



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 11:38 AM JST

PDB ID : 7VZR / pdb_00007vzr
EMDB ID : EMD-32229
Title : Structure of the Acidobacteria homodimeric reaction center bound with cytochrome c (the smaller form)
Authors : Huang, G.Q.; Dong, S.S.; Qin, X.C.; Sui, S.F.
Deposited on : 2021-11-16
Resolution : 2.22 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:

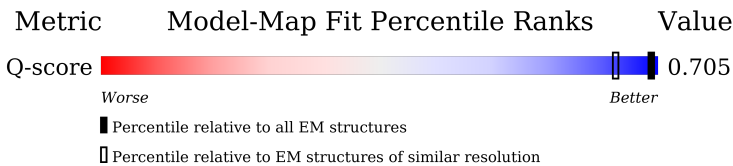
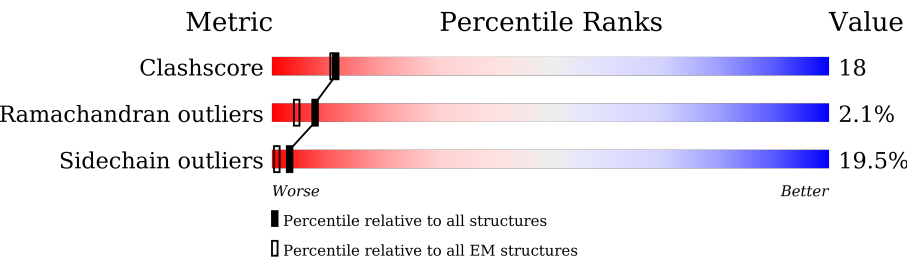
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.22 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.



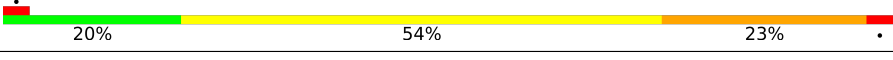
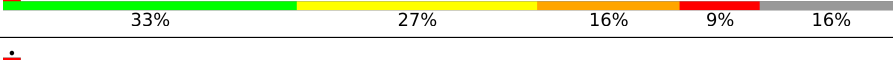
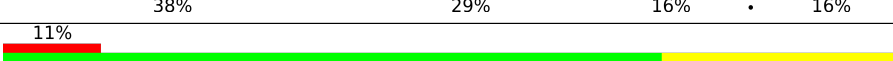
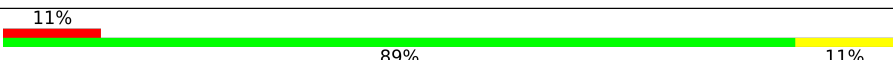
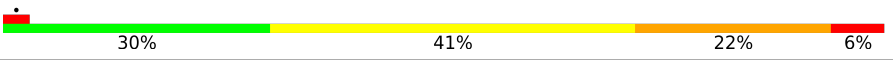
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3277 (1.73 - 2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	865	52%32%11% . .
1	a	865	58%29%9% . .
2	C	221	37%33%11%7%13%
3	E	35	23%60%17%
3	e	35	46%43%9% .

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Mol	Chain	Length	Quality of chain
4	F	35	
4	f	35	
5	G	45	
5	g	45	
6	H	19	
6	h	19	
7	c	145	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	A	910	X	-	-	-
10	CLA	A	911	X	-	-	-
11	LYC	c	201	-	X	-	-
14	UNL	A	922	-	-	X	-
14	UNL	A	923	-	-	X	-
14	UNL	A	927	-	-	X	-
14	UNL	C	302	-	-	X	-
14	UNL	a	926	-	-	X	-
14	UNL	a	930	-	-	X	-
14	UNL	a	931	-	-	X	-
16	HEC	C	301	X	X	-	-
16	HEC	c	202	X	-	-	-
18	SF4	a	917	-	-	X	-
8	2GO	A	901	X	-	-	-
8	2GO	a	903	X	-	-	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 21354 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 Photosynthetic reaction center subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	854	Total	C	N	O	S	0	0
			6960	4602	1155	1170	33		
1	a	858	Total	C	N	O	S	0	0
			6984	4616	1160	1175	33		

- Molecule 2 is a protein called Cytochrome c, mono-and diheme variants.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	193	Total	C	N	O	S	0	0
			1474	900	277	288	9		

- Molecule 3 is a protein called PscE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	35	Total	C	N	O	S	0	0
			258	174	40	42	2		
3	e	35	Total	C	N	O	S	0	0
			258	174	40	42	2		

- Molecule 4 is a protein called PscF.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	35	Total	C	N	O	S	0	0
			273	185	43	43	2		
4	f	35	Total	C	N	O	S	0	0
			273	185	43	43	2		

- Molecule 5 is a protein called PscG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	38	Total	C	N	O	S	0	0
			302	210	45	44	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	38	Total	C	N	O	S	0	0
			302	210	45	44	3		

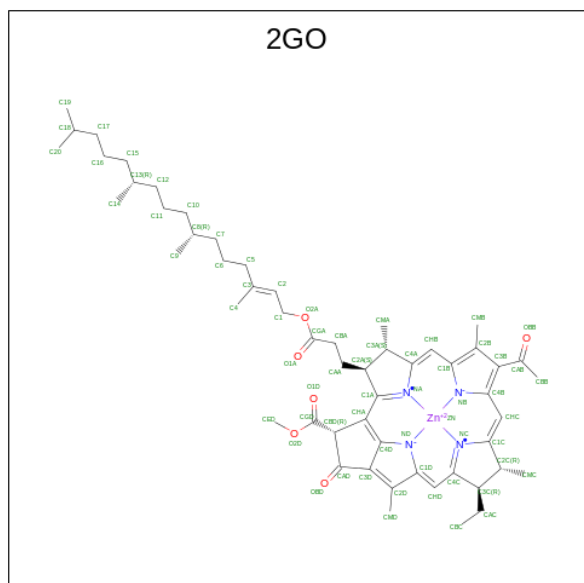
- Molecule 6 is a protein called undefined polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	19	Total	C	N	O	0	0
			95	57	19	19		
6	h	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 7 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	145	Total	C	N	O	S	0	0
			1096	679	200	210	7		

- Molecule 8 is (T-4-S)-[(3S,4S,13R,14R,21R,23R,25R)-9-acetyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-(3-oxo-3-[(2E,7R,11R)-3,7,11,15-tetramethylhexadec-2-en-1-yl]oxy}propyl)-23,25-didehydro-13,14-dihydrophorbine-23,25-diido-kappa 4 N 23 ,N 24 , N 25 ,N 26]zinc (CCD ID: 2GO) (formula: C₅₅H₇₄N₄O₆Zn) (labeled as "Ligand of Interest" by depositor).



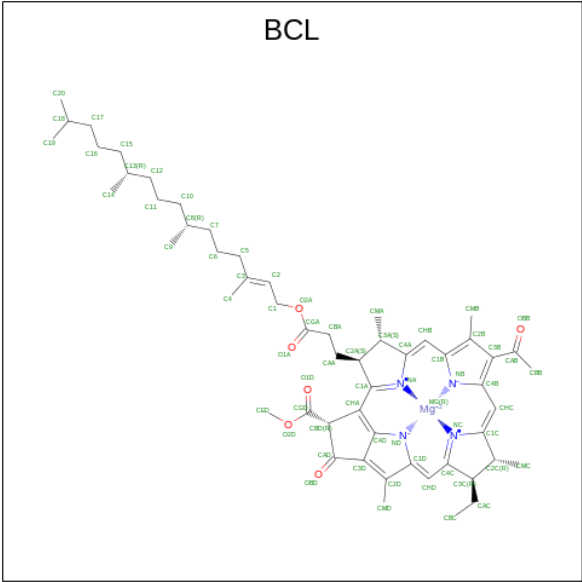
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	Zn	0
			66	55	4	6	1	

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

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



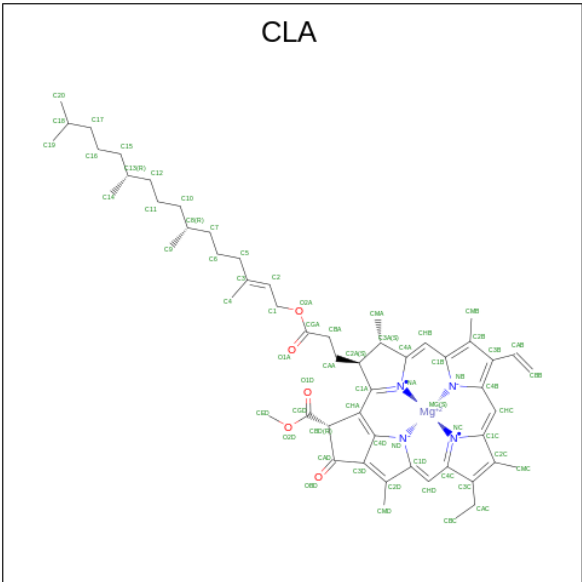
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
9	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



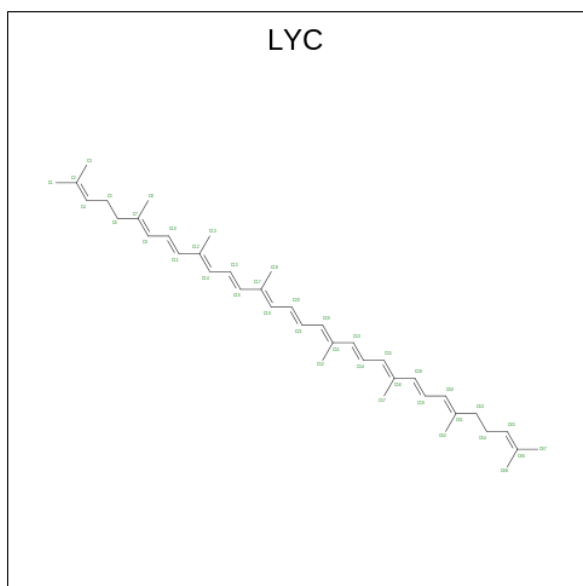
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
10	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
10	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

- Molecule 11 is LYCOPENE (CCD ID: LYC) (formula: $C_{40}H_{56}$).

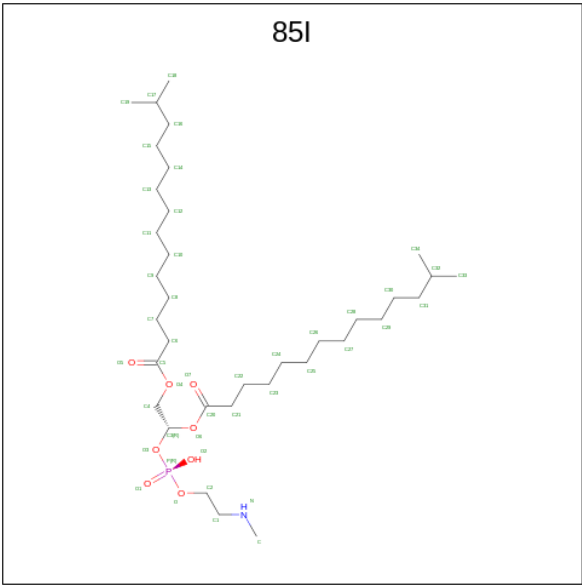


Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	C	0
			40	40	
11	c	1	Total	C	0
			40	40	

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Ca	0
			1	1	
12	a	1	Total	Ca	0
			1	1	

- Molecule 13 is [(2 {R})-2-[2-(methylamino)ethoxy-oxidanyl-phosphoryl]oxy-2-(13-methyltetradecanoyloxy)ethyl] 13-methyltetradecanoate (CCD ID: 85I) (formula: C₃₅H₇₀NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	a	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 14 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

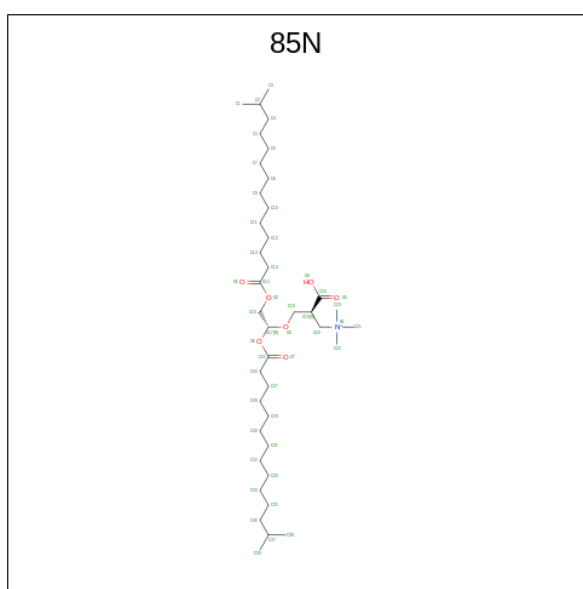
Mol	Chain	Residues	Atoms		AltConf
14	A	13	Total	C	0
			240	240	
14	C	1	Total	C	0
			18	18	
14	E	2	Total	C	0
			26	26	

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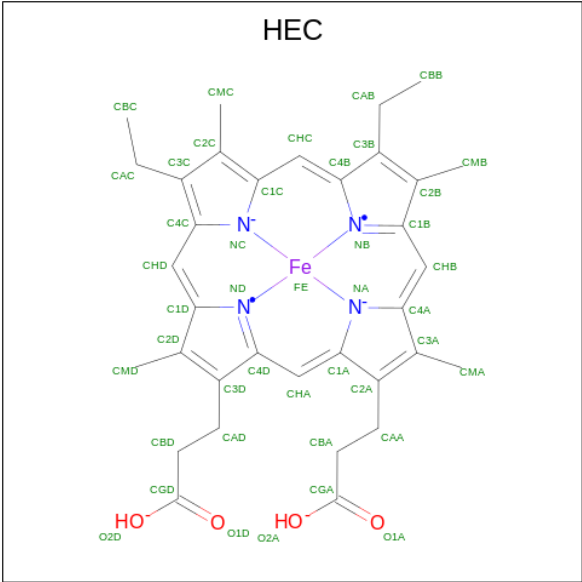
Mol	Chain	Residues	Atoms		AltConf
14	a	13	Total	C	0
			243	243	
14	c	1	Total	C	0
			8	8	
14	e	2	Total	C	0
			26	26	

- Molecule 15 is [(2 {S})-2-[(1 {R})-1,2-bis(13-methyltetradecanoyloxy)ethoxy]methyl]-3-oxidanyl-3-oxidanylidene-propyl]-trimethyl-azanium (CCD ID: 85N) (formula: C₃₉H₇₆NO₇) (labeled as "Ligand of Interest" by depositor).



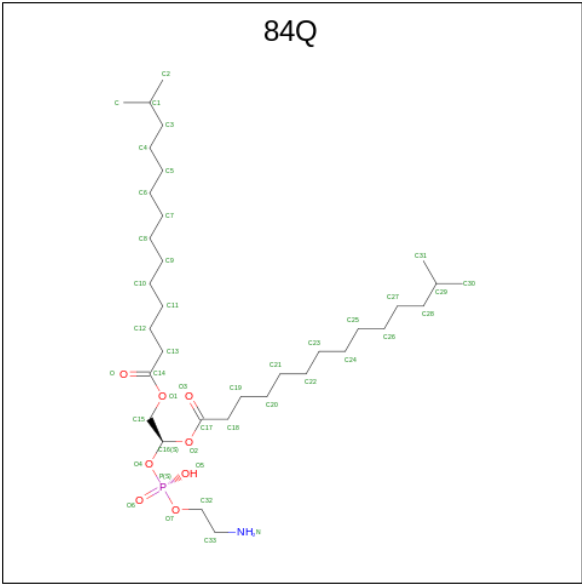
Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total	C	N	O	0
			47	39	1	7	
15	G	1	Total	C	N	O	0
			38	30	1	7	
15	a	1	Total	C	N	O	0
			47	39	1	7	
15	g	1	Total	C	N	O	0
			38	30	1	7	

- Molecule 16 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
16	c	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 17 is [(2S)-2-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-(13-methyltetradecanoxy)ethyl] 13-methyltetradecanoate (CCD ID: 84Q) (formula: C₃₄H₆₈NO₈P) (labeled as "Ligand of Interest" by depositor).



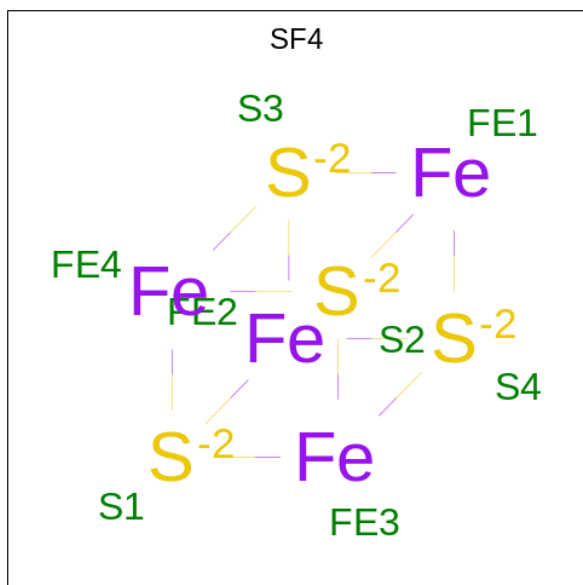
Mol	Chain	Residues	Atoms					AltConf
17	E	1	Total	C	N	O	P	0
			44	34	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	a	1	Total	Fe	S	0
			8	4	4	

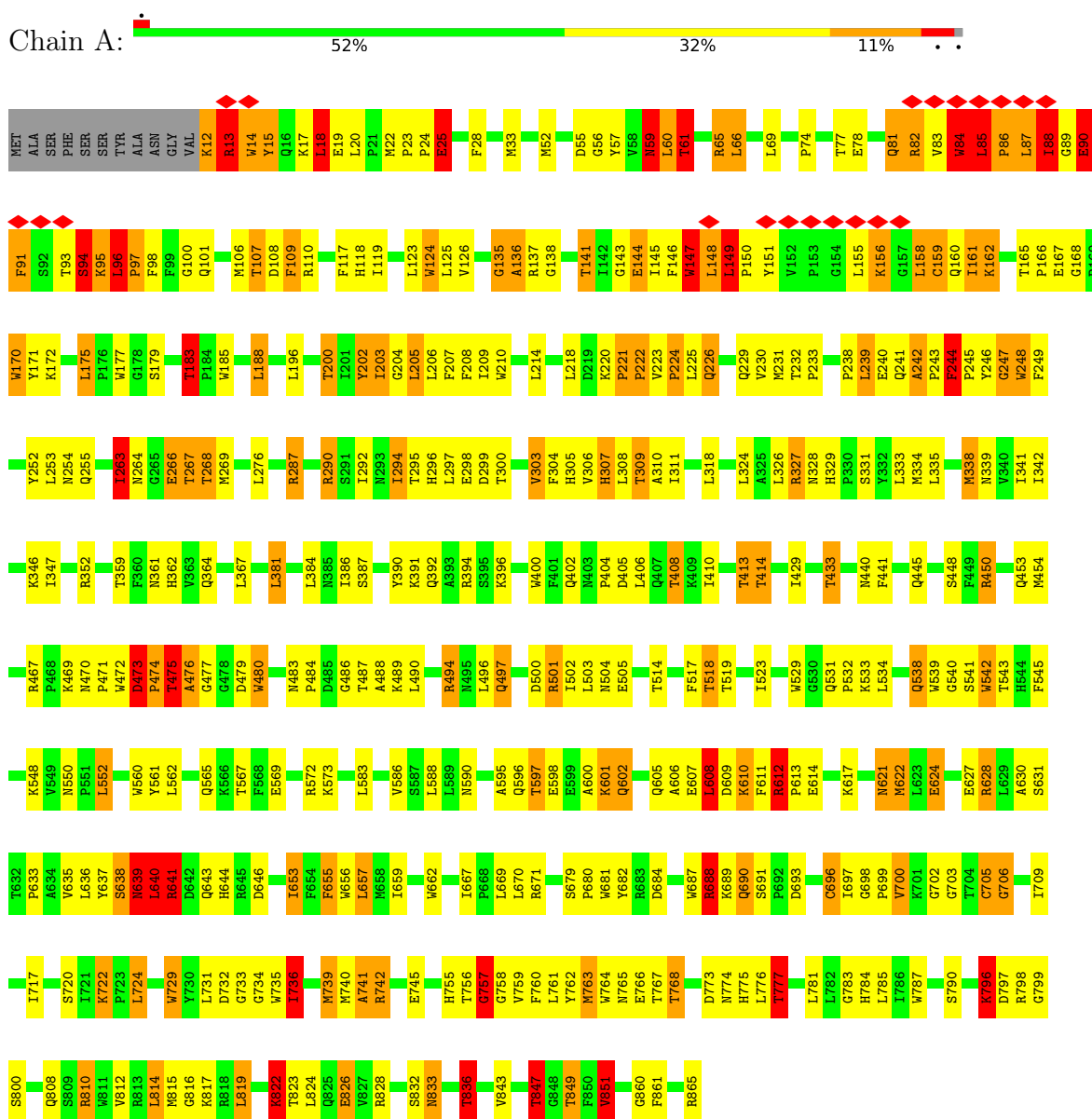
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	A	3	Total	O	0
			3	3	
19	a	3	Total	O	0
			3	3	

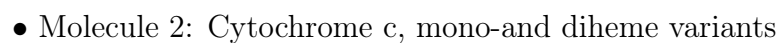
3 Residue-property plots

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: Photosynthetic reaction center subunit M

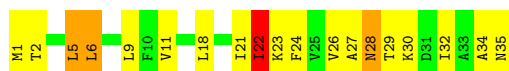


• Molecule 1: Photosynthetic reaction center subunit M

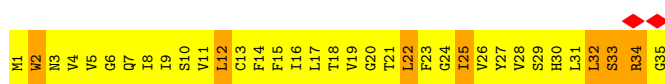
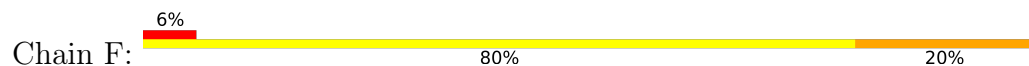




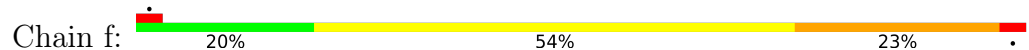
- Molecule 3: PscE



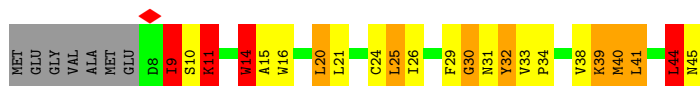
- Molecule 4: PscF



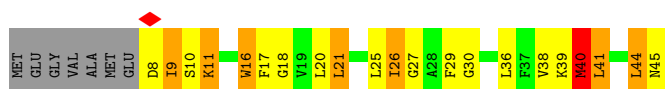
- Molecule 4: PscF



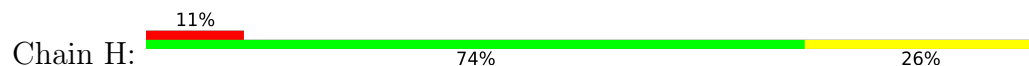
- Molecule 5: PscG



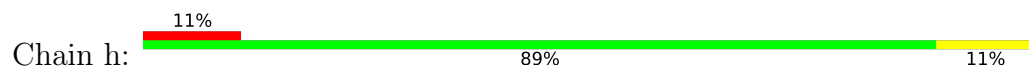
- Molecule 5: PscG



- Molecule 6: undefined polypeptide

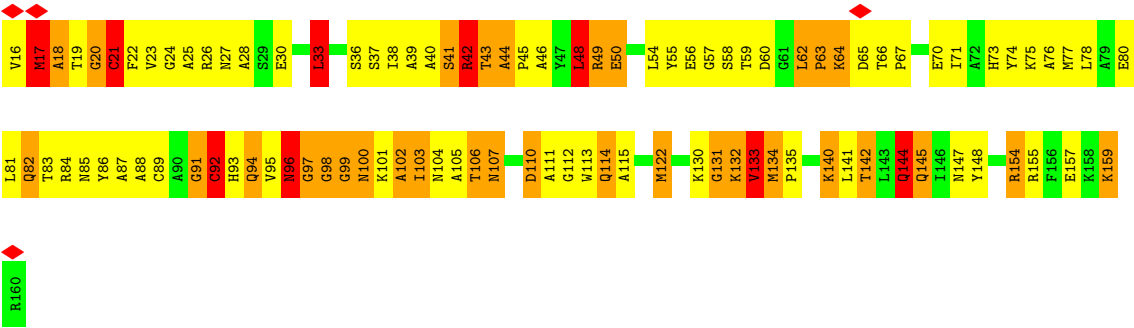


- Molecule 6: undefined polypeptide





• Molecule 7: Cytochrome c domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	490075	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.661	Depositor
Minimum map value	-2.809	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.164	Depositor
Recommended contour level	0.48	Depositor
Map size ($\text{\AA}$)	238.15, 238.15, 238.15	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 85N, 85I, HEC, CA, 84Q, UNL, 2GO, LYC, CLA, BCL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.27	241/7209 (3.3%)	1.57	111/9827 (1.1%)
1	a	2.04	178/7233 (2.5%)	1.42	92/9860 (0.9%)
2	C	3.01	114/1503 (7.6%)	2.06	66/2037 (3.2%)
3	E	3.18	26/262 (9.9%)	1.94	7/356 (2.0%)
3	e	2.23	9/262 (3.4%)	1.83	3/356 (0.8%)
4	F	3.38	34/279 (12.2%)	1.79	8/379 (2.1%)
4	f	2.88	22/279 (7.9%)	1.79	9/379 (2.4%)
5	G	2.13	13/311 (4.2%)	1.93	8/421 (1.9%)
5	g	1.68	1/311 (0.3%)	1.56	7/421 (1.7%)
7	c	3.24	127/1115 (11.4%)	2.20	52/1506 (3.5%)
All	All	2.36	765/18764 (4.1%)	1.63	363/25542 (1.4%)

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	A	0	1
1	a	0	4
2	C	0	2
7	c	0	1
All	All	0	8

The worst 5 of 765 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	539	TRP	C-O	-23.08	0.94	1.23
2	C	141	THR	C-O	-19.02	1.01	1.24
1	a	305	HIS	C-O	-15.89	1.05	1.24
2	C	179	ASN	C-O	-15.84	1.04	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	852	LEU	C-O	-15.74	1.04	1.24

The worst 5 of 363 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	LEU	CA-C-N	22.20	147.59	119.84
1	A	96	LEU	C-N-CA	22.20	147.59	119.84
1	A	473	ASP	CA-C-N	17.04	136.90	120.03
1	A	473	ASP	C-N-CA	17.04	136.90	120.03
2	C	141	THR	CA-C-O	-14.88	104.56	120.63

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	639	ASN	Mainchain
2	C	141	THR	Mainchain
2	C	179	ASN	Mainchain
1	a	92	SER	Peptide
1	a	93	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6960	0	6807	263	0
1	a	6984	0	6830	222	0
2	C	1474	0	1403	57	0
3	E	258	0	279	6	0
3	e	258	0	279	15	0
4	F	273	0	290	9	0
4	f	273	0	290	12	0
5	G	302	0	318	23	0
5	g	302	0	318	27	0
6	H	95	0	23	8	0
6	h	95	0	20	5	0
7	c	1096	0	1079	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	66	0	68	2	0
8	a	66	0	69	1	0
9	A	489	0	507	46	0
9	a	508	0	553	44	0
10	A	292	0	287	20	0
10	a	292	0	284	17	0
11	A	40	0	56	6	0
11	c	40	0	55	5	0
12	A	1	0	0	0	0
12	a	1	0	0	0	0
13	A	135	0	0	5	0
13	a	135	0	0	5	0
14	A	240	0	0	15	0
14	C	18	0	0	2	0
14	E	26	0	0	0	0
14	a	243	0	0	9	0
14	c	8	0	0	1	0
14	e	26	0	0	1	0
15	A	47	0	0	8	0
15	G	38	0	0	7	0
15	a	47	0	0	3	0
15	g	38	0	0	1	0
16	C	43	0	31	9	0
16	c	43	0	31	5	0
17	E	44	0	0	0	0
17	a	44	0	0	0	0
18	a	8	0	0	4	0
19	A	3	0	0	0	0
19	a	3	0	0	0	0
All	All	21354	0	19877	738	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 18.

The worst 5 of 738 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD12	1:A:86:PRO:CD	1.38	1.47
5:G:40:MET:HE1	15:G:101:85N:C22	1.47	1.43
1:a:150:PRO:HA	1:a:156:LYS:NZ	1.27	1.42
1:a:150:PRO:CA	1:a:156:LYS:HZ1	1.32	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:40:MET:CE	15:G:101:85N:C22	1.95	1.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	852/865 (98%)	793 (93%)	41 (5%)	18 (2%)	5	3
1	a	856/865 (99%)	798 (93%)	46 (5%)	12 (1%)	9	7
2	C	189/221 (86%)	174 (92%)	9 (5%)	6 (3%)	3	1
3	E	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
3	e	33/35 (94%)	32 (97%)	0	1 (3%)	3	1
4	F	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
4	f	33/35 (94%)	30 (91%)	2 (6%)	1 (3%)	3	1
5	G	36/45 (80%)	32 (89%)	3 (8%)	1 (3%)	4	2
5	g	36/45 (80%)	32 (89%)	4 (11%)	0	100	100
7	c	143/145 (99%)	127 (89%)	8 (6%)	8 (6%)	1	0
All	All	2244/2326 (96%)	2080 (93%)	117 (5%)	47 (2%)	8	3

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	A	97	PRO
1	A	147	TRP
1	A	170	TRP
1	A	346	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	718/726 (99%)	582 (81%)	136 (19%)	1	1
1	a	720/726 (99%)	583 (81%)	137 (19%)	1	1
2	C	155/180 (86%)	126 (81%)	29 (19%)	1	1
3	E	25/25 (100%)	20 (80%)	5 (20%)	1	1
3	e	25/25 (100%)	18 (72%)	7 (28%)	0	0
4	F	31/31 (100%)	25 (81%)	6 (19%)	1	1
4	f	31/31 (100%)	26 (84%)	5 (16%)	2	2
5	G	31/36 (86%)	22 (71%)	9 (29%)	0	0
5	g	31/36 (86%)	21 (68%)	10 (32%)	0	0
7	c	112/112 (100%)	90 (80%)	22 (20%)	1	1
All	All	1879/1928 (98%)	1513 (80%)	366 (20%)	3	1

5 of 366 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	206	LEU
1	a	588	LEU
1	a	263	ILE
1	a	433	THR
1	a	709	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	602	GLN
7	c	94	GLN
1	a	621	ASN
1	a	765	ASN
7	c	144	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 79 ligands modelled in this entry, 2 are monoatomic and 32 are unknown - leaving 45 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
9	BCL	A	909	1	69,74,74	3.31	29 (42%)	83,115,115	4.39	38 (45%)
11	LYC	A	913	-	39,39,39	2.05	11 (28%)	44,46,46	2.49	18 (40%)
8	2GO	A	901	1	71,74,74	2.80	22 (30%)	83,115,115	2.56	26 (31%)
10	CLA	a	913	1	69,73,73	2.51	21 (30%)	83,113,113	3.96	36 (43%)
15	85N	g	101	-	36,37,46	0.79	1 (2%)	40,45,55	0.58	0
15	85N	G	101	-	36,37,46	0.72	0	40,45,55	0.77	2 (5%)
9	BCL	a	904	1	69,74,74	2.67	20 (28%)	83,115,115	3.47	30 (36%)
17	84Q	E	101	-	42,43,43	2.09	10 (23%)	47,50,50	1.90	8 (17%)
10	CLA	a	901	19	69,73,73	2.63	23 (33%)	83,113,113	3.71	36 (43%)
13	85I	A	915	-	43,44,44	2.29	10 (23%)	47,51,51	2.44	7 (14%)
9	BCL	a	909	1	69,74,74	2.52	26 (37%)	83,115,115	3.88	33 (39%)
10	CLA	A	910	1	69,73,73	2.50	21 (30%)	83,113,113	3.61	40 (48%)
13	85I	a	918	-	43,44,44	1.06	2 (4%)	47,51,51	1.69	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	A	908	1	69,74,74	2.52	30 (43%)	83,115,115	2.99	33 (39%)
9	BCL	A	907	1	64,69,74	3.34	29 (45%)	77,109,115	4.61	43 (55%)
18	SF4	a	917	1	0,12,12	-	-	-	-	-
9	BCL	A	904	1	49,54,74	2.57	22 (44%)	59,91,115	3.09	27 (45%)
10	CLA	A	911	1	69,73,73	2.61	22 (31%)	83,113,113	3.34	34 (40%)
15	85N	a	902	-	45,46,46	0.59	0	50,55,55	0.42	0
13	85I	a	920	-	43,44,44	2.21	2 (4%)	47,51,51	2.04	3 (6%)
10	CLA	a	914	1	50,54,73	2.92	21 (42%)	60,90,113	3.84	30 (50%)
10	CLA	A	933	1	55,59,73	2.81	21 (38%)	66,96,113	4.25	36 (54%)
11	LYC	c	201	-	39,39,39	1.65	9 (23%)	44,46,46	5.75	28 (63%)
9	BCL	A	902	1	69,74,74	2.81	24 (34%)	83,115,115	3.37	36 (43%)
9	BCL	a	905	1	69,74,74	2.82	21 (30%)	83,115,115	3.88	36 (43%)
10	CLA	a	915	1	55,59,73	2.94	21 (38%)	66,96,113	3.54	37 (56%)
16	HEC	c	202	7	50,50,50	3.71	27 (54%)	68,82,82	3.32	33 (48%)
16	HEC	C	301	2	50,50,50	3.85	32 (64%)	68,82,82	3.46	39 (57%)
9	BCL	a	911	1	69,74,74	2.85	28 (40%)	83,115,115	3.50	35 (42%)
10	CLA	A	912	1	50,54,73	2.69	16 (32%)	60,90,113	4.18	31 (51%)
8	2GO	a	903	1	71,74,74	2.46	18 (25%)	83,115,115	2.26	29 (34%)
9	BCL	A	905	1	69,74,74	2.71	21 (30%)	83,115,115	3.98	36 (43%)
9	BCL	A	903	1	69,74,74	2.89	22 (31%)	83,115,115	3.82	36 (43%)
13	85I	A	916	-	43,44,44	2.22	3 (6%)	47,51,51	1.93	6 (12%)
9	BCL	a	908	1	69,74,74	2.96	26 (37%)	83,115,115	4.42	38 (45%)
9	BCL	a	907	1	69,74,74	2.64	27 (39%)	83,115,115	3.82	31 (37%)
10	CLA	A	931	1	69,73,73	3.00	26 (37%)	83,113,113	4.40	44 (53%)
9	BCL	A	906	1	55,60,74	3.00	20 (36%)	66,98,115	4.75	29 (43%)
17	84Q	a	921	-	42,43,43	1.35	2 (4%)	47,50,50	1.04	2 (4%)
10	CLA	a	912	19	69,73,73	2.76	19 (27%)	83,113,113	3.58	42 (50%)
9	BCL	a	910	1	69,74,74	3.21	22 (31%)	83,115,115	4.00	40 (48%)
9	BCL	a	906	1	49,54,74	2.89	22 (44%)	59,91,115	3.46	28 (47%)
15	85N	A	932	-	45,46,46	1.04	1 (2%)	50,55,55	1.82	4 (8%)
13	85I	A	917	-	43,44,44	1.57	2 (4%)	47,51,51	2.42	3 (6%)
13	85I	a	919	-	43,44,44	1.41	2 (4%)	47,51,51	1.66	3 (6%)

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
9	BCL	A	909	1	-	12/41/137/137	-
11	LYC	A	913	-	-	1/43/43/43	-
8	2GO	A	901	1	2/2/21/25	5/41/137/137	-
10	CLA	a	913	1	-	11/39/115/115	-
15	85N	g	101	-	-	19/42/42/51	-
15	85N	G	101	-	-	18/42/42/51	-
9	BCL	a	904	1	-	12/41/137/137	-
17	84Q	E	101	-	-	27/46/47/47	-
10	CLA	a	901	19	-	25/39/115/115	-
13	85I	A	915	-	-	19/47/48/48	-
10	CLA	A	910	1	1/1/15/20	9/39/115/115	-
9	BCL	a	909	1	-	13/41/137/137	-
13	85I	a	918	-	-	21/47/48/48	-
9	BCL	A	908	1	-	14/41/137/137	-
9	BCL	A	907	1	-	16/35/131/137	-
18	SF4	a	917	1	-	-	0/6/5/5
10	CLA	A	911	1	1/1/15/20	11/39/115/115	-
9	BCL	A	904	1	-	6/17/113/137	-
15	85N	a	902	-	-	25/51/51/51	-
13	85I	a	920	-	-	30/47/48/48	-
10	CLA	a	914	1	-	4/17/93/115	-
10	CLA	A	933	1	-	6/23/99/115	-
11	LYC	c	201	-	-	16/43/43/43	-
9	BCL	A	902	1	-	18/41/137/137	-
9	BCL	a	905	1	-	17/41/137/137	-
10	CLA	a	915	1	-	9/23/99/115	-
16	HEC	c	202	7	1/1/3/7	7/14/54/54	-
16	HEC	C	301	2	1/1/3/7	7/14/54/54	-
9	BCL	a	911	1	-	5/41/137/137	-
10	CLA	A	912	1	-	2/17/93/115	-
8	2GO	a	903	1	2/2/21/25	5/41/137/137	-
9	BCL	A	905	1	-	16/41/137/137	-
9	BCL	A	903	1	-	21/41/137/137	-
13	85I	A	916	-	-	27/47/48/48	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	a	908	1	-	20/41/137/137	-
9	BCL	a	907	1	-	12/41/137/137	-
10	CLA	A	931	1	-	18/39/115/115	-
9	BCL	A	906	1	-	6/25/121/137	-
17	84Q	a	921	-	-	32/46/47/47	-
10	CLA	a	912	19	-	12/39/115/115	-
9	BCL	a	910	1	-	11/41/137/137	-
9	BCL	a	906	1	-	6/17/113/137	-
15	85N	A	932	-	-	18/51/51/51	-
13	85I	A	917	-	-	29/47/48/48	-
13	85I	a	919	-	-	36/47/48/48	-

The worst 5 of 754 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	920	85I	O6-C3	-14.01	1.20	1.44
9	a	910	BCL	C4B-NB	-13.44	1.21	1.37
10	A	931	CLA	C4B-NB	-10.59	1.24	1.37
10	a	912	CLA	C3D-C4D	-10.25	1.21	1.44
9	A	909	BCL	C4B-NB	-9.97	1.25	1.37

The worst 5 of 1130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	909	BCL	O2D-CGD-CBD	20.86	148.33	111.27
9	a	908	BCL	C4A-NA-C1A	18.67	115.10	106.71
9	A	906	BCL	O2D-CGD-CBD	18.23	143.67	111.27
10	A	931	CLA	O2D-CGD-CBD	18.08	143.39	111.27
9	a	907	BCL	C4A-NA-C1A	16.53	114.14	106.71

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	901	2GO	CBD
8	A	901	2GO	ND
8	a	903	2GO	CBD
8	a	903	2GO	ND
10	A	910	CLA	C8

5 of 654 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	902	BCL	C1A-C2A-CAA-CBA
9	A	902	BCL	C3A-C2A-CAA-CBA
9	A	902	BCL	CBD-CGD-O2D-CED
9	A	902	BCL	C11-C12-C13-C14
9	A	903	BCL	C1A-C2A-CAA-CBA

There are no ring outliers.

41 monomers are involved in 182 short contacts:

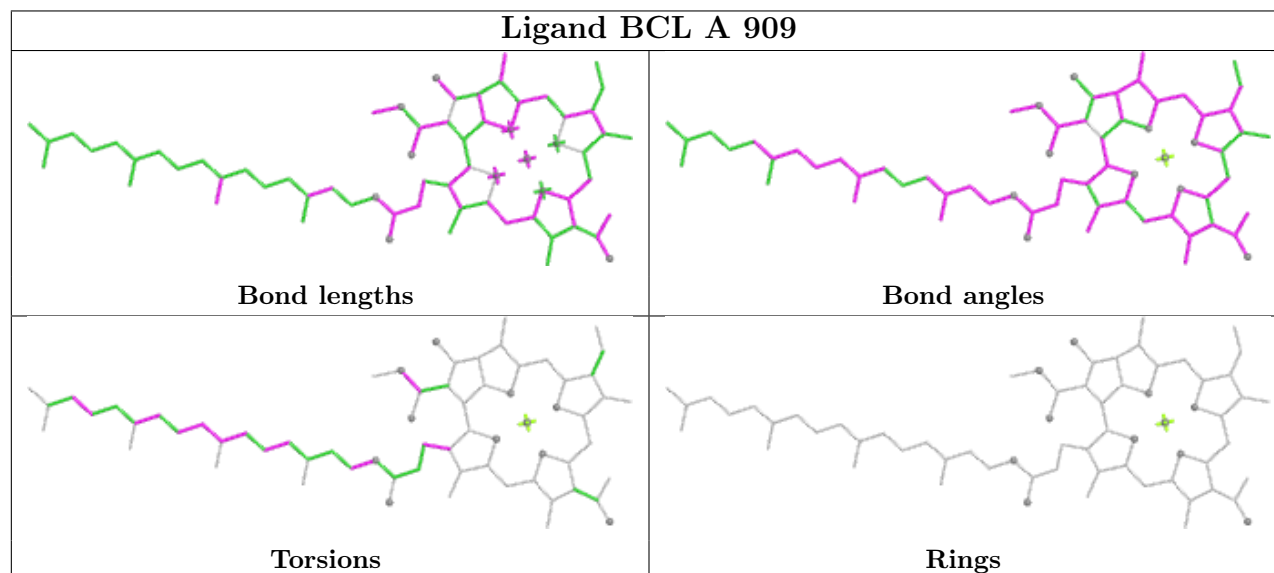
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	909	BCL	2	0
11	A	913	LYC	6	0
8	A	901	2GO	2	0
10	a	913	CLA	6	0
15	g	101	85N	1	0
15	G	101	85N	7	0
9	a	904	BCL	10	0
10	a	901	CLA	3	0
13	A	915	85I	2	0
9	a	909	BCL	5	0
10	A	910	CLA	4	0
9	A	908	BCL	7	0
9	A	907	BCL	6	0
18	a	917	SF4	4	0
9	A	904	BCL	2	0
10	A	911	CLA	7	0
15	a	902	85N	3	0
13	a	920	85I	4	0
10	a	914	CLA	2	0
10	A	933	CLA	1	0
11	c	201	LYC	5	0
9	A	902	BCL	9	0
9	a	905	BCL	8	0
10	a	915	CLA	2	0
16	c	202	HEC	5	0
16	C	301	HEC	9	0
9	a	911	BCL	5	0
10	A	912	CLA	1	0
8	a	903	2GO	1	0
9	A	905	BCL	9	0
9	A	903	BCL	5	0

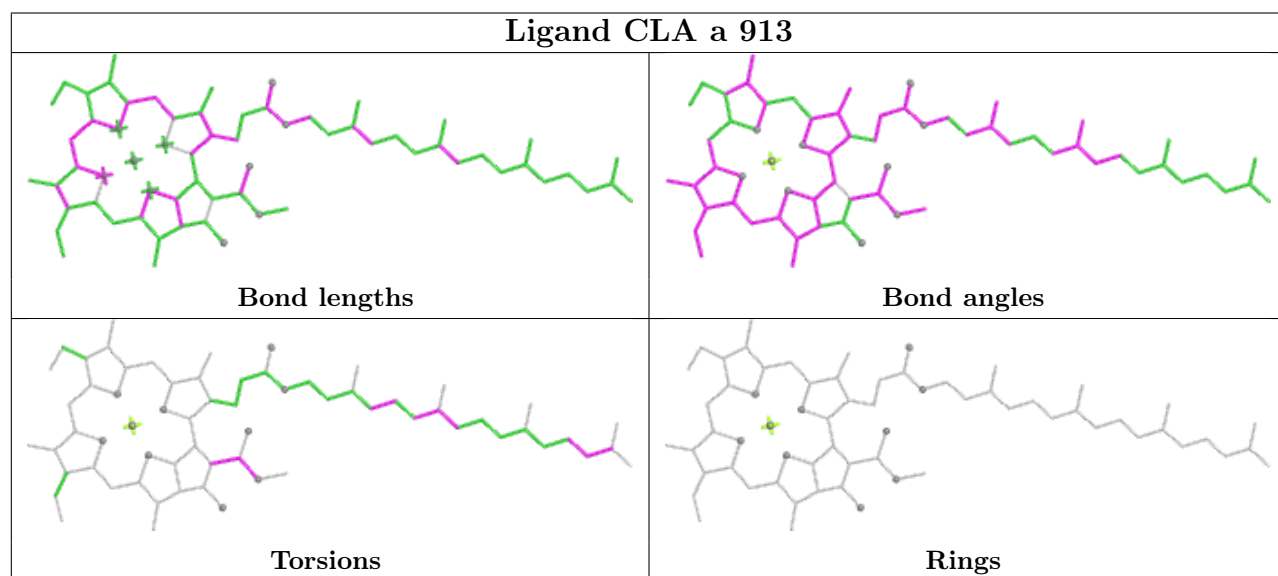
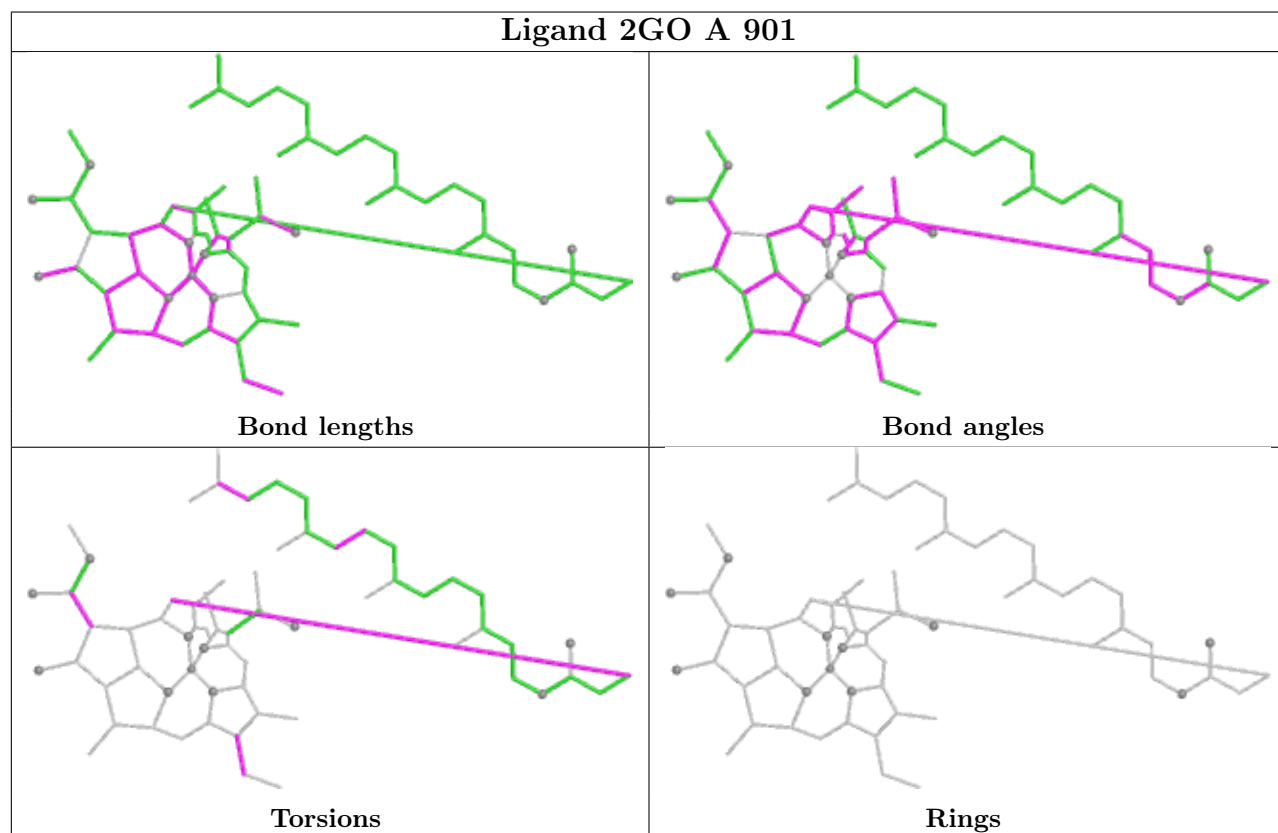
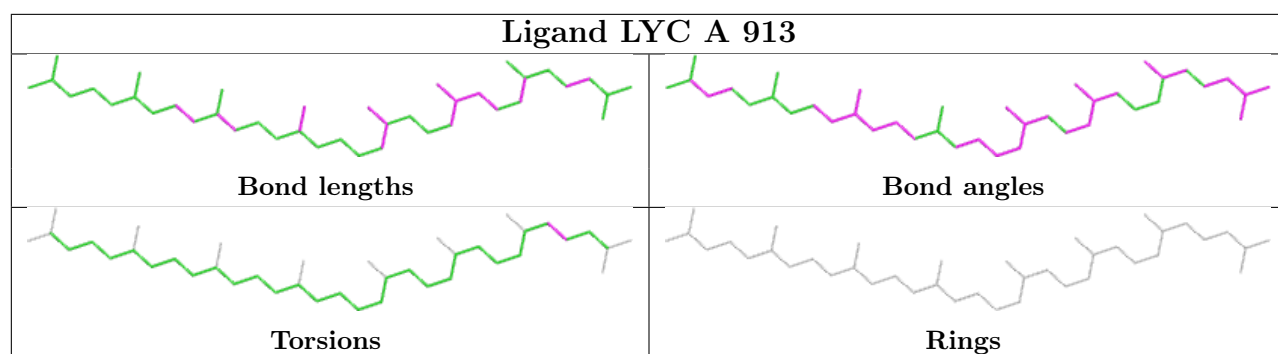
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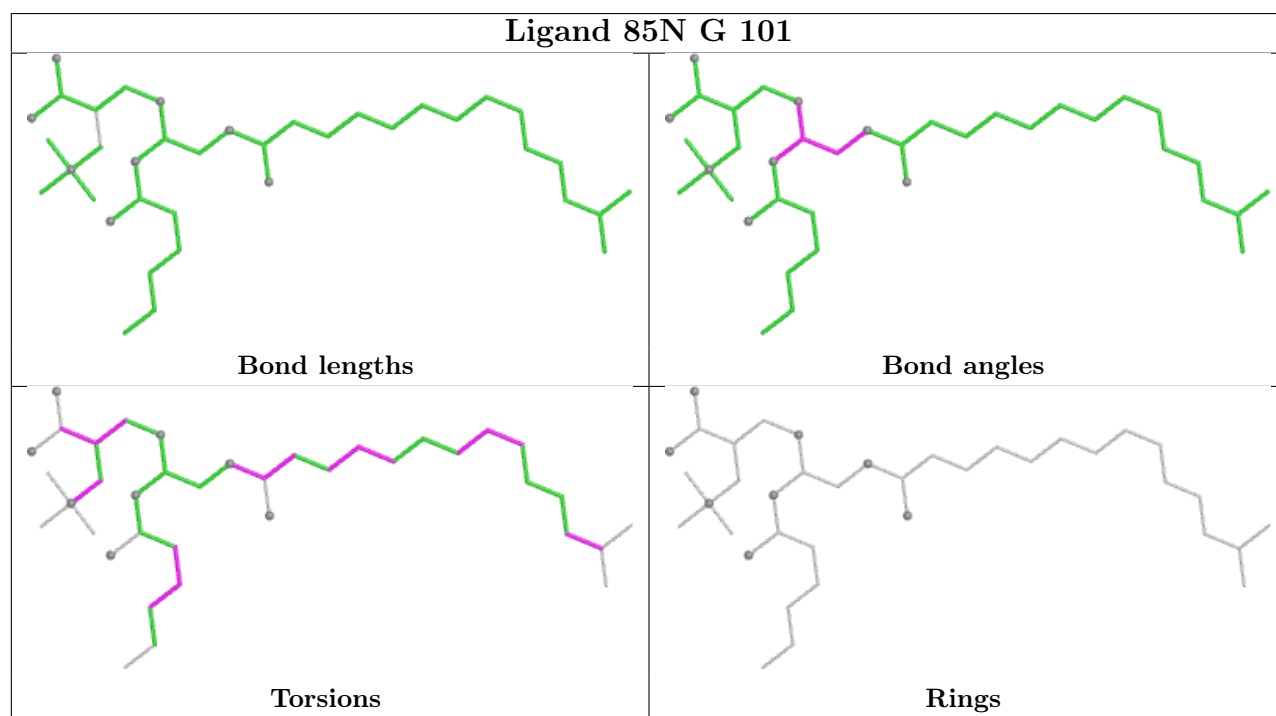
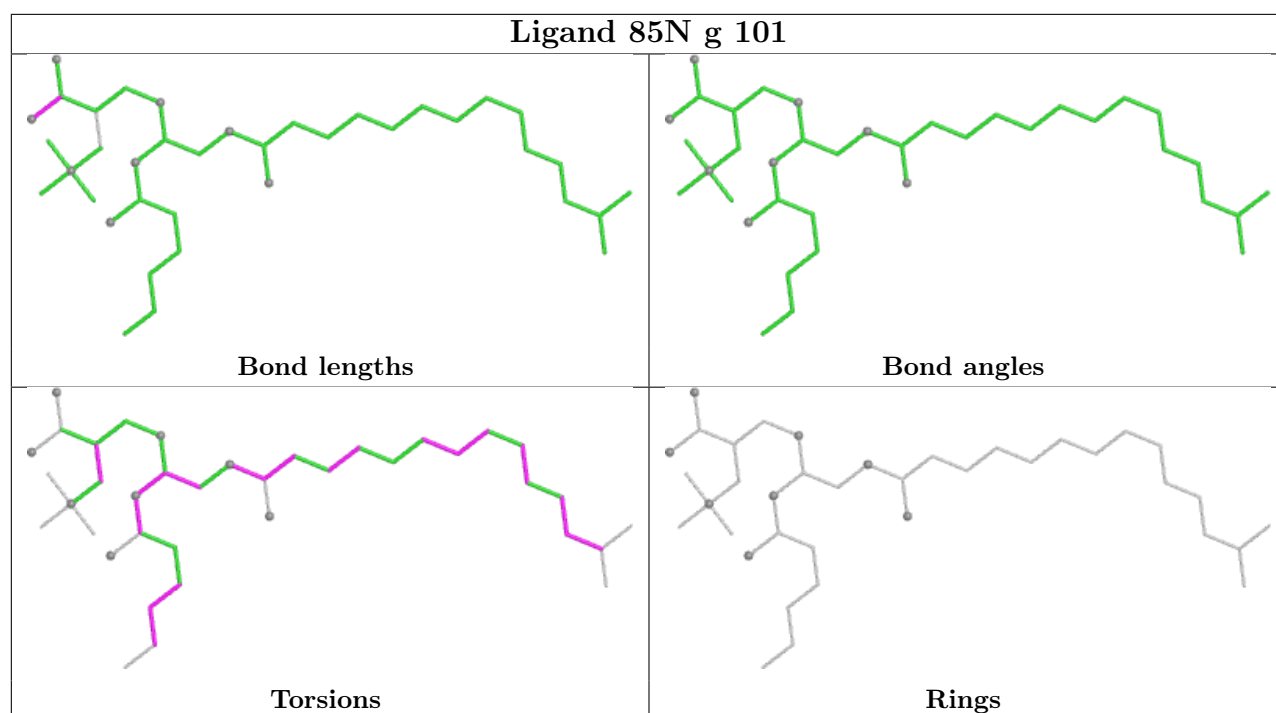
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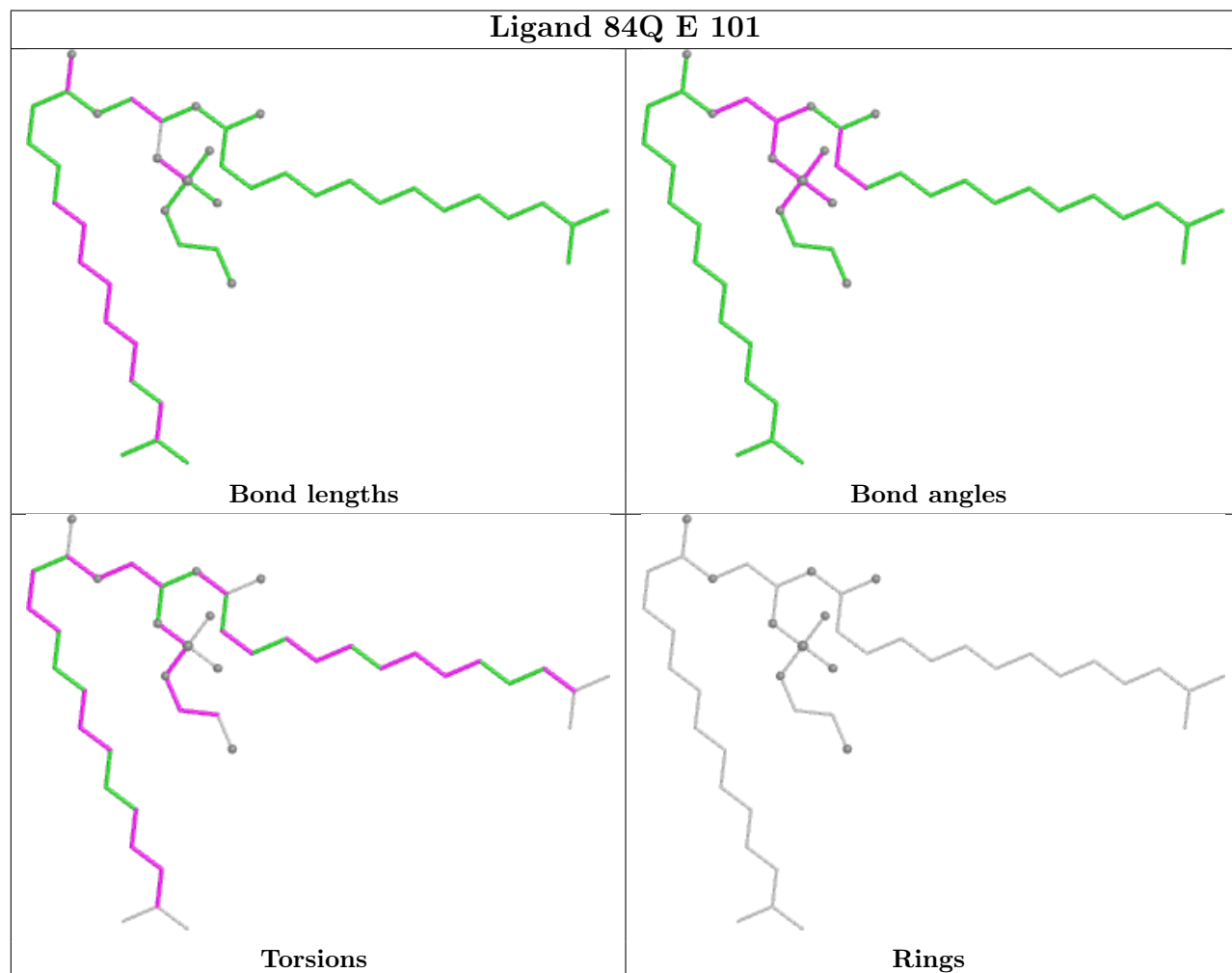
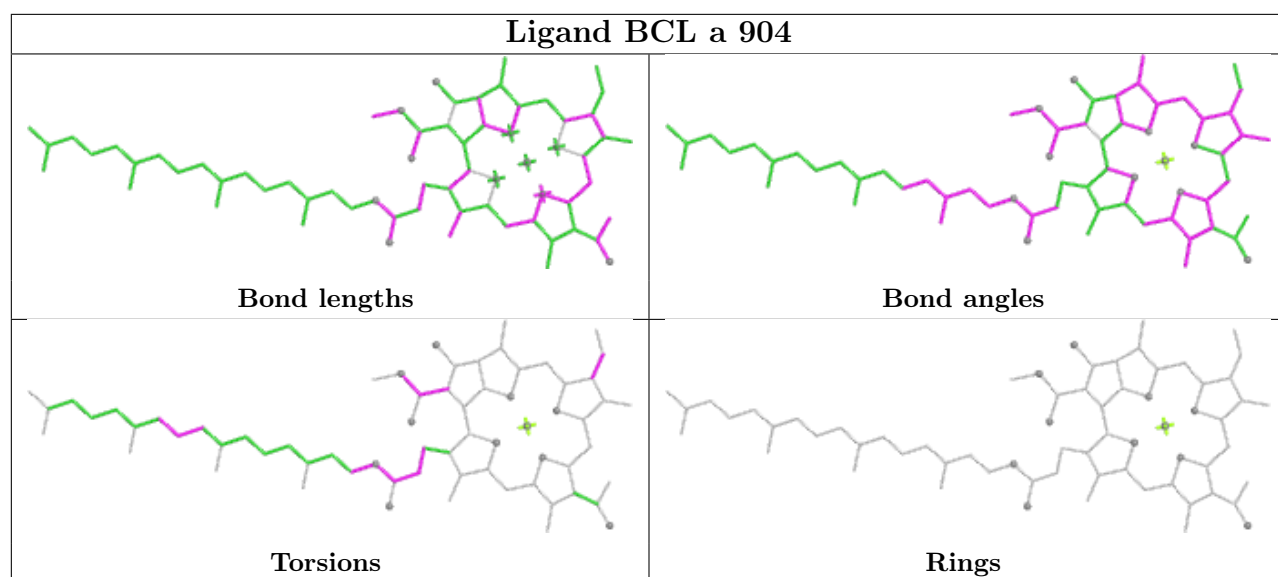
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	916	85I	1	0
9	a	908	BCL	10	0
9	a	907	BCL	4	0
10	A	931	CLA	7	0
9	A	906	BCL	6	0
10	a	912	CLA	4	0
9	a	910	BCL	4	0
15	A	932	85N	8	0
13	A	917	85I	3	0
13	a	919	85I	1	0

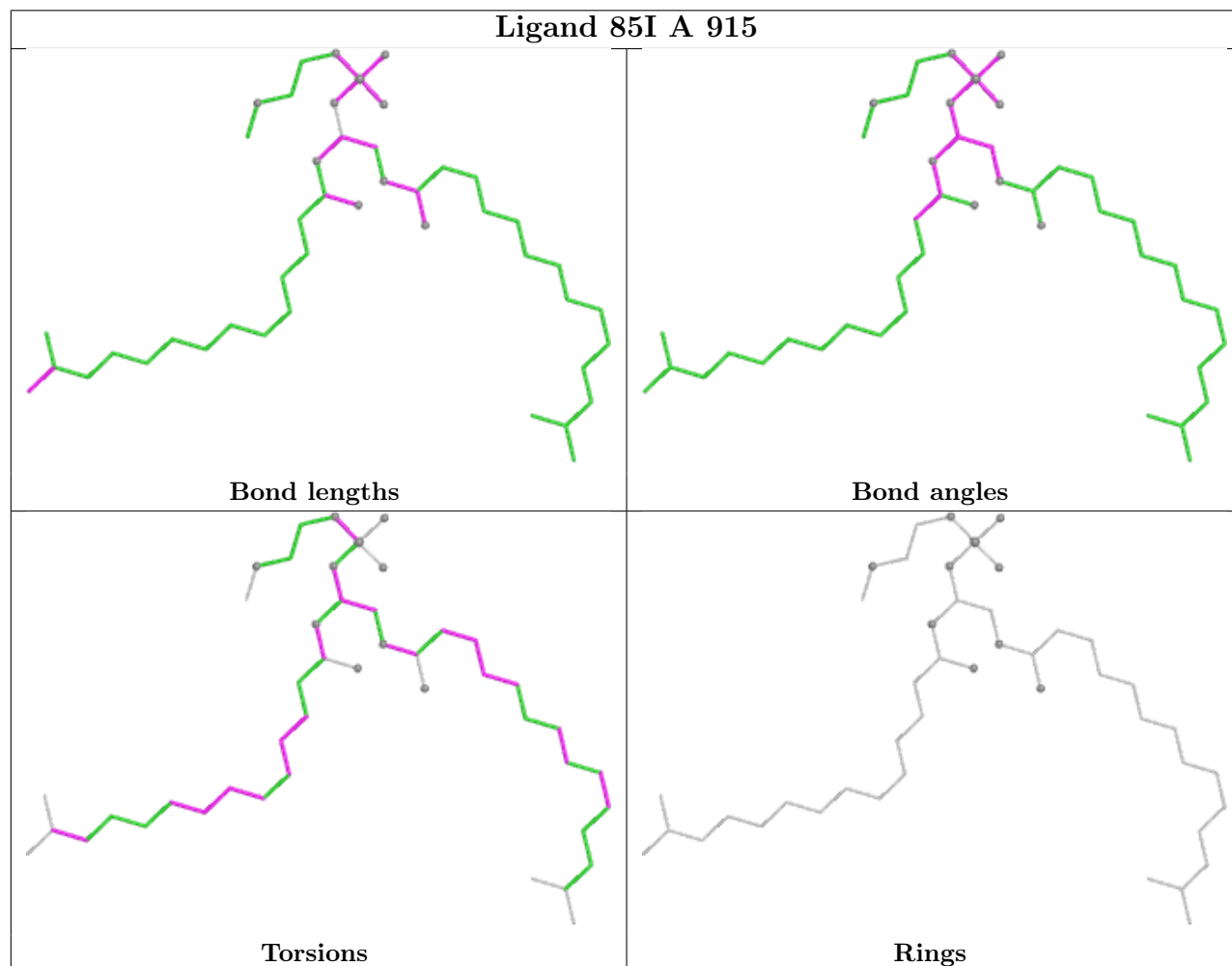
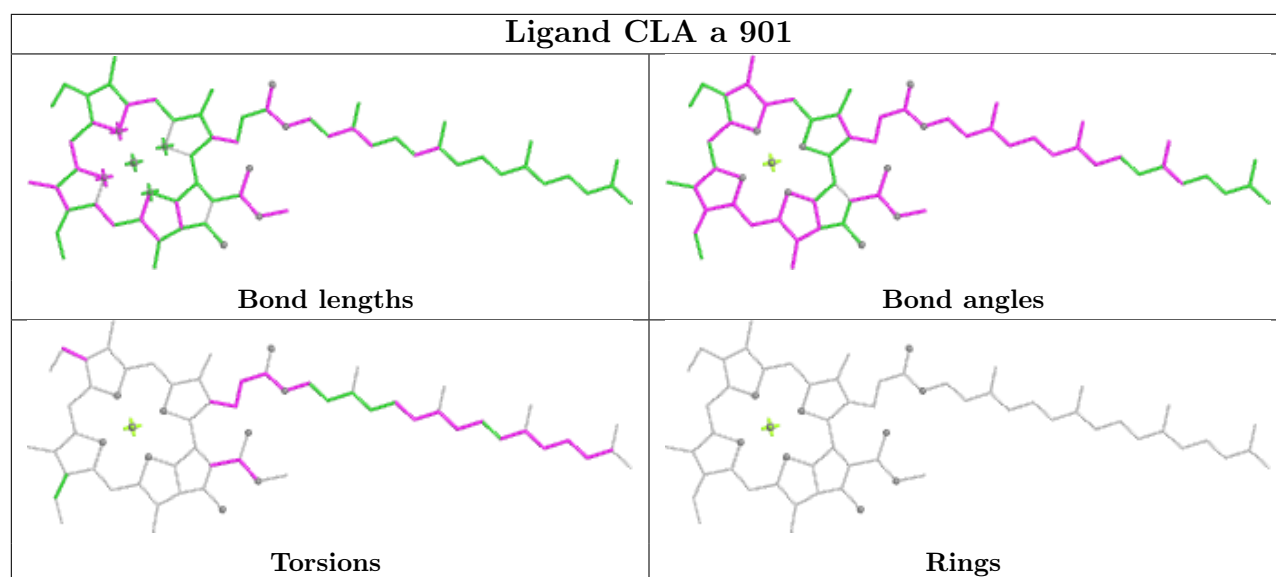
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

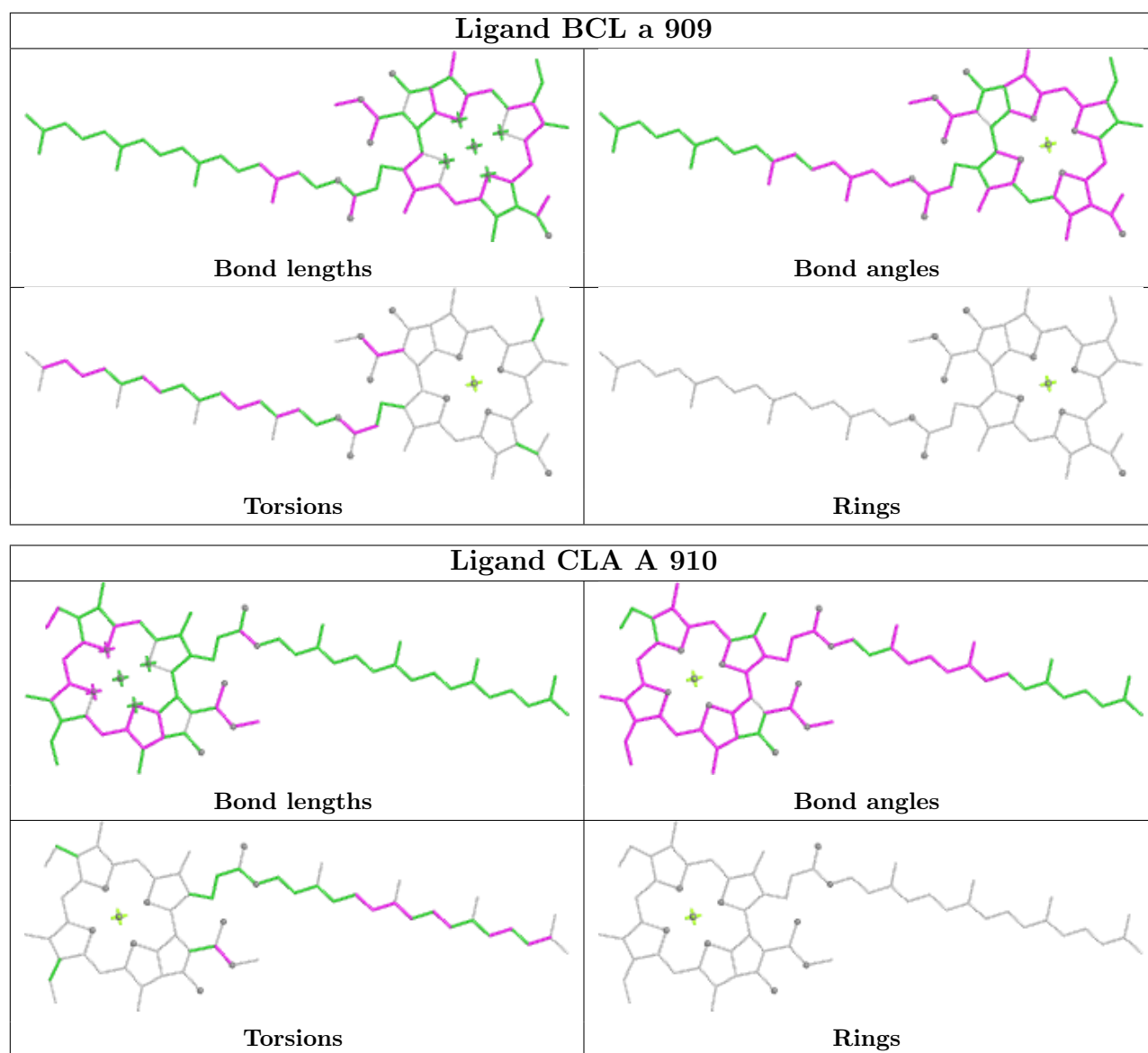


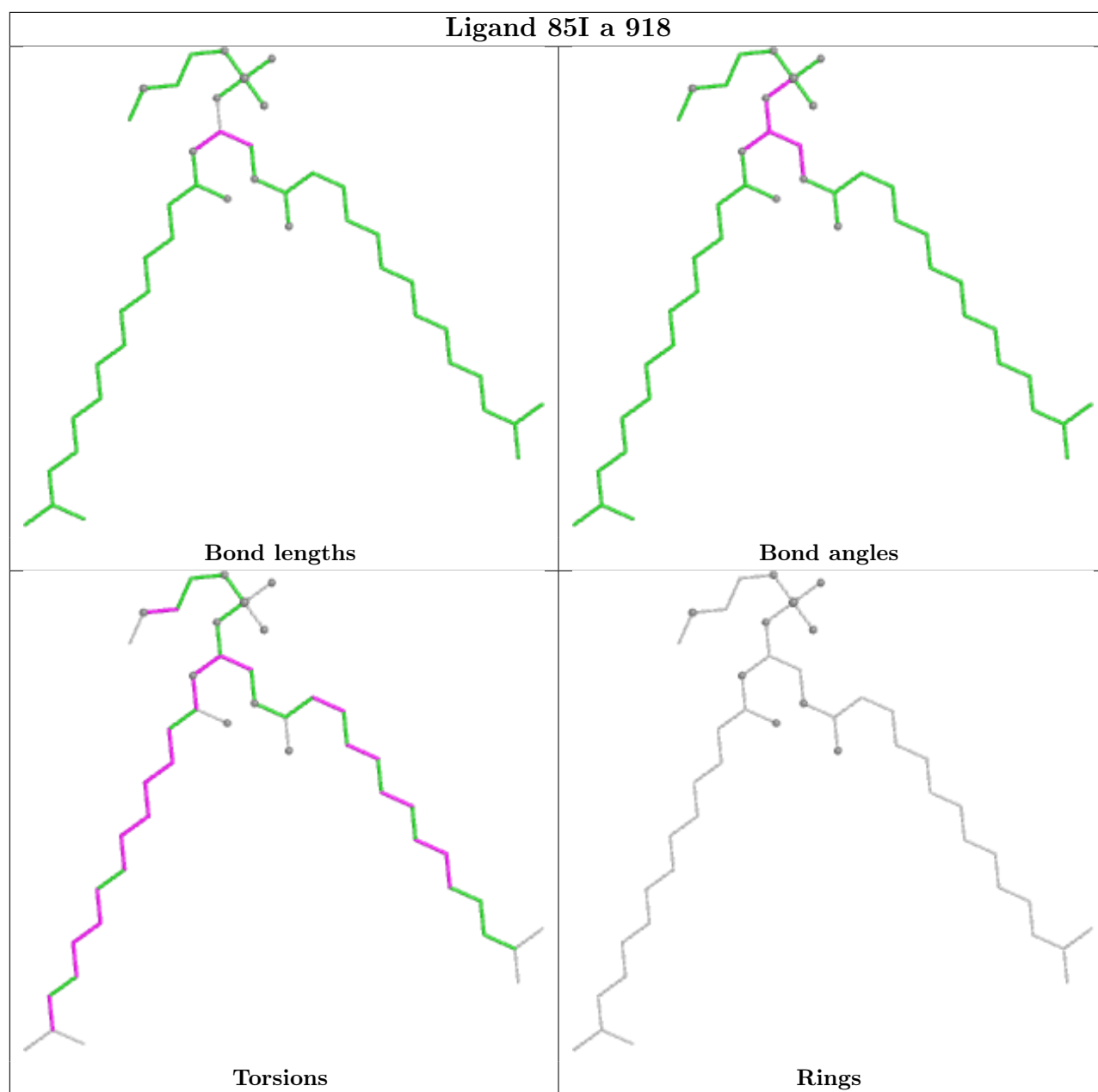


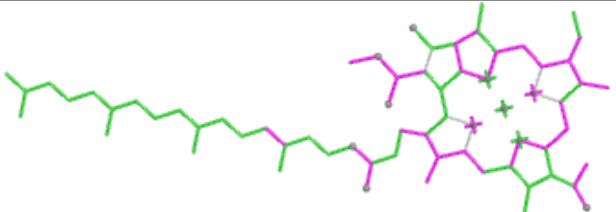
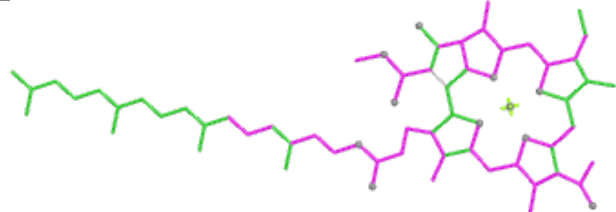
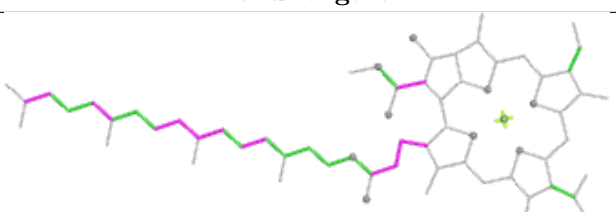
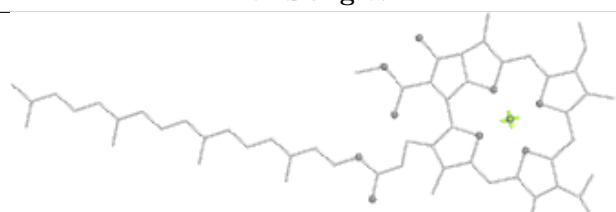
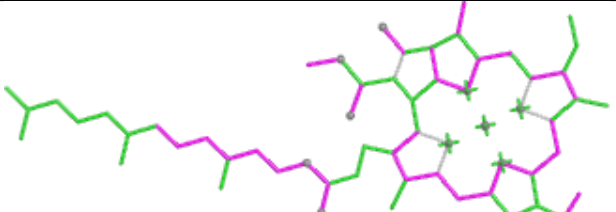
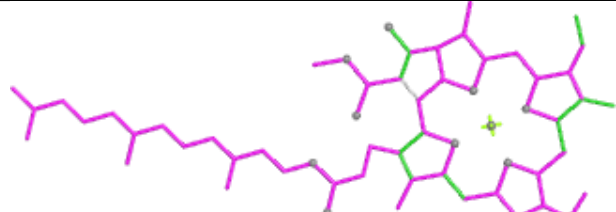
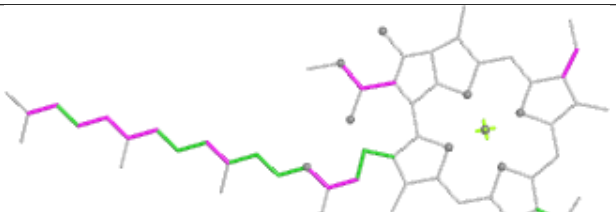
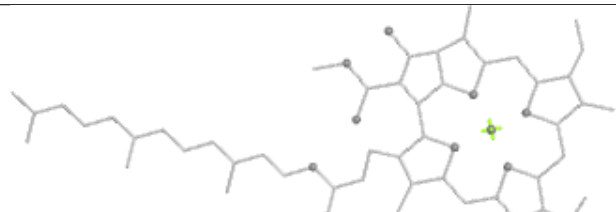


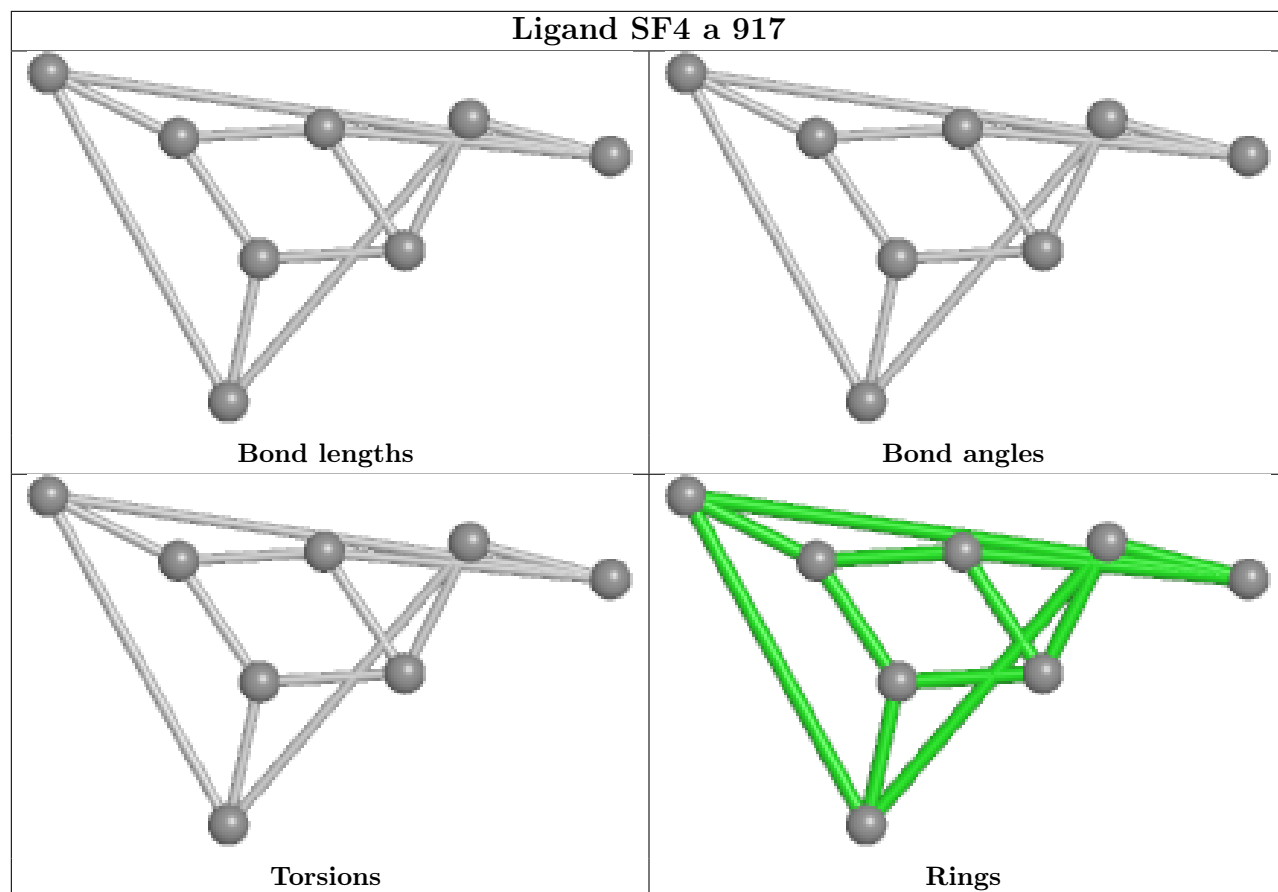


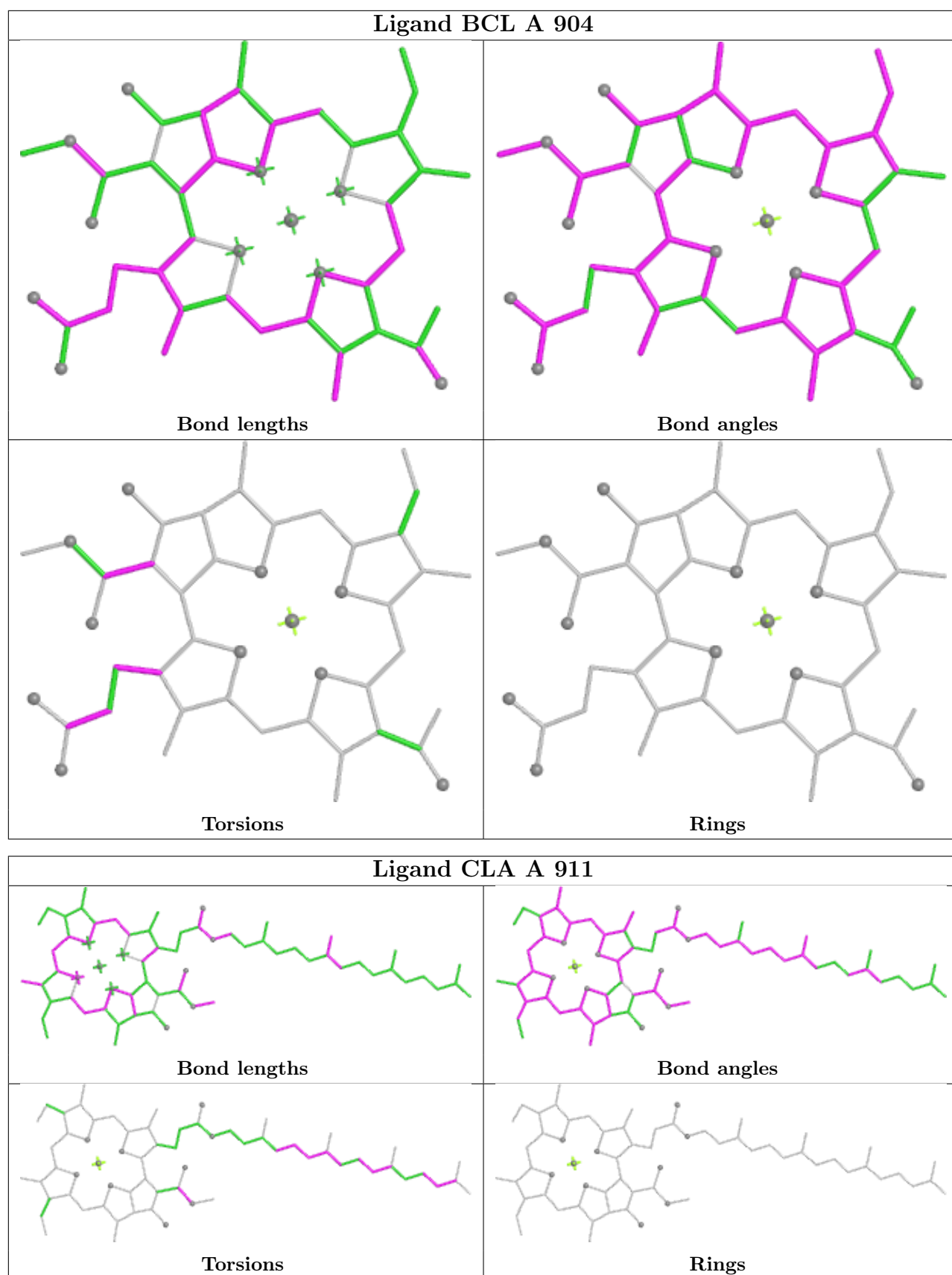


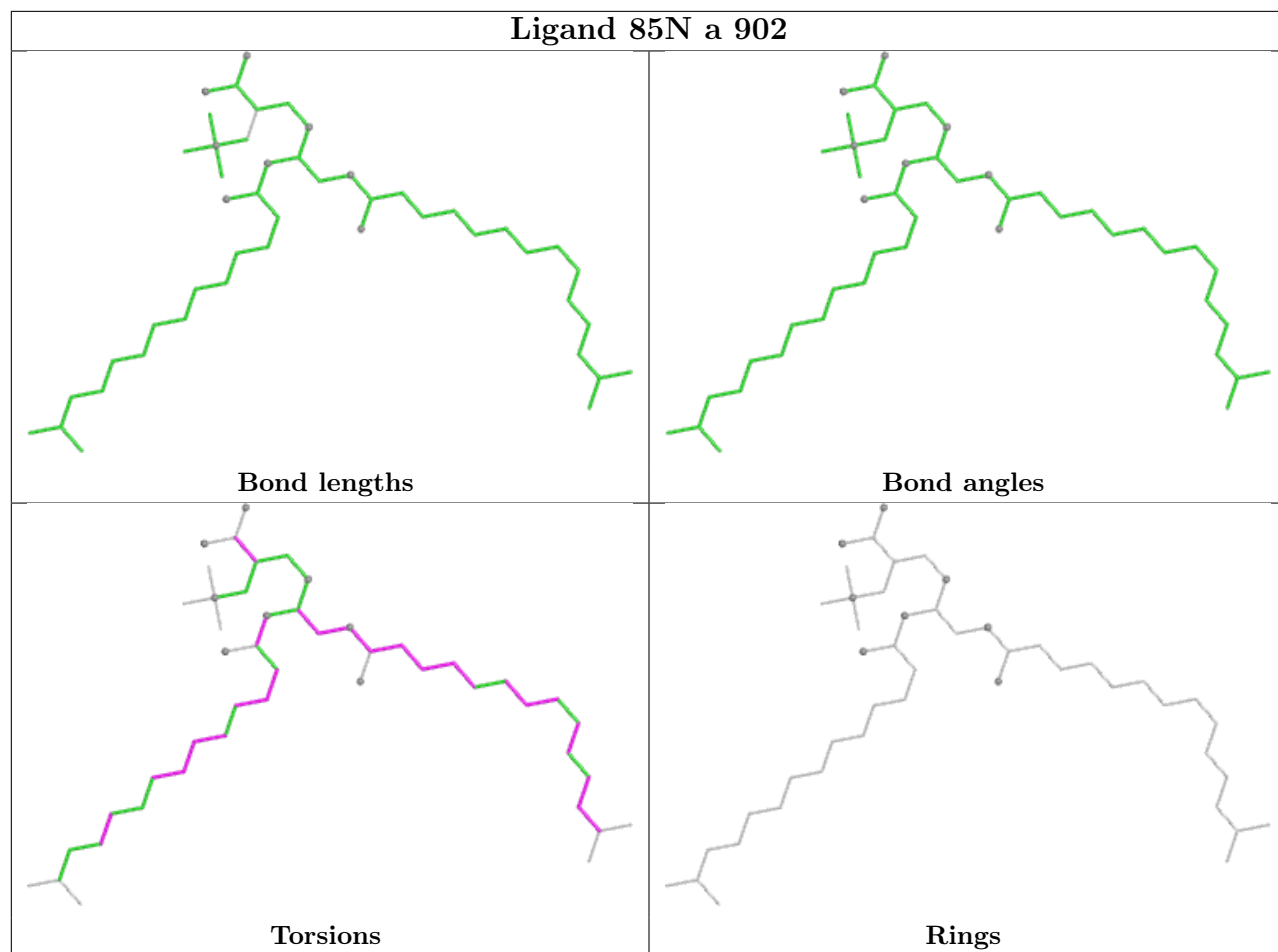


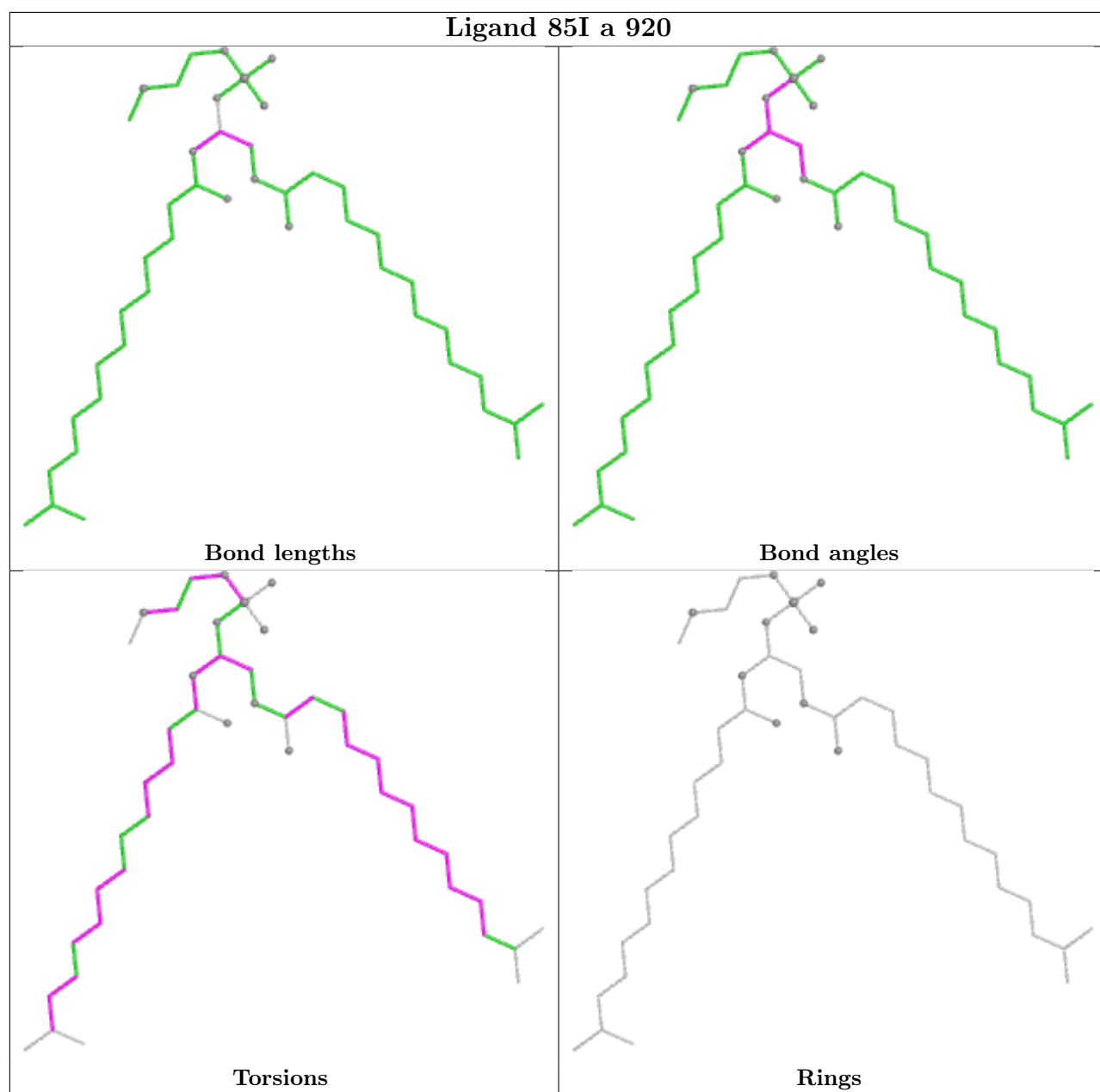


Ligand BCL A 908	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL A 907	
 Bond lengths	 Bond angles
 Torsions	 Rings

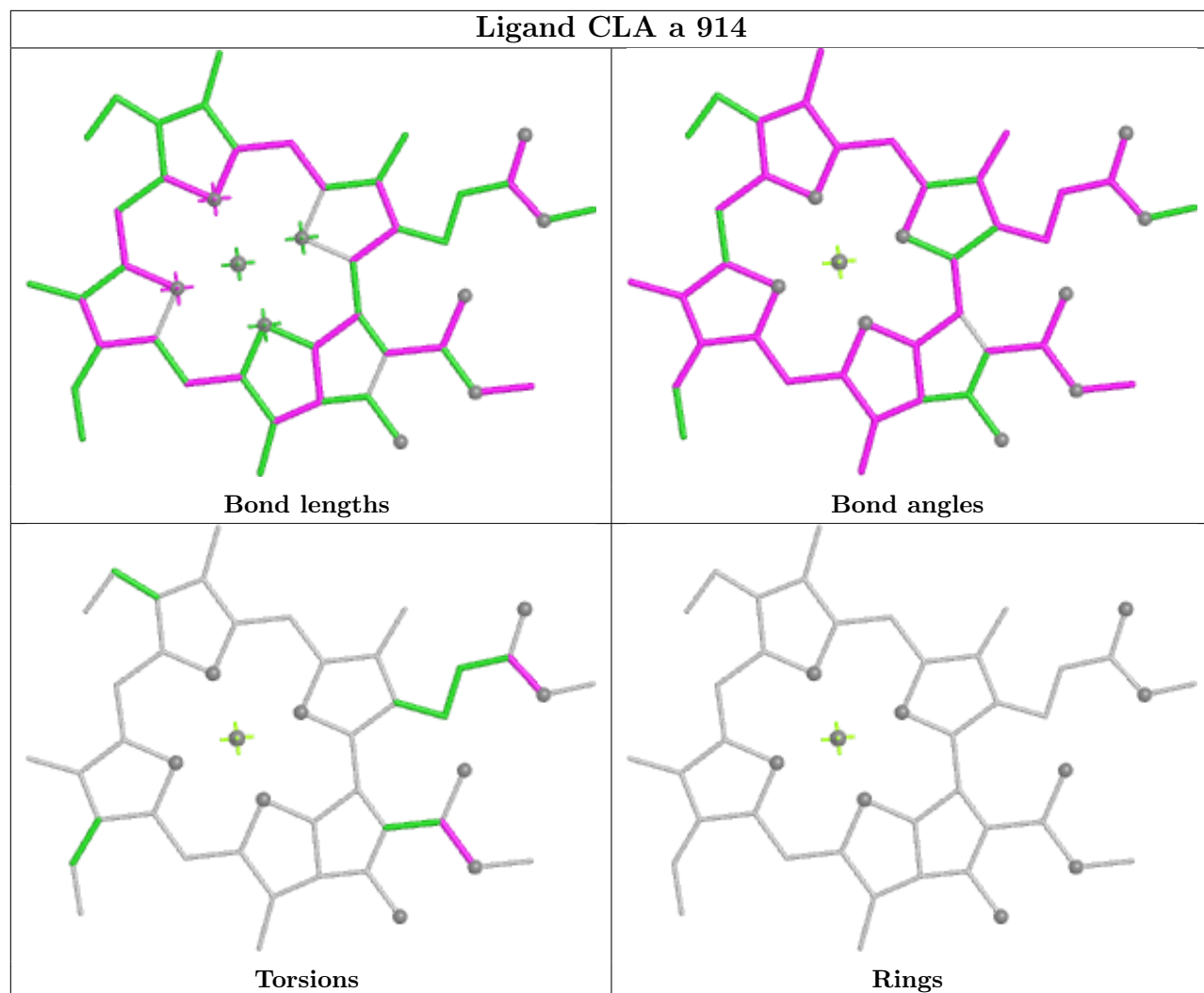


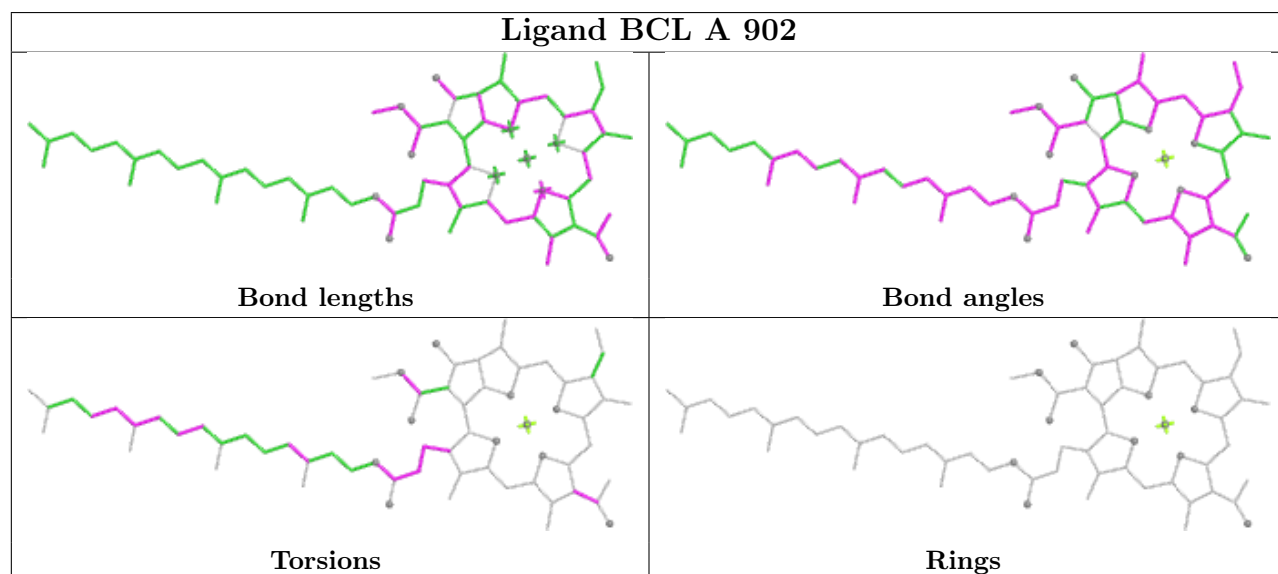
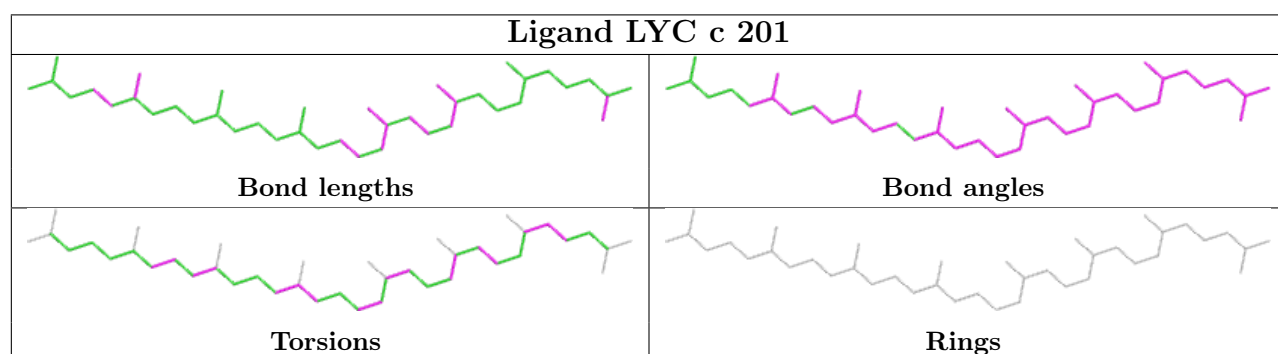
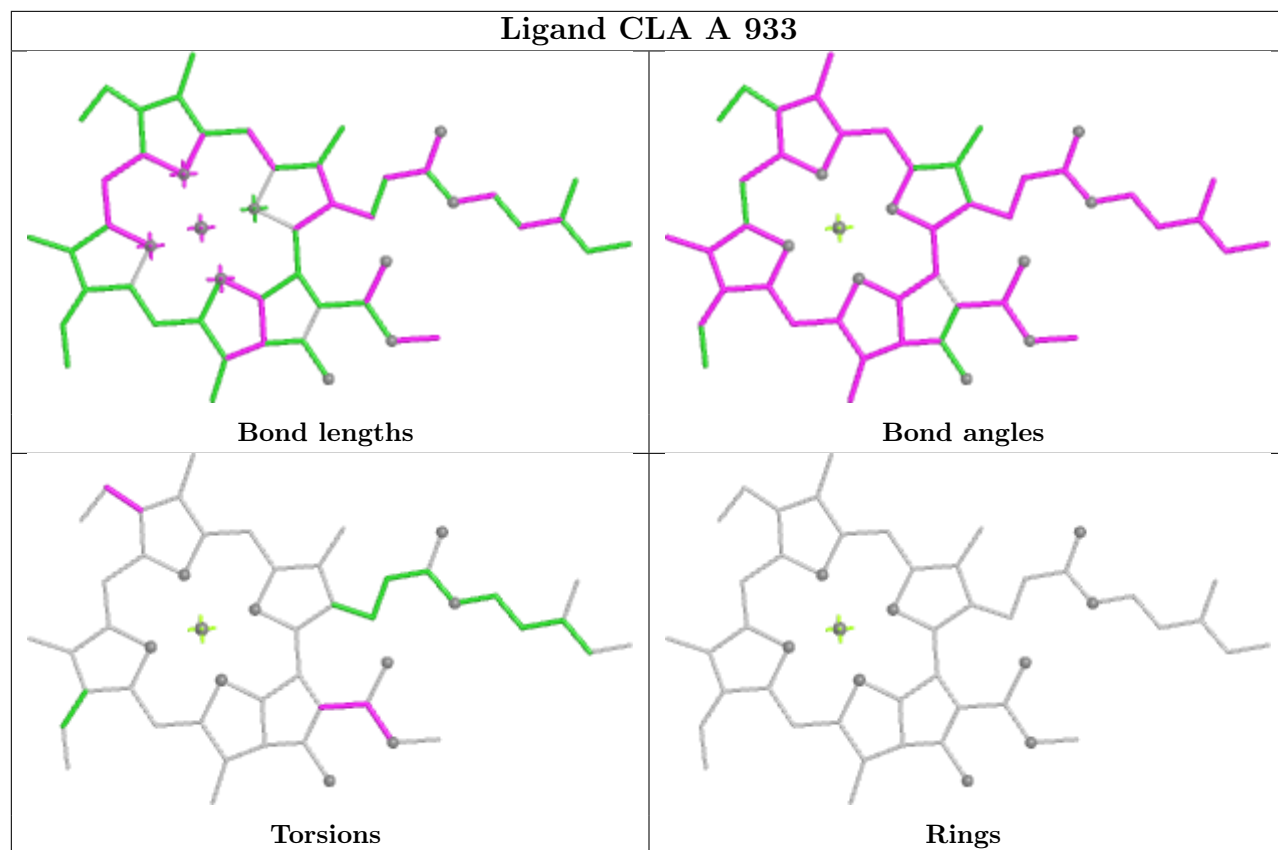


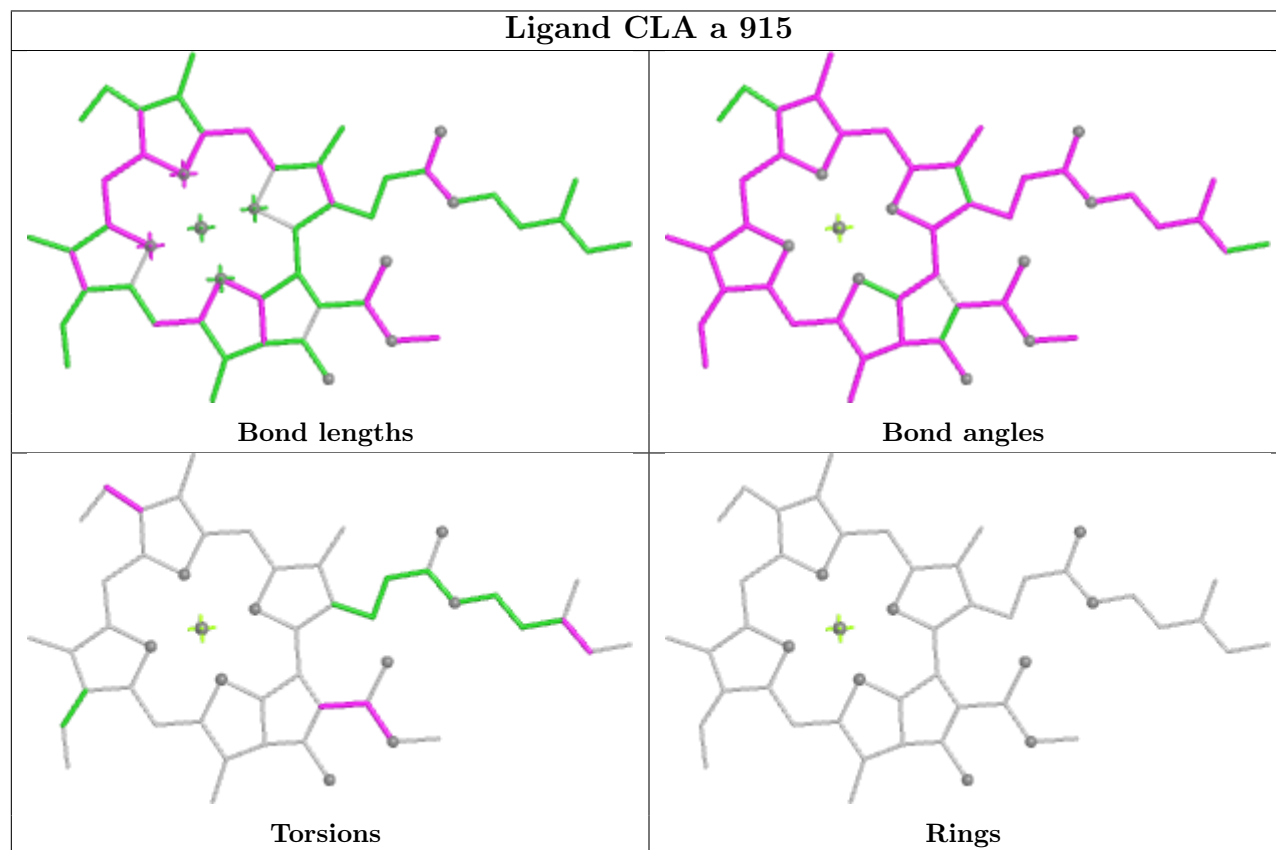
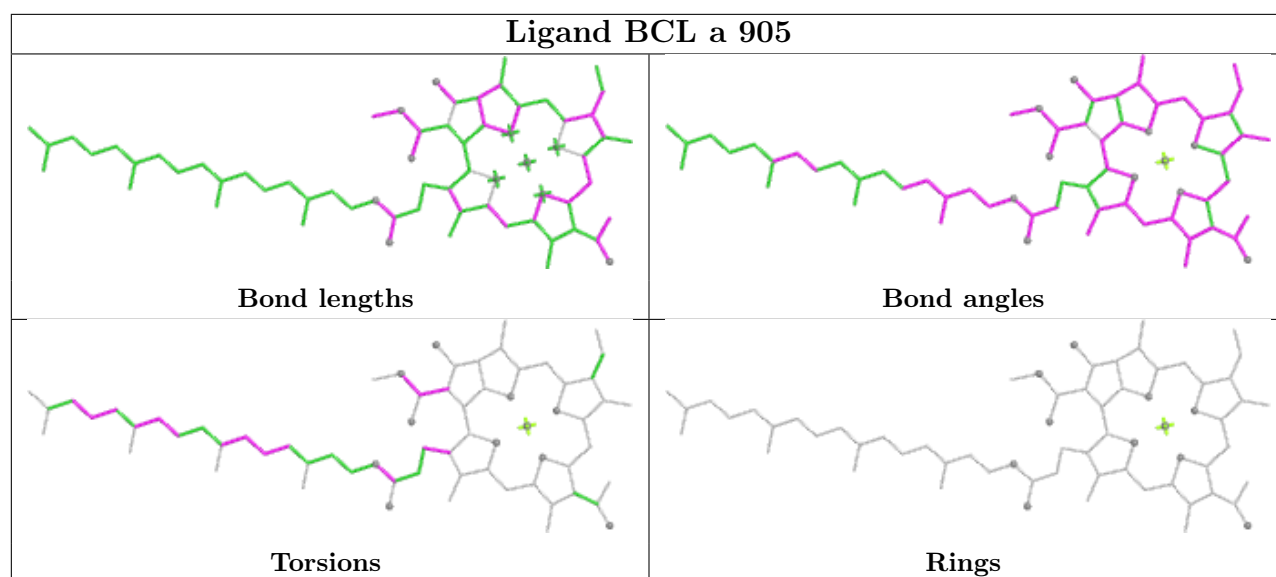




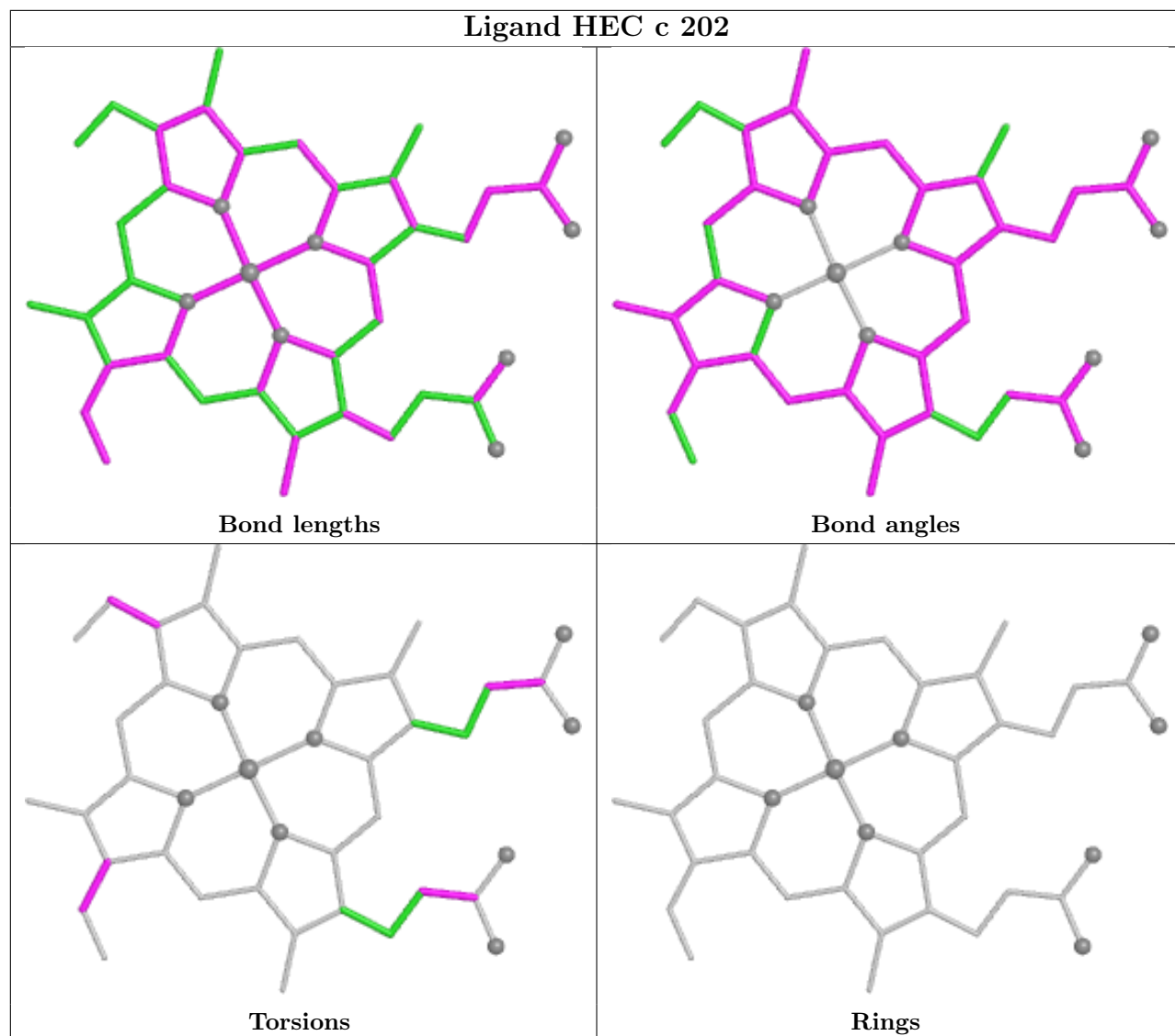
Ligand CLA a 914

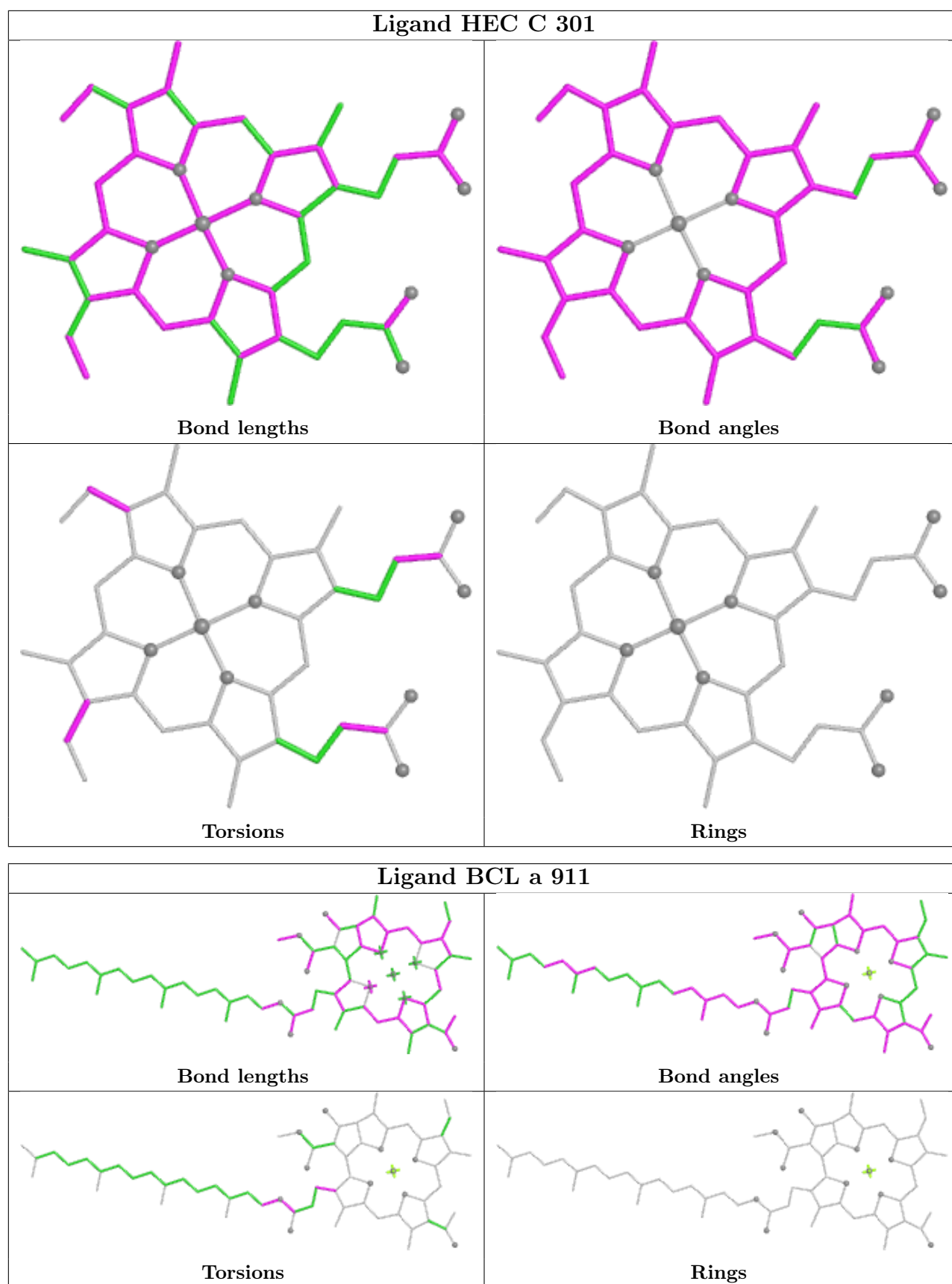


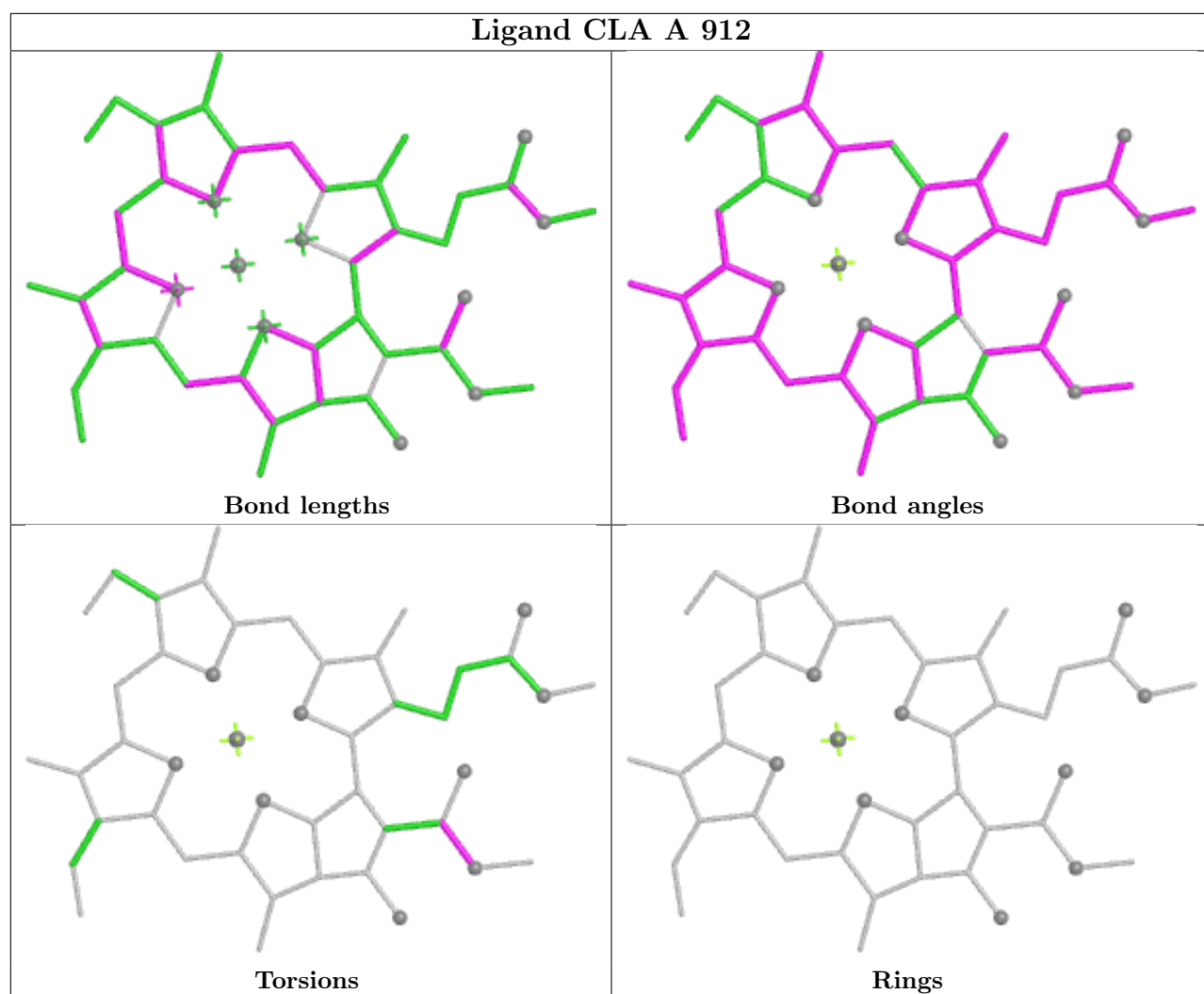


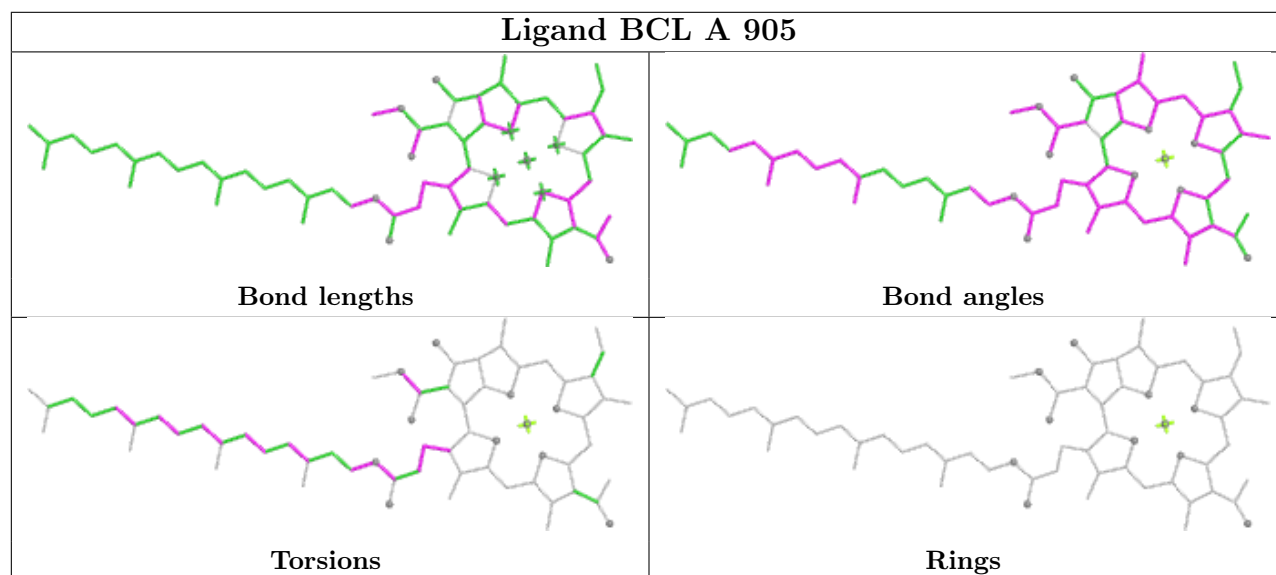
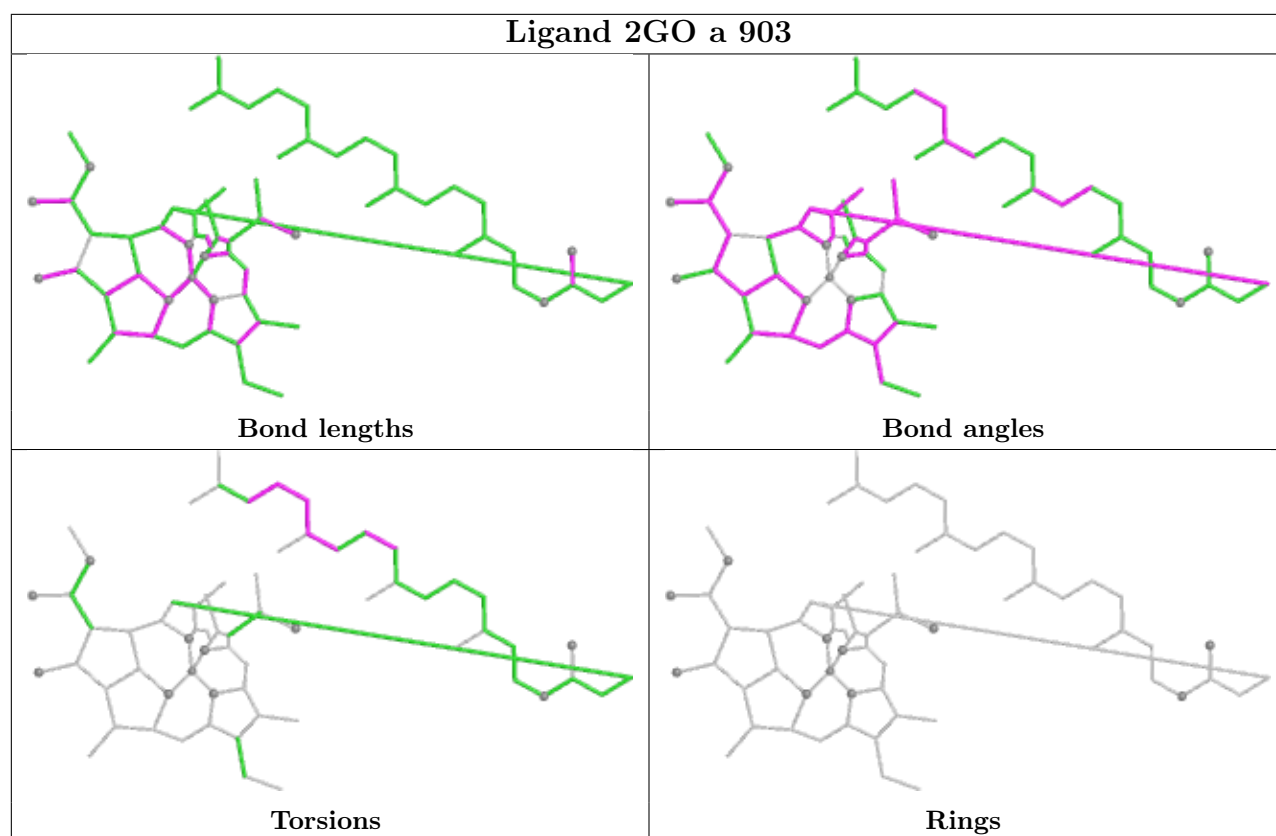


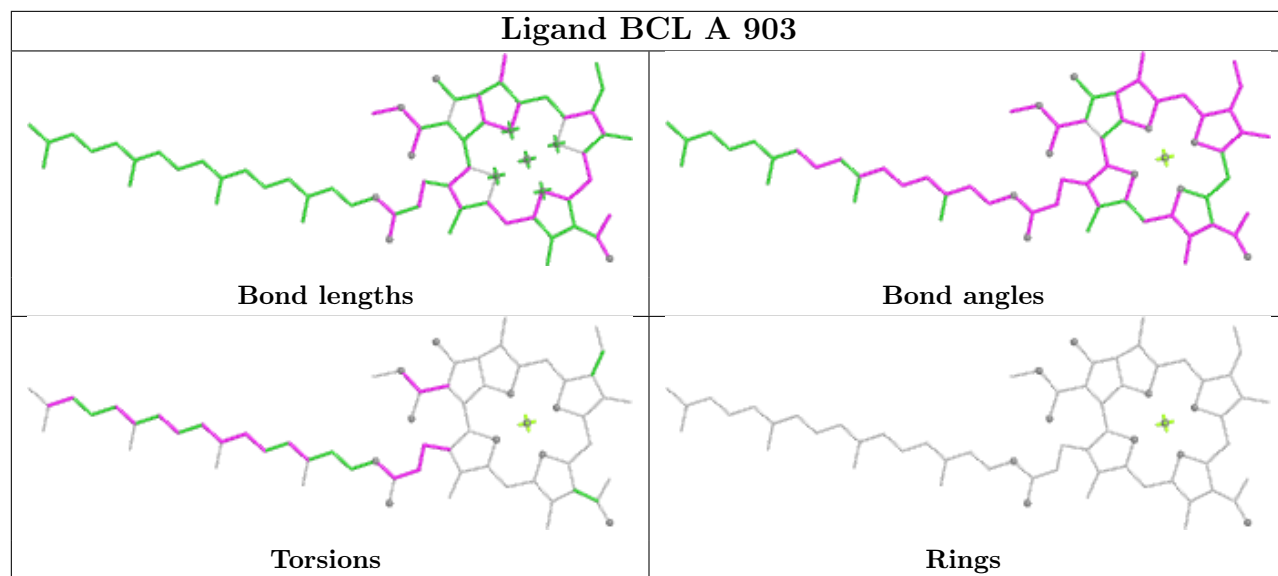
Ligand HEC c 202

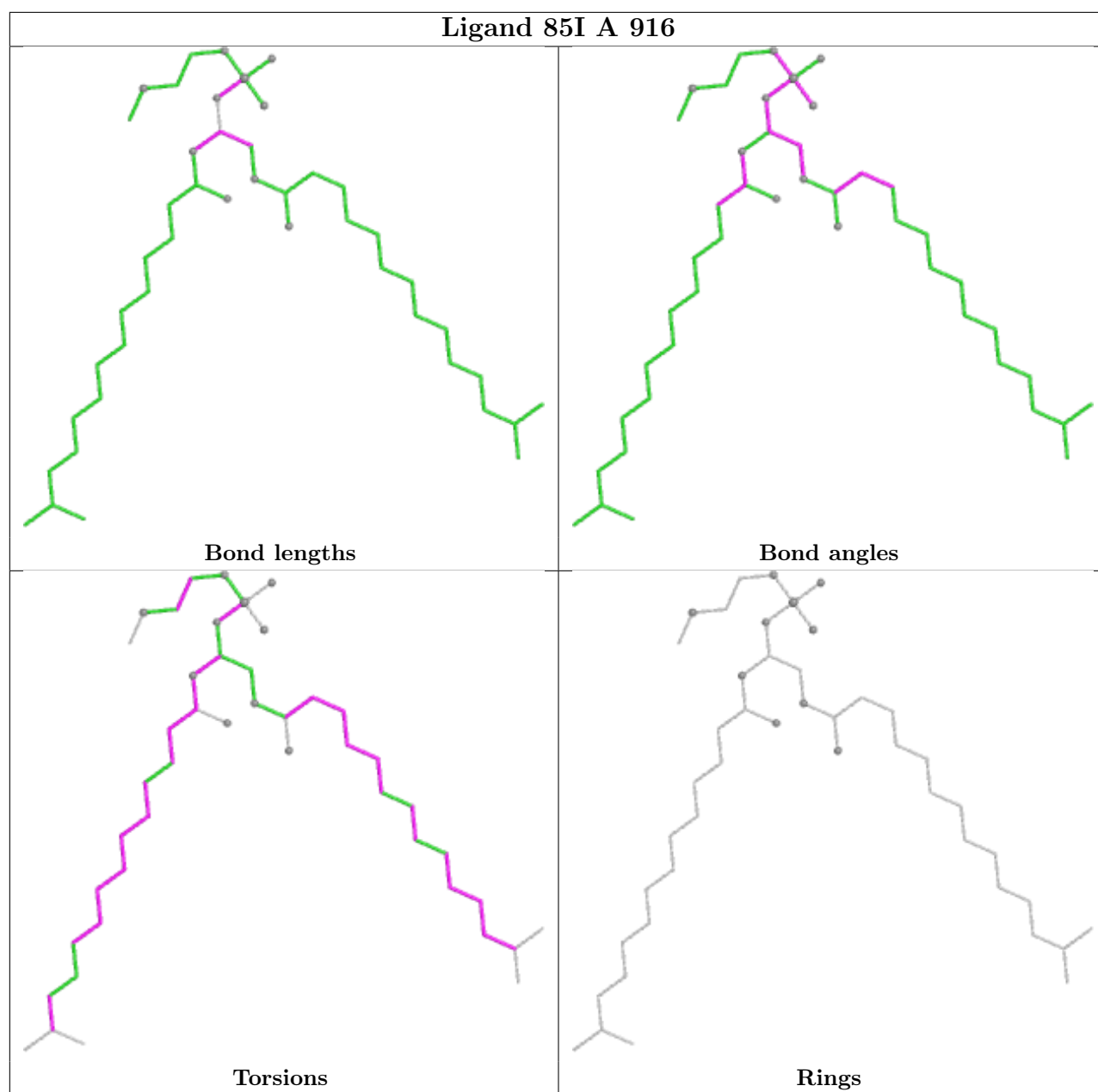


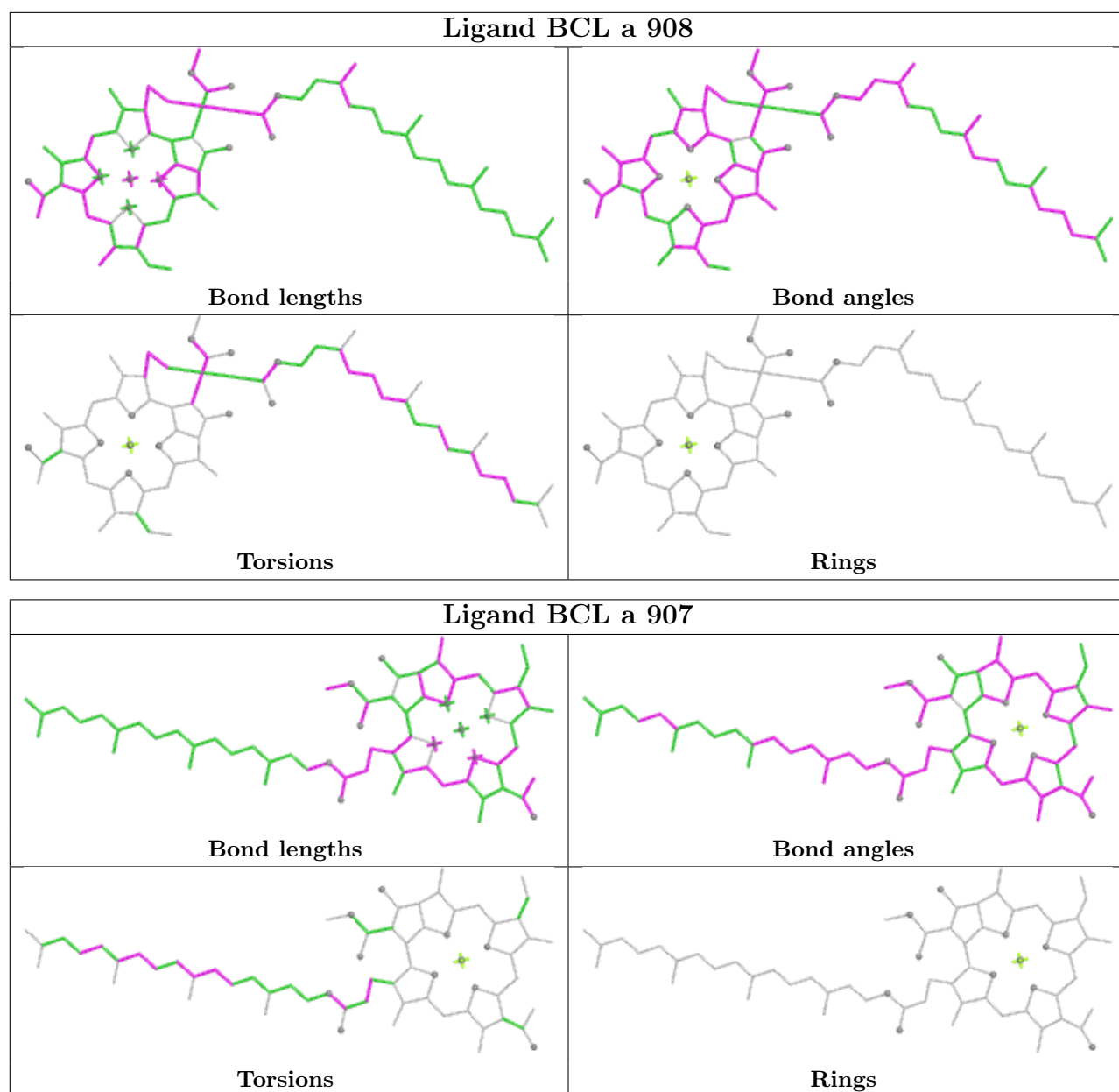


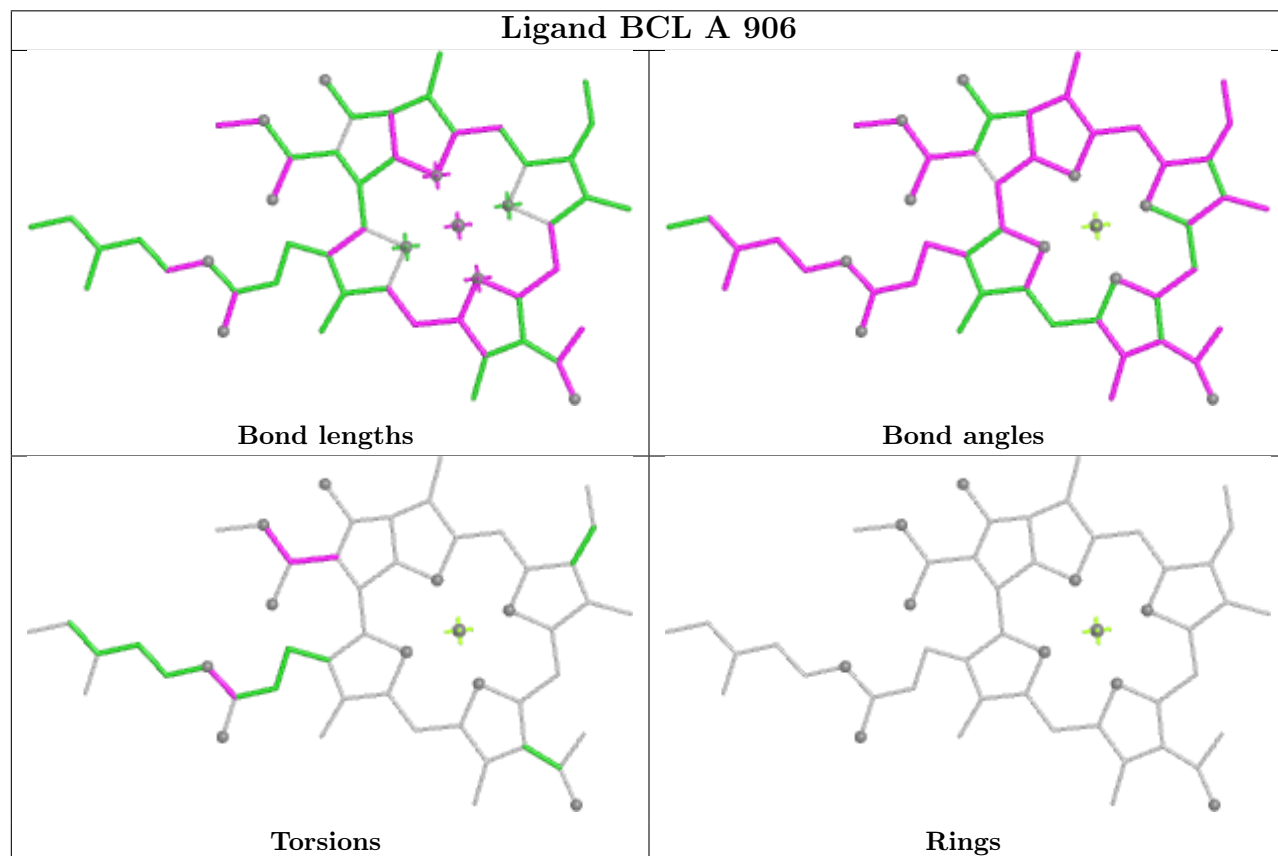
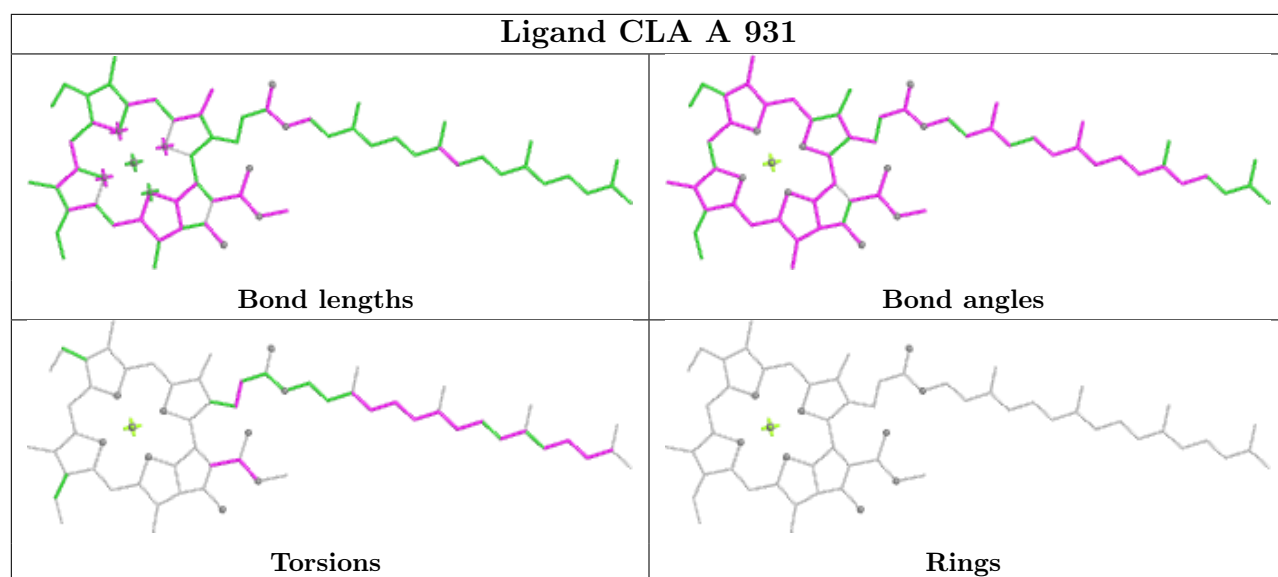


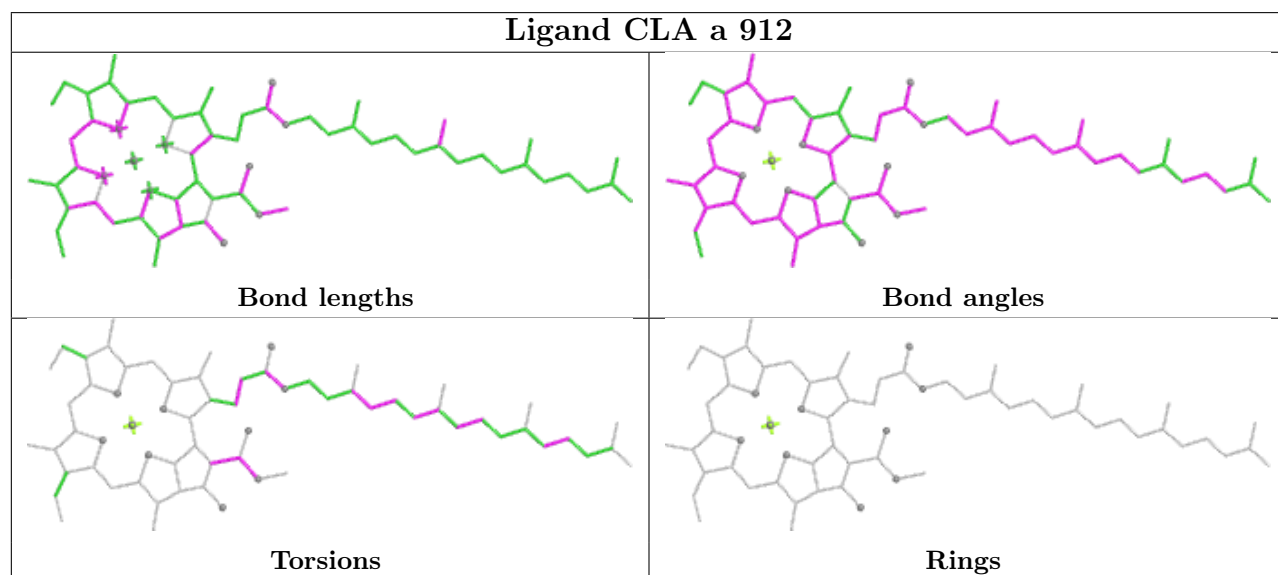
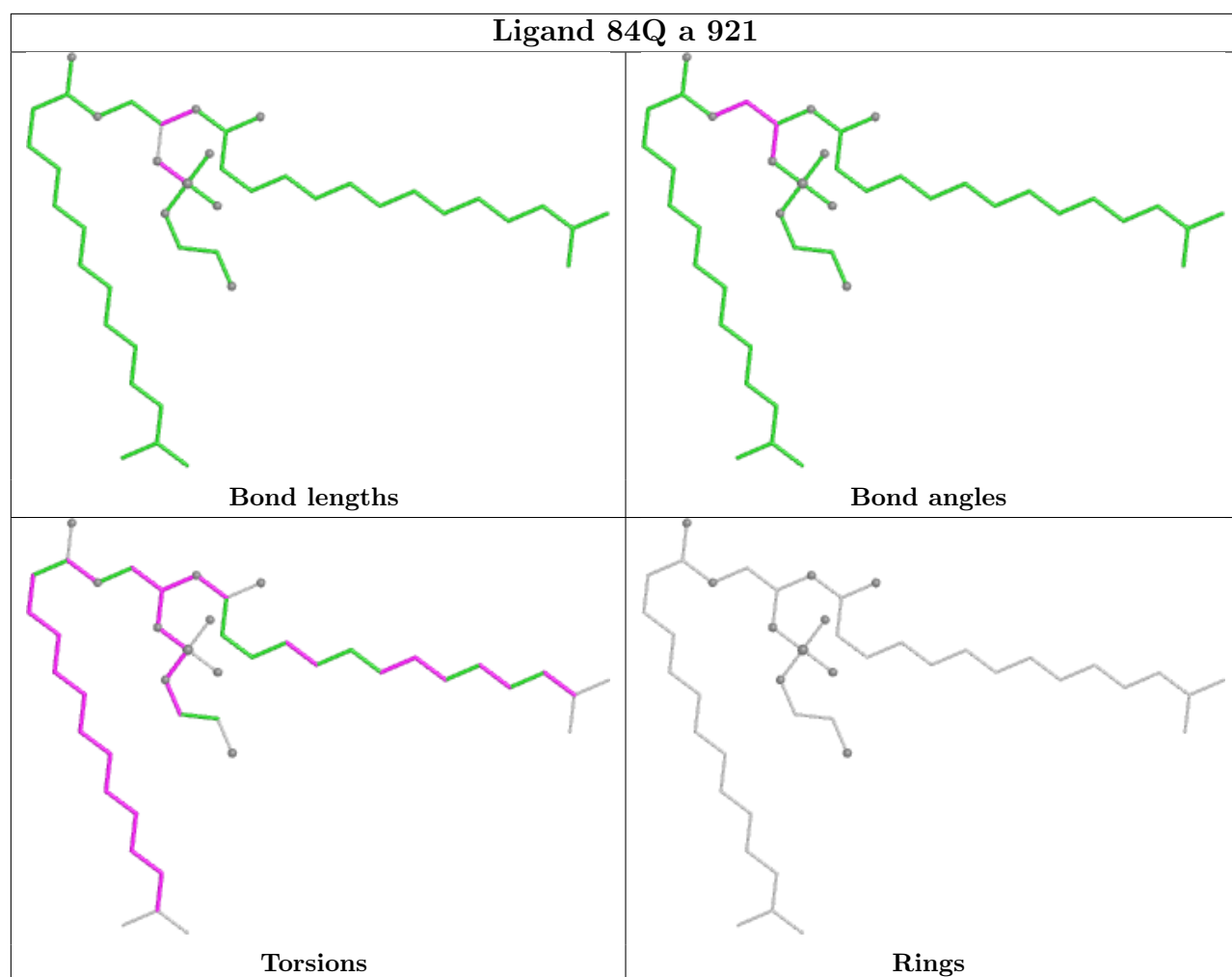


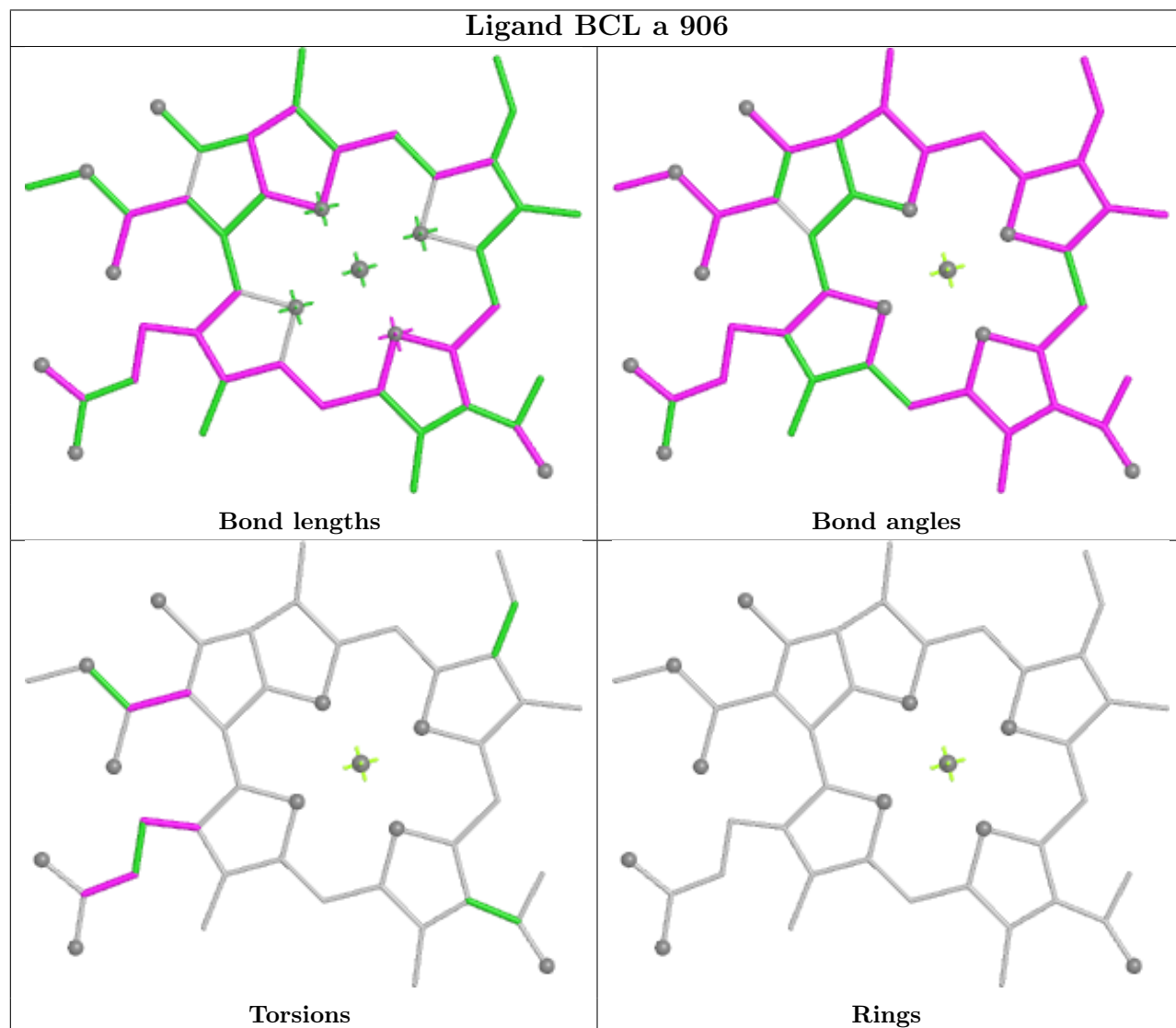
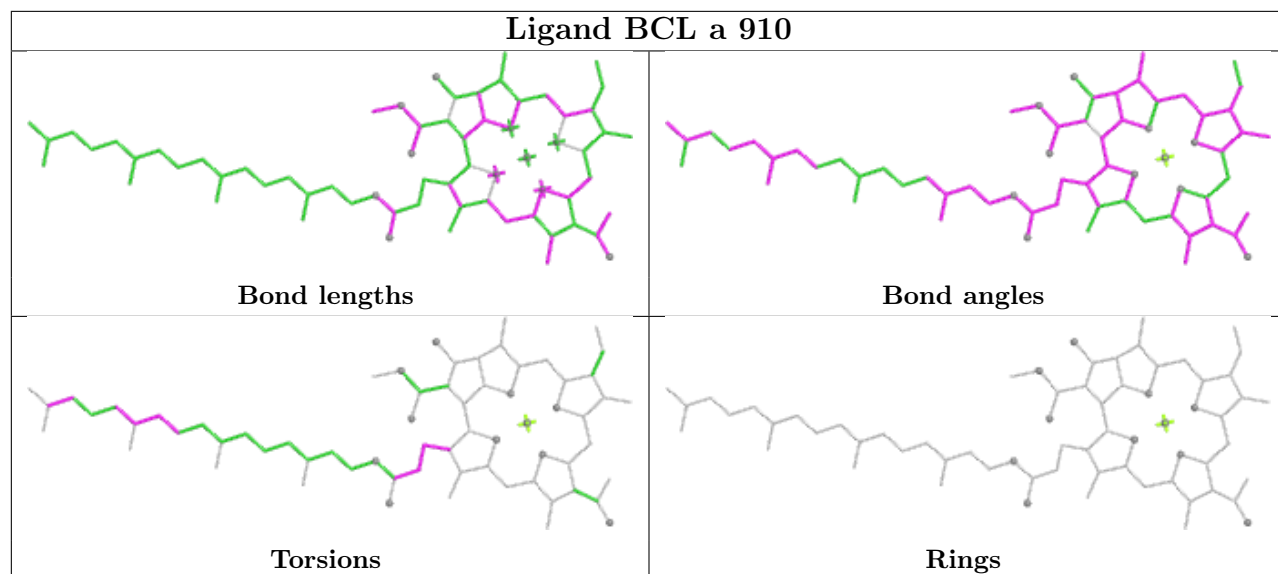


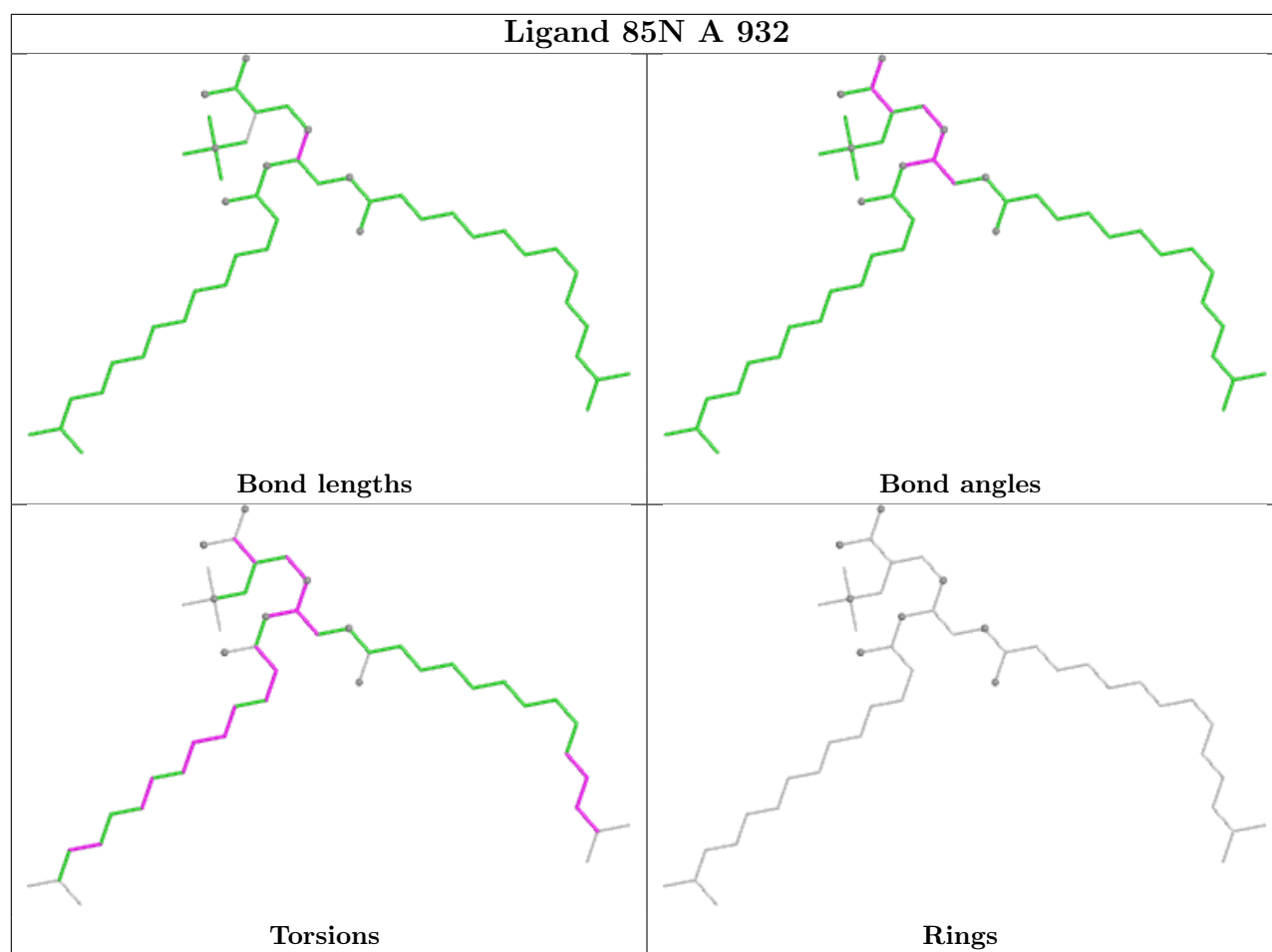








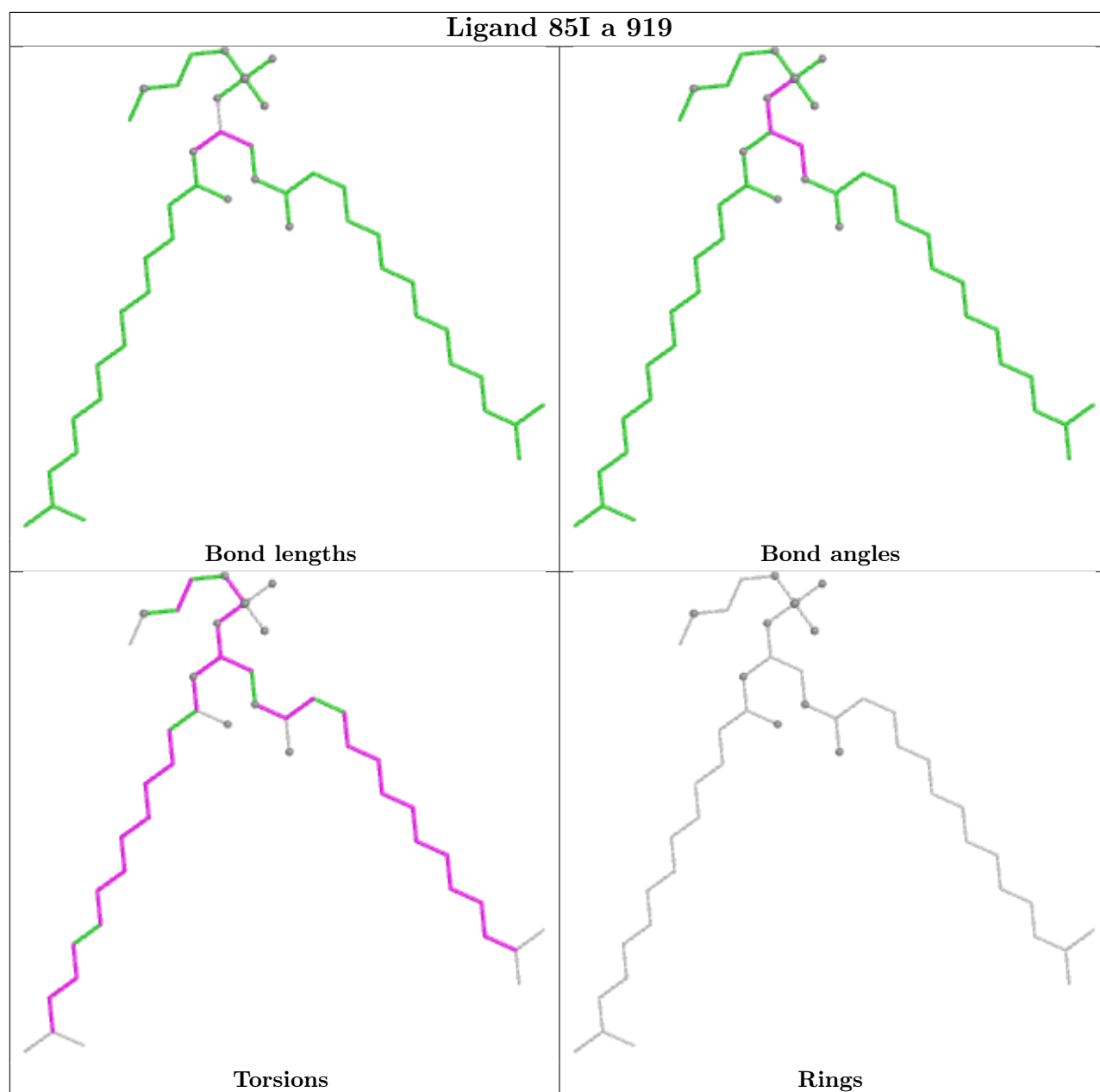




Ligand 85I A 917

The figure displays four panels of geometric analysis for Ligand 85I A 917. The molecule is shown in a stick representation with green and magenta bonds. The panels are:

- Bond lengths:** Shows the molecule with magenta bonds highlighting the C-C and C-H bonds, and green bonds highlighting the C-O and C-N bonds.
- Bond angles:** Shows the molecule with magenta bonds highlighting the C-C and C-H bonds, and green bonds highlighting the C-O and C-N bonds.
- Torsions:** Shows the molecule with magenta bonds highlighting the C-C and C-H bonds, and green bonds highlighting the C-O and C-N bonds.
- Rings:** Shows the molecule with magenta bonds highlighting the C-C and C-H bonds, and green bonds highlighting the C-O and C-N bonds.



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.

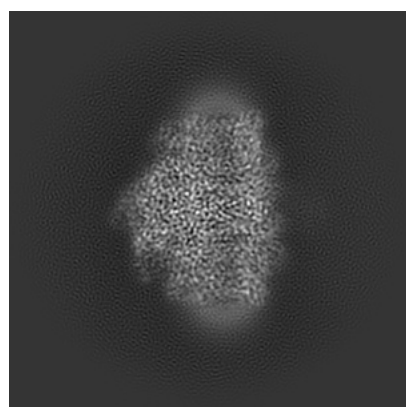
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32229. These allow visual inspection of the internal detail of the map and identification of artifacts.

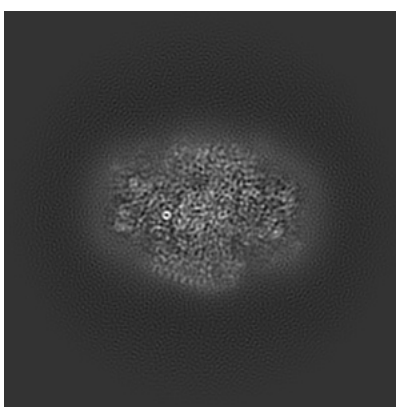
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

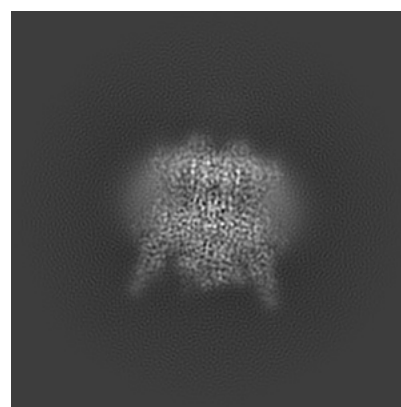
6.1.1 Primary map



X



Y

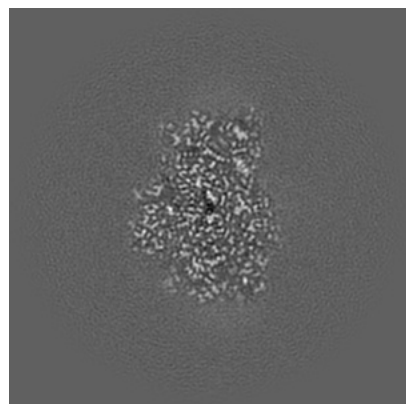


Z

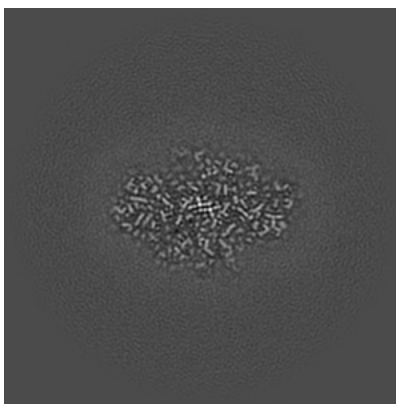
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

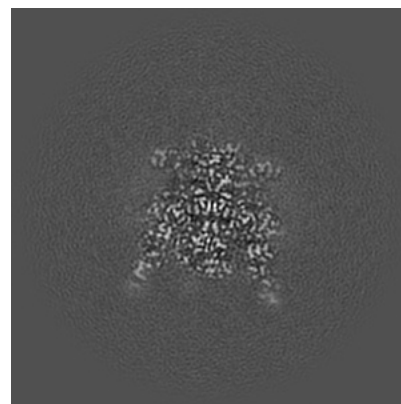
6.2.1 Primary map



X Index: 110



Y Index: 110

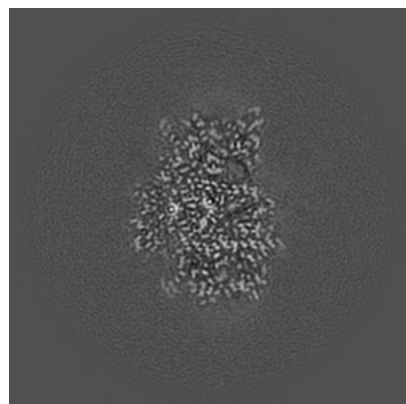


Z Index: 110

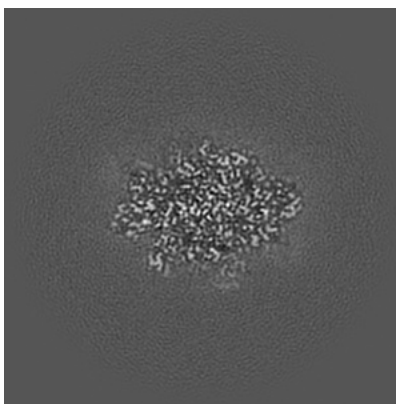
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

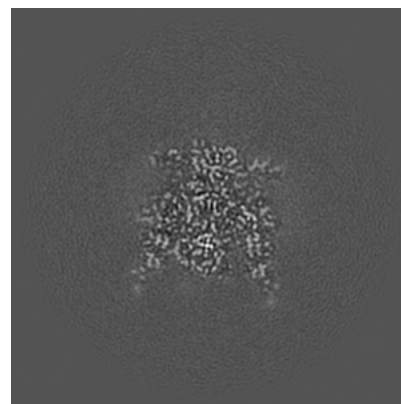
6.3.1 Primary map



X Index: 108



Y Index: 101

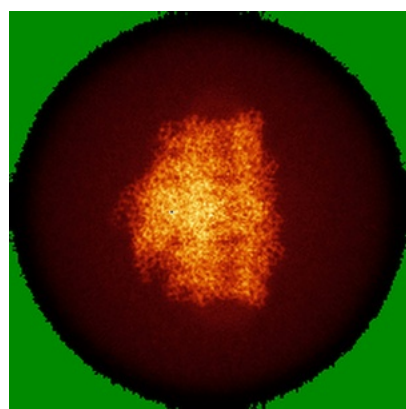


Z Index: 109

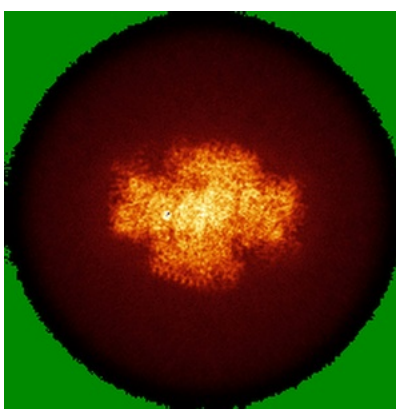
The images above show the largest variance slices of the map in three orthogonal directions.

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

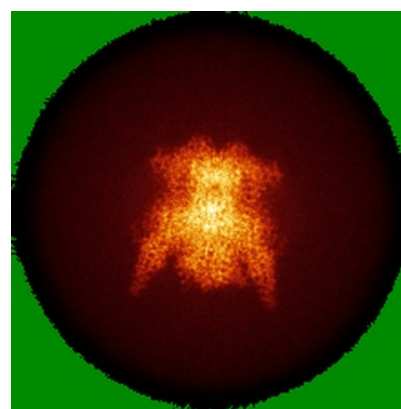
6.4.1 Primary map



X



Y

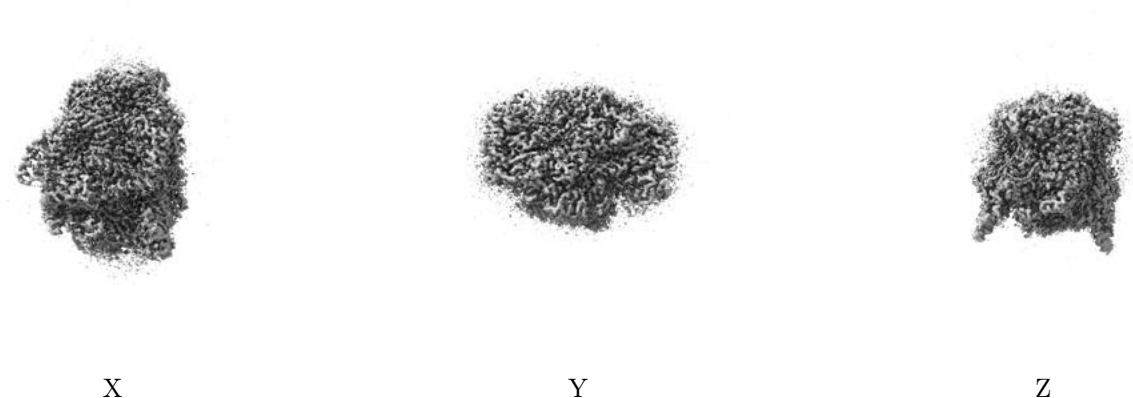


Z

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

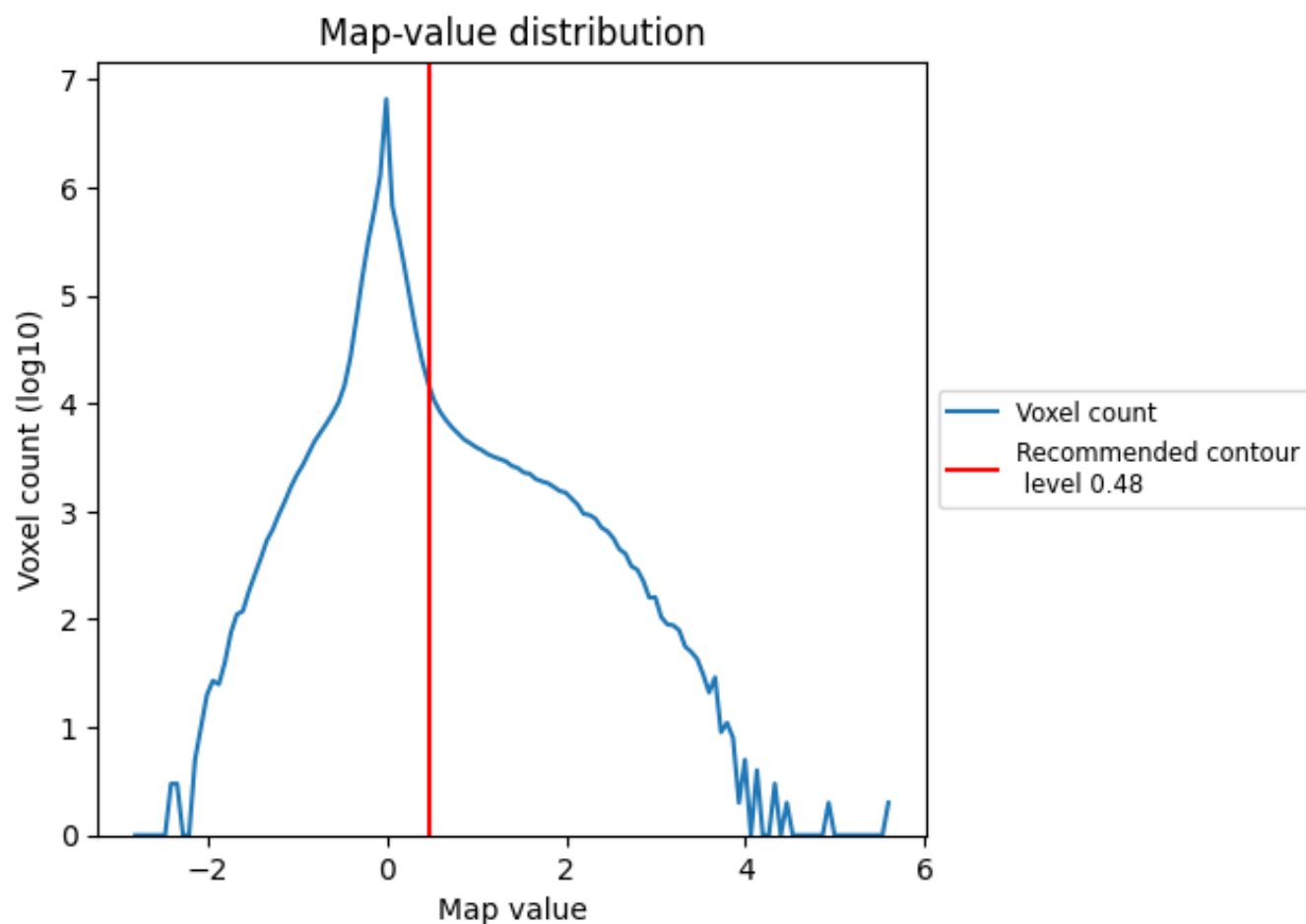
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

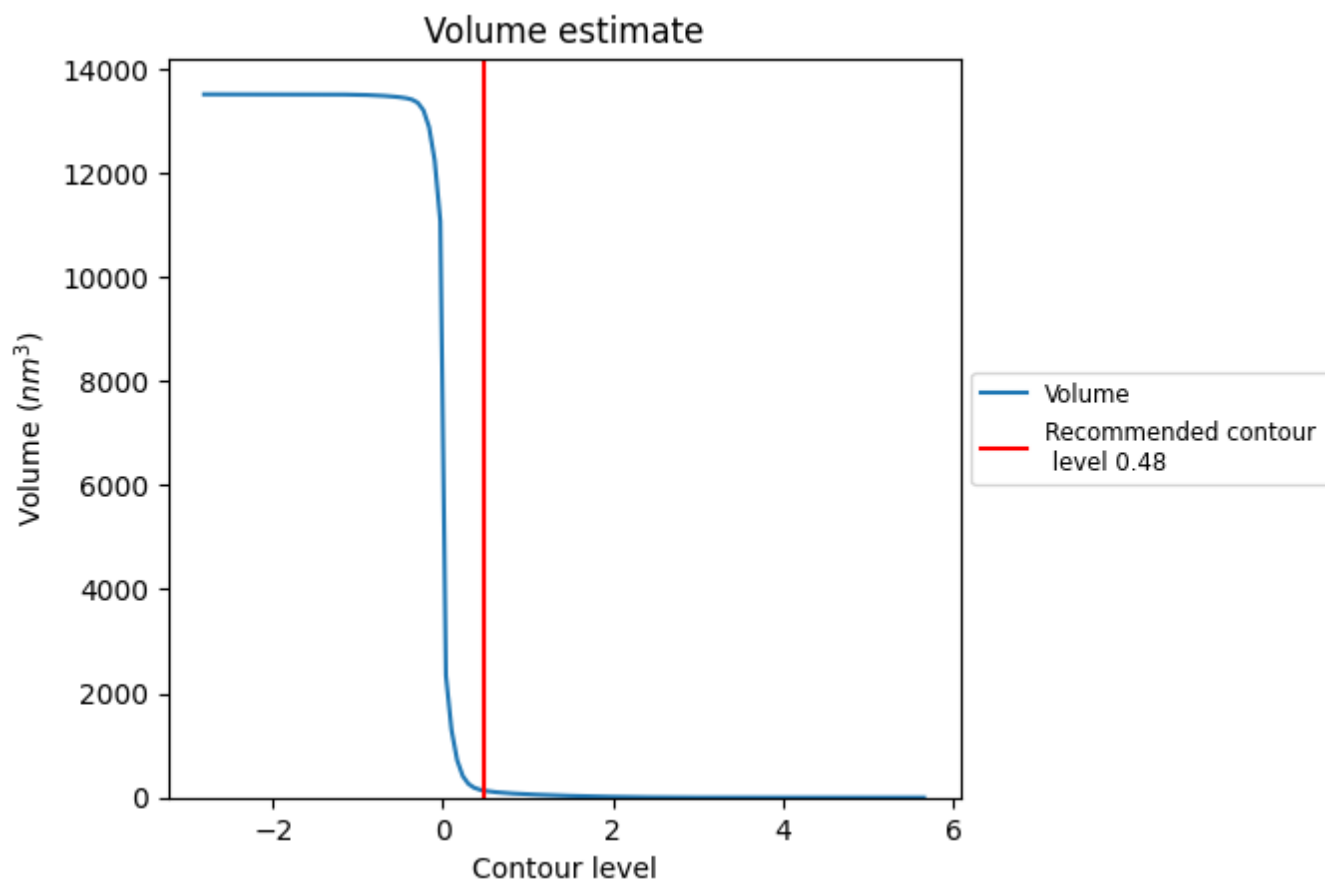
This section contains the results of statistical analysis of the map.

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.

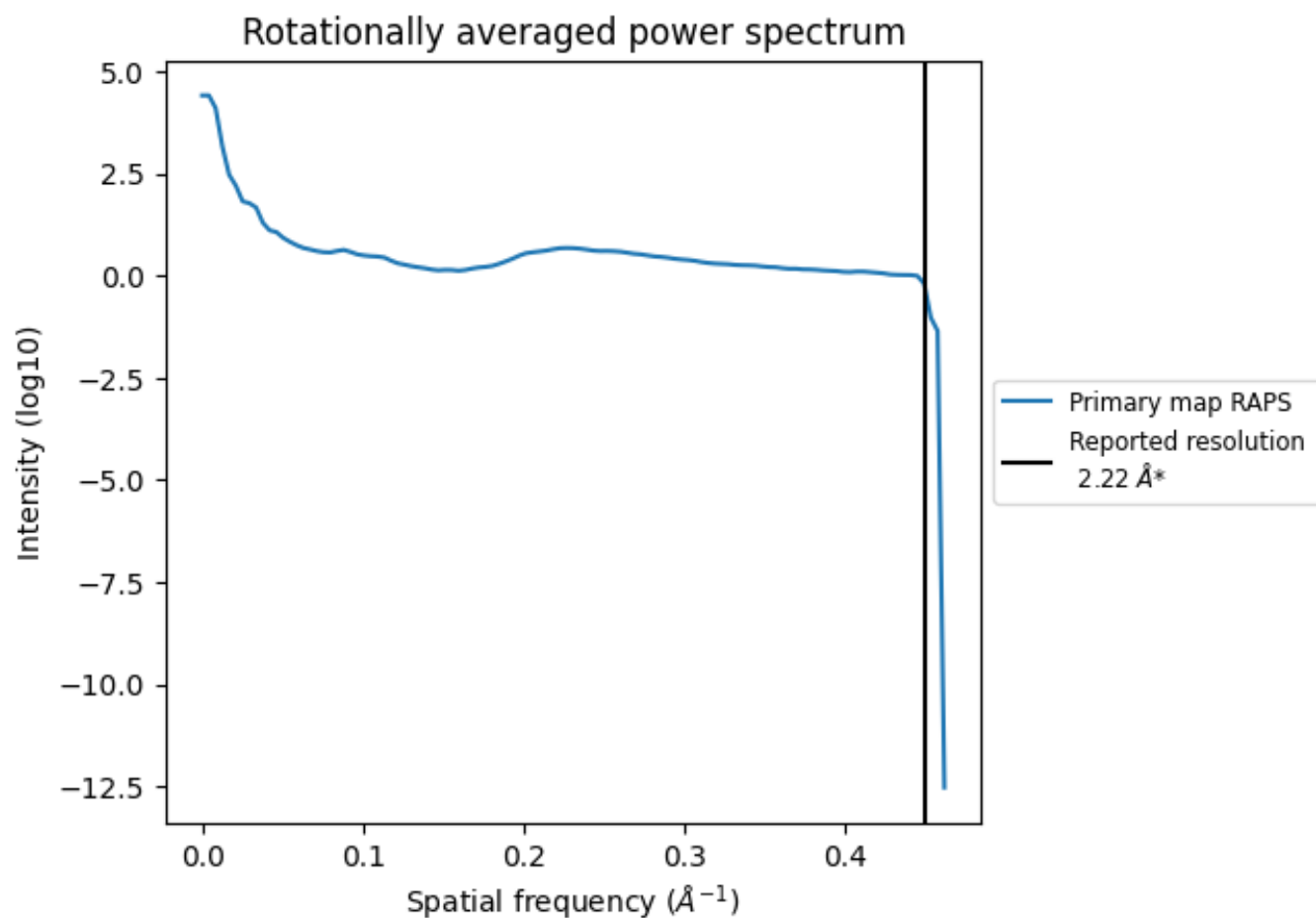
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm³; this corresponds to an approximate mass of 123 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 0.450 Å⁻¹

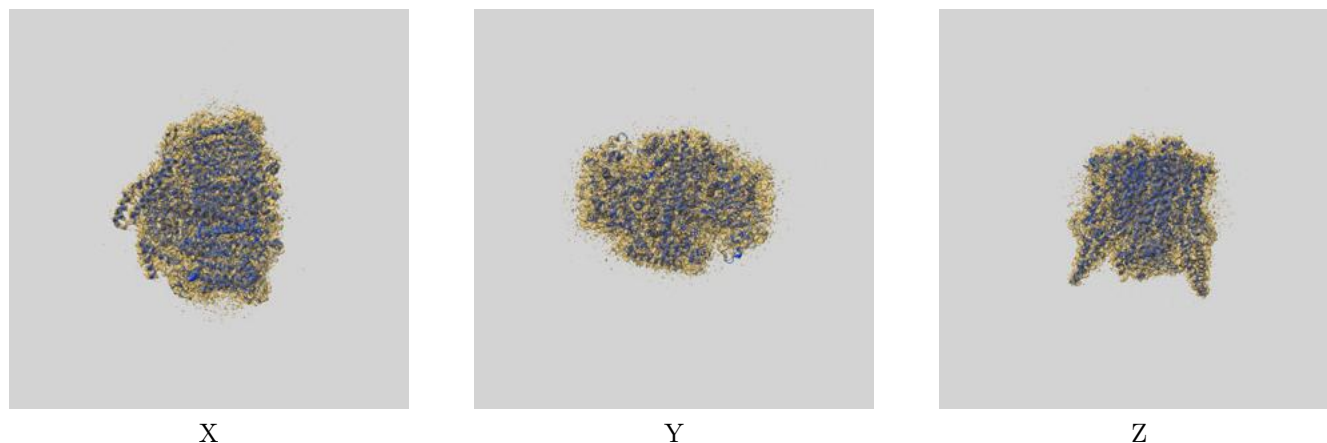
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

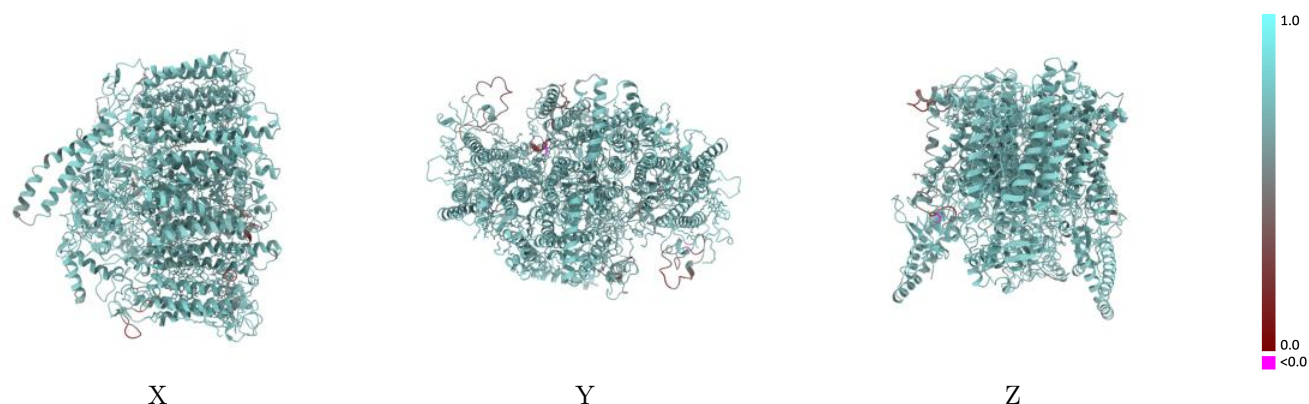
This section contains information regarding the fit between EMDB map EMD-32229 and PDB model 7VZR. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



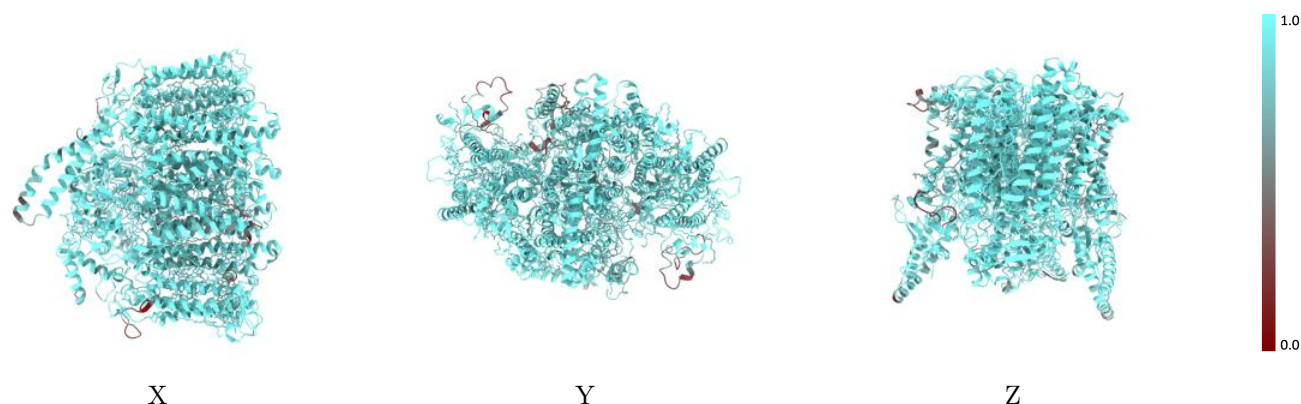
The images above show the 3D surface view of the map at the recommended contour level 0.48 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



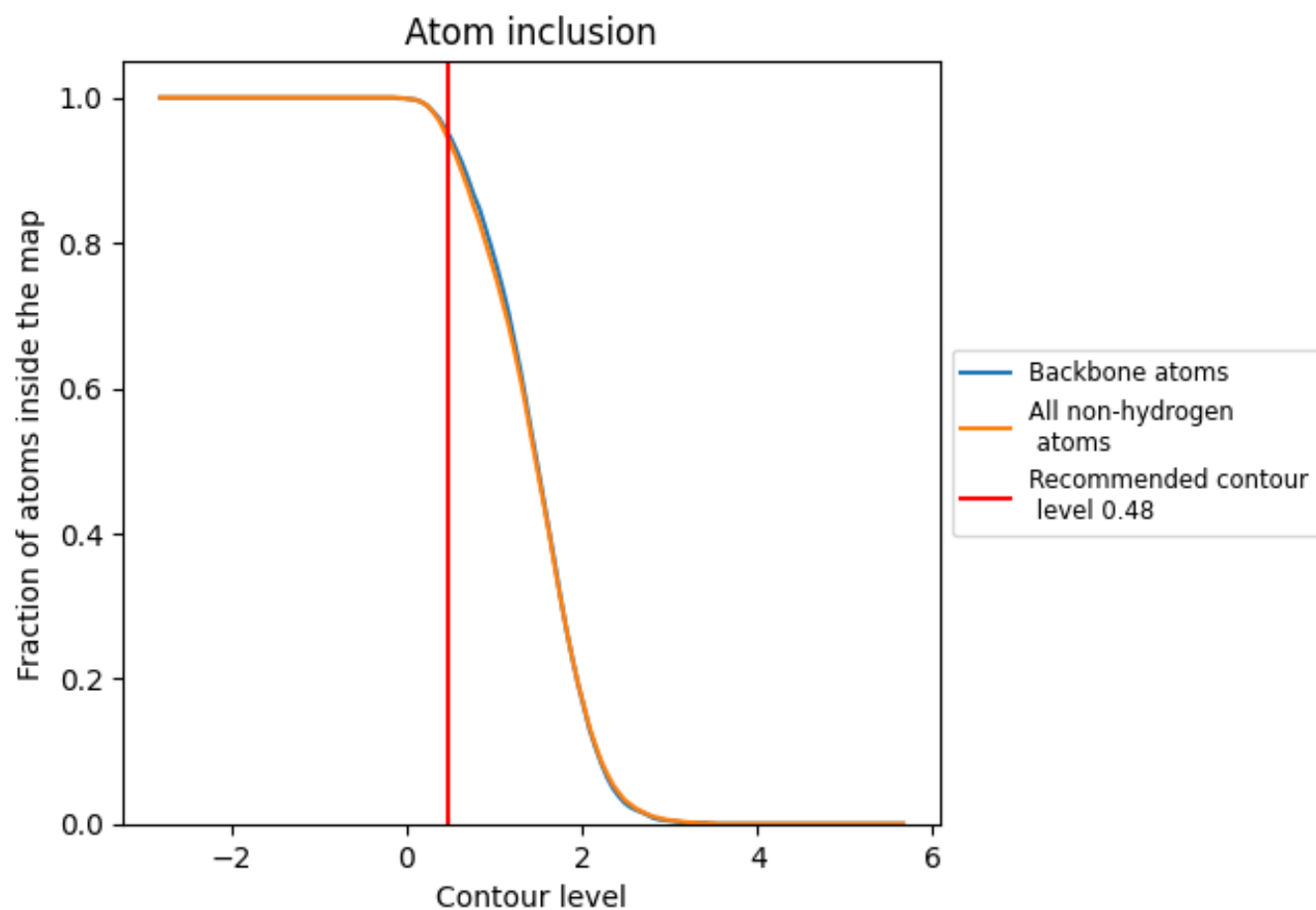
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.48).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9420	0.7050
A	0.9520	0.7100
C	0.9580	0.7210
E	0.9630	0.7140
F	0.9260	0.6700
G	0.7980	0.6490
H	0.8740	0.6670
a	0.9500	0.7060
c	0.9400	0.7060
e	0.9680	0.6970
f	0.9180	0.6770
g	0.7540	0.5870
h	0.8530	0.6610

