLA	Z	612	3	-	6/39/115/115	-
5	CLA	Y	602	2	-	7/31/107/115	-
5	CLA	Y	612	2	-	6/15/91/115	-
4	CHL	Z	606	-	-	4/17/93/117	-
5	CLA	Y	611	9	-	8/13/89/115	-
4	CHL	Z	609	3	-	22/41/117/117	-
5	CLA	X	610	1	-	9/39/115/115	-
4	CHL	Z	601	3	-	21/41/117/117	-
5	CLA	X	614	1	-	6/12/88/115	-
4	CHL	Y	609	2	-	16/41/117/117	-
5	CLA	X	602	1	-	10/39/115/115	-
5	CLA	Z	610	3	-	11/39/115/115	-
4	CHL	Y	608	-	-	6/21/97/117	-
5	CLA	Z	604	-	-	6/30/106/115	-
9	LHG	X	2630	5	-	10/53/53/53	-
7	XAT	Y	1622	-	-	4/31/93/93	0/4/4/4
5	CLA	Z	611	9	-	6/39/115/115	-
5	CLA	Y	604	-	-	5/21/97/115	-

The worst 5 of 502 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	606	CHL	O2D-CGD	5.24	1.46	1.33
4	Z	606	CHL	O2D-CGD	5.20	1.45	1.33
4	Z	605	CHL	O2D-CGD	5.17	1.45	1.33
4	Y	608	CHL	O2D-CGD	5.15	1.45	1.33
4	Z	608	CHL	O2D-CGD	5.15	1.45	1.33

The worst 5 of 786 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Z	1622	XAT	C37-C21-C36	-17.98	80.85	107.37
7	Y	1622	XAT	C37-C21-C36	-17.67	81.31	107.37
7	X	1622	XAT	C37-C21-C36	-17.67	81.31	107.37
7	Y	1622	XAT	C37-C21-C22	-15.13	82.70	108.98
7	X	1622	XAT	C37-C21-C22	-15.12	82.72	108.98

There are no chirality outliers.

5 of 522 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	601	CHL	C2-C3-C5-C6
4	X	601	CHL	C4-C3-C5-C6
4	X	607	CHL	C1C-C2C-CMC-OMC
4	X	607	CHL	C3C-C2C-CMC-OMC
4	X	607	CHL	C6-C7-C8-C9

There are no ring outliers.

36 monomers are involved in 74 short contacts:

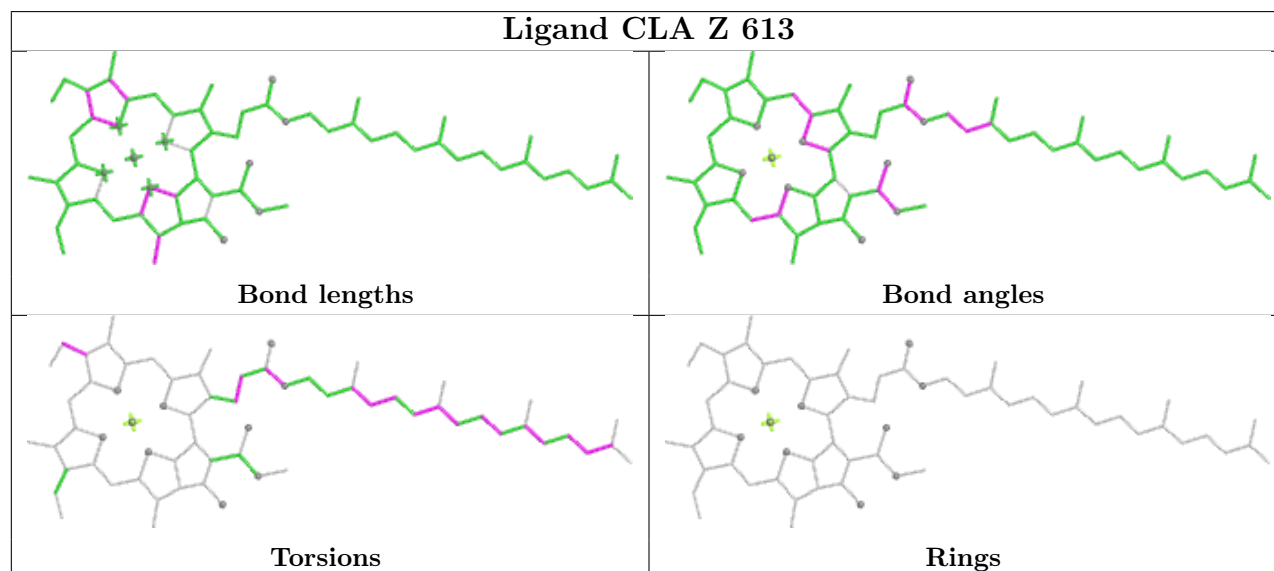
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Z	613	CLA	2	0
4	X	609	CHL	5	0
6	X	1620	LUT	3	0
4	Z	607	CHL	3	0
5	Y	613	CLA	2	0
4	Y	607	CHL	2	0
5	X	603	CLA	1	0
4	X	605	CHL	1	0
4	X	608	CHL	3	0
5	X	613	CLA	2	0
4	Y	606	CHL	2	0
9	Y	2630	LHG	1	0
6	Z	1621	LUT	2	0
6	Z	1620	LUT	3	0
8	Z	1623	NEX	2	0
5	X	611	CLA	3	0
7	Z	1622	XAT	4	0
8	X	1623	NEX	2	0
6	Y	1620	LUT	3	0
4	X	607	CHL	2	0
4	X	601	CHL	2	0
4	Y	601	CHL	6	0
4	Z	605	CHL	1	0
7	X	1622	XAT	3	0
8	Y	1623	NEX	2	0
9	Z	2630	LHG	3	0
4	Z	608	CHL	1	0
4	Y	605	CHL	1	0
4	Z	606	CHL	4	0
5	Y	611	CLA	3	0

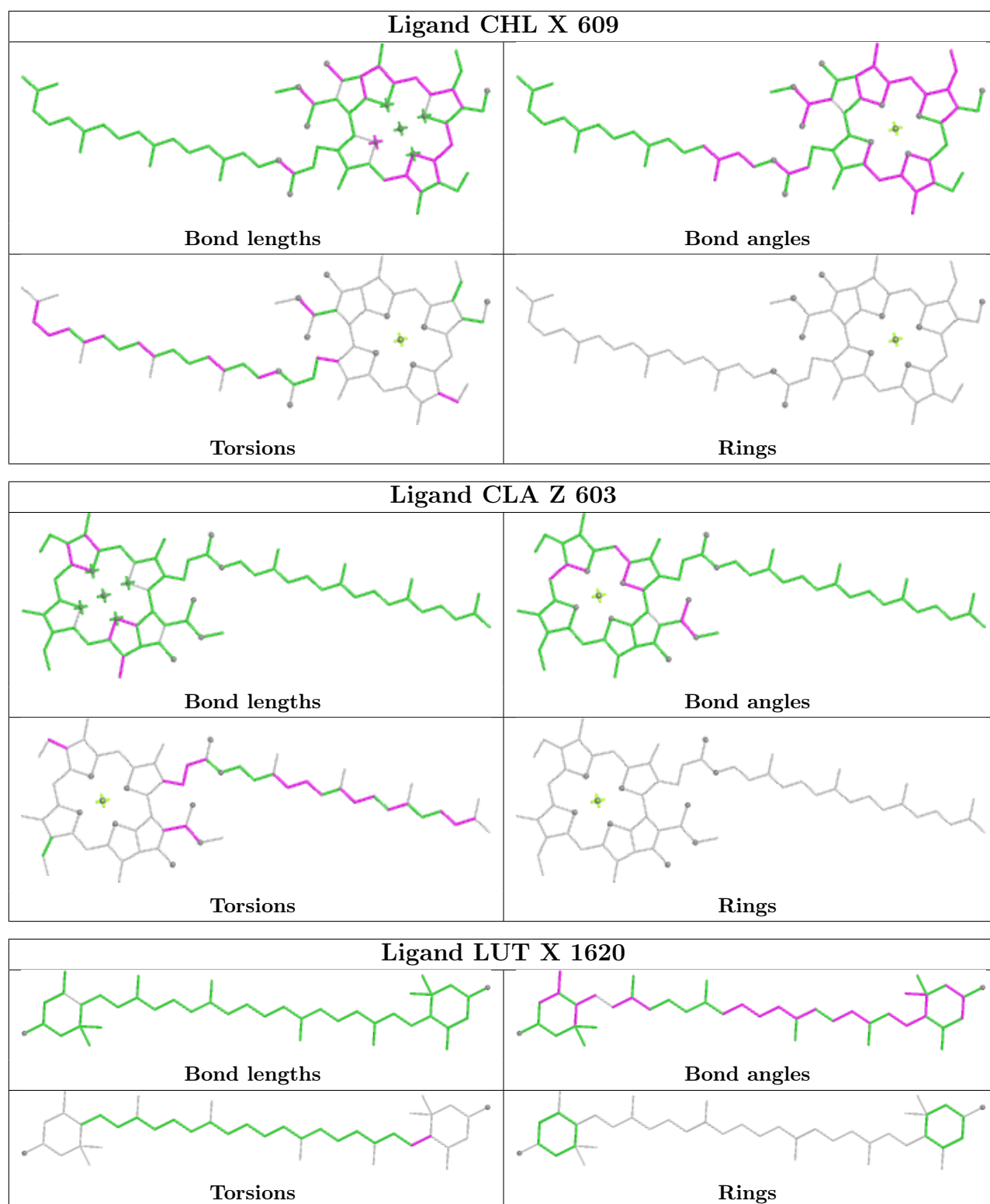
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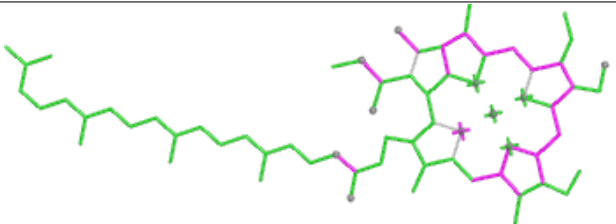
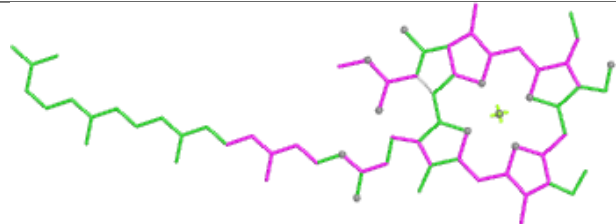
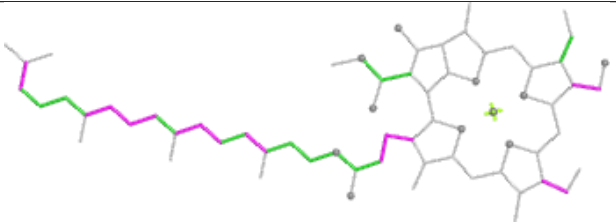
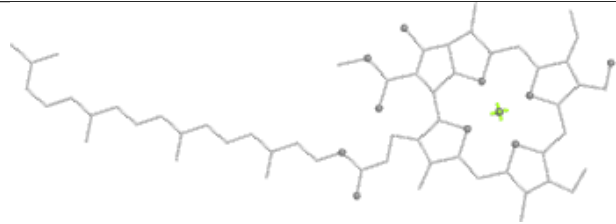
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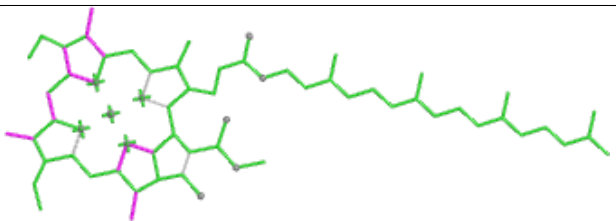
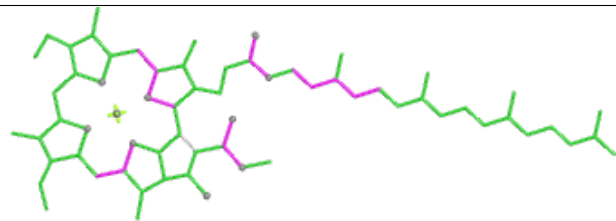
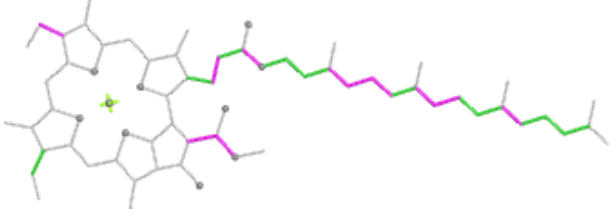
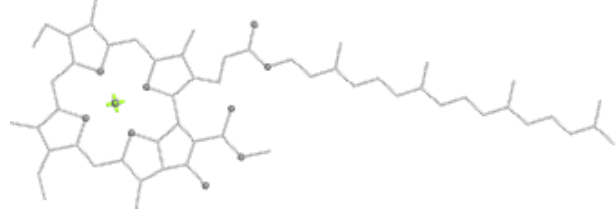
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	609	CHL	5	0
4	Z	601	CHL	3	0
4	Y	609	CHL	4	0
4	Y	608	CHL	1	0
9	X	2630	LHG	1	0
7	Y	1622	XAT	3	0

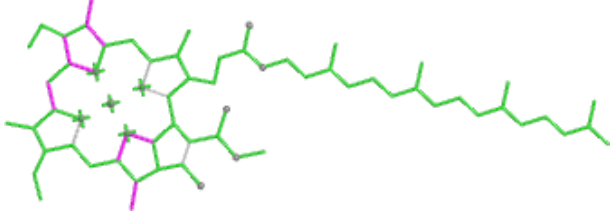
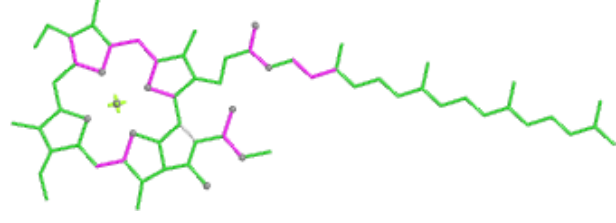
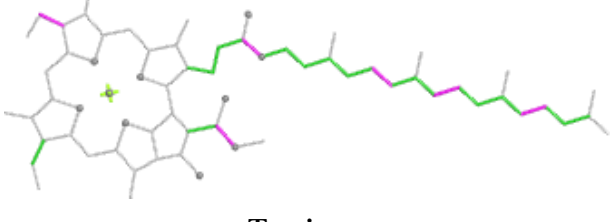
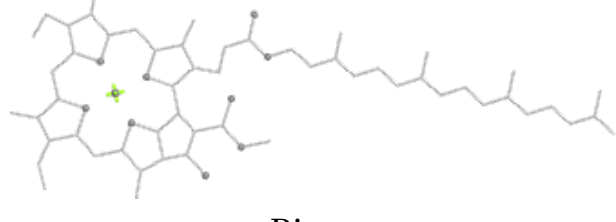
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

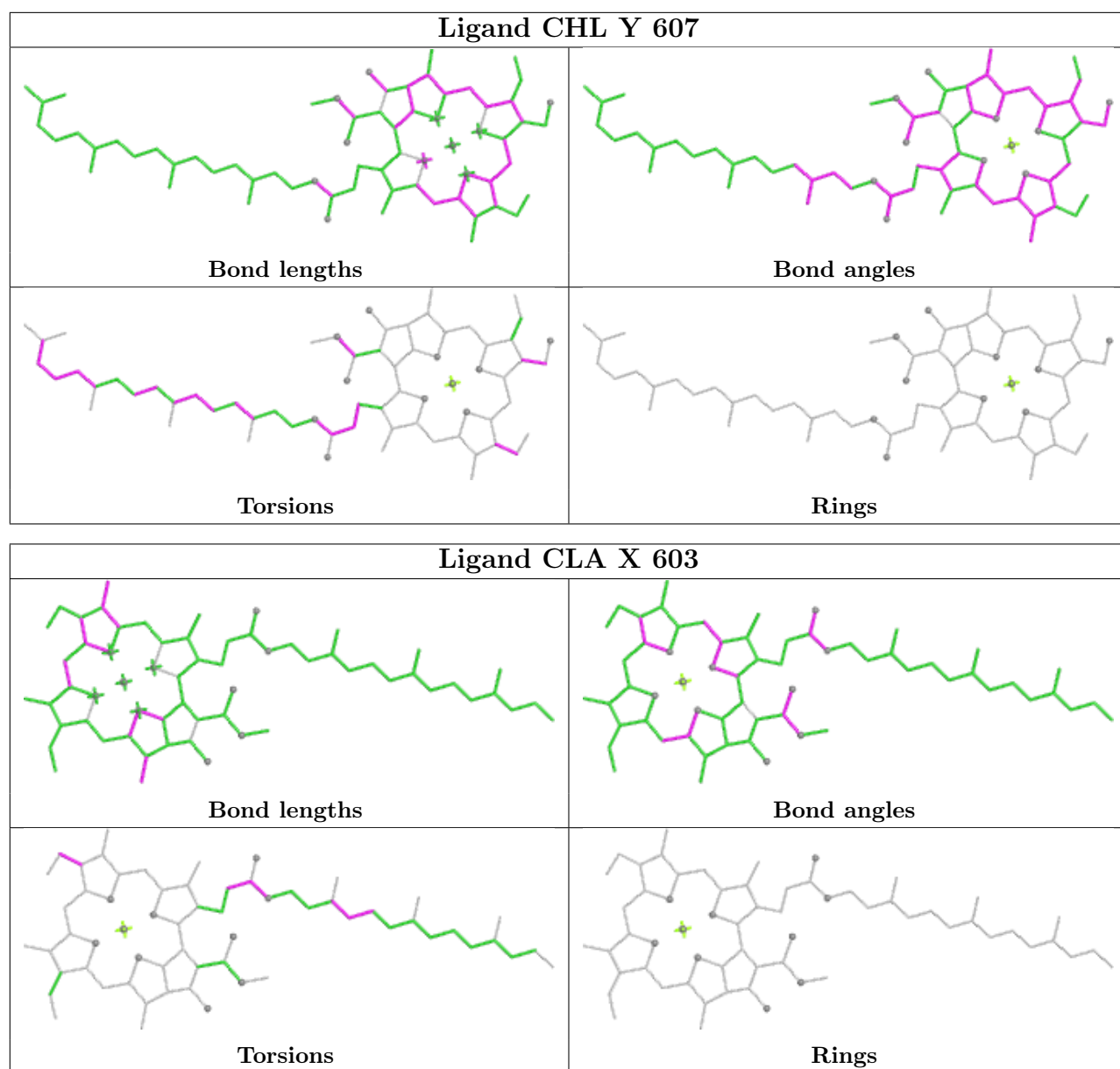


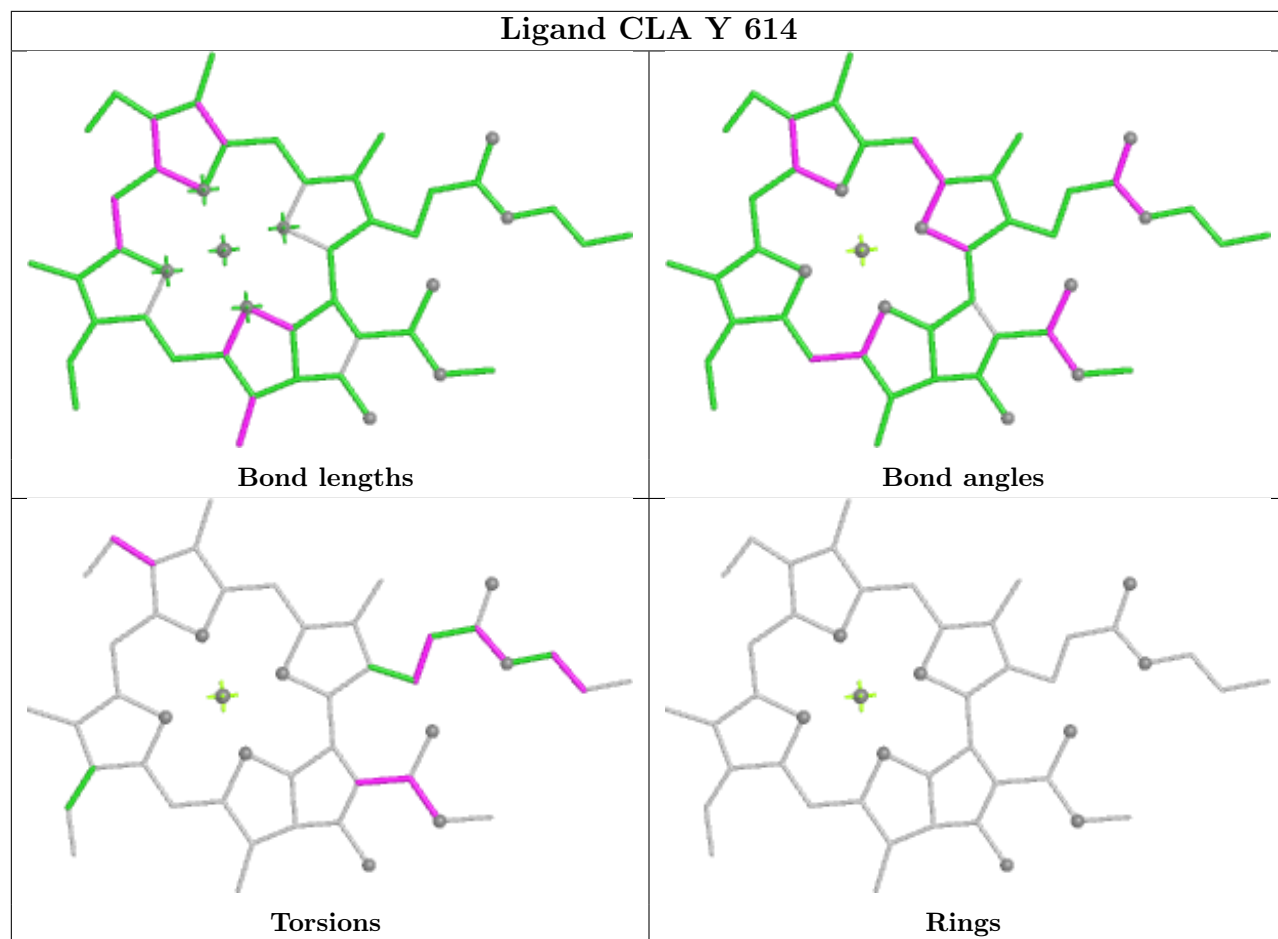


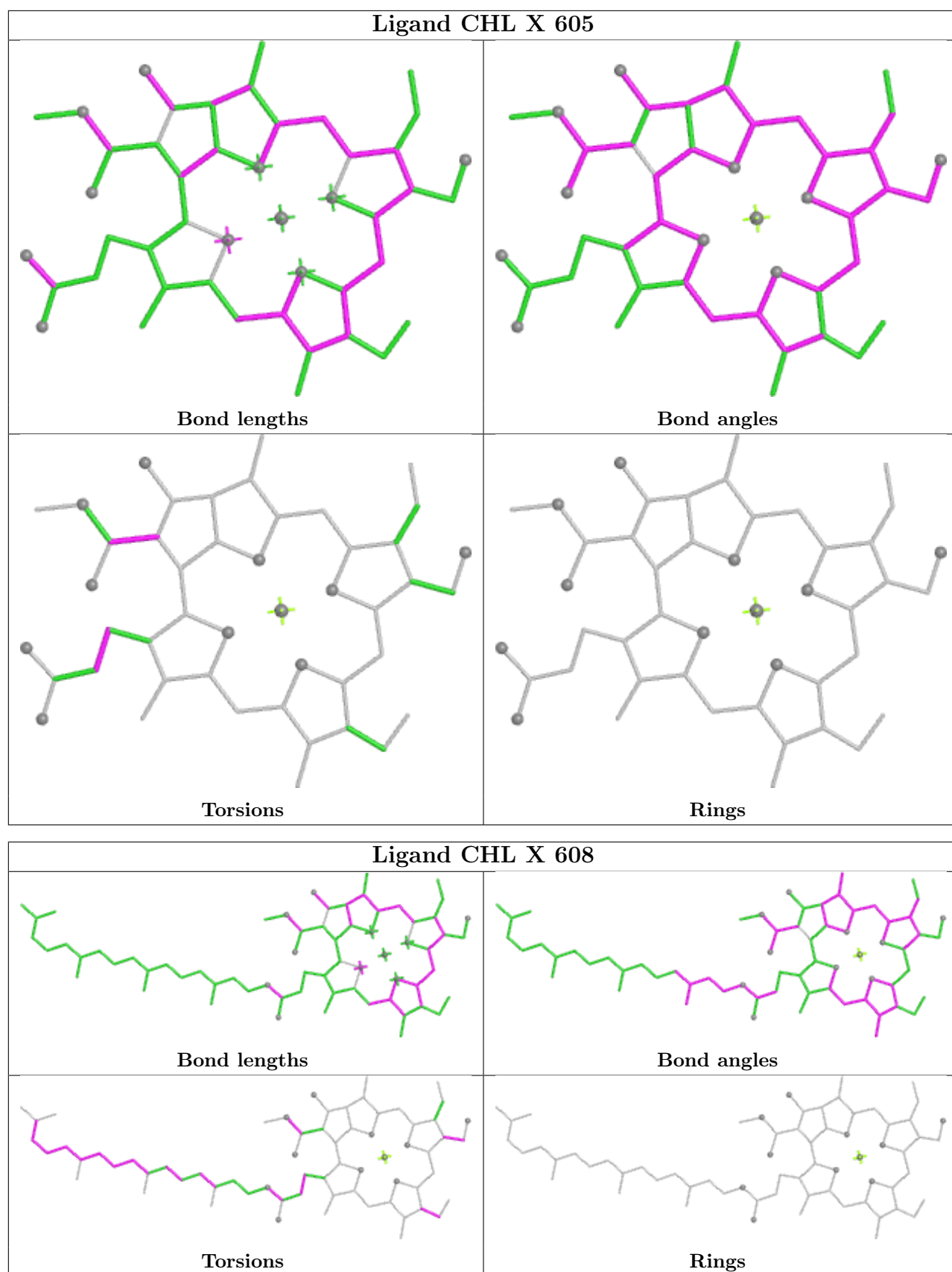
Ligand CHL Z 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

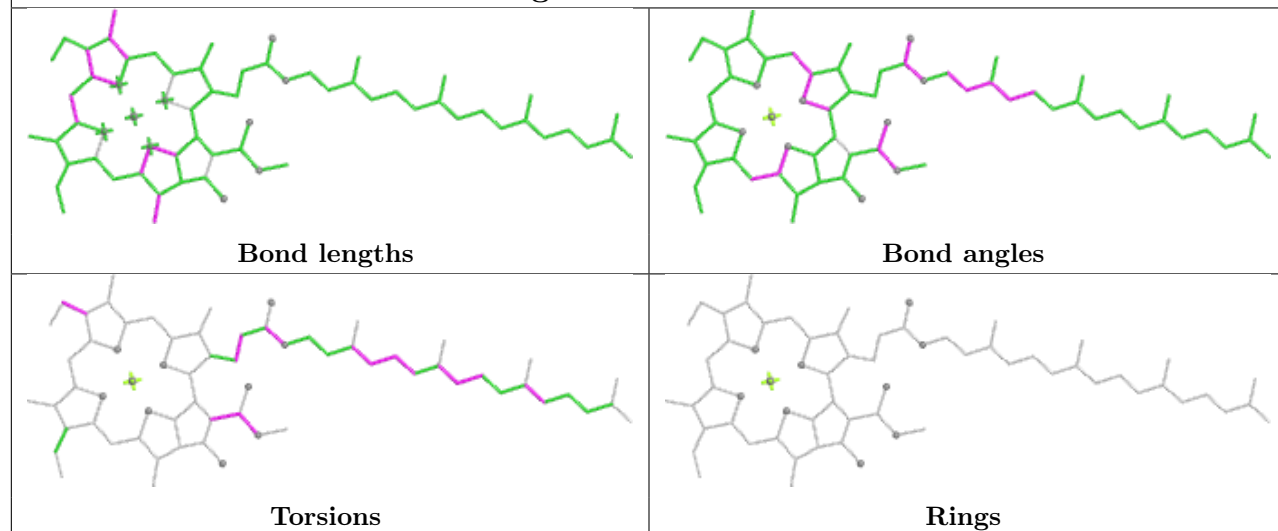
Ligand CLA Y 610	
	
Bond lengths	Bond angles
	
Torsions	Rings



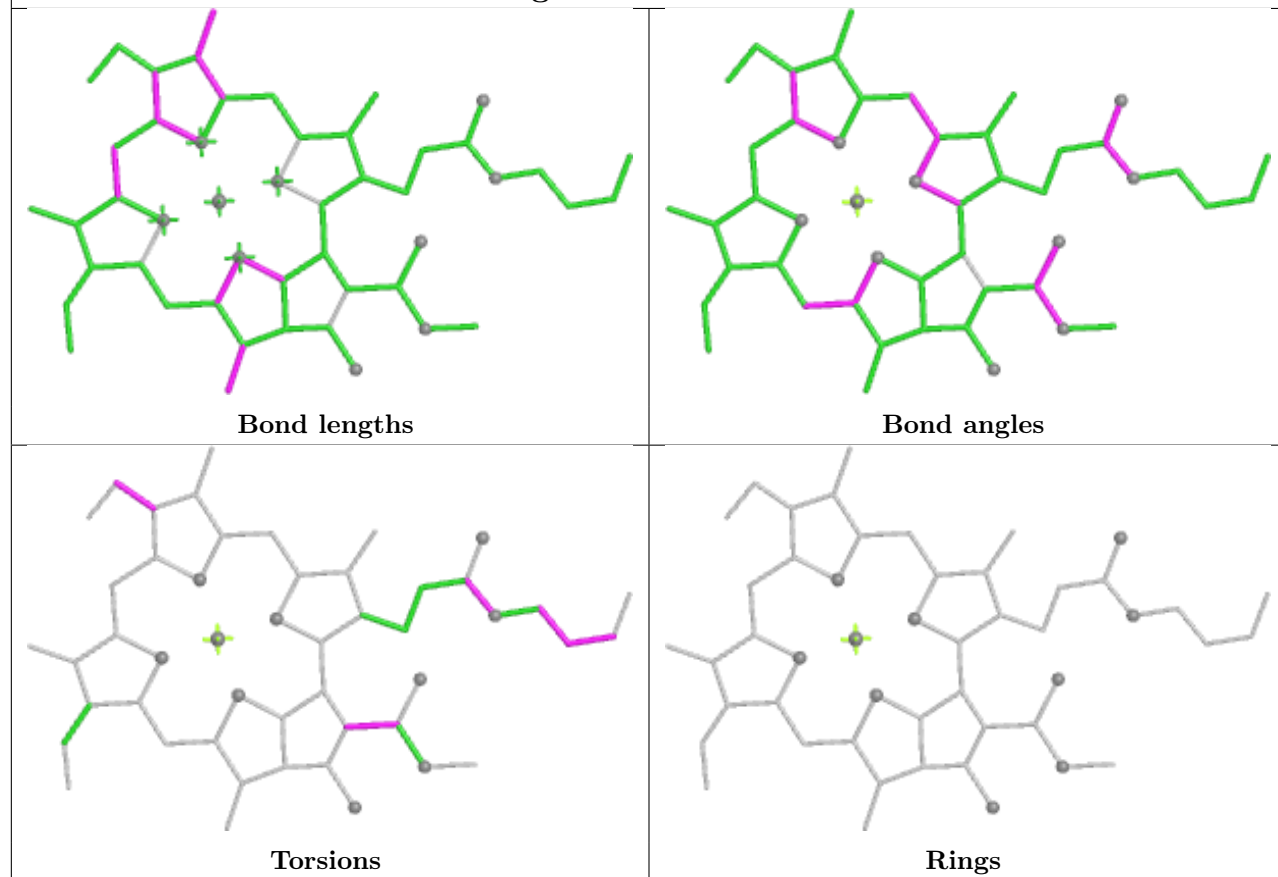


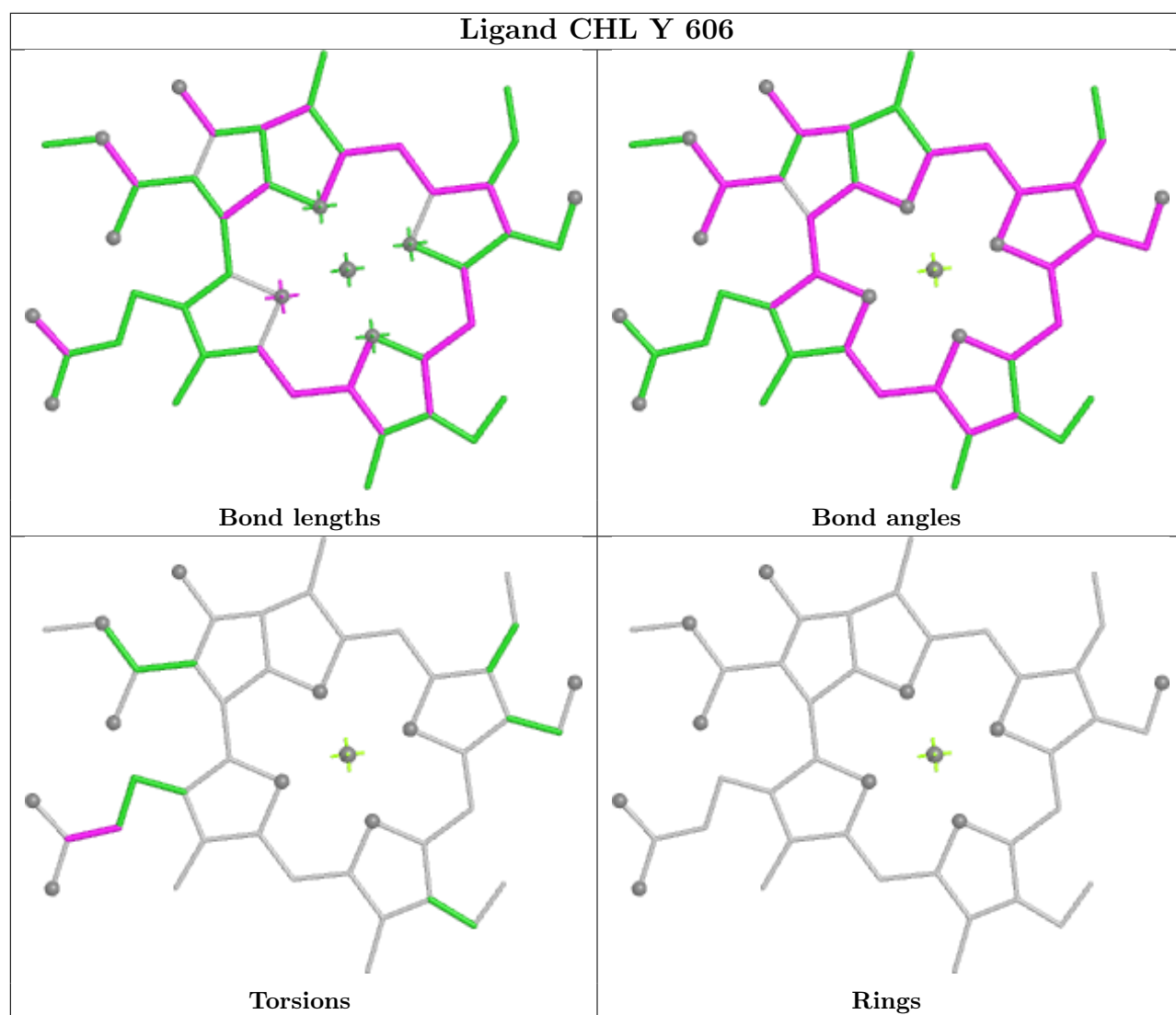


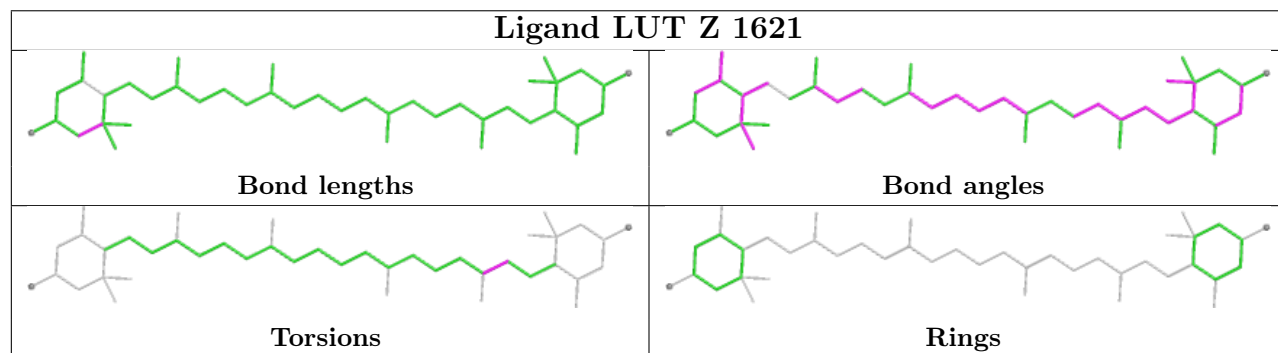
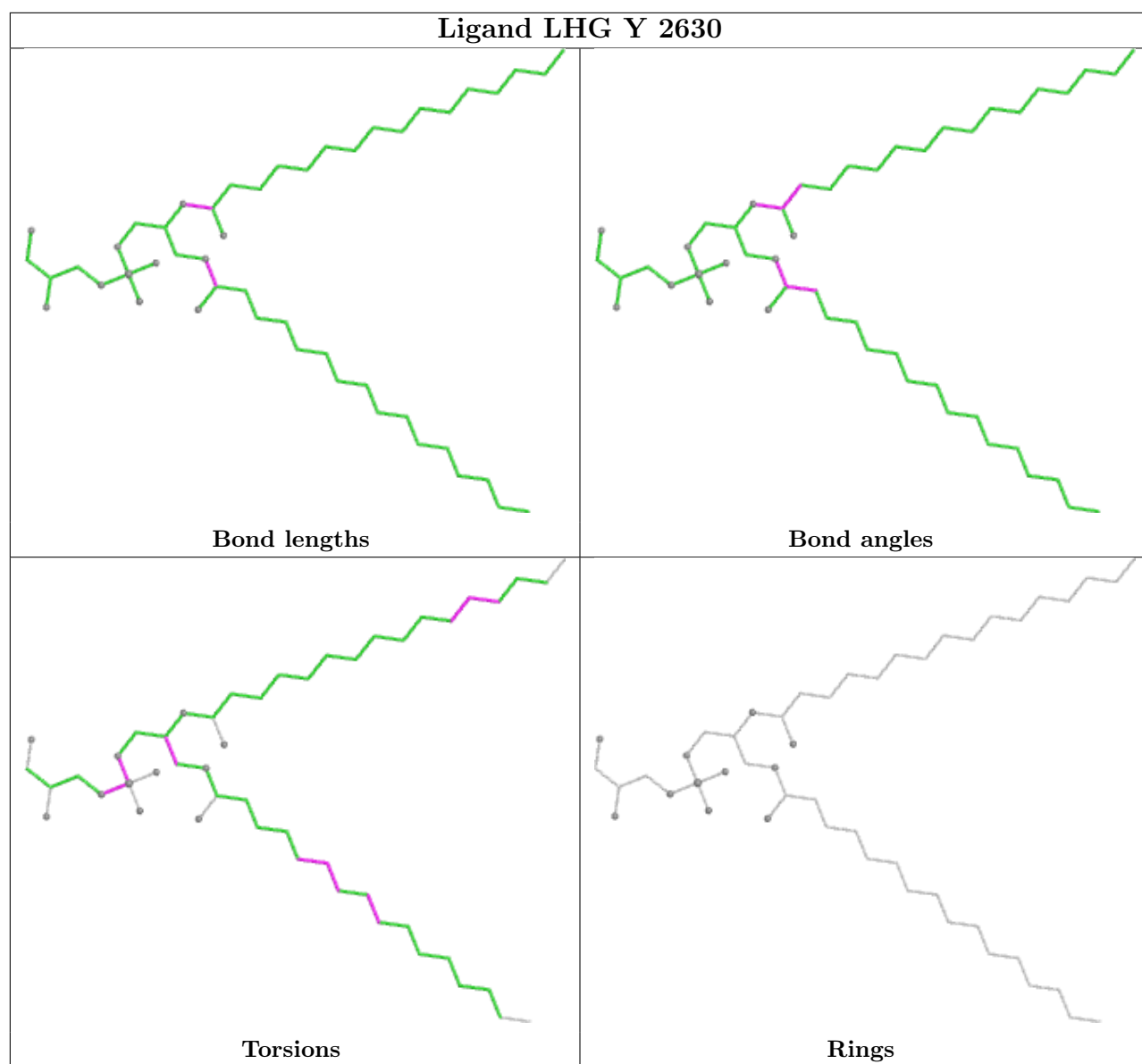
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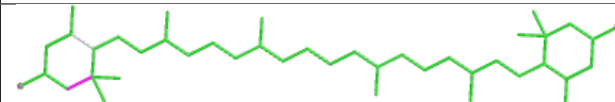
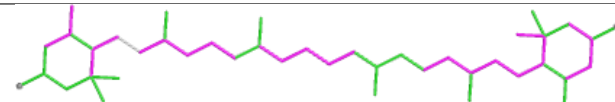
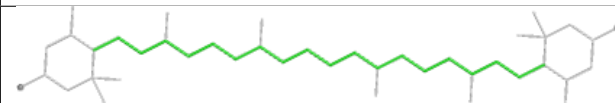
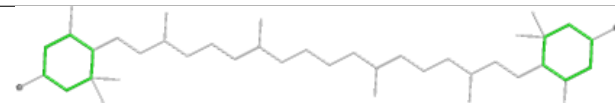


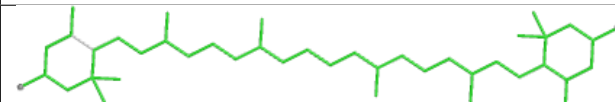
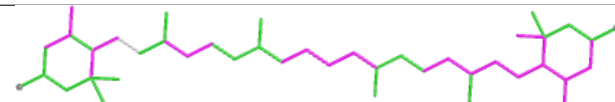
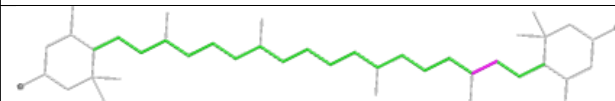
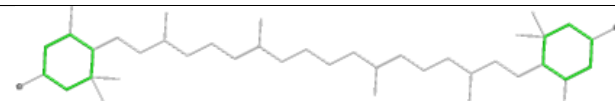
Ligand CLA X 604

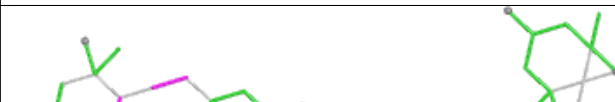
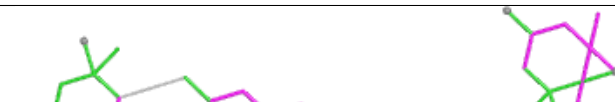
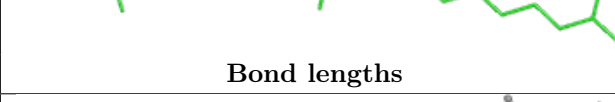
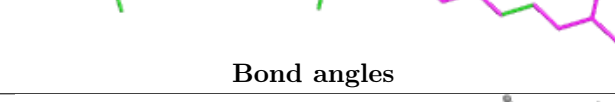


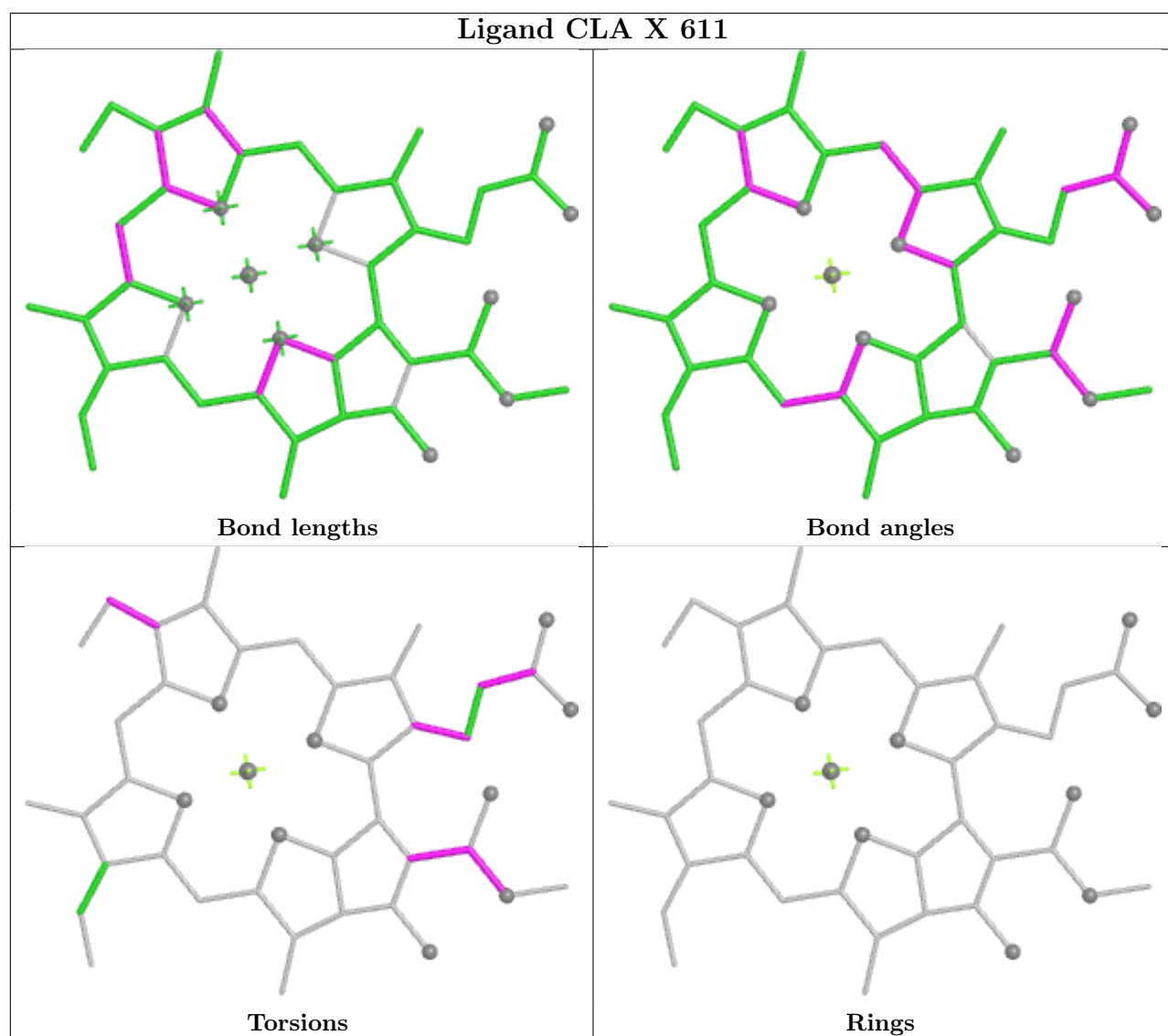


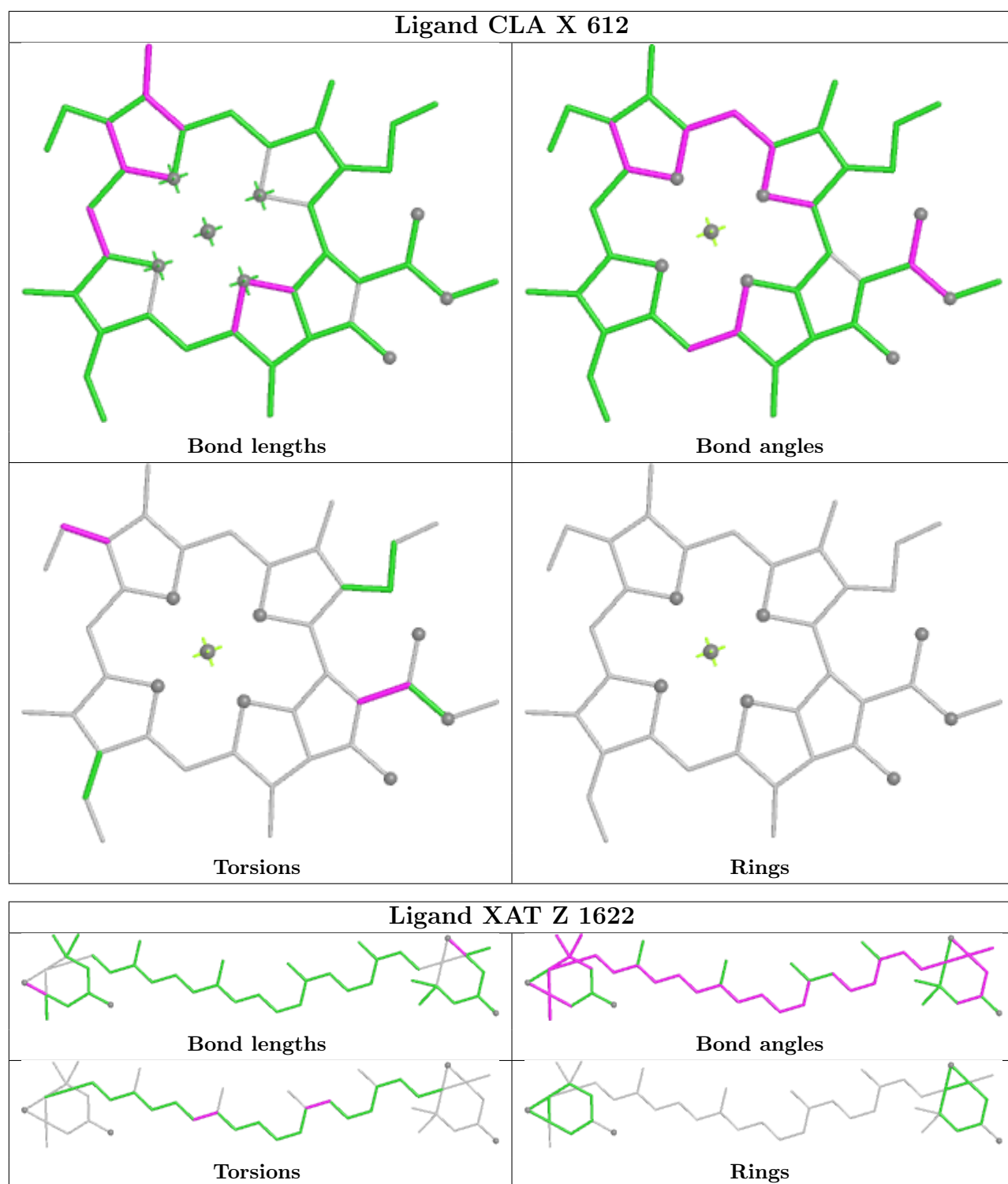


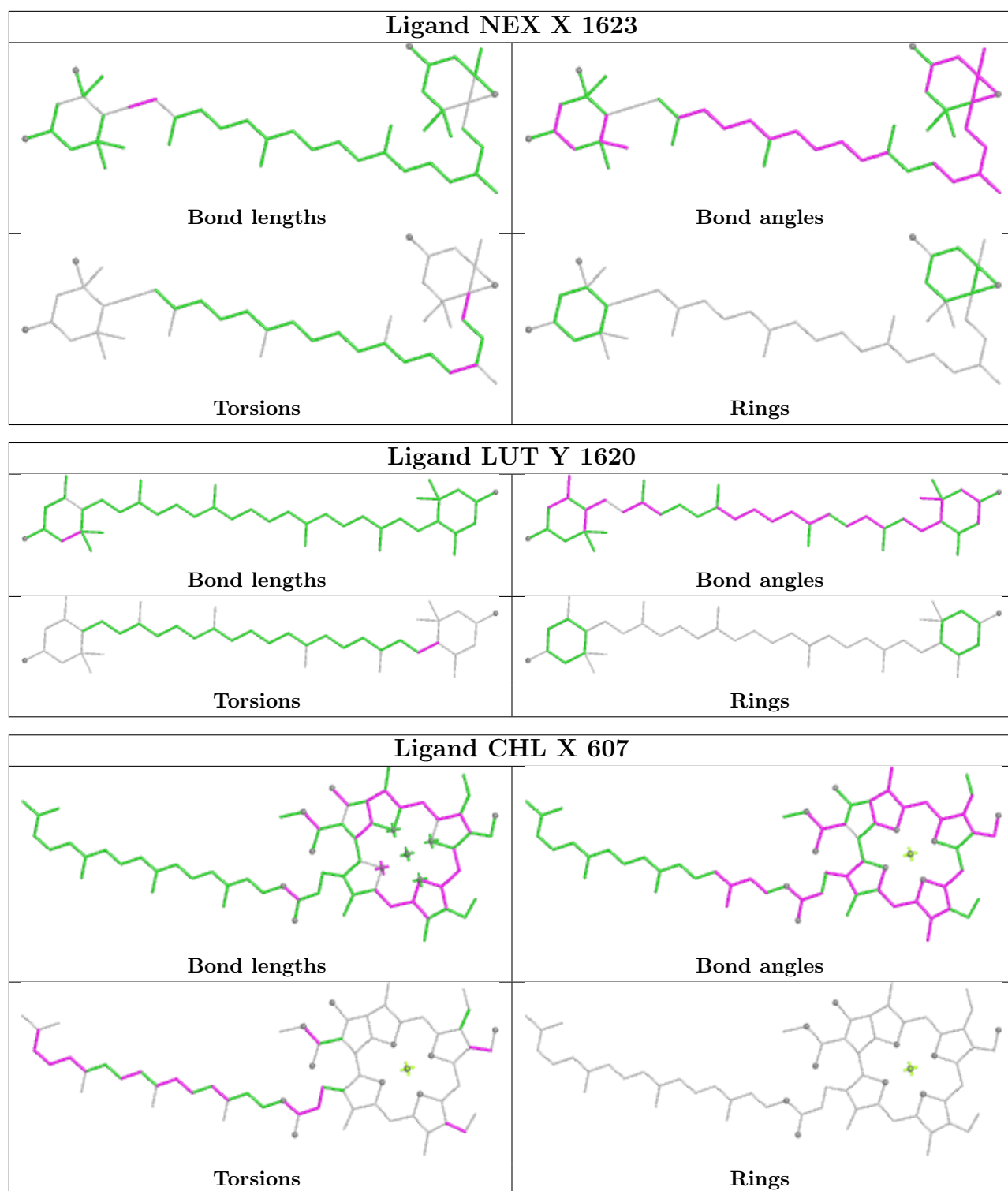
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Bond lengths	Bond angles
	
Torsions	Rings

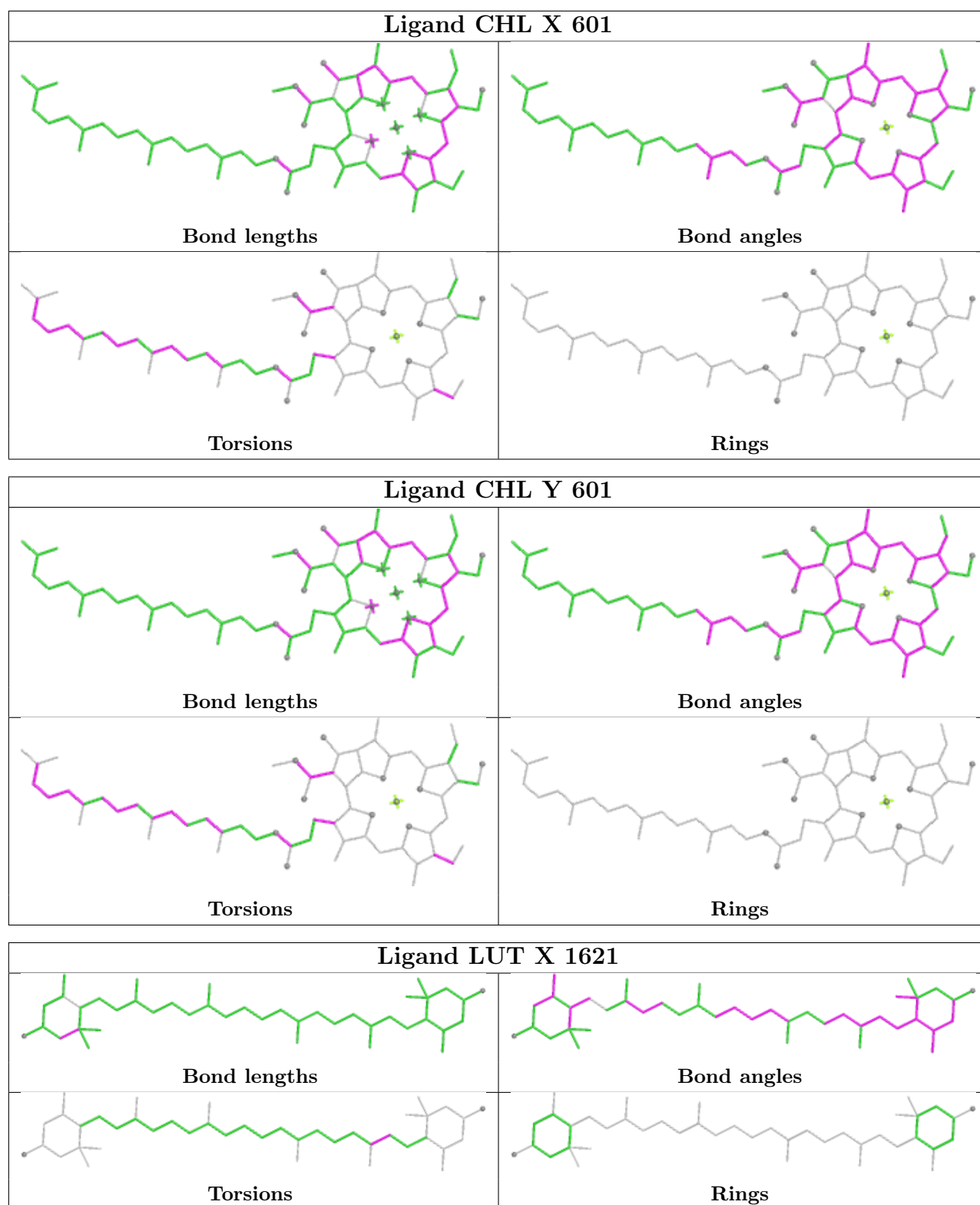
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Bond lengths	Bond angles
	
Torsions	Rings

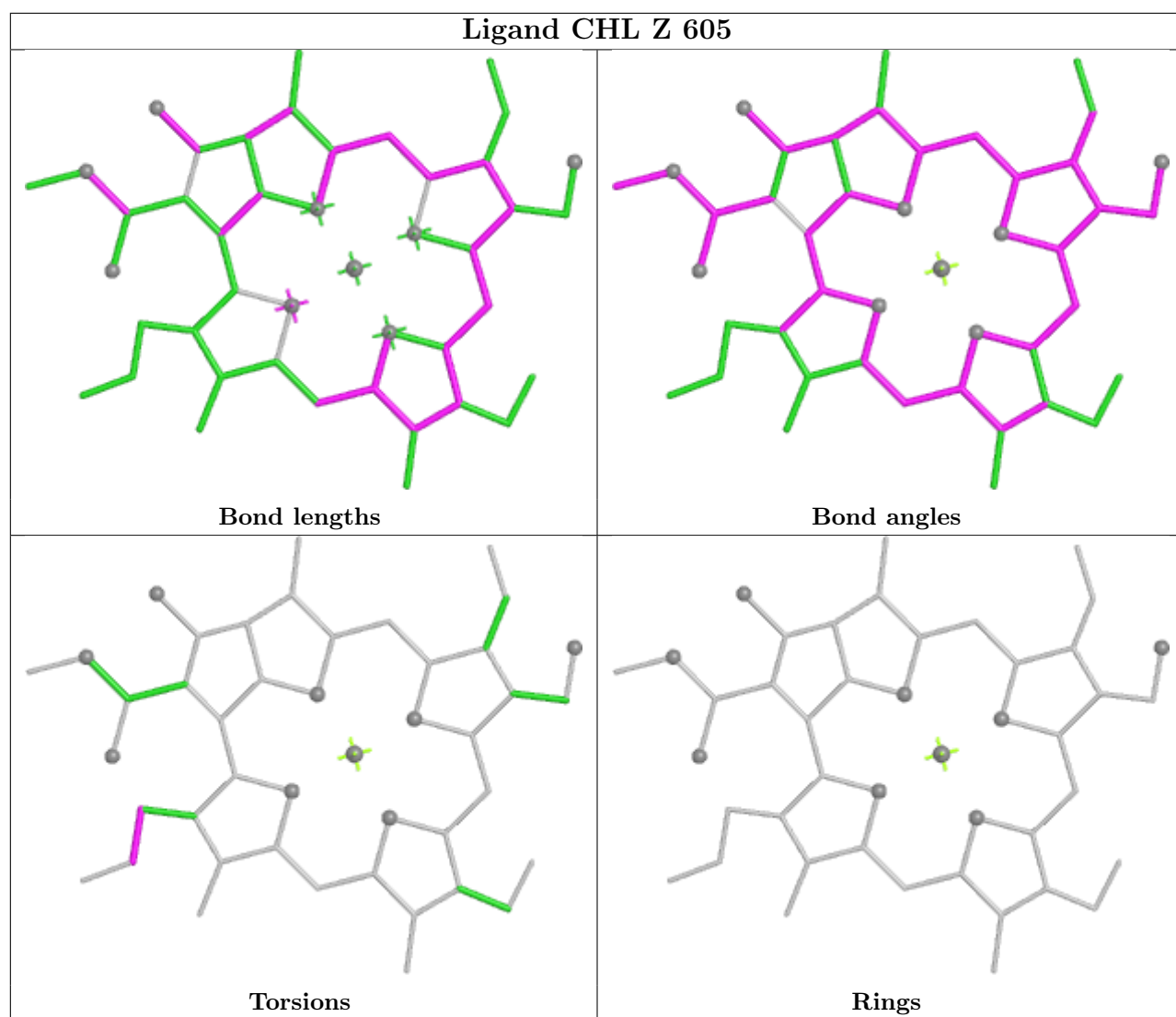
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Bond lengths	Bond angles
	
Torsions	Rings



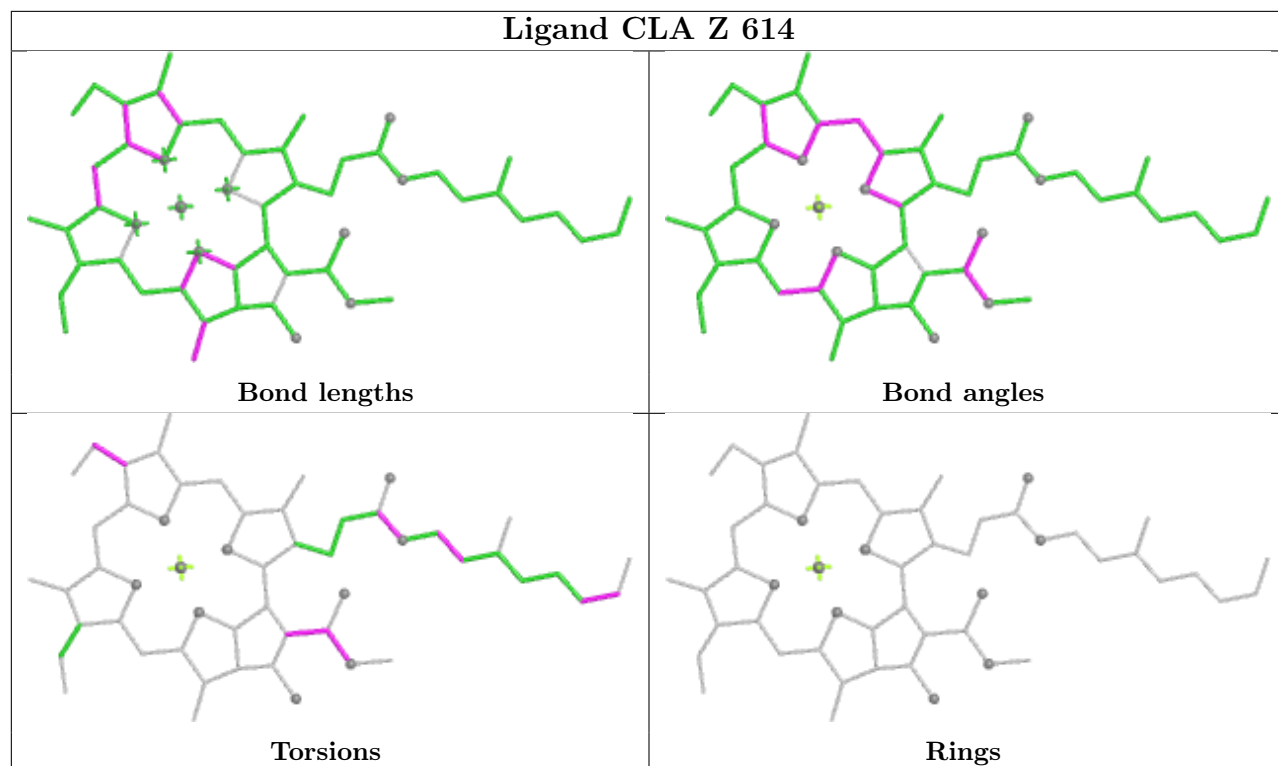




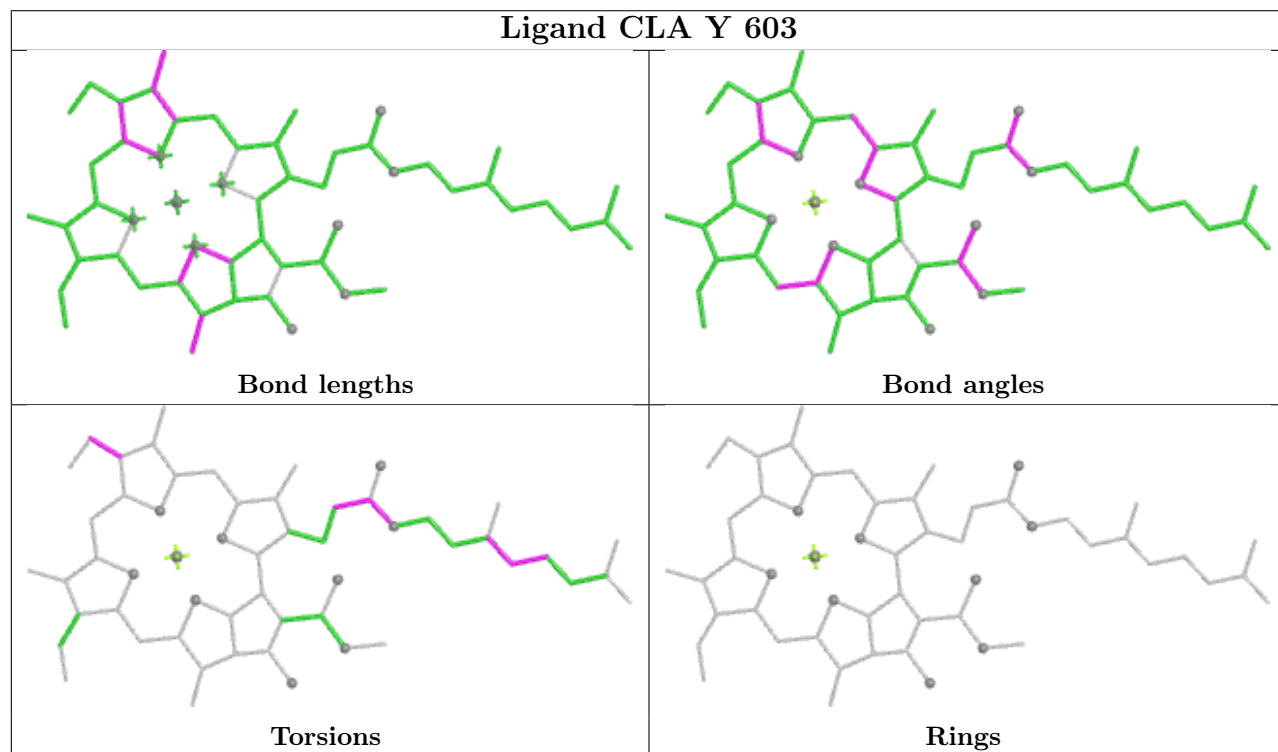


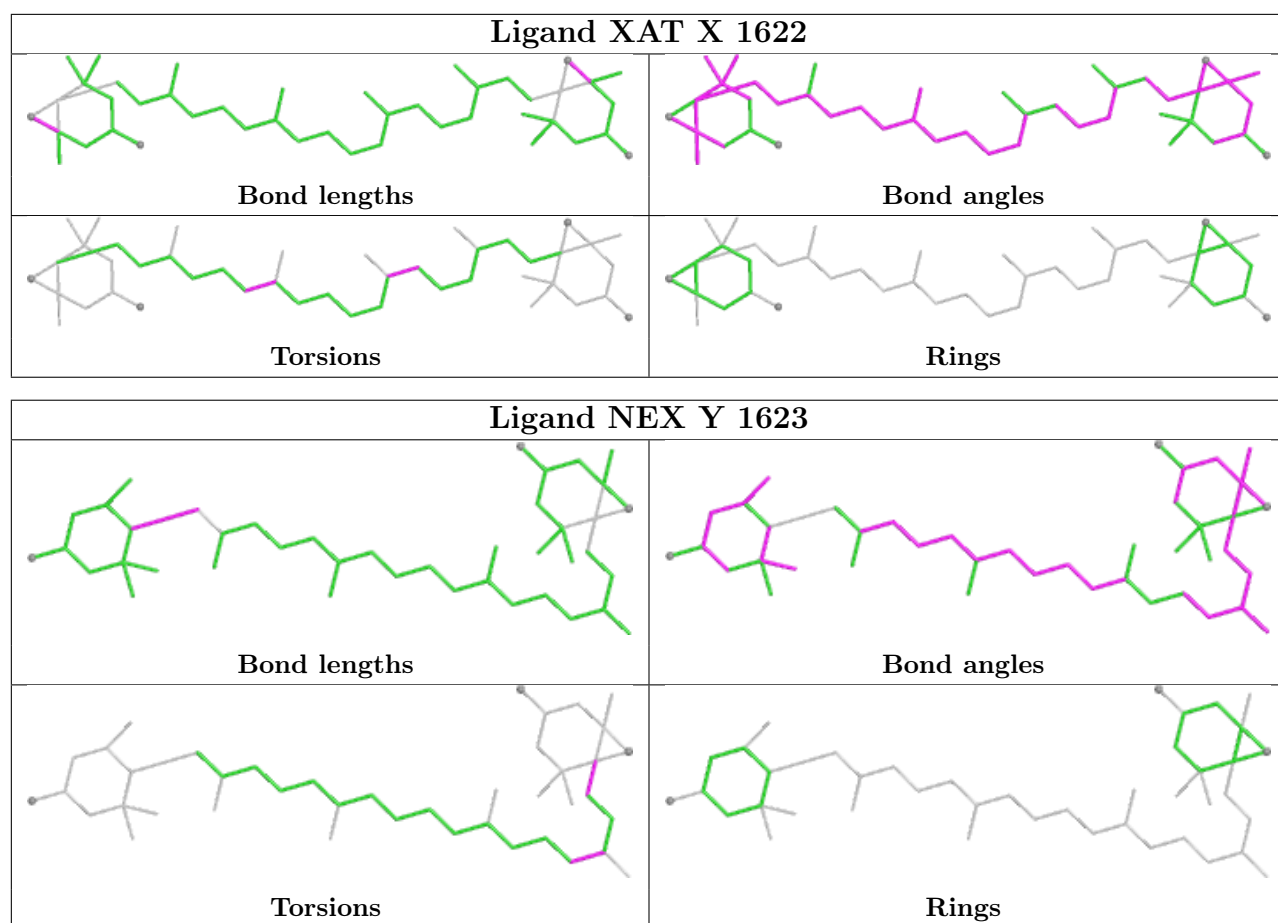


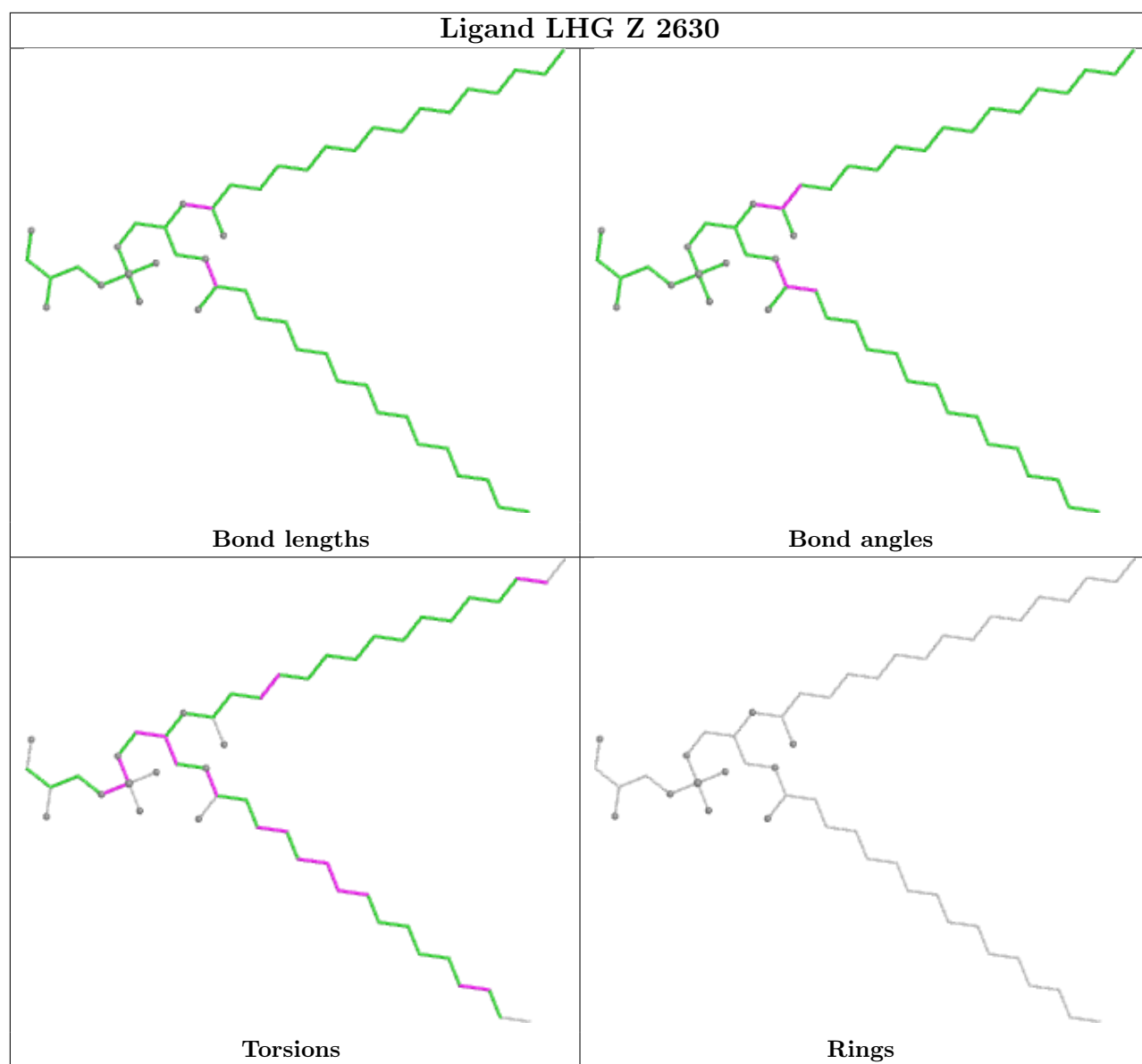
Ligand CLA Z 614



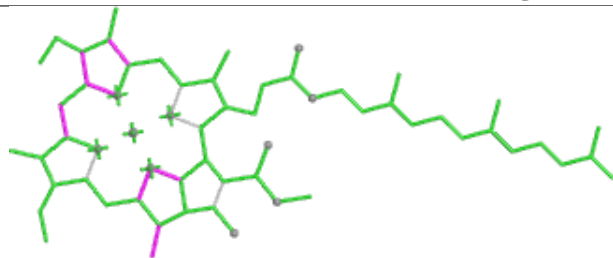
Ligand CLA Y 603



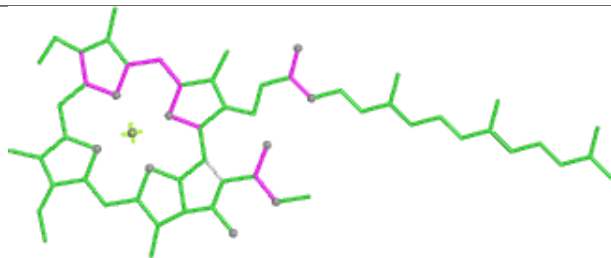




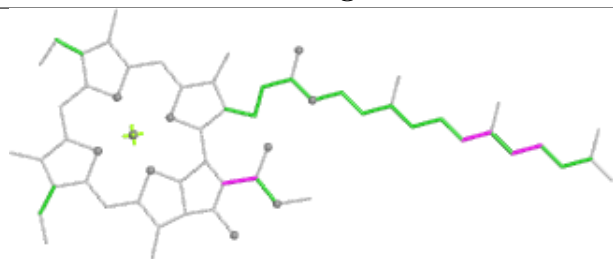
Ligand CLA Z 602



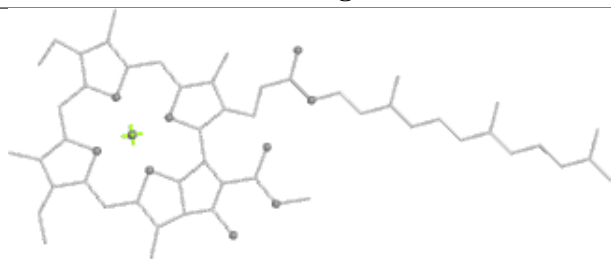
Bond lengths



Bond angles

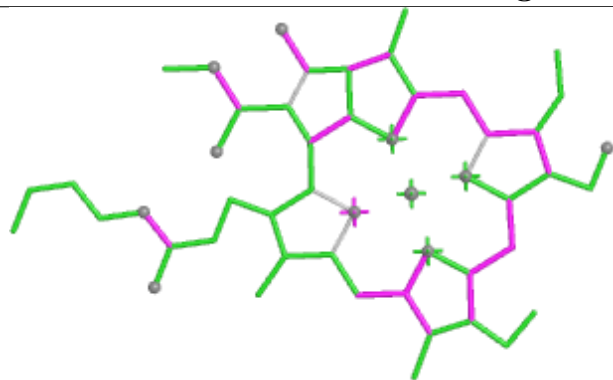


Torsions

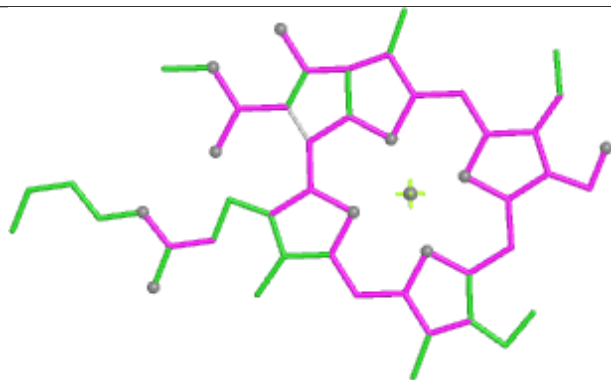


Rings

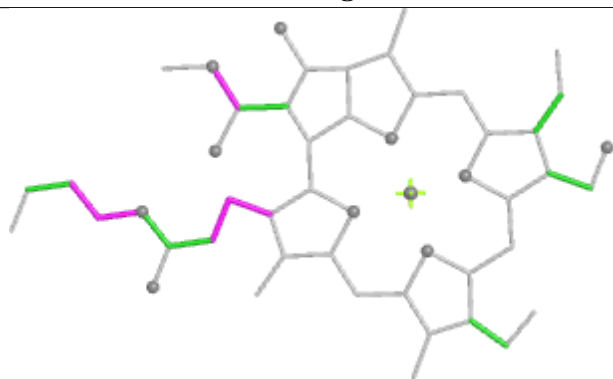
Ligand CHL Z 608



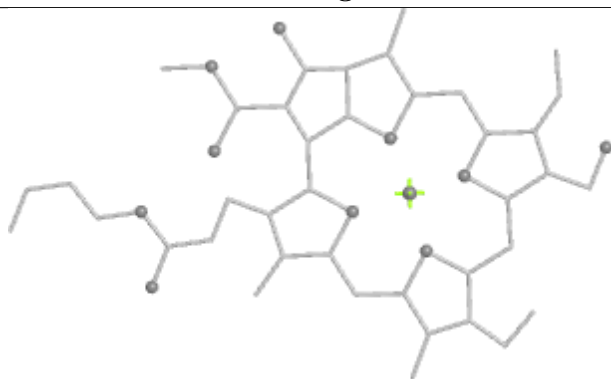
Bond lengths



Bond angles

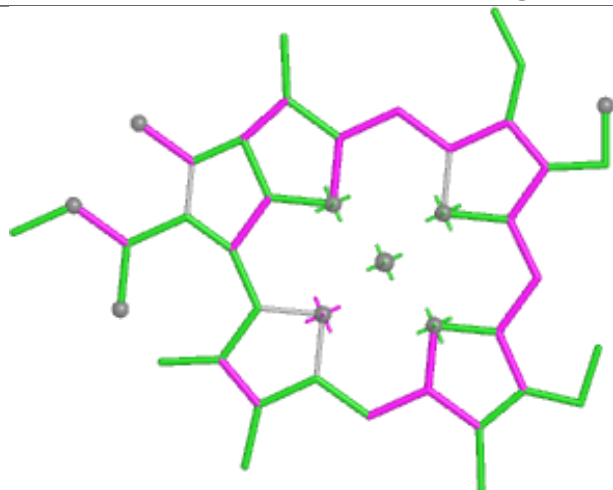


Torsions

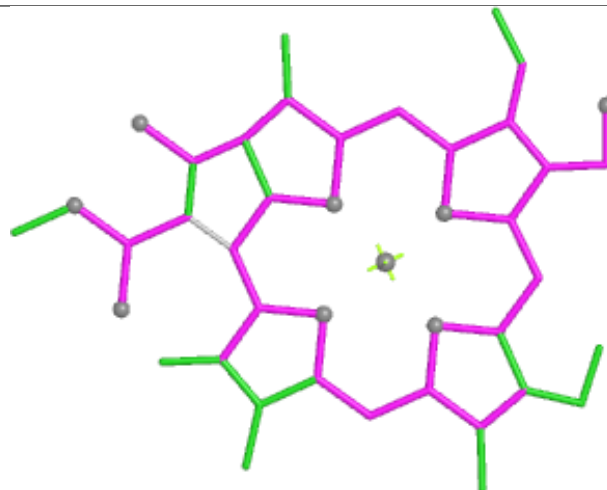


Rings

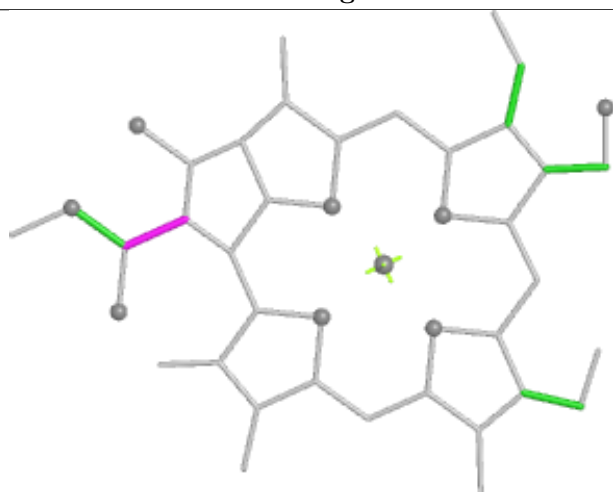
Ligand CHL Y 605



Bond lengths



Bond angles

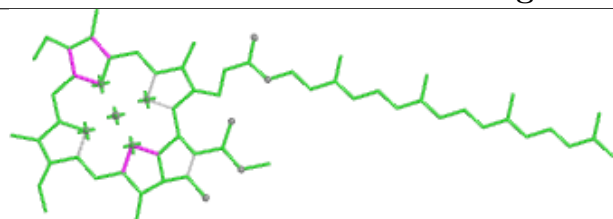


Torsions

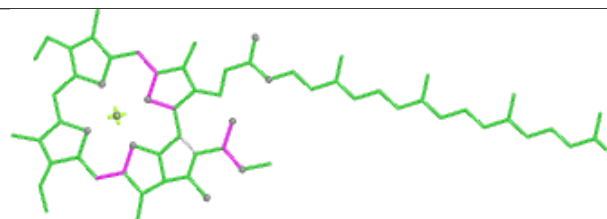


Rings

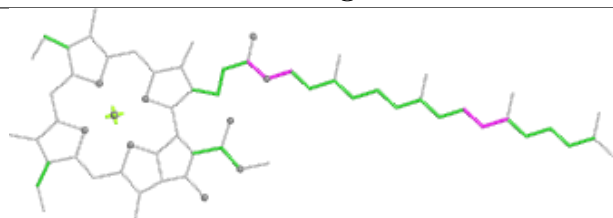
Ligand CLA Z 612



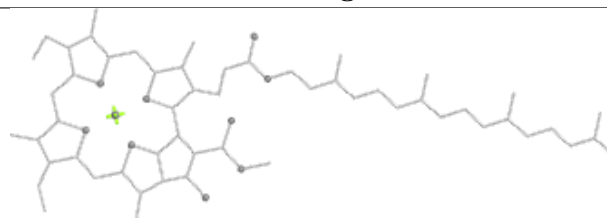
Bond lengths



Bond angles

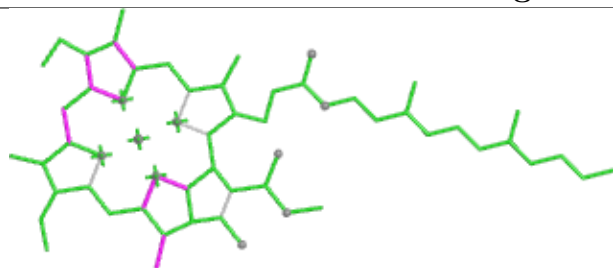


Torsions

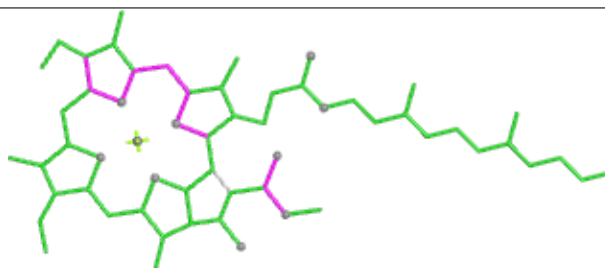


Rings

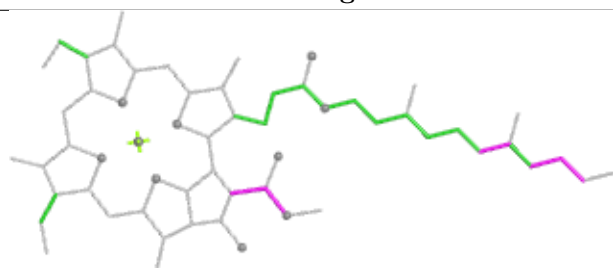
Ligand CLA Y 602



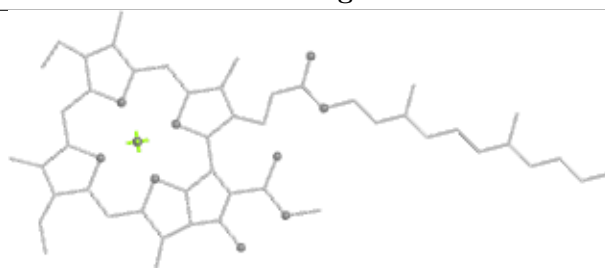
Bond lengths



Bond angles

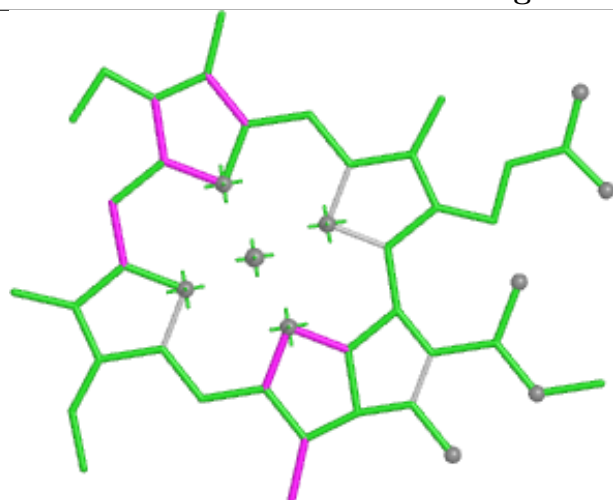


Torsions

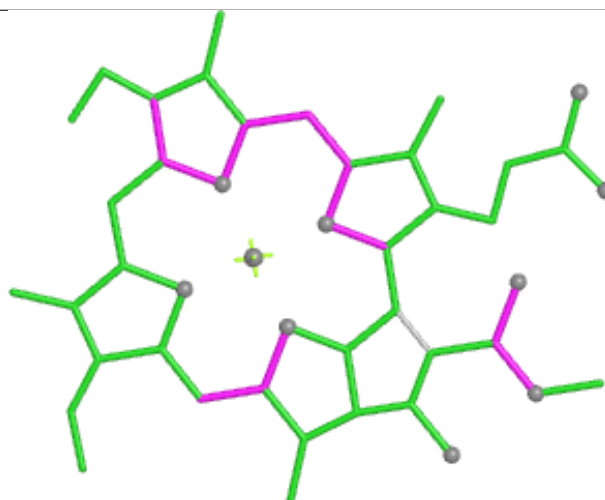


Rings

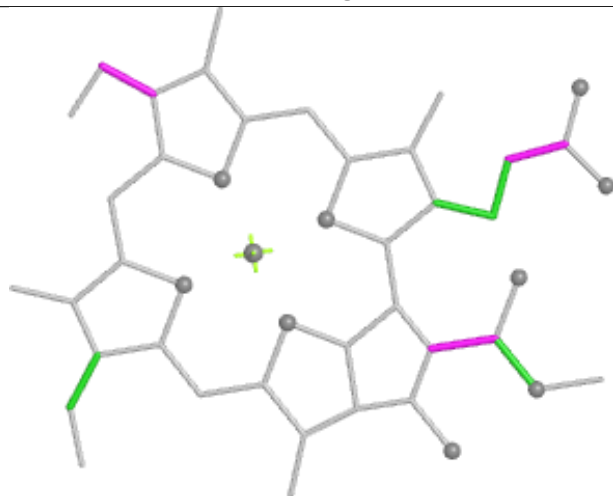
Ligand CLA Y 612



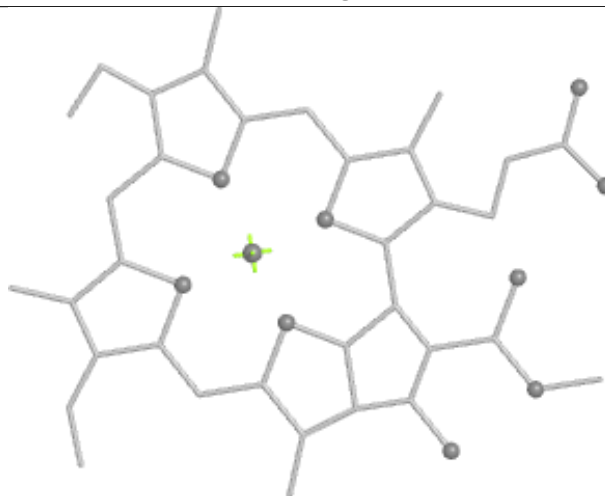
Bond lengths



Bond angles

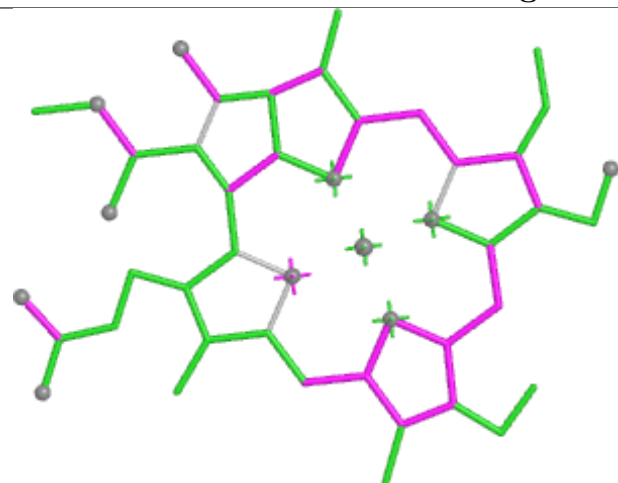


Torsions

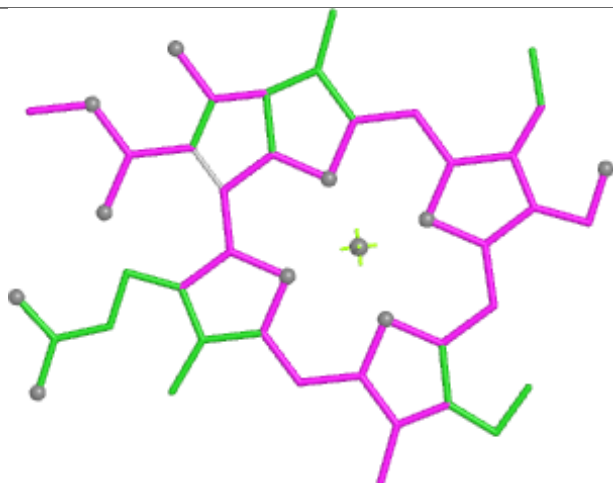


Rings

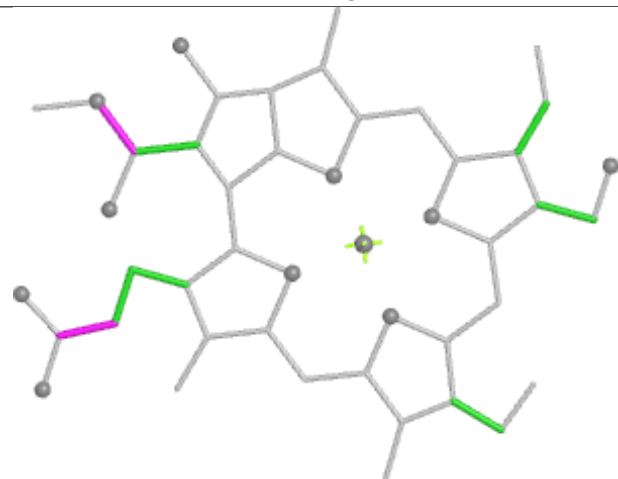
Ligand CHL Z 606



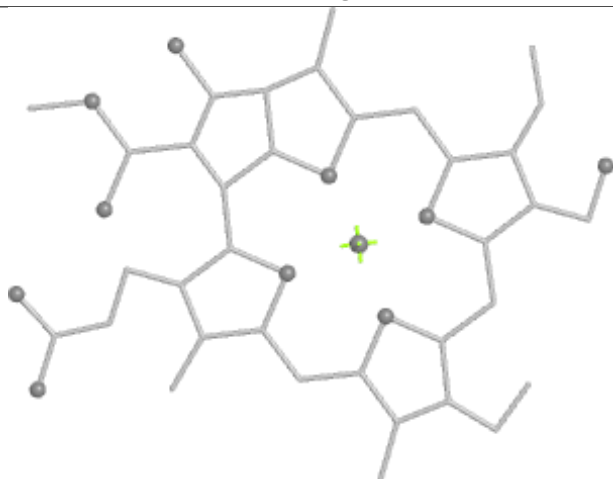
Bond lengths



Bond angles

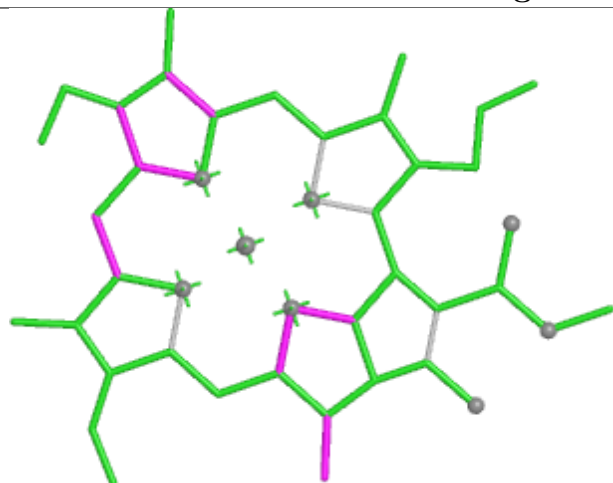


Torsions

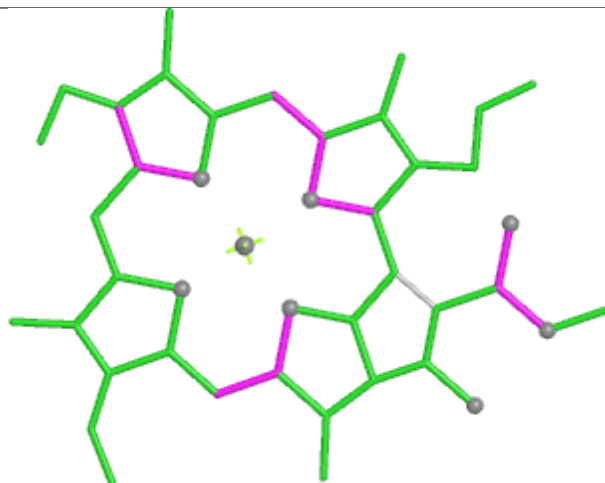


Rings

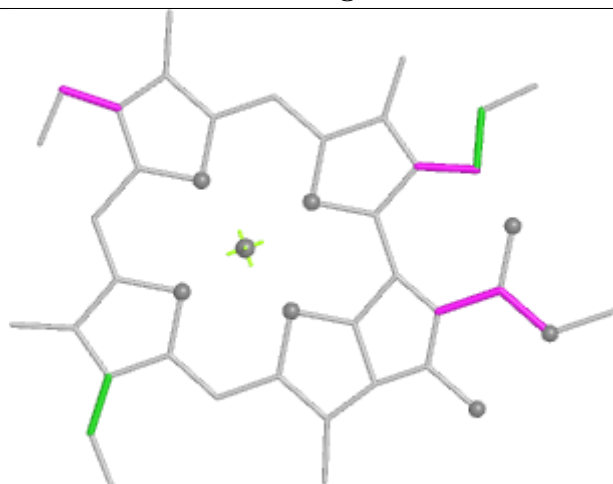
Ligand CLA Y 611



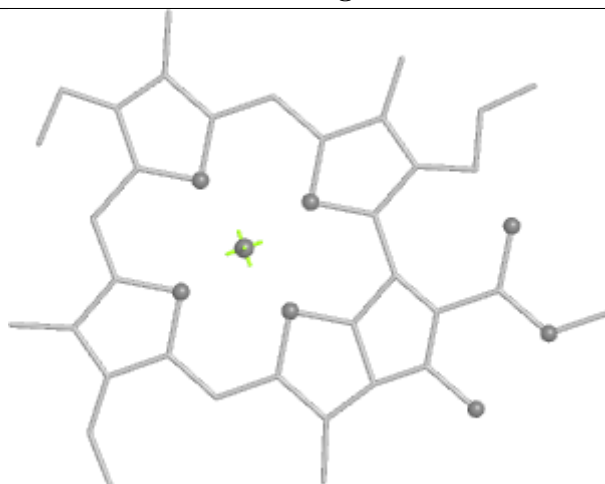
Bond lengths



Bond angles

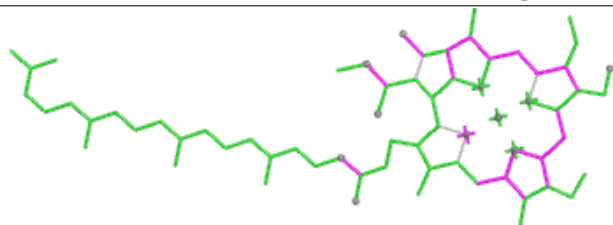


Torsions

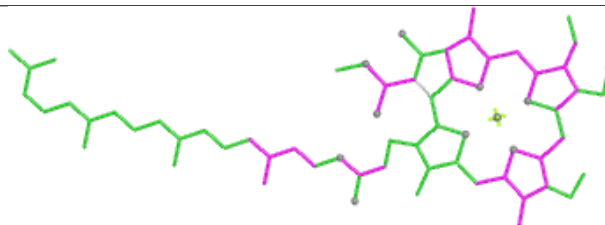


Rings

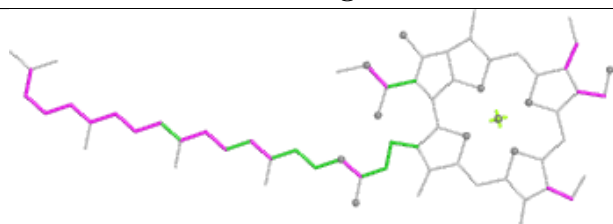
Ligand CHL Z 609



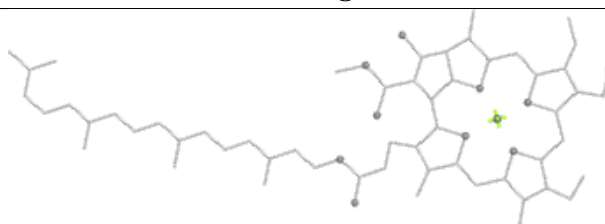
Bond lengths



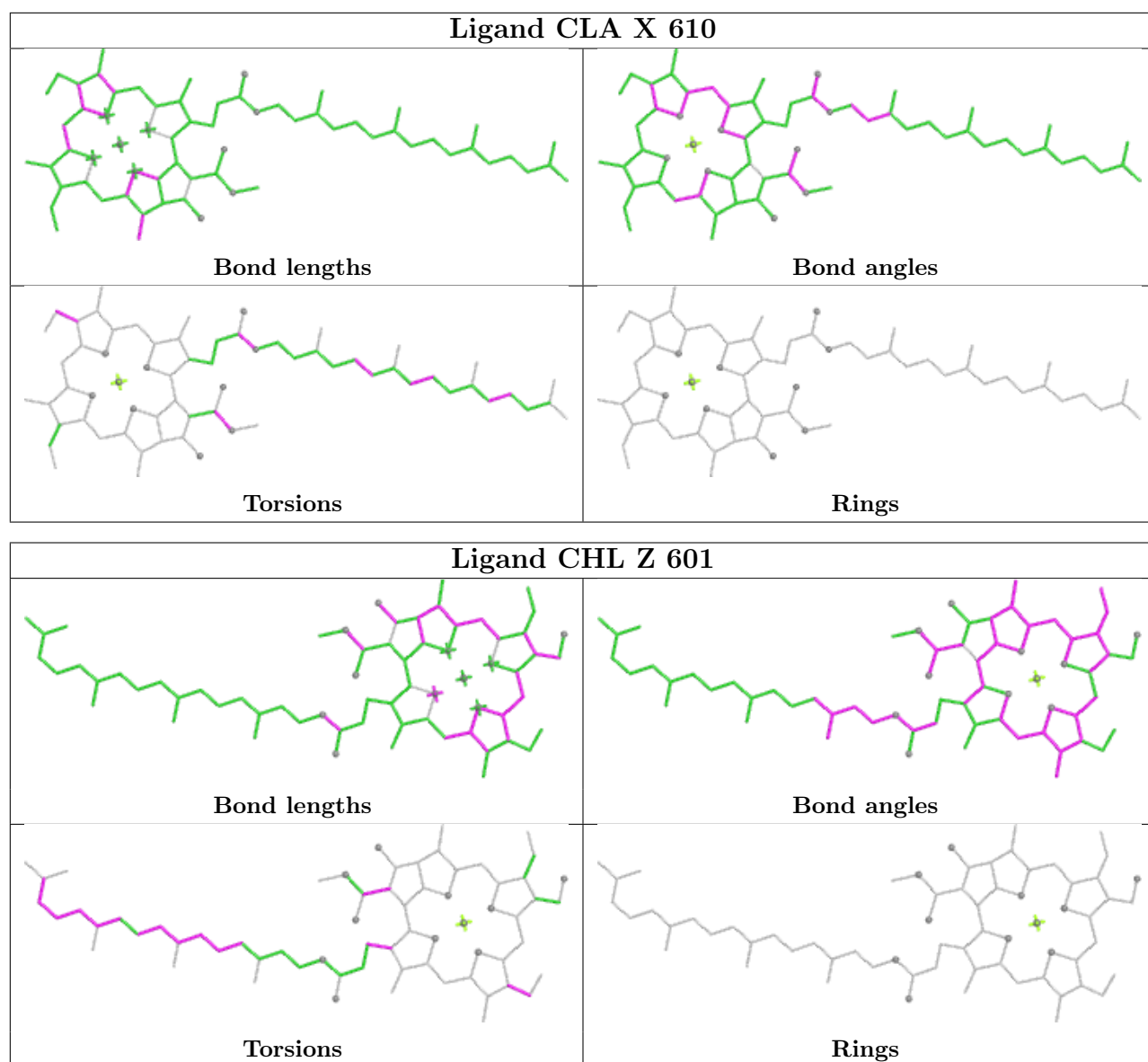
Bond angles



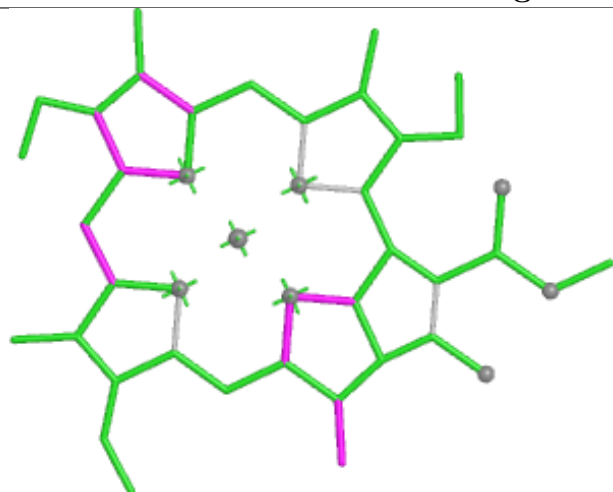
Torsions



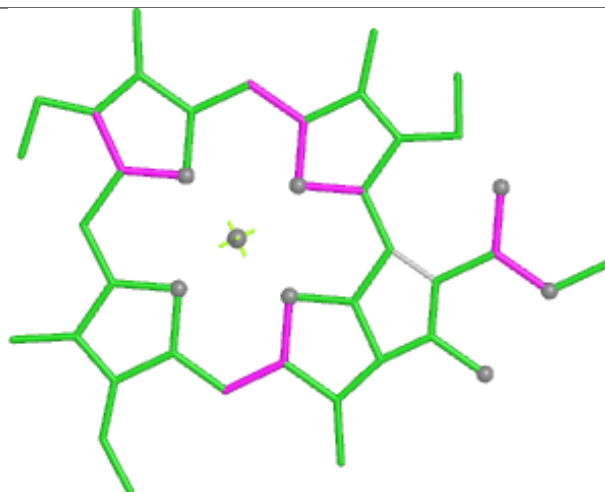
Rings



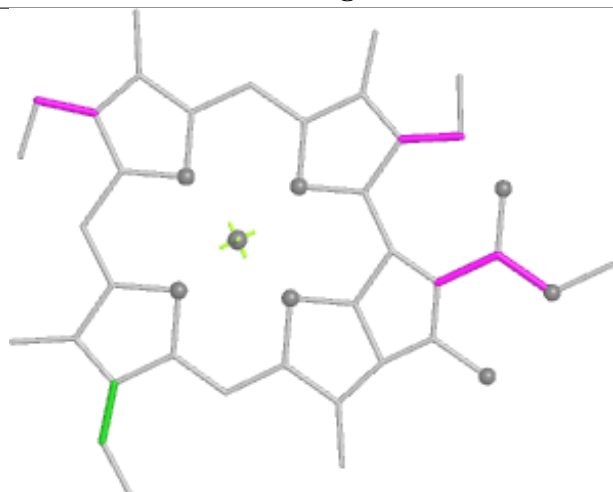
Ligand CLA X 614



Bond lengths



Bond angles

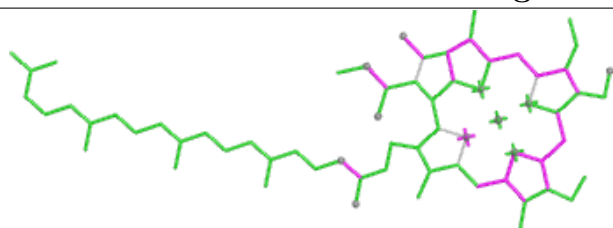


Torsions

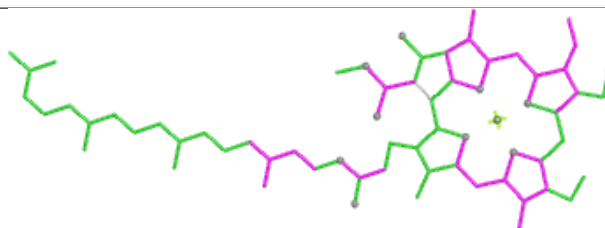


Rings

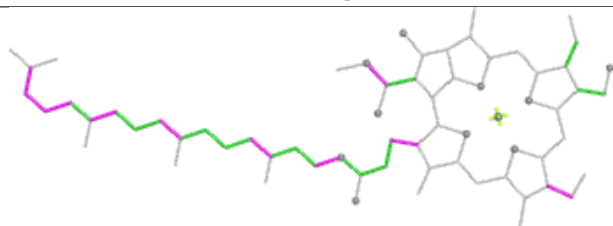
Ligand CHL Y 609



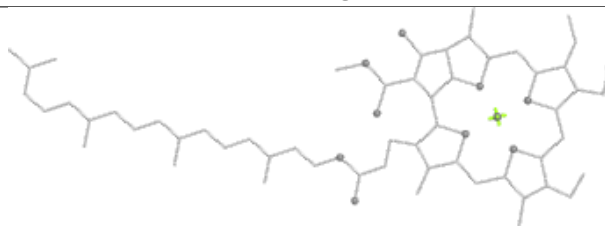
Bond lengths



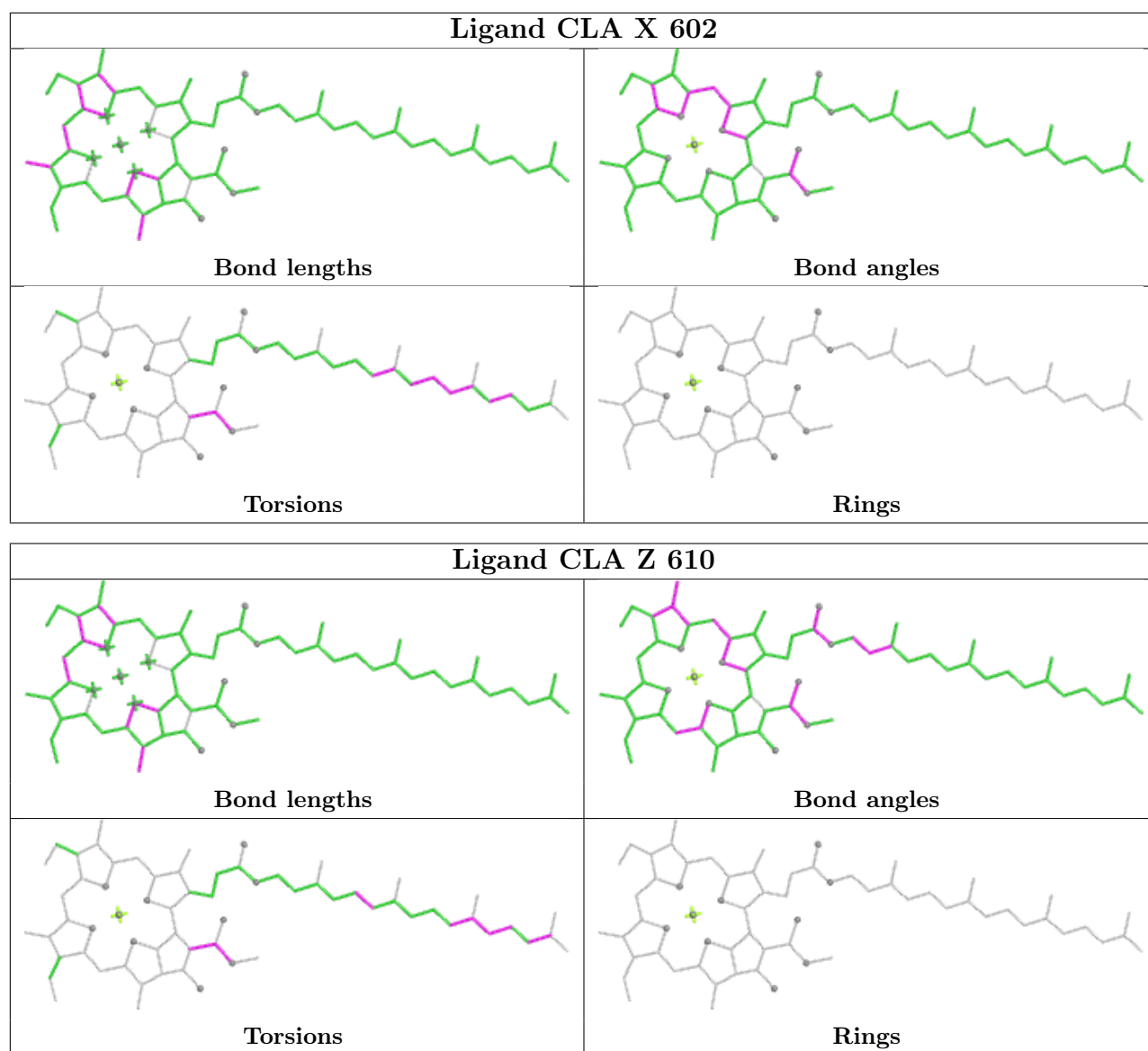
Bond angles

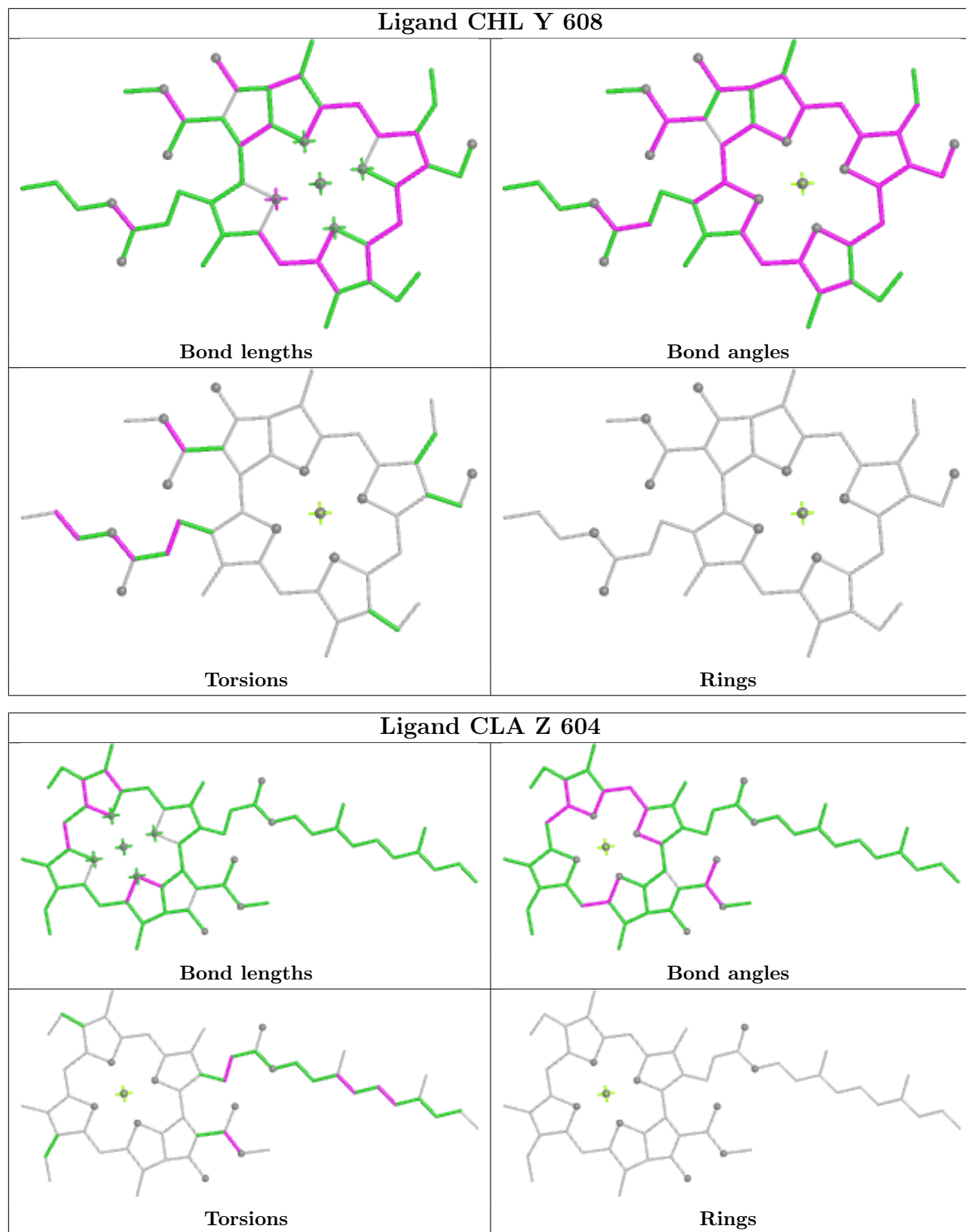


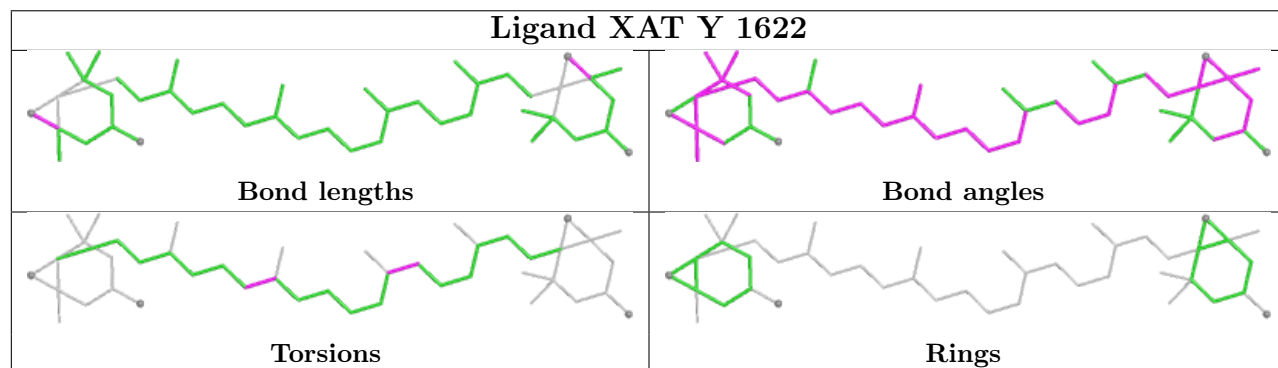
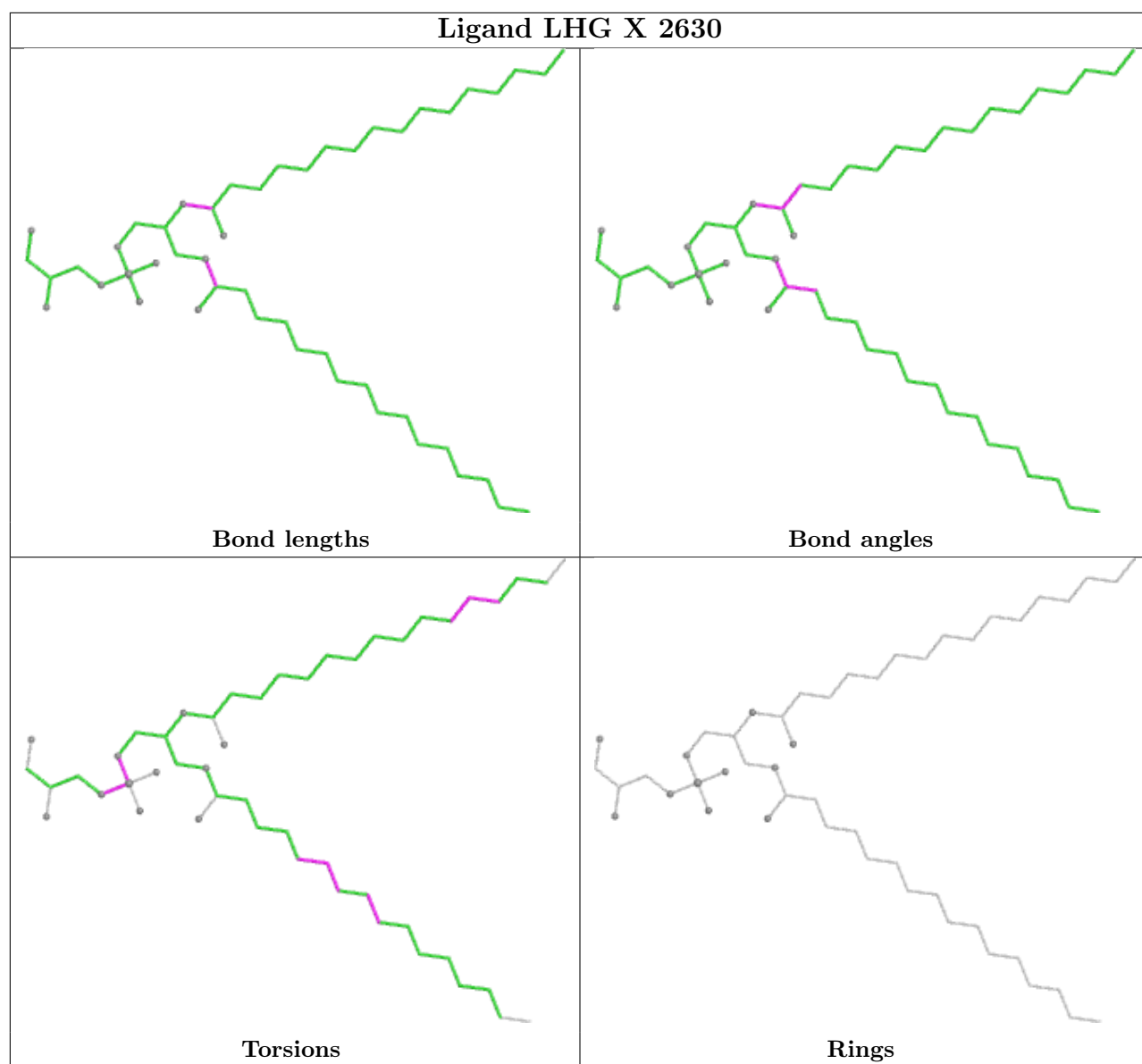
Torsions

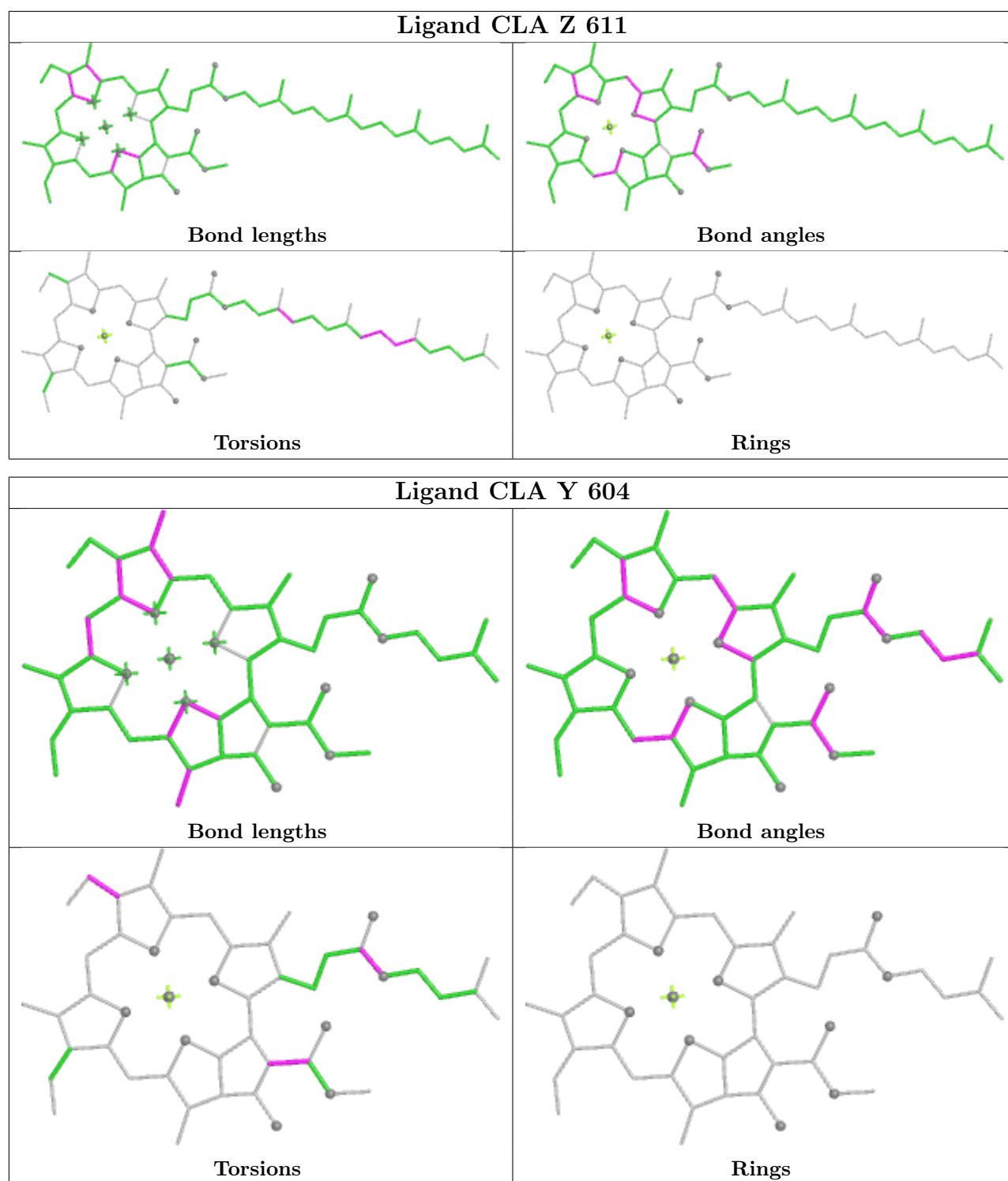


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

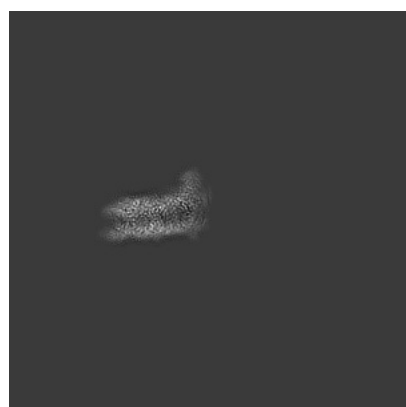
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30934. These allow visual inspection of the internal detail of the map and identification of artifacts.

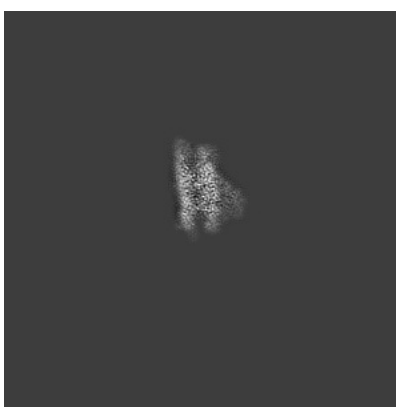
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

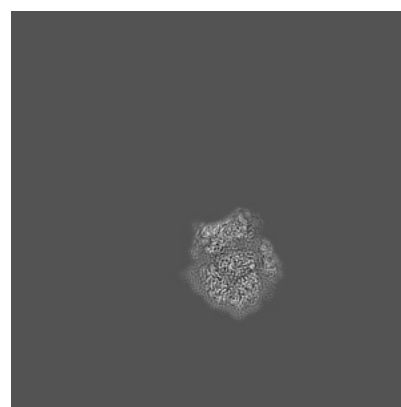
6.1.1 Primary map



X



Y



Z

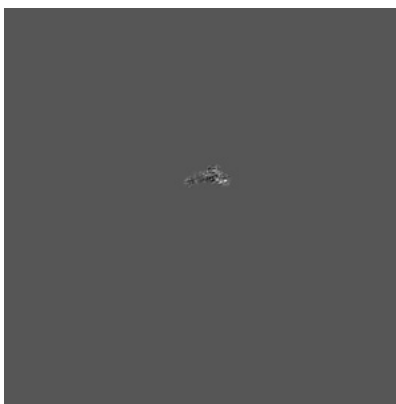
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

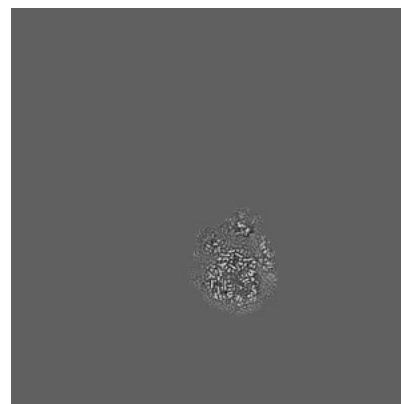
6.2.1 Primary map



X Index: 240



Y Index: 240

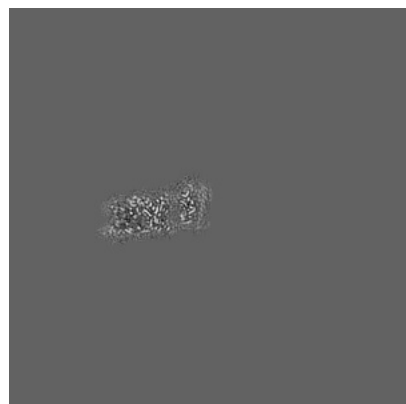


Z Index: 240

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

6.3 Largest variance slices [i](#)

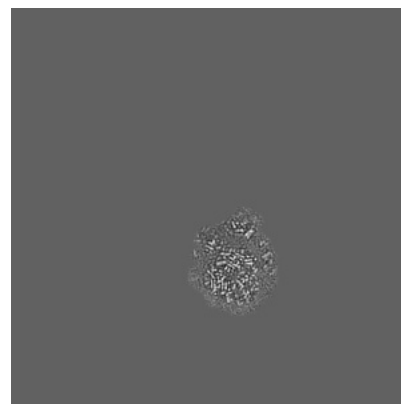
6.3.1 Primary map



X Index: 274



Y Index: 171

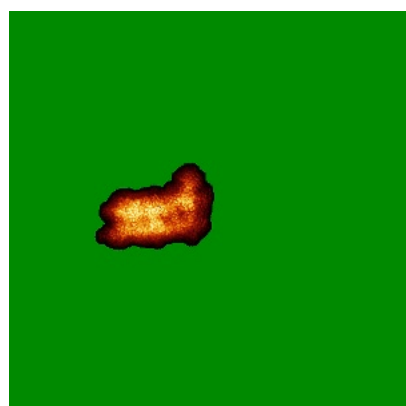


Z Index: 242

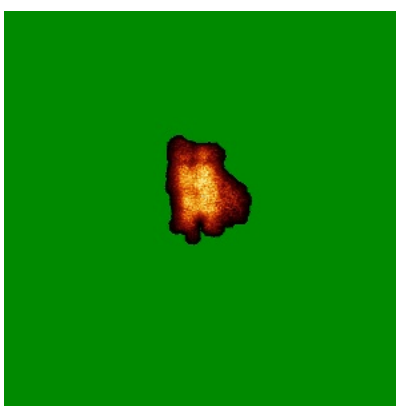
The images above show the largest variance slices of the map in three orthogonal directions.

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

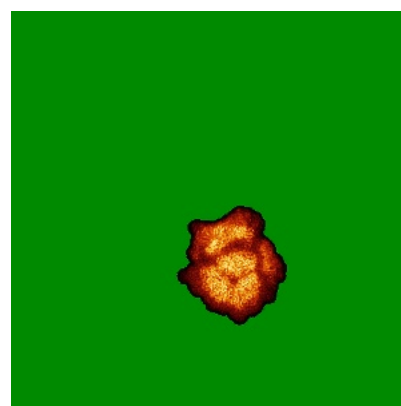
6.4.1 Primary map



X



Y

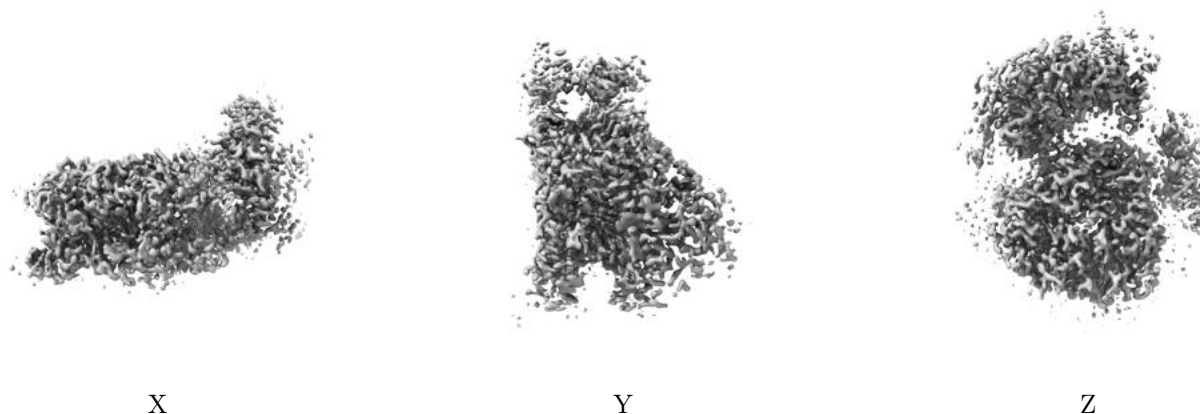


Z

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

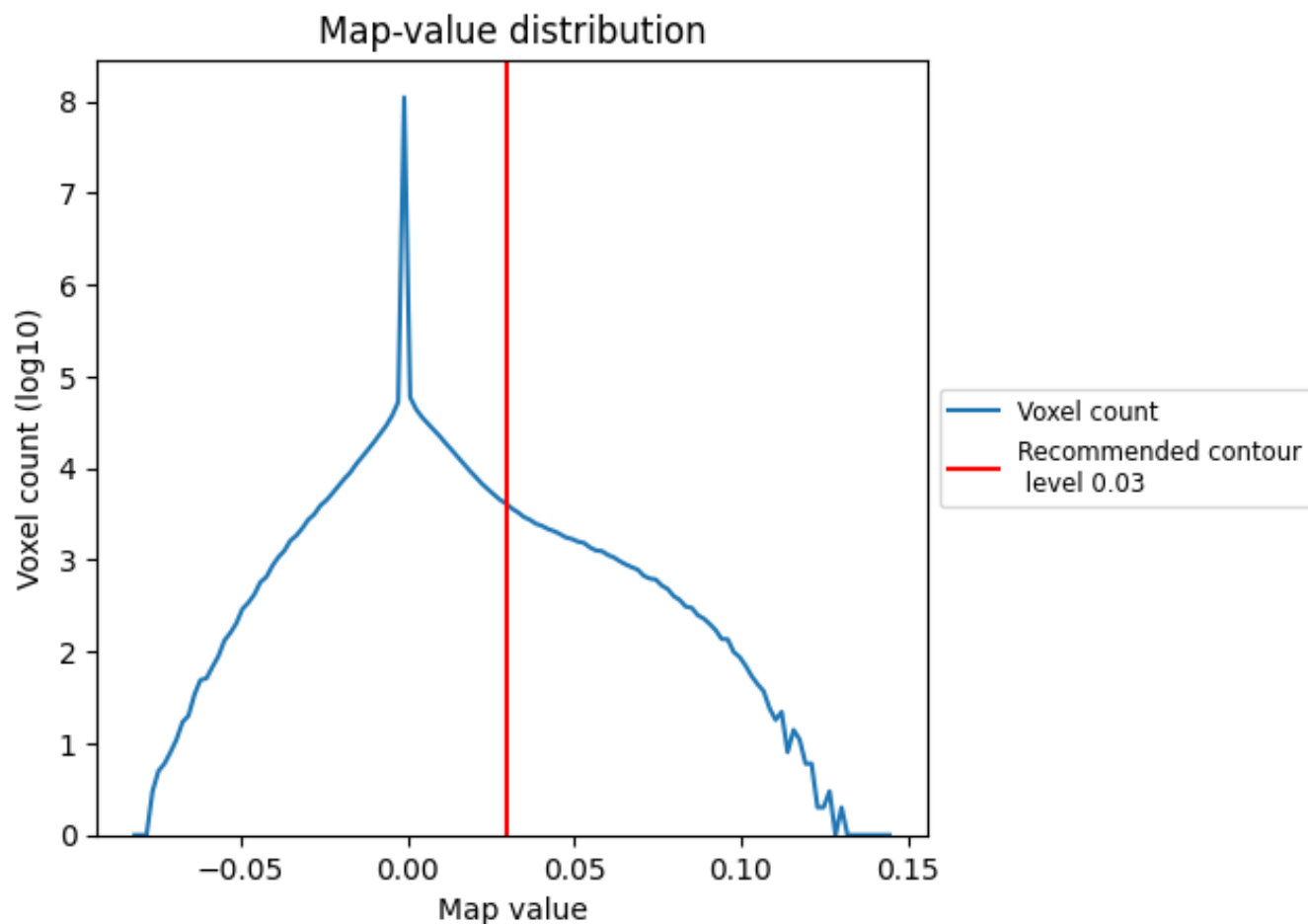
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

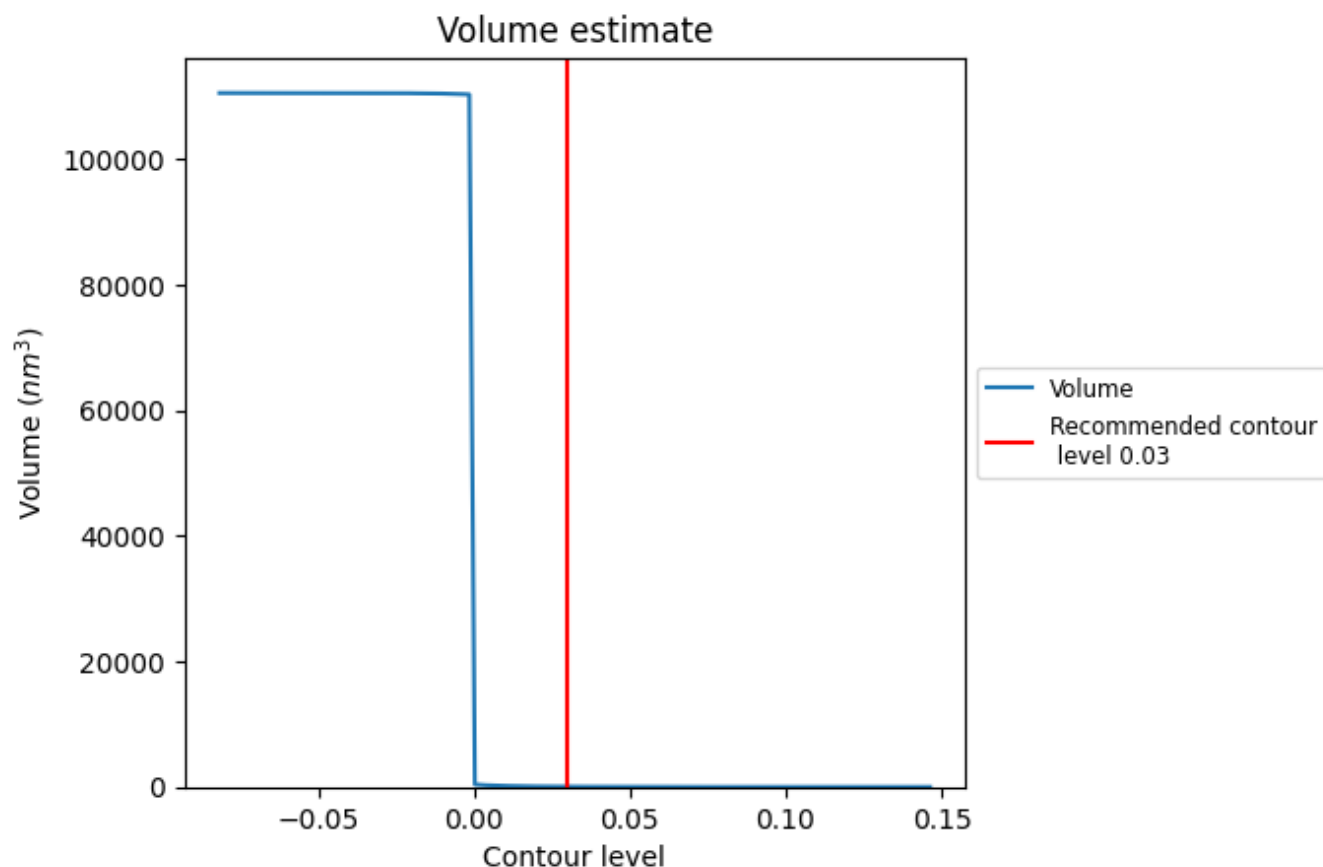
This section contains the results of statistical analysis of the map.

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.

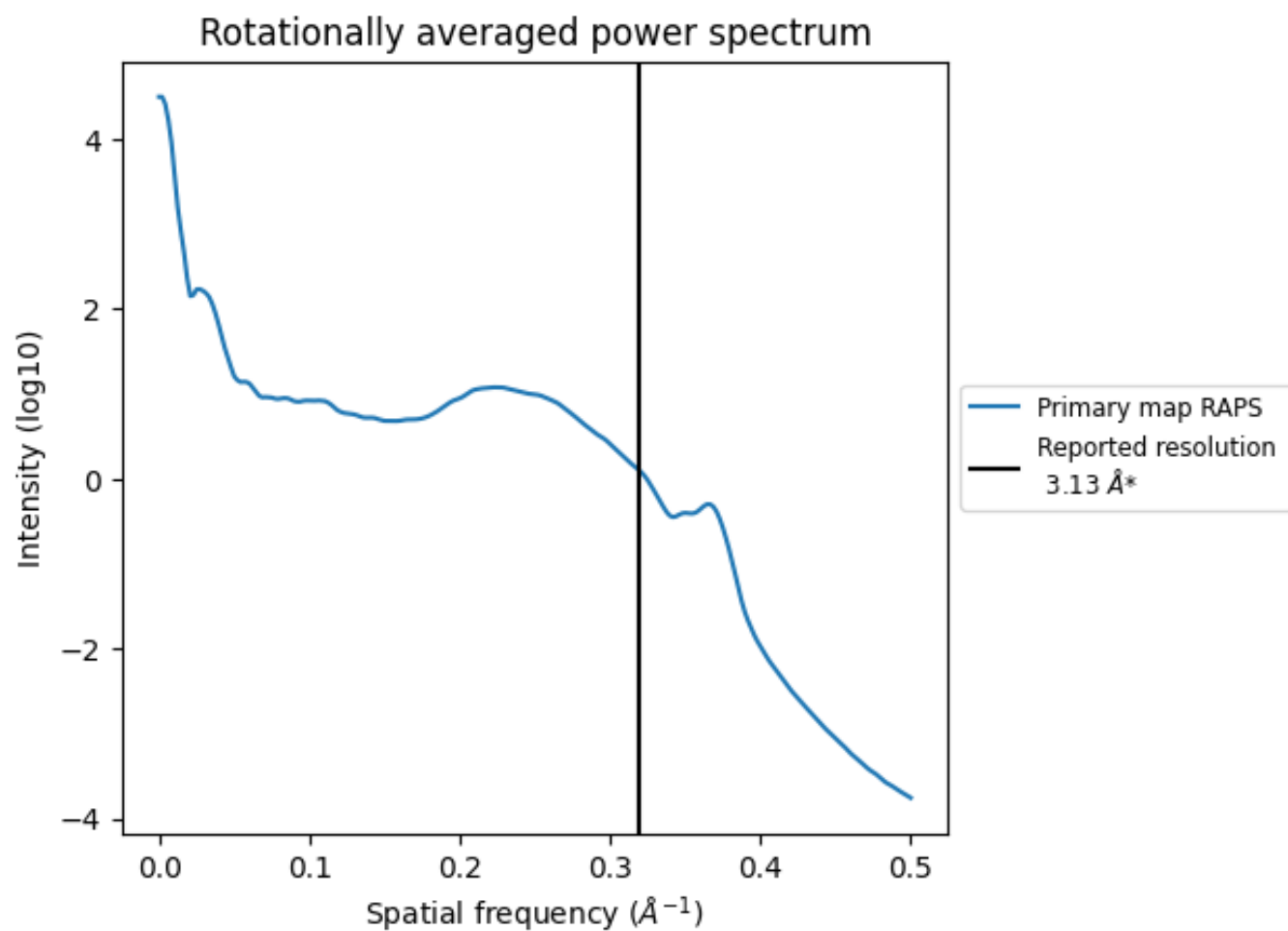
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49 nm^3 ; this corresponds to an approximate mass of 44 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 0.319 Å⁻¹

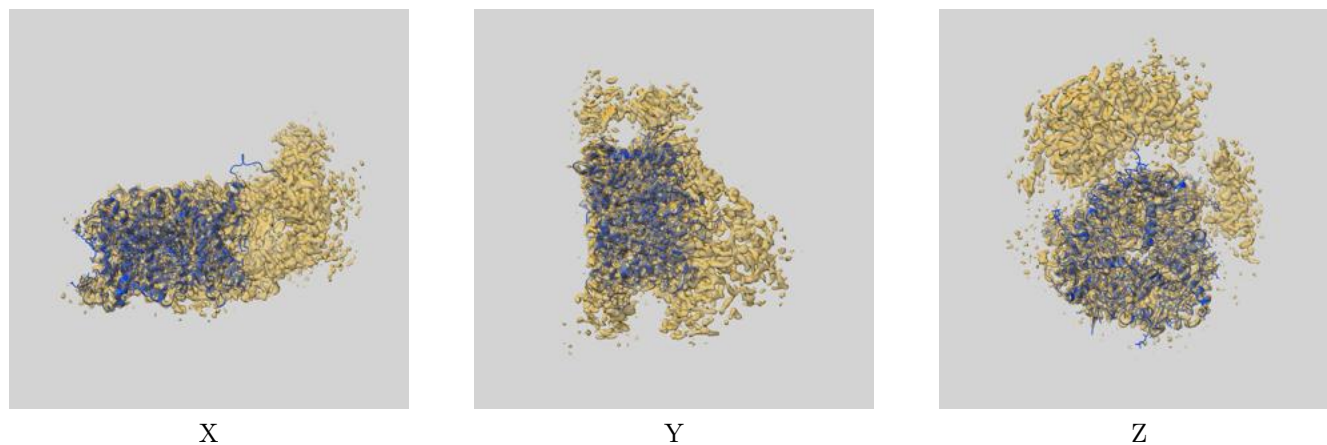
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

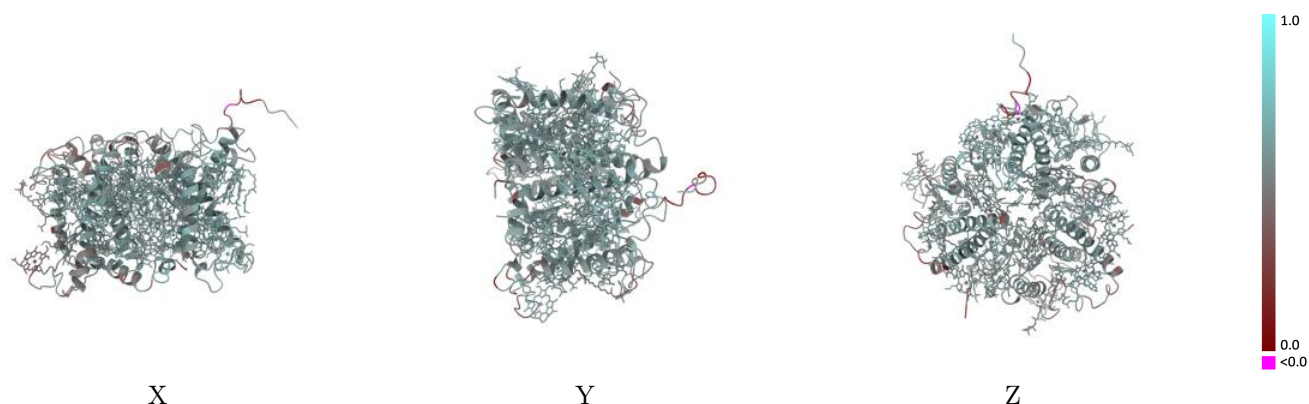
This section contains information regarding the fit between EMDB map EMD-30934 and PDB model 7E0J. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



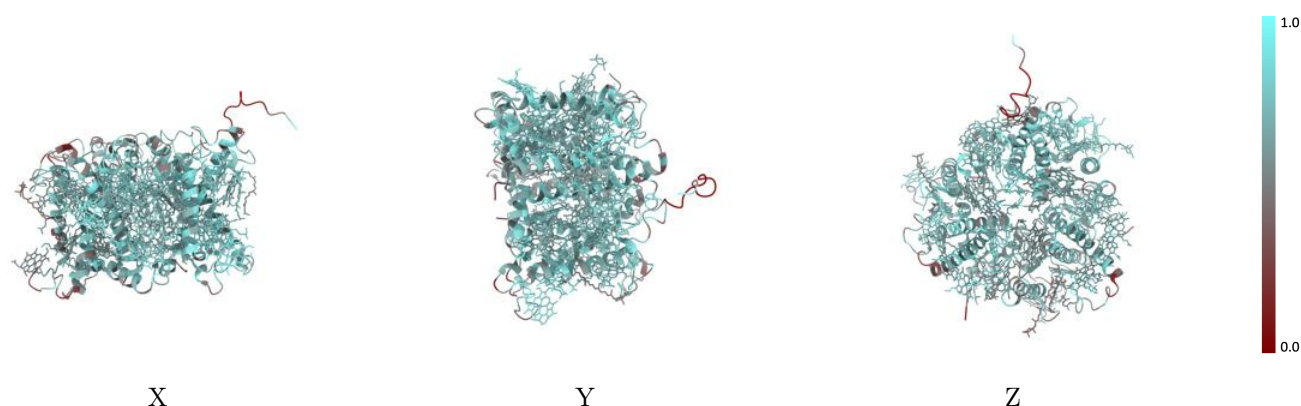
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



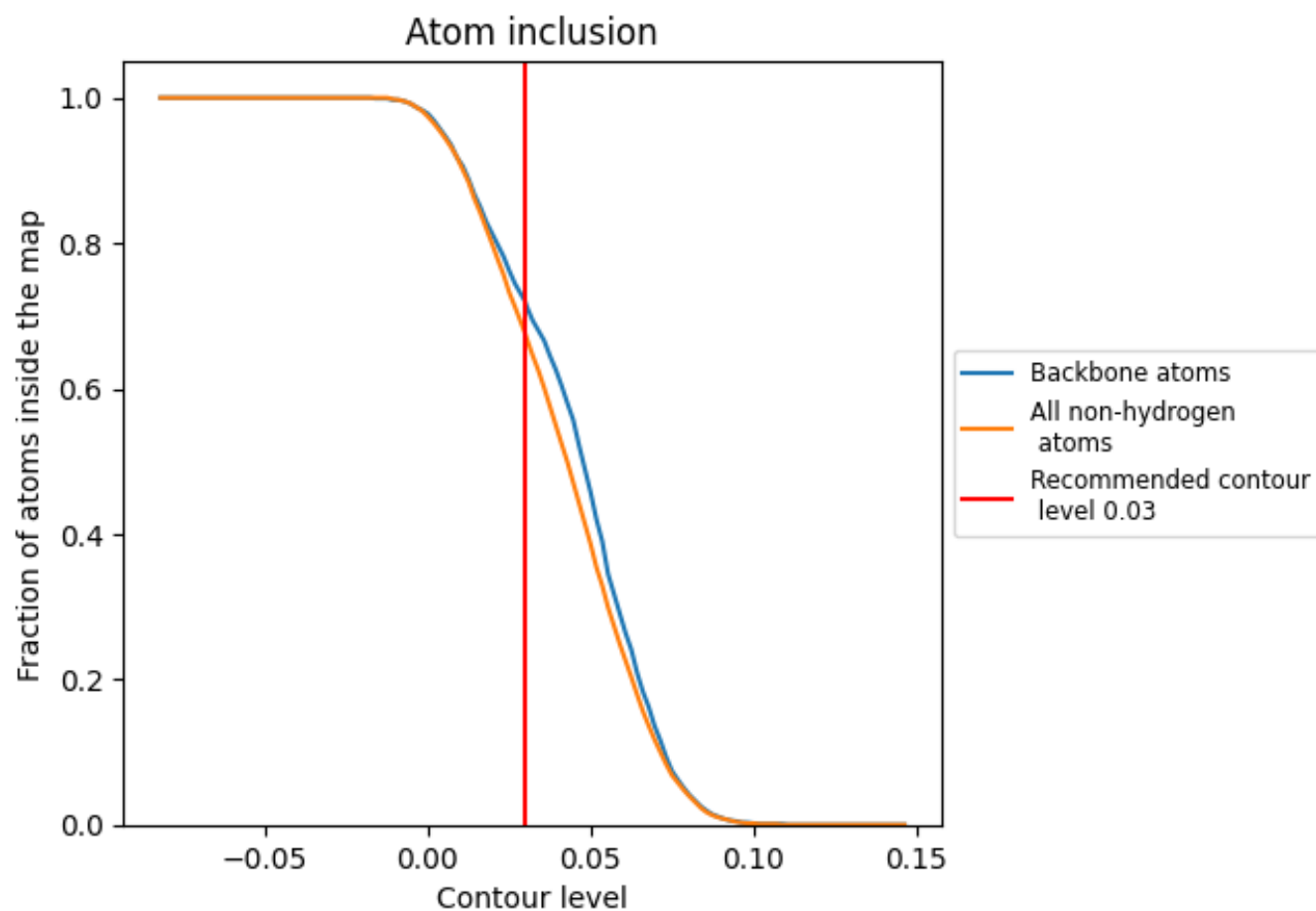
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 68% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6760	0.5440
X	0.6510	0.5290
Y	0.6790	0.5350
Z	0.6960	0.5660

