



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 05:03 pm BST

PDB ID : 9TLA / pdb_00009tla
EMDB ID : EMD-56047
Title : Cryo-EM Structure of the oligomeric LPOR:Chlide:NADPH Complexes RF-21
Authors : Gabruk, M.; Desfosses, A.; Estrozi, L.F.; Pintscher, S.; Rawski, M.
Deposited on : 2025-12-10
Resolution : 3.17 Å(reported)
Based on initial model : 7JK9

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:

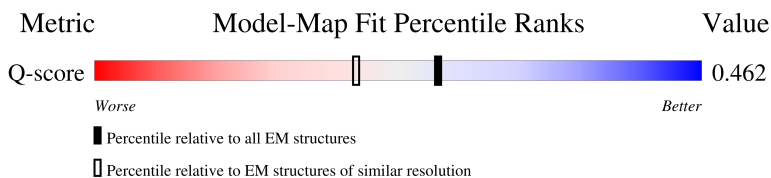
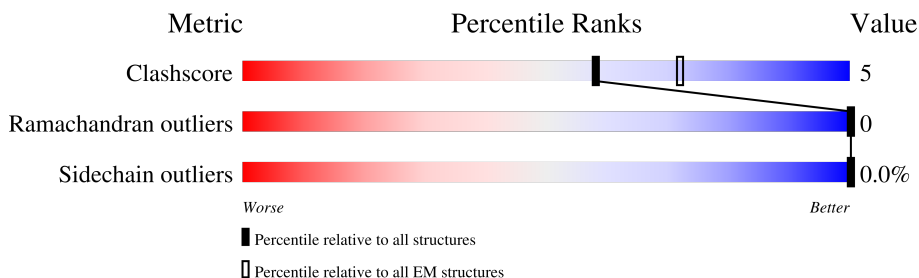
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.17 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	14465 (2.67 - 3.67)

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	YM	353	18% 72% 18% 10%
1	YN	353	85% 5% 10%
1	YO	353	84% 6% 10%
1	YP	353	18% 75% 15% 10%

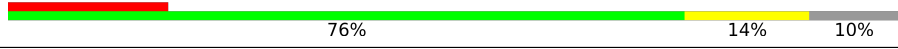
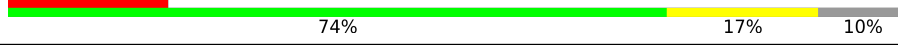
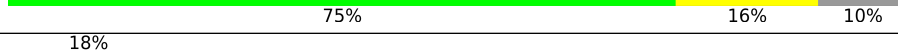
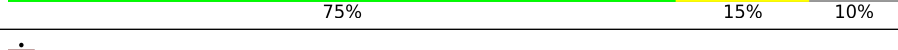
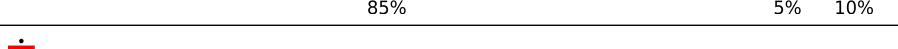
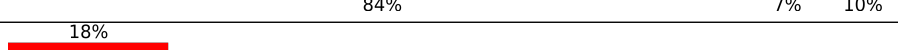
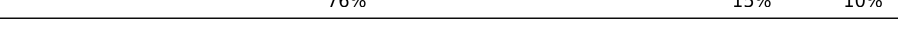
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	YQ	353	
1	YR	353	
1	YS	353	
1	YT	353	
1	YU	353	
1	YV	353	
1	YW	353	
1	YX	353	
1	YY	353	
1	YZ	353	
1	ZA	353	
1	ZB	353	
1	ZC	353	
1	ZD	353	
1	ZE	353	
1	ZF	353	
1	ZG	353	
1	ZH	353	
1	ZI	353	
1	ZJ	353	
1	ZK	353	
1	ZL	353	
1	ZM	353	
1	ZN	353	
1	ZO	353	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	ZP	353	
1	ZQ	353	
1	ZR	353	
1	ZS	353	
1	ZT	353	
1	ZU	353	
1	ZV	353	
1	ZW	353	
1	ZX	353	
1	ZY	353	
1	ZZ	353	

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
3	A1JWG	YM	502	X	-	-	-
3	A1JWG	YN	503	X	-	-	-
3	A1JWG	YO	502	X	-	-	-
3	A1JWG	YP	502	X	-	-	-
3	A1JWG	YQ	502	X	-	-	-
3	A1JWG	YR	503	X	-	-	-
3	A1JWG	YS	502	X	-	-	-
3	A1JWG	YT	502	X	-	-	-
3	A1JWG	YU	502	X	-	-	-
3	A1JWG	YV	503	X	-	-	-
3	A1JWG	YW	502	X	-	-	-
3	A1JWG	YX	502	X	-	-	-
3	A1JWG	YY	502	X	-	-	-
3	A1JWG	YZ	503	X	-	-	-
3	A1JWG	ZA	502	X	-	-	-
3	A1JWG	ZB	502	X	-	-	-
3	A1JWG	ZC	502	X	-	-	-
3	A1JWG	ZD	503	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	A1JWG	ZE	502	X	-	-	-
3	A1JWG	ZF	502	X	-	-	-
3	A1JWG	ZG	502	X	-	-	-
3	A1JWG	ZH	503	X	-	-	-
3	A1JWG	ZI	502	X	-	-	-
3	A1JWG	ZJ	502	X	-	-	-
3	A1JWG	ZK	502	X	-	-	-
3	A1JWG	ZL	503	X	-	-	-
3	A1JWG	ZM	502	X	-	-	-
3	A1JWG	ZN	502	X	-	-	-
3	A1JWG	ZO	502	X	-	-	-
3	A1JWG	ZP	503	X	-	-	-
3	A1JWG	ZQ	502	X	-	-	-
3	A1JWG	ZR	502	X	-	-	-
3	A1JWG	ZS	502	X	-	-	-
3	A1JWG	ZT	503	X	-	-	-
3	A1JWG	ZU	502	X	-	-	-
3	A1JWG	ZV	502	X	-	-	-
3	A1JWG	ZW	502	X	-	-	-
3	A1JWG	ZX	503	X	-	-	-
3	A1JWG	ZY	502	X	-	-	-
3	A1JWG	ZZ	502	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 102450 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 Protochlorophyllide reductase B, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	YM	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	YN	319	Total	C	N	O	S	0	0
			2446	1550	423	463	10		
1	YO	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	YP	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	YQ	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	YR	319	Total	C	N	O	S	0	0
			2446	1550	423	463	10		
1	YS	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	YT	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	YU	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	YV	319	Total	C	N	O	S	0	0
			2446	1550	423	463	10		
1	YW	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	YX	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	YY	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	YZ	319	Total	C	N	O	S	0	0
			2446	1550	423	463	10		
1	ZA	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	ZB	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	ZC	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	ZD	319	Total 2446	C 1550	N 423	O 463	S 10	0	0
1	ZE	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZF	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZG	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZH	319	Total 2446	C 1550	N 423	O 463	S 10	0	0
1	ZI	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZJ	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZK	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZL	319	Total 2446	C 1550	N 423	O 463	S 10	0	0
1	ZM	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZN	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZO	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZP	319	Total 2446	C 1550	N 423	O 463	S 10	0	0
1	ZQ	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZR	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZS	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZT	319	Total 2446	C 1550	N 423	O 463	S 10	0	0
1	ZU	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZV	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZW	319	Total 2445	C 1550	N 422	O 463	S 10	0	0
1	ZX	319	Total 2446	C 1550	N 423	O 463	S 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	ZY	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		
1	ZZ	319	Total	C	N	O	S	0	0
			2445	1550	422	463	10		

There are 760 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
YM	49	MET	-	initiating methionine	UNP P21218
YM	50	GLY	-	expression tag	UNP P21218
YM	51	SER	-	expression tag	UNP P21218
YM	52	SER	-	expression tag	UNP P21218
YM	53	HIS	-	expression tag	UNP P21218
YM	54	HIS	-	expression tag	UNP P21218
YM	55	HIS	-	expression tag	UNP P21218
YM	56	HIS	-	expression tag	UNP P21218
YM	57	HIS	-	expression tag	UNP P21218
YM	58	HIS	-	expression tag	UNP P21218
YM	59	SER	-	expression tag	UNP P21218
YM	60	SER	-	expression tag	UNP P21218
YM	61	GLY	-	expression tag	UNP P21218
YM	62	LEU	-	expression tag	UNP P21218
YM	63	VAL	-	expression tag	UNP P21218
YM	64	PRO	-	expression tag	UNP P21218
YM	65	ARG	-	expression tag	UNP P21218
YM	66	GLY	-	expression tag	UNP P21218
YM	67	SER	-	expression tag	UNP P21218
YN	49	MET	-	initiating methionine	UNP P21218
YN	50	GLY	-	expression tag	UNP P21218
YN	51	SER	-	expression tag	UNP P21218
YN	52	SER	-	expression tag	UNP P21218
YN	53	HIS	-	expression tag	UNP P21218
YN	54	HIS	-	expression tag	UNP P21218
YN	55	HIS	-	expression tag	UNP P21218
YN	56	HIS	-	expression tag	UNP P21218
YN	57	HIS	-	expression tag	UNP P21218
YN	58	HIS	-	expression tag	UNP P21218
YN	59	SER	-	expression tag	UNP P21218
YN	60	SER	-	expression tag	UNP P21218
YN	61	GLY	-	expression tag	UNP P21218
YN	62	LEU	-	expression tag	UNP P21218
YN	63	VAL	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
YN	64	PRO	-	expression tag	UNP P21218
YN	65	ARG	-	expression tag	UNP P21218
YN	66	GLY	-	expression tag	UNP P21218
YN	67	SER	-	expression tag	UNP P21218
YO	49	MET	-	initiating methionine	UNP P21218
YO	50	GLY	-	expression tag	UNP P21218
YO	51	SER	-	expression tag	UNP P21218
YO	52	SER	-	expression tag	UNP P21218
YO	53	HIS	-	expression tag	UNP P21218
YO	54	HIS	-	expression tag	UNP P21218
YO	55	HIS	-	expression tag	UNP P21218
YO	56	HIS	-	expression tag	UNP P21218
YO	57	HIS	-	expression tag	UNP P21218
YO	58	HIS	-	expression tag	UNP P21218
YO	59	SER	-	expression tag	UNP P21218
YO	60	SER	-	expression tag	UNP P21218
YO	61	GLY	-	expression tag	UNP P21218
YO	62	LEU	-	expression tag	UNP P21218
YO	63	VAL	-	expression tag	UNP P21218
YO	64	PRO	-	expression tag	UNP P21218
YO	65	ARG	-	expression tag	UNP P21218
YO	66	GLY	-	expression tag	UNP P21218
YO	67	SER	-	expression tag	UNP P21218
YP	49	MET	-	initiating methionine	UNP P21218
YP	50	GLY	-	expression tag	UNP P21218
YP	51	SER	-	expression tag	UNP P21218
YP	52	SER	-	expression tag	UNP P21218
YP	53	HIS	-	expression tag	UNP P21218
YP	54	HIS	-	expression tag	UNP P21218
YP	55	HIS	-	expression tag	UNP P21218
YP	56	HIS	-	expression tag	UNP P21218
YP	57	HIS	-	expression tag	UNP P21218
YP	58	HIS	-	expression tag	UNP P21218
YP	59	SER	-	expression tag	UNP P21218
YP	60	SER	-	expression tag	UNP P21218
YP	61	GLY	-	expression tag	UNP P21218
YP	62	LEU	-	expression tag	UNP P21218
YP	63	VAL	-	expression tag	UNP P21218
YP	64	PRO	-	expression tag	UNP P21218
YP	65	ARG	-	expression tag	UNP P21218
YP	66	GLY	-	expression tag	UNP P21218
YP	67	SER	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
YQ	49	MET	-	initiating methionine	UNP P21218
YQ	50	GLY	-	expression tag	UNP P21218
YQ	51	SER	-	expression tag	UNP P21218
YQ	52	SER	-	expression tag	UNP P21218
YQ	53	HIS	-	expression tag	UNP P21218
YQ	54	HIS	-	expression tag	UNP P21218
YQ	55	HIS	-	expression tag	UNP P21218
YQ	56	HIS	-	expression tag	UNP P21218
YQ	57	HIS	-	expression tag	UNP P21218
YQ	58	HIS	-	expression tag	UNP P21218
YQ	59	SER	-	expression tag	UNP P21218
YQ	60	SER	-	expression tag	UNP P21218
YQ	61	GLY	-	expression tag	UNP P21218
YQ	62	LEU	-	expression tag	UNP P21218
YQ	63	VAL	-	expression tag	UNP P21218
YQ	64	PRO	-	expression tag	UNP P21218
YQ	65	ARG	-	expression tag	UNP P21218
YQ	66	GLY	-	expression tag	UNP P21218
YQ	67	SER	-	expression tag	UNP P21218
YR	49	MET	-	initiating methionine	UNP P21218
YR	50	GLY	-	expression tag	UNP P21218
YR	51	SER	-	expression tag	UNP P21218
YR	52	SER	-	expression tag	UNP P21218
YR	53	HIS	-	expression tag	UNP P21218
YR	54	HIS	-	expression tag	UNP P21218
YR	55	HIS	-	expression tag	UNP P21218
YR	56	HIS	-	expression tag	UNP P21218
YR	57	HIS	-	expression tag	UNP P21218
YR	58	HIS	-	expression tag	UNP P21218
YR	59	SER	-	expression tag	UNP P21218
YR	60	SER	-	expression tag	UNP P21218
YR	61	GLY	-	expression tag	UNP P21218
YR	62	LEU	-	expression tag	UNP P21218
YR	63	VAL	-	expression tag	UNP P21218
YR	64	PRO	-	expression tag	UNP P21218
YR	65	ARG	-	expression tag	UNP P21218
YR	66	GLY	-	expression tag	UNP P21218
YR	67	SER	-	expression tag	UNP P21218
YS	49	MET	-	initiating methionine	UNP P21218
YS	50	GLY	-	expression tag	UNP P21218
YS	51	SER	-	expression tag	UNP P21218
YS	52	SER	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
YS	53	HIS	-	expression tag	UNP P21218
YS	54	HIS	-	expression tag	UNP P21218
YS	55	HIS	-	expression tag	UNP P21218
YS	56	HIS	-	expression tag	UNP P21218
YS	57	HIS	-	expression tag	UNP P21218
YS	58	HIS	-	expression tag	UNP P21218
YS	59	SER	-	expression tag	UNP P21218
YS	60	SER	-	expression tag	UNP P21218
YS	61	GLY	-	expression tag	UNP P21218
YS	62	LEU	-	expression tag	UNP P21218
YS	63	VAL	-	expression tag	UNP P21218
YS	64	PRO	-	expression tag	UNP P21218
YS	65	ARG	-	expression tag	UNP P21218
YS	66	GLY	-	expression tag	UNP P21218
YS	67	SER	-	expression tag	UNP P21218
YT	49	MET	-	initiating methionine	UNP P21218
YT	50	GLY	-	expression tag	UNP P21218
YT	51	SER	-	expression tag	UNP P21218
YT	52	SER	-	expression tag	UNP P21218
YT	53	HIS	-	expression tag	UNP P21218
YT	54	HIS	-	expression tag	UNP P21218
YT	55	HIS	-	expression tag	UNP P21218
YT	56	HIS	-	expression tag	UNP P21218
YT	57	HIS	-	expression tag	UNP P21218
YT	58	HIS	-	expression tag	UNP P21218
YT	59	SER	-	expression tag	UNP P21218
YT	60	SER	-	expression tag	UNP P21218
YT	61	GLY	-	expression tag	UNP P21218
YT	62	LEU	-	expression tag	UNP P21218
YT	63	VAL	-	expression tag	UNP P21218
YT	64	PRO	-	expression tag	UNP P21218
YT	65	ARG	-	expression tag	UNP P21218
YT	66	GLY	-	expression tag	UNP P21218
YT	67	SER	-	expression tag	UNP P21218
YU	49	MET	-	initiating methionine	UNP P21218
YU	50	GLY	-	expression tag	UNP P21218
YU	51	SER	-	expression tag	UNP P21218
YU	52	SER	-	expression tag	UNP P21218
YU	53	HIS	-	expression tag	UNP P21218
YU	54	HIS	-	expression tag	UNP P21218
YU	55	HIS	-	expression tag	UNP P21218
YU	56	HIS	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
YU	57	HIS	-	expression tag	UNP P21218
YU	58	HIS	-	expression tag	UNP P21218
YU	59	SER	-	expression tag	UNP P21218
YU	60	SER	-	expression tag	UNP P21218
YU	61	GLY	-	expression tag	UNP P21218
YU	62	LEU	-	expression tag	UNP P21218
YU	63	VAL	-	expression tag	UNP P21218
YU	64	PRO	-	expression tag	UNP P21218
YU	65	ARG	-	expression tag	UNP P21218
YU	66	GLY	-	expression tag	UNP P21218
YU	67	SER	-	expression tag	UNP P21218
YV	49	MET	-	initiating methionine	UNP P21218
YV	50	GLY	-	expression tag	UNP P21218
YV	51	SER	-	expression tag	UNP P21218
YV	52	SER	-	expression tag	UNP P21218
YV	53	HIS	-	expression tag	UNP P21218
YV	54	HIS	-	expression tag	UNP P21218
YV	55	HIS	-	expression tag	UNP P21218
YV	56	HIS	-	expression tag	UNP P21218
YV	57	HIS	-	expression tag	UNP P21218
YV	58	HIS	-	expression tag	UNP P21218
YV	59	SER	-	expression tag	UNP P21218
YV	60	SER	-	expression tag	UNP P21218
YV	61	GLY	-	expression tag	UNP P21218
YV	62	LEU	-	expression tag	UNP P21218
YV	63	VAL	-	expression tag	UNP P21218
YV	64	PRO	-	expression tag	UNP P21218
YV	65	ARG	-	expression tag	UNP P21218
YV	66	GLY	-	expression tag	UNP P21218
YV	67	SER	-	expression tag	UNP P21218
YW	49	MET	-	initiating methionine	UNP P21218
YW	50	GLY	-	expression tag	UNP P21218
YW	51	SER	-	expression tag	UNP P21218
YW	52	SER	-	expression tag	UNP P21218
YW	53	HIS	-	expression tag	UNP P21218
YW	54	HIS	-	expression tag	UNP P21218
YW	55	HIS	-	expression tag	UNP P21218
YW	56	HIS	-	expression tag	UNP P21218
YW	57	HIS	-	expression tag	UNP P21218
YW	58	HIS	-	expression tag	UNP P21218
YW	59	SER	-	expression tag	UNP P21218
YW	60	SER	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
YW	61	GLY	-	expression tag	UNP P21218
YW	62	LEU	-	expression tag	UNP P21218
YW	63	VAL	-	expression tag	UNP P21218
YW	64	PRO	-	expression tag	UNP P21218
YW	65	ARG	-	expression tag	UNP P21218
YW	66	GLY	-	expression tag	UNP P21218
YW	67	SER	-	expression tag	UNP P21218
YX	49	MET	-	initiating methionine	UNP P21218
YX	50	GLY	-	expression tag	UNP P21218
YX	51	SER	-	expression tag	UNP P21218
YX	52	SER	-	expression tag	UNP P21218
YX	53	HIS	-	expression tag	UNP P21218
YX	54	HIS	-	expression tag	UNP P21218
YX	55	HIS	-	expression tag	UNP P21218
YX	56	HIS	-	expression tag	UNP P21218
YX	57	HIS	-	expression tag	UNP P21218
YX	58	HIS	-	expression tag	UNP P21218
YX	59	SER	-	expression tag	UNP P21218
YX	60	SER	-	expression tag	UNP P21218
YX	61	GLY	-	expression tag	UNP P21218
YX	62	LEU	-	expression tag	UNP P21218
YX	63	VAL	-	expression tag	UNP P21218
YX	64	PRO	-	expression tag	UNP P21218
YX	65	ARG	-	expression tag	UNP P21218
YX	66	GLY	-	expression tag	UNP P21218
YX	67	SER	-	expression tag	UNP P21218
YY	49	MET	-	initiating methionine	UNP P21218
YY	50	GLY	-	expression tag	UNP P21218
YY	51	SER	-	expression tag	UNP P21218
YY	52	SER	-	expression tag	UNP P21218
YY	53	HIS	-	expression tag	UNP P21218
YY	54	HIS	-	expression tag	UNP P21218
YY	55	HIS	-	expression tag	UNP P21218
YY	56	HIS	-	expression tag	UNP P21218
YY	57	HIS	-	expression tag	UNP P21218
YY	58	HIS	-	expression tag	UNP P21218
YY	59	SER	-	expression tag	UNP P21218
YY	60	SER	-	expression tag	UNP P21218
YY	61	GLY	-	expression tag	UNP P21218
YY	62	LEU	-	expression tag	UNP P21218
YY	63	VAL	-	expression tag	UNP P21218
YY	64	PRO	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
YY	65	ARG	-	expression tag	UNP P21218
YY	66	GLY	-	expression tag	UNP P21218
YY	67	SER	-	expression tag	UNP P21218
YZ	49	MET	-	initiating methionine	UNP P21218
YZ	50	GLY	-	expression tag	UNP P21218
YZ	51	SER	-	expression tag	UNP P21218
YZ	52	SER	-	expression tag	UNP P21218
YZ	53	HIS	-	expression tag	UNP P21218
YZ	54	HIS	-	expression tag	UNP P21218
YZ	55	HIS	-	expression tag	UNP P21218
YZ	56	HIS	-	expression tag	UNP P21218
YZ	57	HIS	-	expression tag	UNP P21218
YZ	58	HIS	-	expression tag	UNP P21218
YZ	59	SER	-	expression tag	UNP P21218
YZ	60	SER	-	expression tag	UNP P21218
YZ	61	GLY	-	expression tag	UNP P21218
YZ	62	LEU	-	expression tag	UNP P21218
YZ	63	VAL	-	expression tag	UNP P21218
YZ	64	PRO	-	expression tag	UNP P21218
YZ	65	ARG	-	expression tag	UNP P21218
YZ	66	GLY	-	expression tag	UNP P21218
YZ	67	SER	-	expression tag	UNP P21218
ZA	49	MET	-	initiating methionine	UNP P21218
ZA	50	GLY	-	expression tag	UNP P21218
ZA	51	SER	-	expression tag	UNP P21218
ZA	52	SER	-	expression tag	UNP P21218
ZA	53	HIS	-	expression tag	UNP P21218
ZA	54	HIS	-	expression tag	UNP P21218
ZA	55	HIS	-	expression tag	UNP P21218
ZA	56	HIS	-	expression tag	UNP P21218
ZA	57	HIS	-	expression tag	UNP P21218
ZA	58	HIS	-	expression tag	UNP P21218
ZA	59	SER	-	expression tag	UNP P21218
ZA	60	SER	-	expression tag	UNP P21218
ZA	61	GLY	-	expression tag	UNP P21218
ZA	62	LEU	-	expression tag	UNP P21218
ZA	63	VAL	-	expression tag	UNP P21218
ZA	64	PRO	-	expression tag	UNP P21218
ZA	65	ARG	-	expression tag	UNP P21218
ZA	66	GLY	-	expression tag	UNP P21218
ZA	67	SER	-	expression tag	UNP P21218
ZB	49	MET	-	initiating methionine	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZB	50	GLY	-	expression tag	UNP P21218
ZB	51	SER	-	expression tag	UNP P21218
ZB	52	SER	-	expression tag	UNP P21218
ZB	53	HIS	-	expression tag	UNP P21218
ZB	54	HIS	-	expression tag	UNP P21218
ZB	55	HIS	-	expression tag	UNP P21218
ZB	56	HIS	-	expression tag	UNP P21218
ZB	57	HIS	-	expression tag	UNP P21218
ZB	58	HIS	-	expression tag	UNP P21218
ZB	59	SER	-	expression tag	UNP P21218
ZB	60	SER	-	expression tag	UNP P21218
ZB	61	GLY	-	expression tag	UNP P21218
ZB	62	LEU	-	expression tag	UNP P21218
ZB	63	VAL	-	expression tag	UNP P21218
ZB	64	PRO	-	expression tag	UNP P21218
ZB	65	ARG	-	expression tag	UNP P21218
ZB	66	GLY	-	expression tag	UNP P21218
ZB	67	SER	-	expression tag	UNP P21218
ZC	49	MET	-	initiating methionine	UNP P21218
ZC	50	GLY	-	expression tag	UNP P21218
ZC	51	SER	-	expression tag	UNP P21218
ZC	52	SER	-	expression tag	UNP P21218
ZC	53	HIS	-	expression tag	UNP P21218
ZC	54	HIS	-	expression tag	UNP P21218
ZC	55	HIS	-	expression tag	UNP P21218
ZC	56	HIS	-	expression tag	UNP P21218
ZC	57	HIS	-	expression tag	UNP P21218
ZC	58	HIS	-	expression tag	UNP P21218
ZC	59	SER	-	expression tag	UNP P21218
ZC	60	SER	-	expression tag	UNP P21218
ZC	61	GLY	-	expression tag	UNP P21218
ZC	62	LEU	-	expression tag	UNP P21218
ZC	63	VAL	-	expression tag	UNP P21218
ZC	64	PRO	-	expression tag	UNP P21218
ZC	65	ARG	-	expression tag	UNP P21218
ZC	66	GLY	-	expression tag	UNP P21218
ZC	67	SER	-	expression tag	UNP P21218
ZD	49	MET	-	initiating methionine	UNP P21218
ZD	50	GLY	-	expression tag	UNP P21218
ZD	51	SER	-	expression tag	UNP P21218
ZD	52	SER	-	expression tag	UNP P21218
ZD	53	HIS	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZD	54	HIS	-	expression tag	UNP P21218
ZD	55	HIS	-	expression tag	UNP P21218
ZD	56	HIS	-	expression tag	UNP P21218
ZD	57	HIS	-	expression tag	UNP P21218
ZD	58	HIS	-	expression tag	UNP P21218
ZD	59	SER	-	expression tag	UNP P21218
ZD	60	SER	-	expression tag	UNP P21218
ZD	61	GLY	-	expression tag	UNP P21218
ZD	62	LEU	-	expression tag	UNP P21218
ZD	63	VAL	-	expression tag	UNP P21218
ZD	64	PRO	-	expression tag	UNP P21218
ZD	65	ARG	-	expression tag	UNP P21218
ZD	66	GLY	-	expression tag	UNP P21218
ZD	67	SER	-	expression tag	UNP P21218
ZE	49	MET	-	initiating methionine	UNP P21218
ZE	50	GLY	-	expression tag	UNP P21218
ZE	51	SER	-	expression tag	UNP P21218
ZE	52	SER	-	expression tag	UNP P21218
ZE	53	HIS	-	expression tag	UNP P21218
ZE	54	HIS	-	expression tag	UNP P21218
ZE	55	HIS	-	expression tag	UNP P21218
ZE	56	HIS	-	expression tag	UNP P21218
ZE	57	HIS	-	expression tag	UNP P21218
ZE	58	HIS	-	expression tag	UNP P21218
ZE	59	SER	-	expression tag	UNP P21218
ZE	60	SER	-	expression tag	UNP P21218
ZE	61	GLY	-	expression tag	UNP P21218
ZE	62	LEU	-	expression tag	UNP P21218
ZE	63	VAL	-	expression tag	UNP P21218
ZE	64	PRO	-	expression tag	UNP P21218
ZE	65	ARG	-	expression tag	UNP P21218
ZE	66	GLY	-	expression tag	UNP P21218
ZE	67	SER	-	expression tag	UNP P21218
ZF	49	MET	-	initiating methionine	UNP P21218
ZF	50	GLY	-	expression tag	UNP P21218
ZF	51	SER	-	expression tag	UNP P21218
ZF	52	SER	-	expression tag	UNP P21218
ZF	53	HIS	-	expression tag	UNP P21218
ZF	54	HIS	-	expression tag	UNP P21218
ZF	55	HIS	-	expression tag	UNP P21218
ZF	56	HIS	-	expression tag	UNP P21218
ZF	57	HIS	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZF	58	HIS	-	expression tag	UNP P21218
ZF	59	SER	-	expression tag	UNP P21218
ZF	60	SER	-	expression tag	UNP P21218
ZF	61	GLY	-	expression tag	UNP P21218
ZF	62	LEU	-	expression tag	UNP P21218
ZF	63	VAL	-	expression tag	UNP P21218
ZF	64	PRO	-	expression tag	UNP P21218
ZF	65	ARG	-	expression tag	UNP P21218
ZF	66	GLY	-	expression tag	UNP P21218
ZF	67	SER	-	expression tag	UNP P21218
ZG	49	MET	-	initiating methionine	UNP P21218
ZG	50	GLY	-	expression tag	UNP P21218
ZG	51	SER	-	expression tag	UNP P21218
ZG	52	SER	-	expression tag	UNP P21218
ZG	53	HIS	-	expression tag	UNP P21218
ZG	54	HIS	-	expression tag	UNP P21218
ZG	55	HIS	-	expression tag	UNP P21218
ZG	56	HIS	-	expression tag	UNP P21218
ZG	57	HIS	-	expression tag	UNP P21218
ZG	58	HIS	-	expression tag	UNP P21218
ZG	59	SER	-	expression tag	UNP P21218
ZG	60	SER	-	expression tag	UNP P21218
ZG	61	GLY	-	expression tag	UNP P21218
ZG	62	LEU	-	expression tag	UNP P21218
ZG	63	VAL	-	expression tag	UNP P21218
ZG	64	PRO	-	expression tag	UNP P21218
ZG	65	ARG	-	expression tag	UNP P21218
ZG	66	GLY	-	expression tag	UNP P21218
ZG	67	SER	-	expression tag	UNP P21218
ZH	49	MET	-	initiating methionine	UNP P21218
ZH	50	GLY	-	expression tag	UNP P21218
ZH	51	SER	-	expression tag	UNP P21218
ZH	52	SER	-	expression tag	UNP P21218
ZH	53	HIS	-	expression tag	UNP P21218
ZH	54	HIS	-	expression tag	UNP P21218
ZH	55	HIS	-	expression tag	UNP P21218
ZH	56	HIS	-	expression tag	UNP P21218
ZH	57	HIS	-	expression tag	UNP P21218
ZH	58	HIS	-	expression tag	UNP P21218
ZH	59	SER	-	expression tag	UNP P21218
ZH	60	SER	-	expression tag	UNP P21218
ZH	61	GLY	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZH	62	LEU	-	expression tag	UNP P21218
ZH	63	VAL	-	expression tag	UNP P21218
ZH	64	PRO	-	expression tag	UNP P21218
ZH	65	ARG	-	expression tag	UNP P21218
ZH	66	GLY	-	expression tag	UNP P21218
ZH	67	SER	-	expression tag	UNP P21218
ZI	49	MET	-	initiating methionine	UNP P21218
ZI	50	GLY	-	expression tag	UNP P21218
ZI	51	SER	-	expression tag	UNP P21218
ZI	52	SER	-	expression tag	UNP P21218
ZI	53	HIS	-	expression tag	UNP P21218
ZI	54	HIS	-	expression tag	UNP P21218
ZI	55	HIS	-	expression tag	UNP P21218
ZI	56	HIS	-	expression tag	UNP P21218
ZI	57	HIS	-	expression tag	UNP P21218
ZI	58	HIS	-	expression tag	UNP P21218
ZI	59	SER	-	expression tag	UNP P21218
ZI	60	SER	-	expression tag	UNP P21218
ZI	61	GLY	-	expression tag	UNP P21218
ZI	62	LEU	-	expression tag	UNP P21218
ZI	63	VAL	-	expression tag	UNP P21218
ZI	64	PRO	-	expression tag	UNP P21218
ZI	65	ARG	-	expression tag	UNP P21218
ZI	66	GLY	-	expression tag	UNP P21218
ZI	67	SER	-	expression tag	UNP P21218
ZJ	49	MET	-	initiating methionine	UNP P21218
ZJ	50	GLY	-	expression tag	UNP P21218
ZJ	51	SER	-	expression tag	UNP P21218
ZJ	52	SER	-	expression tag	UNP P21218
ZJ	53	HIS	-	expression tag	UNP P21218
ZJ	54	HIS	-	expression tag	UNP P21218
ZJ	55	HIS	-	expression tag	UNP P21218
ZJ	56	HIS	-	expression tag	UNP P21218
ZJ	57	HIS	-	expression tag	UNP P21218
ZJ	58	HIS	-	expression tag	UNP P21218
ZJ	59	SER	-	expression tag	UNP P21218
ZJ	60	SER	-	expression tag	UNP P21218
ZJ	61	GLY	-	expression tag	UNP P21218
ZJ	62	LEU	-	expression tag	UNP P21218
ZJ	63	VAL	-	expression tag	UNP P21218
ZJ	64	PRO	-	expression tag	UNP P21218
ZJ	65	ARG	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZJ	66	GLY	-	expression tag	UNP P21218
ZJ	67	SER	-	expression tag	UNP P21218
ZK	49	MET	-	initiating methionine	UNP P21218
ZK	50	GLY	-	expression tag	UNP P21218
ZK	51	SER	-	expression tag	UNP P21218
ZK	52	SER	-	expression tag	UNP P21218
ZK	53	HIS	-	expression tag	UNP P21218
ZK	54	HIS	-	expression tag	UNP P21218
ZK	55	HIS	-	expression tag	UNP P21218
ZK	56	HIS	-	expression tag	UNP P21218
ZK	57	HIS	-	expression tag	UNP P21218
ZK	58	HIS	-	expression tag	UNP P21218
ZK	59	SER	-	expression tag	UNP P21218
ZK	60	SER	-	expression tag	UNP P21218
ZK	61	GLY	-	expression tag	UNP P21218
ZK	62	LEU	-	expression tag	UNP P21218
ZK	63	VAL	-	expression tag	UNP P21218
ZK	64	PRO	-	expression tag	UNP P21218
ZK	65	ARG	-	expression tag	UNP P21218
ZK	66	GLY	-	expression tag	UNP P21218
ZK	67	SER	-	expression tag	UNP P21218
ZL	49	MET	-	initiating methionine	UNP P21218
ZL	50	GLY	-	expression tag	UNP P21218
ZL	51	SER	-	expression tag	UNP P21218
ZL	52	SER	-	expression tag	UNP P21218
ZL	53	HIS	-	expression tag	UNP P21218
ZL	54	HIS	-	expression tag	UNP P21218
ZL	55	HIS	-	expression tag	UNP P21218
ZL	56	HIS	-	expression tag	UNP P21218
ZL	57	HIS	-	expression tag	UNP P21218
ZL	58	HIS	-	expression tag	UNP P21218
ZL	59	SER	-	expression tag	UNP P21218
ZL	60	SER	-	expression tag	UNP P21218
ZL	61	GLY	-	expression tag	UNP P21218
ZL	62	LEU	-	expression tag	UNP P21218
ZL	63	VAL	-	expression tag	UNP P21218
ZL	64	PRO	-	expression tag	UNP P21218
ZL	65	ARG	-	expression tag	UNP P21218
ZL	66	GLY	-	expression tag	UNP P21218
ZL	67	SER	-	expression tag	UNP P21218
ZM	49	MET	-	initiating methionine	UNP P21218
ZM	50	GLY	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZM	51	SER	-	expression tag	UNP P21218
ZM	52	SER	-	expression tag	UNP P21218
ZM	53	HIS	-	expression tag	UNP P21218
ZM	54	HIS	-	expression tag	UNP P21218
ZM	55	HIS	-	expression tag	UNP P21218
ZM	56	HIS	-	expression tag	UNP P21218
ZM	57	HIS	-	expression tag	UNP P21218
ZM	58	HIS	-	expression tag	UNP P21218
ZM	59	SER	-	expression tag	UNP P21218
ZM	60	SER	-	expression tag	UNP P21218
ZM	61	GLY	-	expression tag	UNP P21218
ZM	62	LEU	-	expression tag	UNP P21218
ZM	63	VAL	-	expression tag	UNP P21218
ZM	64	PRO	-	expression tag	UNP P21218
ZM	65	ARG	-	expression tag	UNP P21218
ZM	66	GLY	-	expression tag	UNP P21218
ZM	67	SER	-	expression tag	UNP P21218
ZN	49	MET	-	initiating methionine	UNP P21218
ZN	50	GLY	-	expression tag	UNP P21218
ZN	51	SER	-	expression tag	UNP P21218
ZN	52	SER	-	expression tag	UNP P21218
ZN	53	HIS	-	expression tag	UNP P21218
ZN	54	HIS	-	expression tag	UNP P21218
ZN	55	HIS	-	expression tag	UNP P21218
ZN	56	HIS	-	expression tag	UNP P21218
ZN	57	HIS	-	expression tag	UNP P21218
ZN	58	HIS	-	expression tag	UNP P21218
ZN	59	SER	-	expression tag	UNP P21218
ZN	60	SER	-	expression tag	UNP P21218
ZN	61	GLY	-	expression tag	UNP P21218
ZN	62	LEU	-	expression tag	UNP P21218
ZN	63	VAL	-	expression tag	UNP P21218
ZN	64	PRO	-	expression tag	UNP P21218
ZN	65	ARG	-	expression tag	UNP P21218
ZN	66	GLY	-	expression tag	UNP P21218
ZN	67	SER	-	expression tag	UNP P21218
ZO	49	MET	-	initiating methionine	UNP P21218
ZO	50	GLY	-	expression tag	UNP P21218
ZO	51	SER	-	expression tag	UNP P21218
ZO	52	SER	-	expression tag	UNP P21218
ZO	53	HIS	-	expression tag	UNP P21218
ZO	54	HIS	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZO	55	HIS	-	expression tag	UNP P21218
ZO	56	HIS	-	expression tag	UNP P21218
ZO	57	HIS	-	expression tag	UNP P21218
ZO	58	HIS	-	expression tag	UNP P21218
ZO	59	SER	-	expression tag	UNP P21218
ZO	60	SER	-	expression tag	UNP P21218
ZO	61	GLY	-	expression tag	UNP P21218
ZO	62	LEU	-	expression tag	UNP P21218
ZO	63	VAL	-	expression tag	UNP P21218
ZO	64	PRO	-	expression tag	UNP P21218
ZO	65	ARG	-	expression tag	UNP P21218
ZO	66	GLY	-	expression tag	UNP P21218
ZO	67	SER	-	expression tag	UNP P21218
ZP	49	MET	-	initiating methionine	UNP P21218
ZP	50	GLY	-	expression tag	UNP P21218
ZP	51	SER	-	expression tag	UNP P21218
ZP	52	SER	-	expression tag	UNP P21218
ZP	53	HIS	-	expression tag	UNP P21218
ZP	54	HIS	-	expression tag	UNP P21218
ZP	55	HIS	-	expression tag	UNP P21218
ZP	56	HIS	-	expression tag	UNP P21218
ZP	57	HIS	-	expression tag	UNP P21218
ZP	58	HIS	-	expression tag	UNP P21218
ZP	59	SER	-	expression tag	UNP P21218
ZP	60	SER	-	expression tag	UNP P21218
ZP	61	GLY	-	expression tag	UNP P21218
ZP	62	LEU	-	expression tag	UNP P21218
ZP	63	VAL	-	expression tag	UNP P21218
ZP	64	PRO	-	expression tag	UNP P21218
ZP	65	ARG	-	expression tag	UNP P21218
ZP	66	GLY	-	expression tag	UNP P21218
ZP	67	SER	-	expression tag	UNP P21218
ZQ	49	MET	-	initiating methionine	UNP P21218
ZQ	50	GLY	-	expression tag	UNP P21218
ZQ	51	SER	-	expression tag	UNP P21218
ZQ	52	SER	-	expression tag	UNP P21218
ZQ	53	HIS	-	expression tag	UNP P21218
ZQ	54	HIS	-	expression tag	UNP P21218
ZQ	55	HIS	-	expression tag	UNP P21218
ZQ	56	HIS	-	expression tag	UNP P21218
ZQ	57	HIS	-	expression tag	UNP P21218
ZQ	58	HIS	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZQ	59	SER	-	expression tag	UNP P21218
ZQ	60	SER	-	expression tag	UNP P21218
ZQ	61	GLY	-	expression tag	UNP P21218
ZQ	62	LEU	-	expression tag	UNP P21218
ZQ	63	VAL	-	expression tag	UNP P21218
ZQ	64	PRO	-	expression tag	UNP P21218
ZQ	65	ARG	-	expression tag	UNP P21218
ZQ	66	GLY	-	expression tag	UNP P21218
ZQ	67	SER	-	expression tag	UNP P21218
ZR	49	MET	-	initiating methionine	UNP P21218
ZR	50	GLY	-	expression tag	UNP P21218
ZR	51	SER	-	expression tag	UNP P21218
ZR	52	SER	-	expression tag	UNP P21218
ZR	53	HIS	-	expression tag	UNP P21218
ZR	54	HIS	-	expression tag	UNP P21218
ZR	55	HIS	-	expression tag	UNP P21218
ZR	56	HIS	-	expression tag	UNP P21218
ZR	57	HIS	-	expression tag	UNP P21218
ZR	58	HIS	-	expression tag	UNP P21218
ZR	59	SER	-	expression tag	UNP P21218
ZR	60	SER	-	expression tag	UNP P21218
ZR	61	GLY	-	expression tag	UNP P21218
ZR	62	LEU	-	expression tag	UNP P21218
ZR	63	VAL	-	expression tag	UNP P21218
ZR	64	PRO	-	expression tag	UNP P21218
ZR	65	ARG	-	expression tag	UNP P21218
ZR	66	GLY	-	expression tag	UNP P21218
ZR	67	SER	-	expression tag	UNP P21218
ZS	49	MET	-	initiating methionine	UNP P21218
ZS	50	GLY	-	expression tag	UNP P21218
ZS	51	SER	-	expression tag	UNP P21218
ZS	52	SER	-	expression tag	UNP P21218
ZS	53	HIS	-	expression tag	UNP P21218
ZS	54	HIS	-	expression tag	UNP P21218
ZS	55	HIS	-	expression tag	UNP P21218
ZS	56	HIS	-	expression tag	UNP P21218
ZS	57	HIS	-	expression tag	UNP P21218
ZS	58	HIS	-	expression tag	UNP P21218
ZS	59	SER	-	expression tag	UNP P21218
ZS	60	SER	-	expression tag	UNP P21218
ZS	61	GLY	-	expression tag	UNP P21218
ZS	62	LEU	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZS	63	VAL	-	expression tag	UNP P21218
ZS	64	PRO	-	expression tag	UNP P21218
ZS	65	ARG	-	expression tag	UNP P21218
ZS	66	GLY	-	expression tag	UNP P21218
ZS	67	SER	-	expression tag	UNP P21218
ZT	49	MET	-	initiating methionine	UNP P21218
ZT	50	GLY	-	expression tag	UNP P21218
ZT	51	SER	-	expression tag	UNP P21218
ZT	52	SER	-	expression tag	UNP P21218
ZT	53	HIS	-	expression tag	UNP P21218
ZT	54	HIS	-	expression tag	UNP P21218
ZT	55	HIS	-	expression tag	UNP P21218
ZT	56	HIS	-	expression tag	UNP P21218
ZT	57	HIS	-	expression tag	UNP P21218
ZT	58	HIS	-	expression tag	UNP P21218
ZT	59	SER	-	expression tag	UNP P21218
ZT	60	SER	-	expression tag	UNP P21218
ZT	61	GLY	-	expression tag	UNP P21218
ZT	62	LEU	-	expression tag	UNP P21218
ZT	63	VAL	-	expression tag	UNP P21218
ZT	64	PRO	-	expression tag	UNP P21218
ZT	65	ARG	-	expression tag	UNP P21218
ZT	66	GLY	-	expression tag	UNP P21218
ZT	67	SER	-	expression tag	UNP P21218
ZU	49	MET	-	initiating methionine	UNP P21218
ZU	50	GLY	-	expression tag	UNP P21218
ZU	51	SER	-	expression tag	UNP P21218
ZU	52	SER	-	expression tag	UNP P21218
ZU	53	HIS	-	expression tag	UNP P21218
ZU	54	HIS	-	expression tag	UNP P21218
ZU	55	HIS	-	expression tag	UNP P21218
ZU	56	HIS	-	expression tag	UNP P21218
ZU	57	HIS	-	expression tag	UNP P21218
ZU	58	HIS	-	expression tag	UNP P21218
ZU	59	SER	-	expression tag	UNP P21218
ZU	60	SER	-	expression tag	UNP P21218
ZU	61	GLY	-	expression tag	UNP P21218
ZU	62	LEU	-	expression tag	UNP P21218
ZU	63	VAL	-	expression tag	UNP P21218
ZU	64	PRO	-	expression tag	UNP P21218
ZU	65	ARG	-	expression tag	UNP P21218
ZU	66	GLY	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZU	67	SER	-	expression tag	UNP P21218
ZV	49	MET	-	initiating methionine	UNP P21218
ZV	50	GLY	-	expression tag	UNP P21218
ZV	51	SER	-	expression tag	UNP P21218
ZV	52	SER	-	expression tag	UNP P21218
ZV	53	HIS	-	expression tag	UNP P21218
ZV	54	HIS	-	expression tag	UNP P21218
ZV	55	HIS	-	expression tag	UNP P21218
ZV	56	HIS	-	expression tag	UNP P21218
ZV	57	HIS	-	expression tag	UNP P21218
ZV	58	HIS	-	expression tag	UNP P21218
ZV	59	SER	-	expression tag	UNP P21218
ZV	60	SER	-	expression tag	UNP P21218
ZV	61	GLY	-	expression tag	UNP P21218
ZV	62	LEU	-	expression tag	UNP P21218
ZV	63	VAL	-	expression tag	UNP P21218
ZV	64	PRO	-	expression tag	UNP P21218
ZV	65	ARG	-	expression tag	UNP P21218
ZV	66	GLY	-	expression tag	UNP P21218
ZV	67	SER	-	expression tag	UNP P21218
ZW	49	MET	-	initiating methionine	UNP P21218
ZW	50	GLY	-	expression tag	UNP P21218
ZW	51	SER	-	expression tag	UNP P21218
ZW	52	SER	-	expression tag	UNP P21218
ZW	53	HIS	-	expression tag	UNP P21218
ZW	54	HIS	-	expression tag	UNP P21218
ZW	55	HIS	-	expression tag	UNP P21218
ZW	56	HIS	-	expression tag	UNP P21218
ZW	57	HIS	-	expression tag	UNP P21218
ZW	58	HIS	-	expression tag	UNP P21218
ZW	59	SER	-	expression tag	UNP P21218
ZW	60	SER	-	expression tag	UNP P21218
ZW	61	GLY	-	expression tag	UNP P21218
ZW	62	LEU	-	expression tag	UNP P21218
ZW	63	VAL	-	expression tag	UNP P21218
ZW	64	PRO	-	expression tag	UNP P21218
ZW	65	ARG	-	expression tag	UNP P21218
ZW	66	GLY	-	expression tag	UNP P21218
ZW	67	SER	-	expression tag	UNP P21218
ZX	49	MET	-	initiating methionine	UNP P21218
ZX	50	GLY	-	expression tag	UNP P21218
ZX	51	SER	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

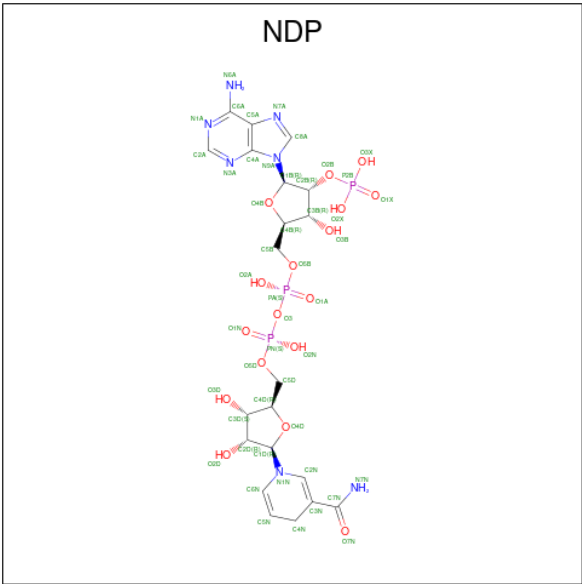
Chain	Residue	Modelled	Actual	Comment	Reference
ZX	52	SER	-	expression tag	UNP P21218
ZX	53	HIS	-	expression tag	UNP P21218
ZX	54	HIS	-	expression tag	UNP P21218
ZX	55	HIS	-	expression tag	UNP P21218
ZX	56	HIS	-	expression tag	UNP P21218
ZX	57	HIS	-	expression tag	UNP P21218
ZX	58	HIS	-	expression tag	UNP P21218
ZX	59	SER	-	expression tag	UNP P21218
ZX	60	SER	-	expression tag	UNP P21218
ZX	61	GLY	-	expression tag	UNP P21218
ZX	62	LEU	-	expression tag	UNP P21218
ZX	63	VAL	-	expression tag	UNP P21218
ZX	64	PRO	-	expression tag	UNP P21218
ZX	65	ARG	-	expression tag	UNP P21218
ZX	66	GLY	-	expression tag	UNP P21218
ZX	67	SER	-	expression tag	UNP P21218
ZY	49	MET	-	initiating methionine	UNP P21218
ZY	50	GLY	-	expression tag	UNP P21218
ZY	51	SER	-	expression tag	UNP P21218
ZY	52	SER	-	expression tag	UNP P21218
ZY	53	HIS	-	expression tag	UNP P21218
ZY	54	HIS	-	expression tag	UNP P21218
ZY	55	HIS	-	expression tag	UNP P21218
ZY	56	HIS	-	expression tag	UNP P21218
ZY	57	HIS	-	expression tag	UNP P21218
ZY	58	HIS	-	expression tag	UNP P21218
ZY	59	SER	-	expression tag	UNP P21218
ZY	60	SER	-	expression tag	UNP P21218
ZY	61	GLY	-	expression tag	UNP P21218
ZY	62	LEU	-	expression tag	UNP P21218
ZY	63	VAL	-	expression tag	UNP P21218
ZY	64	PRO	-	expression tag	UNP P21218
ZY	65	ARG	-	expression tag	UNP P21218
ZY	66	GLY	-	expression tag	UNP P21218
ZY	67	SER	-	expression tag	UNP P21218
ZZ	49	MET	-	initiating methionine	UNP P21218
ZZ	50	GLY	-	expression tag	UNP P21218
ZZ	51	SER	-	expression tag	UNP P21218
ZZ	52	SER	-	expression tag	UNP P21218
ZZ	53	HIS	-	expression tag	UNP P21218
ZZ	54	HIS	-	expression tag	UNP P21218
ZZ	55	HIS	-	expression tag	UNP P21218

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZZ	56	HIS	-	expression tag	UNP P21218
ZZ	57	HIS	-	expression tag	UNP P21218
ZZ	58	HIS	-	expression tag	UNP P21218
ZZ	59	SER	-	expression tag	UNP P21218
ZZ	60	SER	-	expression tag	UNP P21218
ZZ	61	GLY	-	expression tag	UNP P21218
ZZ	62	LEU	-	expression tag	UNP P21218
ZZ	63	VAL	-	expression tag	UNP P21218
ZZ	64	PRO	-	expression tag	UNP P21218
ZZ	65	ARG	-	expression tag	UNP P21218
ZZ	66	GLY	-	expression tag	UNP P21218
ZZ	67	SER	-	expression tag	UNP P21218

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	YM	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	YN	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	YO	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	YP	1	Total	C	N	O	P	0
			48	21	7	17	3	

Continued on next page...

Continued from previous page...

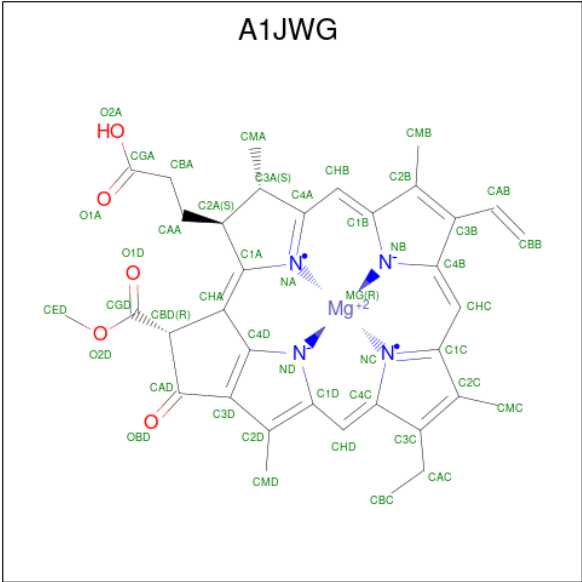
Mol	Chain	Residues	Atoms					AltConf
2	YQ	1	Total 48	C 21	N 7	O 17	P 3	0
2	YR	1	Total 48	C 21	N 7	O 17	P 3	0
2	YS	1	Total 48	C 21	N 7	O 17	P 3	0
2	YT	1	Total 48	C 21	N 7	O 17	P 3	0
2	YU	1	Total 48	C 21	N 7	O 17	P 3	0
2	YV	1	Total 48	C 21	N 7	O 17	P 3	0
2	YW	1	Total 48	C 21	N 7	O 17	P 3	0
2	YX	1	Total 48	C 21	N 7	O 17	P 3	0
2	YY	1	Total 48	C 21	N 7	O 17	P 3	0
2	YZ	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZA	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZB	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZC	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZD	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZE	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZF	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZG	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZH	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZI	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZJ	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZK	1	Total 48	C 21	N 7	O 17	P 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	ZL	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZM	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZN	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZO	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZP	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZQ	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZR	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZS	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZT	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZU	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZV	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZW	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZX	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZY	1	Total 48	C 21	N 7	O 17	P 3	0
2	ZZ	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 3 is Chlorophyllide a (CCD ID: A1JWG) (formula: $C_{35}H_{34}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	YM	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YO	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YP	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YQ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YR	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YS	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YT	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YU	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YV	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YW	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YY	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	YZ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

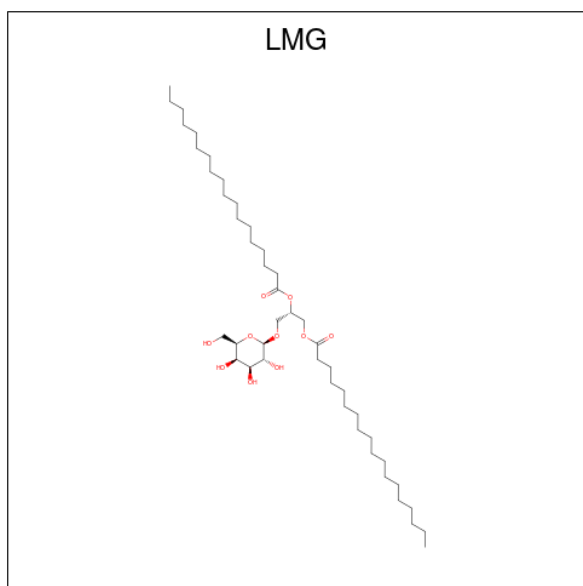
Mol	Chain	Residues	Atoms					AltConf
3	ZA	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZB	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZC	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZD	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZE	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZF	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZG	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZH	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZI	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZK	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZL	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZM	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZN	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZO	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZP	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZQ	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZR	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZS	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZT	1	Total 45	C 35	Mg 1	N 4	O 5	0
3	ZU	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
3	ZV	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	ZW	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	ZX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	ZY	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
3	ZZ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 4 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	YM	1	Total	C	O	0
			23	13	10	
4	YN	1	Total	C	O	0
			23	13	10	
4	YO	1	Total	C	O	0
			23	13	10	
4	YP	1	Total	C	O	0
			23	13	10	
4	YQ	1	Total	C	O	0
			23	13	10	
4	YR	1	Total	C	O	0
			23	13	10	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
4	YS	1	Total 23	C 13	O 10	0
4	YT	1	Total 23	C 13	O 10	0
4	YU	1	Total 23	C 13	O 10	0
4	YV	1	Total 23	C 13	O 10	0
4	YW	1	Total 23	C 13	O 10	0
4	YX	1	Total 23	C 13	O 10	0
4	YY	1	Total 23	C 13	O 10	0
4	YZ	1	Total 23	C 13	O 10	0
4	ZA	1	Total 23	C 13	O 10	0
4	ZB	1	Total 23	C 13	O 10	0
4	ZC	1	Total 23	C 13	O 10	0
4	ZD	1	Total 23	C 13	O 10	0
4	ZE	1	Total 23	C 13	O 10	0
4	ZF	1	Total 23	C 13	O 10	0
4	ZG	1	Total 23	C 13	O 10	0
4	ZH	1	Total 23	C 13	O 10	0
4	ZI	1	Total 23	C 13	O 10	0
4	ZJ	1	Total 23	C 13	O 10	0
4	ZK	1	Total 23	C 13	O 10	0
4	ZL	1	Total 23	C 13	O 10	0
4	ZM	1	Total 23	C 13	O 10	0

Continued on next page...

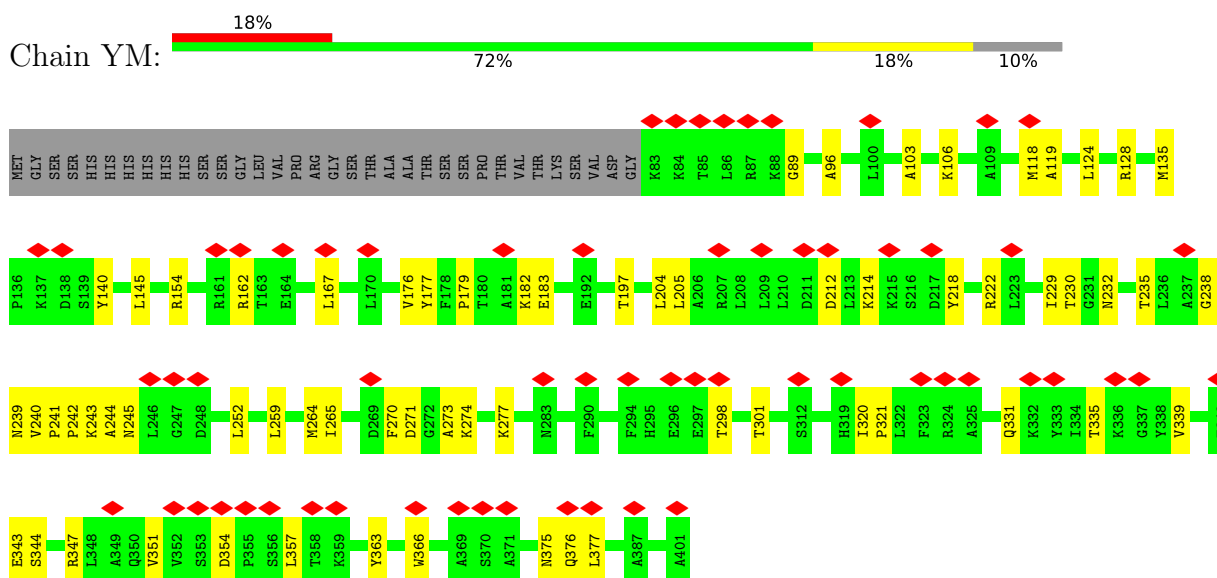
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
4	ZN	1	Total	C	O	0
			23	13	10	
4	ZO	1	Total	C	O	0
			23	13	10	
4	ZP	1	Total	C	O	0
			23	13	10	
4	ZQ	1	Total	C	O	0
			23	13	10	
4	ZR	1	Total	C	O	0
			23	13	10	
4	ZS	1	Total	C	O	0
			23	13	10	
4	ZT	1	Total	C	O	0
			23	13	10	
4	ZU	1	Total	C	O	0
			23	13	10	
4	ZV	1	Total	C	O	0
			23	13	10	
4	ZW	1	Total	C	O	0
			23	13	10	
4	ZX	1	Total	C	O	0
			23	13	10	
4	ZY	1	Total	C	O	0
			23	13	10	
4	ZZ	1	Total	C	O	0
			23	13	10	

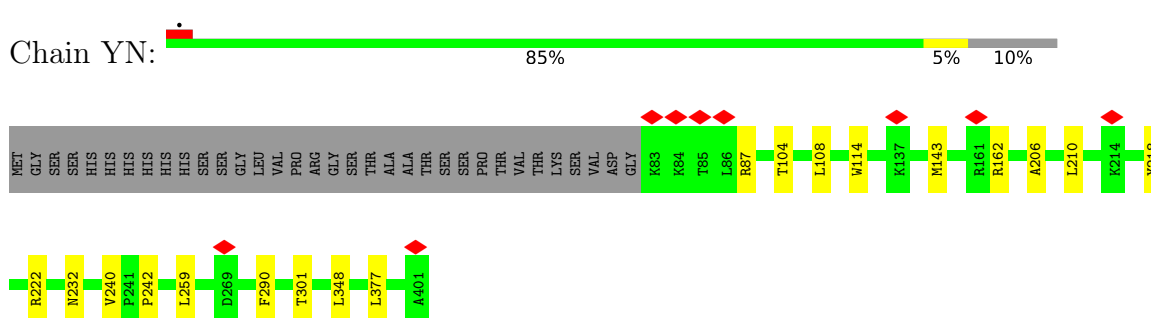
3 Residue-property plots [i](#)

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

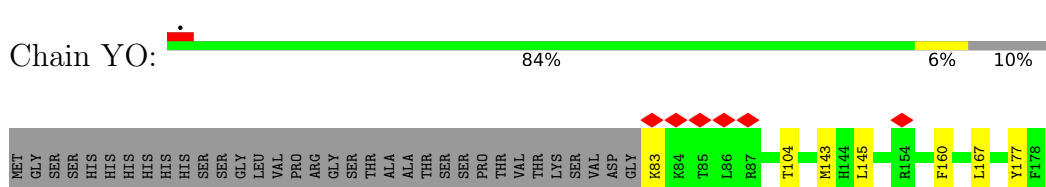
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

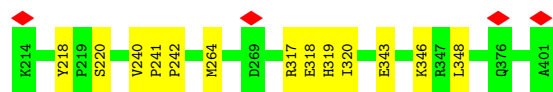


- Molecule 1: Protochlorophyllide reductase B, chloroplastic

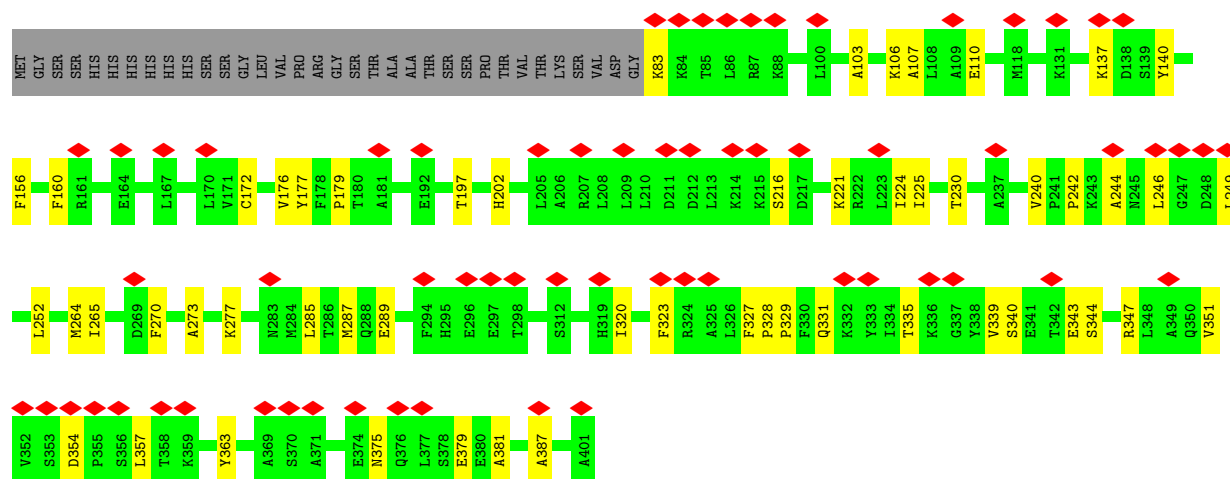
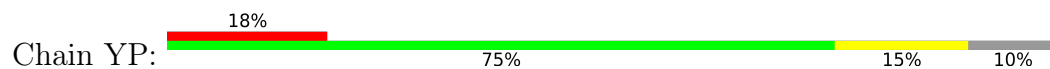


- Molecule 1: Protochlorophyllide reductase B, chloroplastic

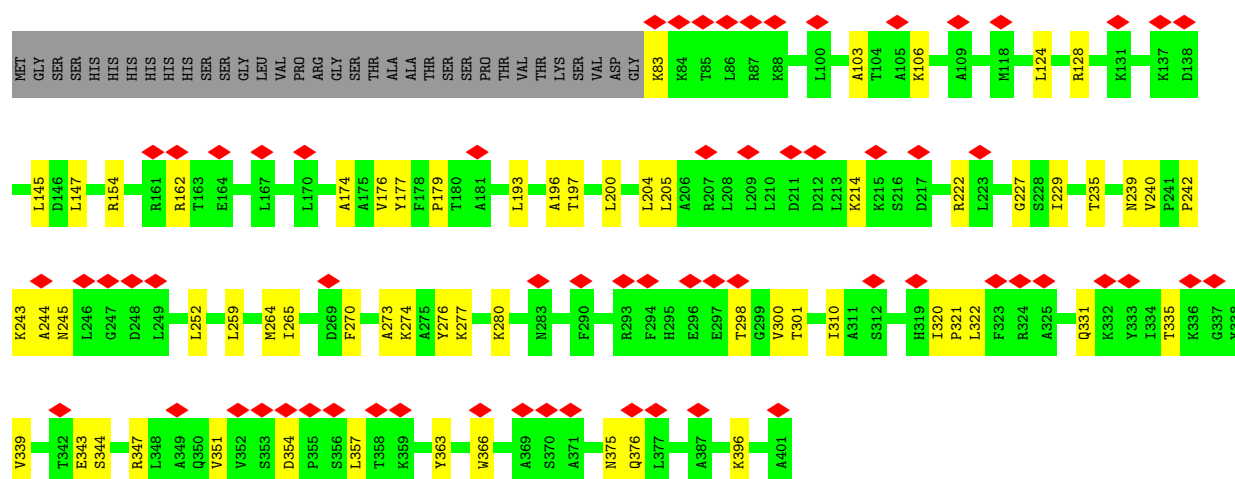
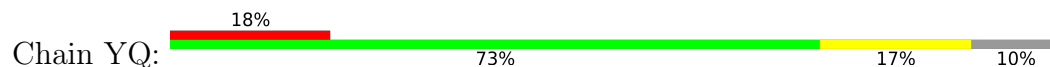




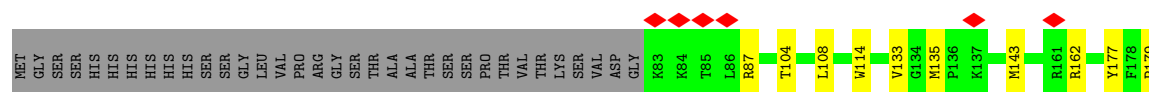
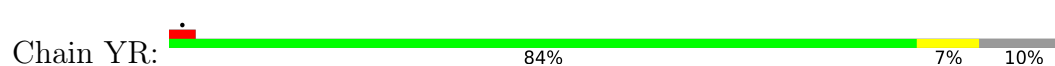
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

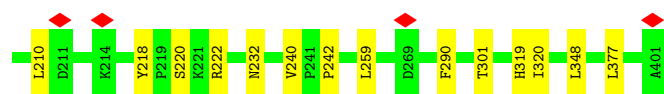


- Molecule 1: Protochlorophyllide reductase B, chloroplastic

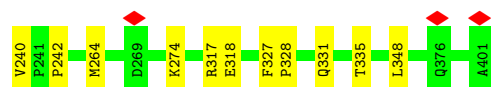
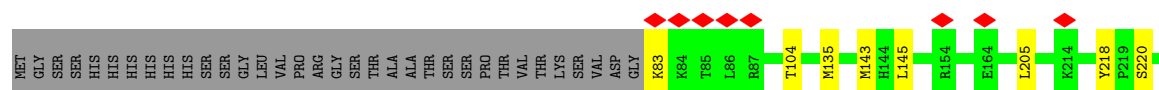
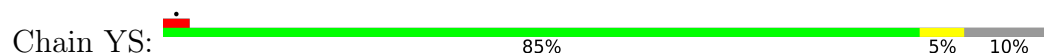


- Molecule 1: Protochlorophyllide reductase B, chloroplastic

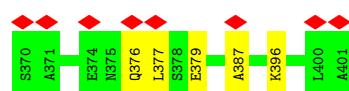
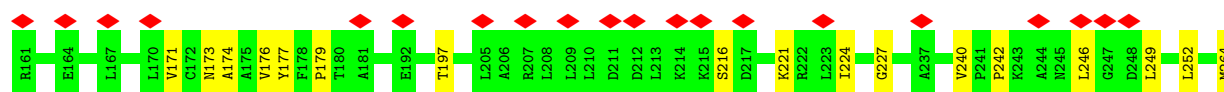
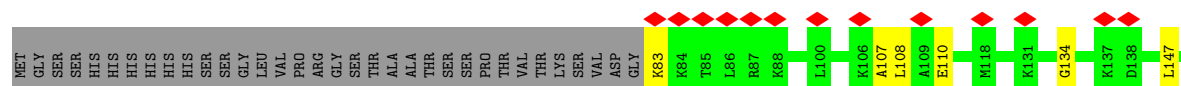
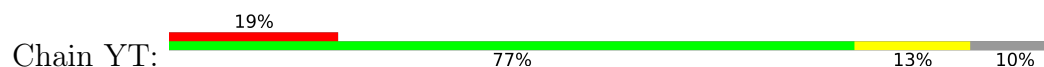




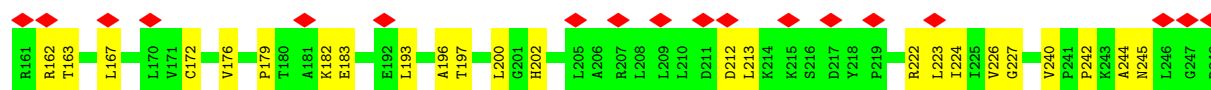
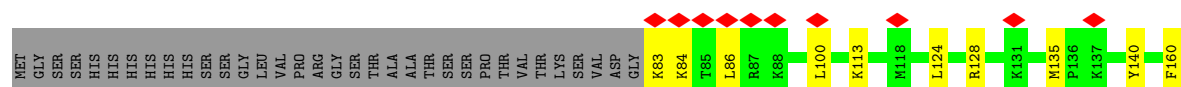
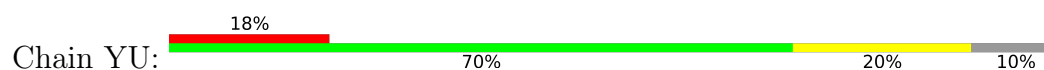
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

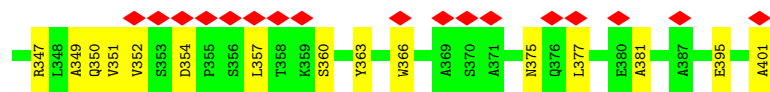


- Molecule 1: Protochlorophyllide reductase B, chloroplastic



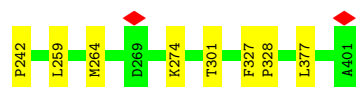
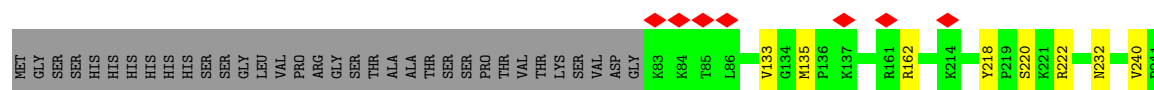
- Molecule 1: Protochlorophyllide reductase B, chloroplastic





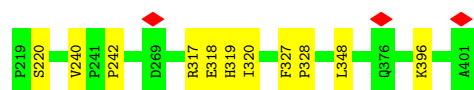
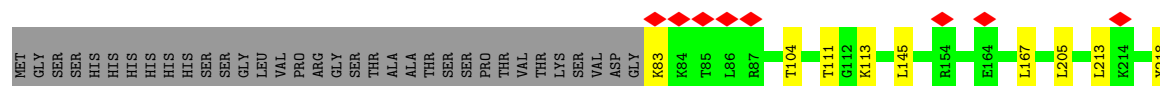
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain YV: 86% 5% 10%



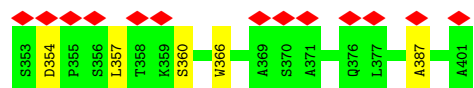
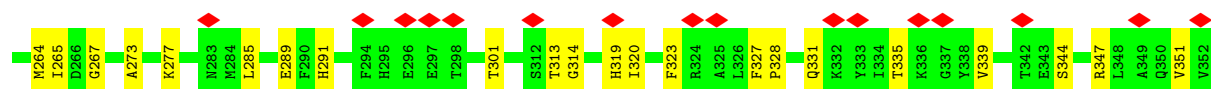
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain YW: 85% 6% 10%



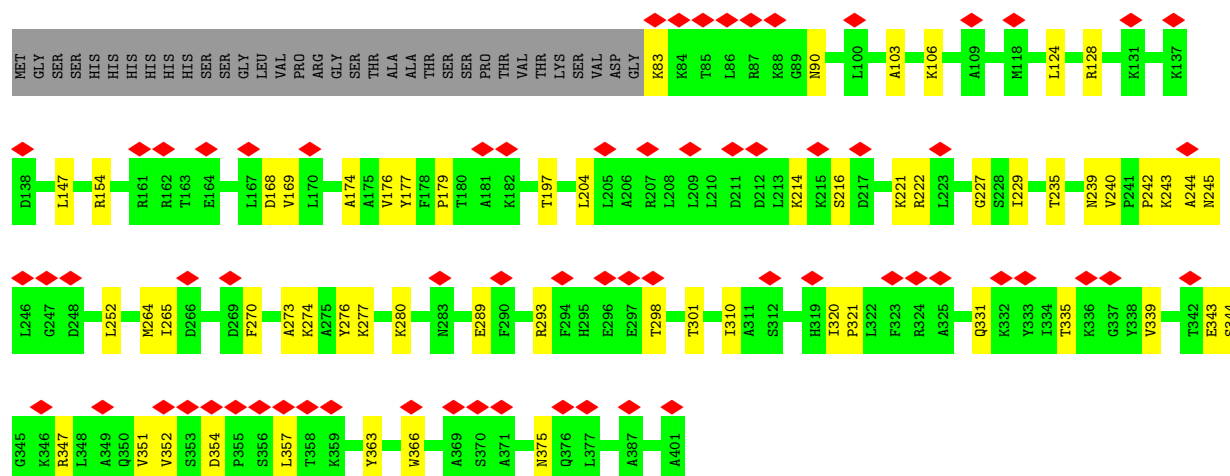
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain YX: 17% 75% 15% 10%



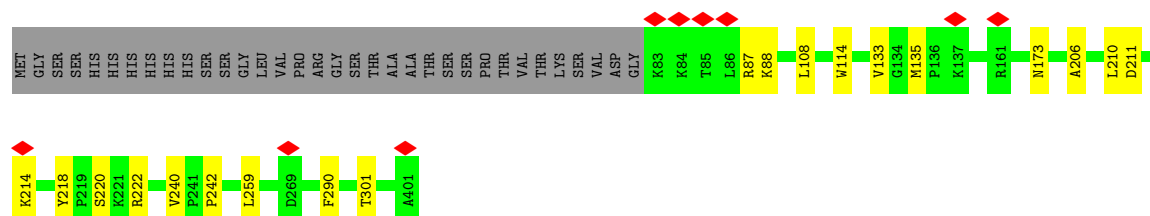
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain YY: 19% 74% 16% 10%



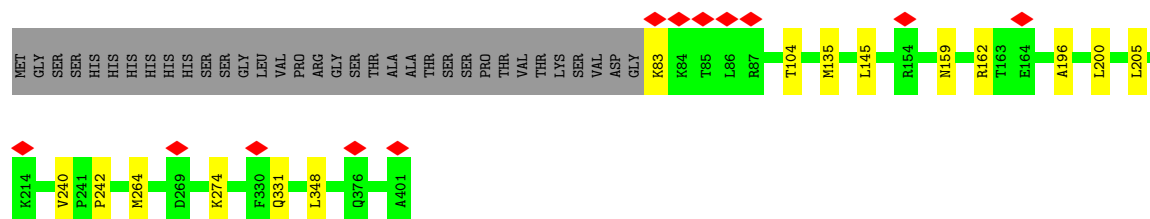
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain YZ: 85% 5% 10%



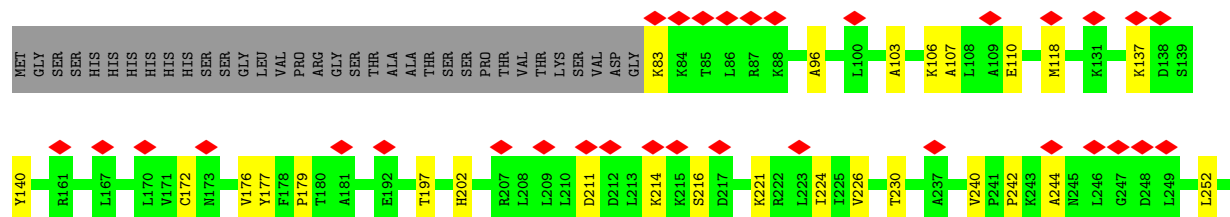
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

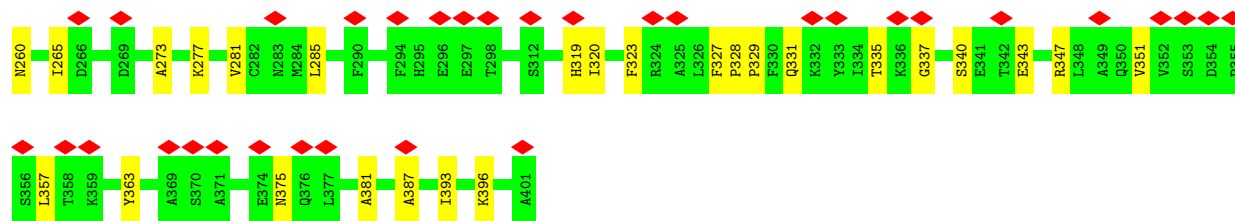
Chain ZA: 86% 10%



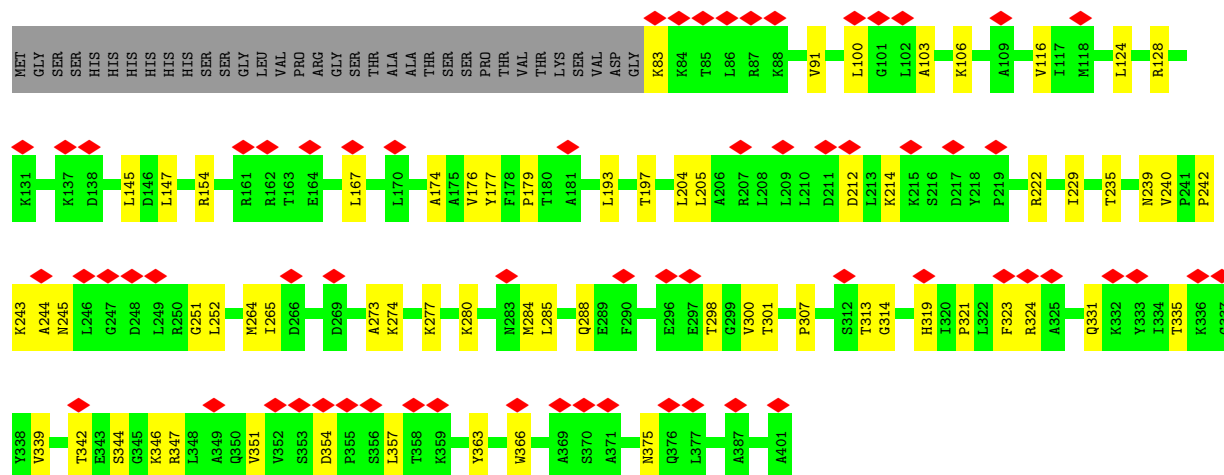
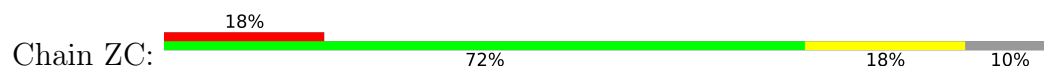
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain ZB: 18% 76% 15% 10%

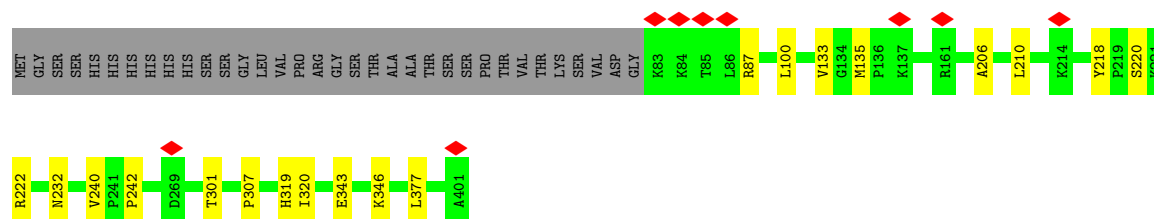
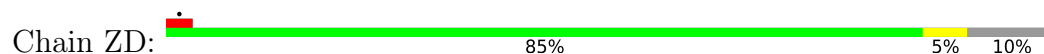




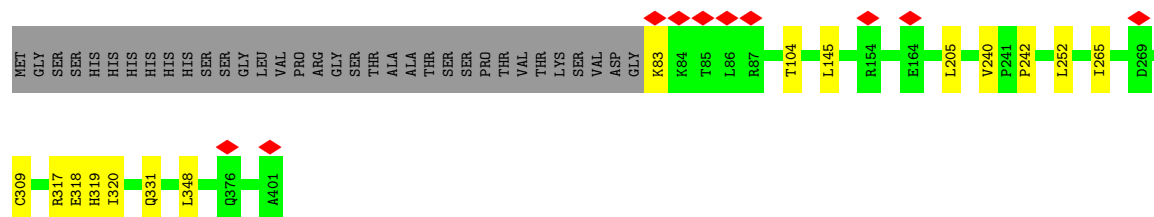
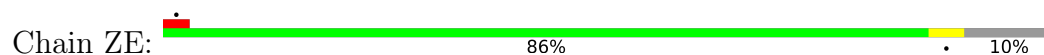
- Molecule 1: Protochlorophyllide reductase B, chloroplastic



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

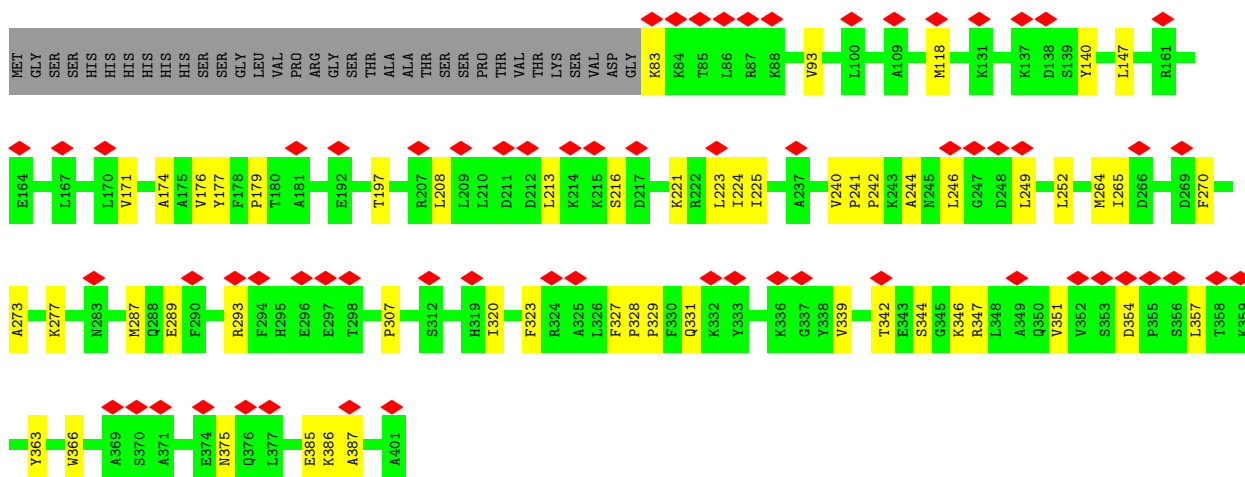


- Molecule 1: Protochlorophyllide reductase B, chloroplastic



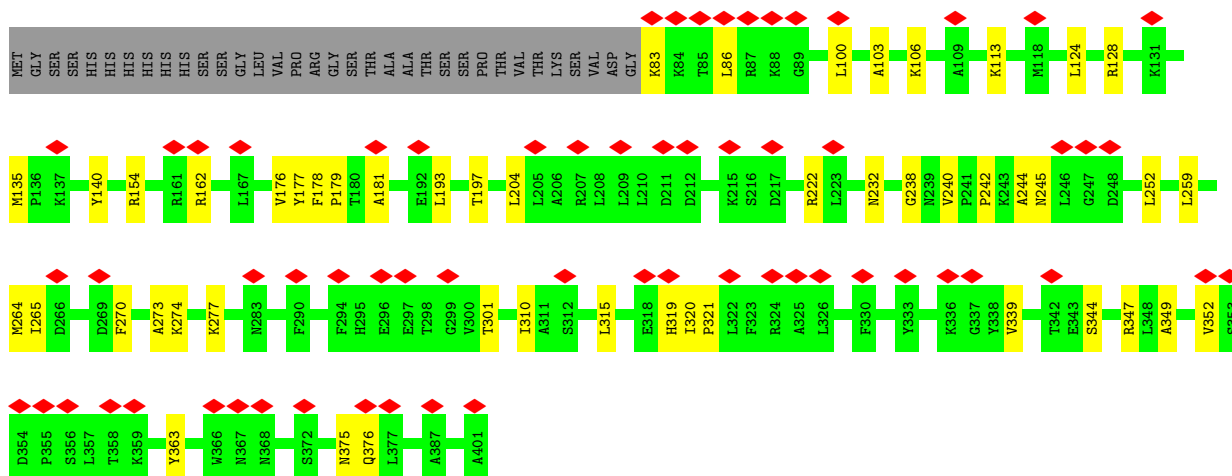
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain ZF: 



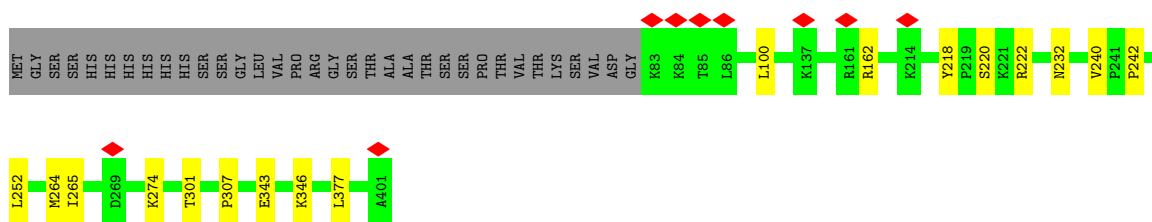
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain ZG: 



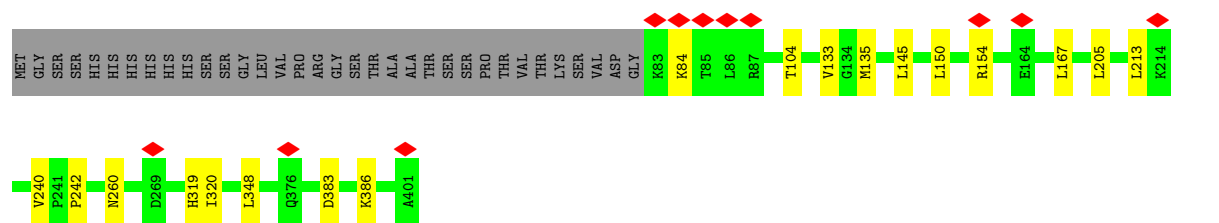
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain ZH: 

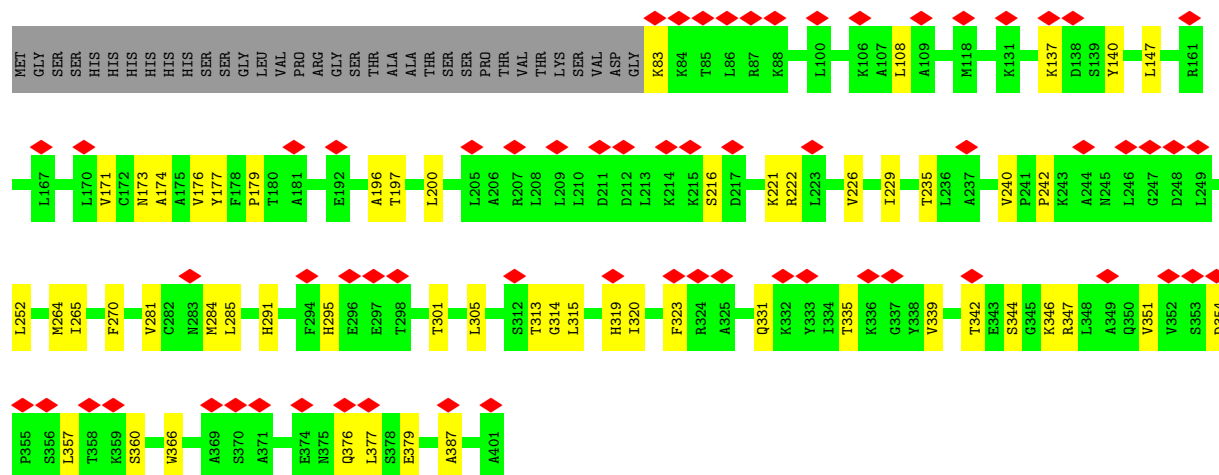
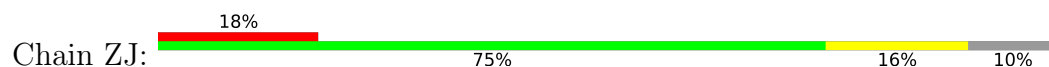


- Molecule 1: Protochlorophyllide reductase B, chloroplastic

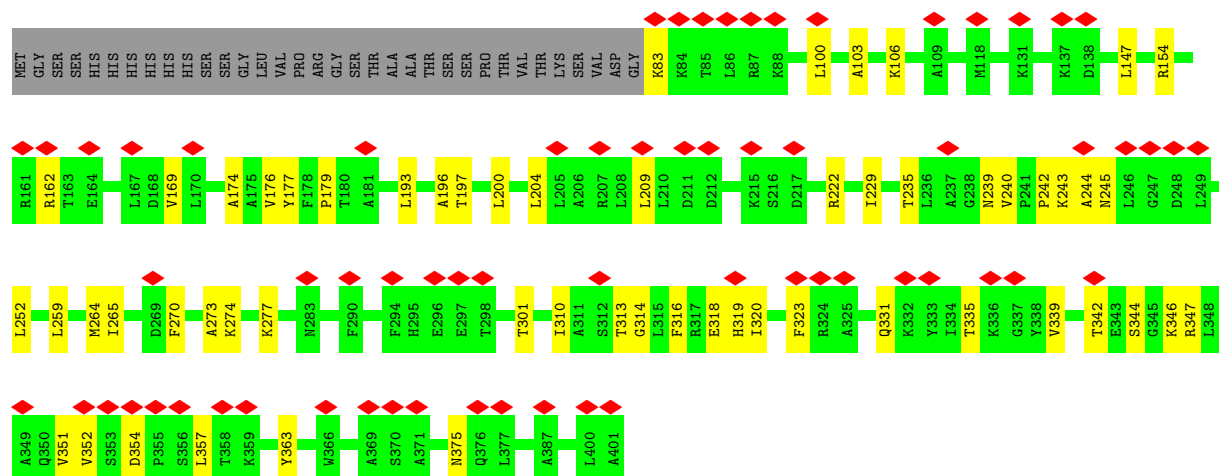
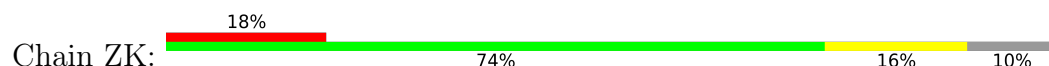
Chain ZI: 



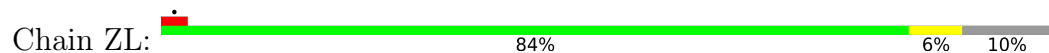
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

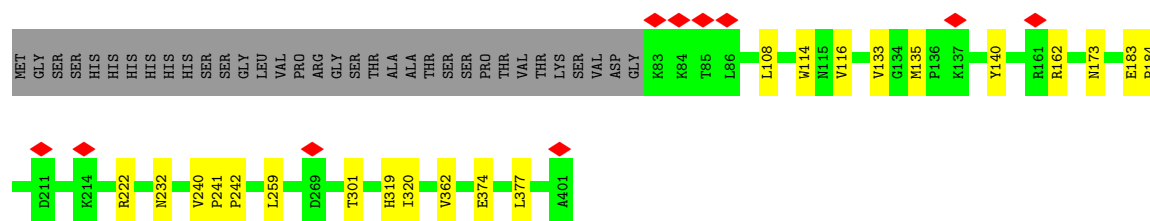


- Molecule 1: Protochlorophyllide reductase B, chloroplastic

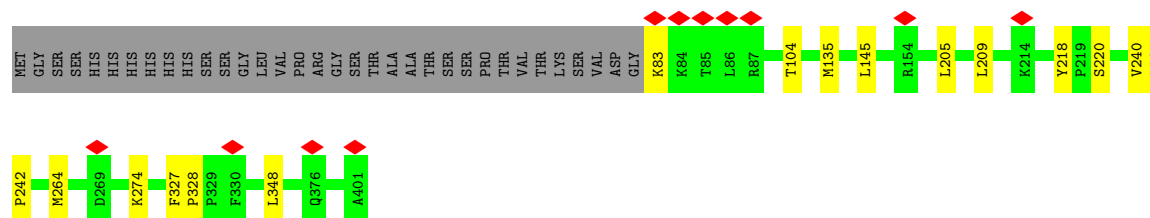


- Molecule 1: Protochlorophyllide reductase B, chloroplastic

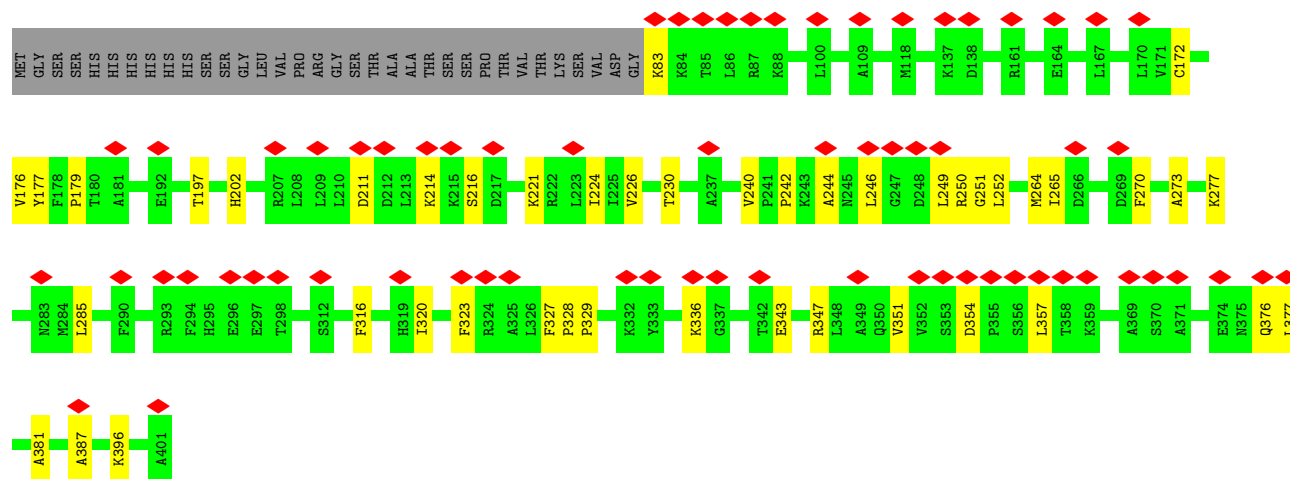
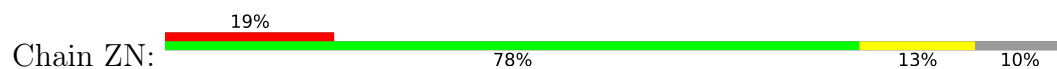




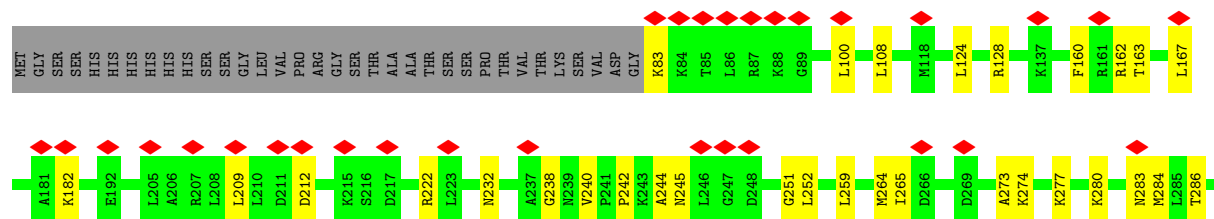
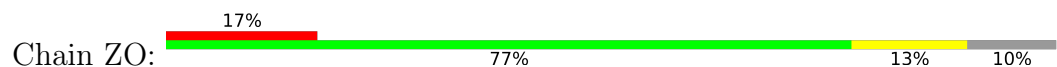
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

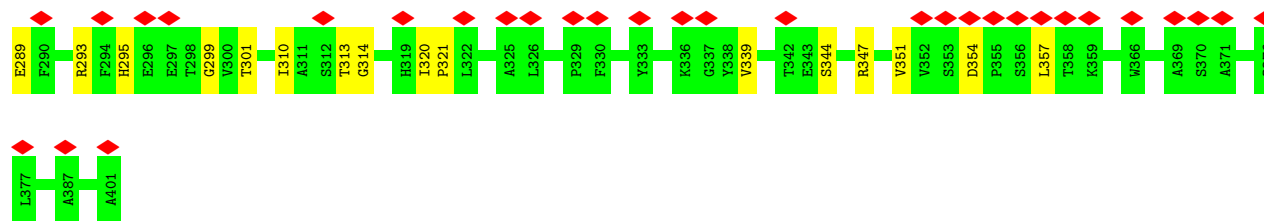


- Molecule 1: Protochlorophyllide reductase B, chloroplastic



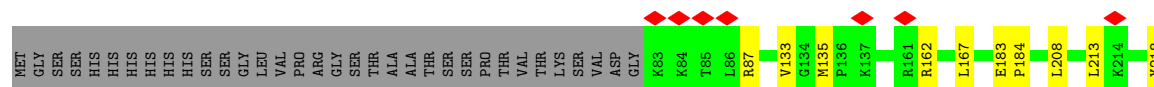
- Molecule 1: Protochlorophyllide reductase B, chloroplastic





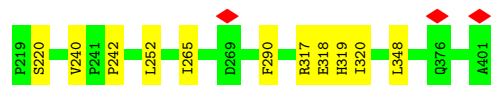
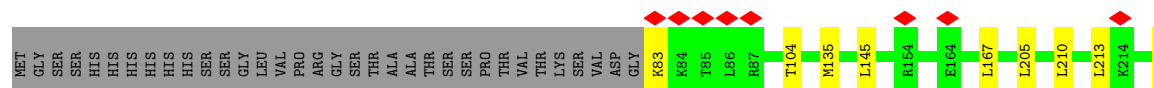
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain ZP: 83% 7% 10%



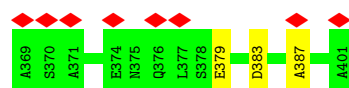
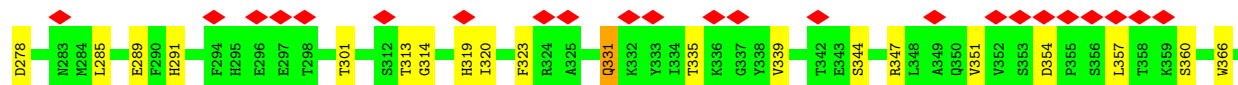
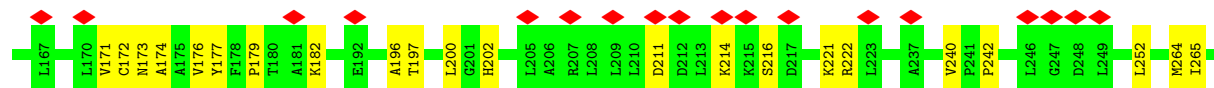
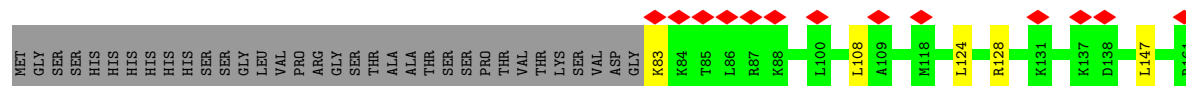
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain ZQ: 85% 6% 10%



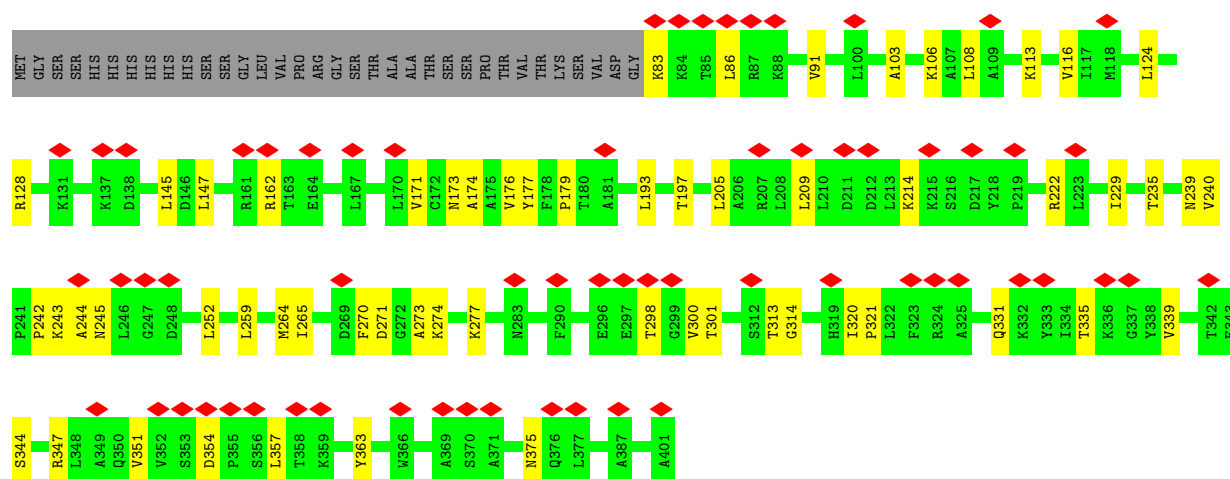
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain ZR: 18% 76% 14% 10%



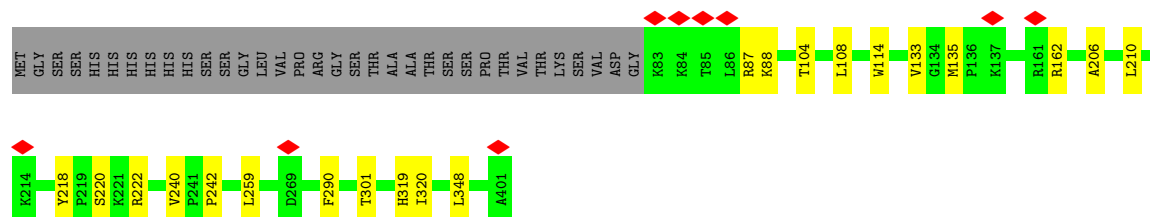
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain ZS: 18% 74% 17% 10%



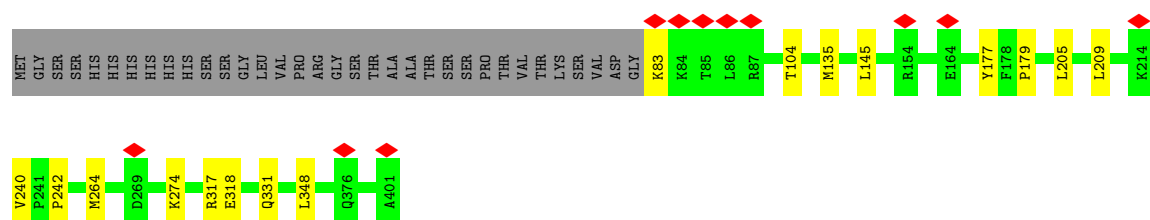
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain ZT: 84% 6% 10%



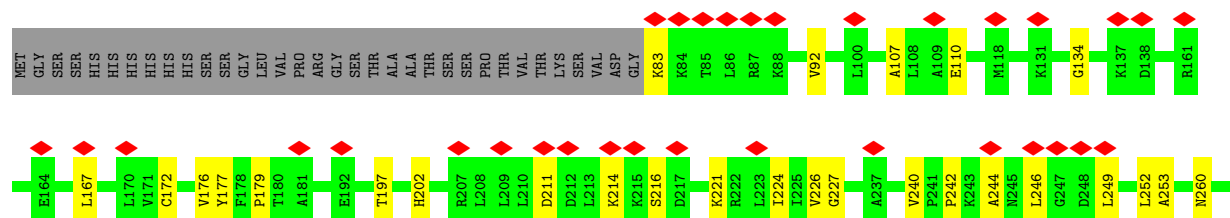
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

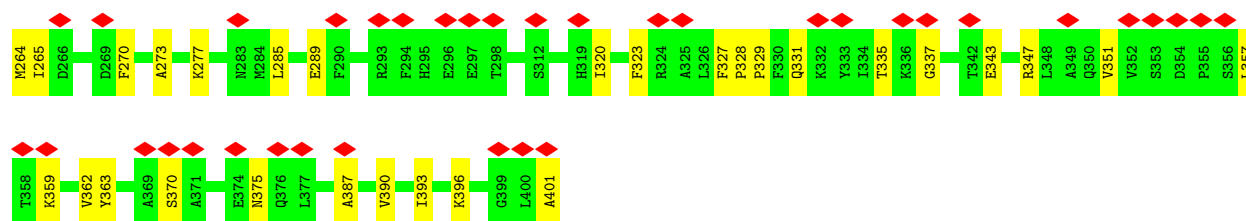
Chain ZU: 86% 5% 10%



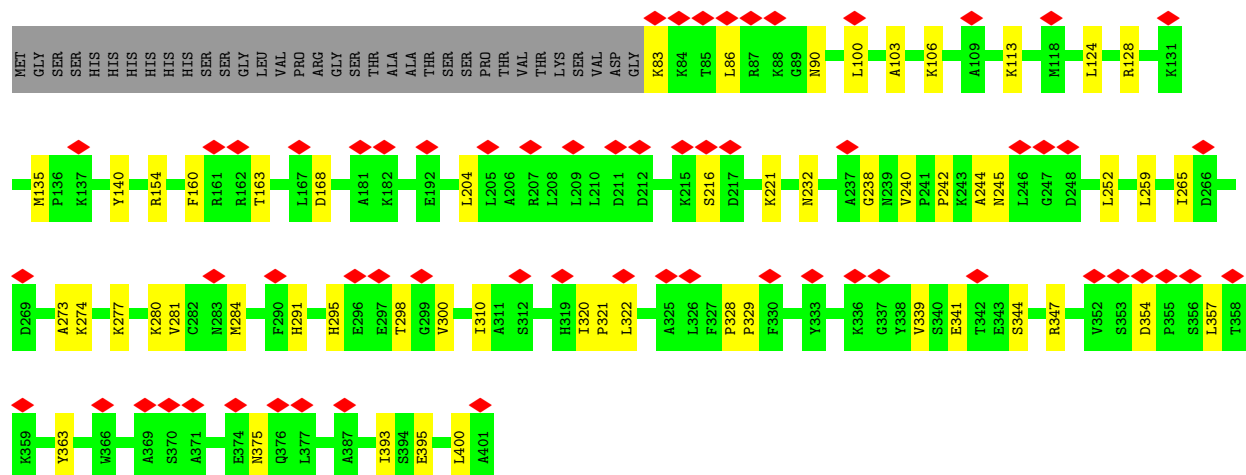
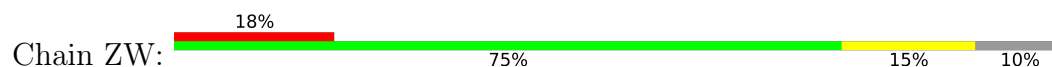
• Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain ZV: 19% 75% 16% 10%

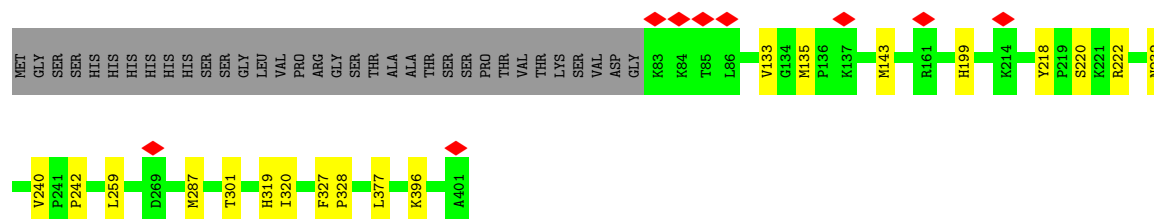
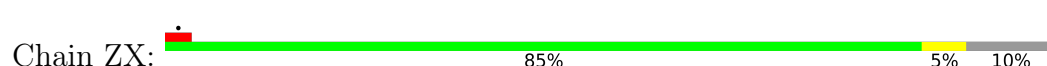




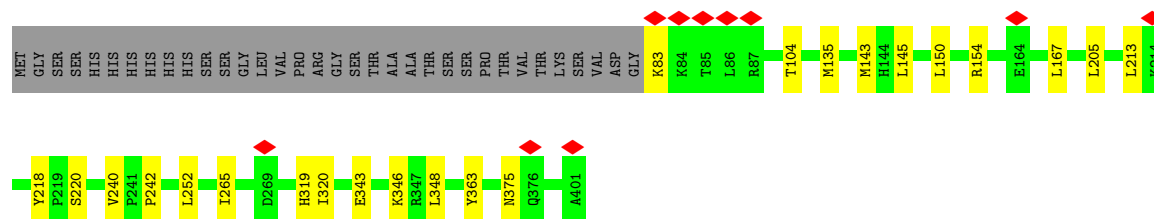
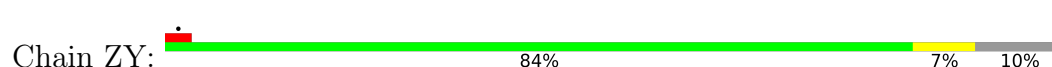
- Molecule 1: Protochlorophyllide reductase B, chloroplastic



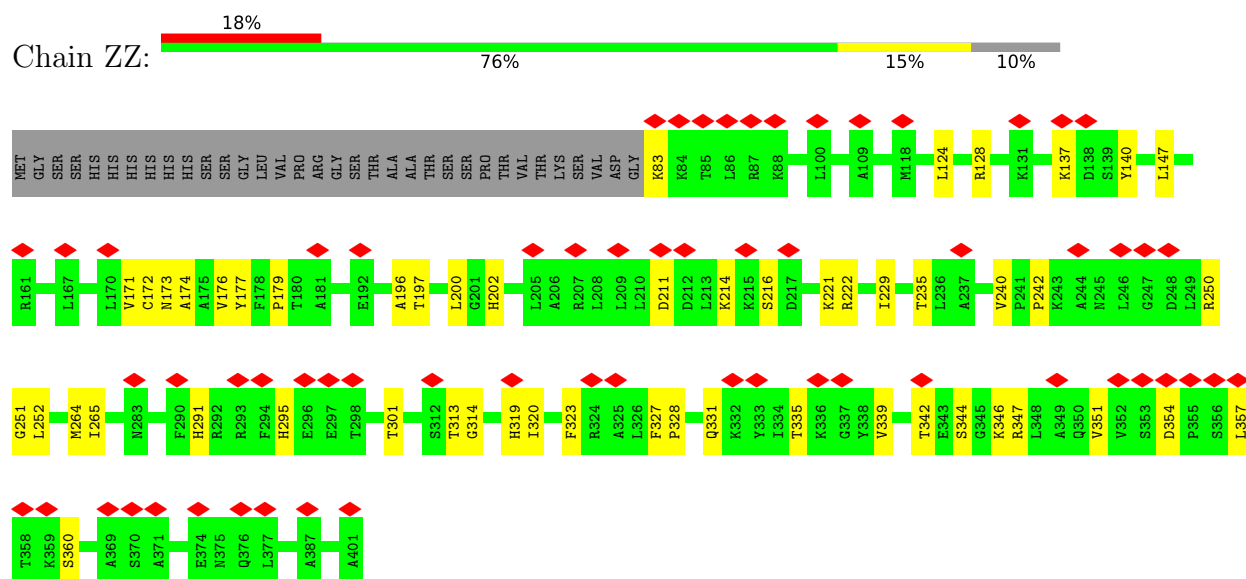
- Molecule 1: Protochlorophyllide reductase B, chloroplastic



- Molecule 1: Protochlorophyllide reductase B, chloroplastic



- Molecule 1: Protochlorophyllide reductase B, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=14.6°, rise=153.242 Å, axial sym=D10	Depositor
Number of segments used	21895	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.396	Depositor
Minimum map value	-0.156	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	550.4, 550.4, 550.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, A1JWG, NDP

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	YM	0.14	0/2494	0.38	0/3372
1	YN	0.13	0/2495	0.33	0/3374
1	YO	0.13	0/2494	0.34	0/3372
1	YP	0.15	0/2494	0.40	0/3372
1	YQ	0.14	0/2494	0.38	0/3372
1	YR	0.14	0/2495	0.35	0/3374
1	YS	0.13	0/2494	0.34	0/3372
1	YT	0.14	0/2494	0.38	0/3372
1	YU	0.15	0/2494	0.37	0/3372
1	YV	0.13	0/2495	0.32	0/3374
1	YW	0.13	0/2494	0.34	0/3372
1	YX	0.13	0/2494	0.35	0/3372
1	YY	0.14	0/2494	0.37	0/3372
1	YZ	0.13	0/2495	0.33	0/3374
1	ZA	0.13	0/2494	0.34	0/3372
1	ZB	0.14	0/2494	0.39	0/3372
1	ZC	0.14	0/2494	0.38	0/3372
1	ZD	0.14	0/2495	0.35	0/3374
1	ZE	0.13	0/2494	0.34	0/3372
1	ZF	0.14	0/2494	0.38	0/3372
1	ZG	0.14	0/2494	0.37	0/3372
1	ZH	0.13	0/2495	0.32	0/3374
1	ZI	0.13	0/2494	0.34	0/3372
1	ZJ	0.13	0/2494	0.35	0/3372
1	ZK	0.14	0/2494	0.36	0/3372
1	ZL	0.14	0/2495	0.33	0/3374
1	ZM	0.13	0/2494	0.34	0/3372
1	ZN	0.14	0/2494	0.39	0/3372
1	ZO	0.15	0/2494	0.37	0/3372
1	ZP	0.13	0/2495	0.32	0/3374
1	ZQ	0.13	0/2494	0.34	0/3372
1	ZR	0.13	0/2494	0.35	0/3372

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	ZS	0.14	0/2494	0.37	0/3372
1	ZT	0.13	0/2495	0.33	0/3374
1	ZU	0.13	0/2494	0.34	0/3372
1	ZV	0.14	0/2494	0.38	0/3372
1	ZW	0.14	0/2494	0.37	0/3372
1	ZX	0.13	0/2495	0.32	0/3374
1	ZY	0.13	0/2494	0.33	0/3372
1	ZZ	0.13	0/2494	0.35	0/3372
All	All	0.14	0/99770	0.35	0/134900

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

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	YM	2445	0	2449	43	0
1	YN	2446	0	2450	12	0
1	YO	2445	0	2449	13	0
1	YP	2445	0	2449	35	0
1	YQ	2445	0	2449	39	0
1	YR	2446	0	2450	17	0
1	YS	2445	0	2449	11	0
1	YT	2445	0	2449	29	0
1	YU	2445	0	2449	45	0
1	YV	2446	0	2450	9	0
1	YW	2445	0	2449	11	0
1	YX	2445	0	2449	35	0
1	YY	2445	0	2449	36	0
1	YZ	2446	0	2450	12	0
1	ZA	2445	0	2449	9	0
1	ZB	2445	0	2449	34	0
1	ZC	2445	0	2449	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	ZD	2446	0	2450	11	0
1	ZE	2445	0	2449	9	0
1	ZF	2445	0	2449	35	0
1	ZG	2445	0	2449	29	0
1	ZH	2446	0	2450	11	0
1	ZI	2445	0	2449	10	0
1	ZJ	2445	0	2449	34	0
1	ZK	2445	0	2449	35	0
1	ZL	2446	0	2450	14	0
1	ZM	2445	0	2449	10	0
1	ZN	2445	0	2449	30	0
1	ZO	2445	0	2449	29	0
1	ZP	2446	0	2450	15	0
1	ZQ	2445	0	2449	12	0
1	ZR	2445	0	2449	35	0
1	ZS	2445	0	2449	39	0
1	ZT	2446	0	2450	12	0
1	ZU	2445	0	2449	10	0
1	ZV	2445	0	2449	35	0
1	ZW	2445	0	2449	32	0
1	ZX	2446	0	2450	11	0
1	ZY	2445	0	2449	13	0
1	ZZ	2445	0	2449	32	0
2	YM	48	0	26	0	0
2	YN	48	0	26	1	0
2	YO	48	0	26	2	0
2	YP	48	0	26	0	0
2	YQ	48	0	26	1	0
2	YR	48	0	26	1	0
2	YS	48	0	26	1	0
2	YT	48	0	26	2	0
2	YU	48	0	26	1	0
2	YV	48	0	26	1	0
2	YW	48	0	26	1	0
2	YX	48	0	26	1	0
2	YY	48	0	26	1	0
2	YZ	48	0	26	3	0
2	ZA	48	0	26	1	0
2	ZB	48	0	26	0	0
2	ZC	48	0	26	0	0
2	ZD	48	0	26	1	0
2	ZE	48	0	26	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	ZF	48	0	26	0	0
2	ZG	48	0	26	1	0
2	ZH	48	0	26	0	0
2	ZI	48	0	26	1	0
2	ZJ	48	0	26	2	0
2	ZK	48	0	26	1	0
2	ZL	48	0	26	2	0
2	ZM	48	0	26	1	0
2	ZN	48	0	26	1	0
2	ZO	48	0	26	0	0
2	ZP	48	0	26	0	0
2	ZQ	48	0	26	1	0
2	ZR	48	0	26	1	0
2	ZS	48	0	26	0	0
2	ZT	48	0	26	0	0
2	ZU	48	0	26	1	0
2	ZV	48	0	26	1	0
2	ZW	48	0	26	0	0
2	ZX	48	0	26	1	0
2	ZY	48	0	26	1	0
2	ZZ	48	0	26	0	0
3	YM	45	0	0	0	0
3	YN	45	0	0	1	0
3	YO	45	0	0	0	0
3	YP	45	0	0	0	0
3	YQ	45	0	0	0	0
3	YR	45	0	0	1	0
3	YS	45	0	0	1	0
3	YT	45	0	0	0	0
3	YU	45	0	0	0	0
3	YV	45	0	0	1	0
3	YW	45	0	0	1	0
3	YX	45	0	0	0	0
3	YY	45	0	0	0	0
3	YZ	45	0	0	1	0
3	ZA	45	0	0	2	0
3	ZB	45	0	0	0	0
3	ZC	45	0	0	0	0
3	ZD	45	0	0	1	0
3	ZE	45	0	0	1	0
3	ZF	45	0	0	1	0
3	ZG	45	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	ZH	45	0	0	0	0
3	ZI	45	0	0	1	0
3	ZJ	45	0	0	1	0
3	ZK	45	0	0	1	0
3	ZL	45	0	0	0	0
3	ZM	45	0	0	1	0
3	ZN	45	0	0	0	0
3	ZO	45	0	0	0	0
3	ZP	45	0	0	0	0
3	ZQ	45	0	0	1	0
3	ZR	45	0	0	0	0
3	ZS	45	0	0	0	0
3	ZT	45	0	0	0	0
3	ZU	45	0	0	2	0
3	ZV	45	0	0	1	0
3	ZW	45	0	0	0	0
3	ZX	45	0	0	1	0
3	ZY	45	0	0	1	0
3	ZZ	45	0	0	0	0
4	YM	23	0	16	1	0
4	YN	23	0	16	1	0
4	YO	23	0	16	0	0
4	YP	23	0	16	0	0
4	YQ	23	0	16	0	0
4	YR	23	0	16	1	0
4	YS	23	0	16	0	0
4	YT	23	0	16	0	0
4	YU	23	0	16	0	0
4	YV	23	0	16	0	0
4	YW	23	0	16	0	0
4	YX	23	0	16	0	0
4	YY	23	0	16	0	0
4	YZ	23	0	16	0	0
4	ZA	23	0	16	0	0
4	ZB	23	0	16	0	0
4	ZC	23	0	16	0	0
4	ZD	23	0	16	0	0
4	ZE	23	0	16	0	0
4	ZF	23	0	16	0	0
4	ZG	23	0	16	0	0
4	ZH	23	0	16	2	0
4	ZI	23	0	16	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	ZJ	23	0	16	0	0
4	ZK	23	0	16	0	0
4	ZL	23	0	16	0	0
4	ZM	23	0	16	0	0
4	ZN	23	0	16	0	0
4	ZO	23	0	16	0	0
4	ZP	23	0	16	0	0
4	ZQ	23	0	16	0	0
4	ZR	23	0	16	0	0
4	ZS	23	0	16	0	0
4	ZT	23	0	16	0	0
4	ZU	23	0	16	0	0
4	ZV	23	0	16	0	0
4	ZW	23	0	16	0	0
4	ZX	23	0	16	0	0
4	ZY	23	0	16	0	0
4	ZZ	23	0	16	0	0
All	All	102450	0	99650	939	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 5.

The worst 5 of 939 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:YP:285:LEU:HD12	1:YP:387:ALA:HB2	1.58	0.84
1:YT:285:LEU:HD12	1:YT:387:ALA:HB2	1.59	0.82
1:ZS:344:SER:HA	1:ZS:347:ARG:HD2	1.63	0.80
1:YM:118:MET:HE3	1:YM:119:ALA:H	1.46	0.79
1:ZJ:344:SER:HA	1:ZJ:347:ARG:HD2	1.65	0.79

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	YM	317/353 (90%)	315 (99%)	2 (1%)	0	100	100
1	YN	317/353 (90%)	311 (98%)	6 (2%)	0	100	100
1	YO	317/353 (90%)	313 (99%)	4 (1%)	0	100	100
1	YP	317/353 (90%)	312 (98%)	5 (2%)	0	100	100
1	YQ	317/353 (90%)	312 (98%)	5 (2%)	0	100	100
1	YR	317/353 (90%)	311 (98%)	6 (2%)	0	100	100
1	YS	317/353 (90%)	311 (98%)	6 (2%)	0	100	100
1	YT	317/353 (90%)	316 (100%)	1 (0%)	0	100	100
1	YU	317/353 (90%)	313 (99%)	4 (1%)	0	100	100
1	YV	317/353 (90%)	311 (98%)	6 (2%)	0	100	100
1	YW	317/353 (90%)	311 (98%)	6 (2%)	0	100	100
1	YX	317/353 (90%)	312 (98%)	5 (2%)	0	100	100
1	YY	317/353 (90%)	312 (98%)	5 (2%)	0	100	100
1	YZ	317/353 (90%)	311 (98%)	6 (2%)	0	100	100
1	ZA	317/353 (90%)	313 (99%)	4 (1%)	0	100	100
1	ZB	317/353 (90%)	313 (99%)	4 (1%)	0	100	100
1	ZC	317/353 (90%)	313 (99%)	4 (1%)	0	100	100
1	ZD	317/353 (90%)	309 (98%)	8 (2%)	0	100	100
1	ZE	317/353 (90%)	311 (98%)	6 (2%)	0	100	100
1	ZF	317/353 (90%)	315 (99%)	2 (1%)	0	100	100
1	ZG	317/353 (90%)	314 (99%)	3 (1%)	0	100	100
1	ZH	317/353 (90%)	308 (97%)	9 (3%)	0	100	100
1	ZI	317/353 (90%)	313 (99%)	4 (1%)	0	100	100
1	ZJ	317/353 (90%)	310 (98%)	7 (2%)	0	100	100
1	ZK	317/353 (90%)	312 (98%)	5 (2%)	0	100	100
1	ZL	317/353 (90%)	310 (98%)	7 (2%)	0	100	100
1	ZM	317/353 (90%)	312 (98%)	5 (2%)	0	100	100
1	ZN	317/353 (90%)	312 (98%)	5 (2%)	0	100	100
1	ZO	317/353 (90%)	310 (98%)	7 (2%)	0	100	100
1	ZP	317/353 (90%)	311 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ZQ	317/353 (90%)	311 (98%)	6 (2%)	0	100	100
1	ZR	317/353 (90%)	313 (99%)	4 (1%)	0	100	100
1	ZS	317/353 (90%)	315 (99%)	2 (1%)	0	100	100
1	ZT	317/353 (90%)	310 (98%)	7 (2%)	0	100	100
1	ZU	317/353 (90%)	314 (99%)	3 (1%)	0	100	100
1	ZV	317/353 (90%)	315 (99%)	2 (1%)	0	100	100
1	ZW	317/353 (90%)	312 (98%)	5 (2%)	0	100	100
1	ZX	317/353 (90%)	311 (98%)	6 (2%)	0	100	100
1	ZY	317/353 (90%)	312 (98%)	5 (2%)	0	100	100
1	ZZ	317/353 (90%)	315 (99%)	2 (1%)	0	100	100
All	All	12680/14120 (90%)	12485 (98%)	195 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	YM	261/290 (90%)	261 (100%)	0	100	100
1	YN	262/290 (90%)	262 (100%)	0	100	100
1	YO	261/290 (90%)	261 (100%)	0	100	100
1	YP	261/290 (90%)	261 (100%)	0	100	100
1	YQ	261/290 (90%)	261 (100%)	0	100	100
1	YR	262/290 (90%)	262 (100%)	0	100	100
1	YS	261/290 (90%)	261 (100%)	0	100	100
1	YT	261/290 (90%)	261 (100%)	0	100	100
1	YU	261/290 (90%)	261 (100%)	0	100	100
1	YV	262/290 (90%)	262 (100%)	0	100	100
1	YW	261/290 (90%)	261 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	YX	261/290 (90%)	261 (100%)	0	100	100
1	YY	261/290 (90%)	261 (100%)	0	100	100
1	YZ	262/290 (90%)	262 (100%)	0	100	100
1	ZA	261/290 (90%)	261 (100%)	0	100	100
1	ZB	261/290 (90%)	261 (100%)	0	100	100
1	ZC	261/290 (90%)	261 (100%)	0	100	100
1	ZD	262/290 (90%)	262 (100%)	0	100	100
1	ZE	261/290 (90%)	261 (100%)	0	100	100
1	ZF	261/290 (90%)	261 (100%)	0	100	100
1	ZG	261/290 (90%)	261 (100%)	0	100	100
1	ZH	262/290 (90%)	262 (100%)	0	100	100
1	ZI	261/290 (90%)	261 (100%)	0	100	100
1	ZJ	261/290 (90%)	261 (100%)	0	100	100
1	ZK	261/290 (90%)	261 (100%)	0	100	100
1	ZL	262/290 (90%)	262 (100%)	0	100	100
1	ZM	261/290 (90%)	261 (100%)	0	100	100
1	ZN	261/290 (90%)	261 (100%)	0	100	100
1	ZO	261/290 (90%)	261 (100%)	0	100	100
1	ZP	262/290 (90%)	262 (100%)	0	100	100
1	ZQ	261/290 (90%)	261 (100%)	0	100	100
1	ZR	261/290 (90%)	260 (100%)	1 (0%)	84	85
1	ZS	261/290 (90%)	261 (100%)	0	100	100
1	ZT	262/290 (90%)	262 (100%)	0	100	100
1	ZU	261/290 (90%)	261 (100%)	0	100	100
1	ZV	261/290 (90%)	261 (100%)	0	100	100
1	ZW	261/290 (90%)	261 (100%)	0	100	100
1	ZX	262/290 (90%)	261 (100%)	1 (0%)	84	85
1	ZY	261/290 (90%)	261 (100%)	0	100	100
1	ZZ	261/290 (90%)	261 (100%)	0	100	100
All	All	10450/11600 (90%)	10448 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	ZR	331	GLN
1	ZX	199	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	ZR	291	HIS
1	ZZ	295	HIS
1	ZS	144	HIS
1	ZX	239	ASN
1	YW	295	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

120 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	$\# Z > 2$
4	LMG	YO	503	-	23,23,55	0.70	0	31,31,63	0.76	0
4	LMG	YY	503	-	23,23,55	0.67	0	31,31,63	0.83	0
4	LMG	YP	503	-	23,23,55	0.67	0	31,31,63	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	ZH	501	-	49,52,52	2.21	5 (10%)	66,80,80	1.66	14 (21%)
2	NDP	YO	501	-	49,52,52	2.18	6 (12%)	66,80,80	1.63	13 (19%)
2	NDP	ZQ	501	-	49,52,52	2.18	5 (10%)	66,80,80	1.66	13 (19%)
3	A1JWG	YV	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.17	3 (4%)
4	LMG	ZU	503	-	23,23,55	0.69	0	31,31,63	0.77	0
3	A1JWG	ZK	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.23	3 (4%)
2	NDP	YM	501	-	49,52,52	2.21	6 (12%)	66,80,80	1.66	13 (19%)
2	NDP	YQ	501	-	49,52,52	2.26	6 (12%)	66,80,80	1.65	14 (21%)
3	A1JWG	YQ	502	-	48,53,53	1.39	6 (12%)	62,89,89	1.22	3 (4%)
2	NDP	ZE	501	-	49,52,52	2.18	5 (10%)	66,80,80	1.64	13 (19%)
3	A1JWG	ZR	502	-	48,53,53	1.38	5 (10%)	62,89,89	1.20	2 (3%)
2	NDP	ZP	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.67	13 (19%)
2	NDP	ZR	501	-	49,52,52	2.24	6 (12%)	66,80,80	1.68	14 (21%)
3	A1JWG	ZB	502	-	48,53,53	1.38	5 (10%)	62,89,89	1.01	2 (3%)
3	A1JWG	YP	502	-	48,53,53	1.38	5 (10%)	62,89,89	1.24	2 (3%)
2	NDP	ZV	501	-	49,52,52	2.26	6 (12%)	66,80,80	1.63	14 (21%)
3	A1JWG	YT	502	-	48,53,53	1.39	6 (12%)	62,89,89	1.22	2 (3%)
2	NDP	YT	501	-	49,52,52	2.26	6 (12%)	66,80,80	1.65	13 (19%)
3	A1JWG	YS	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.10	3 (4%)
3	A1JWG	ZA	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	3 (4%)
4	LMG	ZB	503	-	23,23,55	0.67	0	31,31,63	0.80	0
4	LMG	YN	502	-	23,23,55	0.71	0	31,31,63	0.82	0
2	NDP	ZB	501	-	49,52,52	2.25	6 (12%)	66,80,80	1.68	15 (22%)
2	NDP	ZI	501	-	49,52,52	2.19	5 (10%)	66,80,80	1.67	13 (19%)
3	A1JWG	YN	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.13	3 (4%)
3	A1JWG	ZW	502	-	48,53,53	1.40	5 (10%)	62,89,89	0.93	2 (3%)
4	LMG	ZA	503	-	23,23,55	0.71	0	31,31,63	0.78	0
2	NDP	ZF	501	-	49,52,52	2.27	6 (12%)	66,80,80	1.69	15 (22%)
4	LMG	ZZ	503	-	23,23,55	0.67	0	31,31,63	0.81	0
4	LMG	ZD	502	-	23,23,55	0.71	0	31,31,63	0.76	0
4	LMG	ZJ	503	-	23,23,55	0.68	0	31,31,63	0.87	0
3	A1JWG	ZM	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.14	3 (4%)
4	LMG	ZV	503	-	23,23,55	0.67	0	31,31,63	0.79	0
3	A1JWG	ZD	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.15	3 (4%)
2	NDP	ZJ	501	-	49,52,52	2.23	5 (10%)	66,80,80	1.66	15 (22%)
4	LMG	ZH	502	-	23,23,55	0.70	0	31,31,63	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1JWG	ZH	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.15	3 (4%)
3	A1JWG	ZQ	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.11	3 (4%)
3	A1JWG	ZG	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.14	3 (4%)
2	NDP	YU	501	-	49,52,52	2.21	5 (10%)	66,80,80	1.63	13 (19%)
3	A1JWG	YU	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.18	3 (4%)
4	LMG	ZO	503	-	23,23,55	0.69	0	31,31,63	0.75	0
3	A1JWG	ZZ	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.23	3 (4%)
2	NDP	YR	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.65	14 (21%)
2	NDP	ZW	501	-	49,52,52	2.27	5 (10%)	66,80,80	1.62	12 (18%)
4	LMG	ZQ	503	-	23,23,55	0.69	0	31,31,63	0.76	0
3	A1JWG	ZV	502	-	48,53,53	1.38	6 (12%)	62,89,89	1.12	3 (4%)
3	A1JWG	YW	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	3 (4%)
4	LMG	YM	503	-	23,23,55	0.69	0	31,31,63	0.83	0
2	NDP	ZY	501	-	49,52,52	2.18	5 (10%)	66,80,80	1.67	13 (19%)
4	LMG	YU	503	-	23,23,55	0.68	0	31,31,63	0.88	1 (3%)
4	LMG	ZY	503	-	23,23,55	0.70	0	31,31,63	0.82	0
4	LMG	YZ	502	-	23,23,55	0.68	0	31,31,63	0.93	1 (3%)
4	LMG	YX	503	-	23,23,55	0.68	0	31,31,63	0.84	0
2	NDP	ZL	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.65	16 (24%)
4	LMG	ZL	502	-	23,23,55	0.69	0	31,31,63	0.79	0
2	NDP	ZO	501	-	49,52,52	2.26	5 (10%)	66,80,80	1.66	14 (21%)
2	NDP	YV	501	-	49,52,52	2.21	5 (10%)	66,80,80	1.67	15 (22%)
4	LMG	YV	502	-	23,23,55	0.70	0	31,31,63	0.80	0
4	LMG	ZP	502	-	23,23,55	0.71	0	31,31,63	0.90	1 (3%)
2	NDP	ZK	501	-	49,52,52	2.23	6 (12%)	66,80,80	1.65	13 (19%)
3	A1JWG	ZL	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.13	2 (3%)
3	A1JWG	ZP	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.19	3 (4%)
4	LMG	ZR	503	-	23,23,55	0.69	0	31,31,63	0.75	0
2	NDP	ZT	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.65	15 (22%)
4	LMG	ZT	502	-	23,23,55	0.70	0	31,31,63	0.86	0
2	NDP	YS	501	-	49,52,52	2.19	5 (10%)	66,80,80	1.67	13 (19%)
2	NDP	YP	501	-	49,52,52	2.25	5 (10%)	66,80,80	1.68	15 (22%)
3	A1JWG	YX	502	-	48,53,53	1.37	5 (10%)	62,89,89	1.23	1 (1%)
3	A1JWG	YZ	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.16	3 (4%)
3	A1JWG	ZT	503	-	48,53,53	1.37	5 (10%)	62,89,89	1.17	2 (3%)
4	LMG	ZI	503	-	23,23,55	0.71	0	31,31,63	0.82	0
3	A1JWG	ZJ	502	-	48,53,53	1.38	5 (10%)	62,89,89	1.18	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1JWG	ZF	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.08	3 (4%)
3	A1JWG	ZS	502	-	48,53,53	1.38	5 (10%)	62,89,89	1.25	3 (4%)
2	NDP	YW	501	-	49,52,52	2.18	5 (10%)	66,80,80	1.65	13 (19%)
2	NDP	ZZ	501	-	49,52,52	2.23	5 (10%)	66,80,80	1.67	14 (21%)
3	A1JWG	ZE	502	-	48,53,53	1.38	5 (10%)	62,89,89	1.14	1 (1%)
4	LMG	ZW	503	-	23,23,55	0.69	0	31,31,63	0.77	0
2	NDP	ZX	501	-	49,52,52	2.23	5 (10%)	66,80,80	1.65	15 (22%)
2	NDP	ZC	501	-	49,52,52	2.25	5 (10%)	66,80,80	1.66	14 (21%)
4	LMG	ZF	503	-	23,23,55	0.67	0	31,31,63	0.81	0
2	NDP	ZM	501	-	49,52,52	2.18	5 (10%)	66,80,80	1.66	14 (21%)
4	LMG	YR	502	-	23,23,55	0.70	0	31,31,63	0.81	0
4	LMG	ZK	503	-	23,23,55	0.67	0	31,31,63	0.78	0
2	NDP	ZS	501	-	49,52,52	2.20	5 (10%)	66,80,80	1.64	13 (19%)
3	A1JWG	YR	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.16	3 (4%)
3	A1JWG	ZY	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	3 (4%)
3	A1JWG	ZO	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	3 (4%)
4	LMG	ZG	503	-	23,23,55	0.69	0	31,31,63	0.84	0
2	NDP	ZU	501	-	49,52,52	2.20	5 (10%)	66,80,80	1.66	13 (19%)
2	NDP	YX	501	-	49,52,52	2.23	5 (10%)	66,80,80	1.67	14 (21%)
4	LMG	ZS	503	-	23,23,55	0.67	0	31,31,63	0.86	0
2	NDP	YN	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.66	14 (21%)
3	A1JWG	YY	502	-	48,53,53	1.38	5 (10%)	62,89,89	1.21	3 (4%)
2	NDP	YY	501	-	49,52,52	2.27	6 (12%)	66,80,80	1.64	14 (21%)
3	A1JWG	ZN	502	-	48,53,53	1.39	6 (12%)	62,89,89	1.19	1 (1%)
2	NDP	ZD	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.65	15 (22%)
3	A1JWG	YM	502	-	48,53,53	1.37	5 (10%)	62,89,89	1.24	2 (3%)
4	LMG	ZX	502	-	23,23,55	0.71	0	31,31,63	0.79	0
4	LMG	YQ	503	-	23,23,55	0.70	0	31,31,63	0.77	0
3	A1JWG	ZC	502	-	48,53,53	1.38	5 (10%)	62,89,89	1.20	3 (4%)
4	LMG	ZC	503	-	23,23,55	0.67	0	31,31,63	0.82	0
4	LMG	ZE	503	-	23,23,55	0.70	0	31,31,63	0.81	0
2	NDP	ZG	501	-	49,52,52	2.24	4 (8%)	66,80,80	1.70	16 (24%)
4	LMG	ZN	503	-	23,23,55	0.67	0	31,31,63	0.85	0
3	A1JWG	ZI	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.11	3 (4%)
3	A1JWG	ZX	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.14	3 (4%)
4	LMG	ZM	503	-	23,23,55	0.70	0	31,31,63	0.84	0
2	NDP	YZ	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.65	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LMG	YT	503	-	23,23,55	0.68	0	31,31,63	0.80	0
2	NDP	ZA	501	-	49,52,52	2.20	5 (10%)	66,80,80	1.66	13 (19%)
4	LMG	YS	503	-	23,23,55	0.70	0	31,31,63	0.81	0
4	LMG	YW	503	-	23,23,55	0.70	0	31,31,63	0.81	0
3	A1JWG	YO	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	3 (4%)
2	NDP	ZN	501	-	49,52,52	2.27	7 (14%)	66,80,80	1.63	13 (19%)
3	A1JWG	ZU	502	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMG	YO	503	-	-	5/16/36/70	0/1/1/1
4	LMG	YY	503	-	-	3/16/36/70	0/1/1/1
4	LMG	YP	503	-	-	3/16/36/70	0/1/1/1
2	NDP	ZH	501	-	-	9/34/77/77	0/5/5/5
2	NDP	YO	501	-	-	12/34/77/77	0/5/5/5
3	A1JWG	YV	503	-	3/3/11/15	7/15/91/91	-
2	NDP	ZQ	501	-	-	10/34/77/77	0/5/5/5
4	LMG	ZU	503	-	-	2/16/36/70	0/1/1/1
3	A1JWG	ZK	502	-	3/3/11/15	9/15/91/91	-
3	A1JWG	YQ	502	-	3/3/11/15	4/15/91/91	-
2	NDP	YM	501	-	-	8/34/77/77	0/5/5/5
2	NDP	YQ	501	-	-	11/34/77/77	0/5/5/5
2	NDP	ZE	501	-	-	15/34/77/77	0/5/5/5
3	A1JWG	ZR	502	-	3/3/11/15	8/15/91/91	-
2	NDP	ZP	501	-	-	9/34/77/77	0/5/5/5
2	NDP	ZR	501	-	-	11/34/77/77	0/5/5/5
3	A1JWG	ZB	502	-	3/3/11/15	6/15/91/91	-
3	A1JWG	YP	502	-	3/3/11/15	6/15/91/91	-
2	NDP	ZV	501	-	-	12/34/77/77	0/5/5/5
3	A1JWG	YT	502	-	3/3/11/15	3/15/91/91	-
2	NDP	YT	501	-	-	8/34/77/77	0/5/5/5
3	A1JWG	YS	502	-	3/3/11/15	7/15/91/91	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1JWG	ZA	502	-	3/3/11/15	7/15/91/91	-
4	LMG	ZB	503	-	-	10/16/36/70	0/1/1/1
4	LMG	YN	502	-	-	5/16/36/70	0/1/1/1
2	NDP	ZB	501	-	-	9/34/77/77	0/5/5/5
3	A1JWG	YN	503	-	3/3/11/15	7/15/91/91	-
3	A1JWG	ZW	502	-	2/2/11/15	9/15/91/91	-
2	NDP	ZI	501	-	-	10/34/77/77	0/5/5/5
4	LMG	ZA	503	-	-	4/16/36/70	0/1/1/1
2	NDP	ZF	501	-	-	7/34/77/77	0/5/5/5
4	LMG	ZZ	503	-	-	7/16/36/70	0/1/1/1
4	LMG	ZD	502	-	-	1/16/36/70	0/1/1/1
4	LMG	ZJ	503	-	-	9/16/36/70	0/1/1/1
3	A1JWG	ZM	502	-	3/3/11/15	7/15/91/91	-
4	LMG	ZV	503	-	-	4/16/36/70	0/1/1/1
3	A1JWG	ZD	503	-	3/3/11/15	9/15/91/91	-
2	NDP	ZJ	501	-	-	6/34/77/77	0/5/5/5
4	LMG	ZH	502	-	-	4/16/36/70	0/1/1/1
3	A1JWG	ZH	503	-	3/3/11/15	5/15/91/91	-
3	A1JWG	ZQ	502	-	3/3/11/15	7/15/91/91	-
3	A1JWG	ZG	502	-	3/3/11/15	9/15/91/91	-
2	NDP	YU	501	-	-	13/34/77/77	0/5/5/5
3	A1JWG	YU	502	-	3/3/11/15	8/15/91/91	-
4	LMG	ZO	503	-	-	3/16/36/70	0/1/1/1
3	A1JWG	ZZ	502	-	3/3/11/15	10/15/91/91	-
2	NDP	YR	501	-	-	12/34/77/77	0/5/5/5
2	NDP	ZW	501	-	-	12/34/77/77	0/5/5/5
4	LMG	ZQ	503	-	-	6/16/36/70	0/1/1/1
3	A1JWG	ZV	502	-	3/3/11/15	8/15/91/91	-
3	A1JWG	YW	502	-	3/3/11/15	10/15/91/91	-
4	LMG	YM	503	-	-	7/16/36/70	0/1/1/1
2	NDP	ZY	501	-	-	11/34/77/77	0/5/5/5
4	LMG	YU	503	-	-	4/16/36/70	0/1/1/1
4	LMG	ZY	503	-	-	2/16/36/70	0/1/1/1
4	LMG	YZ	502	-	-	6/16/36/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMG	YX	503	-	-	4/16/36/70	0/1/1/1
2	NDP	ZL	501	-	-	14/34/77/77	0/5/5/5
4	LMG	ZL	502	-	-	7/16/36/70	0/1/1/1
2	NDP	ZO	501	-	-	10/34/77/77	0/5/5/5
2	NDP	YV	501	-	-	9/34/77/77	0/5/5/5
4	LMG	YV	502	-	-	6/16/36/70	0/1/1/1
4	LMG	ZP	502	-	-	10/16/36/70	0/1/1/1
3	A1JWG	ZL	503	-	3/3/11/15	6/15/91/91	-
2	NDP	ZK	501	-	-	11/34/77/77	0/5/5/5
3	A1JWG	ZP	503	-	3/3/11/15	5/15/91/91	-
4	LMG	ZR	503	-	-	4/16/36/70	0/1/1/1
2	NDP	ZT	501	-	-	10/34/77/77	0/5/5/5
4	LMG	ZT	502	-	-	8/16/36/70	0/1/1/1
3	A1JWG	YX	502	-	3/3/11/15	5/15/91/91	-
2	NDP	YP	501	-	-	9/34/77/77	0/5/5/5
2	NDP	YS	501	-	-	10/34/77/77	0/5/5/5
3	A1JWG	YZ	503	-	3/3/11/15	6/15/91/91	-
3	A1JWG	ZT	503	-	3/3/11/15	6/15/91/91	-
4	LMG	ZI	503	-	-	5/16/36/70	0/1/1/1
3	A1JWG	ZJ	502	-	3/3/11/15	5/15/91/91	-
3	A1JWG	ZF	502	-	3/3/11/15	4/15/91/91	-
3	A1JWG	ZS	502	-	3/3/11/15	4/15/91/91	-
3	A1JWG	ZE	502	-	3/3/11/15	8/15/91/91	-
2	NDP	YW	501	-	-	9/34/77/77	0/5/5/5
2	NDP	ZZ	501	-	-	11/34/77/77	0/5/5/5
4	LMG	ZW	503	-	-	4/16/36/70	0/1/1/1
2	NDP	ZX	501	-	-	9/34/77/77	0/5/5/5
2	NDP	ZC	501	-	-	8/34/77/77	0/5/5/5
4	LMG	ZF	503	-	-	6/16/36/70	0/1/1/1
2	NDP	ZM	501	-	-	10/34/77/77	0/5/5/5
4	LMG	YR	502	-	-	3/16/36/70	0/1/1/1
4	LMG	ZK	503	-	-	4/16/36/70	0/1/1/1
2	NDP	ZS	501	-	-	15/34/77/77	0/5/5/5
3	A1JWG	YR	503	-	3/3/11/15	8/15/91/91	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1JWG	ZY	502	-	3/3/11/15	7/15/91/91	-
3	A1JWG	ZO	502	-	3/3/11/15	5/15/91/91	-
4	LMG	ZG	503	-	-	8/16/36/70	0/1/1/1
2	NDP	ZU	501	-	-	12/34/77/77	0/5/5/5
2	NDP	YX	501	-	-	8/34/77/77	0/5/5/5
4	LMG	ZS	503	-	-	10/16/36/70	0/1/1/1
2	NDP	YN	501	-	-	10/34/77/77	0/5/5/5
3	A1JWG	YY	502	-	3/3/11/15	4/15/91/91	-
2	NDP	YY	501	-	-	13/34/77/77	0/5/5/5
3	A1JWG	ZN	502	-	3/3/11/15	1/15/91/91	-
2	NDP	ZD	501	-	-	10/34/77/77	0/5/5/5
3	A1JWG	YM	502	-	3/3/11/15	5/15/91/91	-
4	LMG	ZX	502	-	-	2/16/36/70	0/1/1/1
4	LMG	YQ	503	-	-	9/16/36/70	0/1/1/1
3	A1JWG	ZC	502	-	3/3/11/15	6/15/91/91	-
4	LMG	ZC	503	-	-	5/16/36/70	0/1/1/1
4	LMG	ZE	503	-	-	5/16/36/70	0/1/1/1
2	NDP	ZG	501	-	-	8/34/77/77	0/5/5/5
4	LMG	ZN	503	-	-	9/16/36/70	0/1/1/1
3	A1JWG	ZI	502	-	3/3/11/15	10/15/91/91	-
3	A1JWG	ZX	503	-	3/3/11/15	9/15/91/91	-
4	LMG	ZM	503	-	-	5/16/36/70	0/1/1/1
2	NDP	YZ	501	-	-	12/34/77/77	0/5/5/5
4	LMG	YT	503	-	-	6/16/36/70	0/1/1/1
2	NDP	ZA	501	-	-	9/34/77/77	0/5/5/5
4	LMG	YS	503	-	-	2/16/36/70	0/1/1/1
4	LMG	YW	503	-	-	2/16/36/70	0/1/1/1
3	A1JWG	YO	502	-	3/3/11/15	5/15/91/91	-
2	NDP	ZN	501	-	-	15/34/77/77	0/5/5/5
3	A1JWG	ZU	502	-	3/3/11/15	8/15/91/91	-

The worst 5 of 415 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	YY	501	NDP	P2B-O2B	13.01	1.83	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	YQ	501	NDP	P2B-O2B	13.00	1.83	1.59
2	ZW	501	NDP	P2B-O2B	12.99	1.83	1.59
2	ZF	501	NDP	P2B-O2B	12.98	1.83	1.59
2	ZO	501	NDP	P2B-O2B	12.96	1.83	1.59

The worst 5 of 663 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	ZB	501	NDP	PN-O3-PA	-7.29	107.81	132.83
2	YM	501	NDP	PN-O3-PA	-7.22	108.04	132.83
2	ZF	501	NDP	PN-O3-PA	-7.22	108.05	132.83
2	ZY	501	NDP	PN-O3-PA	-7.18	108.20	132.83
2	ZR	501	NDP	PN-O3-PA	-7.17	108.22	132.83

5 of 119 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	YM	502	A1JWG	NA
3	YM	502	A1JWG	NB
3	YM	502	A1JWG	NC
3	YN	503	A1JWG	NA
3	YN	503	A1JWG	NB

5 of 889 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	YM	501	NDP	C2B-O2B-P2B-O1X
2	YM	501	NDP	O4D-C1D-N1N-C6N
2	YM	501	NDP	C2N-C3N-C7N-N7N
2	YN	501	NDP	C5B-O5B-PA-O2A
2	YN	501	NDP	C5B-O5B-PA-O3

There are no ring outliers.

51 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	YO	501	NDP	2	0
2	ZQ	501	NDP	1	0
3	YV	503	A1JWG	1	0
3	ZK	502	A1JWG	1	0
2	YQ	501	NDP	1	0

Continued on next page...

Continued from previous page...

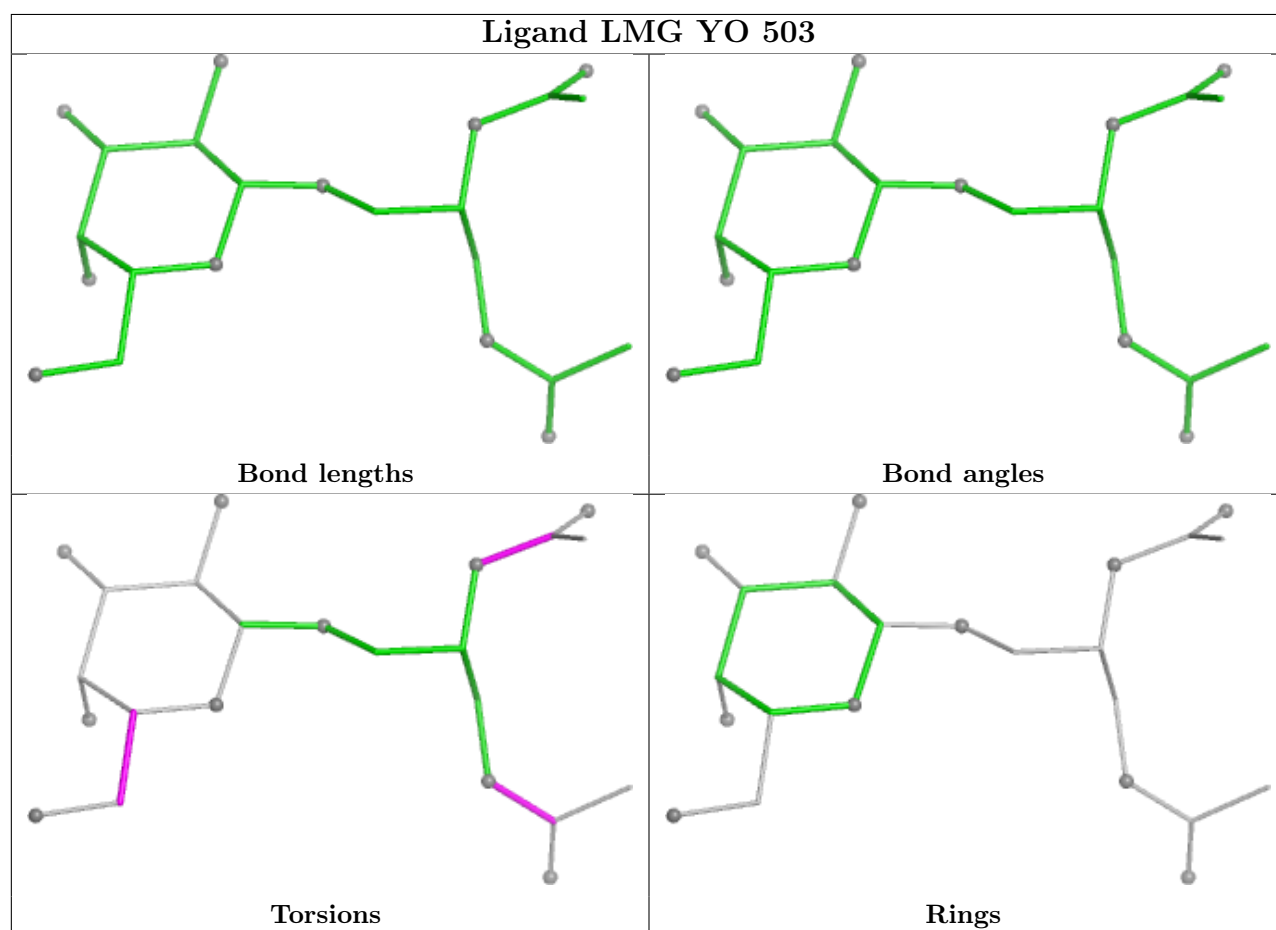
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	ZE	501	NDP	2	0
2	ZR	501	NDP	1	0
2	ZV	501	NDP	1	0
2	YT	501	NDP	2	0
3	YS	502	A1JWG	1	0
3	ZA	502	A1JWG	2	0
4	YN	502	LMG	1	0
2	ZI	501	NDP	1	0
3	YN	503	A1JWG	1	0
3	ZM	502	A1JWG	1	0
3	ZD	503	A1JWG	1	0
2	ZJ	501	NDP	2	0
4	ZH	502	LMG	2	0
3	ZQ	502	A1JWG	1	0
2	YU	501	NDP	1	0
2	YR	501	NDP	1	0
3	ZV	502	A1JWG	1	0
3	YW	502	A1JWG	1	0
4	YM	503	LMG	1	0
2	ZY	501	NDP	1	0
2	ZL	501	NDP	2	0
2	YV	501	NDP	1	0
2	ZK	501	NDP	1	0
2	YS	501	NDP	1	0
3	YZ	503	A1JWG	1	0
3	ZJ	502	A1JWG	1	0
3	ZF	502	A1JWG	1	0
2	YW	501	NDP	1	0
3	ZE	502	A1JWG	1	0
2	ZX	501	NDP	1	0
2	ZM	501	NDP	1	0
4	YR	502	LMG	1	0
3	YR	503	A1JWG	1	0
3	ZY	502	A1JWG	1	0
2	ZU	501	NDP	1	0
2	YX	501	NDP	1	0
2	YN	501	NDP	1	0
2	YY	501	NDP	1	0
2	ZD	501	NDP	1	0
2	ZG	501	NDP	1	0
3	ZI	502	A1JWG	1	0
3	ZX	503	A1JWG	1	0

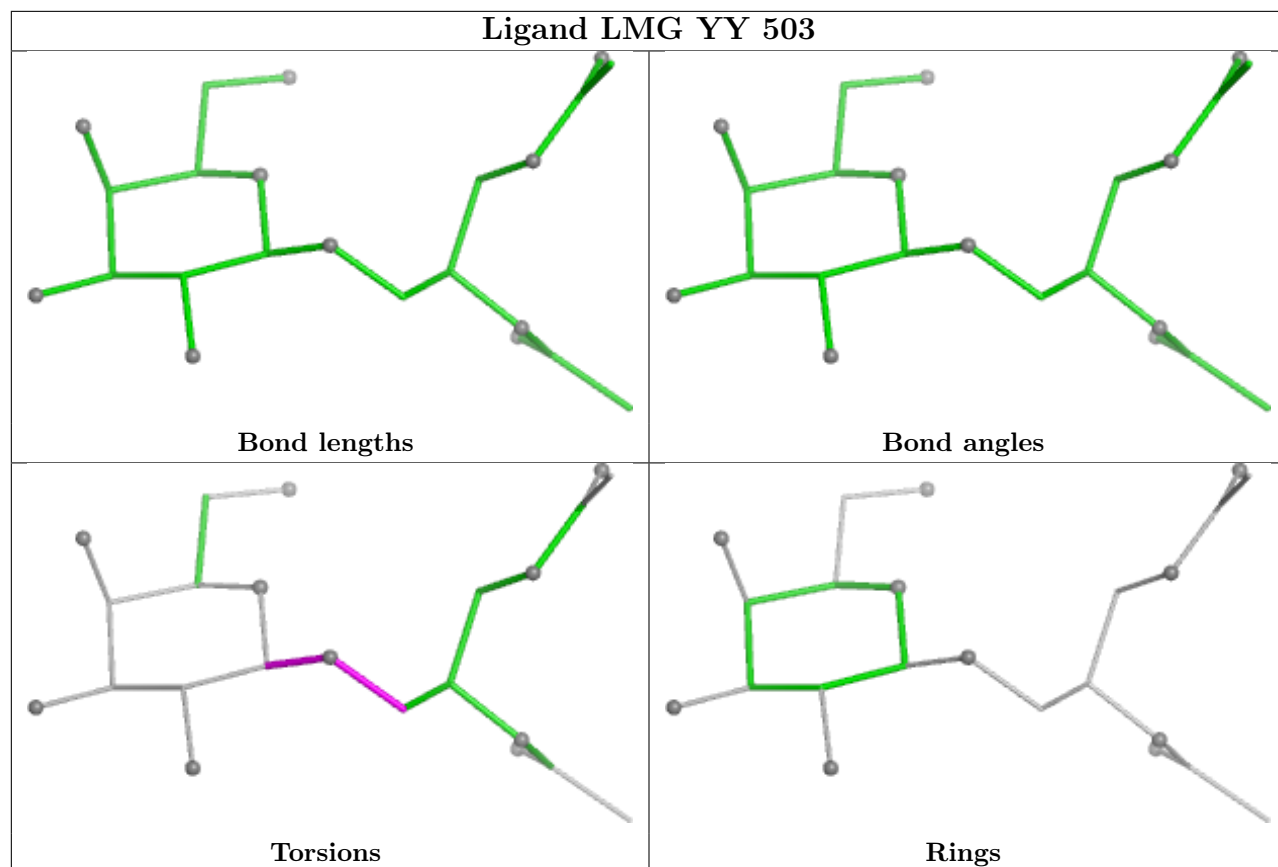
Continued on next page...

Continued from previous page...

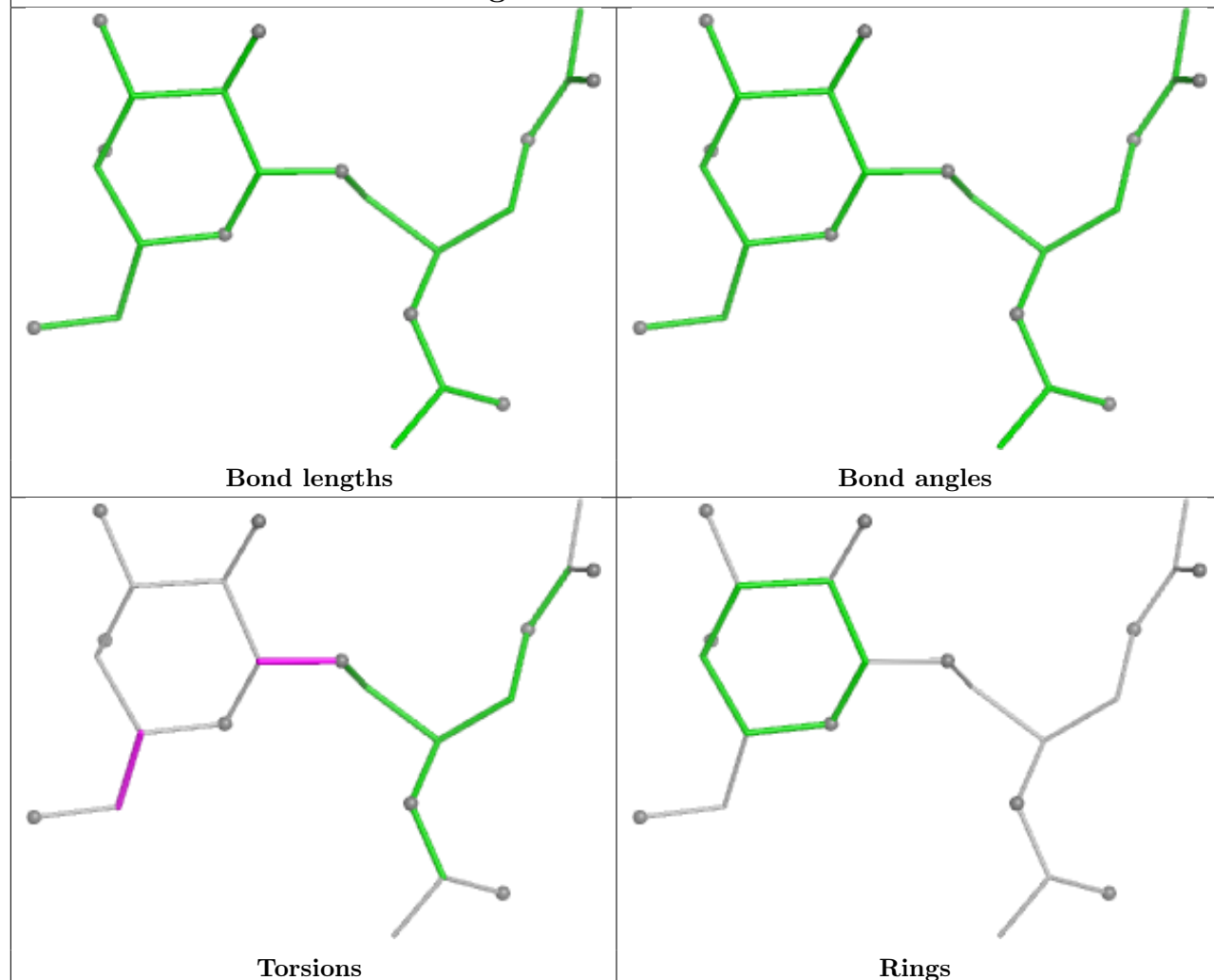
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	YZ	501	NDP	3	0
2	ZA	501	NDP	1	0
2	ZN	501	NDP	1	0
3	ZU	502	A1JWG	2	0

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

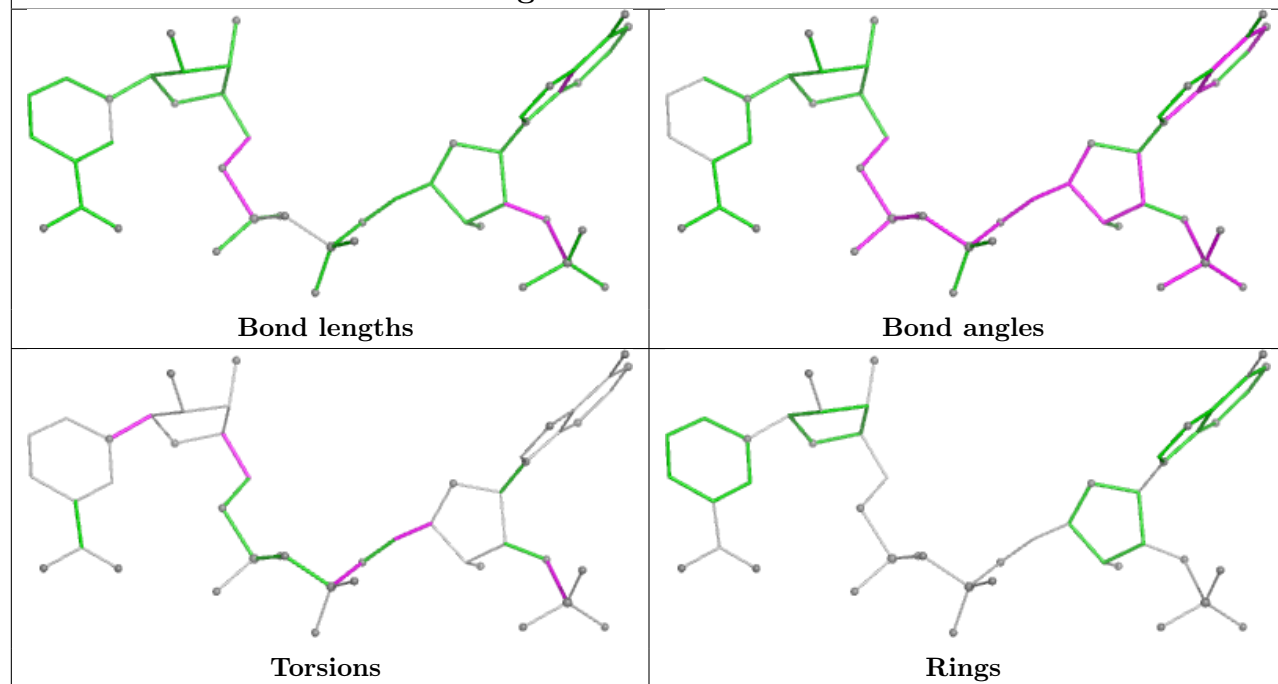




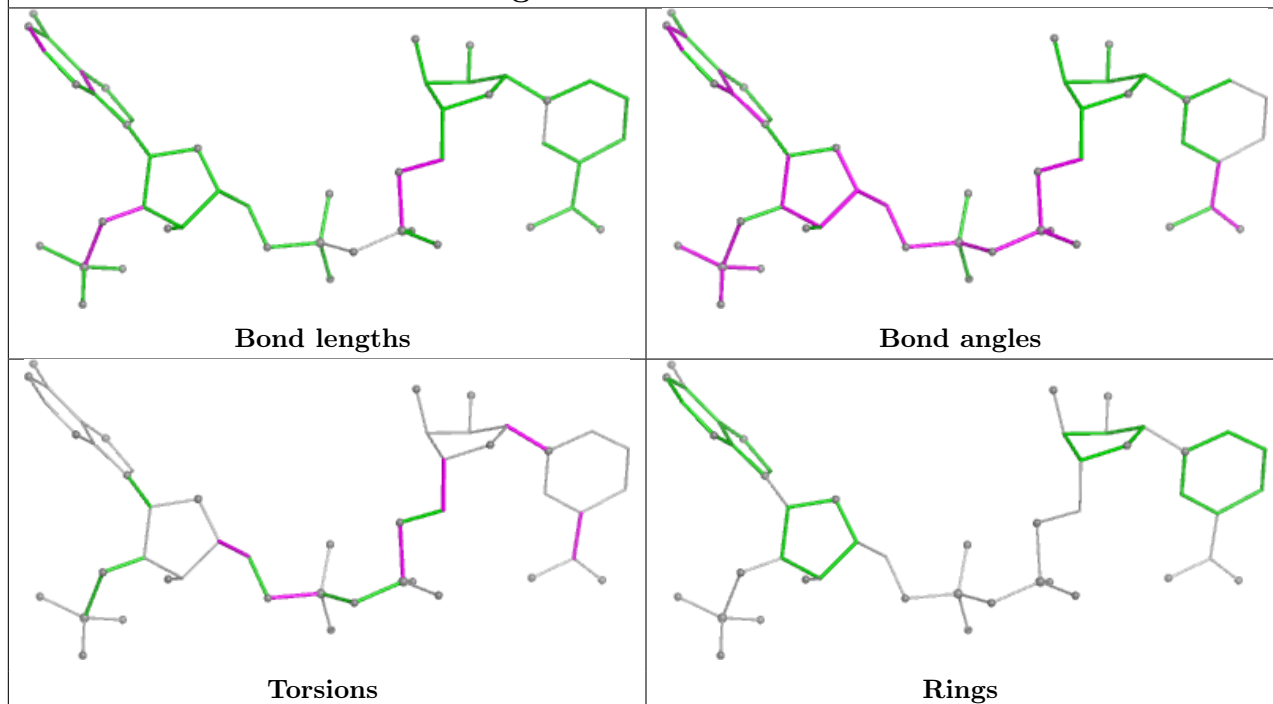
Ligand LMG YP 503



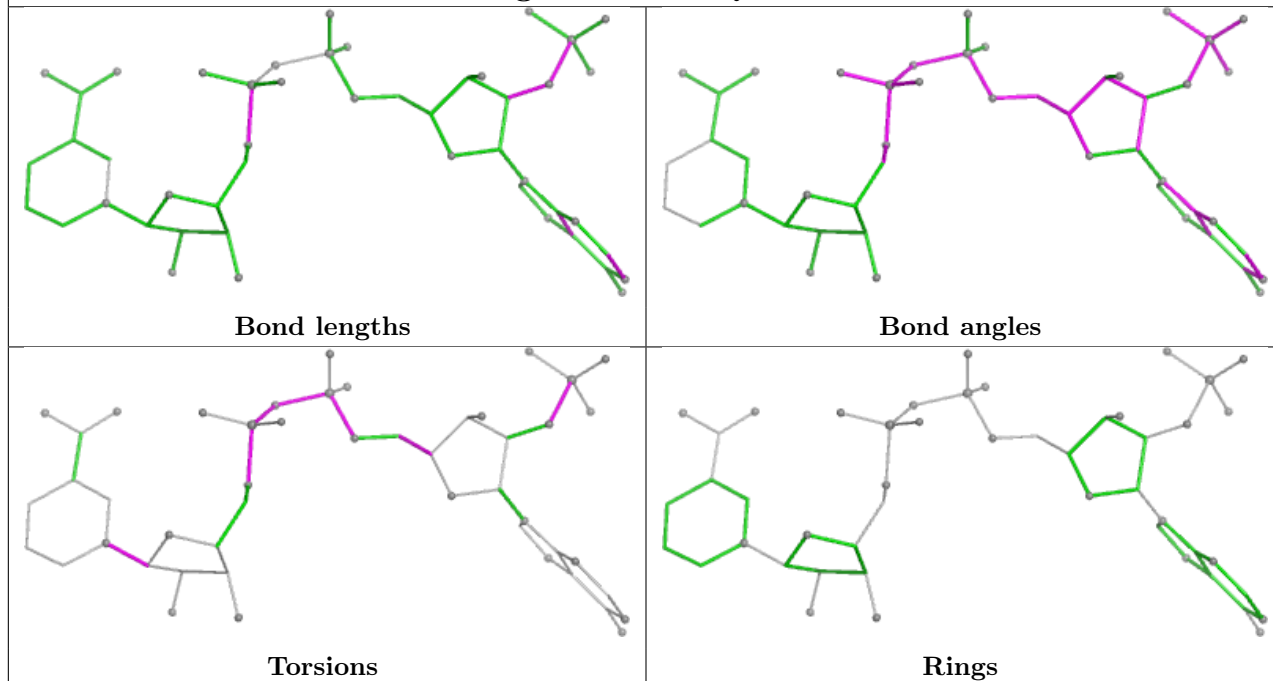
Ligand NDP ZH 501



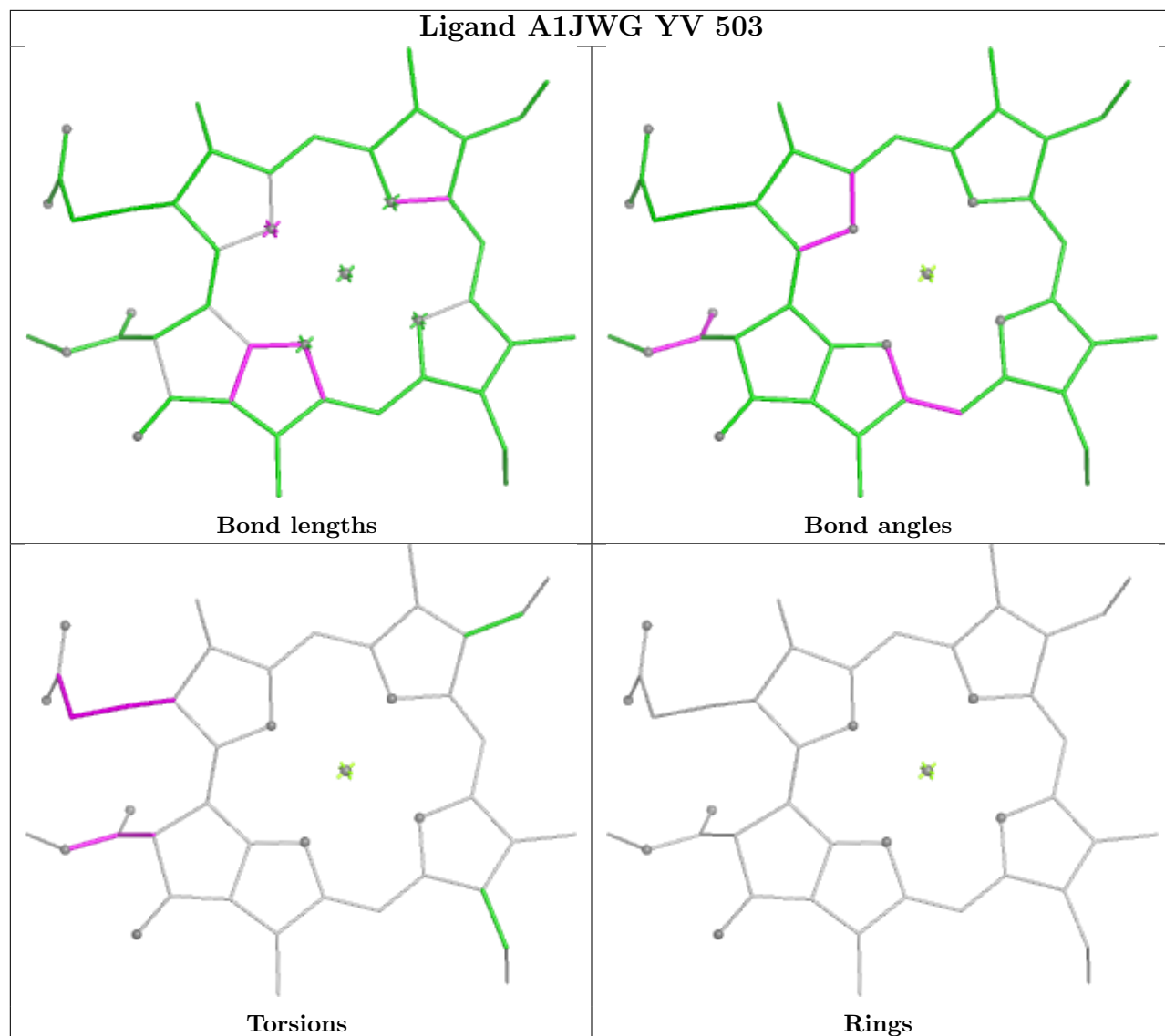
Ligand NDP YO 501

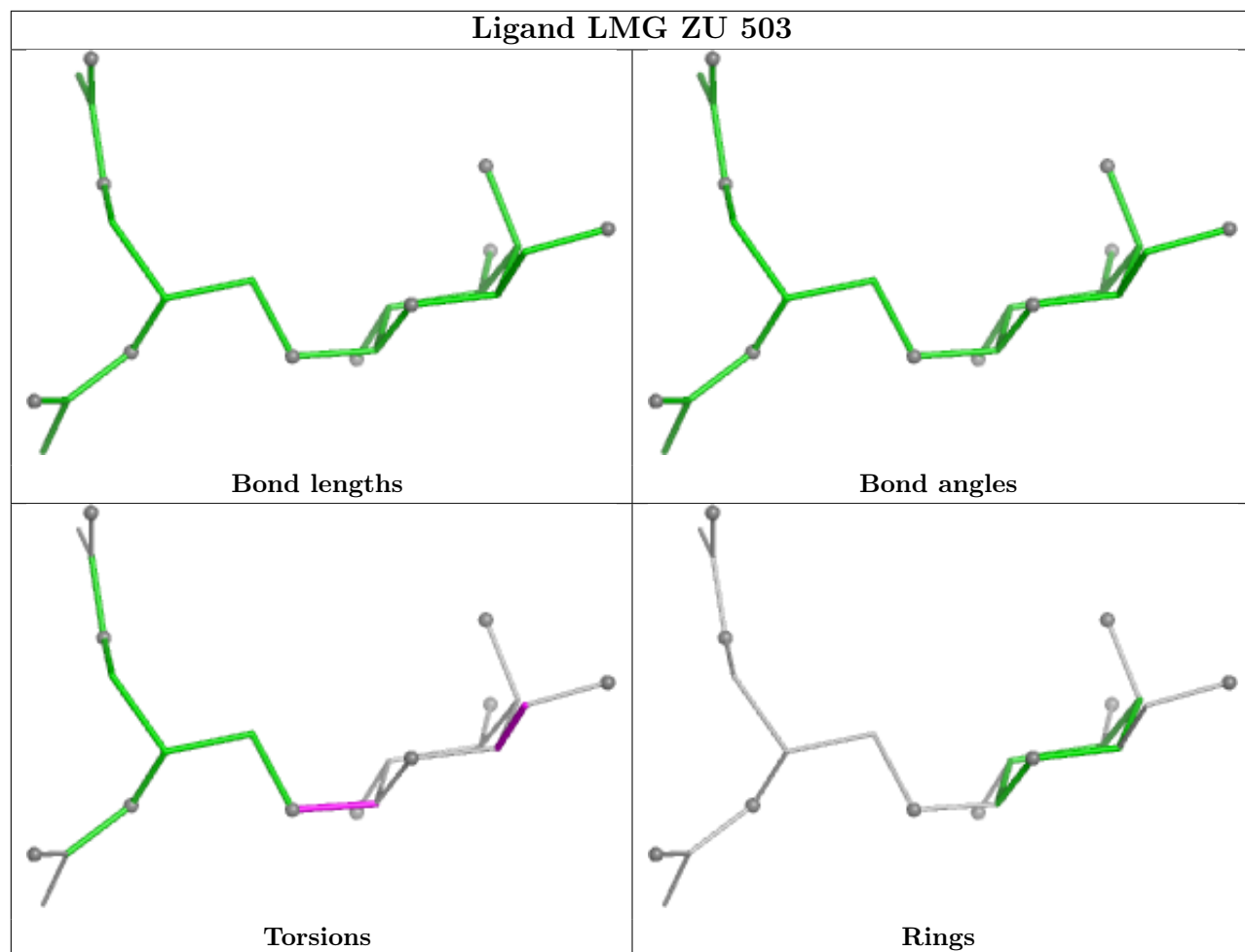


Ligand NDP ZQ 501

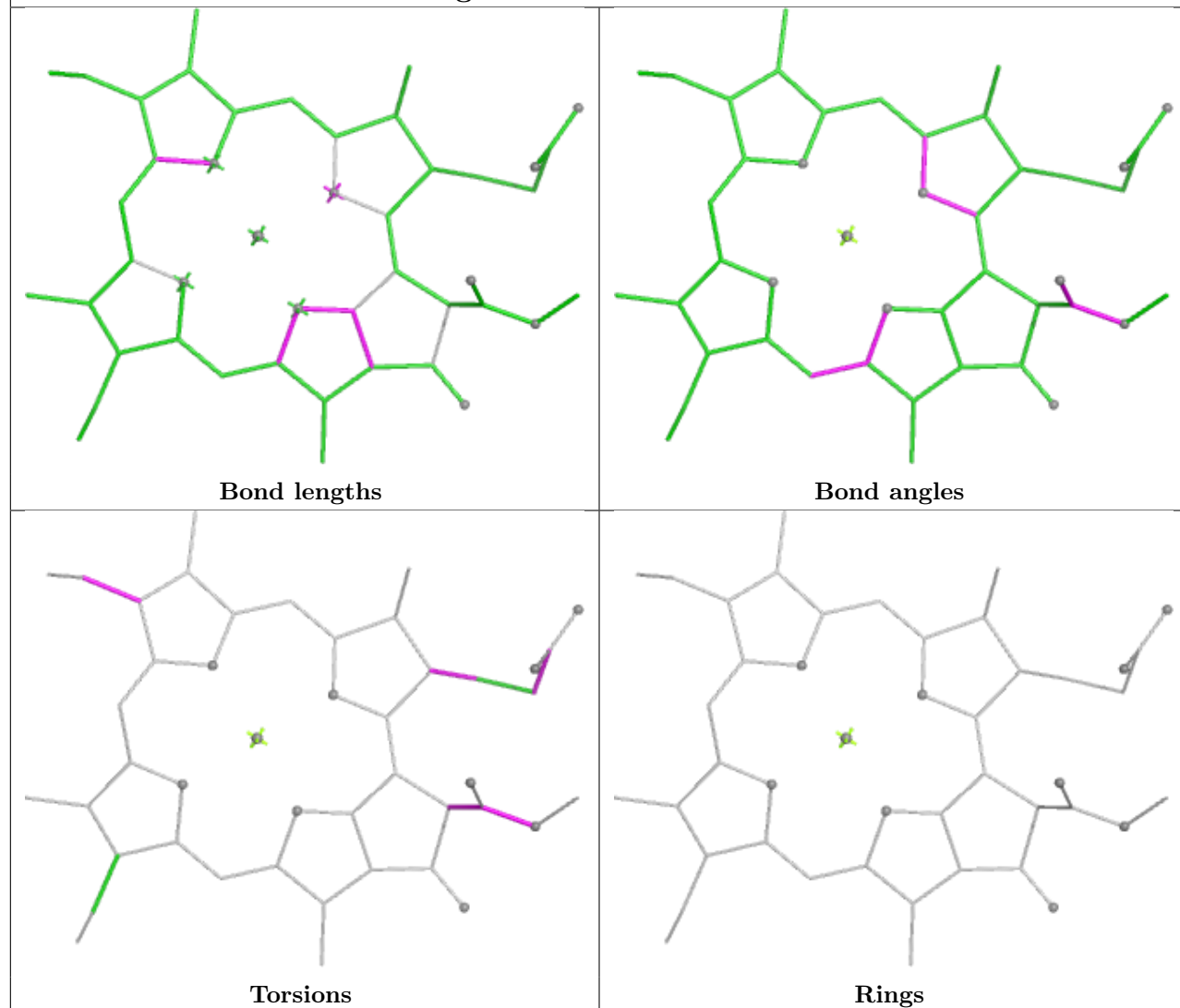


Ligand A1JWG YV 503

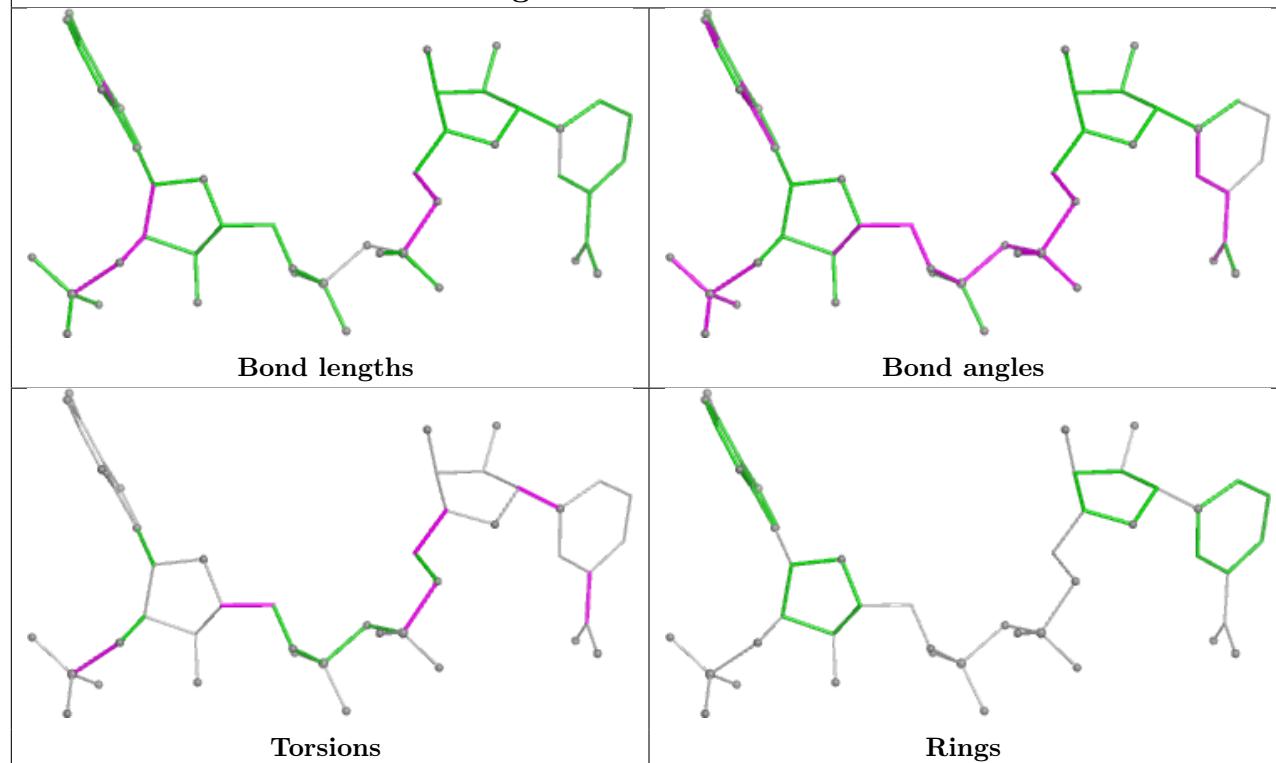




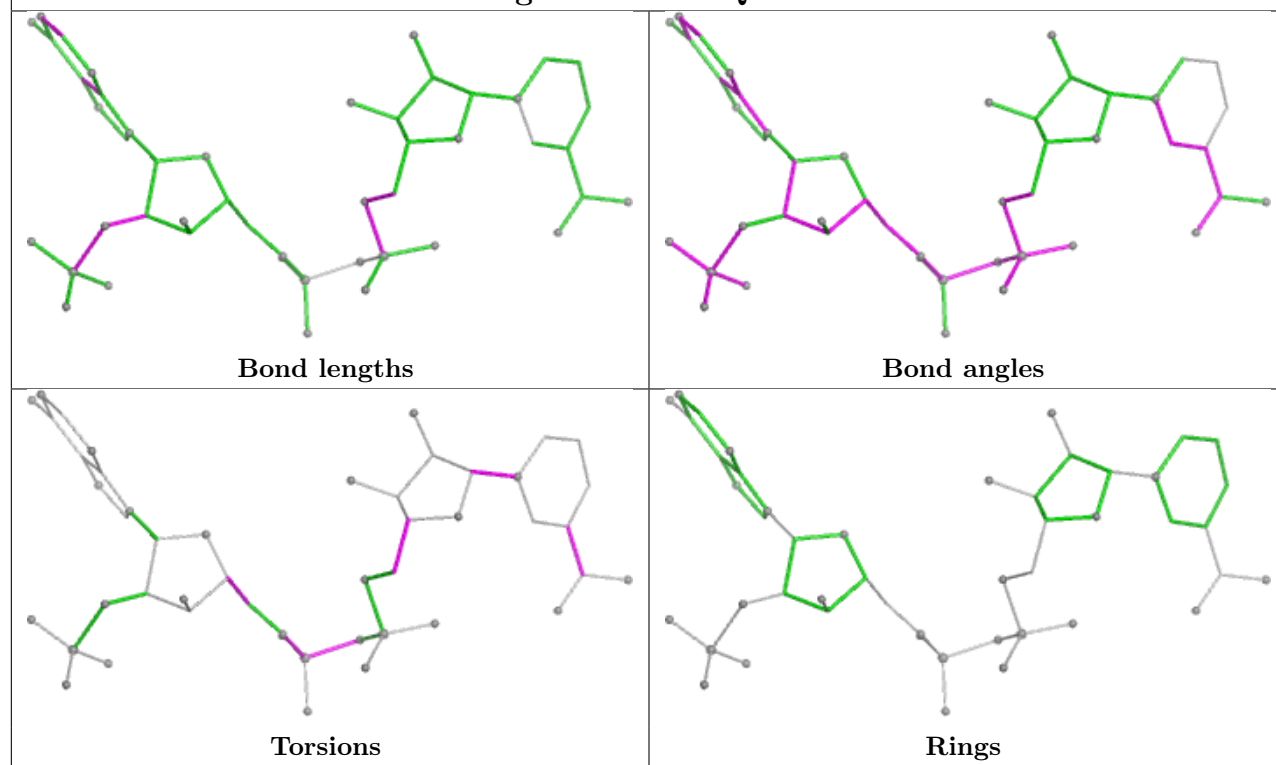
Ligand A1JWG ZK 502



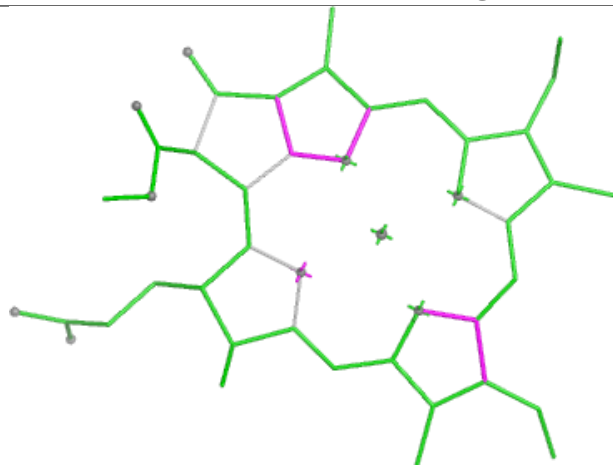
Ligand NDP YM 501



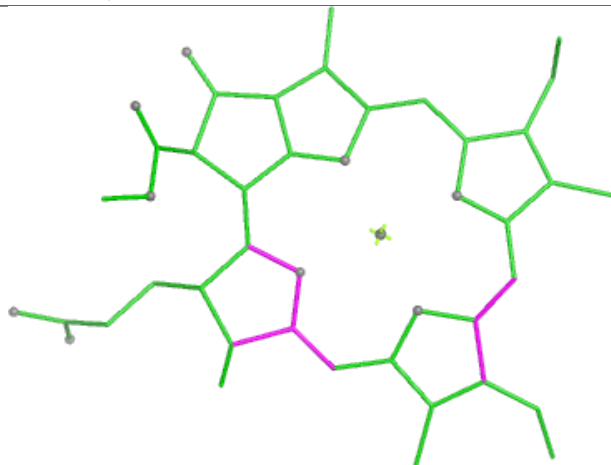
Ligand NDP YQ 501



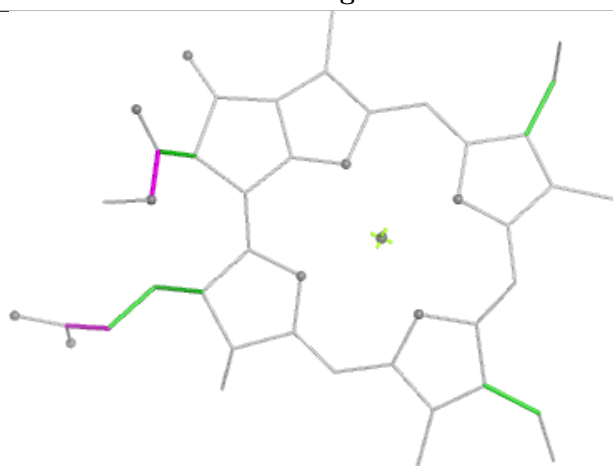
Ligand A1JWG YQ 502



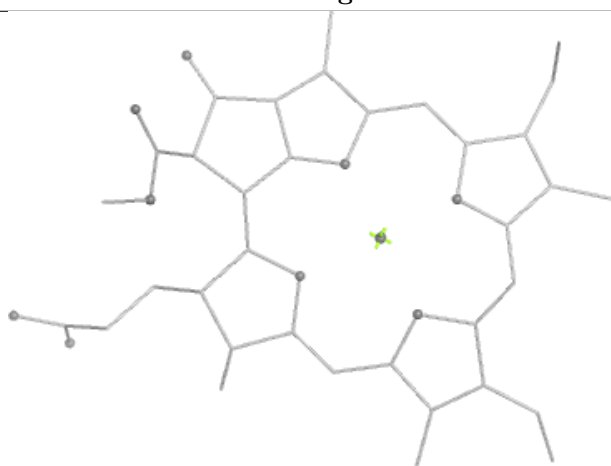
Bond lengths



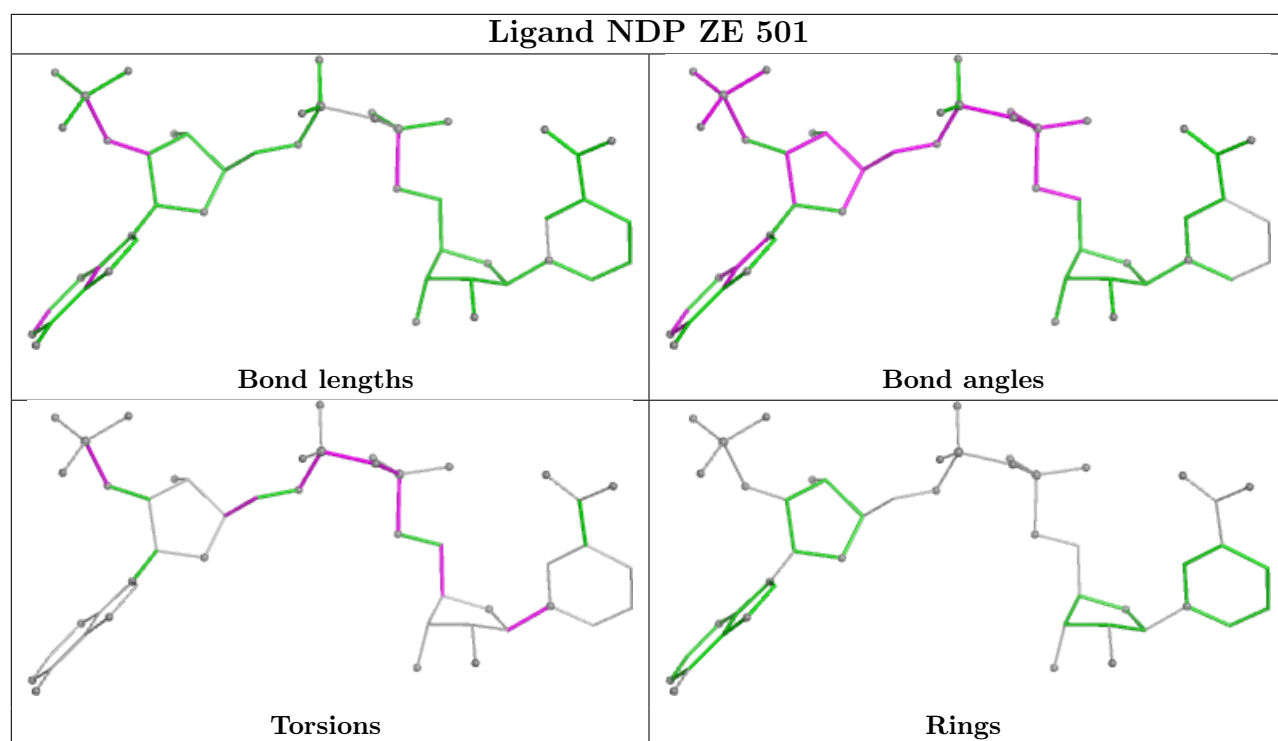
Bond angles



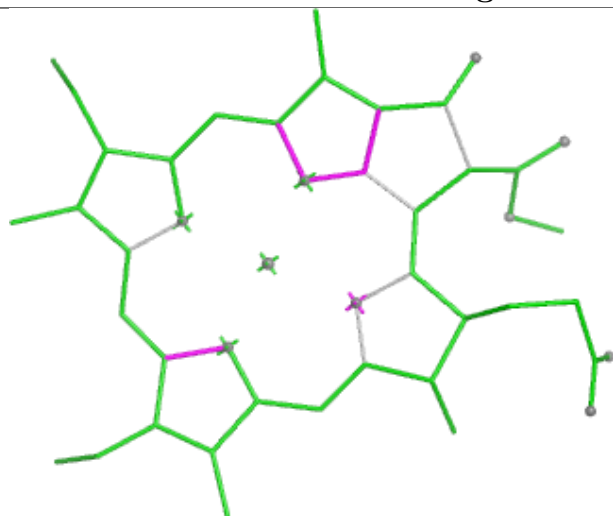
Torsions



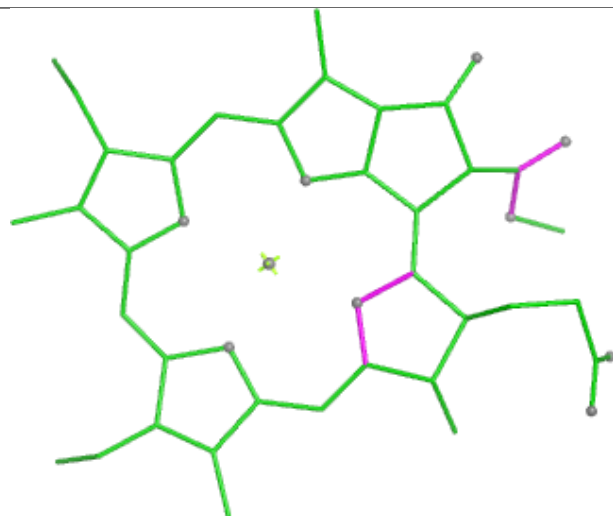
Rings



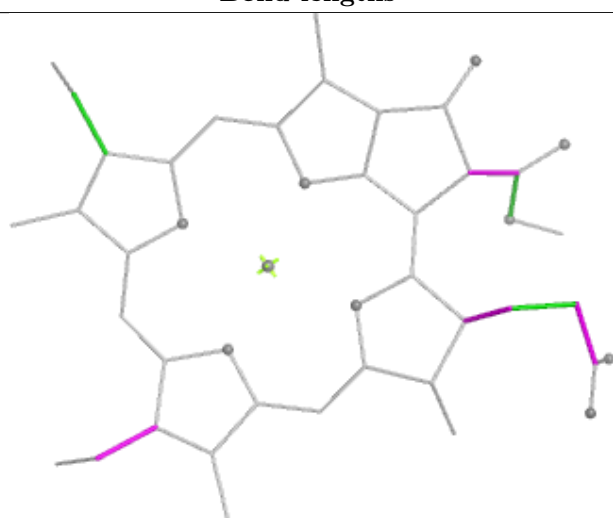
Ligand A1JWG ZR 502



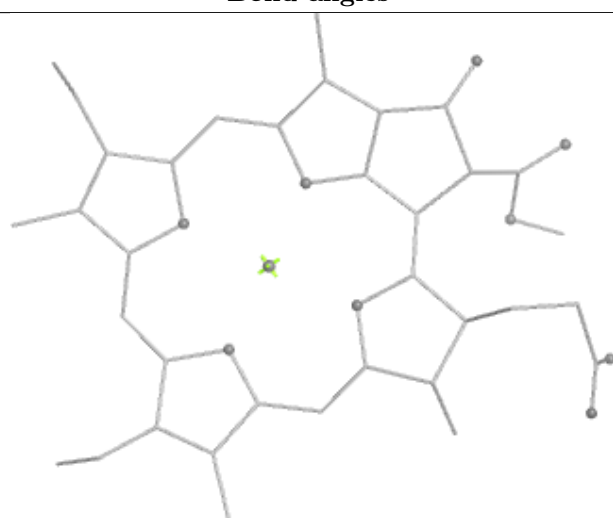
Bond lengths



Bond angles

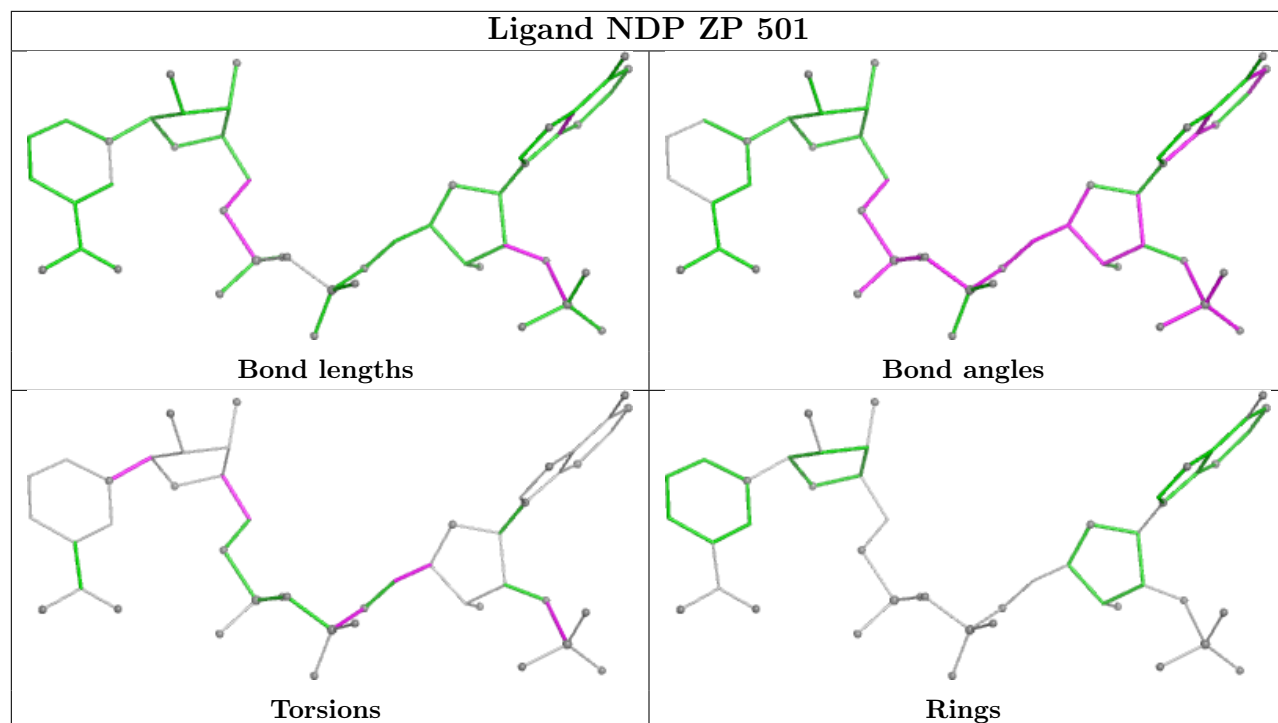


Torsions

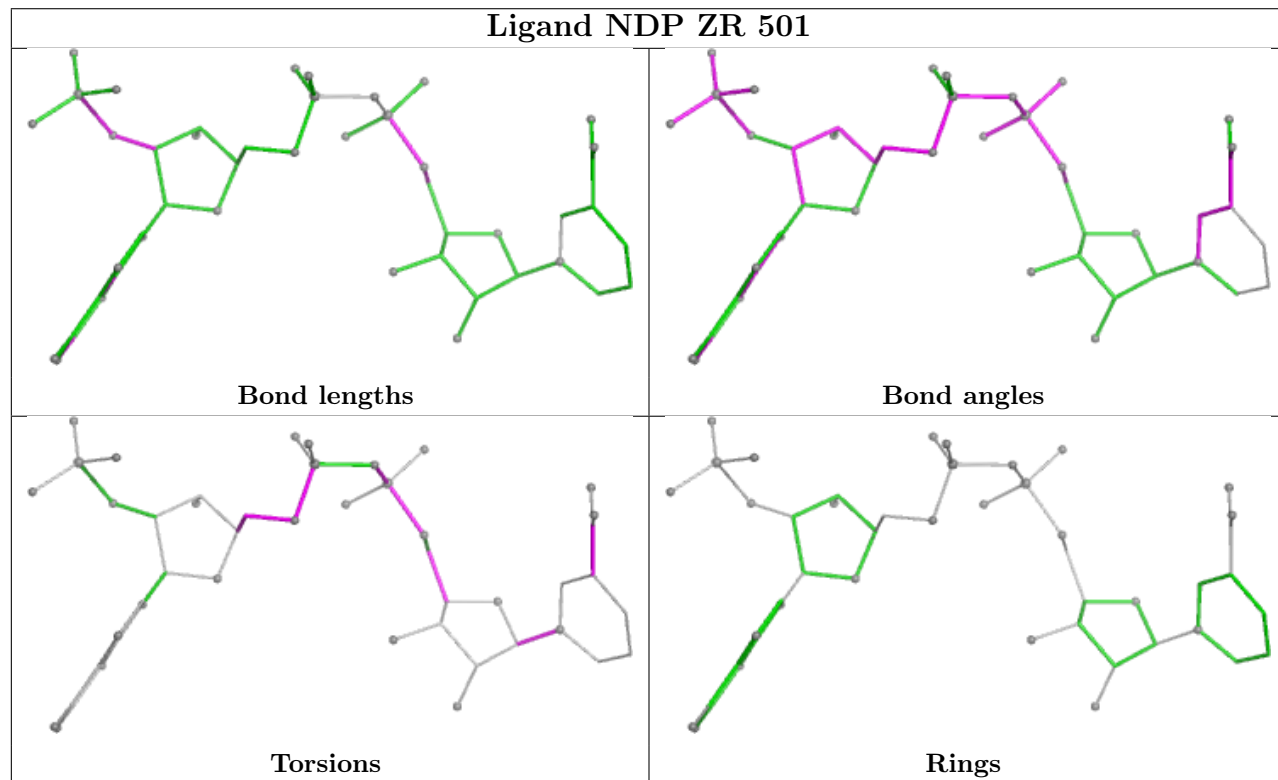


Rings

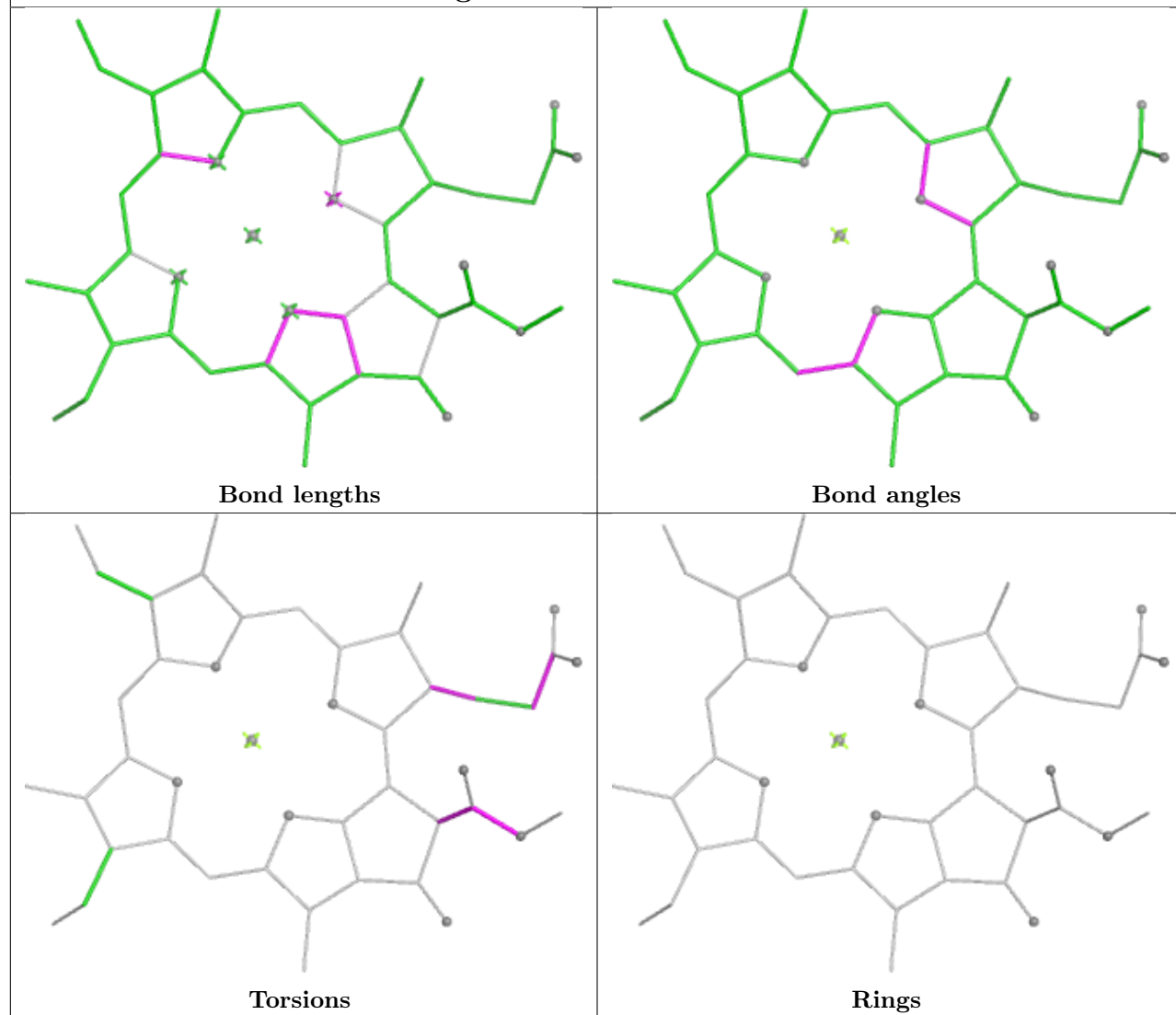
Ligand NDP ZP 501



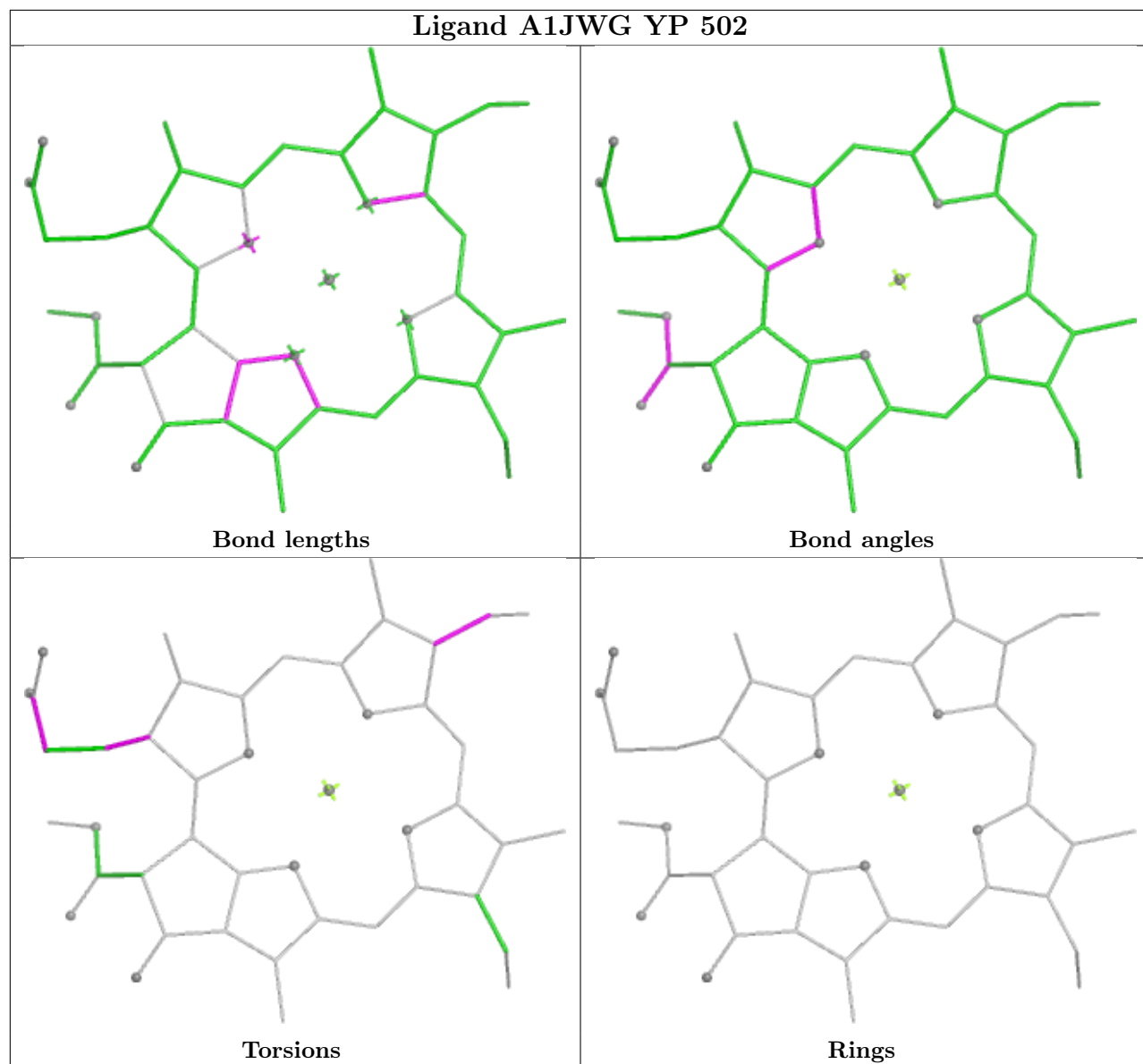
Ligand NDP ZR 501

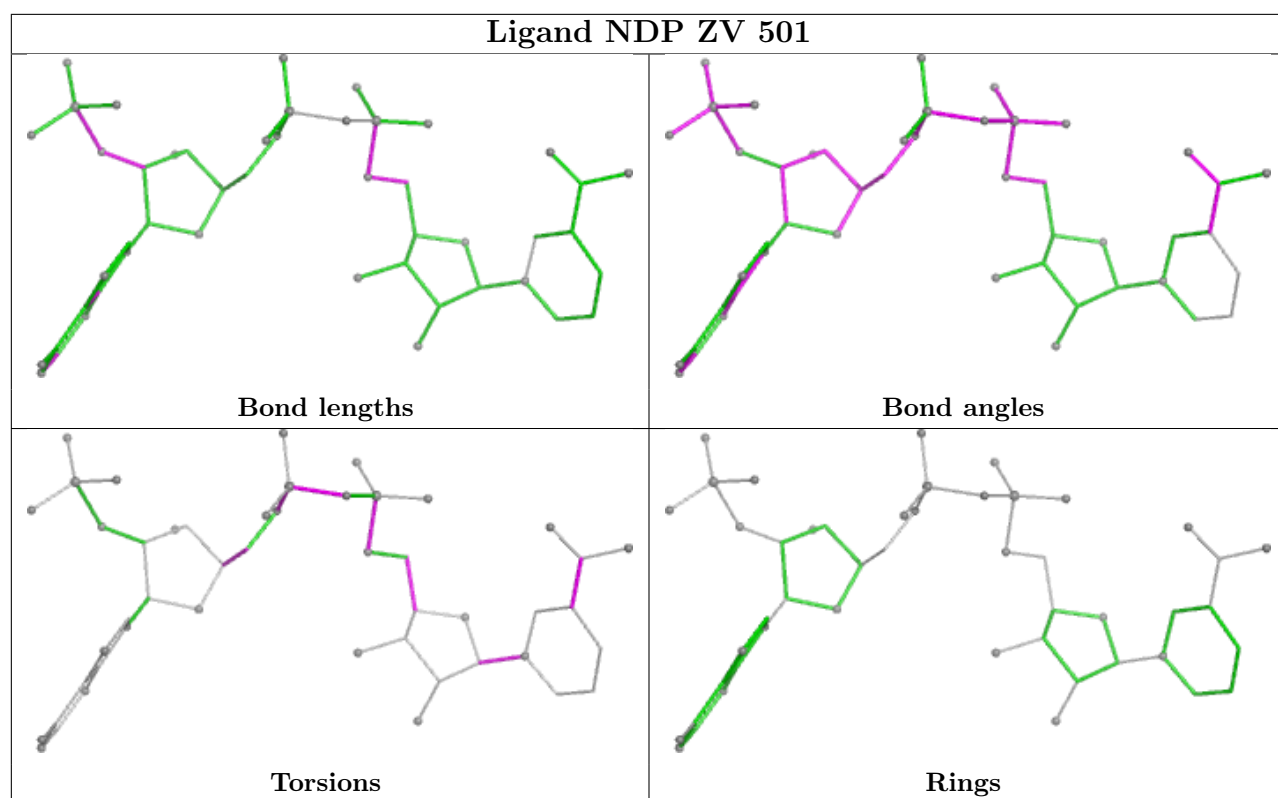


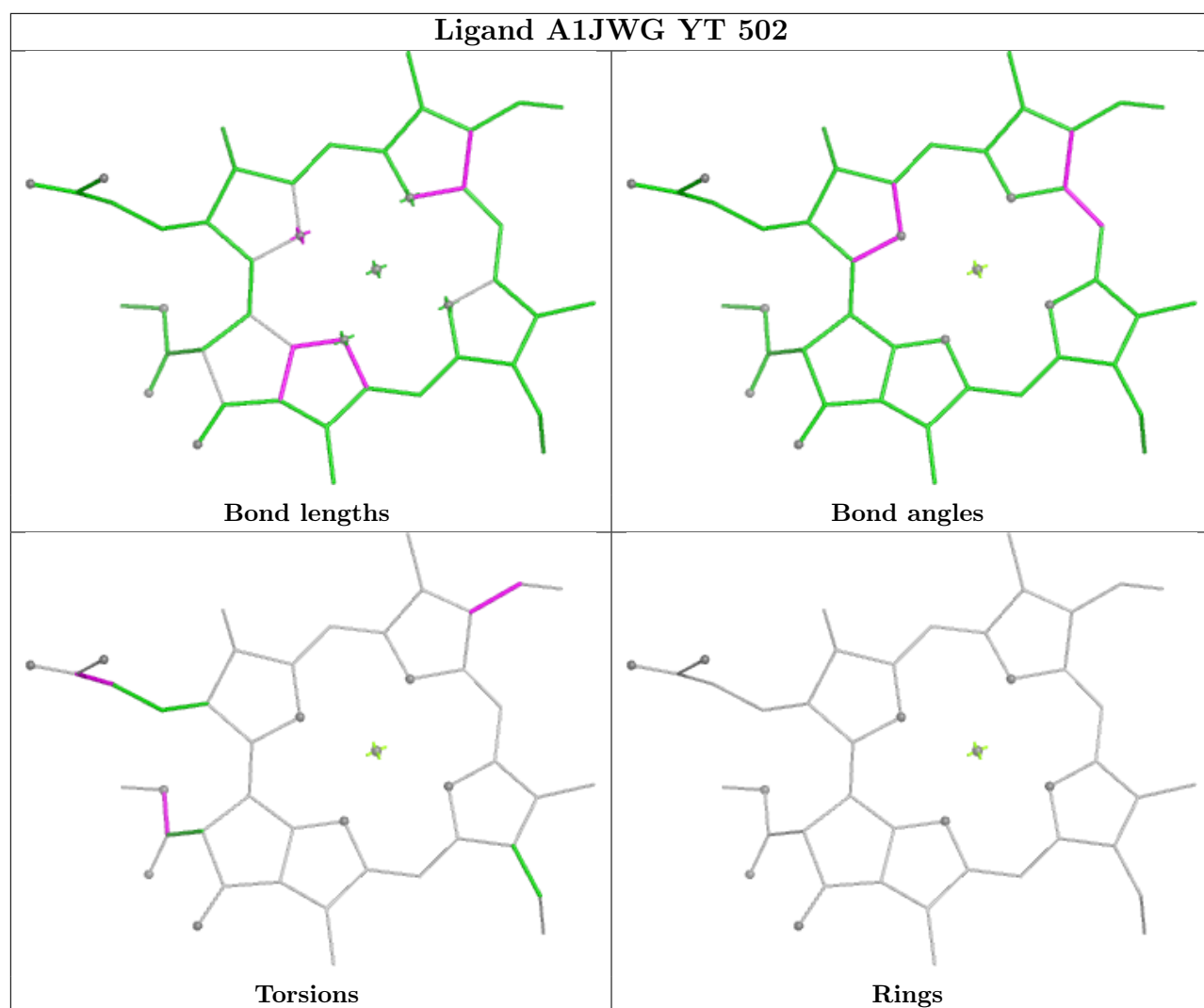
Ligand A1JWG ZB 502

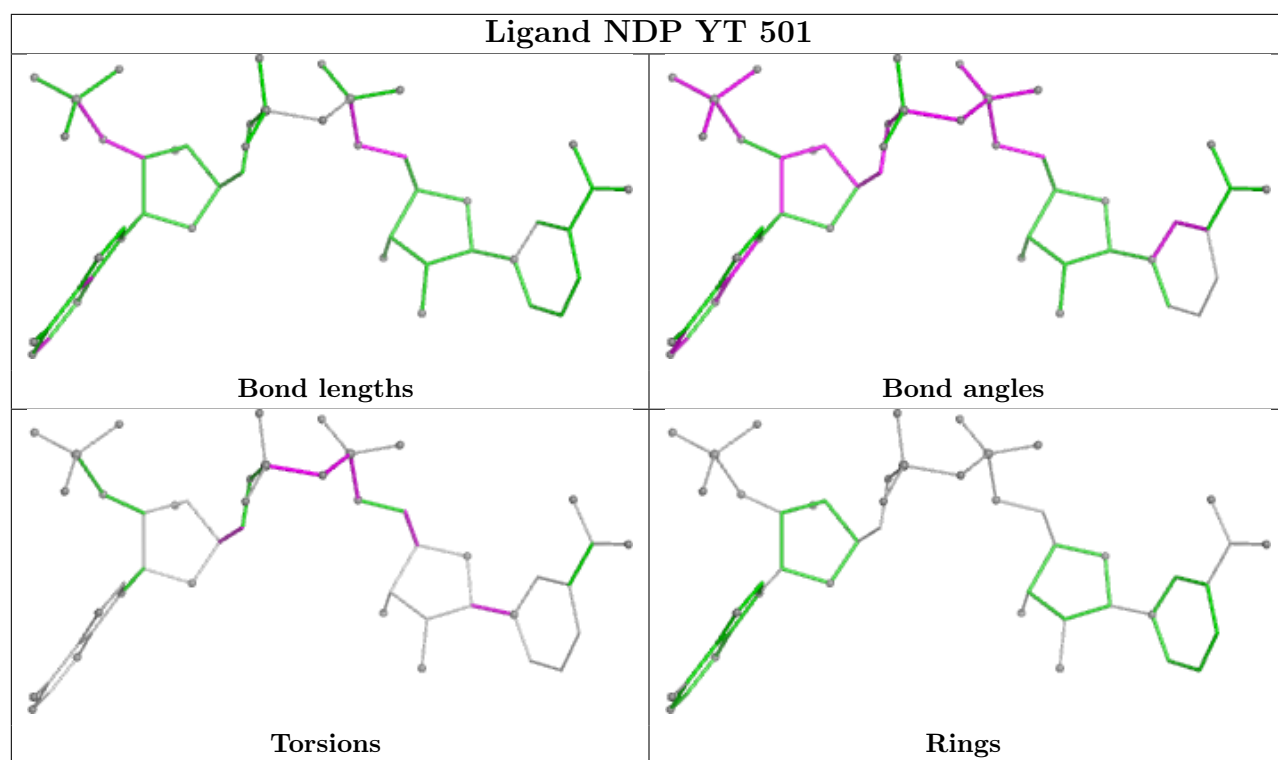


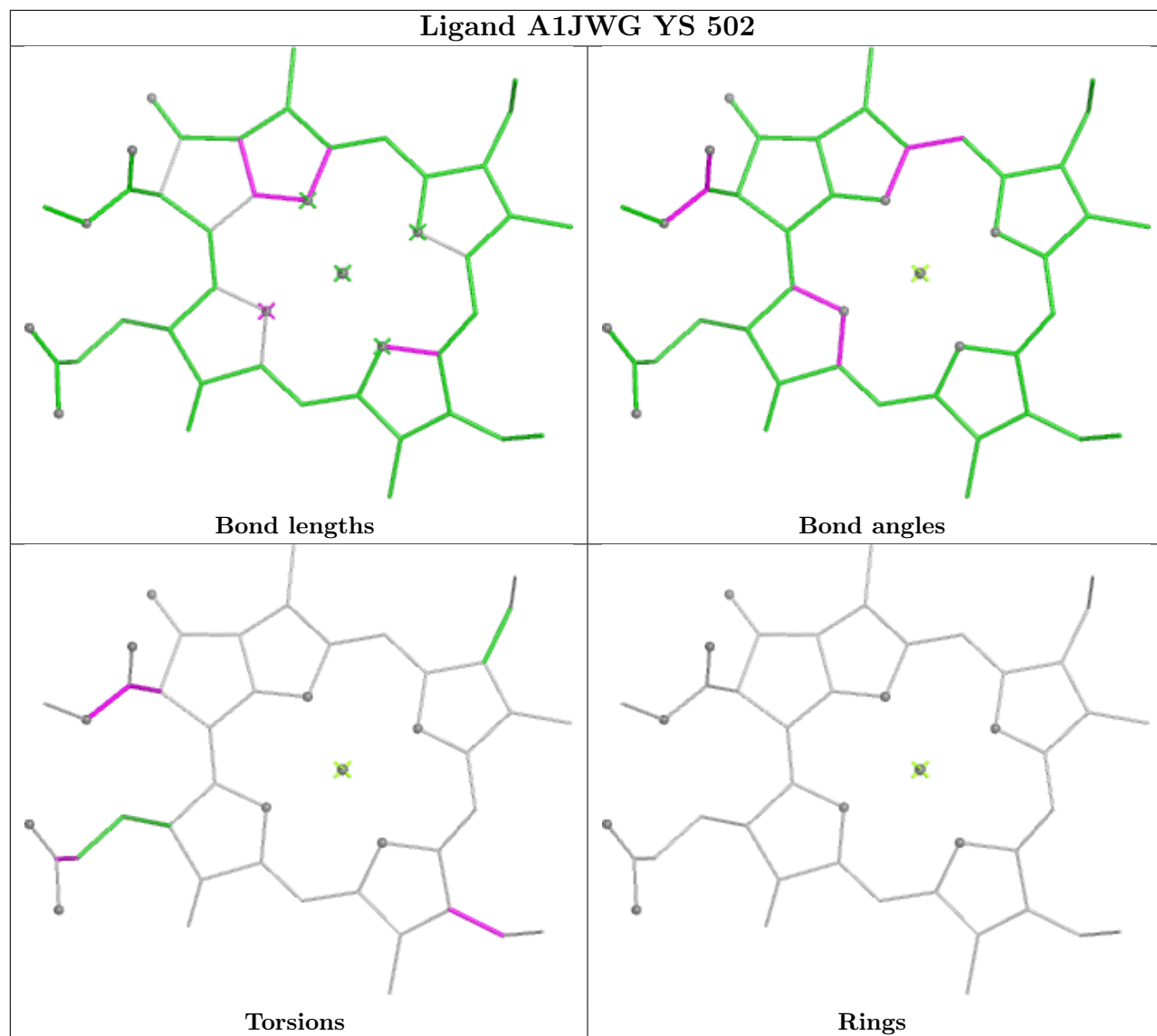
Ligand A1JWG YP 502



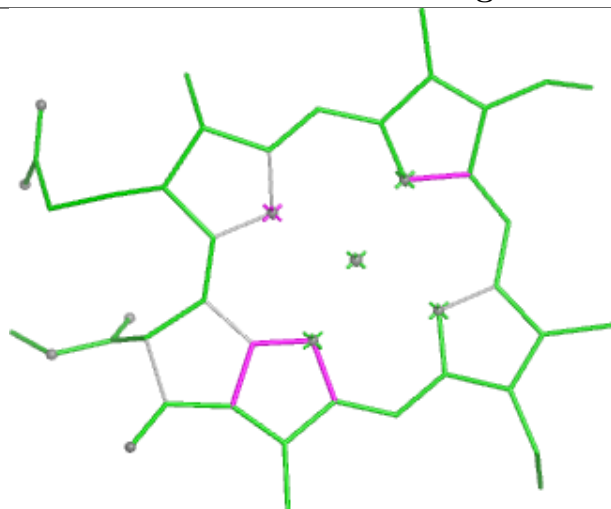




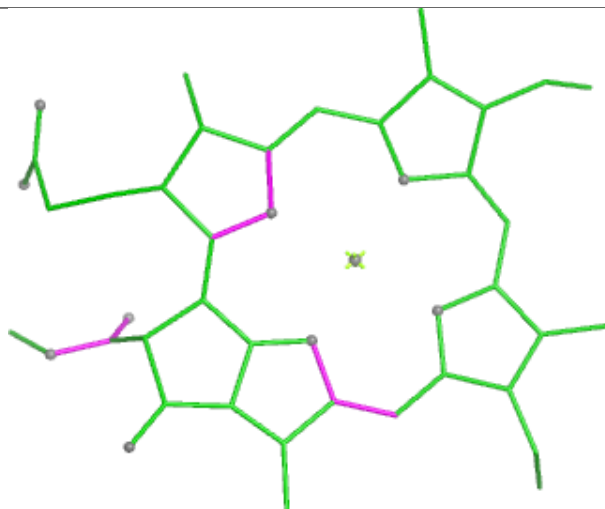




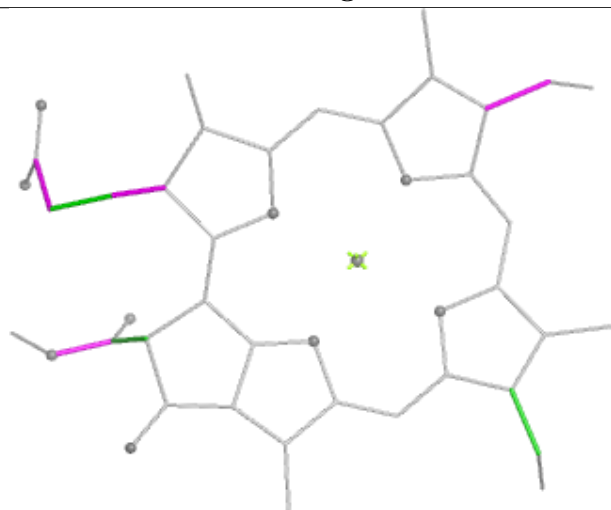
Ligand A1JWG ZA 502



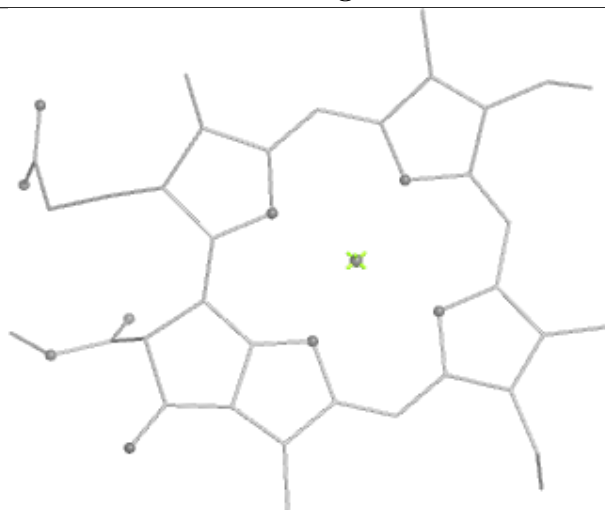
Bond lengths



Bond angles

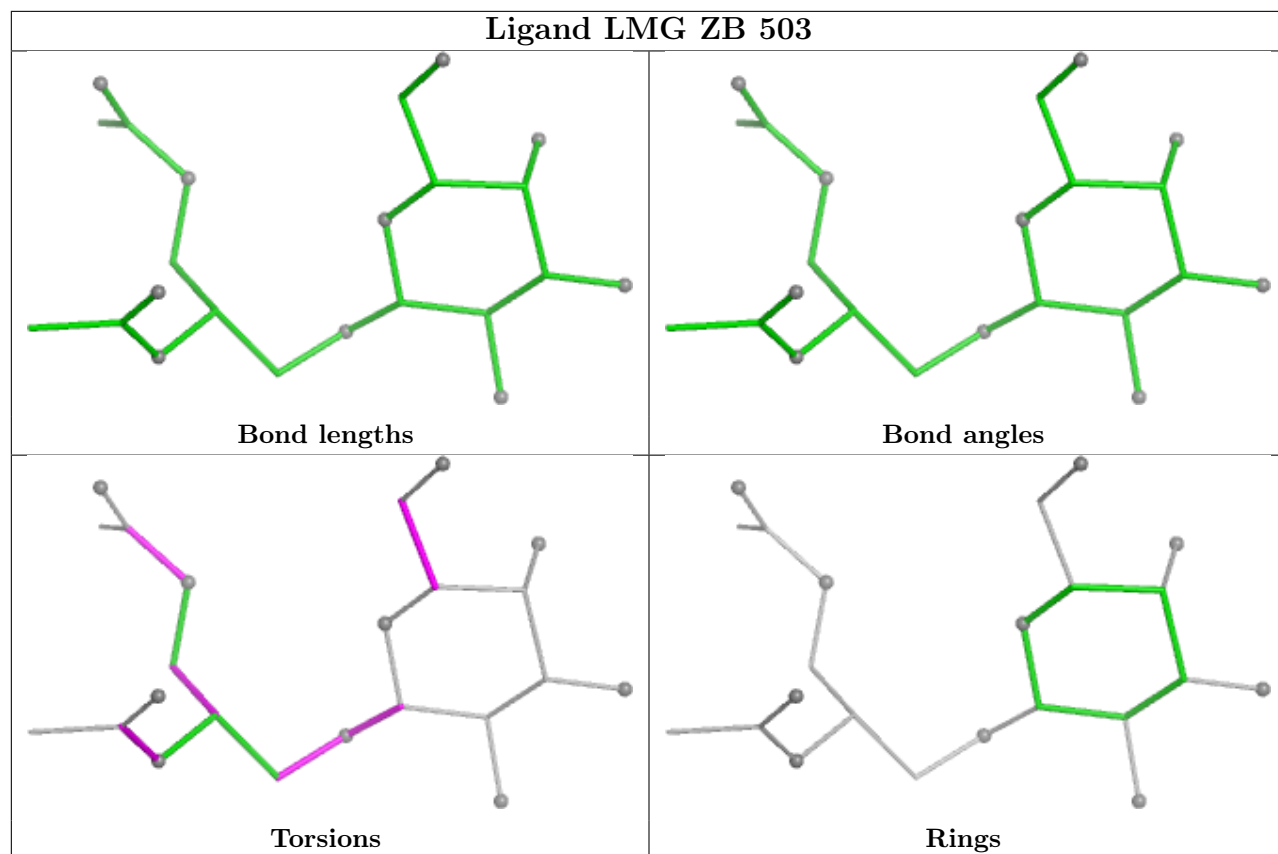


Torsions

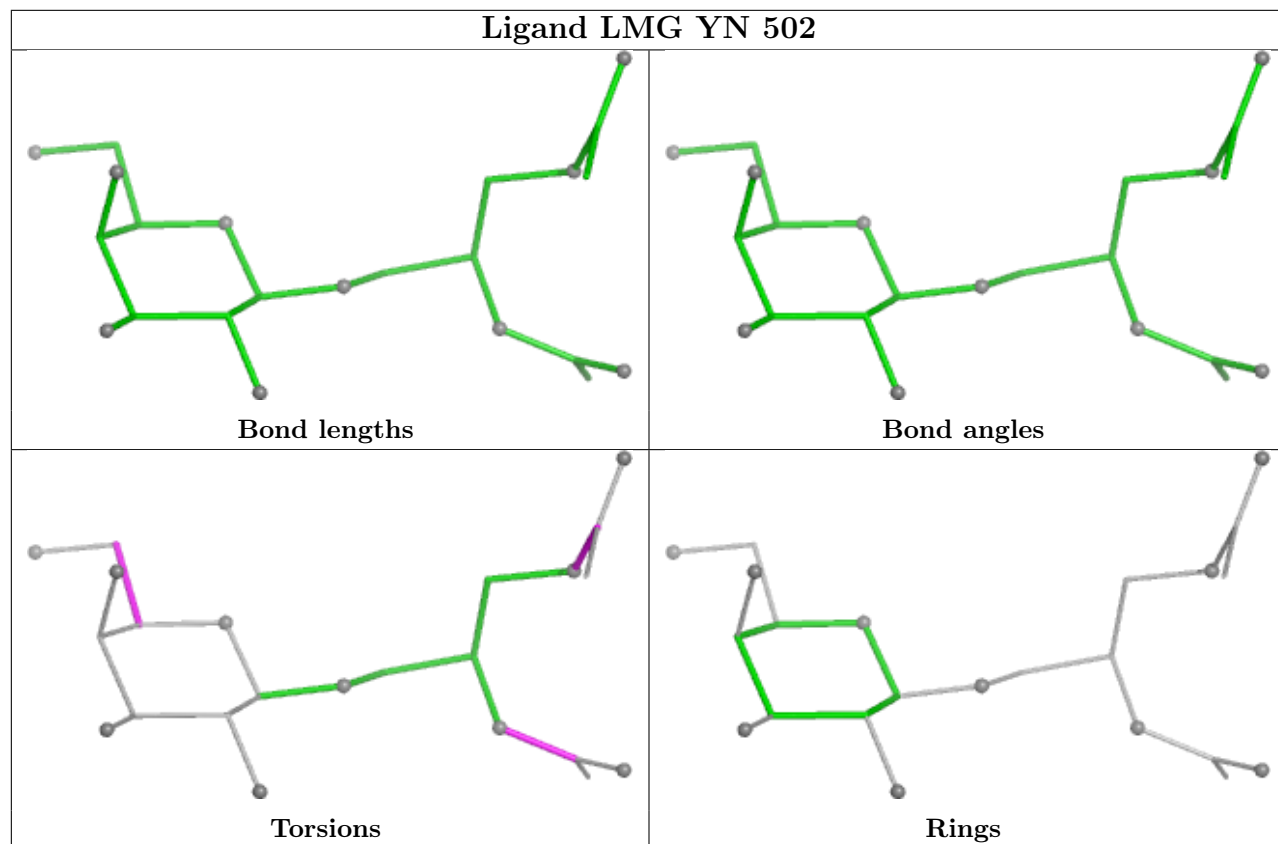


Rings

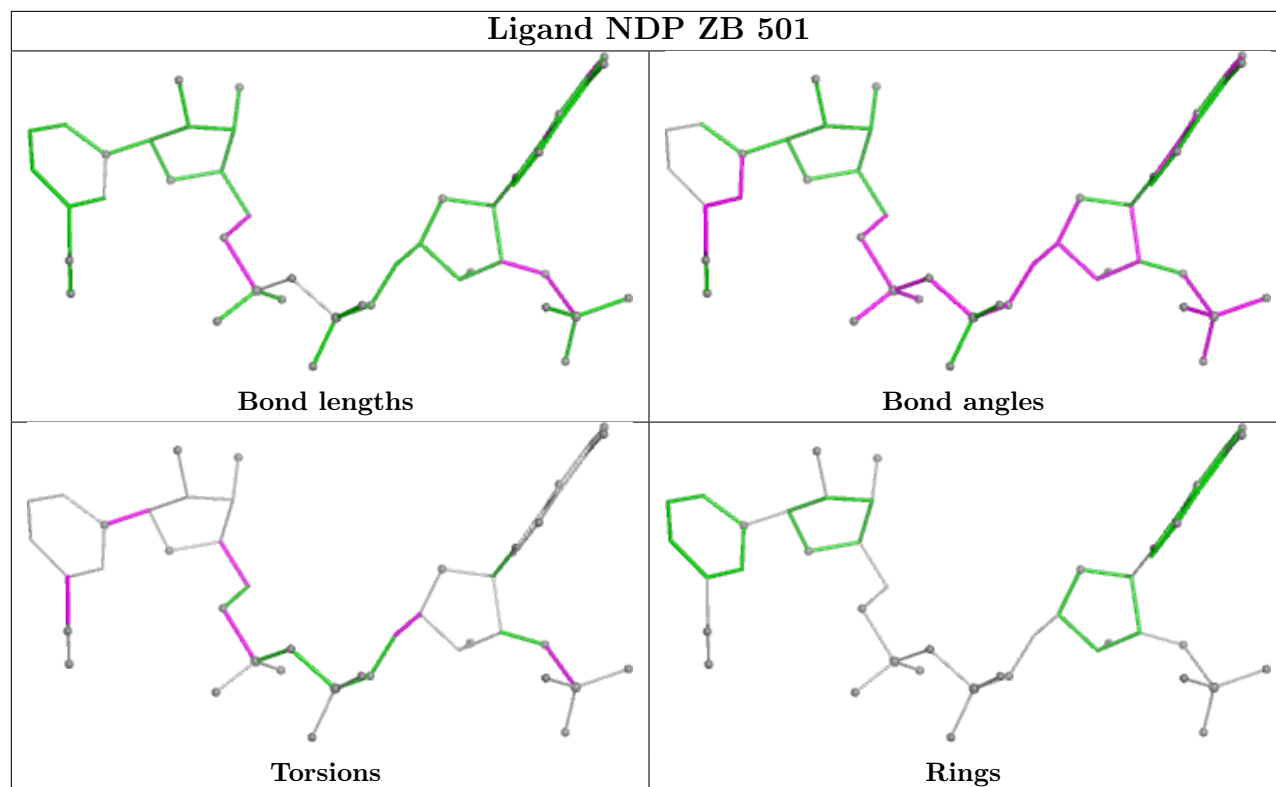
Ligand LMG ZB 503



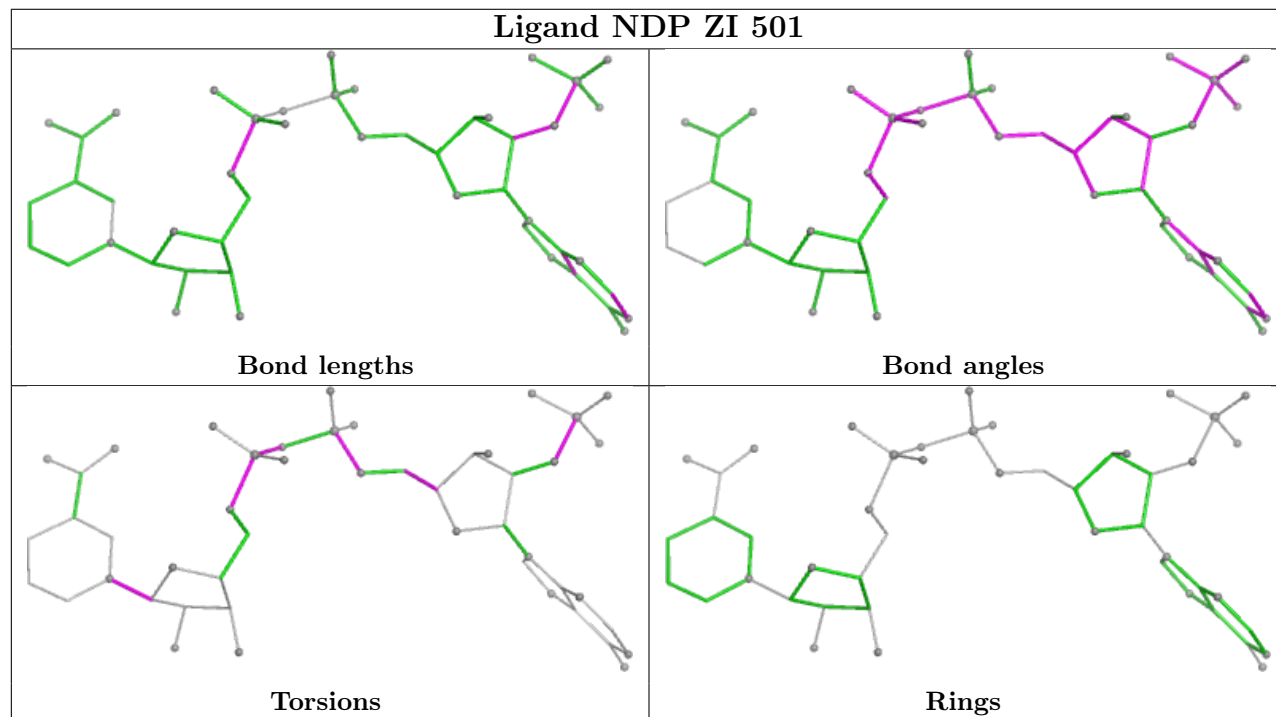
Ligand LMG YN 502



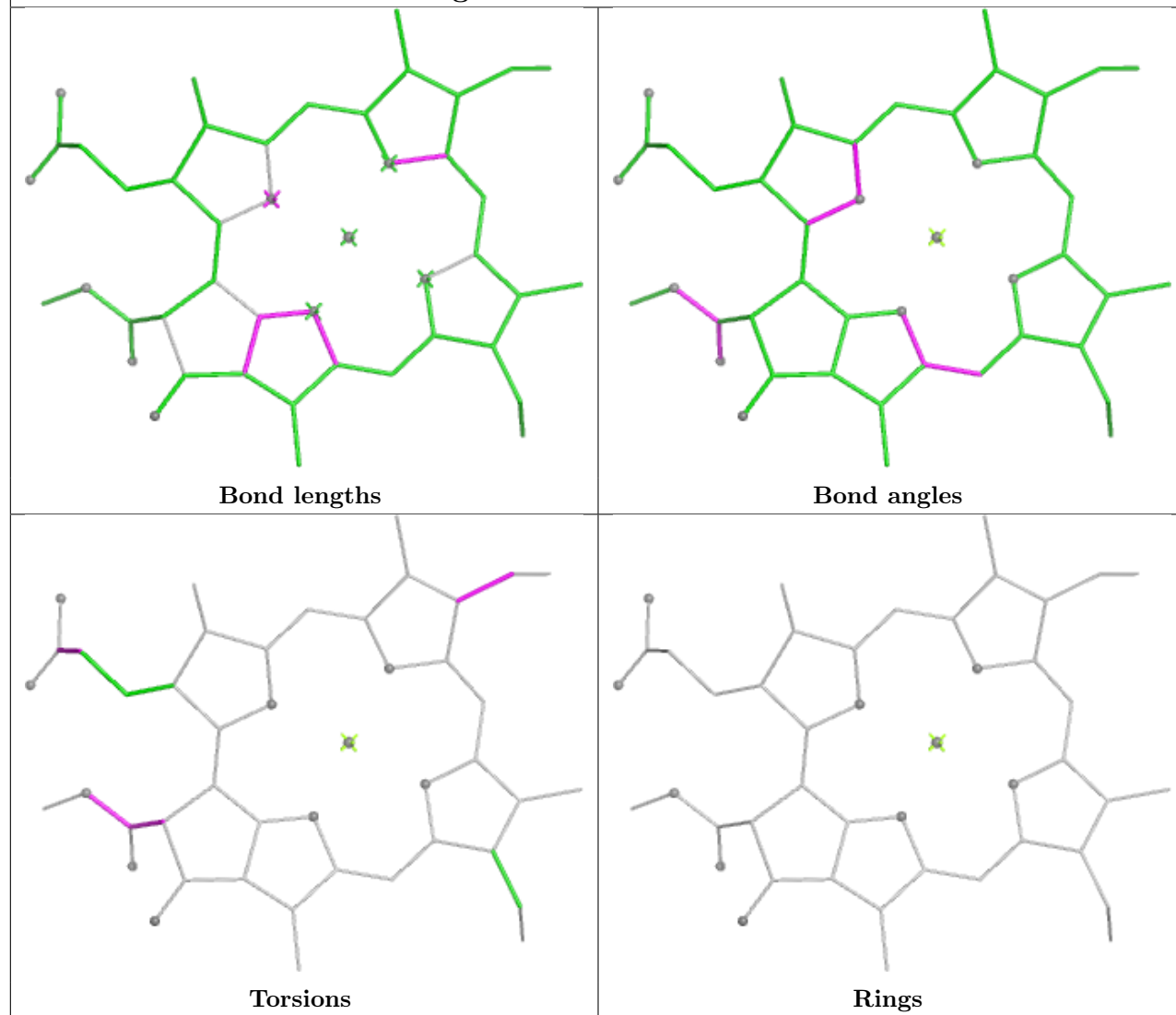
Ligand NDP ZB 501



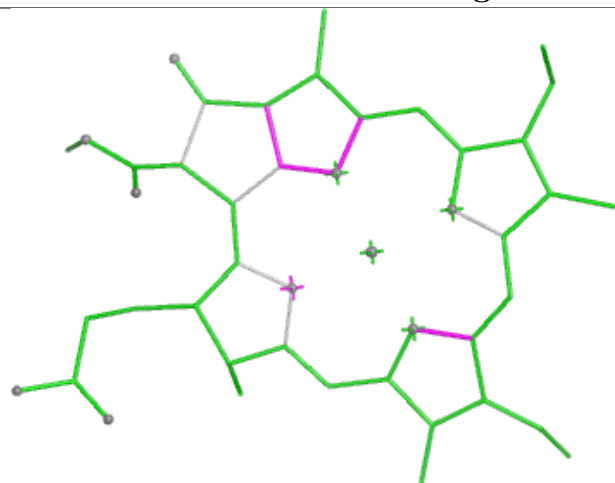
Ligand NDP ZI 501



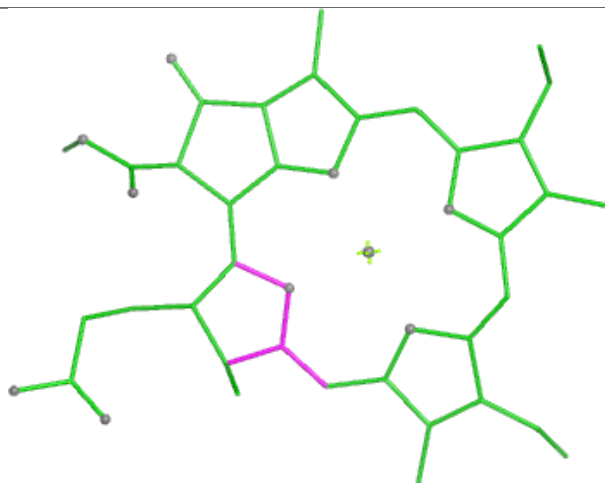
Ligand A1JWG YN 503



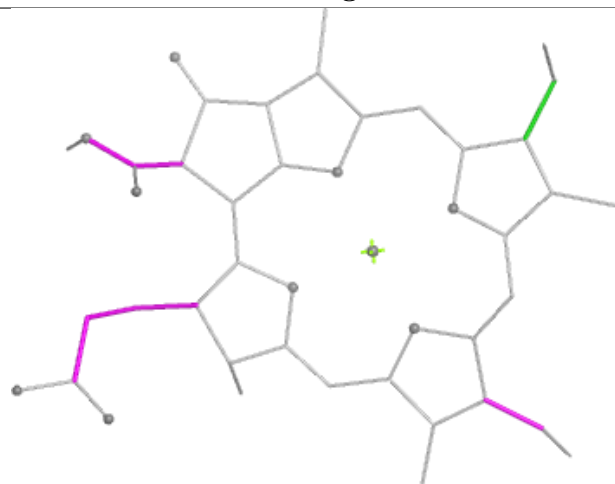
Ligand A1JWG ZW 502



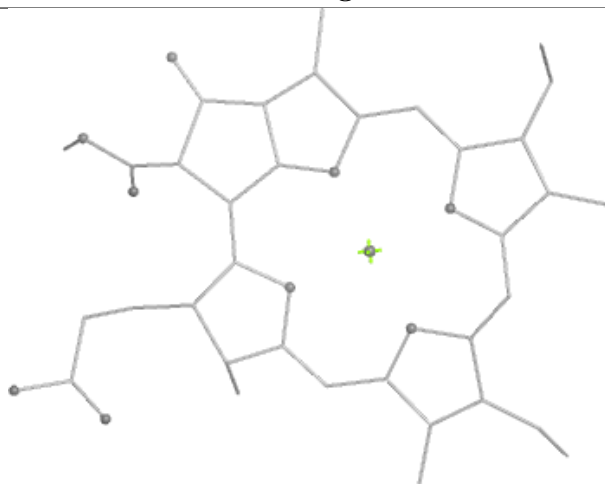
Bond lengths



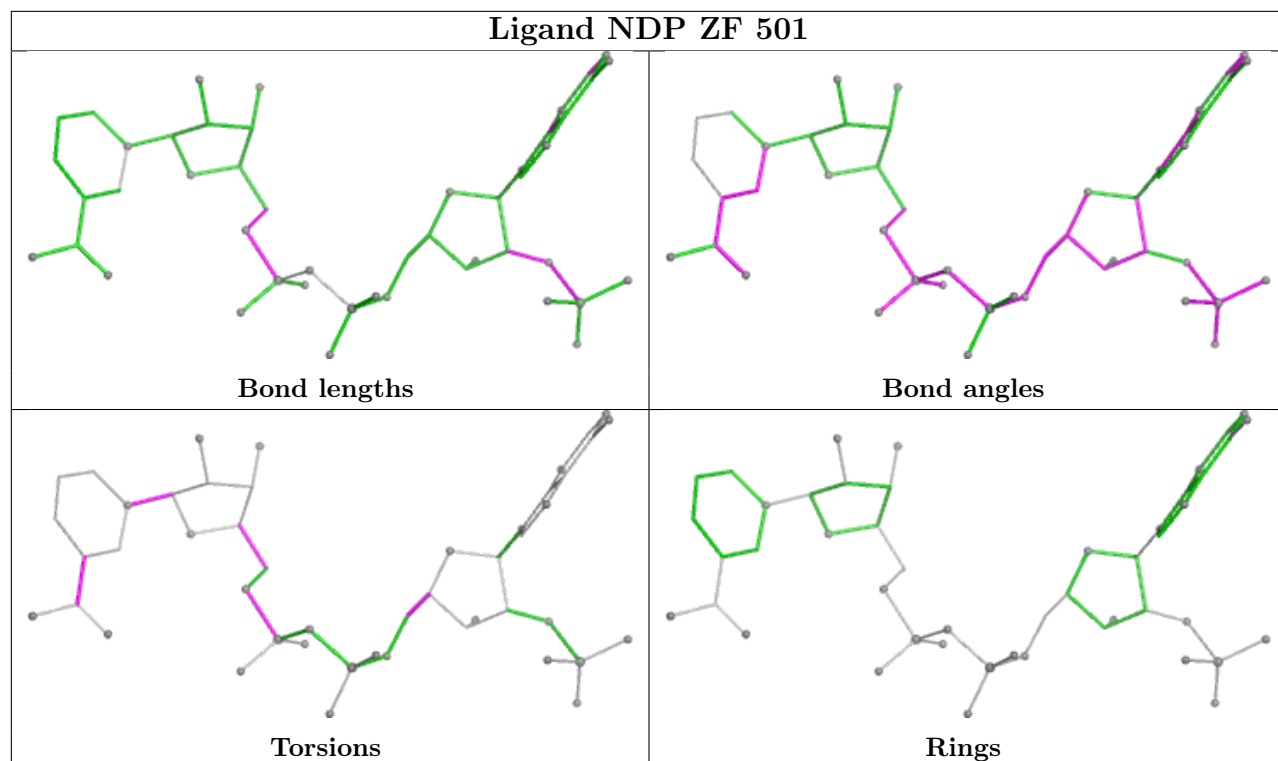
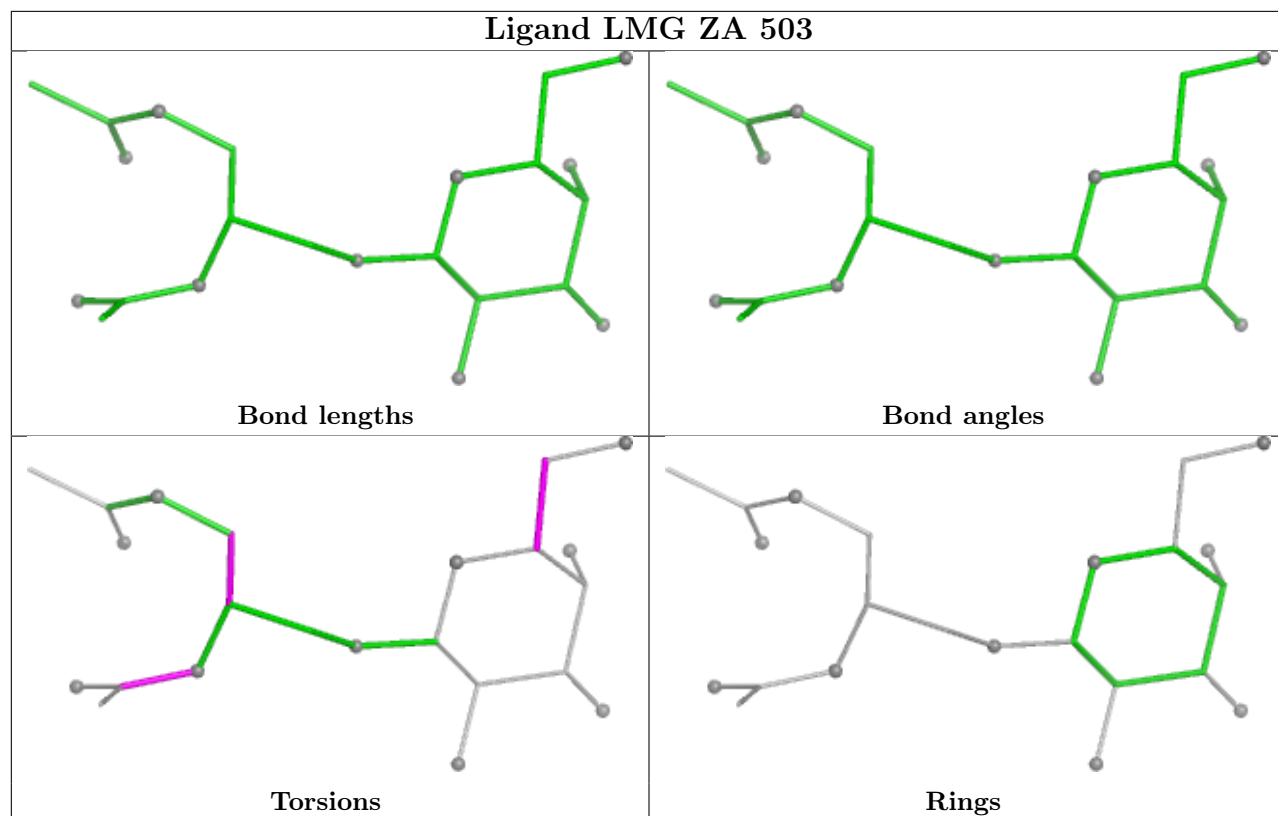
Bond angles

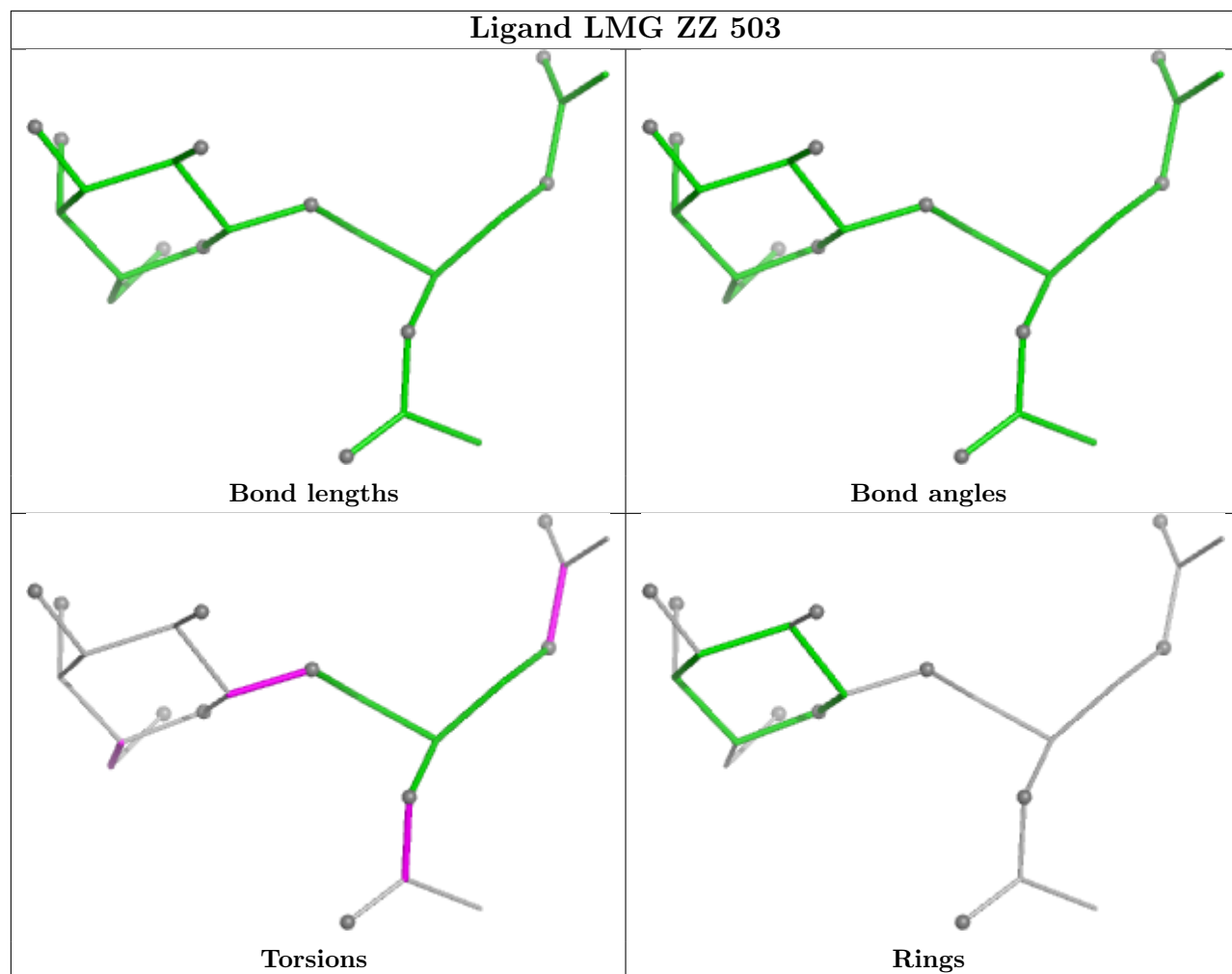


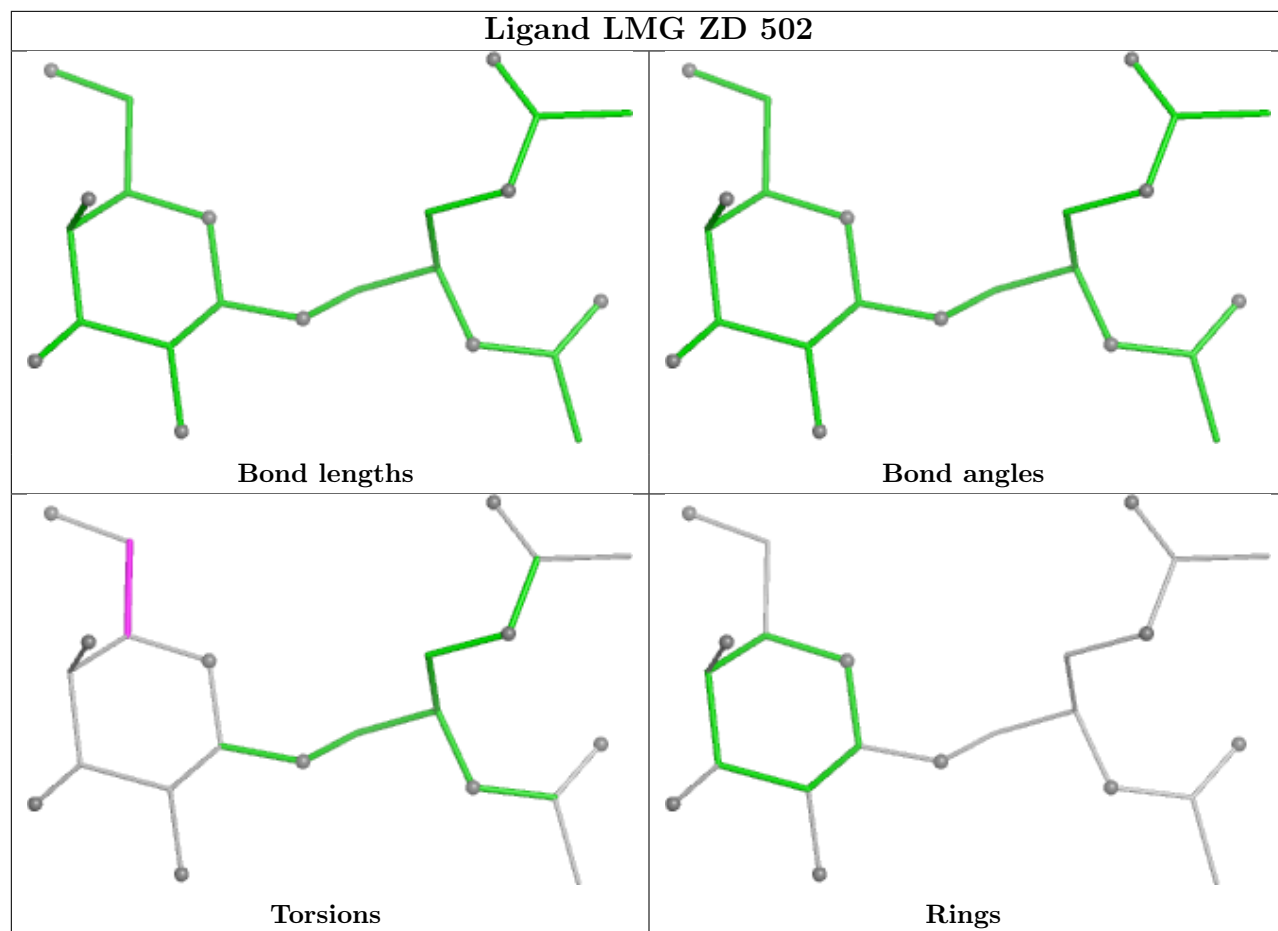
Torsions

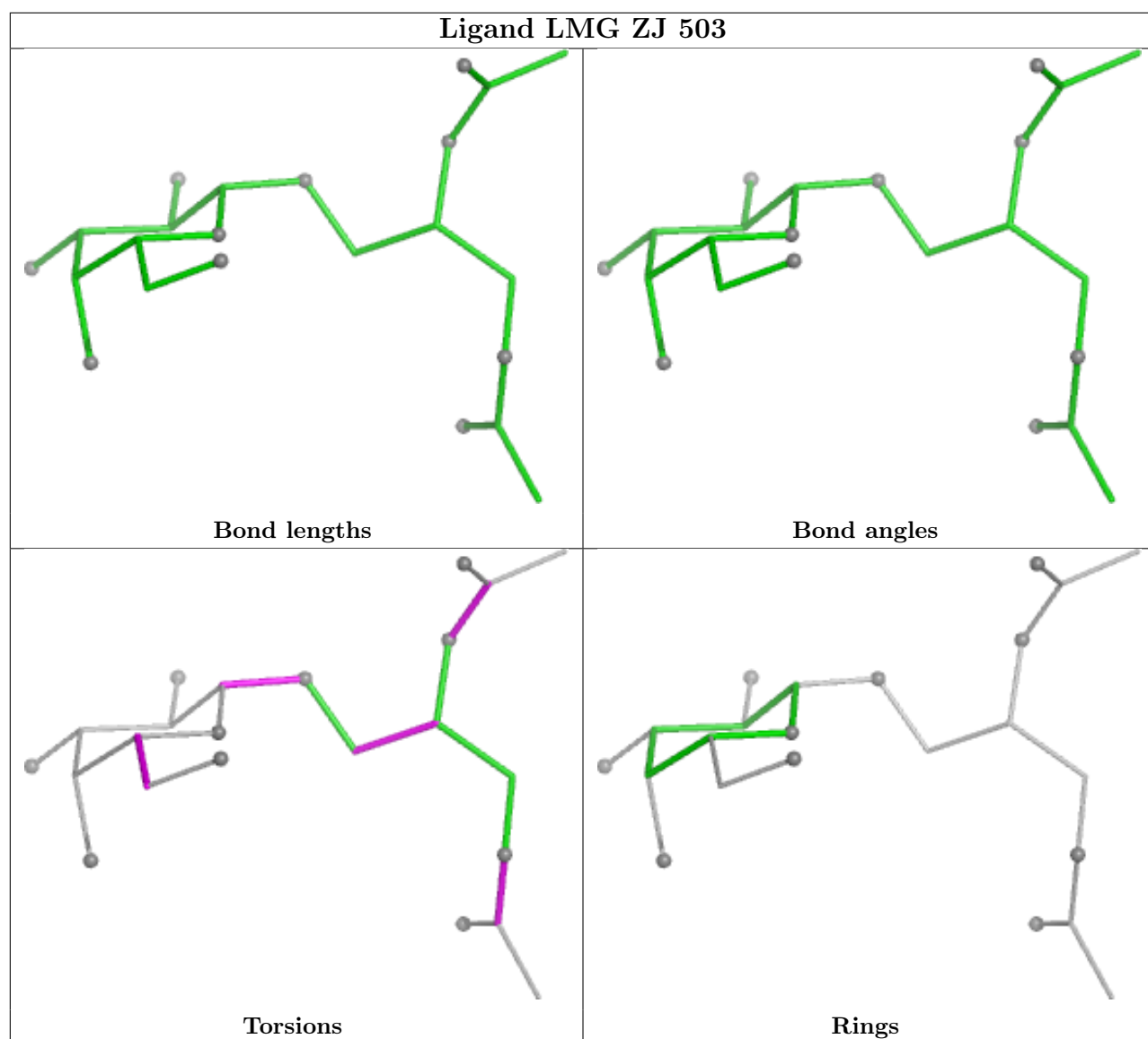


Rings

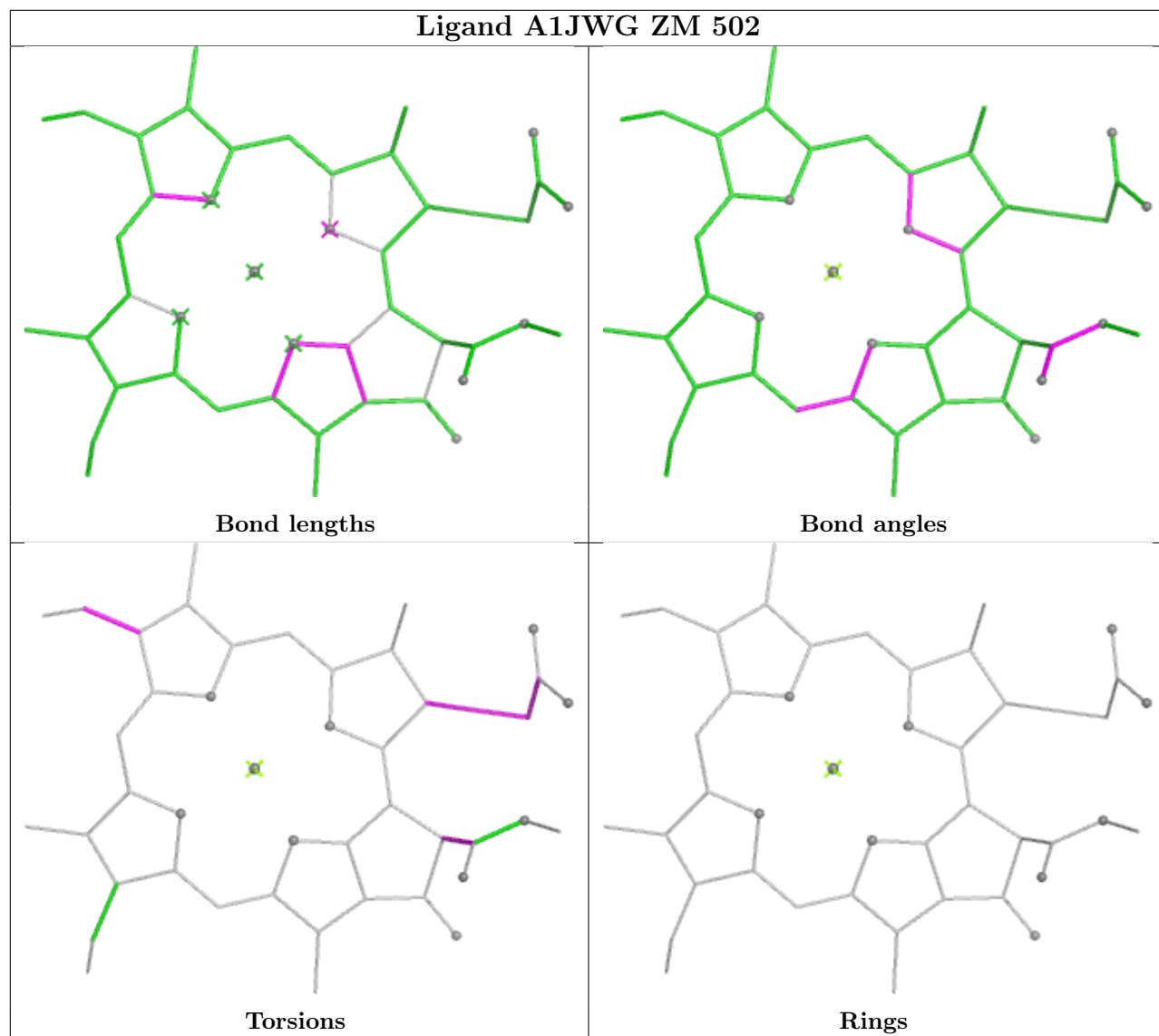




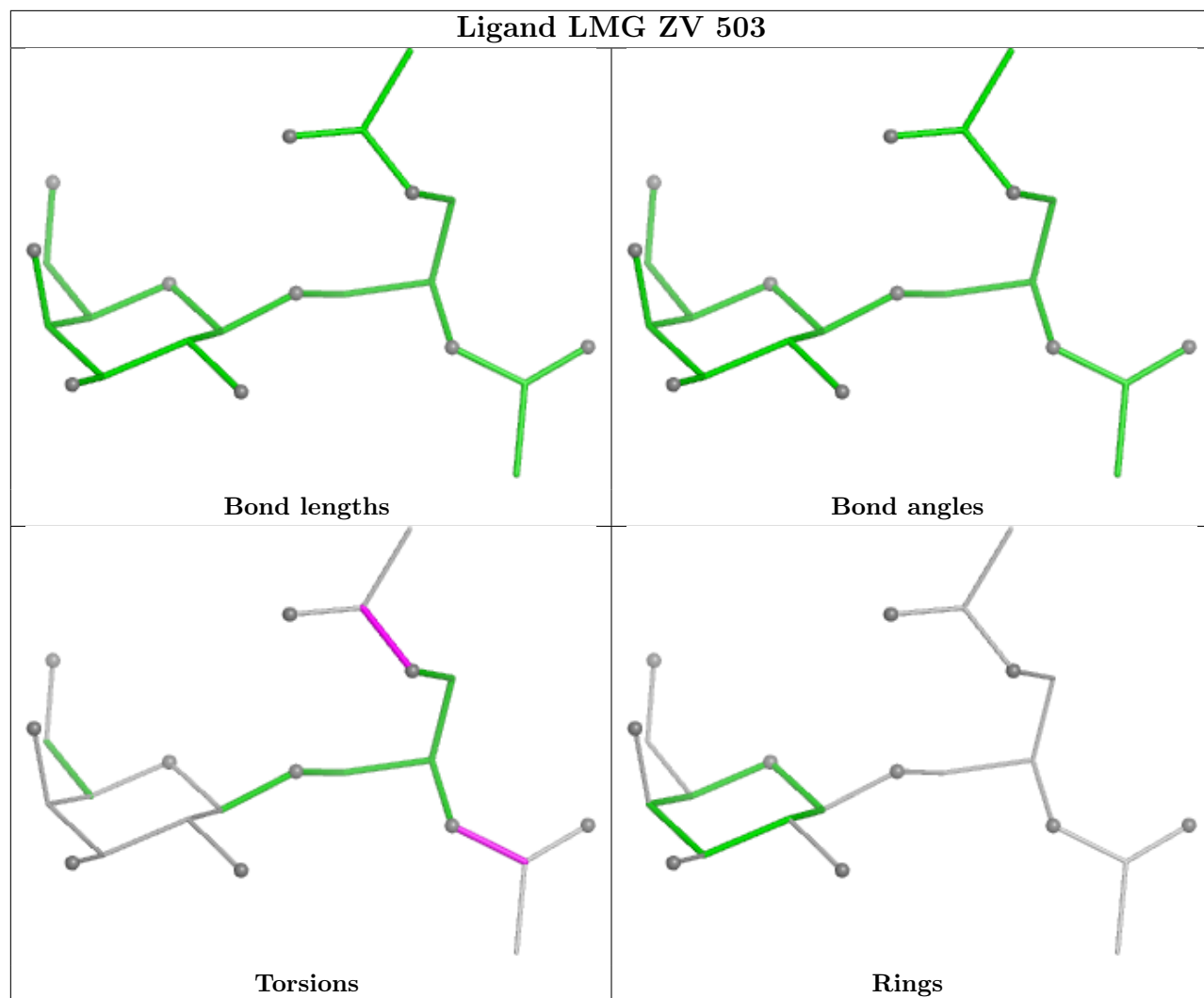




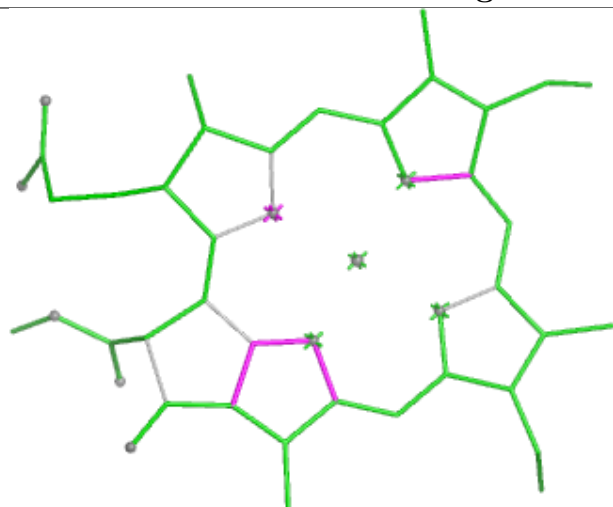
Ligand A1JWG ZM 502



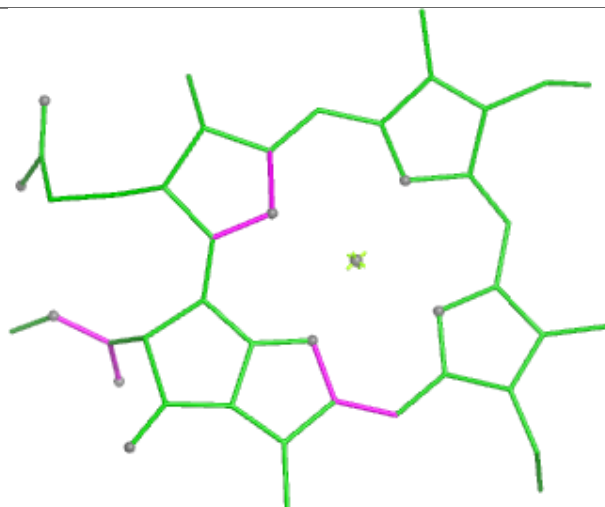
Ligand LMG ZV 503



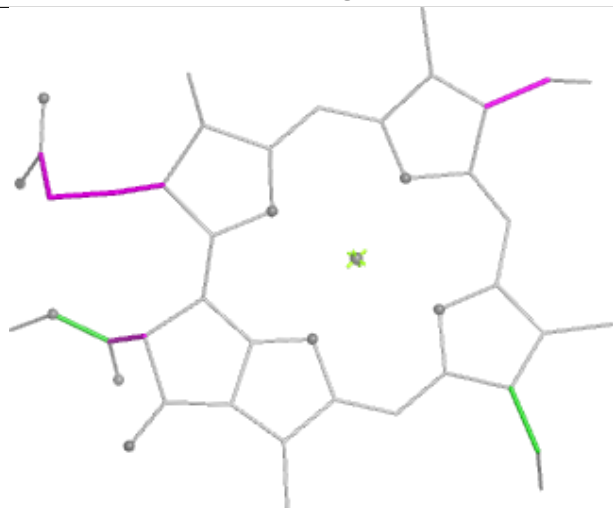
Ligand A1JWG ZD 503



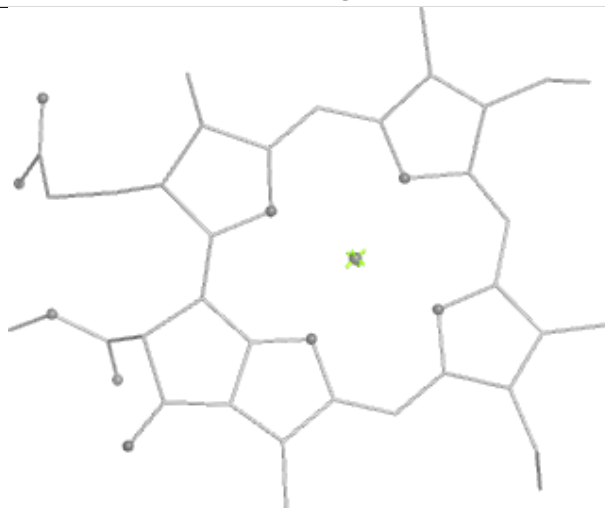
Bond lengths



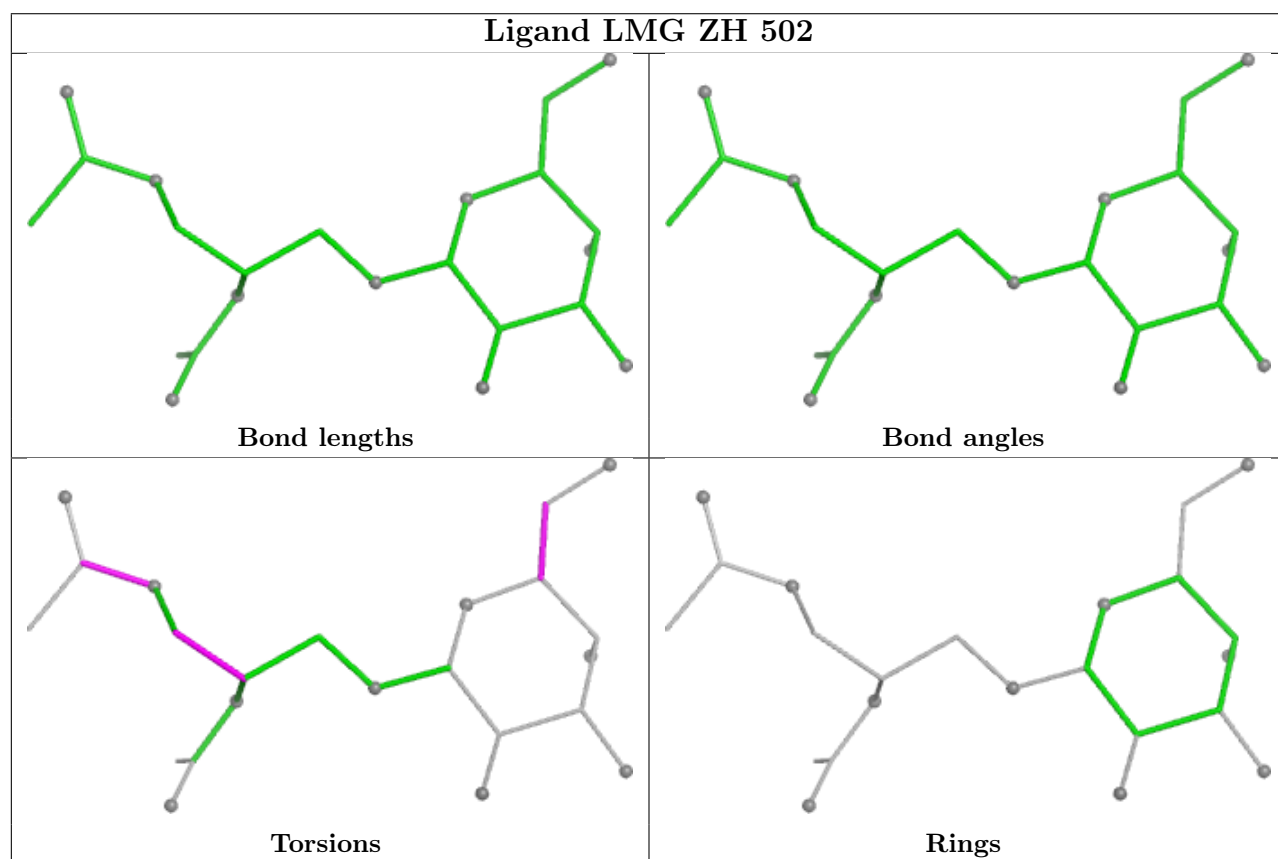
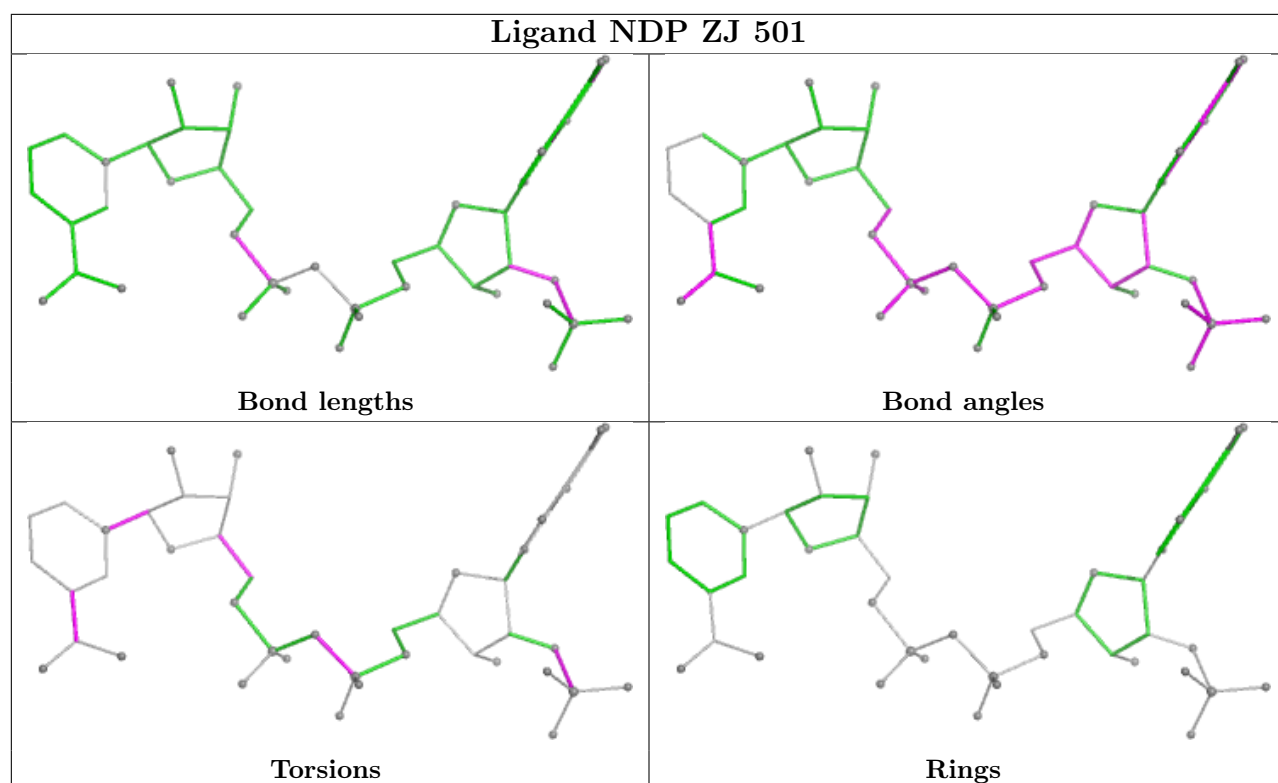
Bond angles



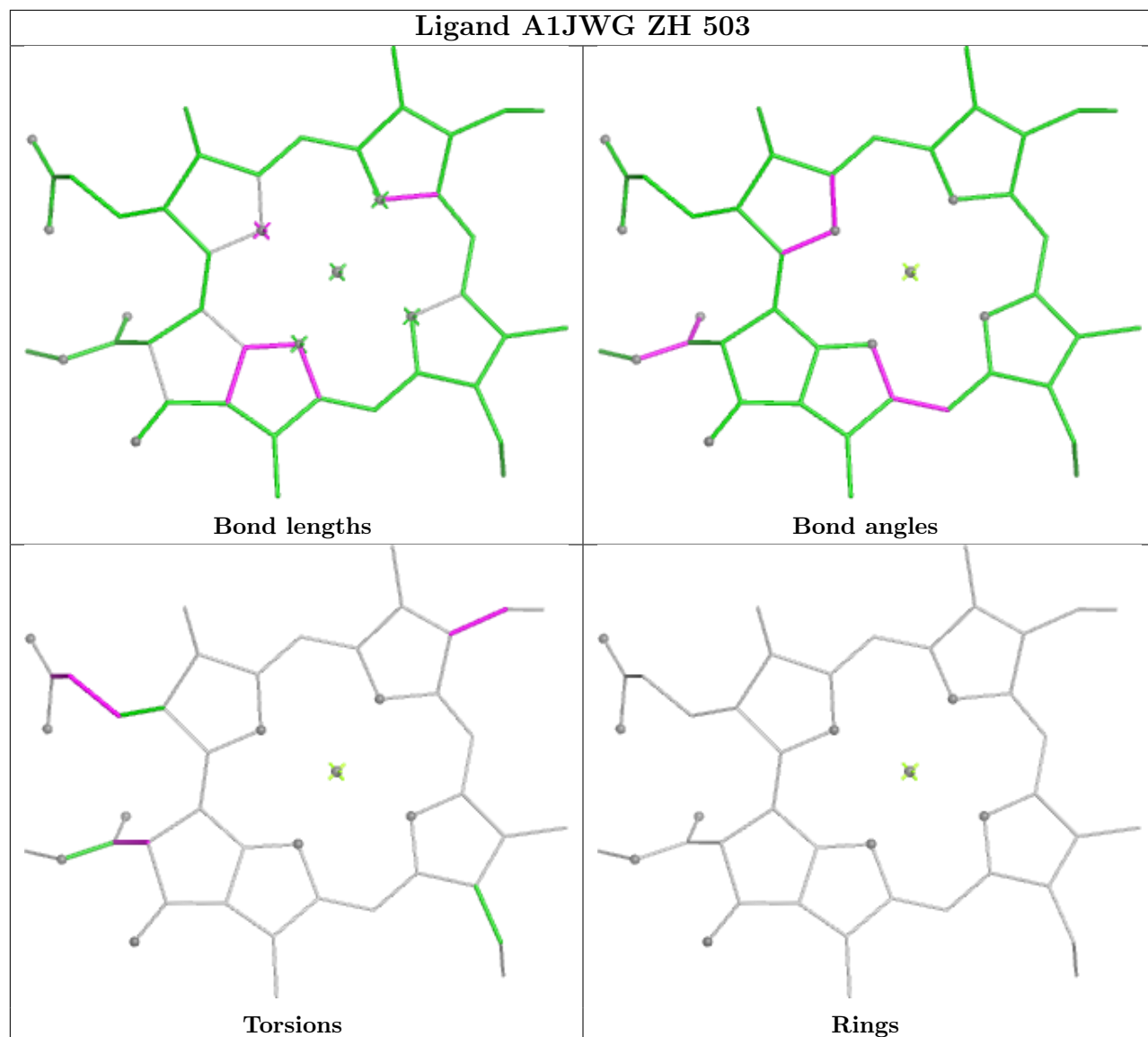
Torsions



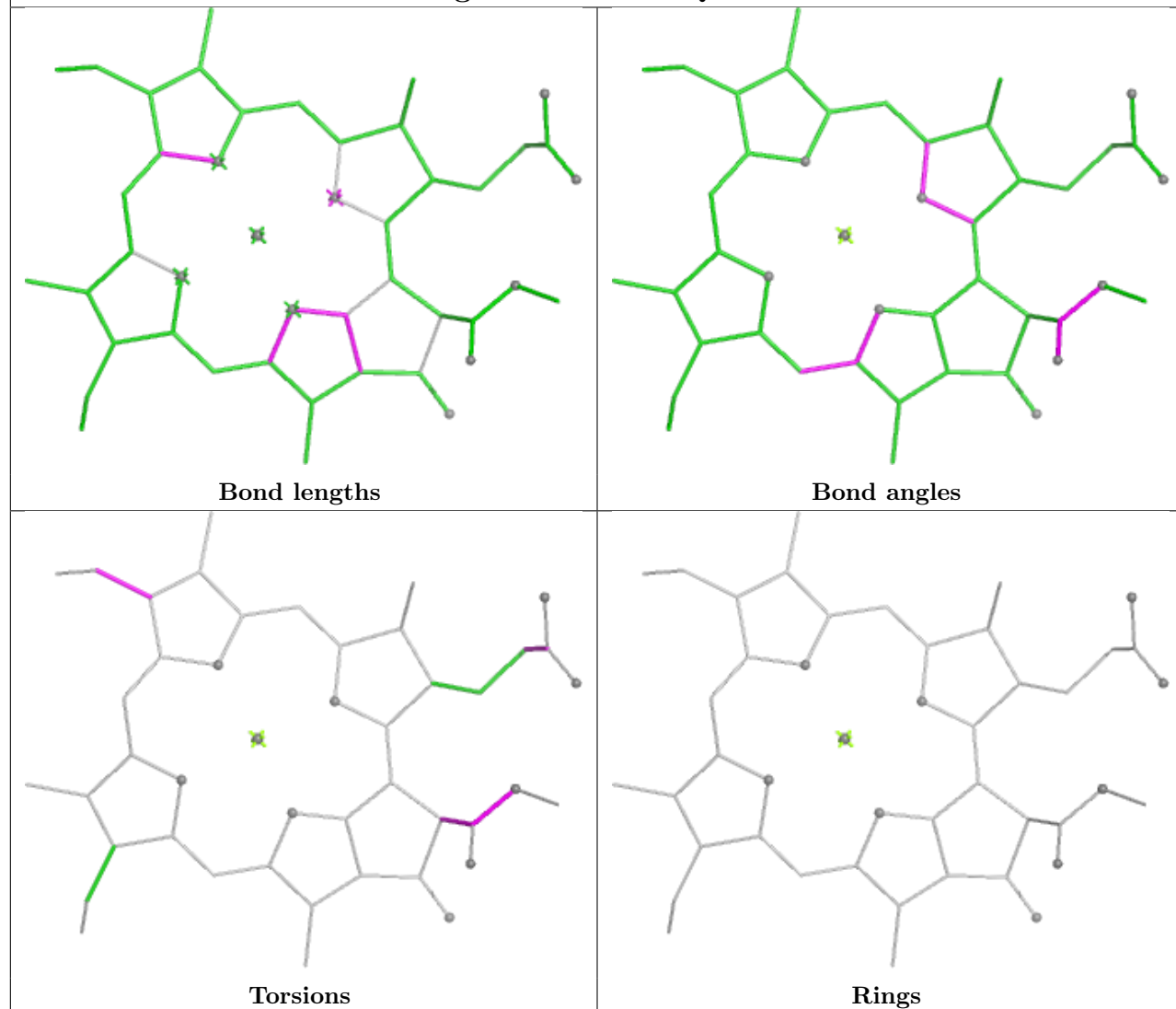
Rings



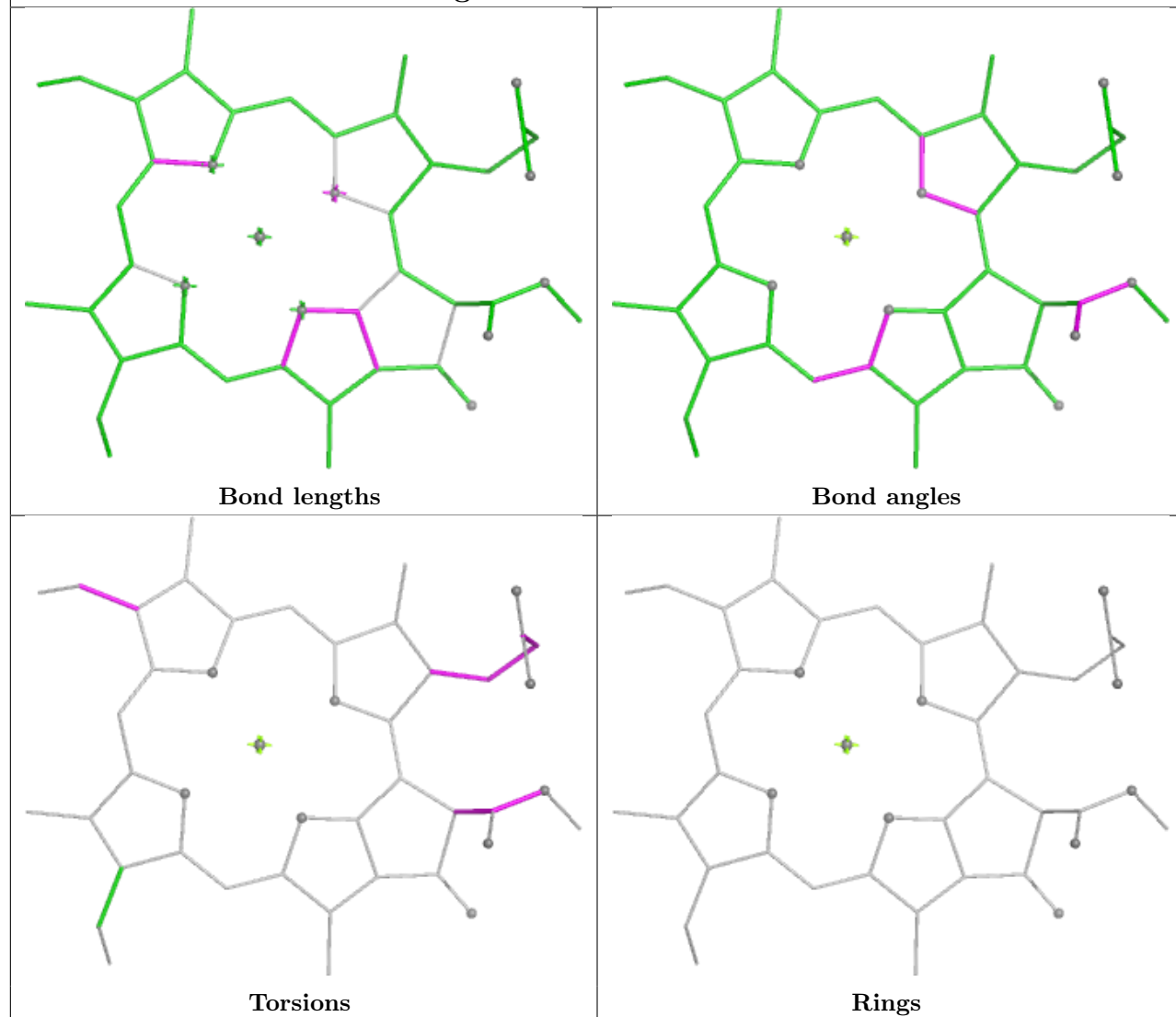
Ligand A1JWG ZH 503

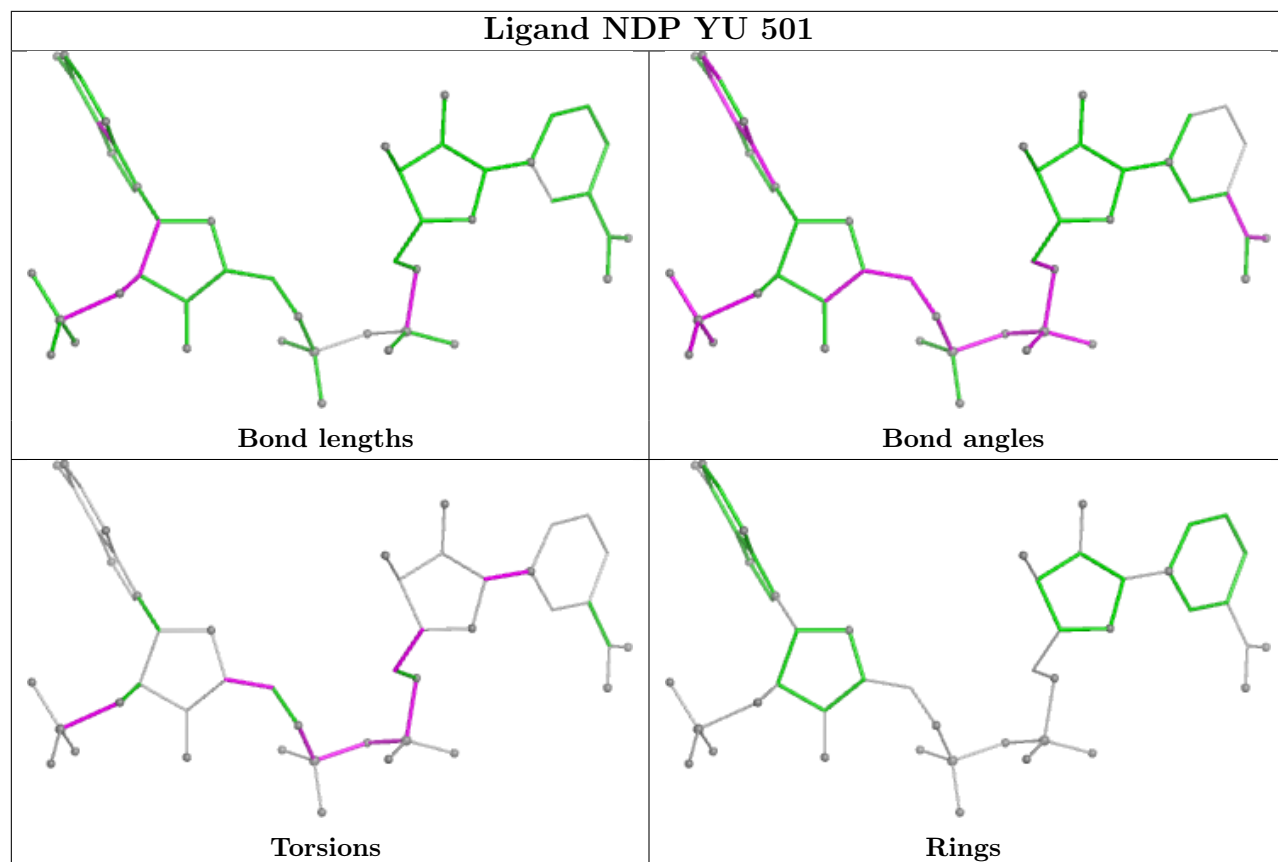


Ligand A1JWG ZQ 502

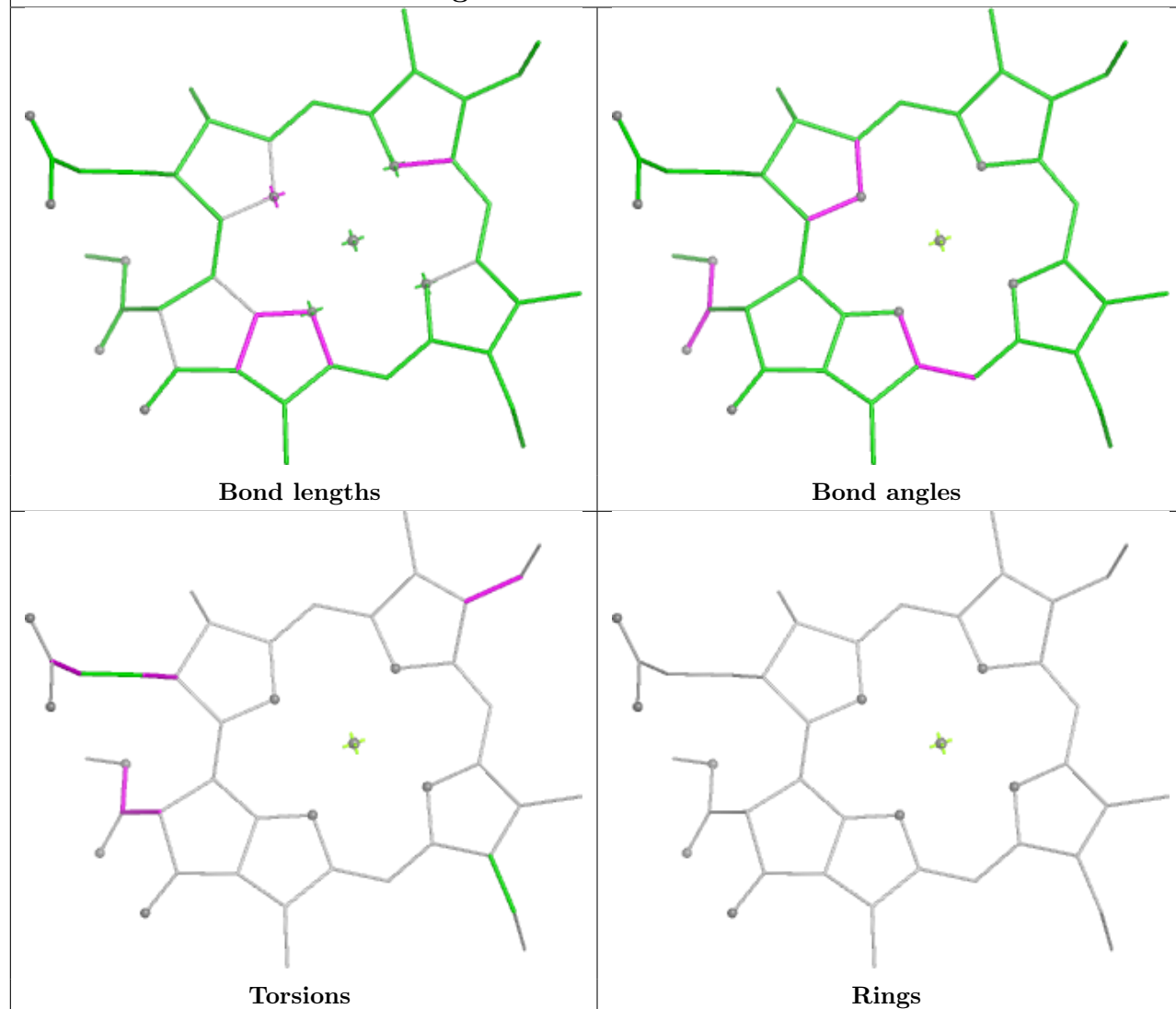


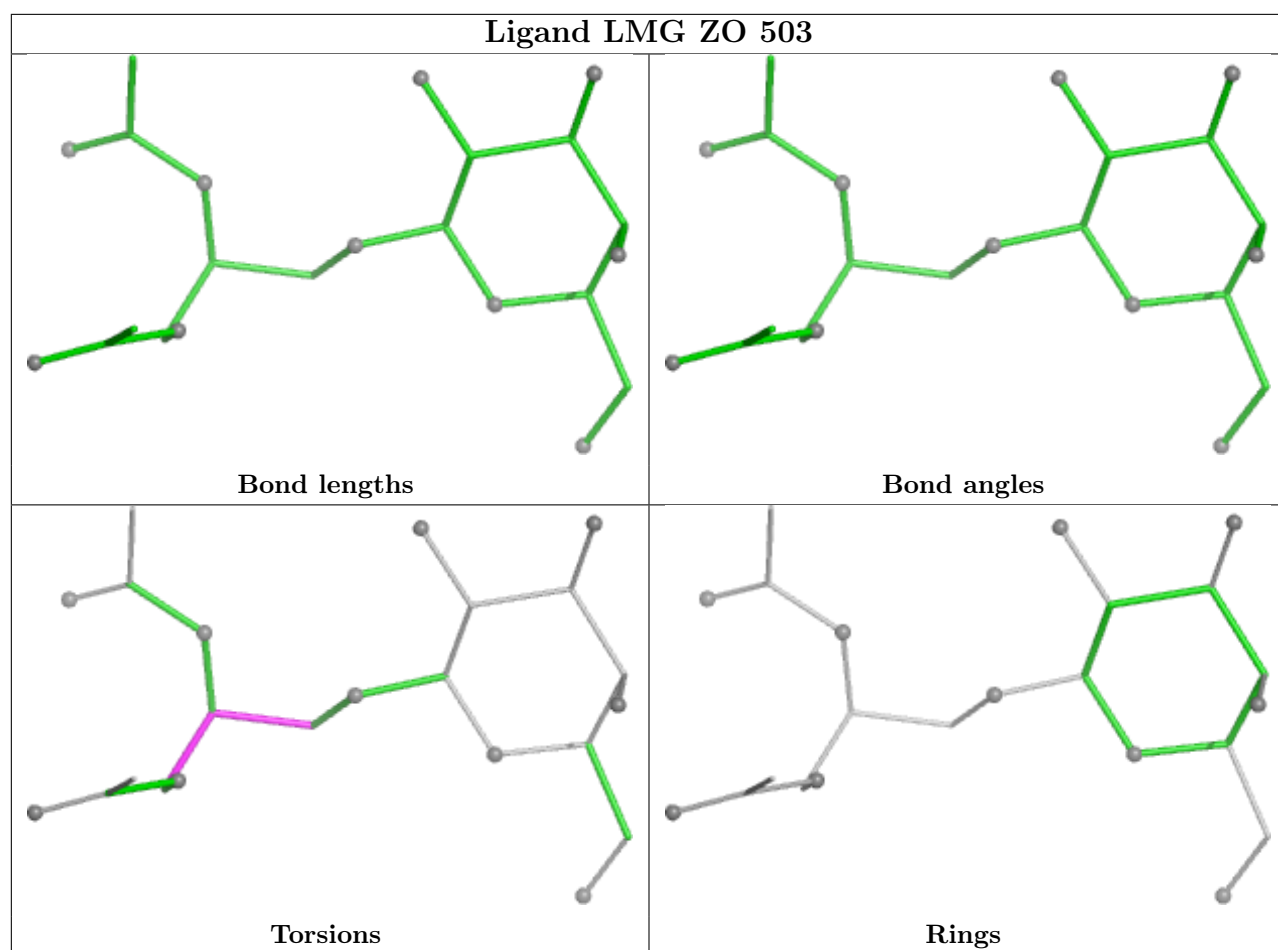
Ligand A1JWG ZG 502



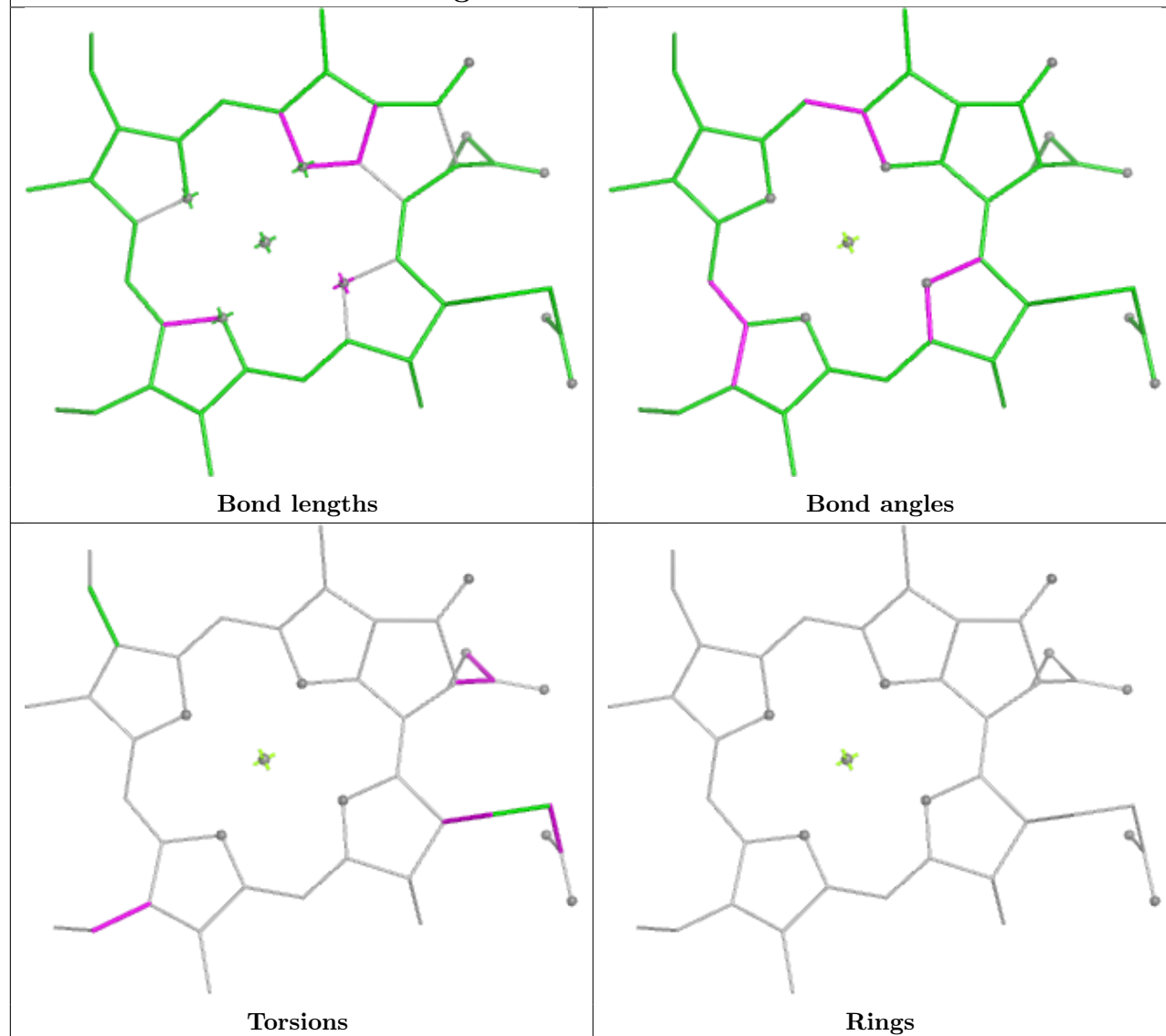


Ligand A1JWG YU 502

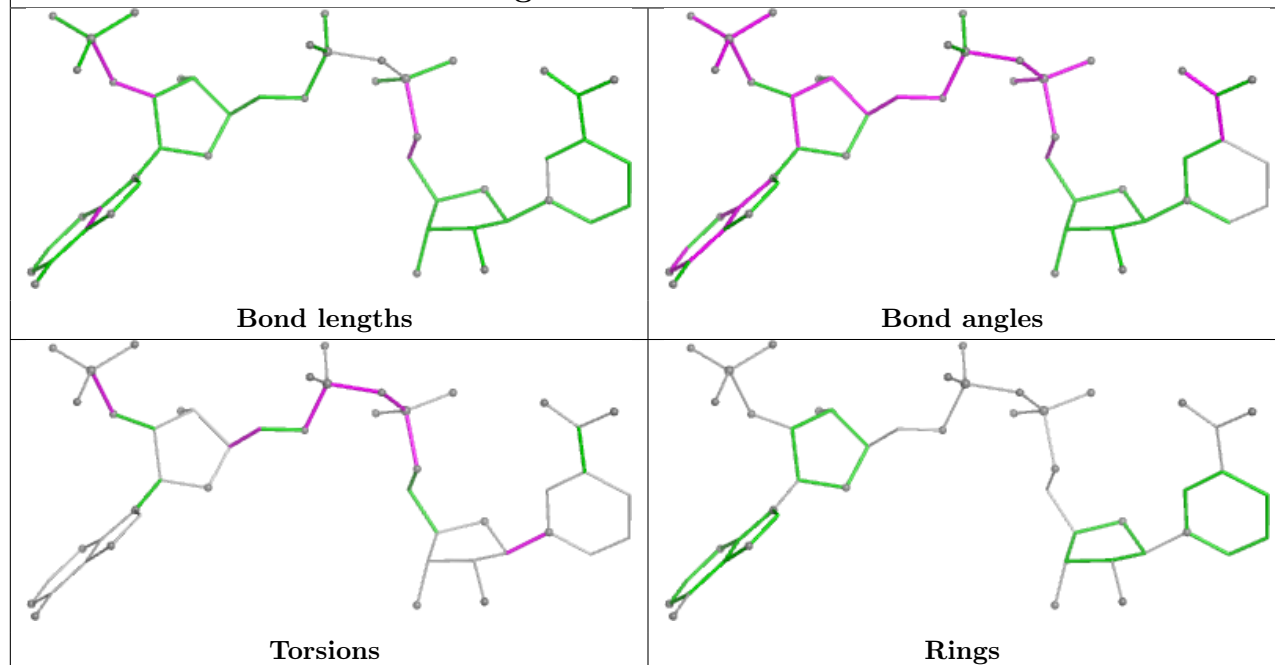




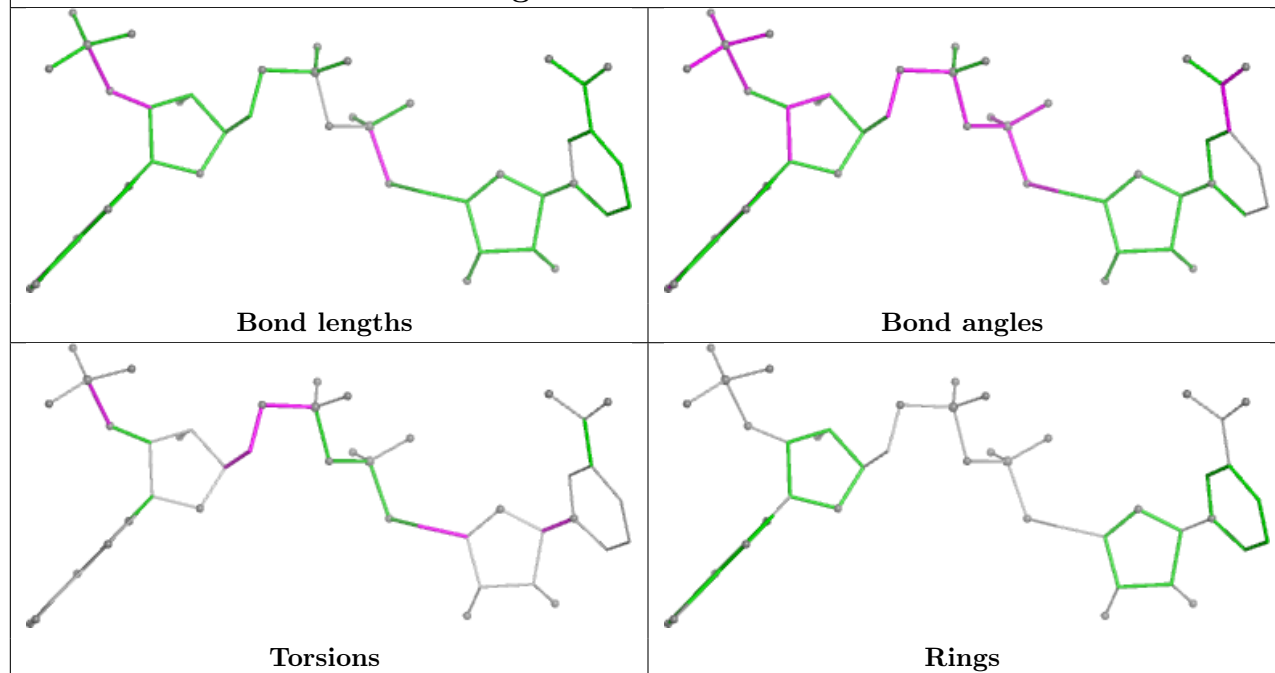
Ligand A1JWG ZZ 502

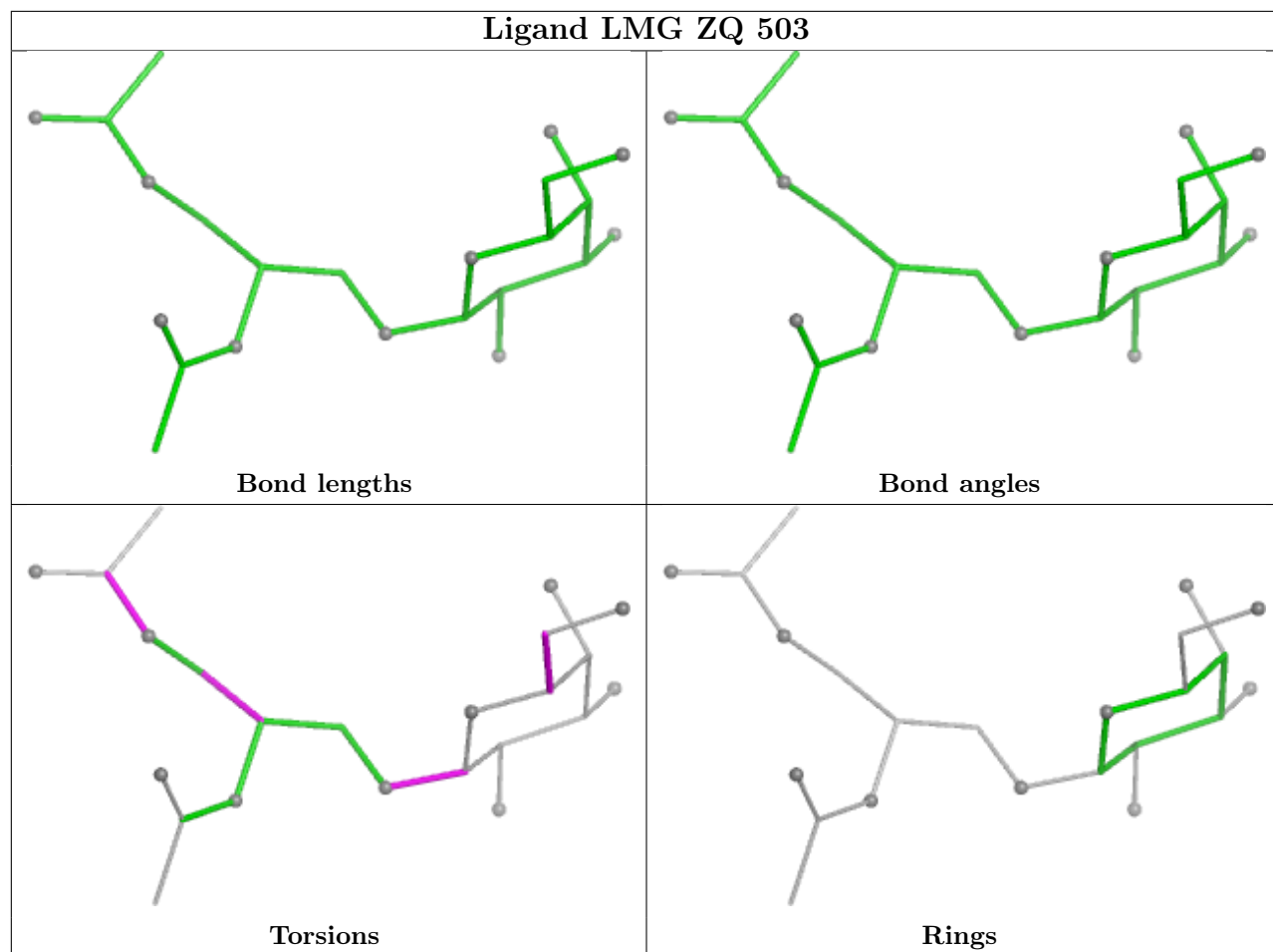


Ligand NDP YR 501

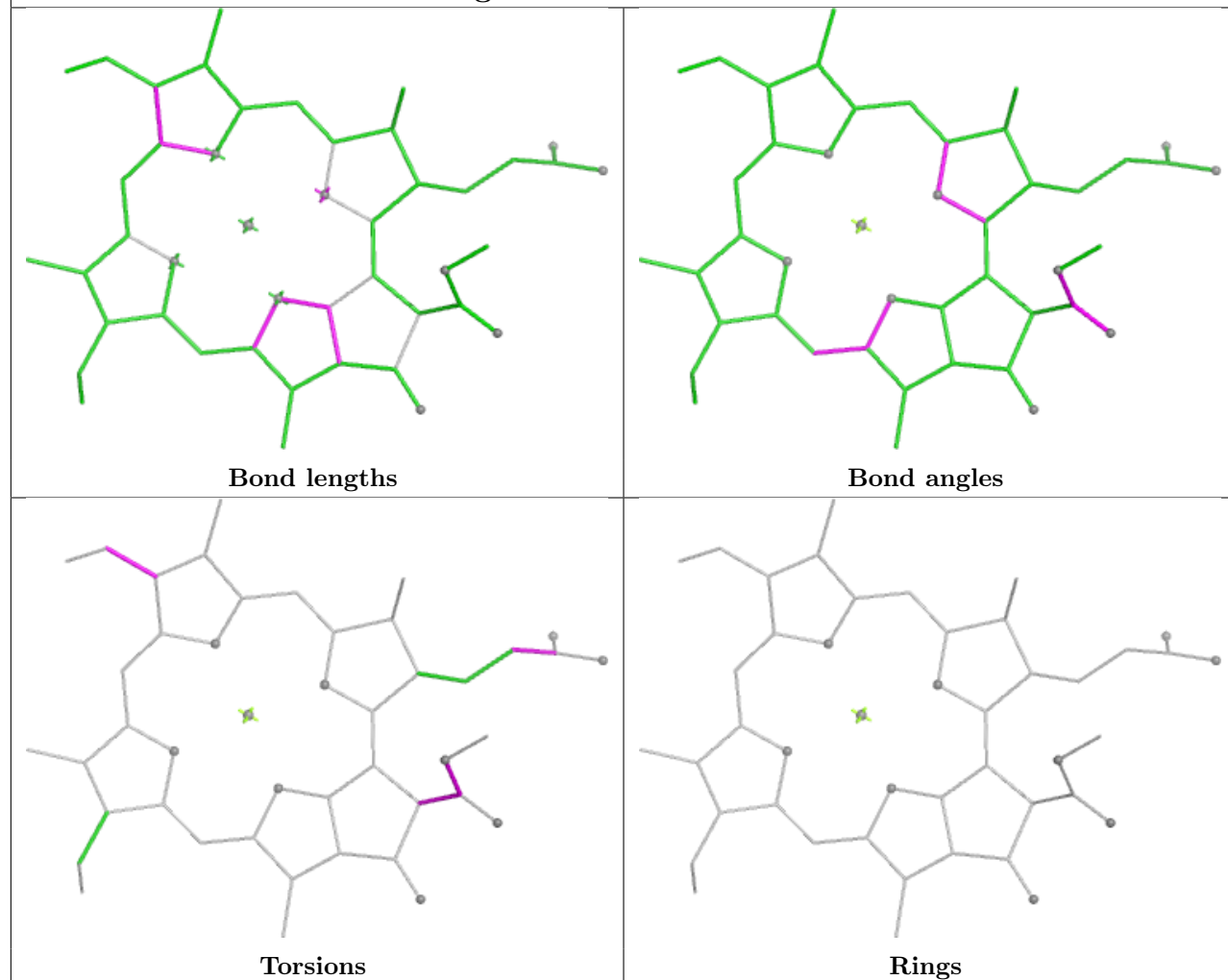


Ligand NDP ZW 501

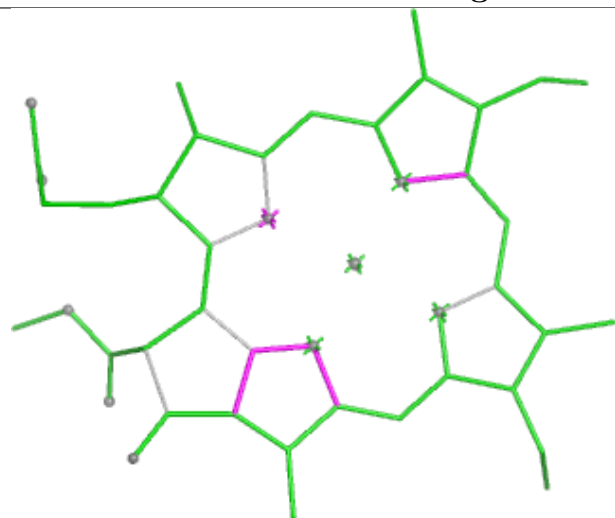




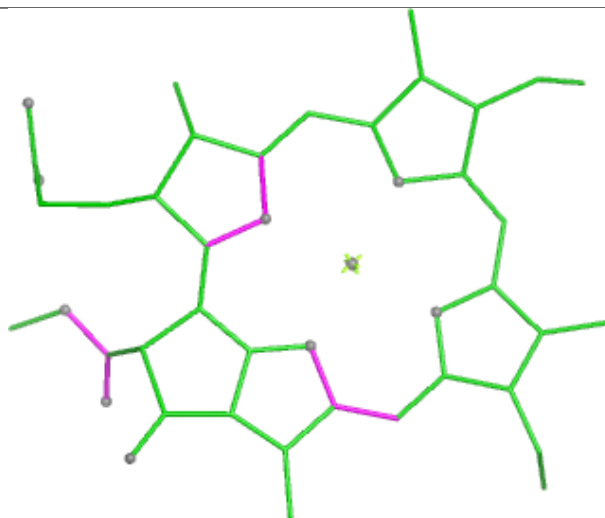
Ligand A1JWG ZV 502



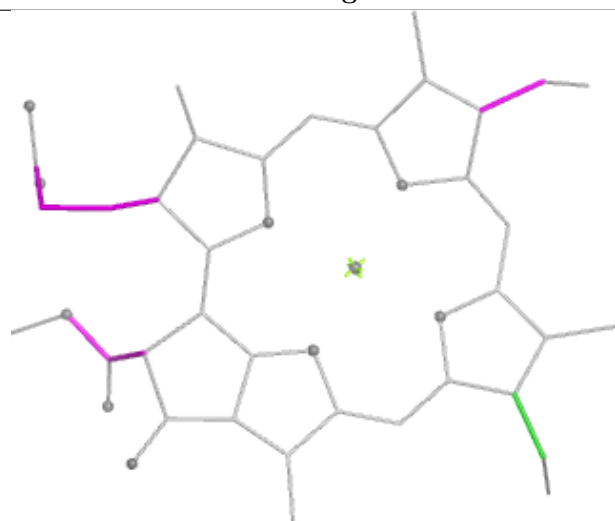
Ligand A1JWG YW 502



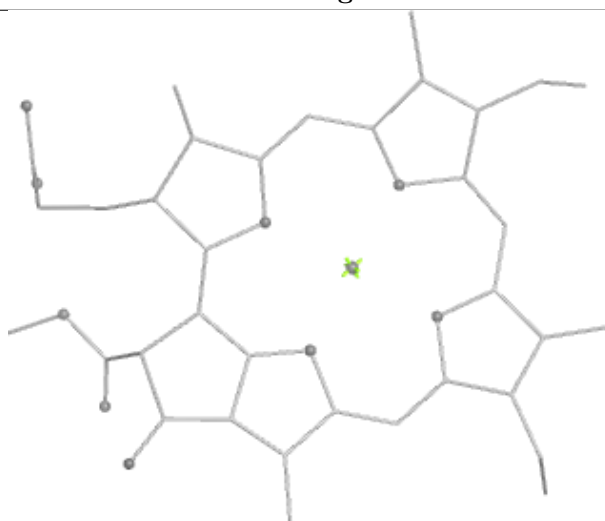
Bond lengths



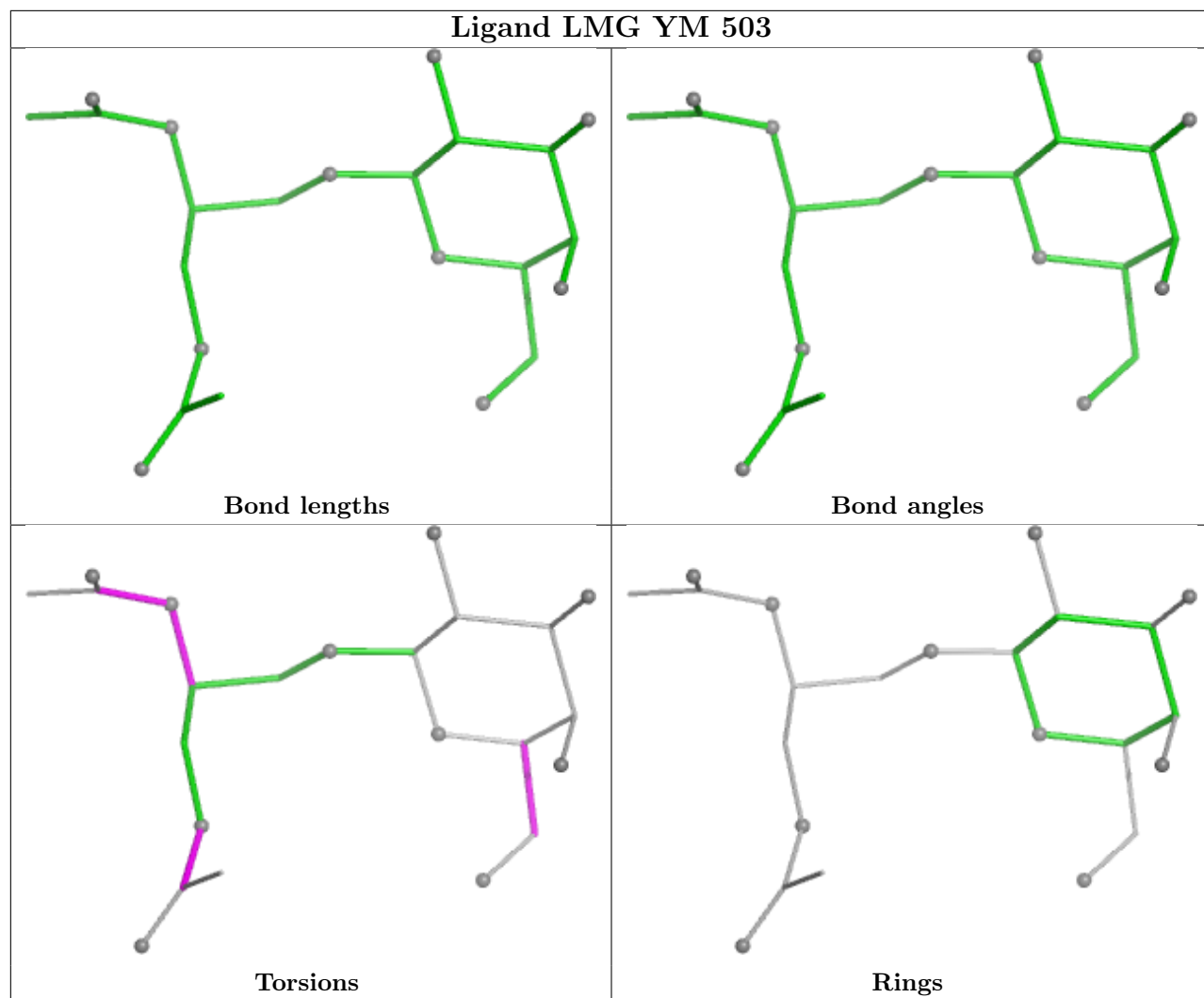
Bond angles



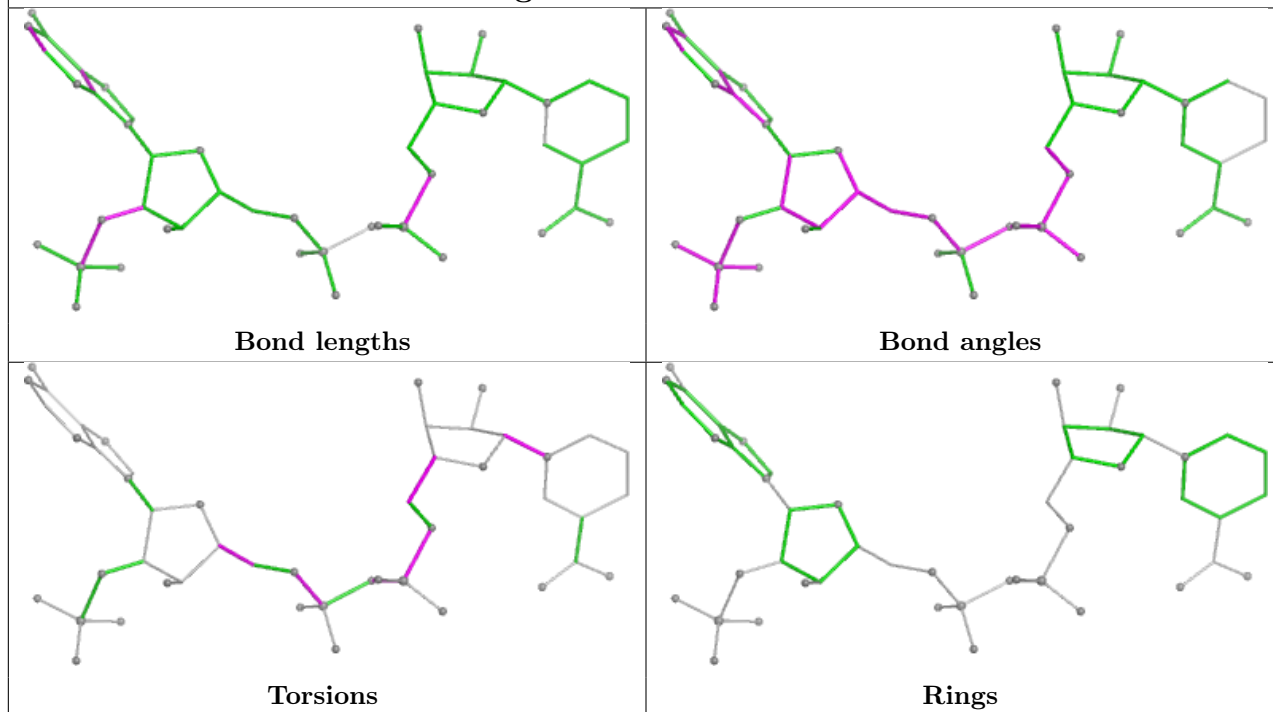
Torsions



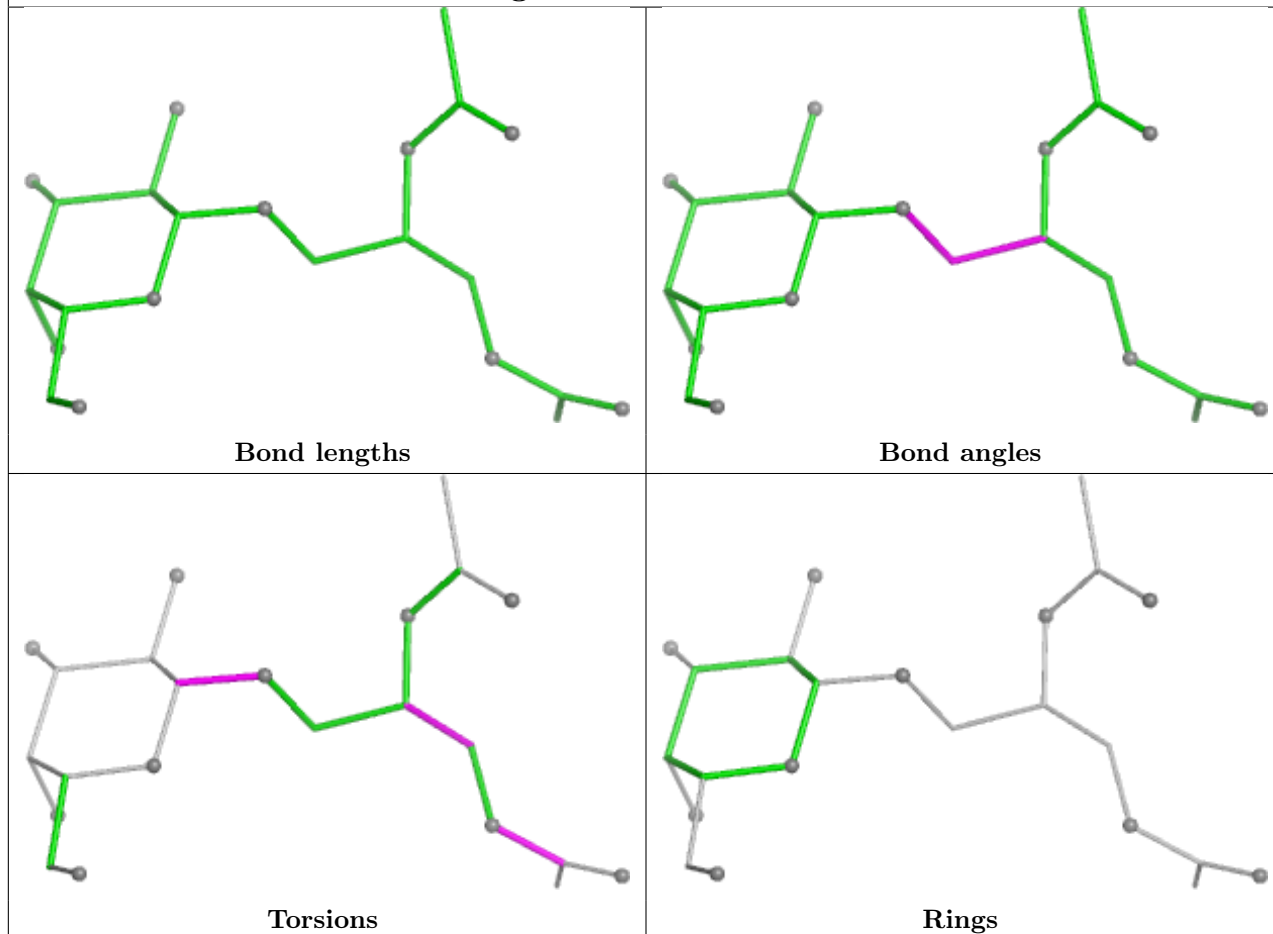
Rings

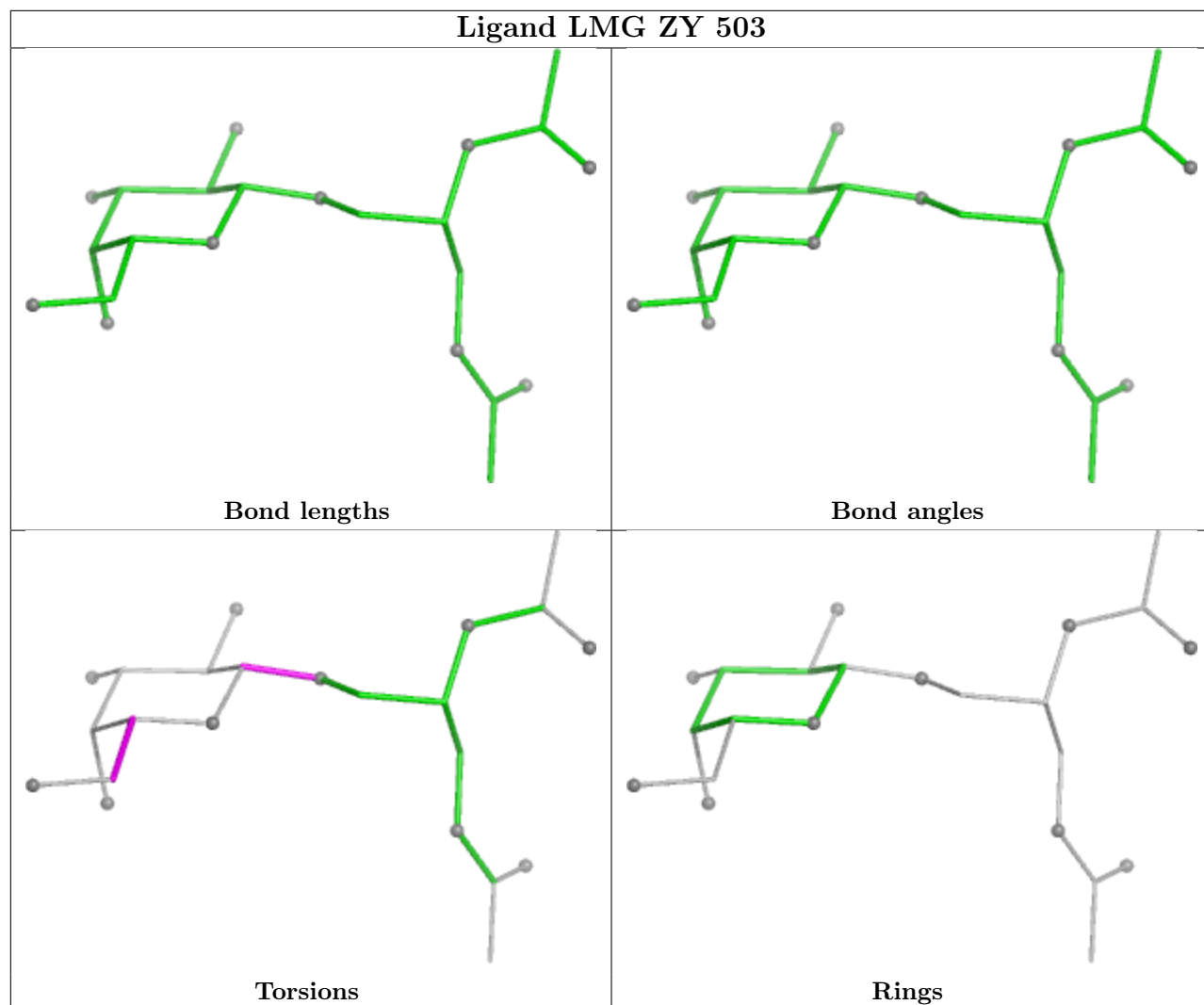


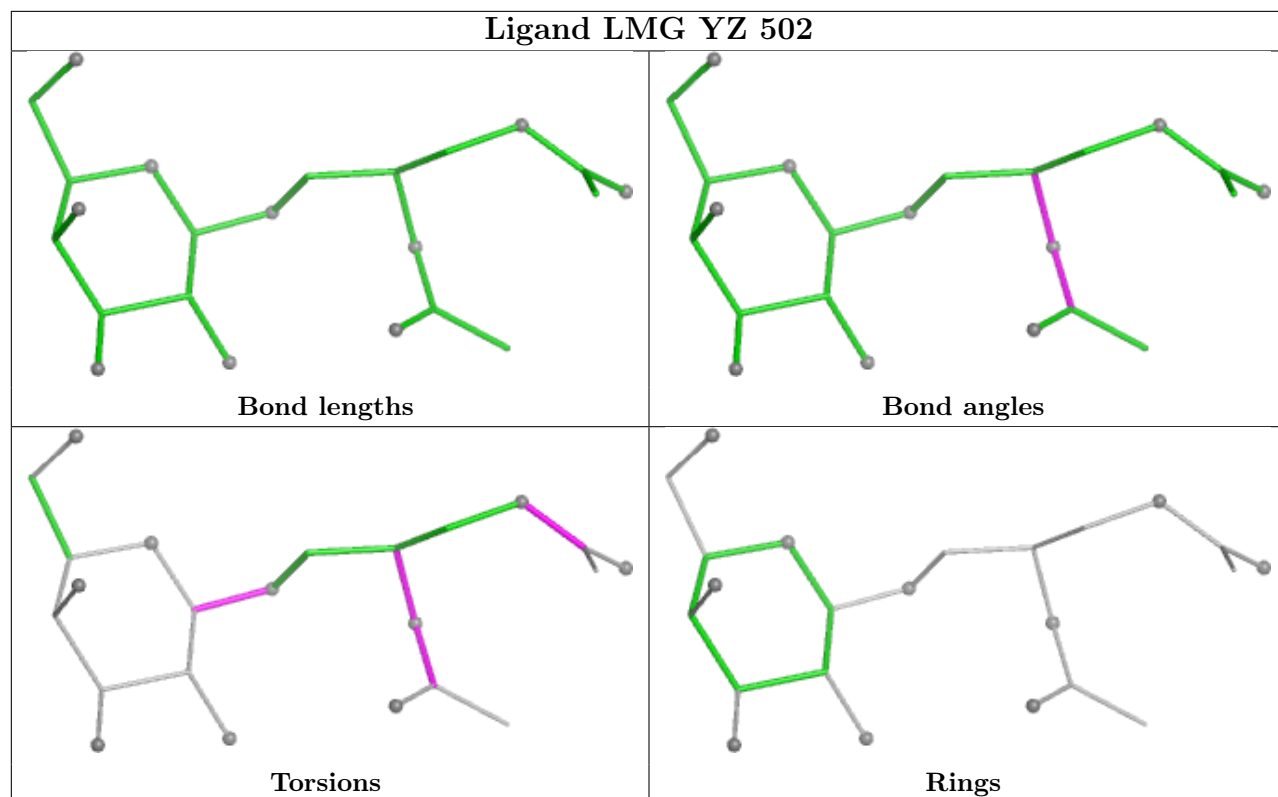
Ligand NDP ZY 501



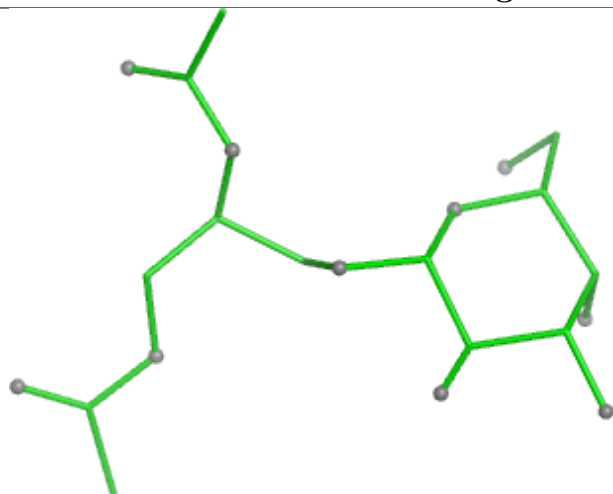
Ligand LMG YU 503



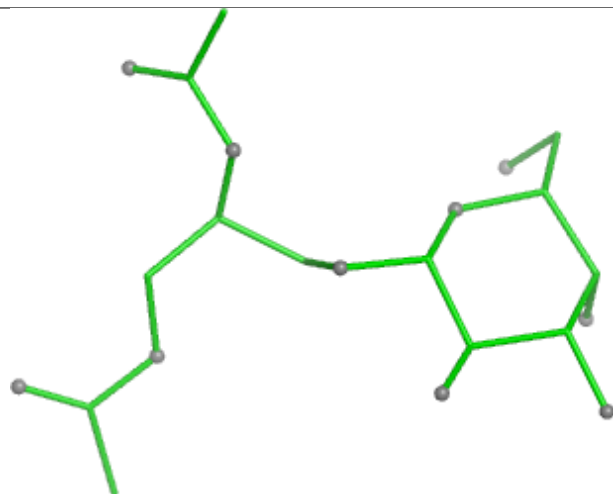




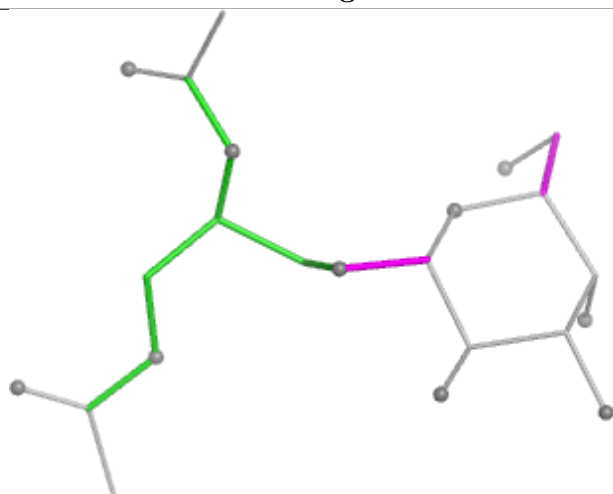
Ligand LMG YX 503



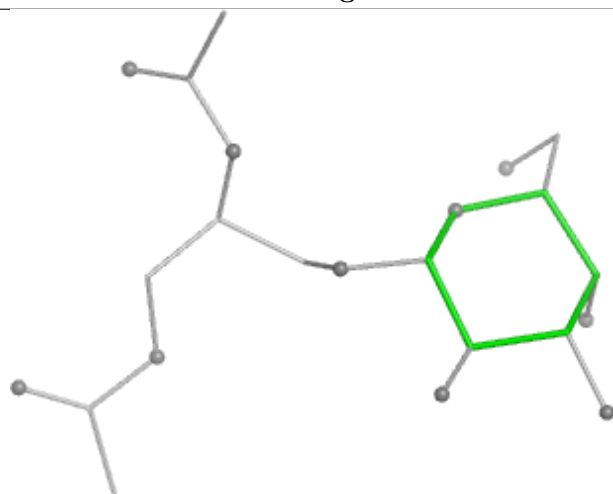
Bond lengths



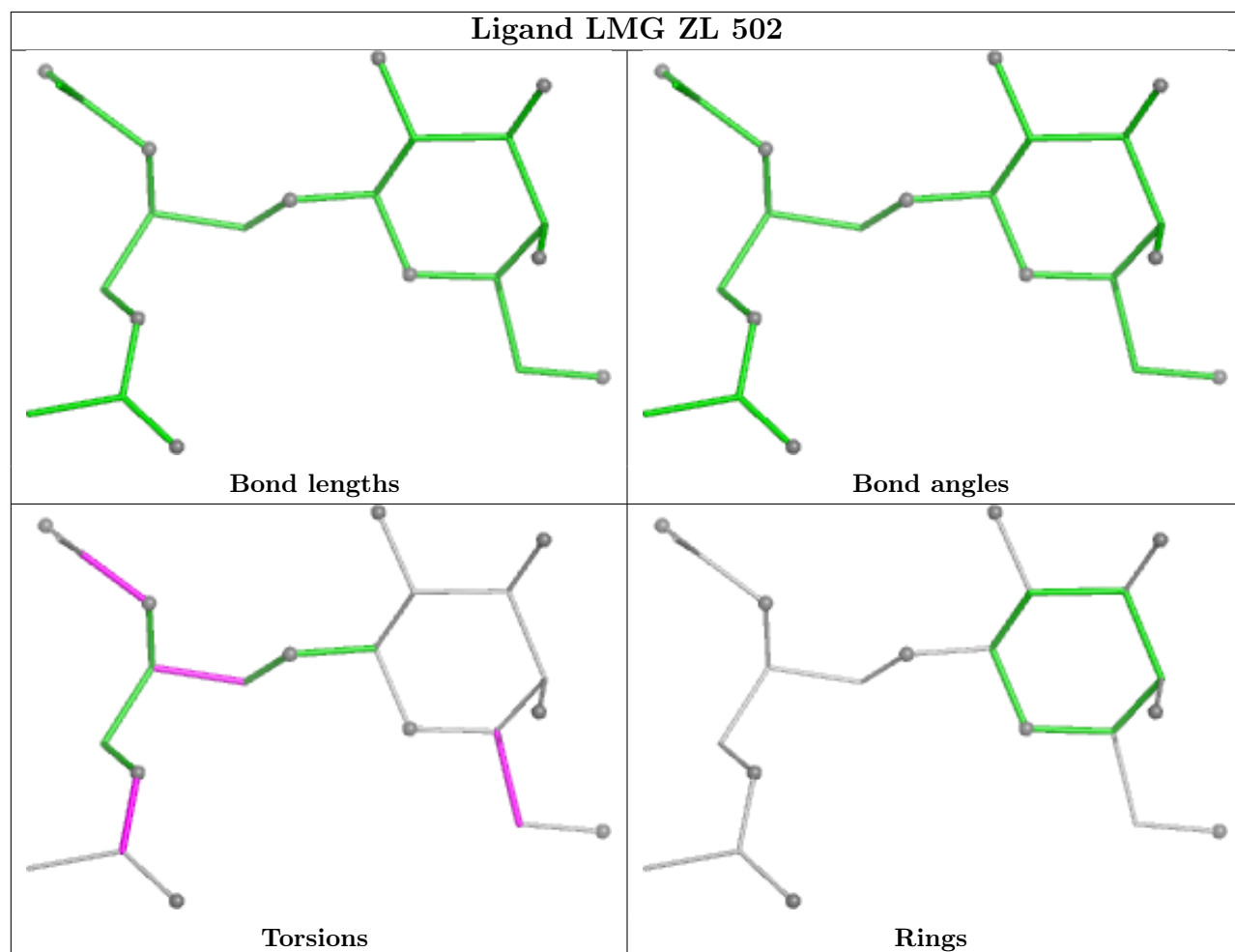
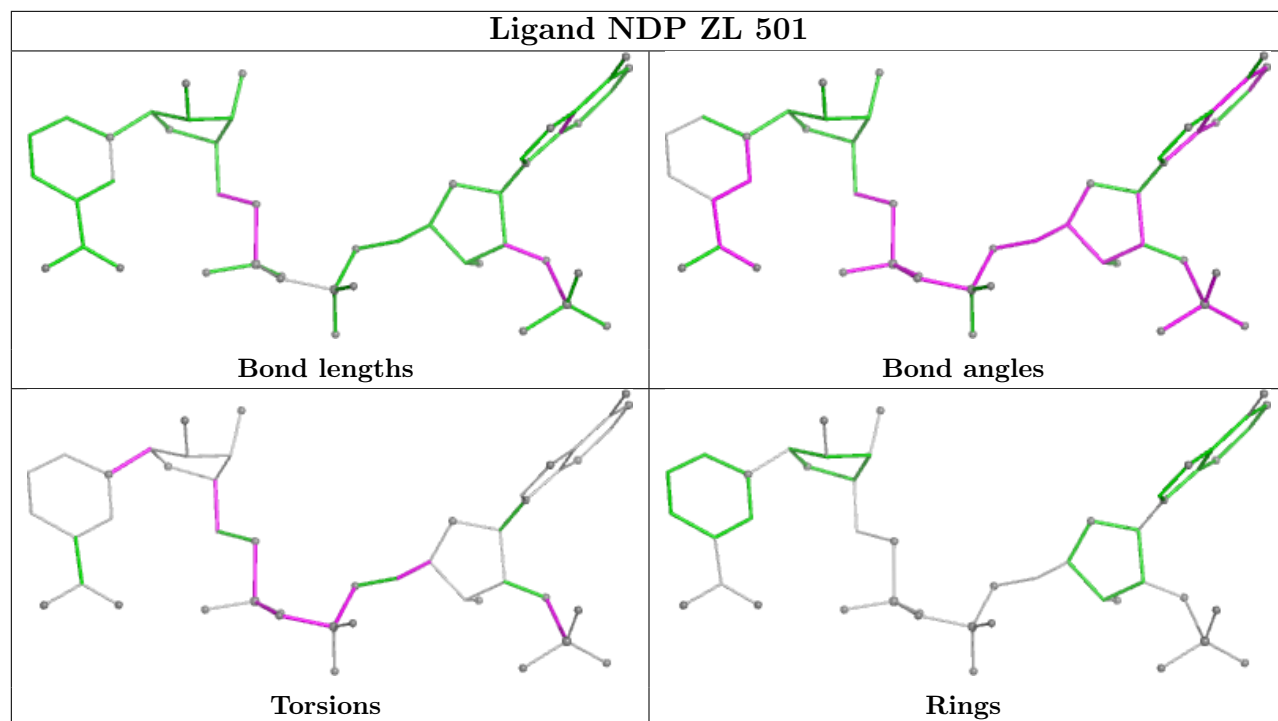
Bond angles



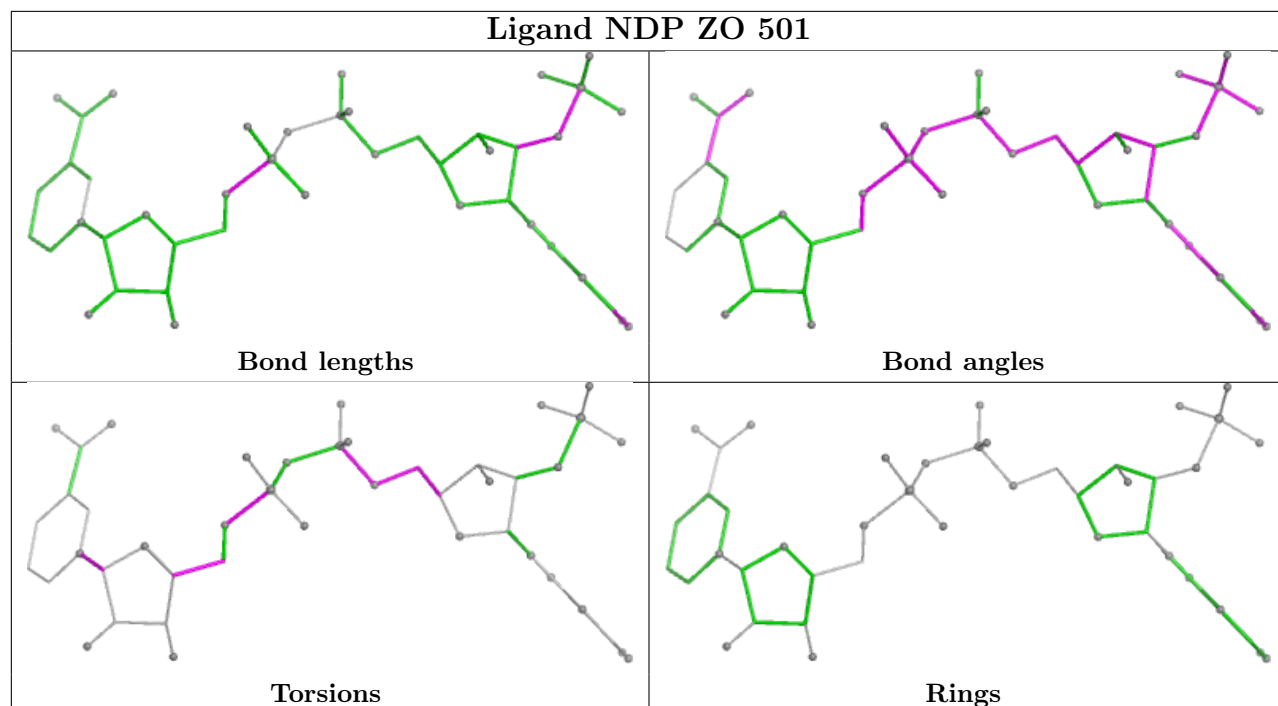
Torsions



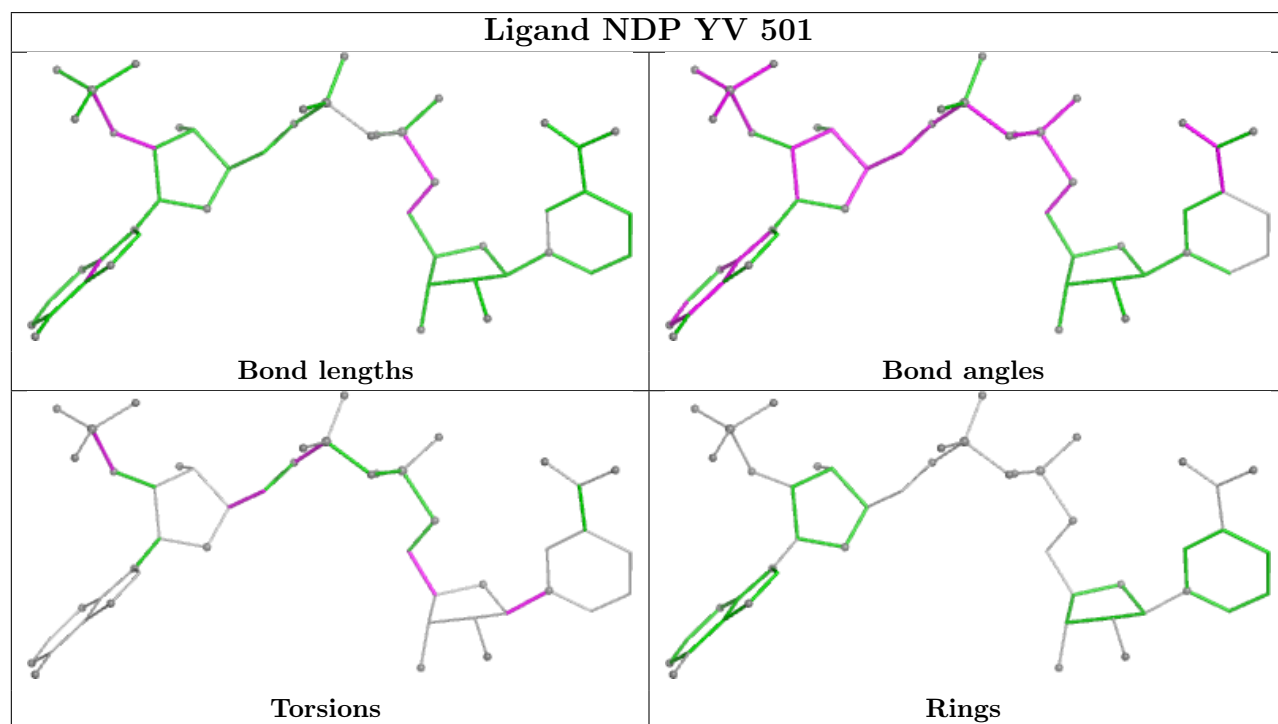
Rings



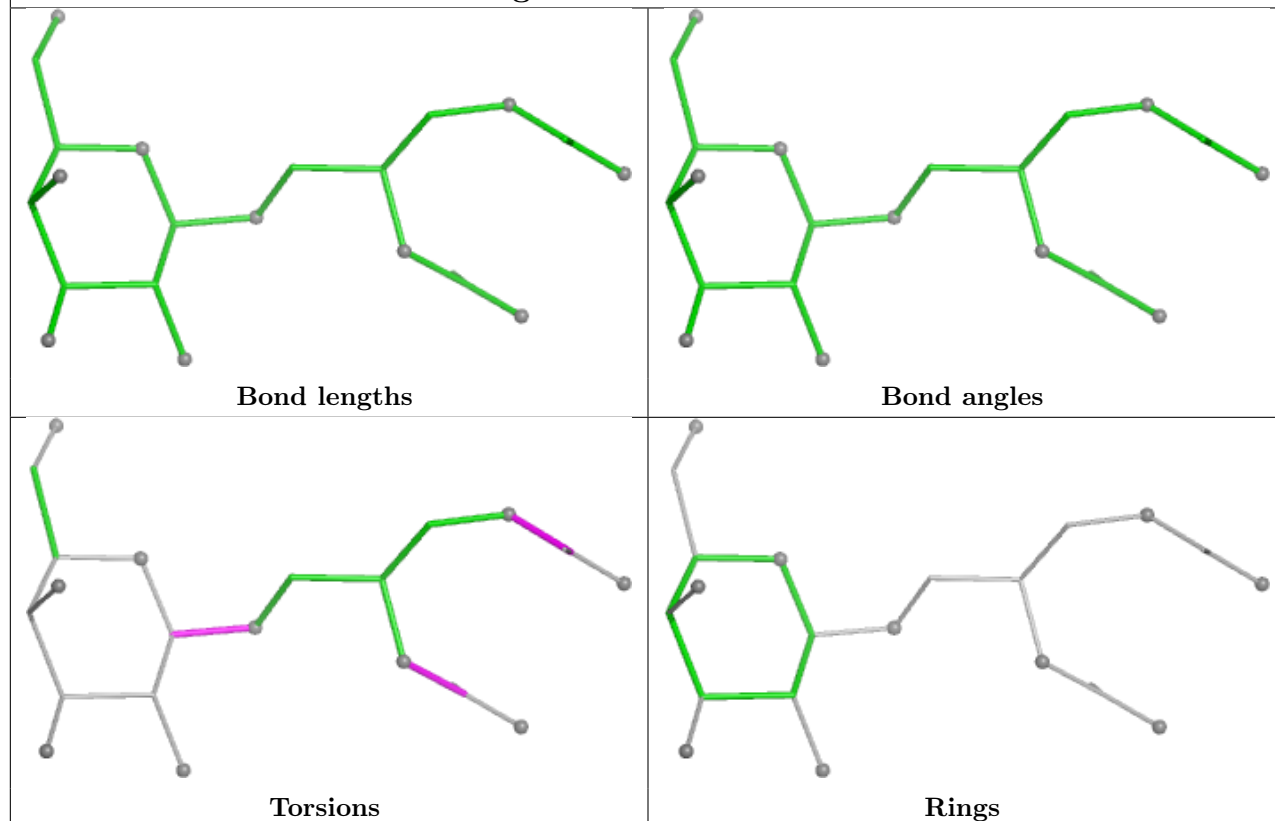
Ligand NDP ZO 501



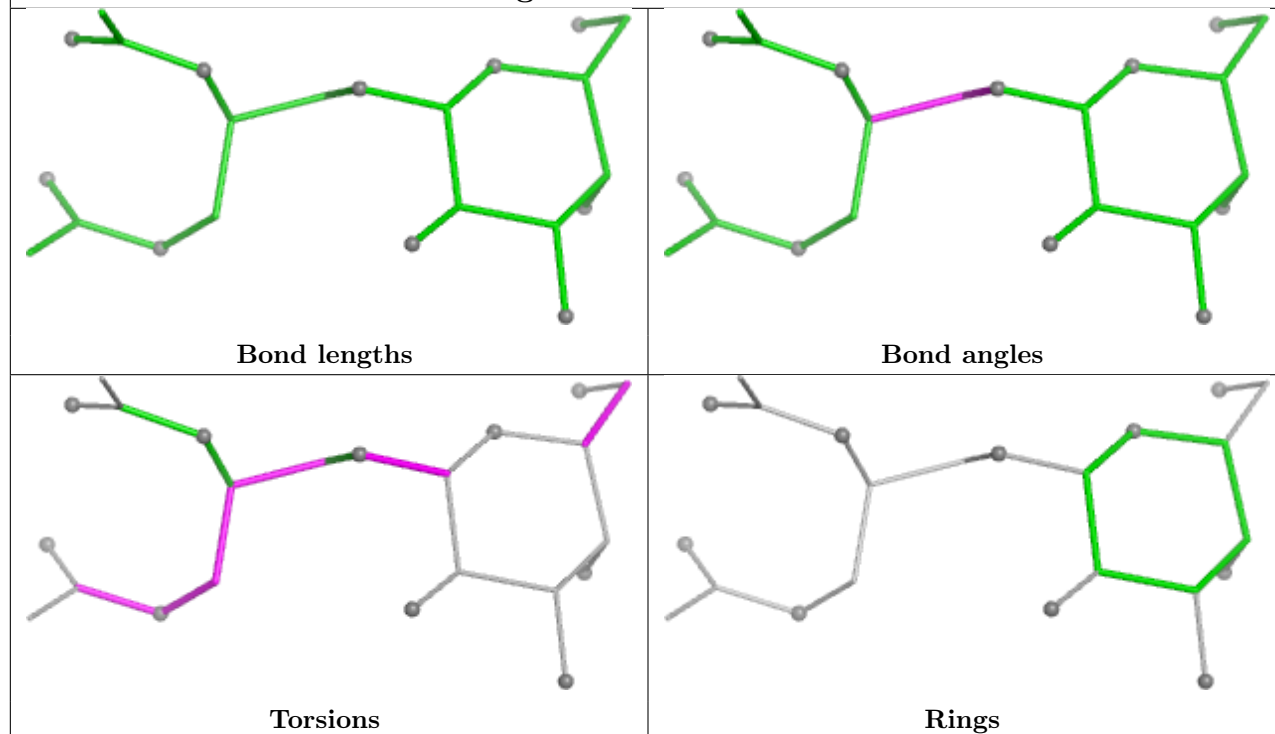
Ligand NDP YV 501

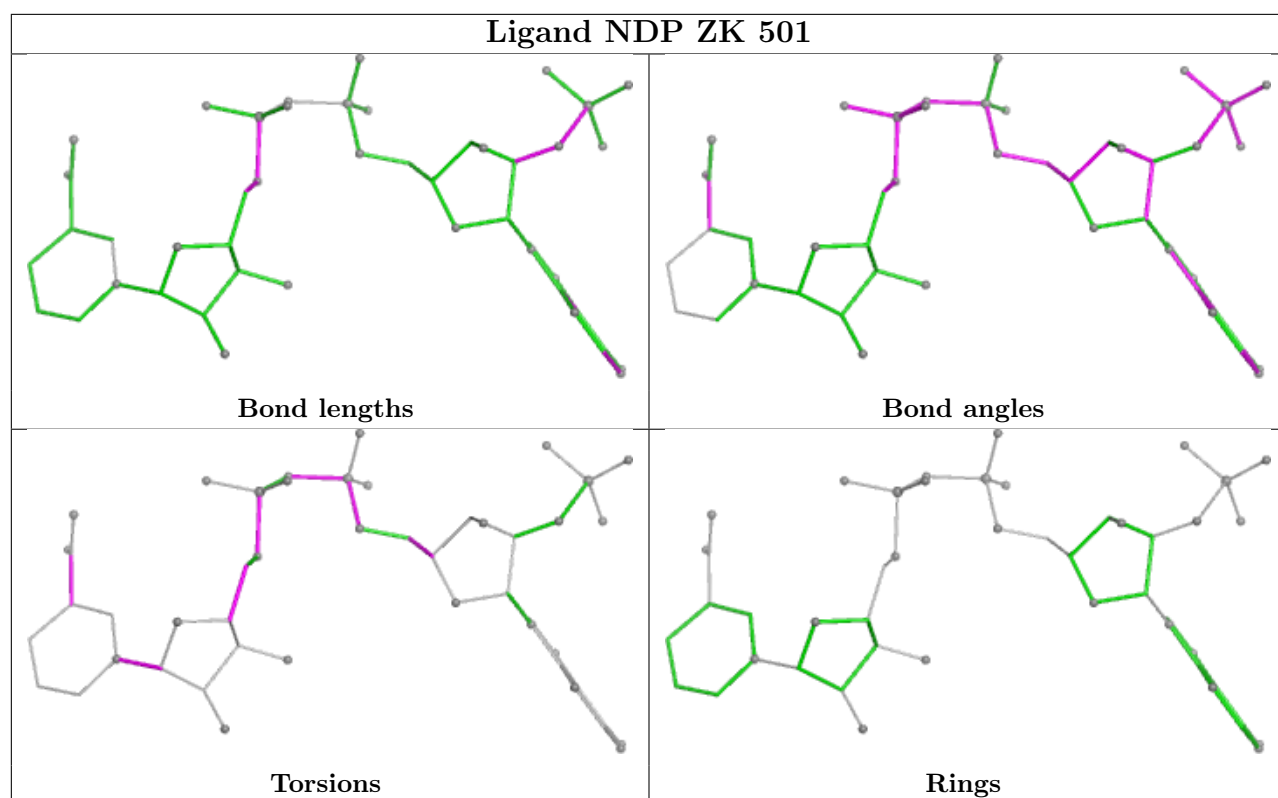


Ligand LMG YV 502

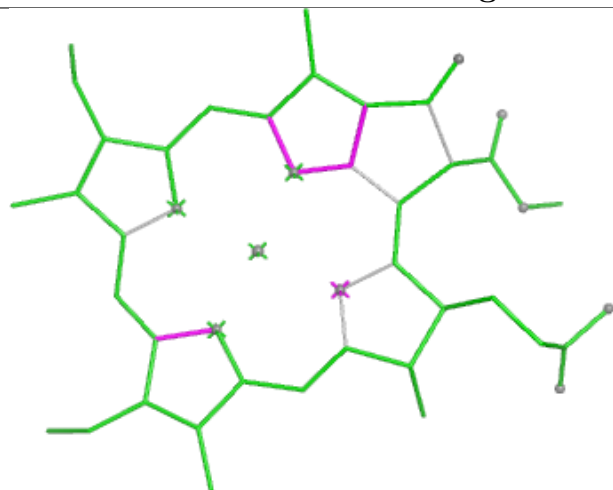


Ligand LMG ZP 502

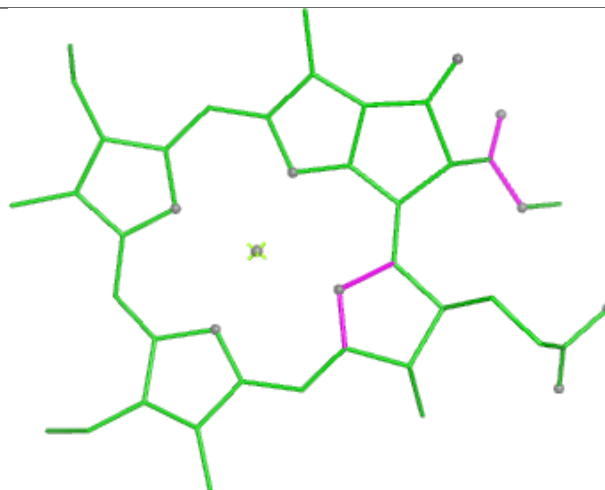




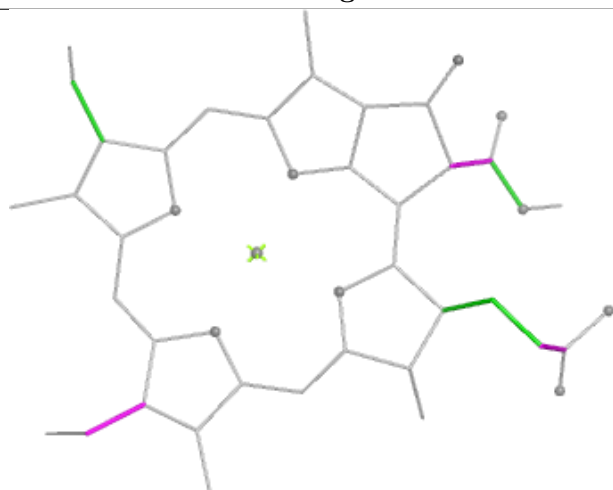
Ligand A1JWG ZL 503



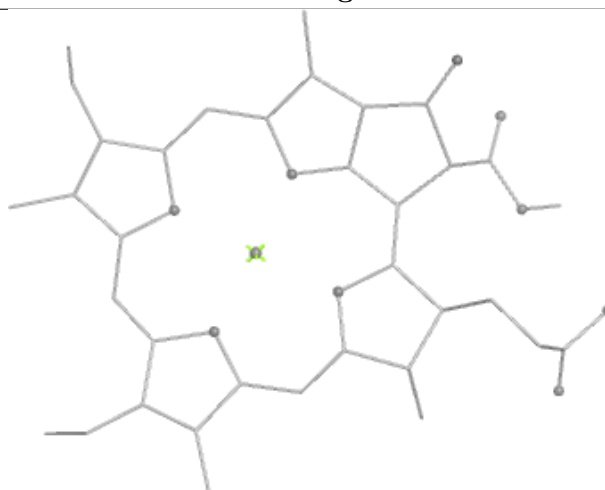
Bond lengths



Bond angles

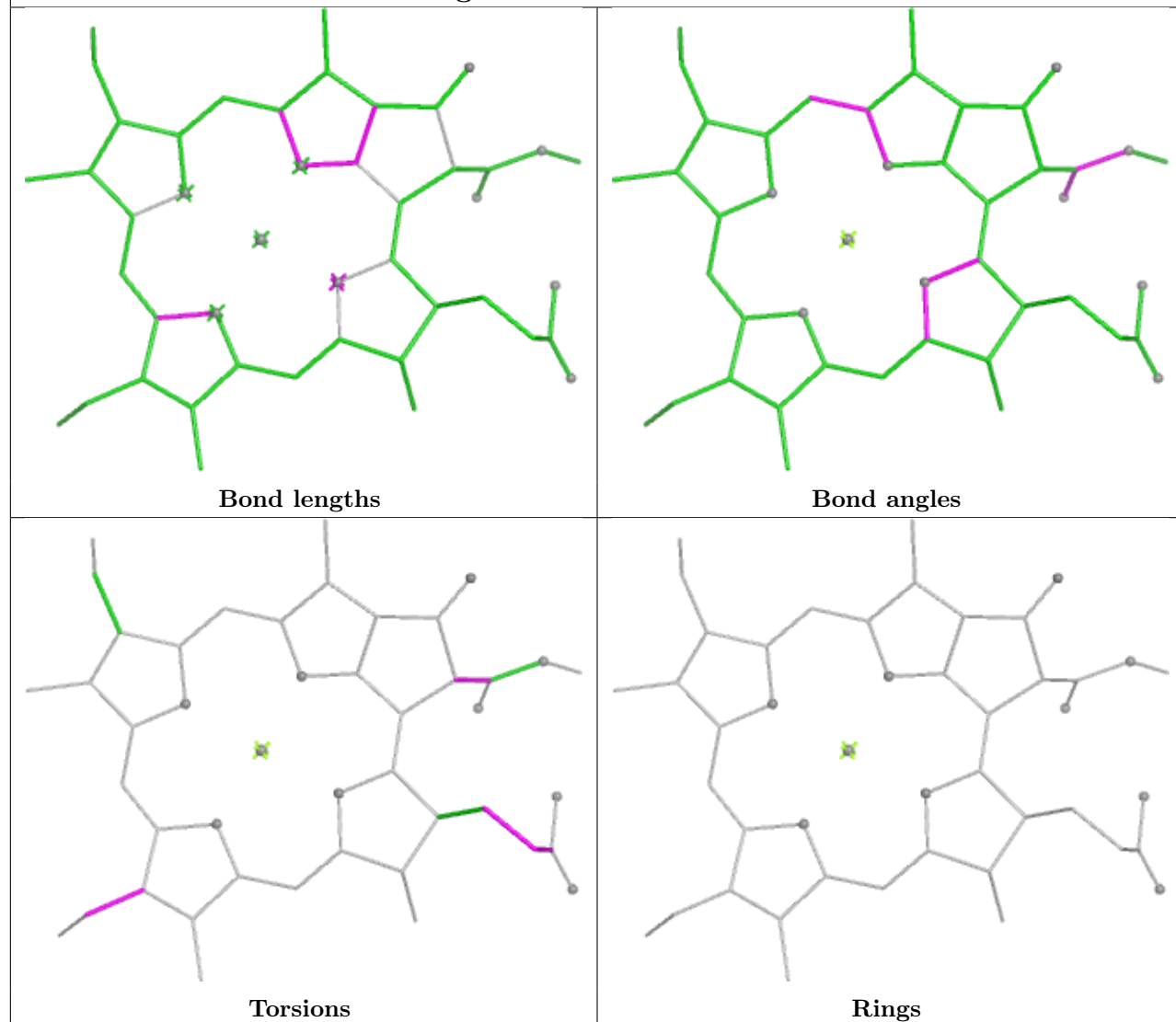


Torsions

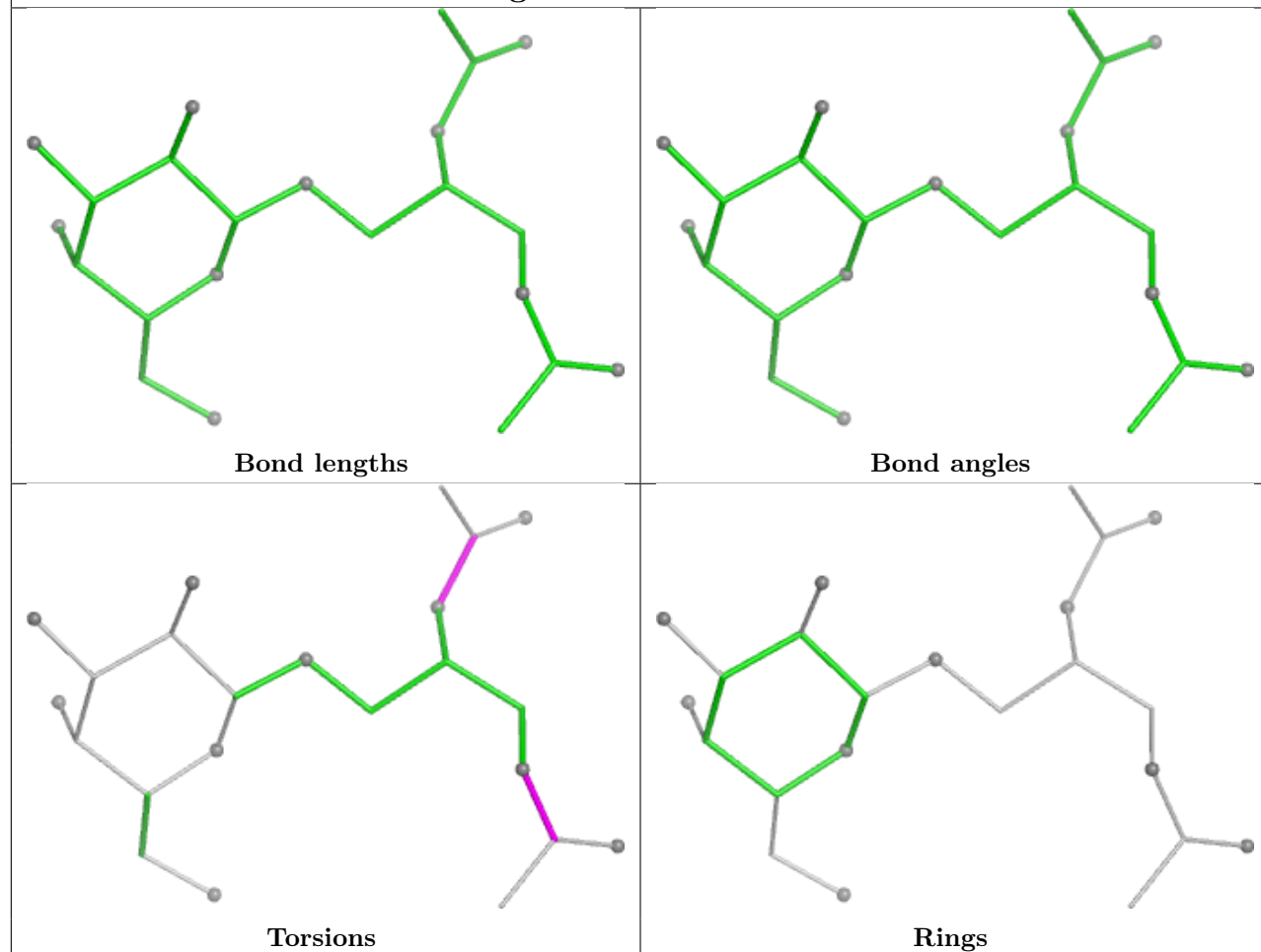


Rings

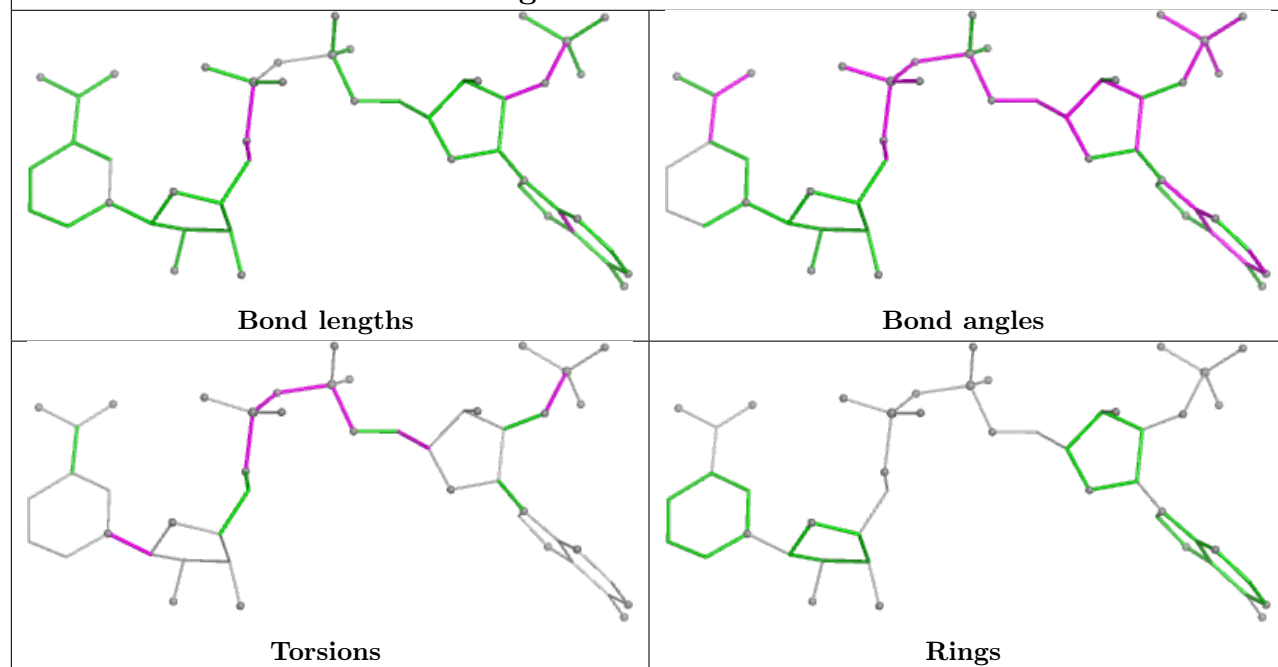
Ligand A1JWG ZP 503



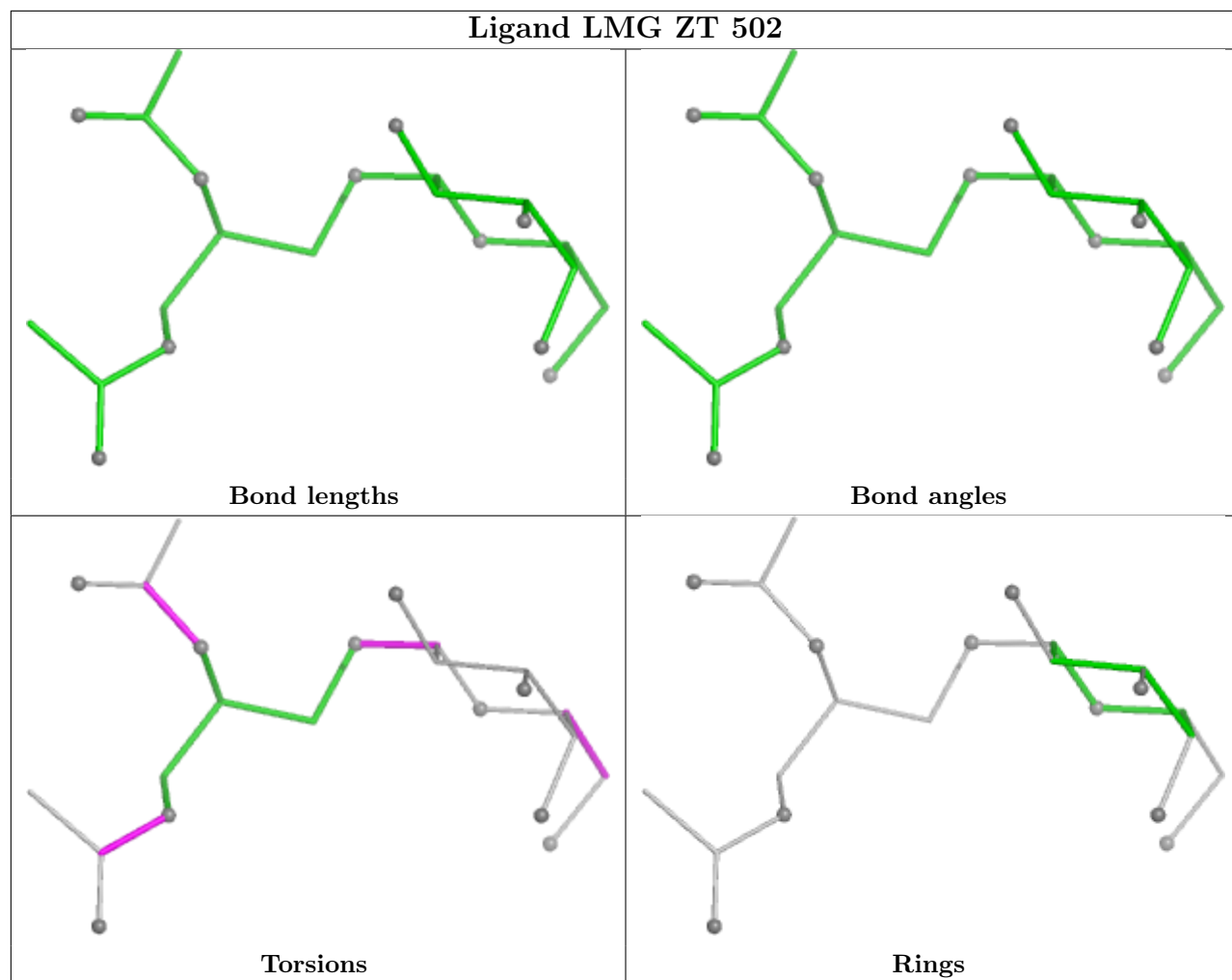
Ligand LMG ZR 503



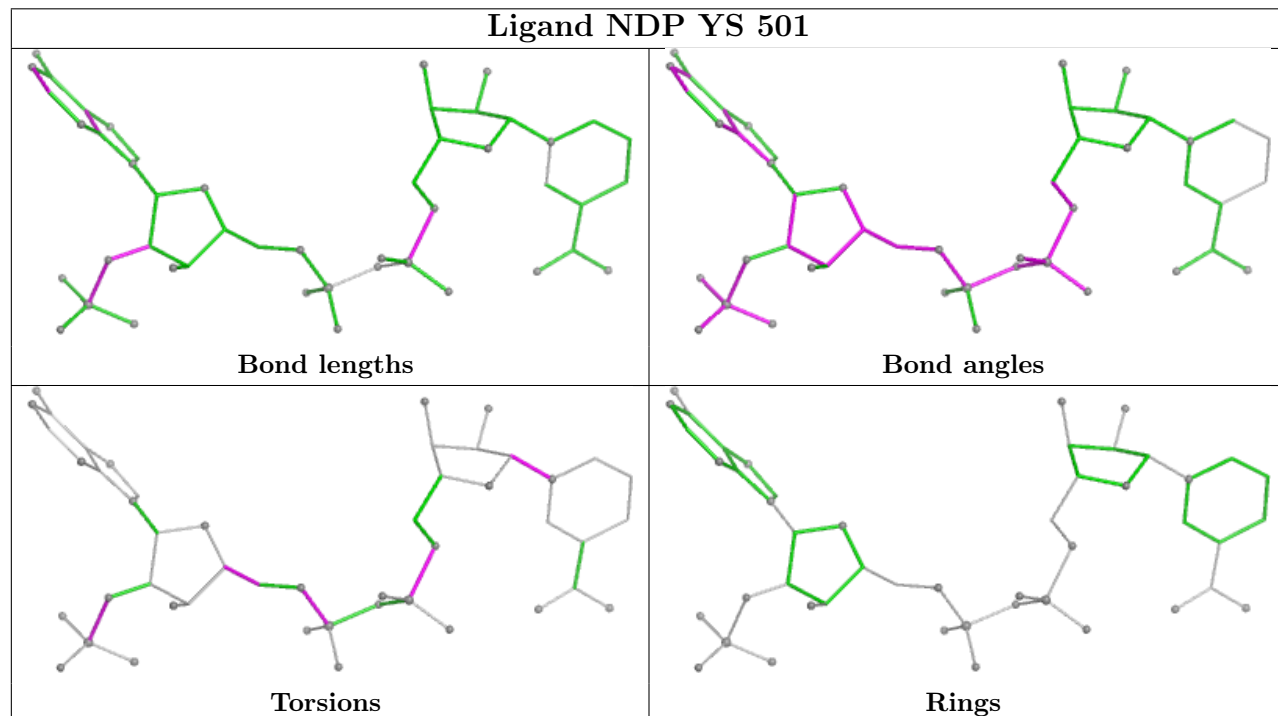
Ligand NDP ZT 501

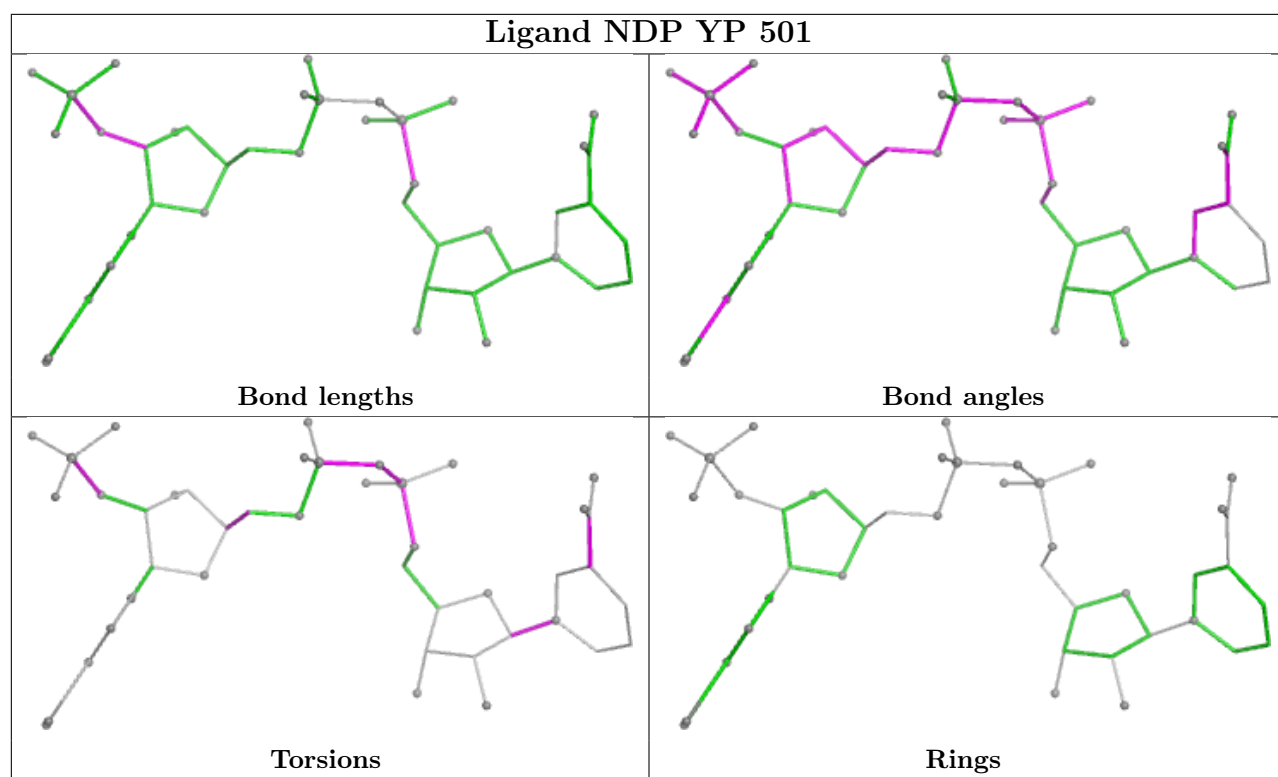


Ligand LMG ZT 502

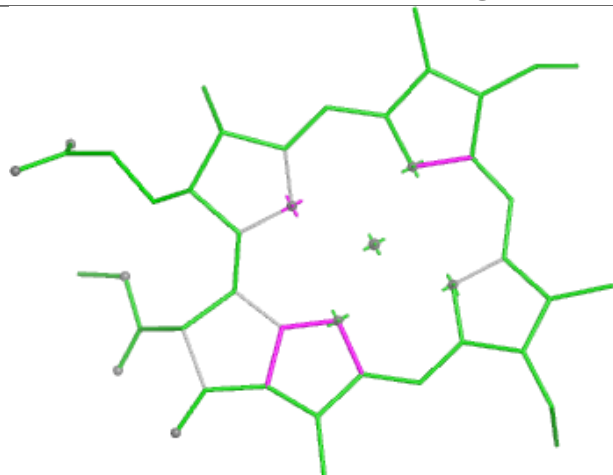


Ligand NDP YS 501

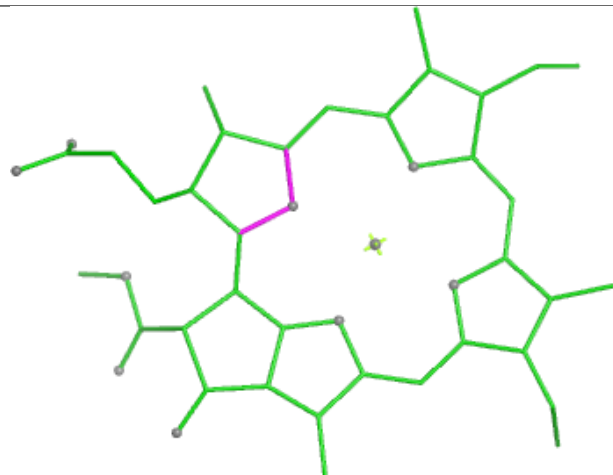




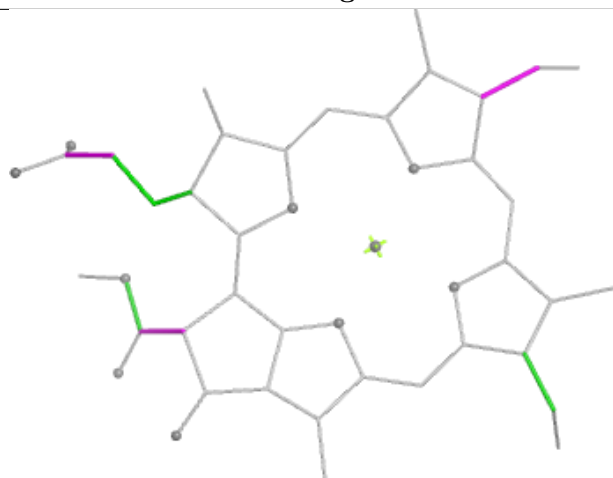
Ligand A1JWG YX 502



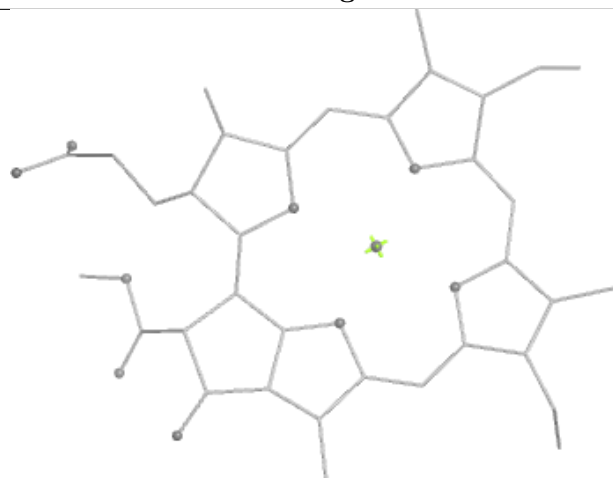
Bond lengths



Bond angles

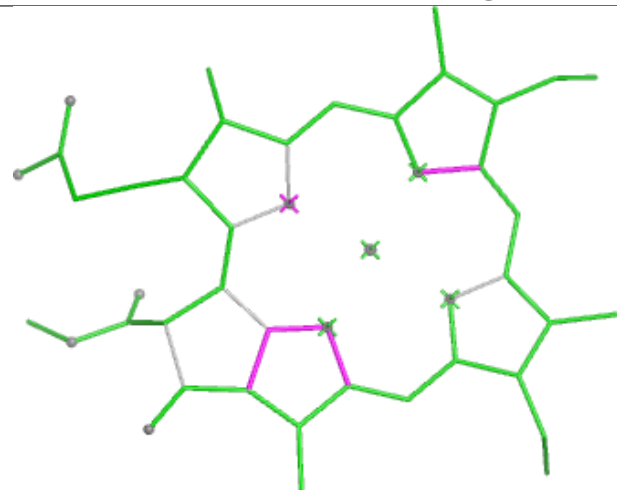


Torsions

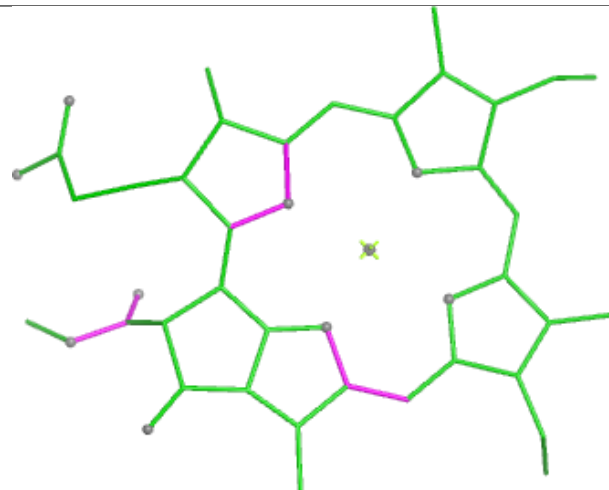


Rings

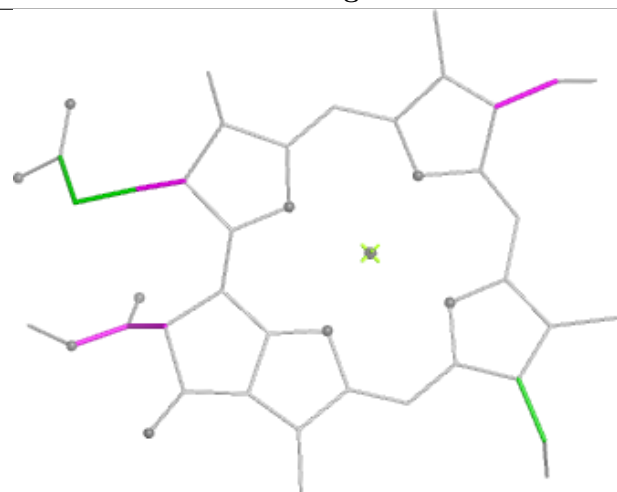
Ligand A1JWG YZ 503



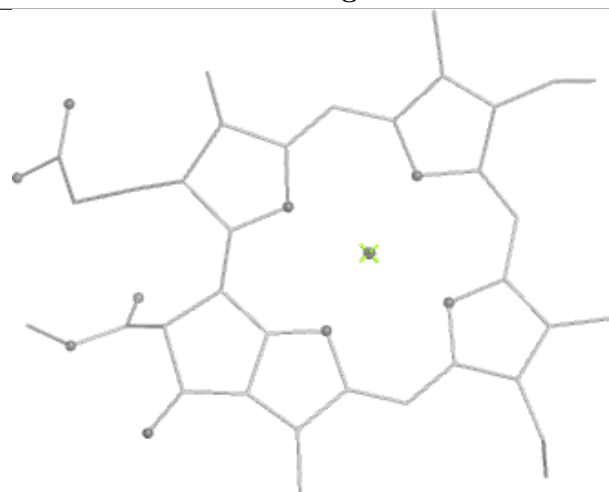
Bond lengths



Bond angles

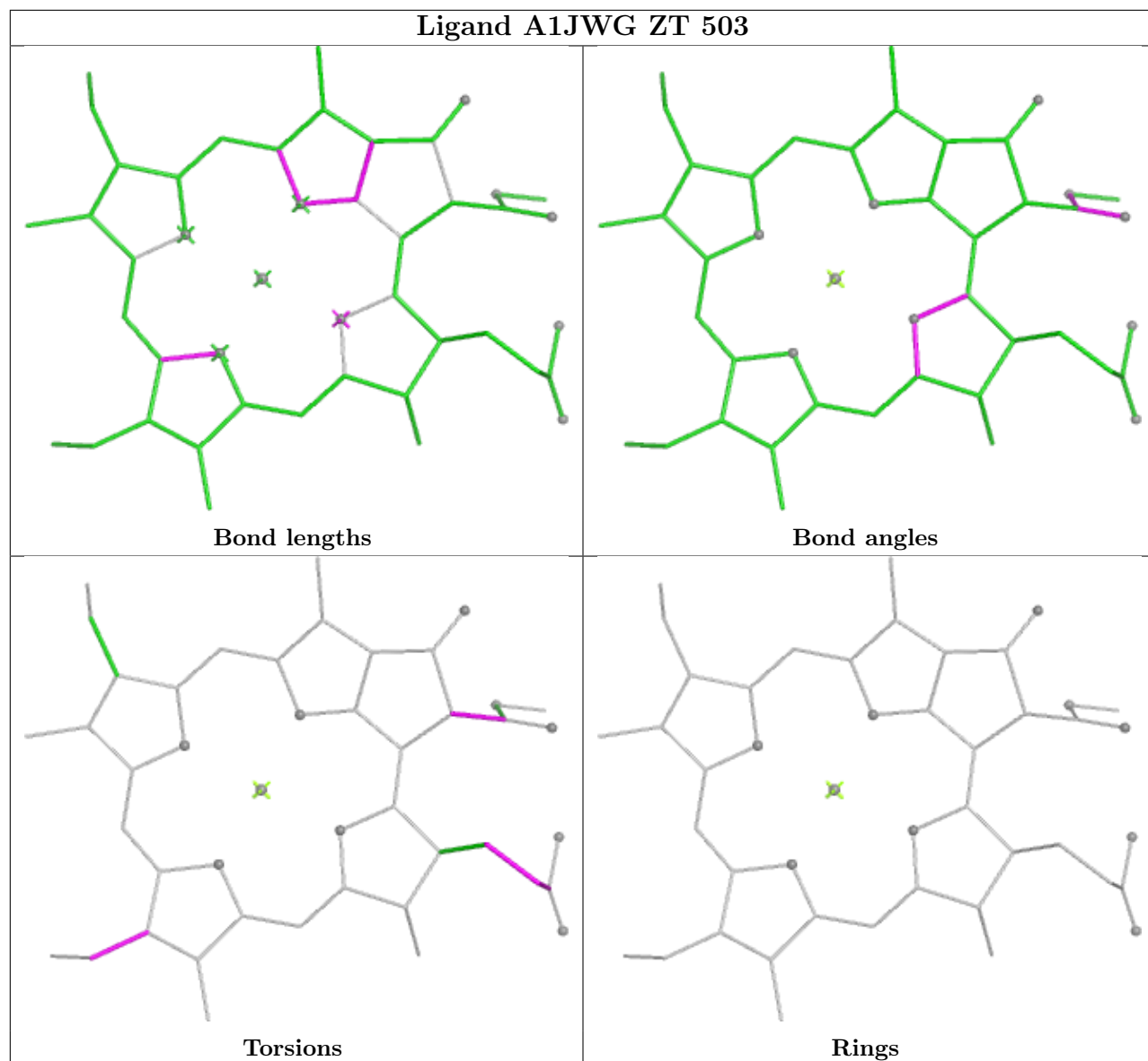


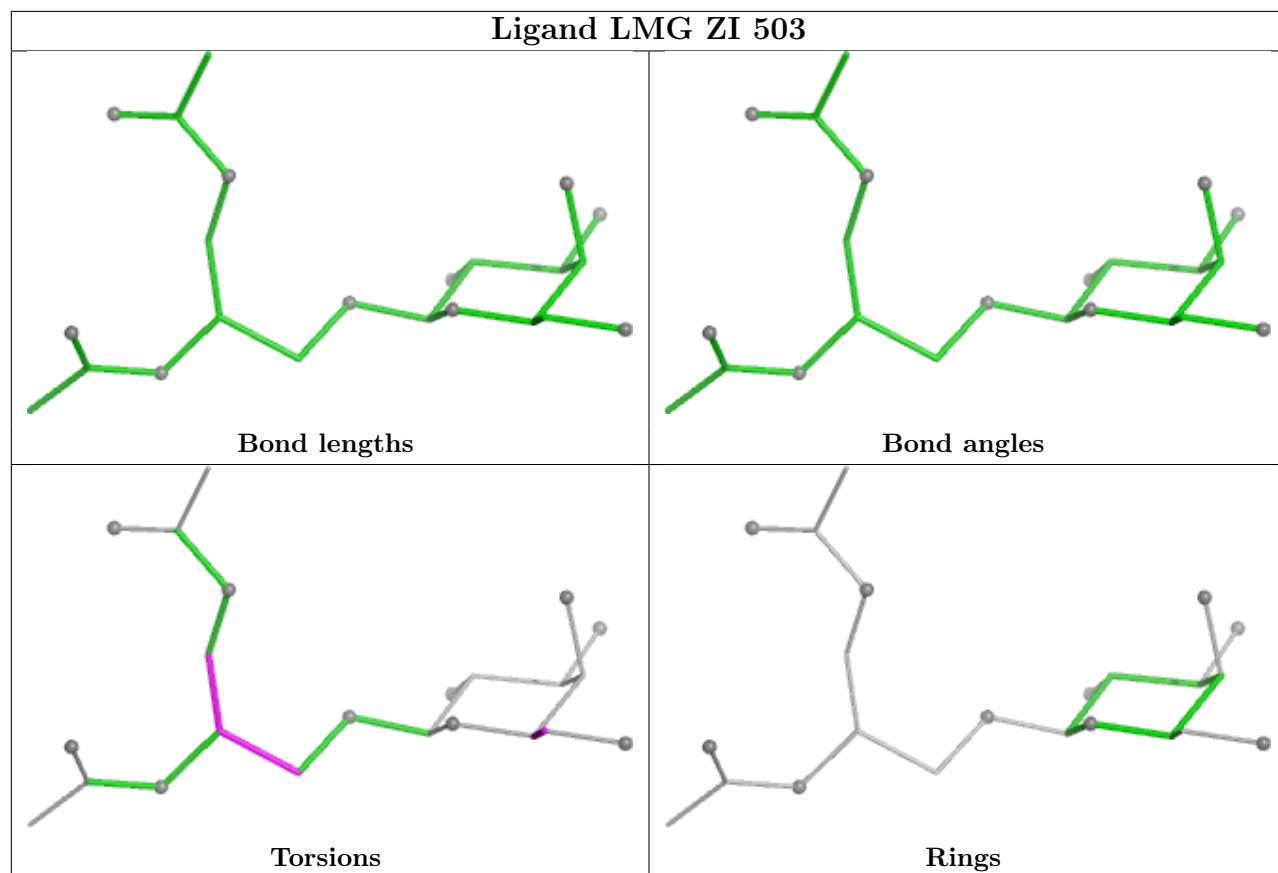
Torsions



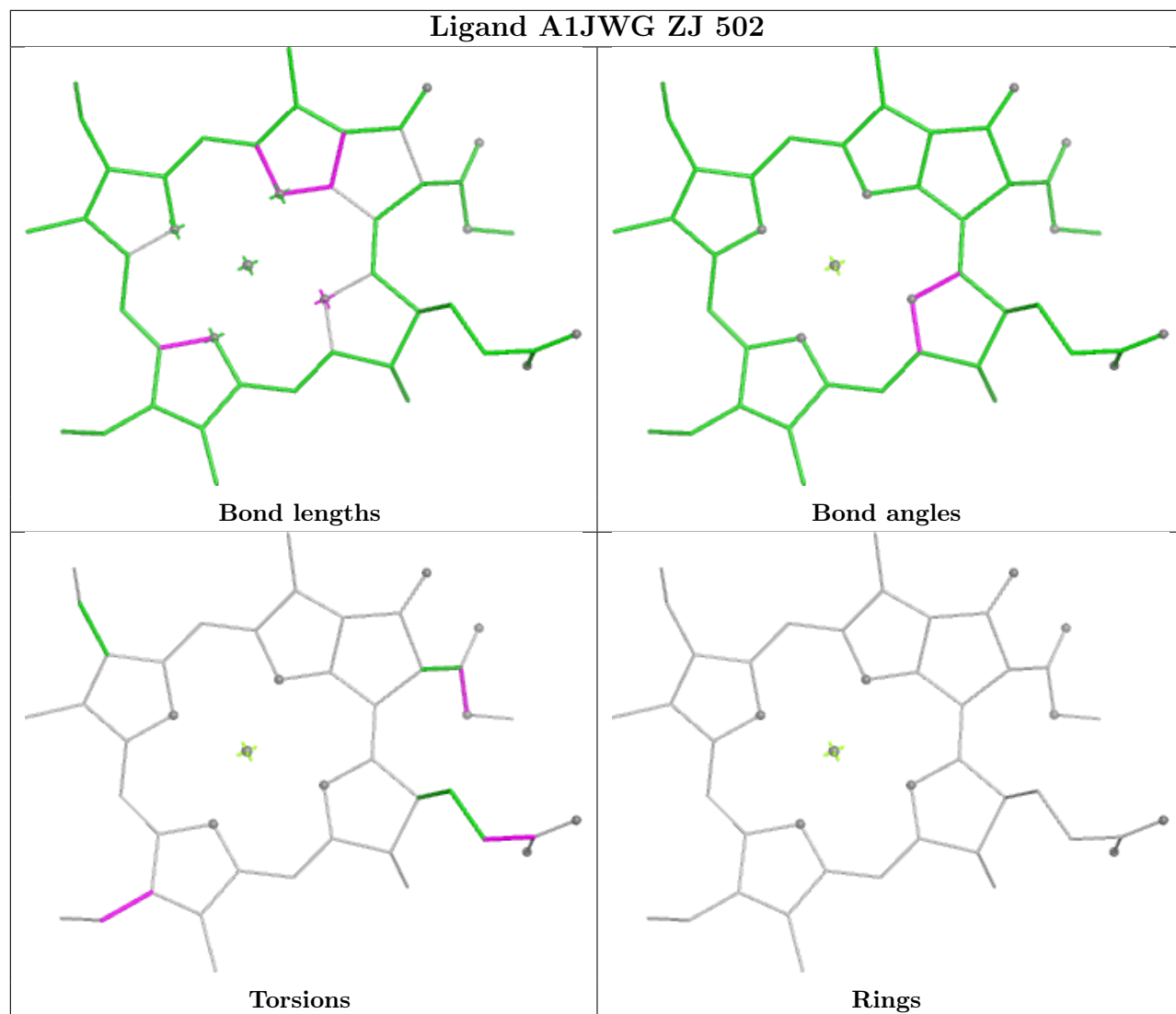
Rings

Ligand A1JWG ZT 503

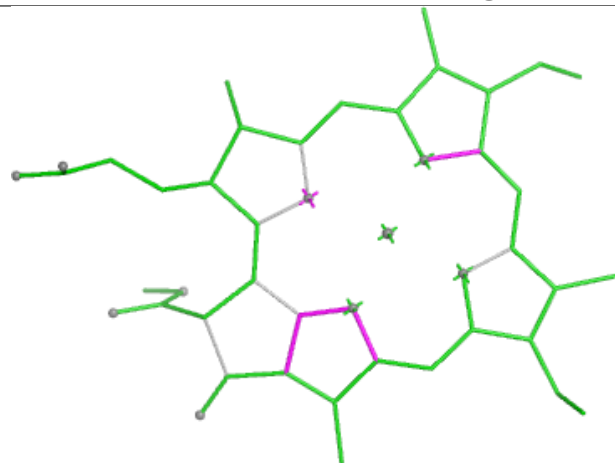




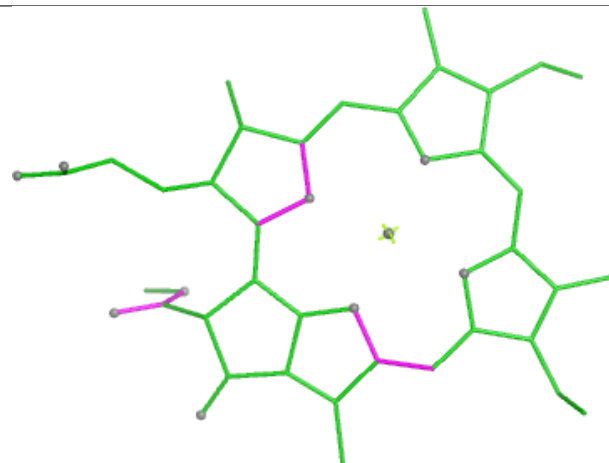
Ligand A1JWG ZJ 502



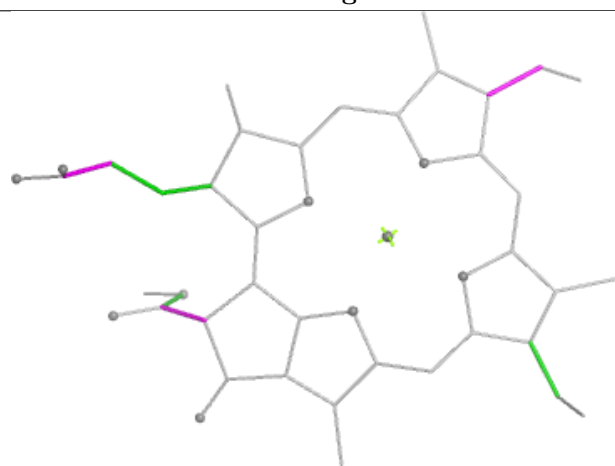
Ligand A1JWG ZF 502



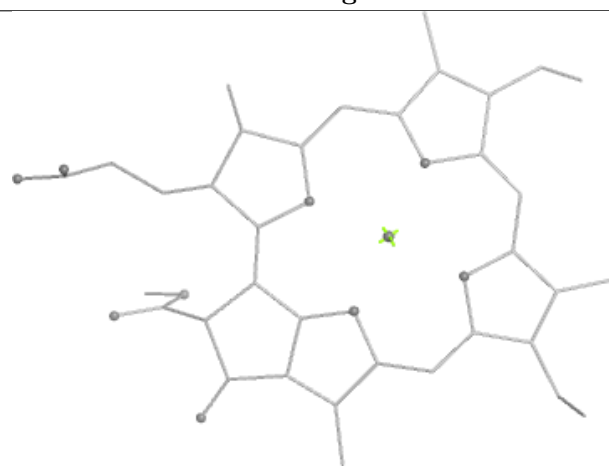
Bond lengths



Bond angles

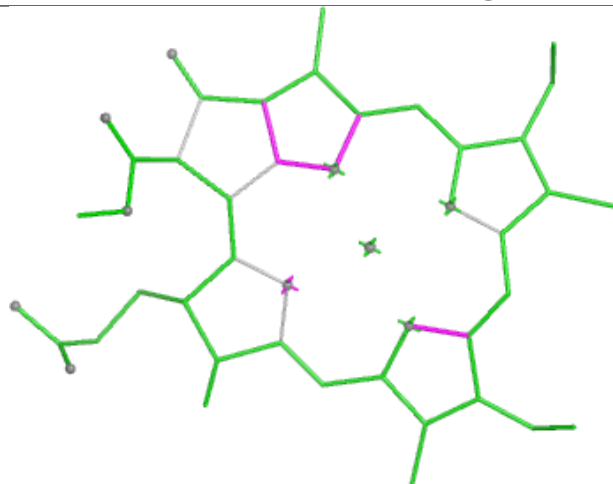


Torsions

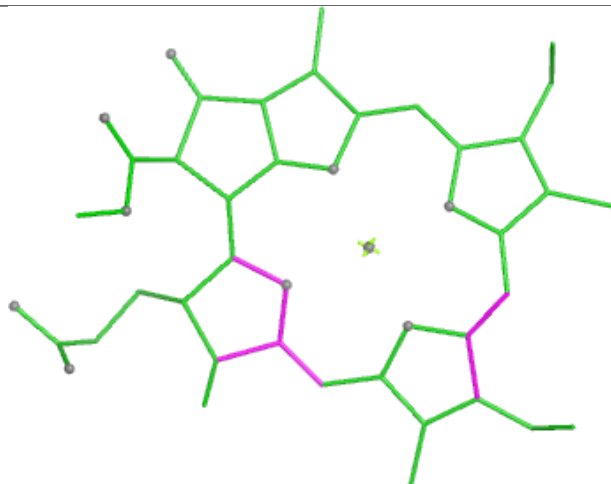


Rings

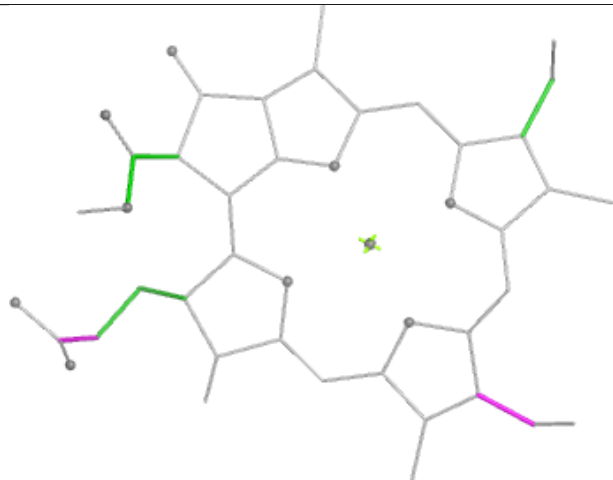
Ligand A1JWG ZS 502



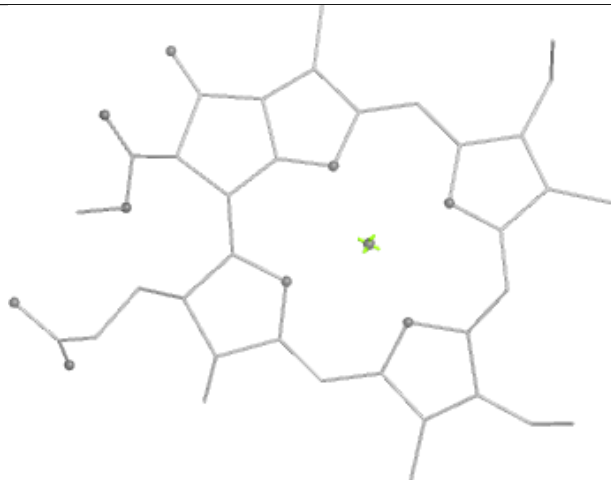
Bond lengths



Bond angles

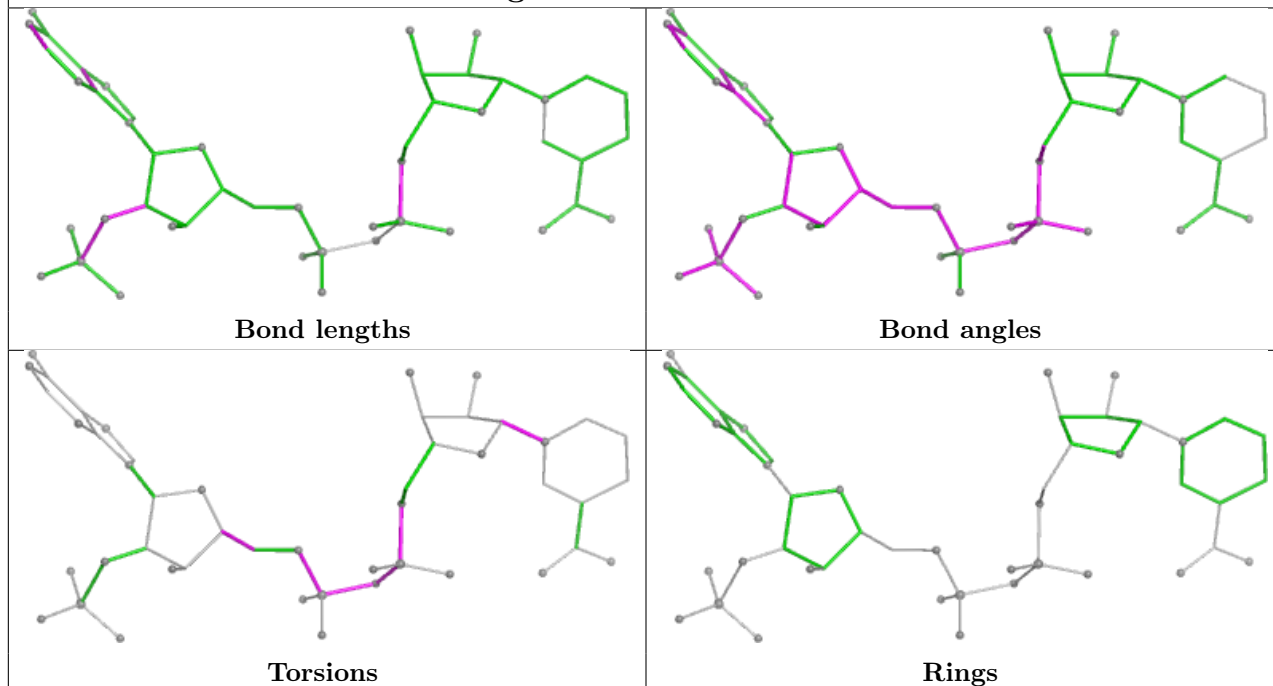


Torsions

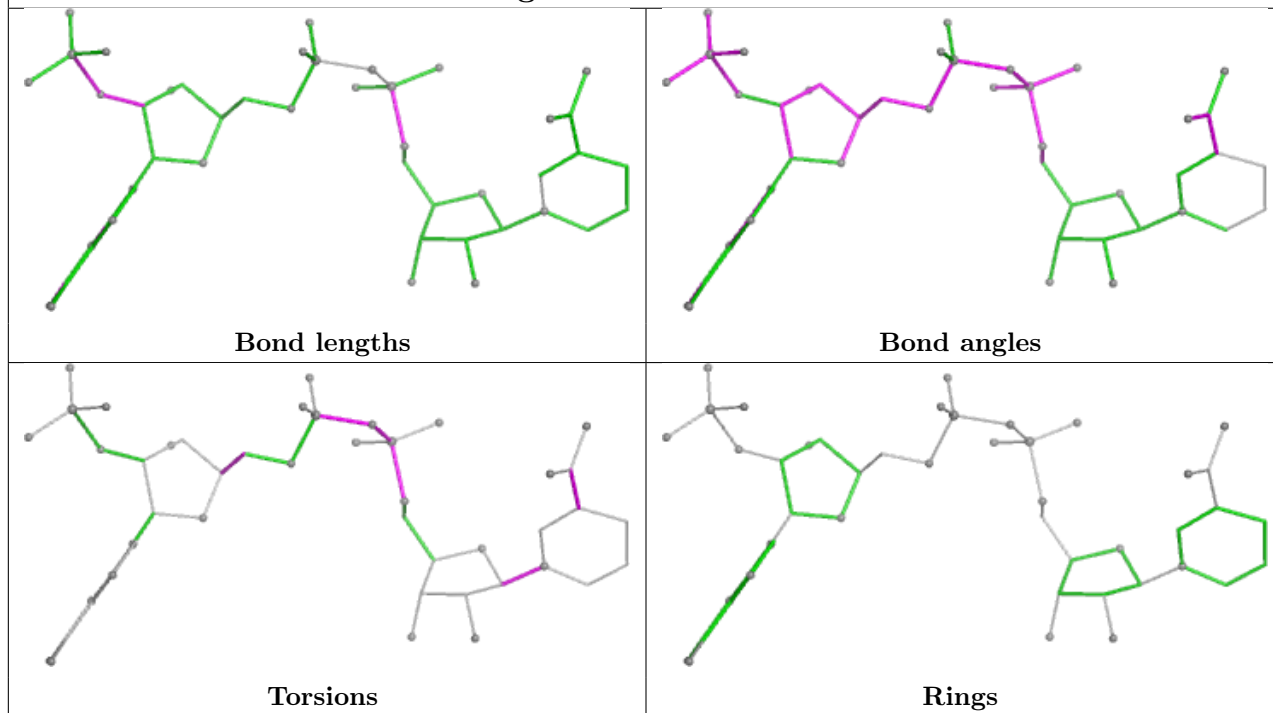


Rings

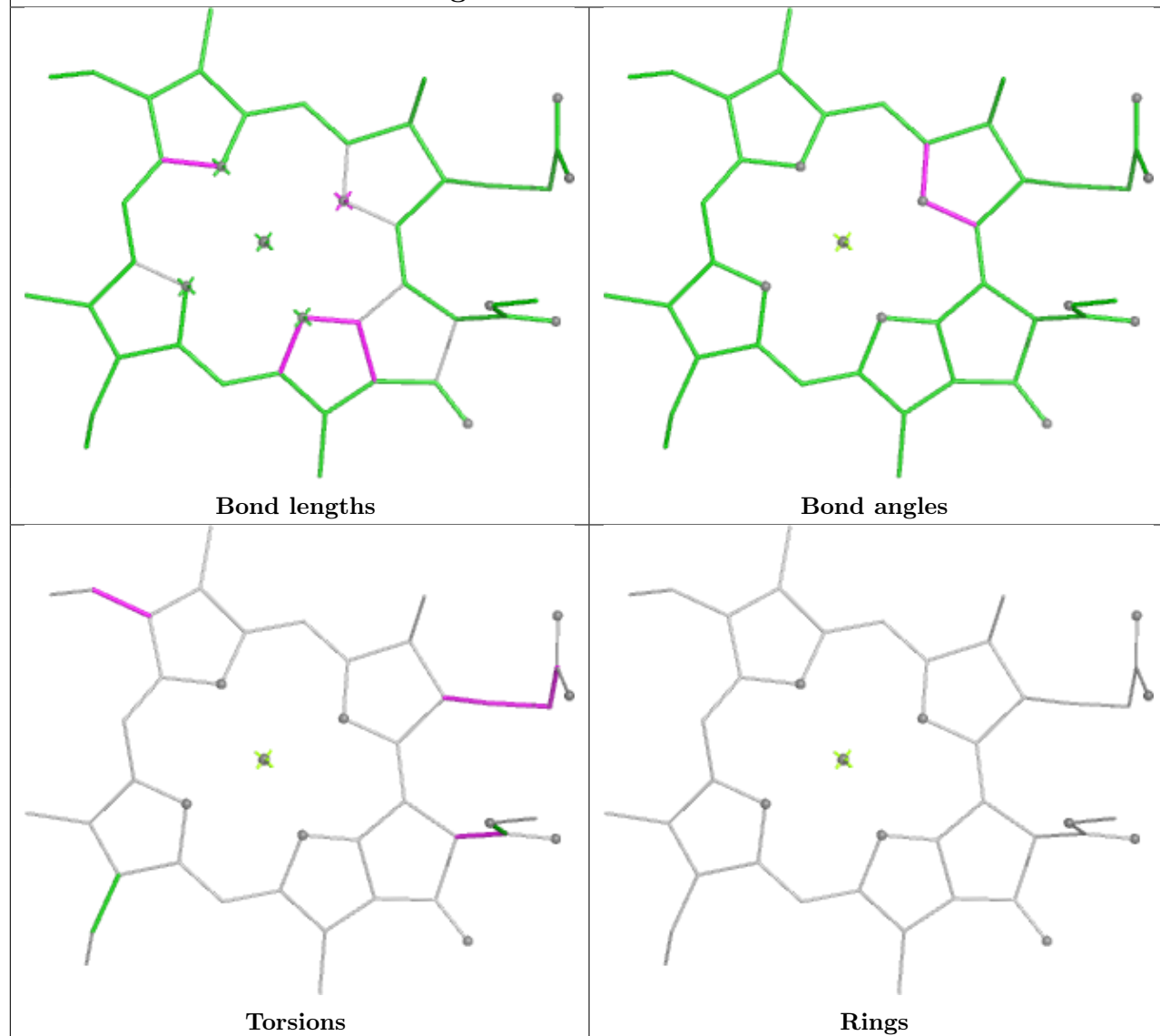
Ligand NDP YW 501



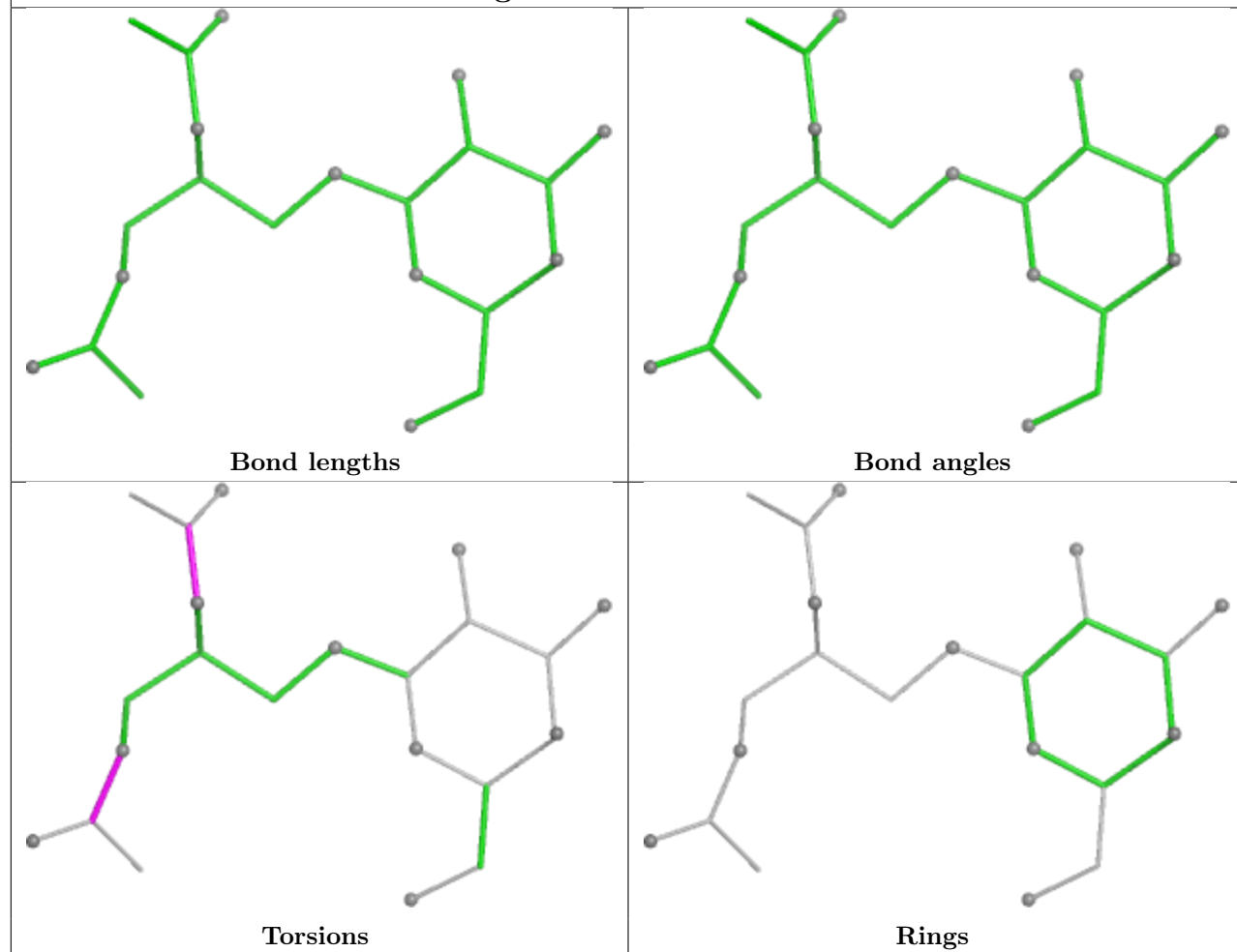
Ligand NDP ZZ 501



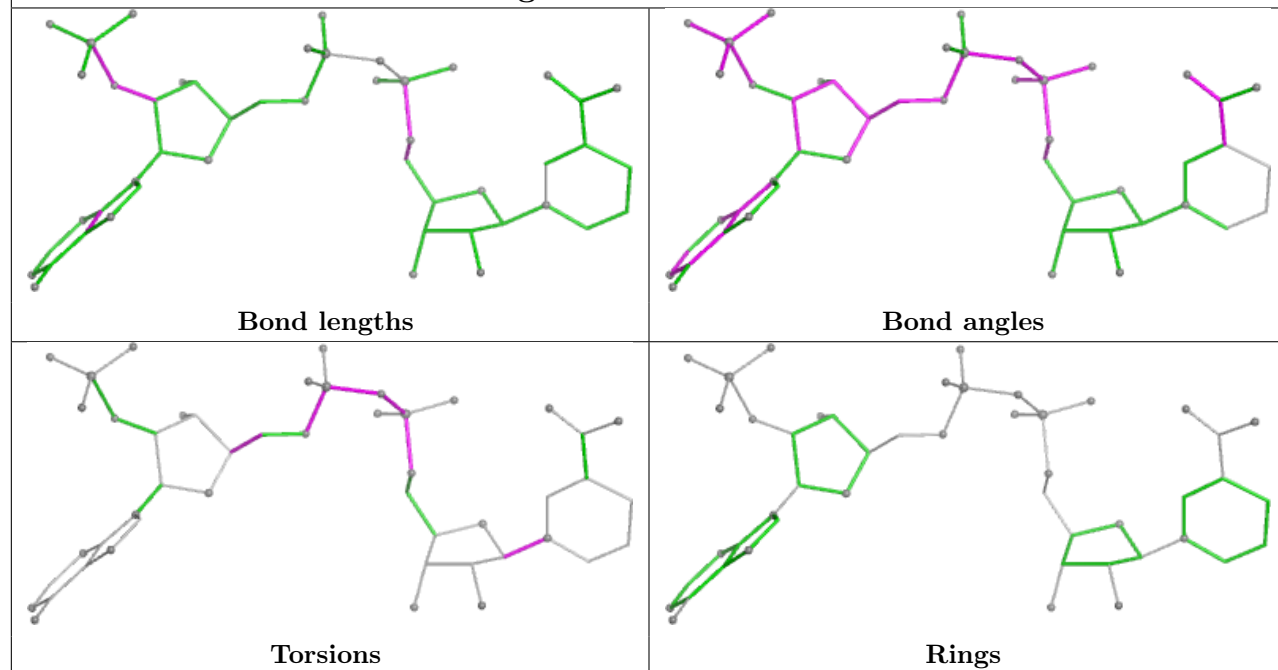
Ligand A1JWG ZE 502



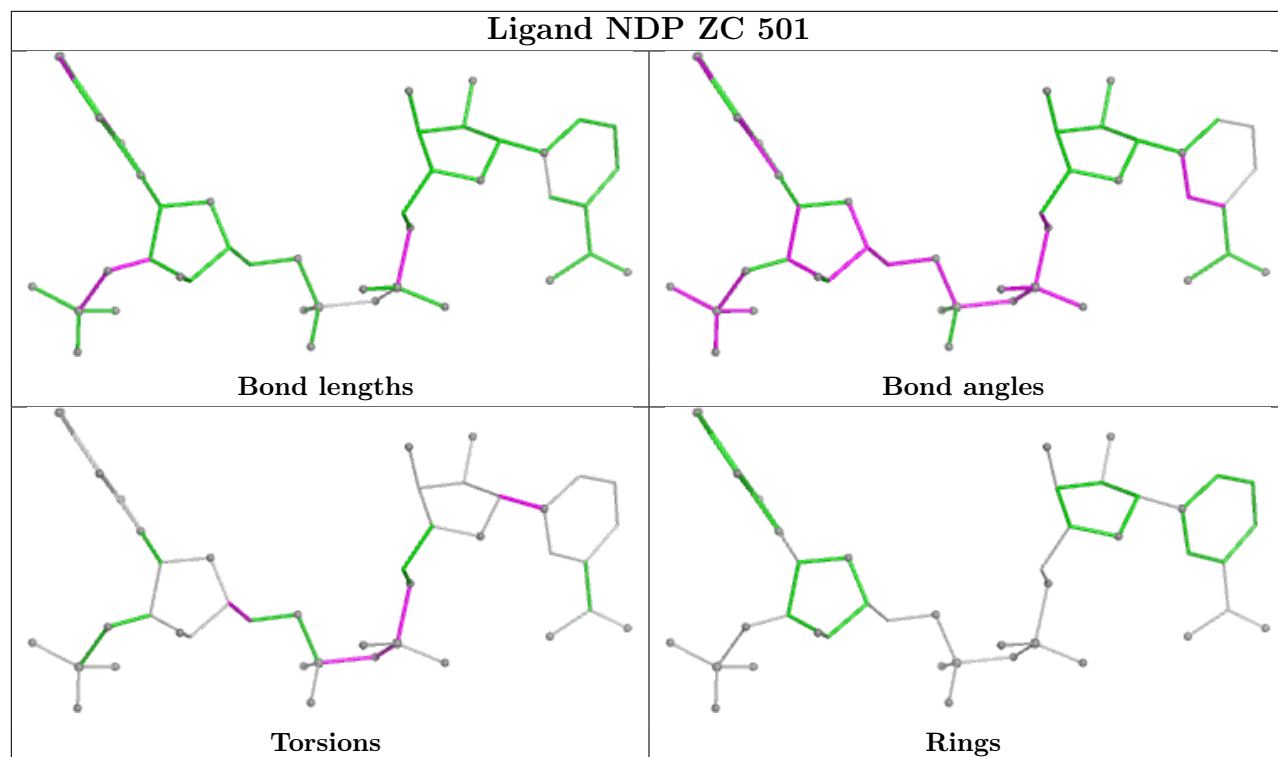
Ligand LMG ZW 503



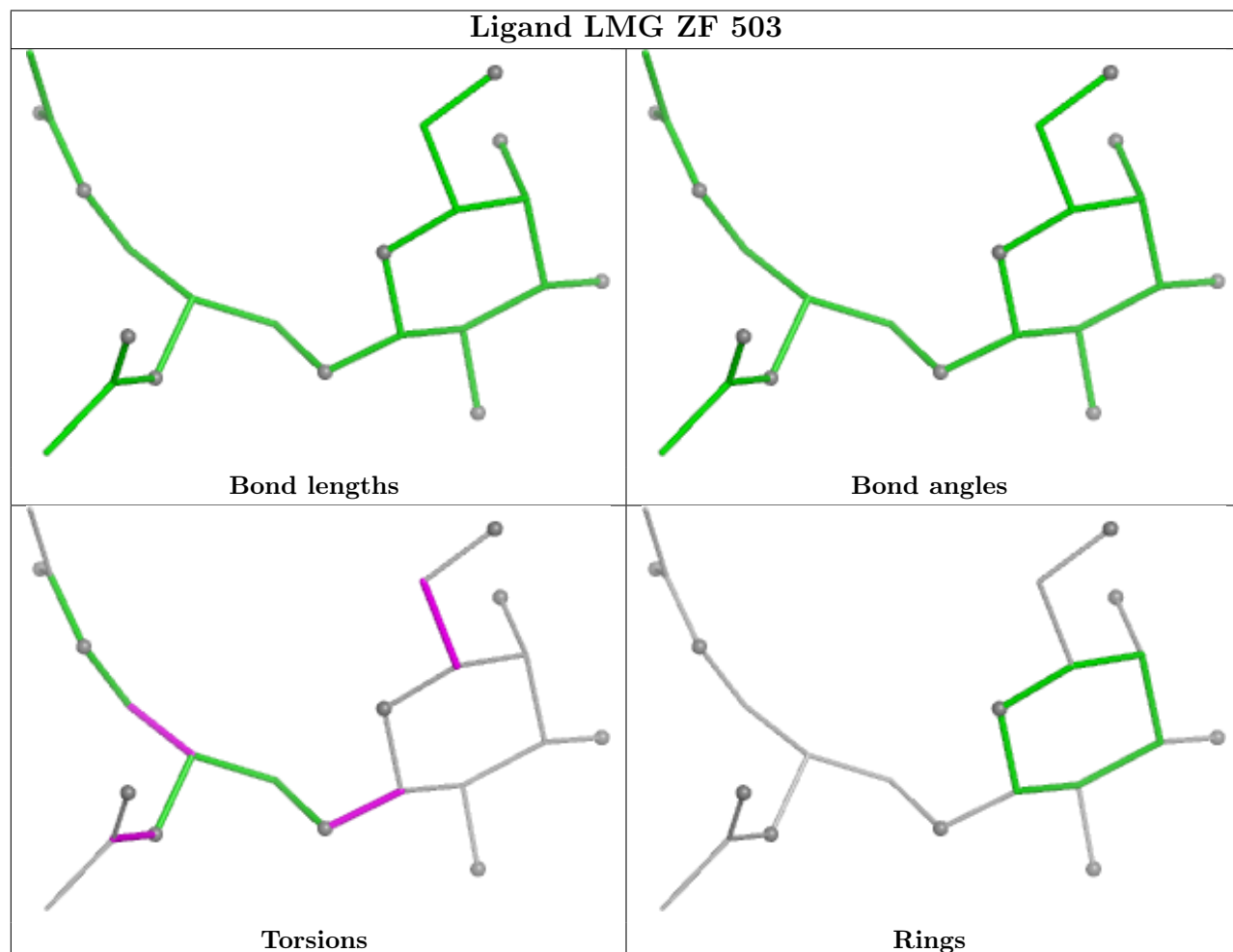
Ligand NDP ZX 501

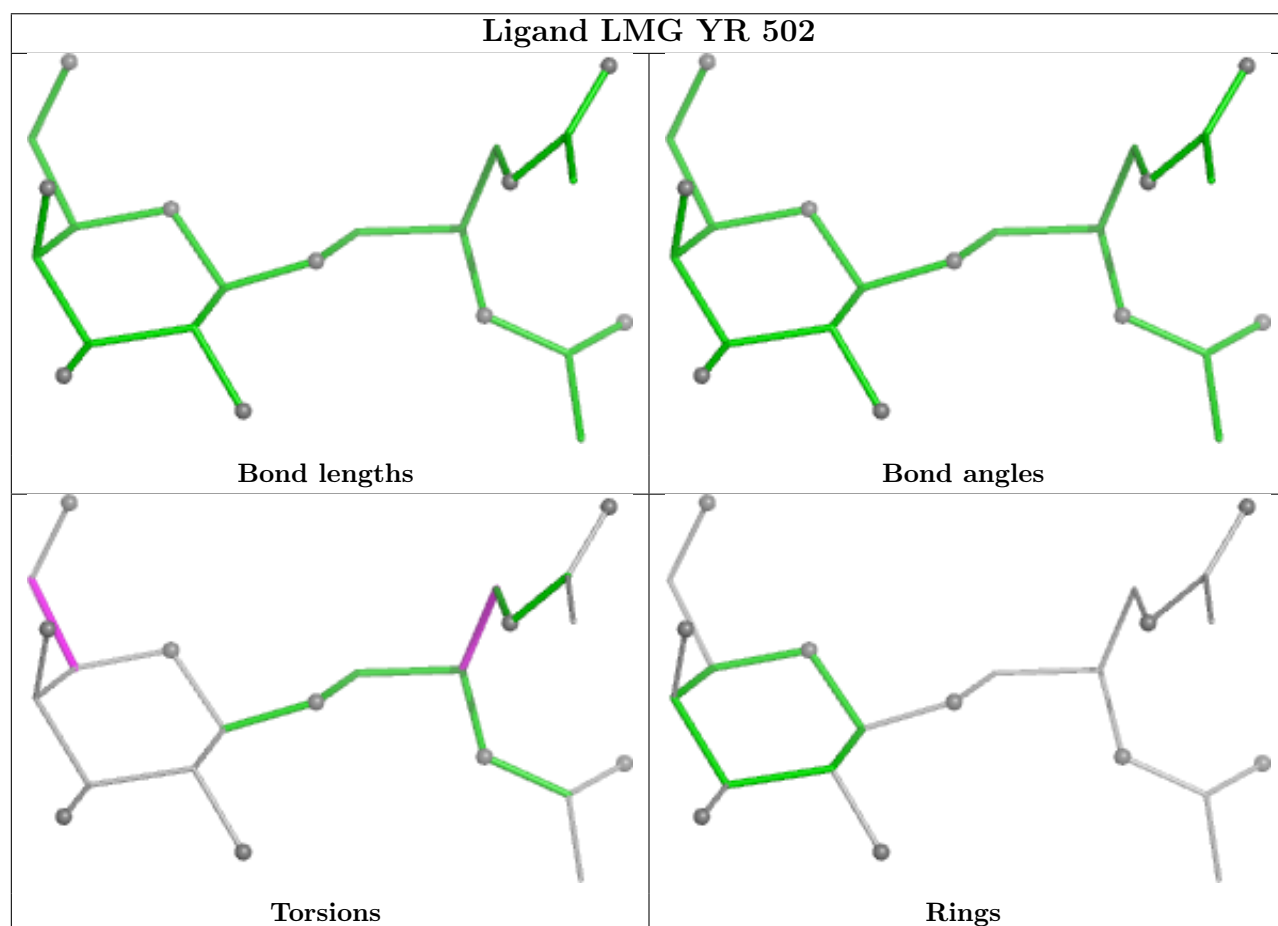
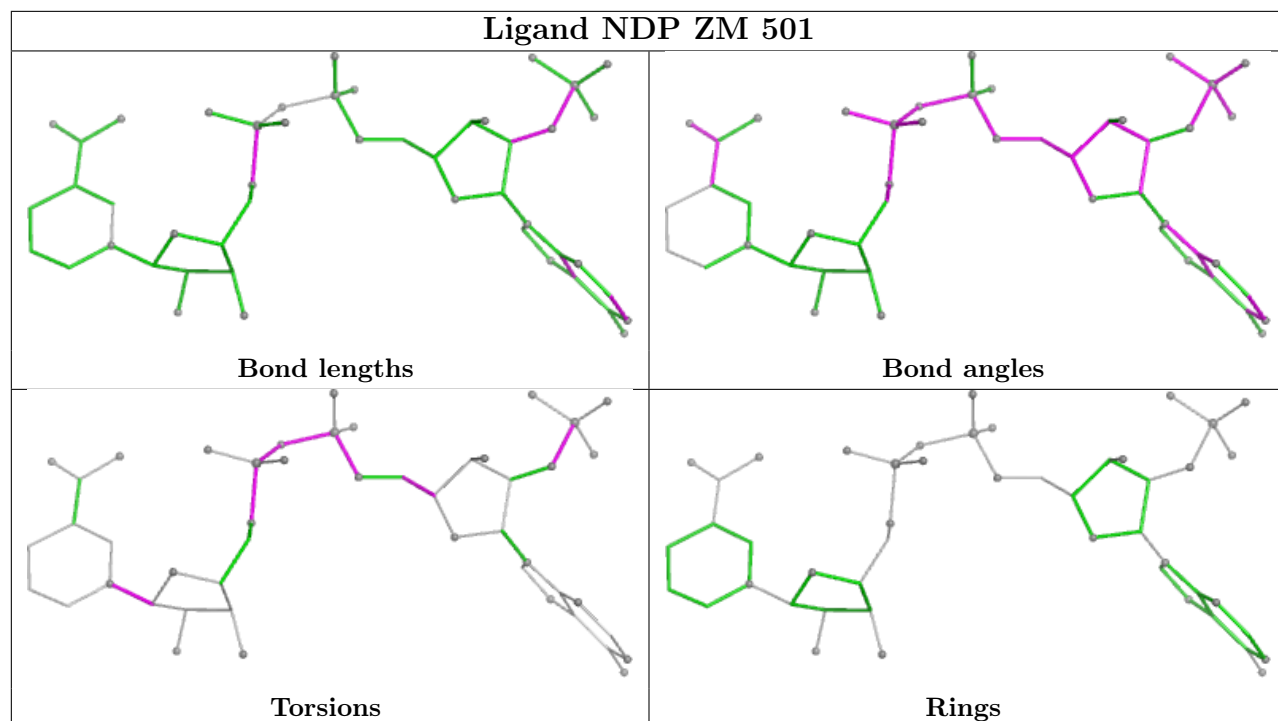


Ligand NDP ZC 501

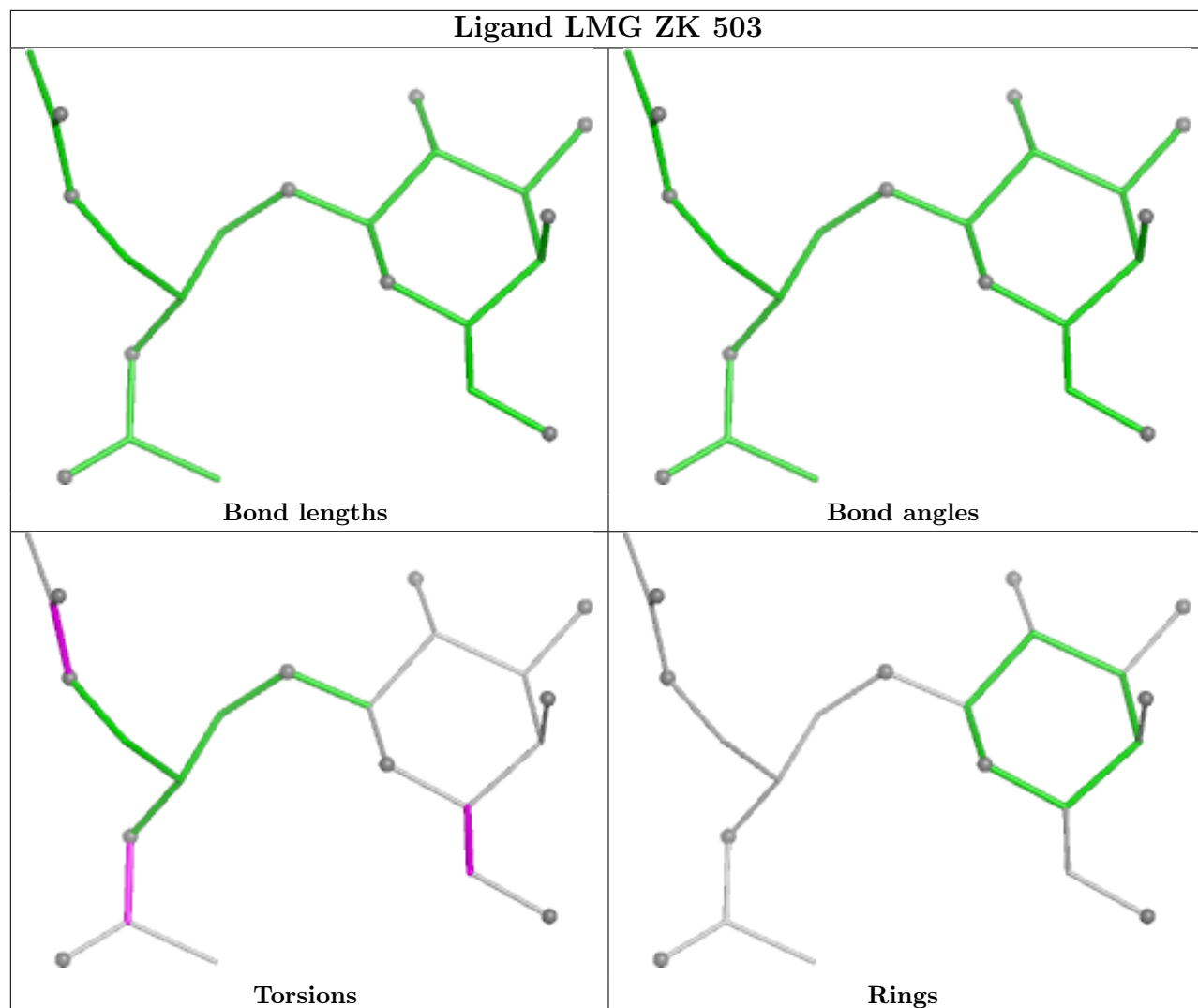


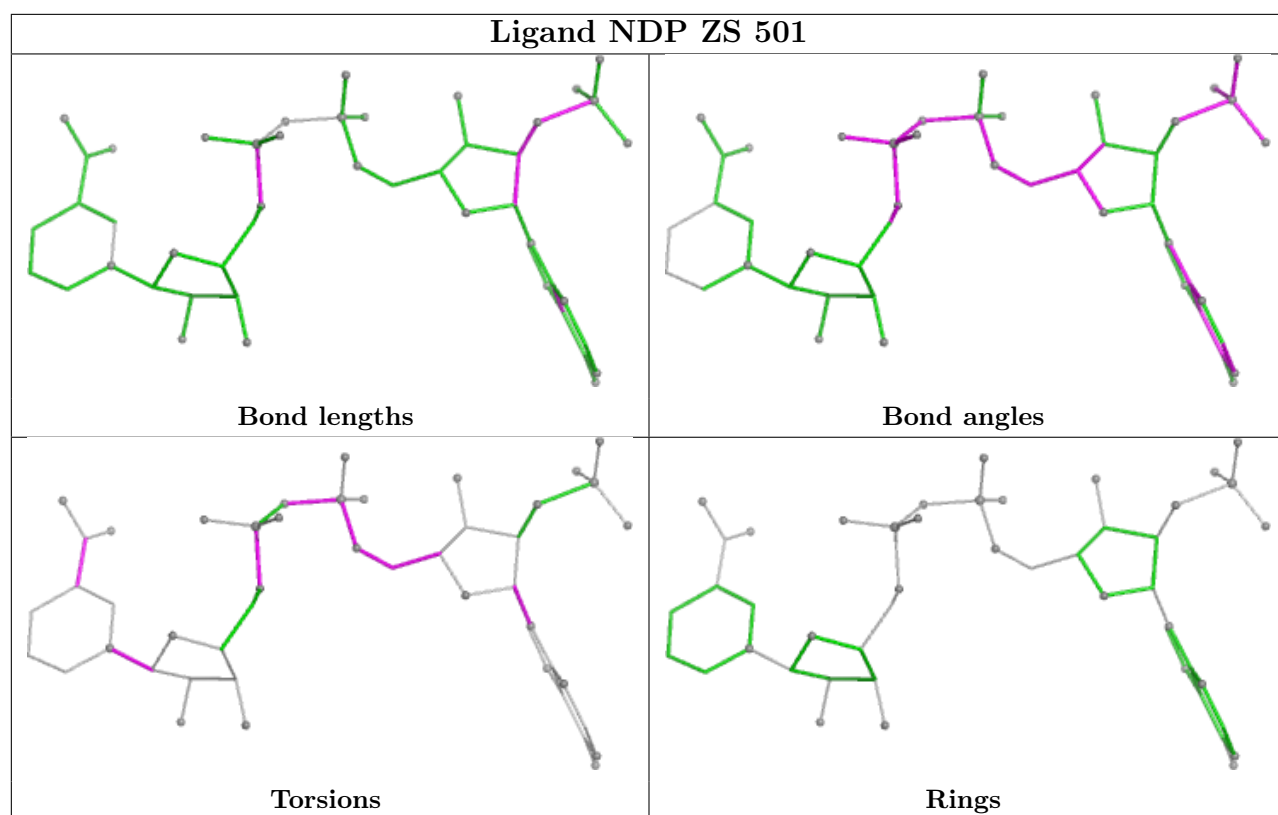
Ligand LMG ZF 503



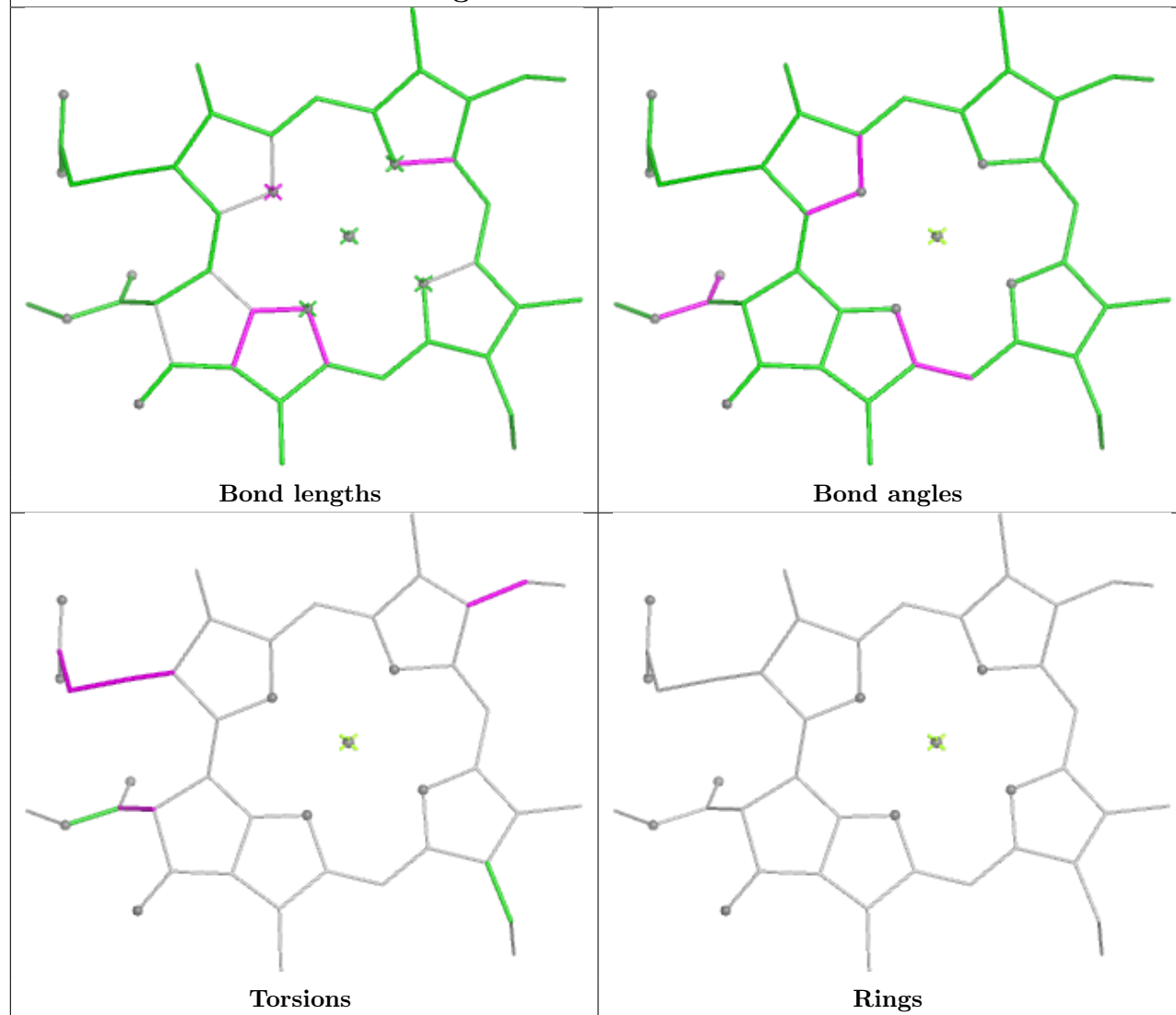


Ligand LMG ZK 503

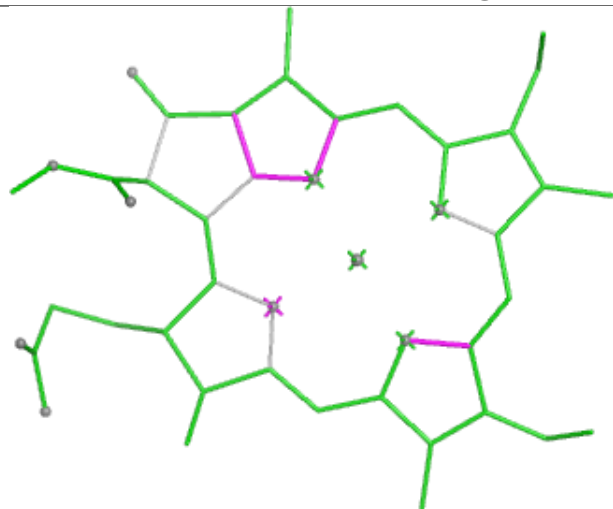




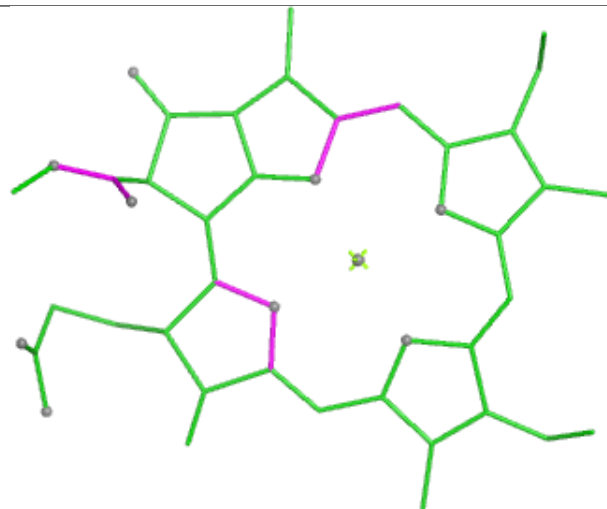
Ligand A1JWG YR 503



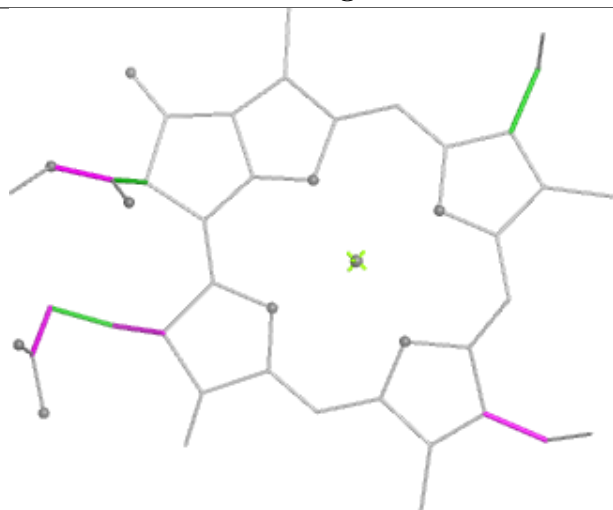
Ligand A1JWG ZY 502



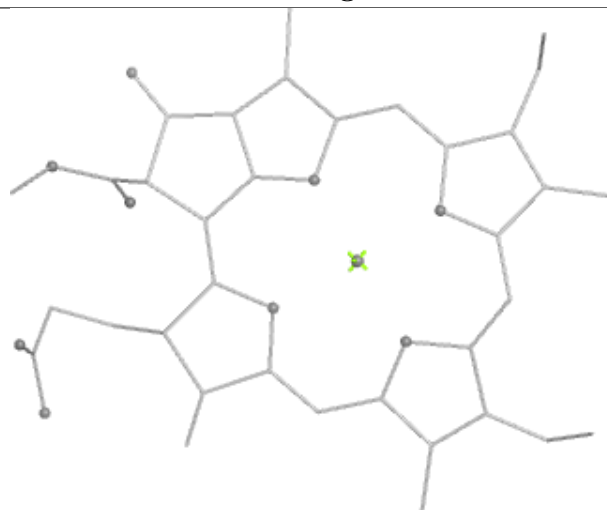
Bond lengths



Bond angles

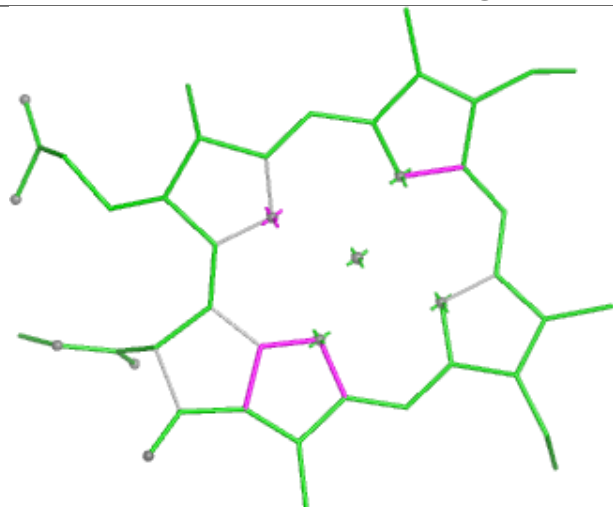


Torsions

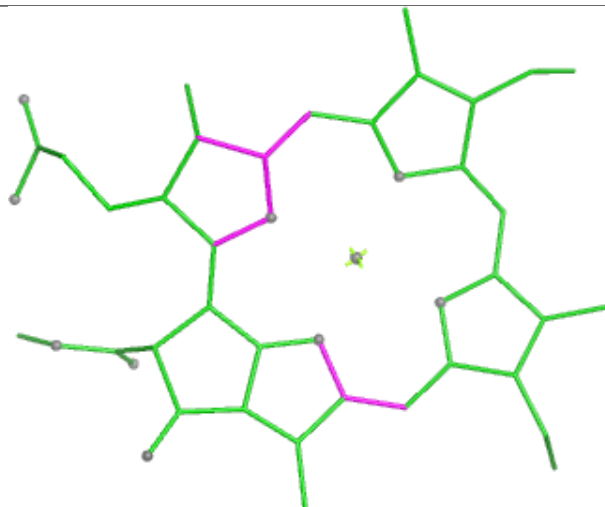


Rings

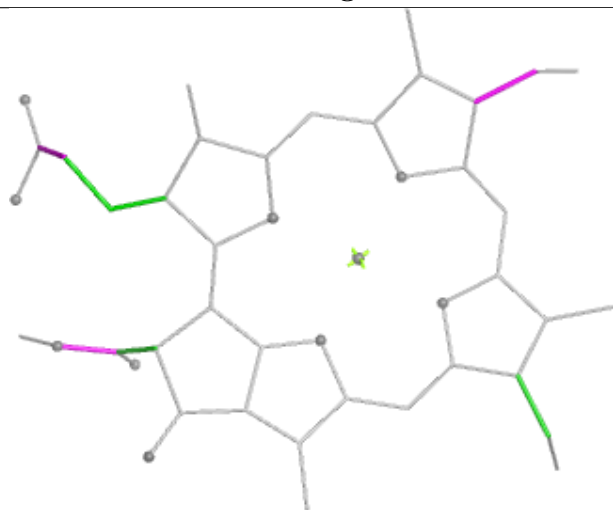
Ligand A1JWG ZO 502



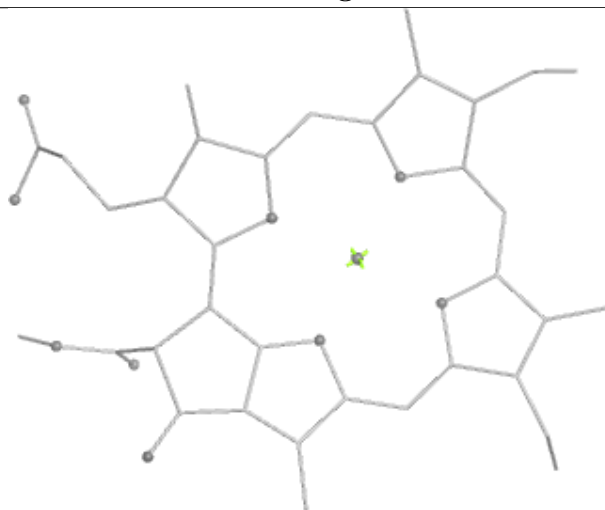
Bond lengths



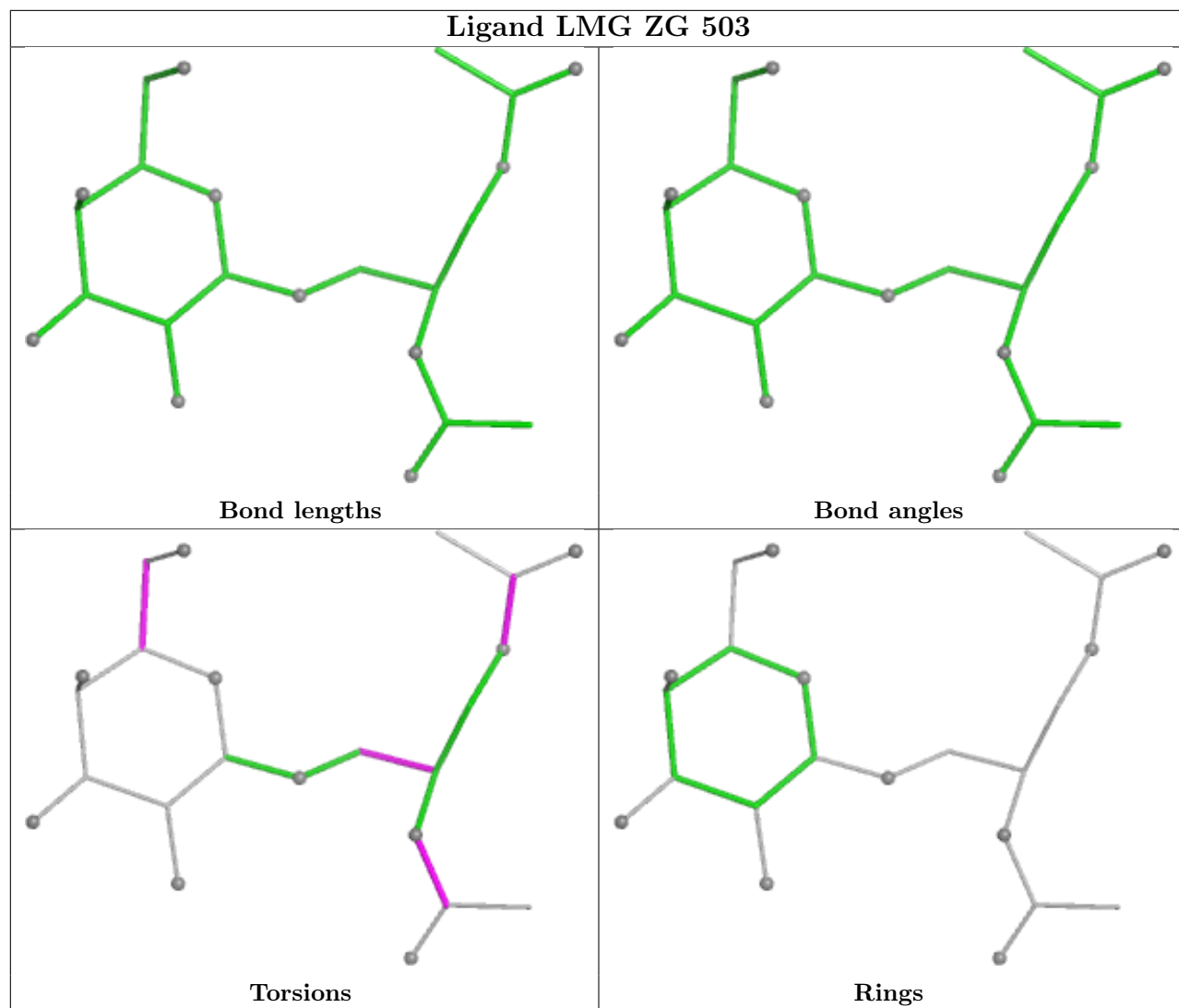
Bond angles

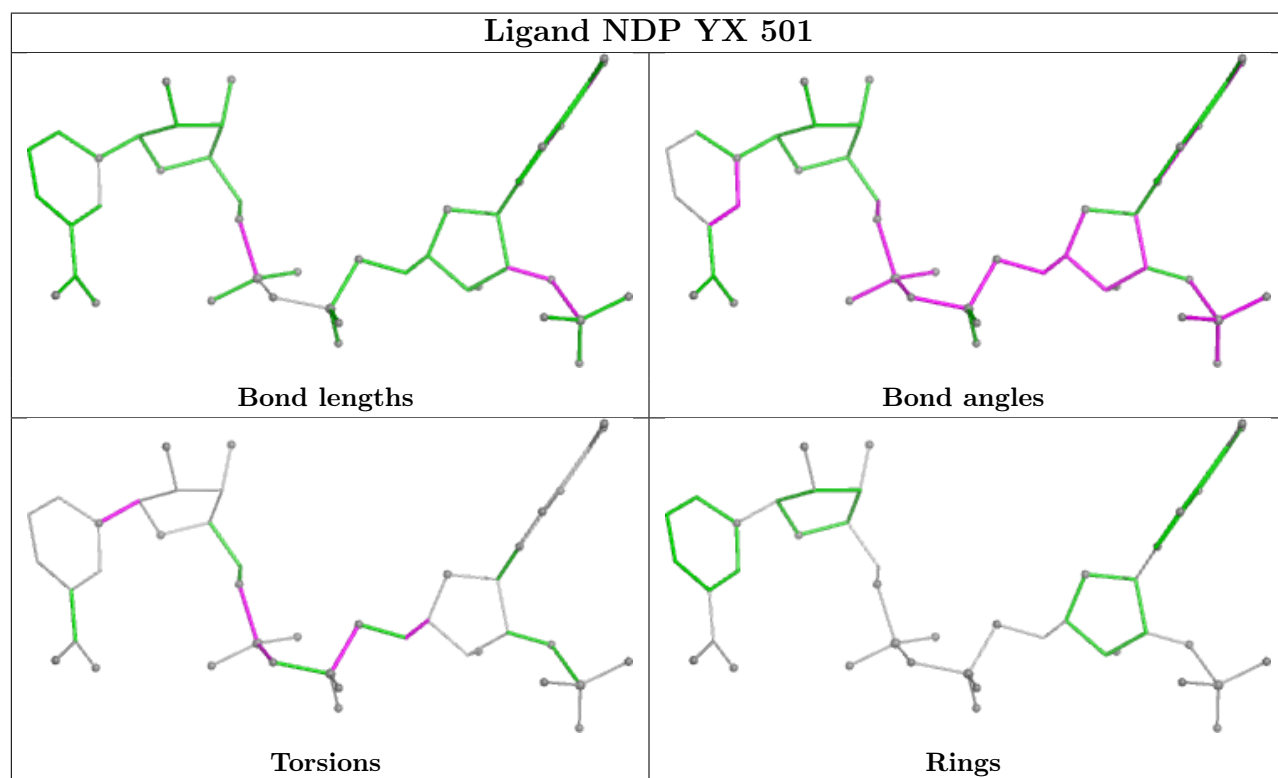
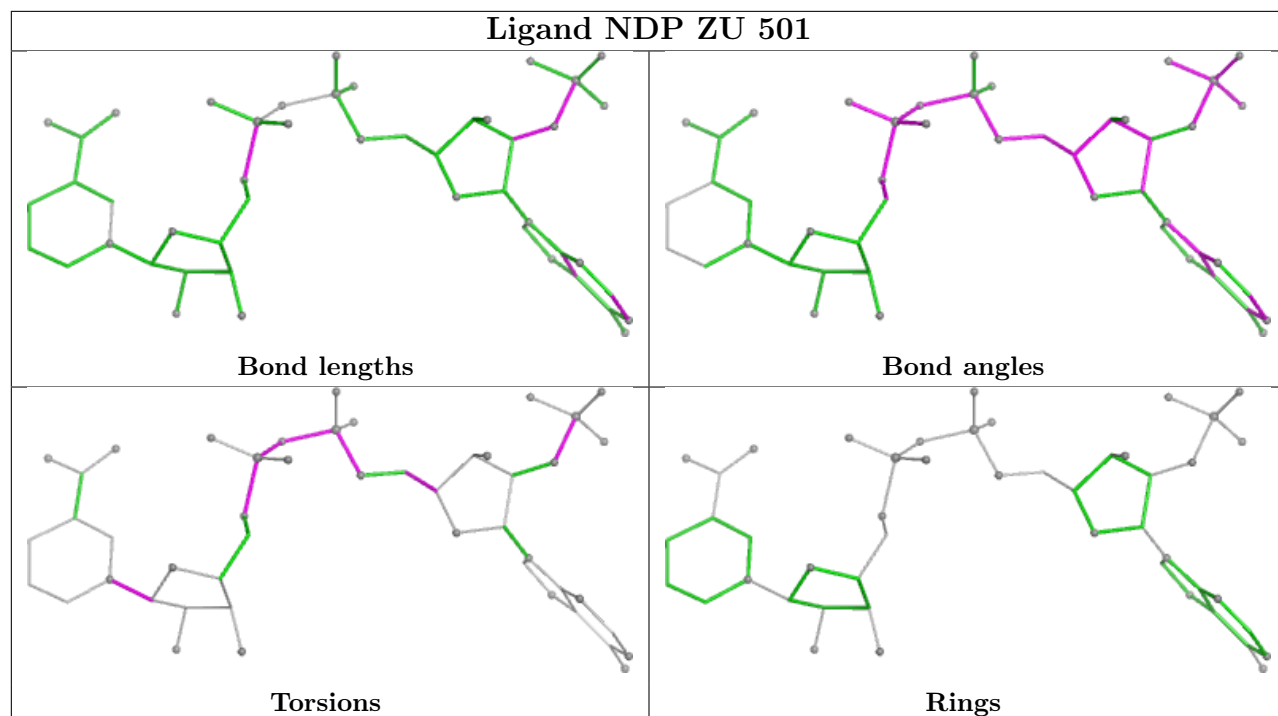


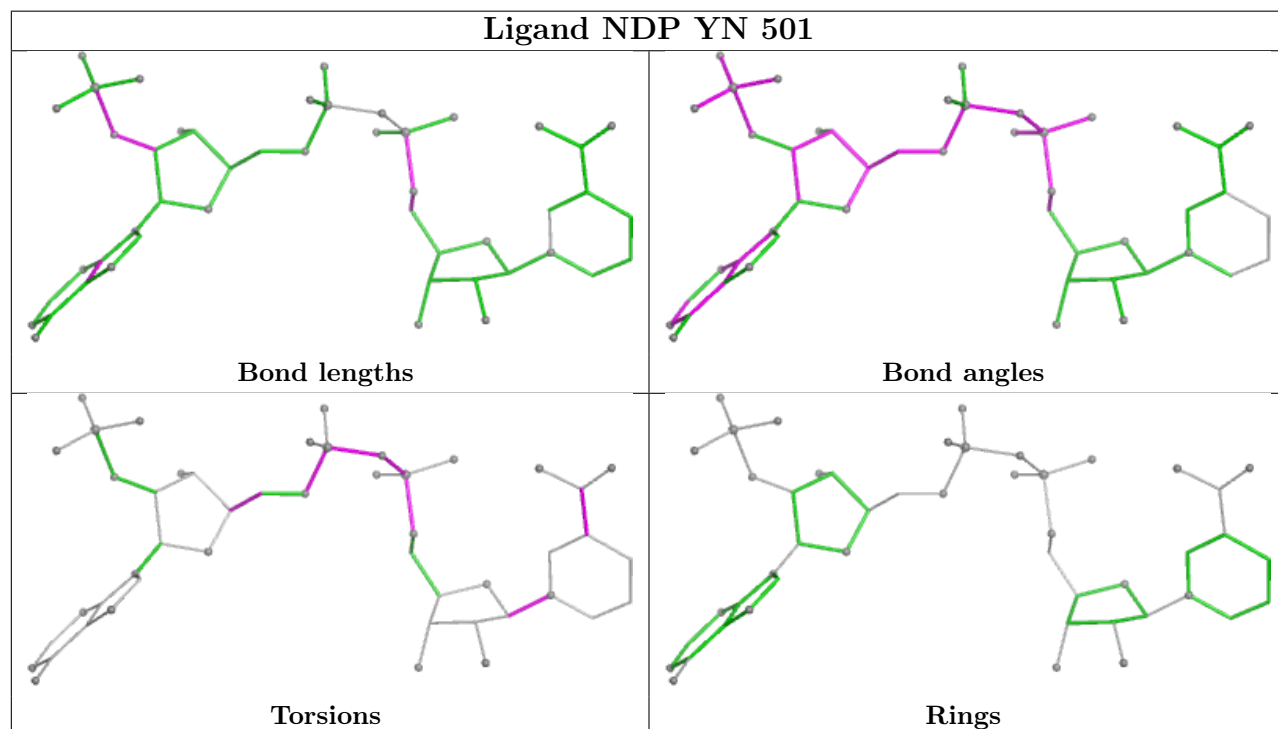
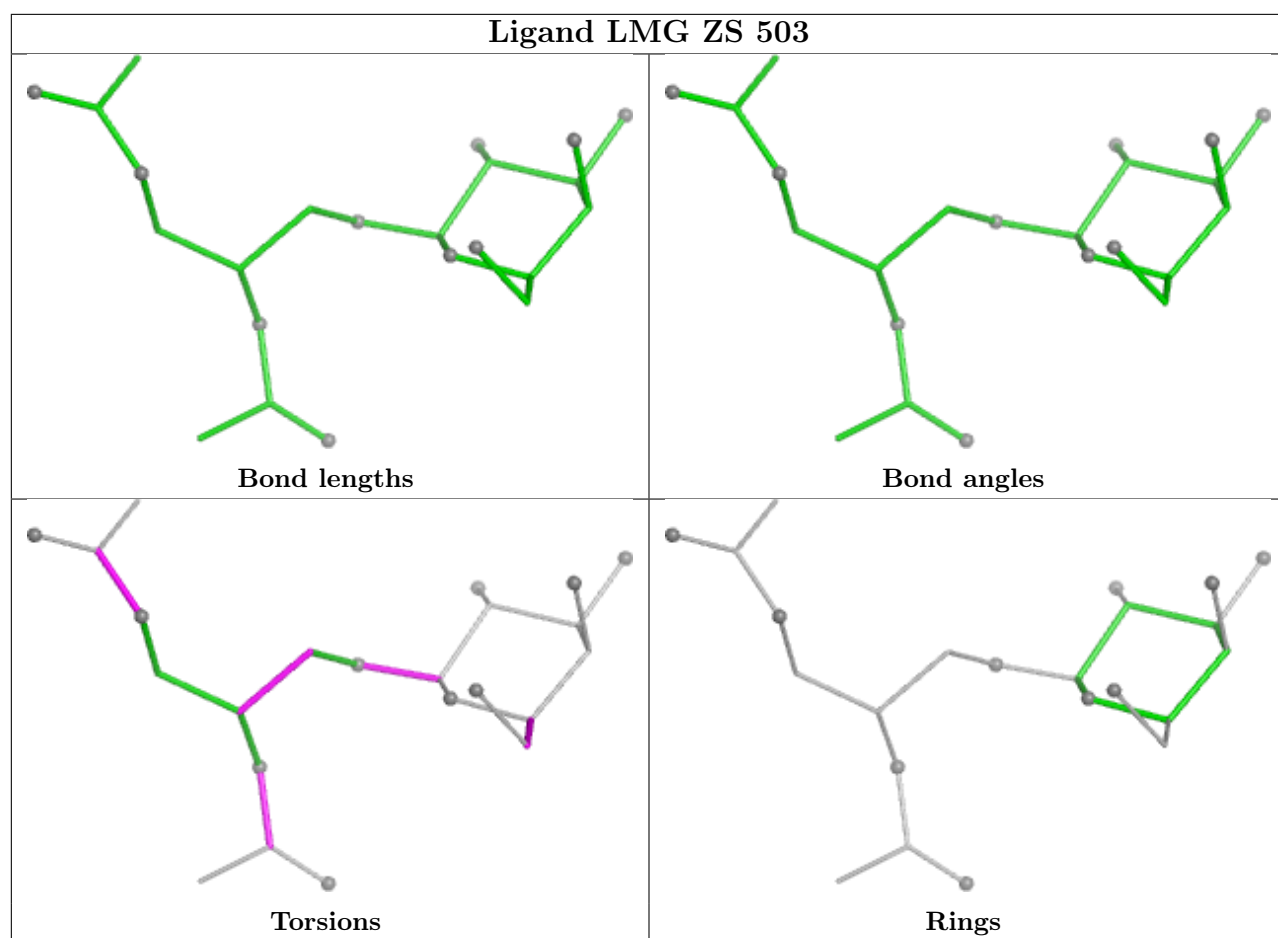
Torsions



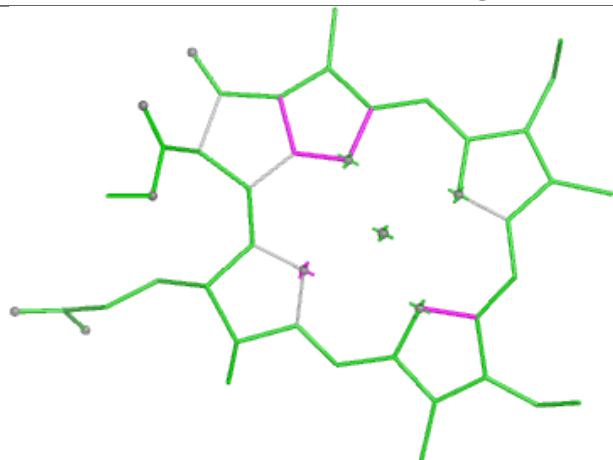
Rings



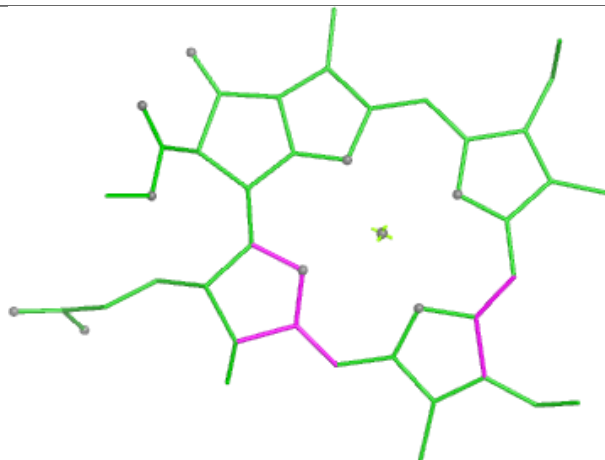




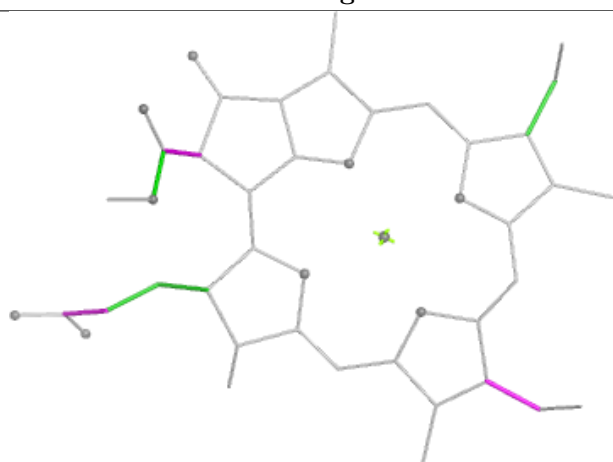
Ligand A1JWG YY 502



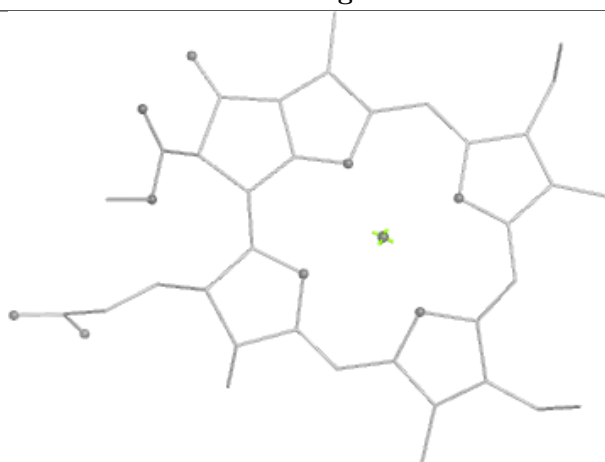
Bond lengths



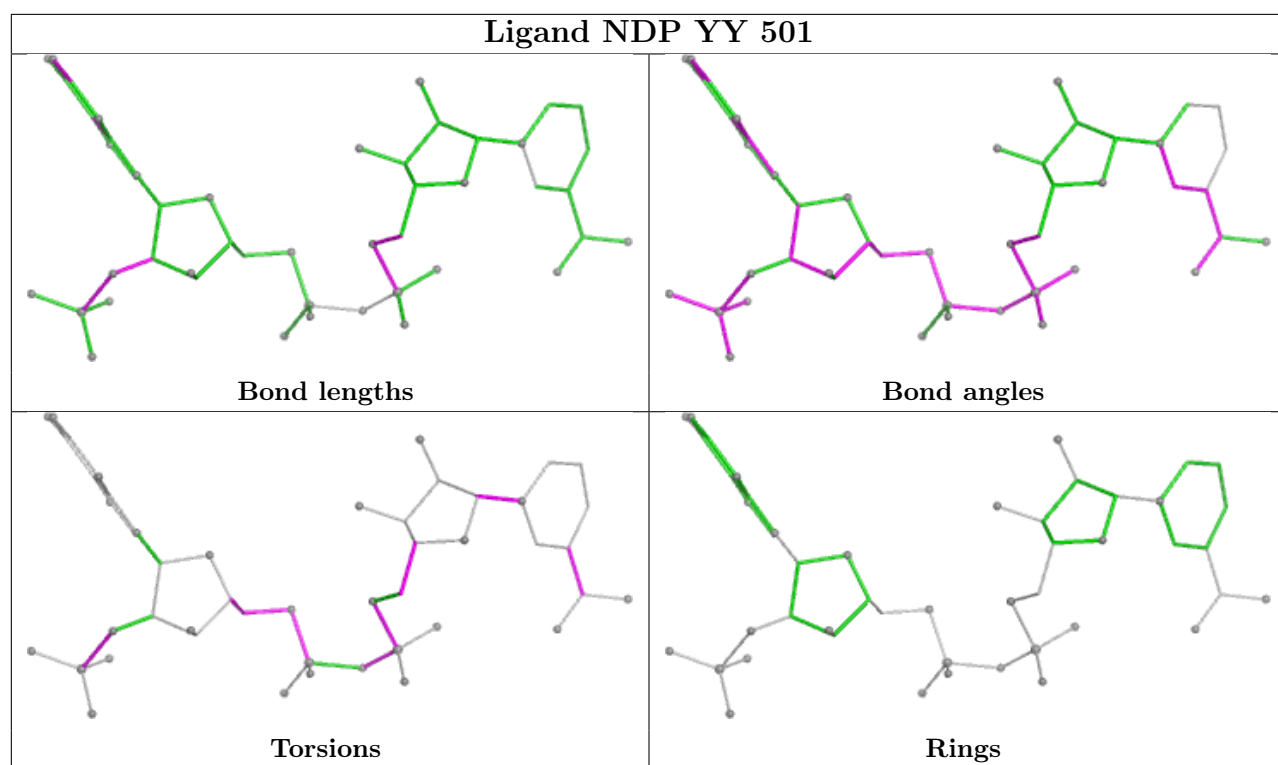
Bond angles



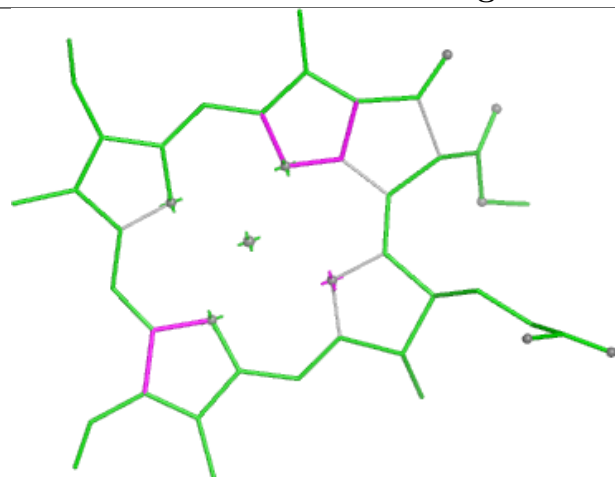
Torsions



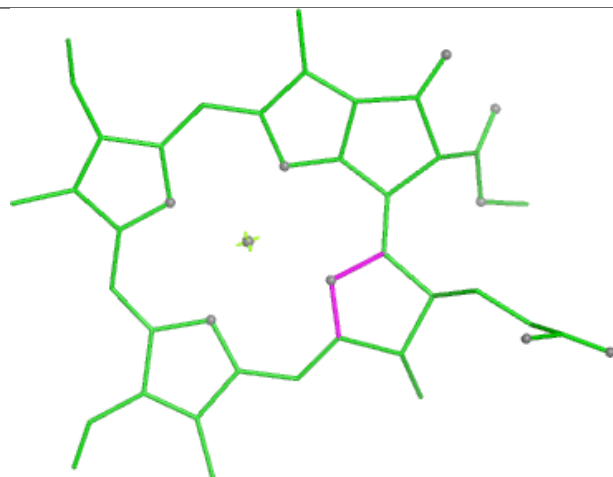
Rings



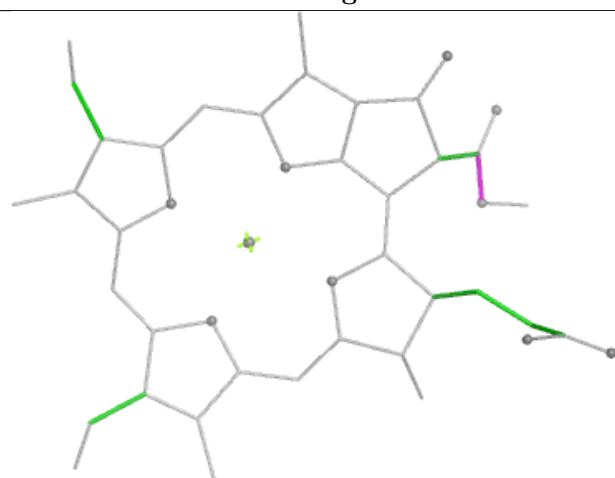
Ligand A1JWG ZN 502



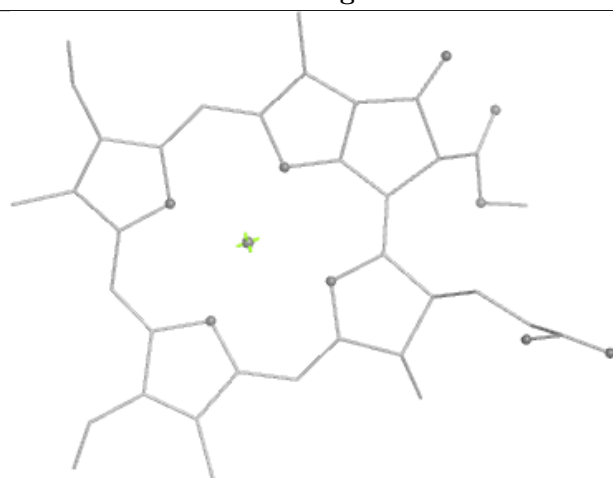
Bond lengths



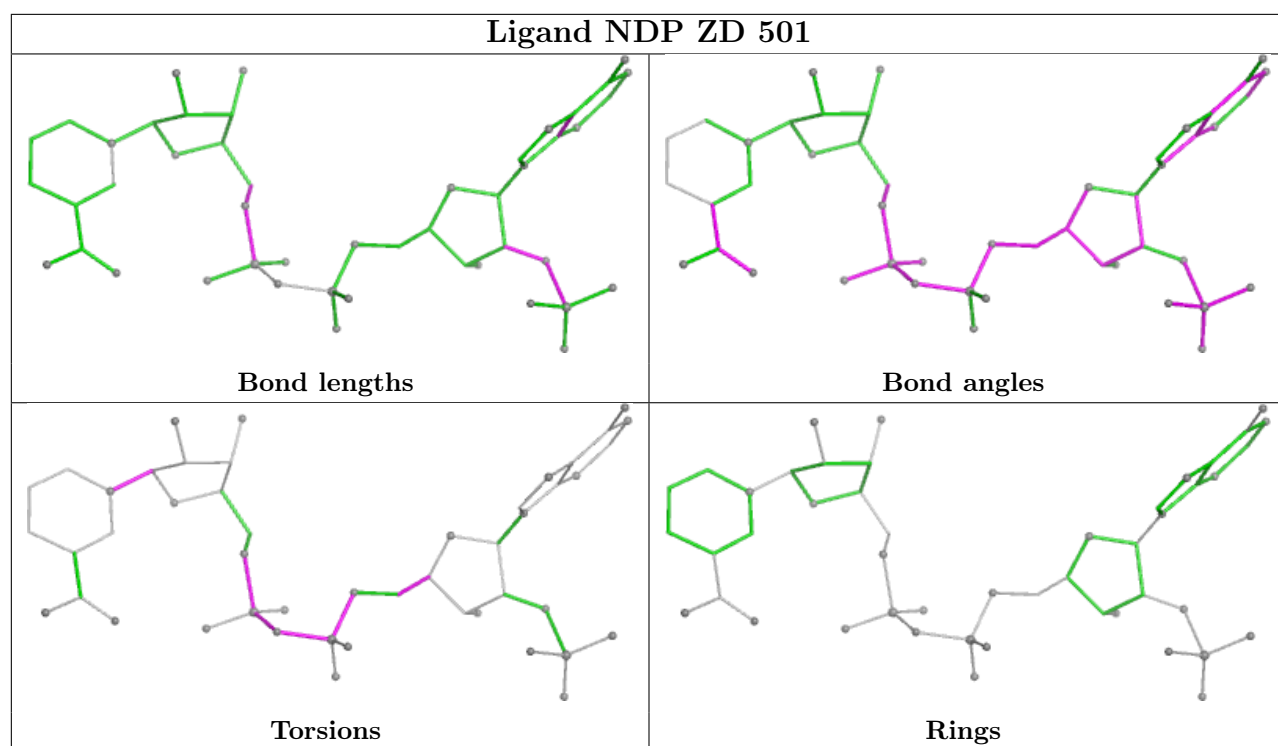
Bond angles



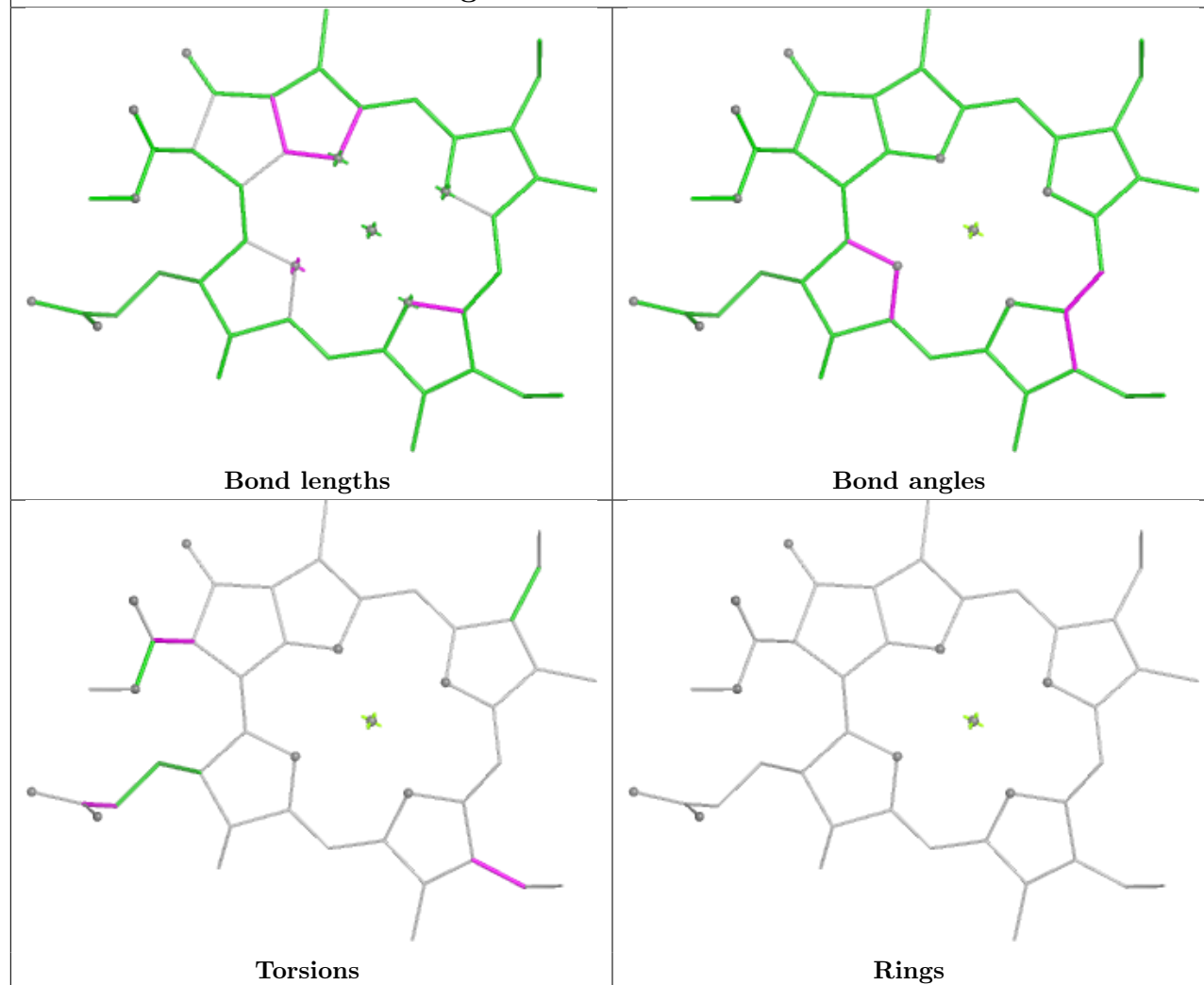
Torsions

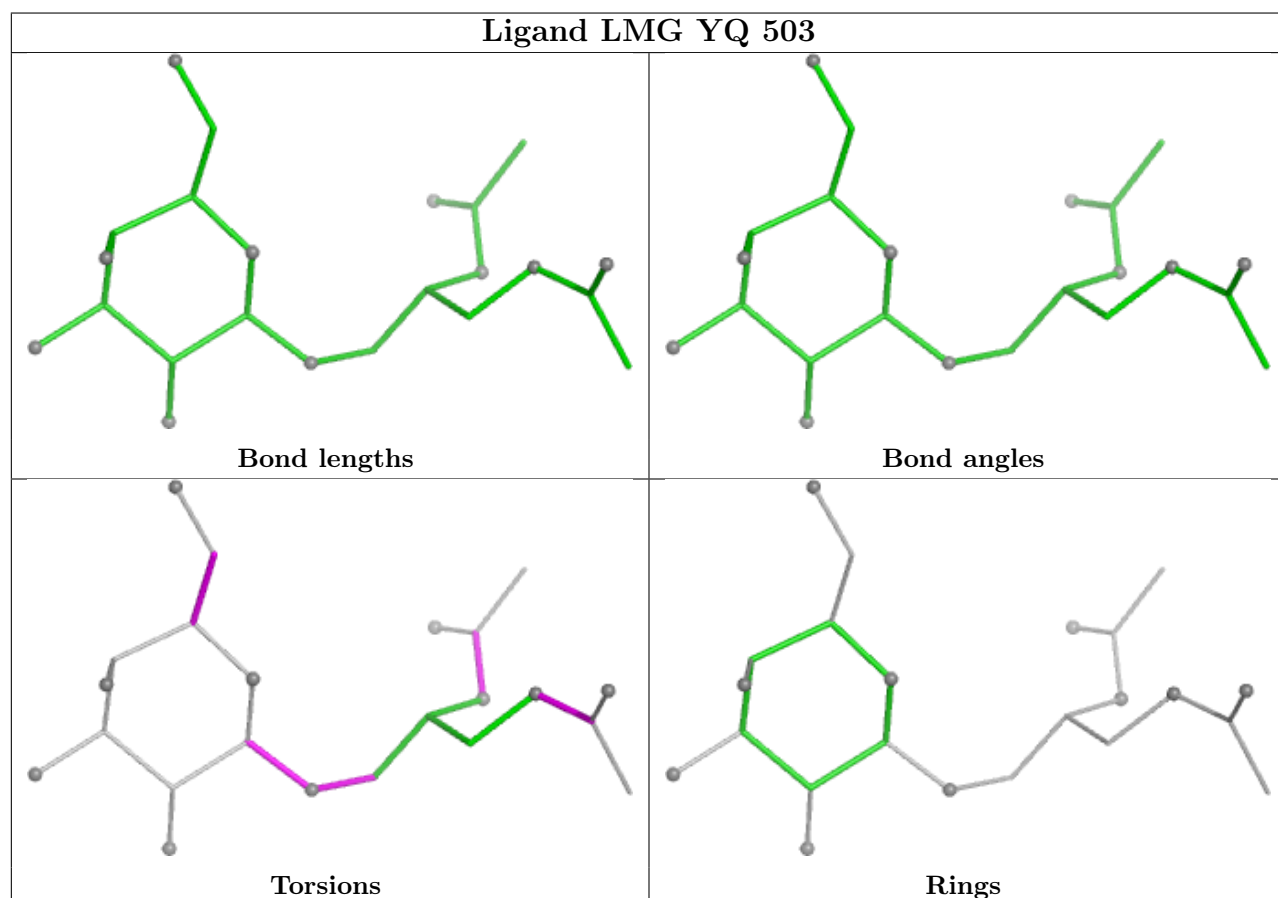
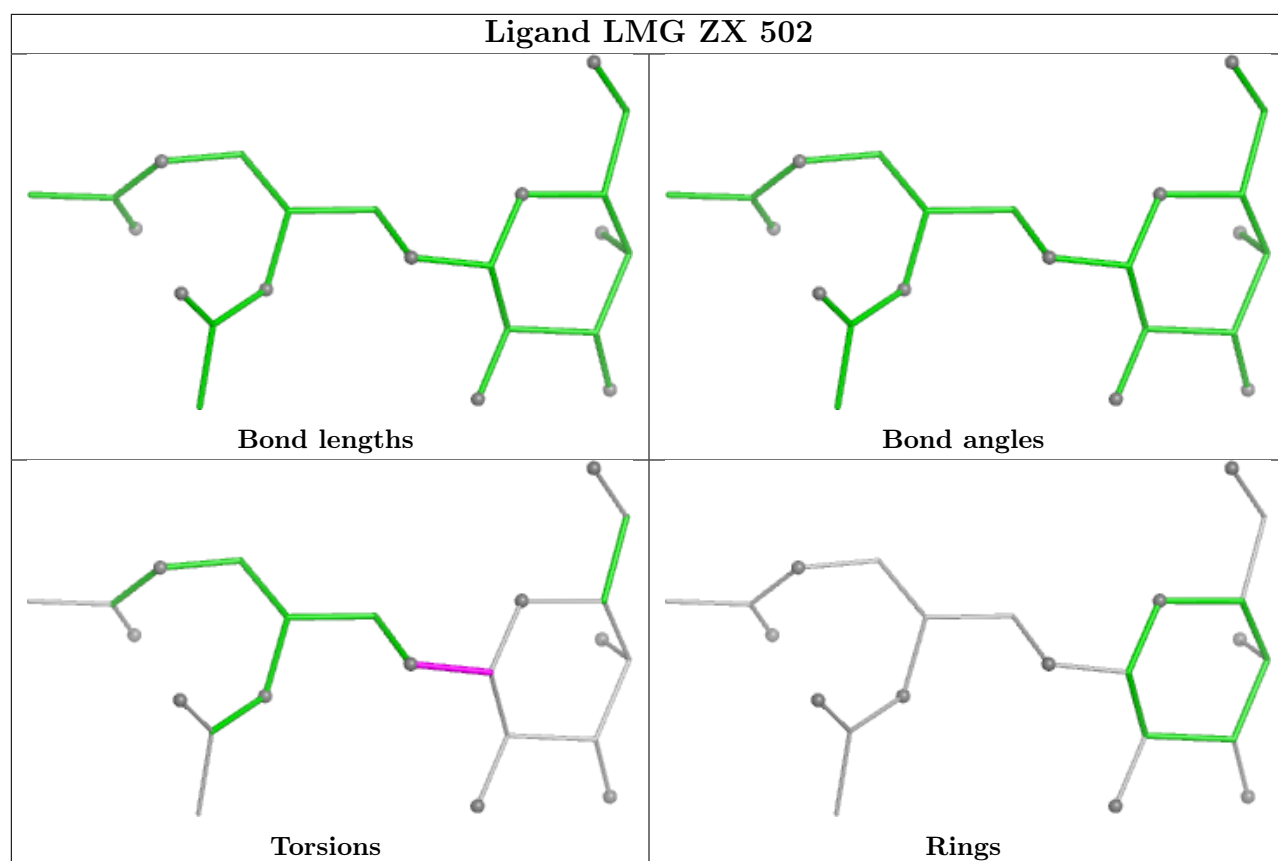


Rings

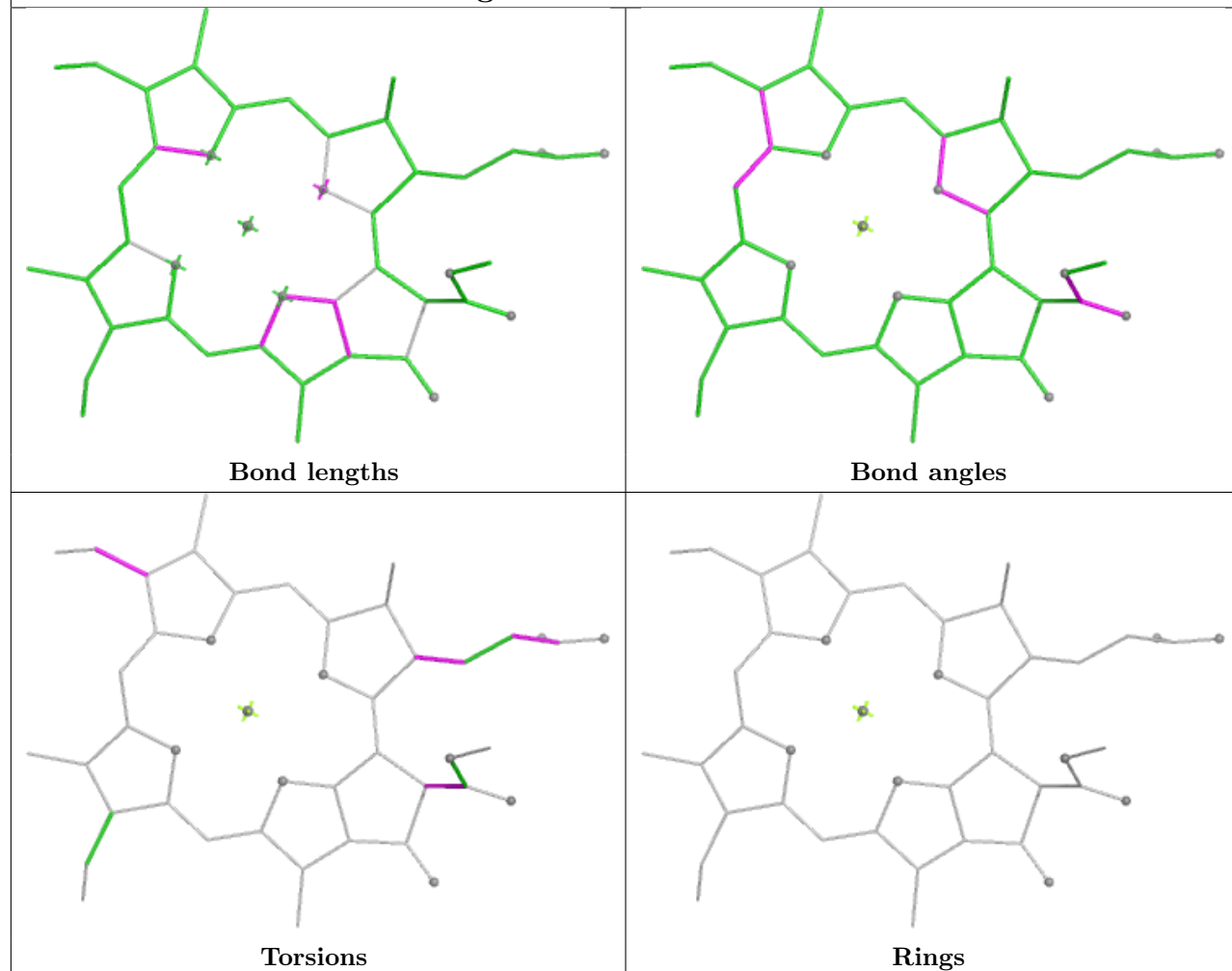


Ligand A1JWG YM 502

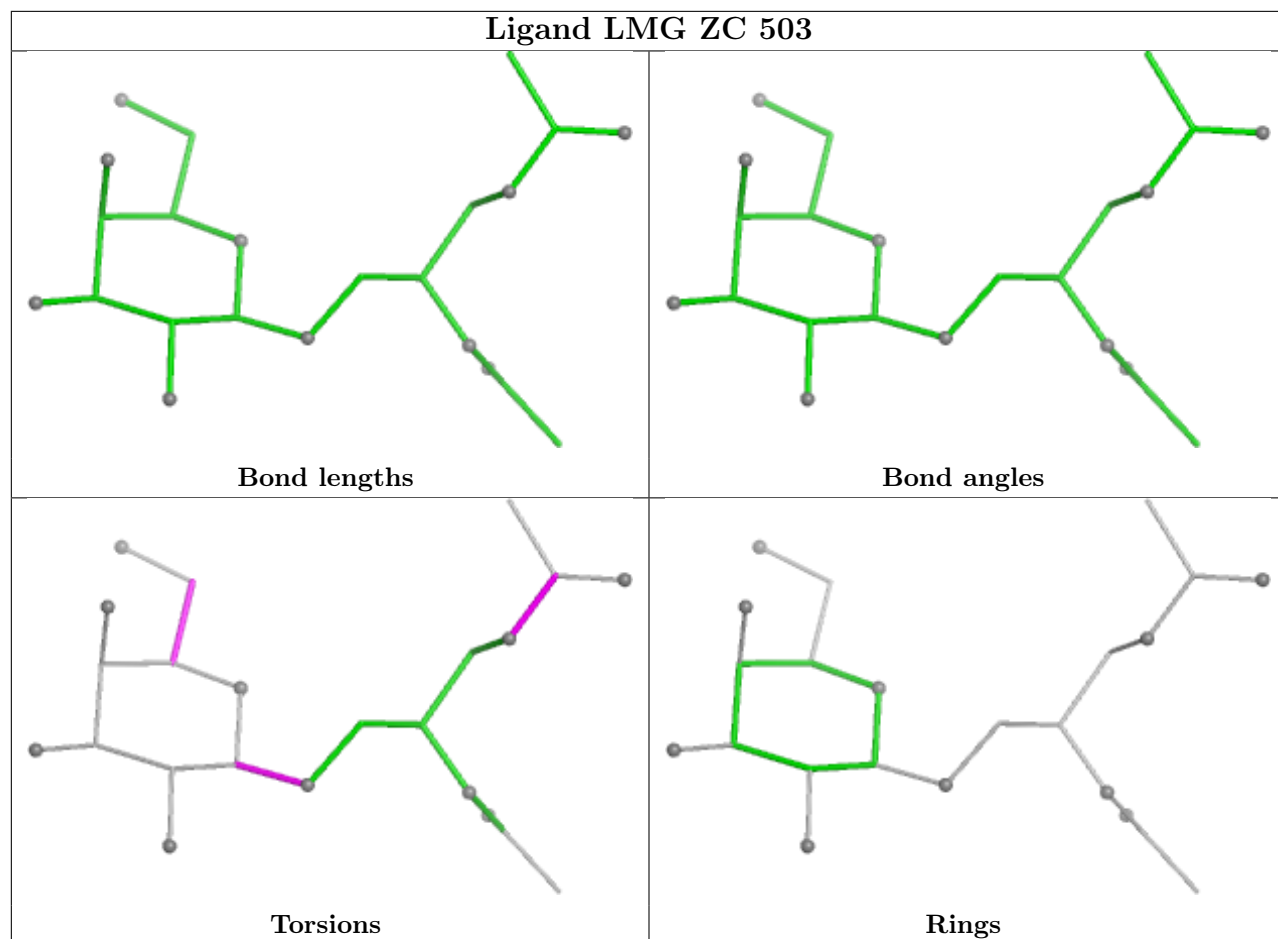




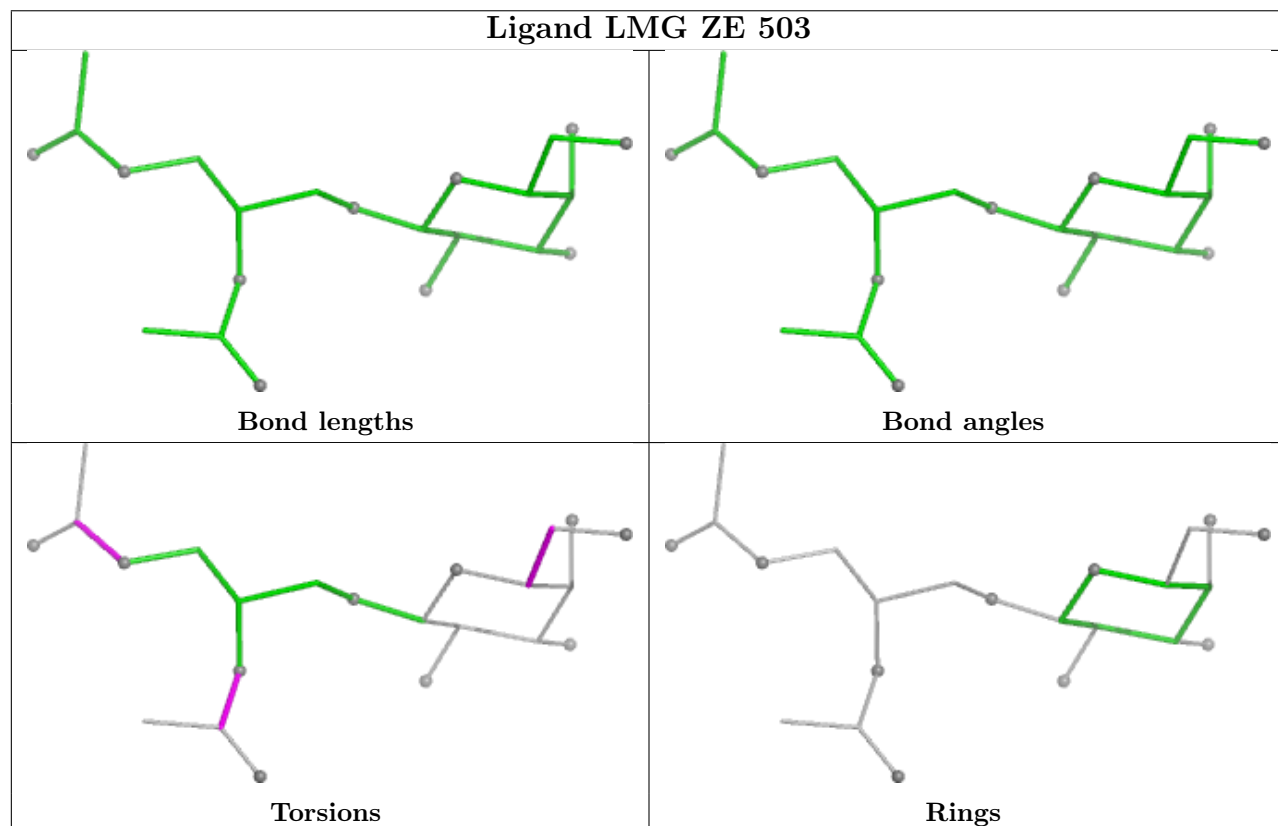
Ligand A1JWG ZC 502

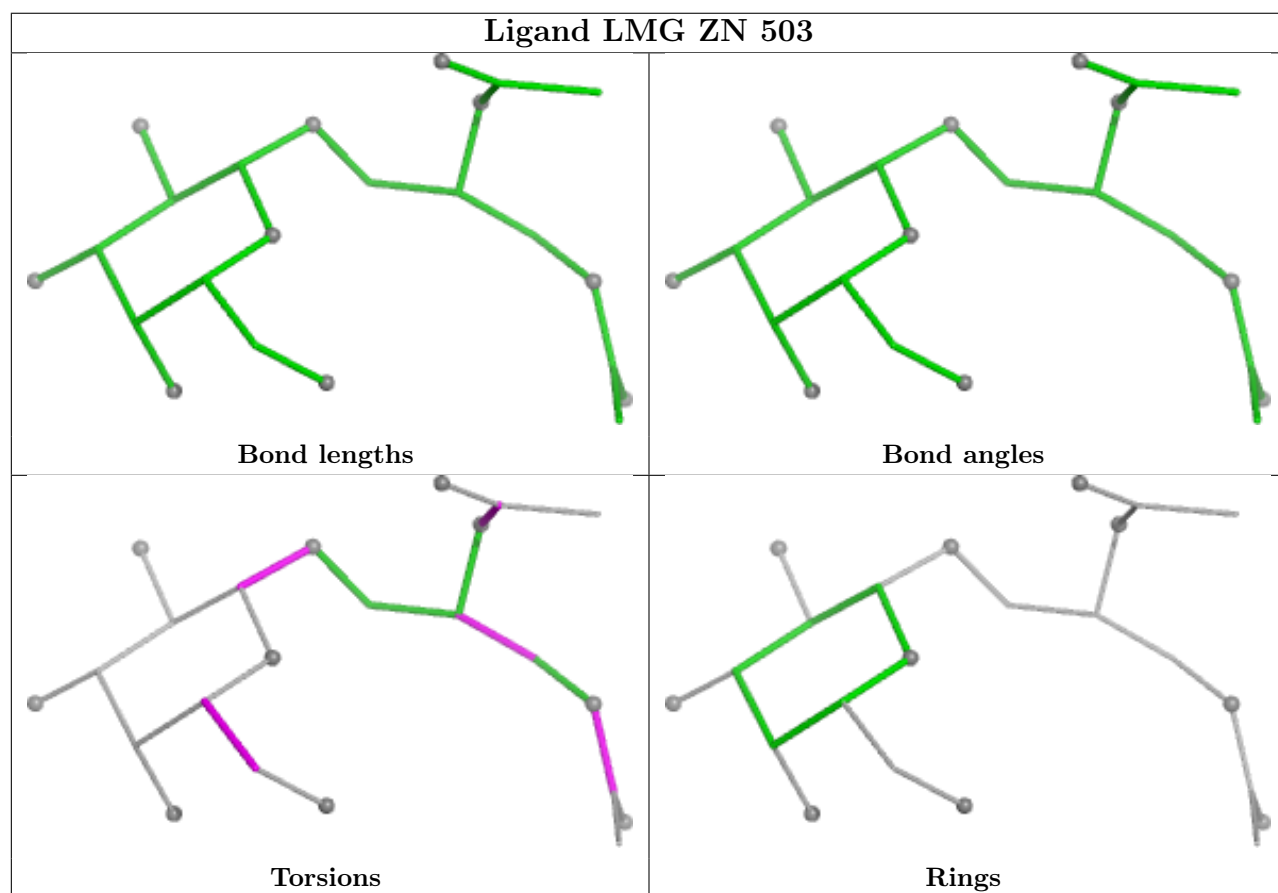
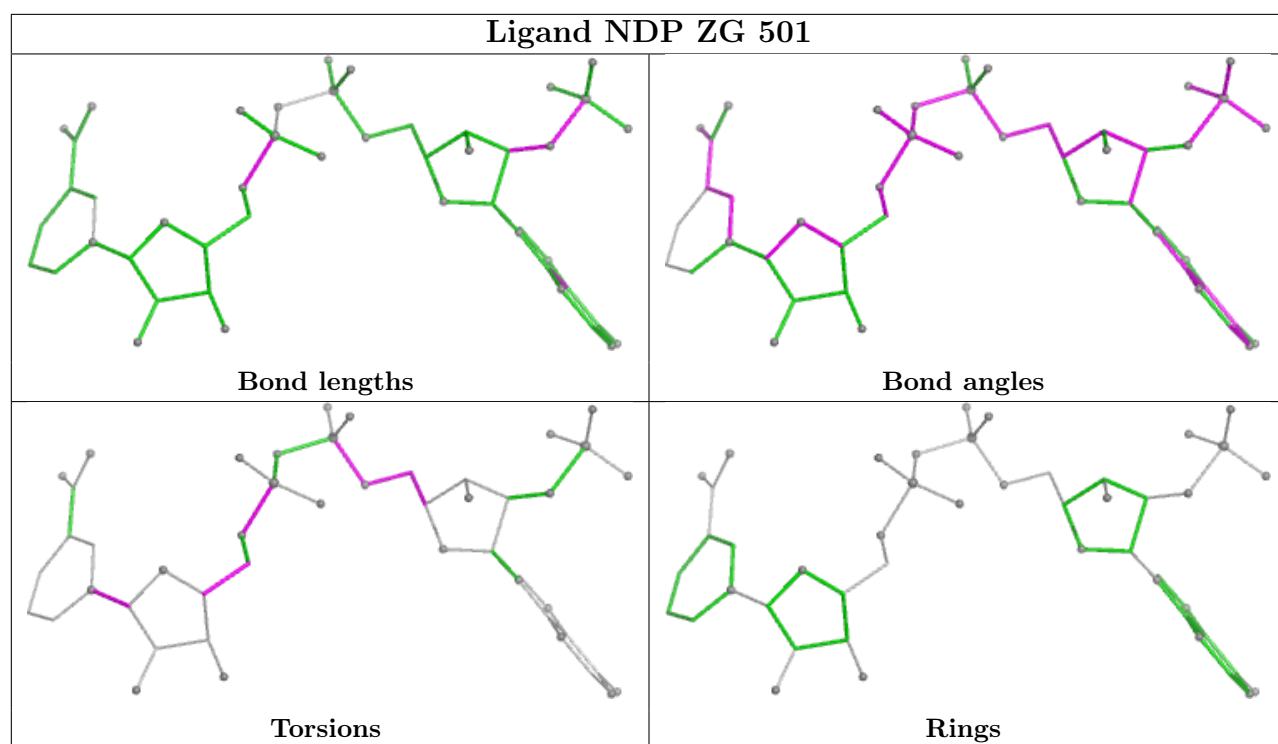


Ligand LMG ZC 503

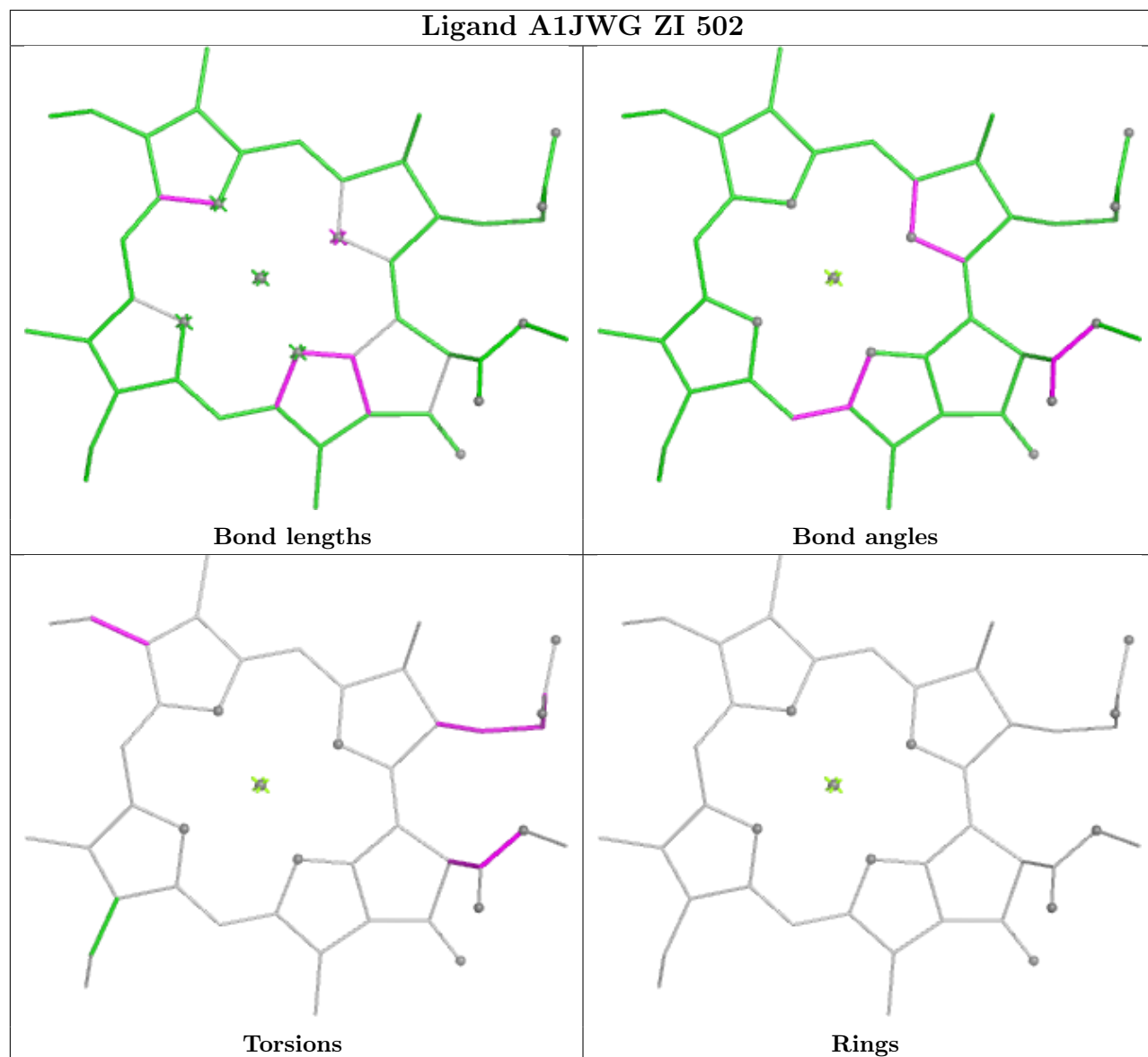


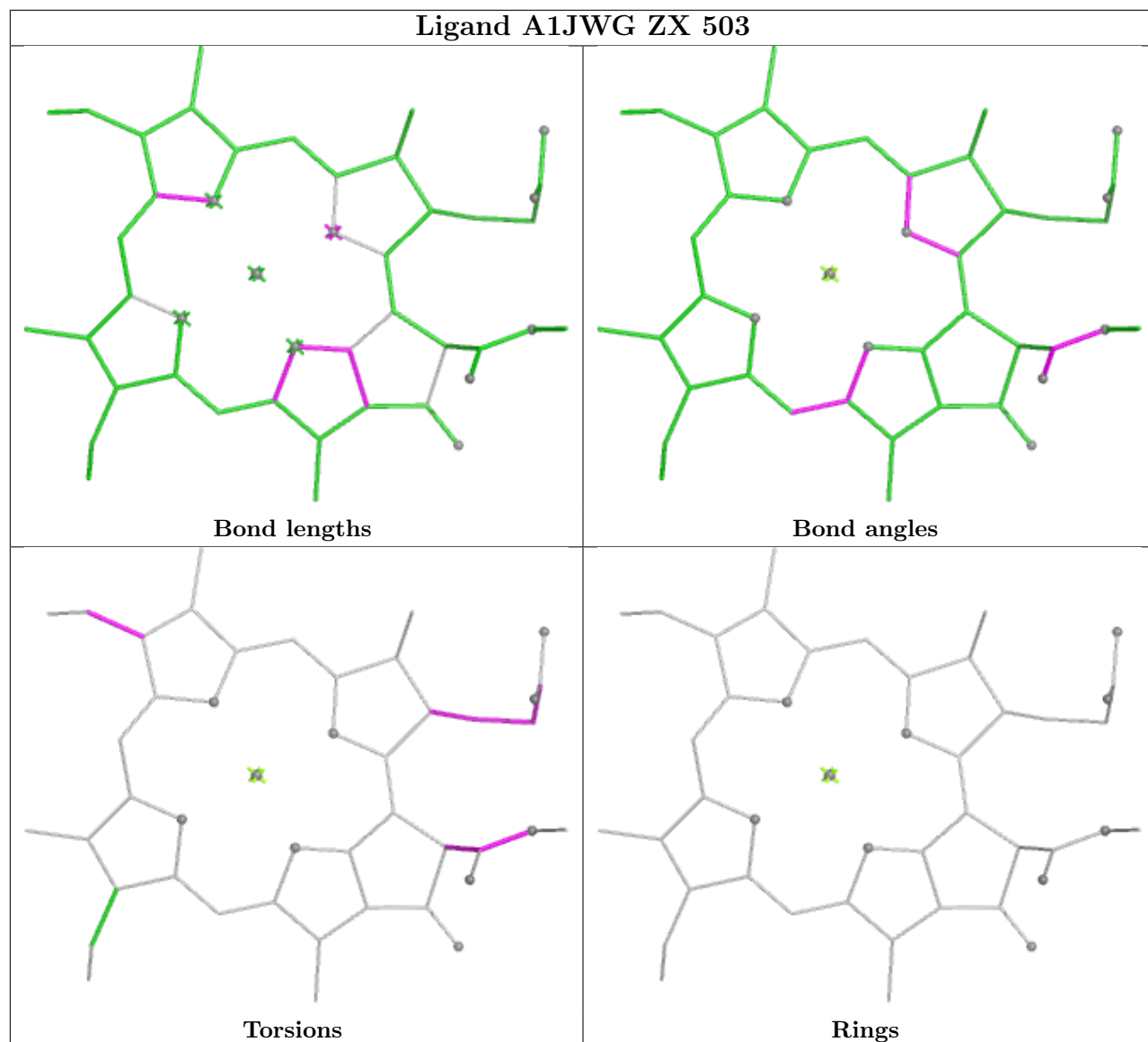
Ligand LMG ZE 503



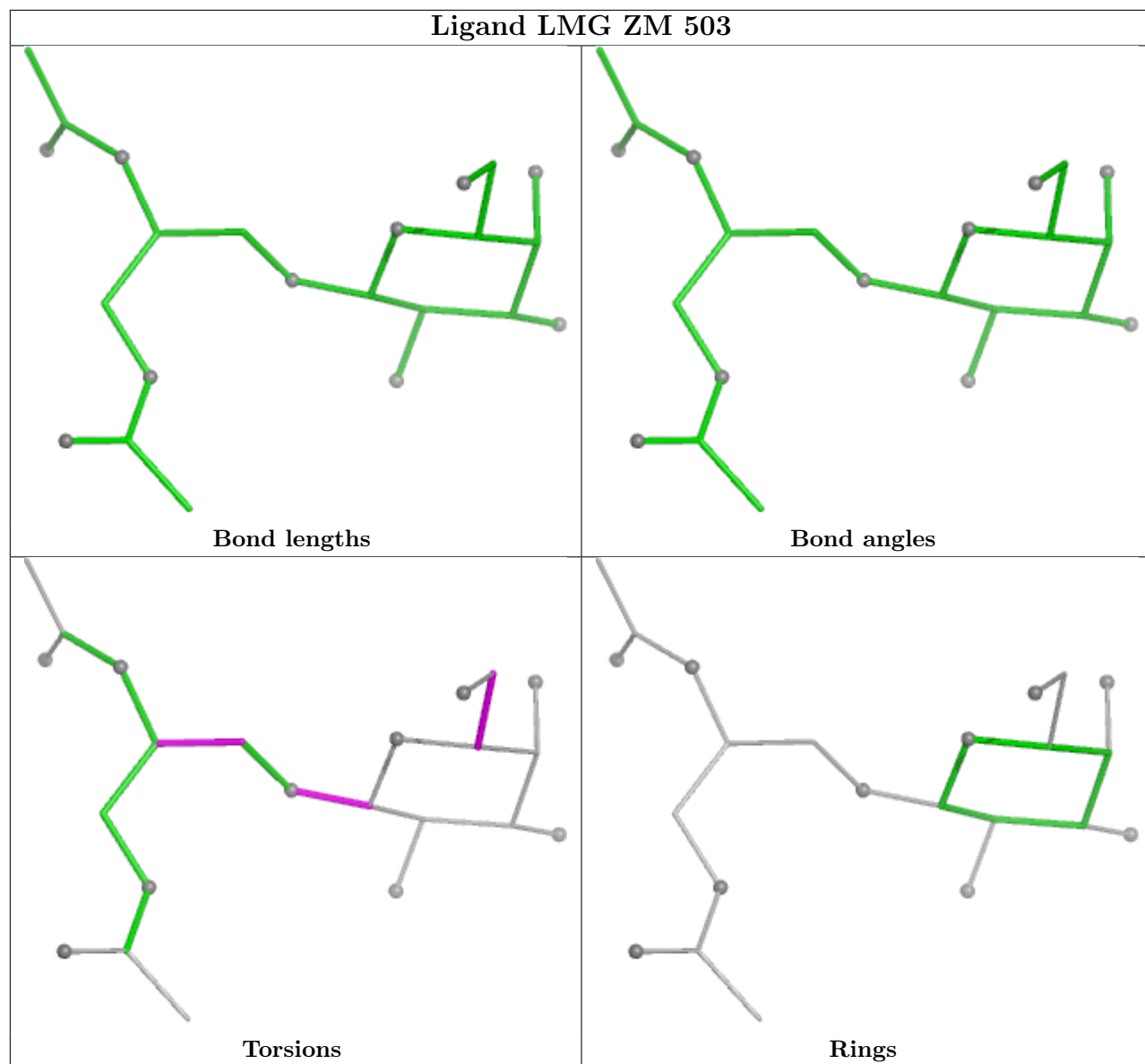


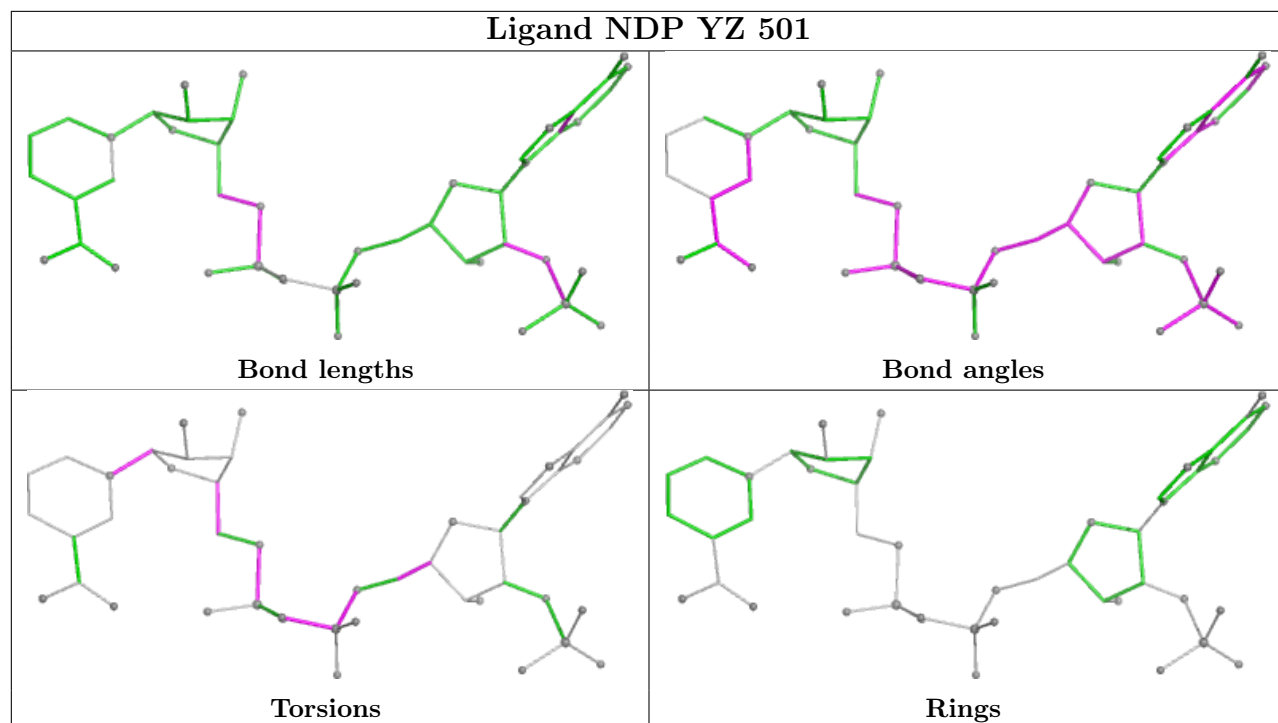
Ligand A1JWG ZI 502



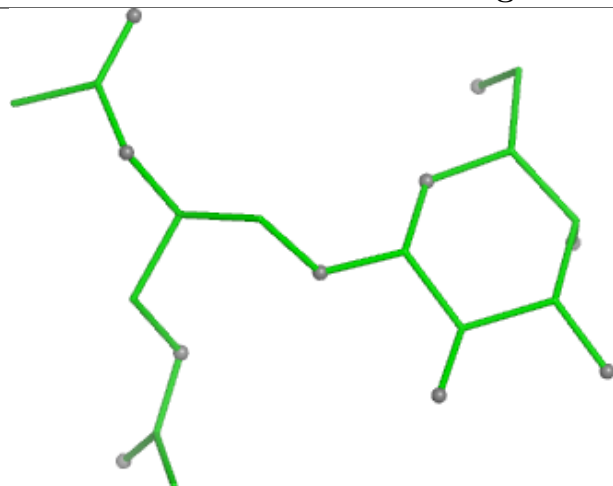


Ligand LMG ZM 503

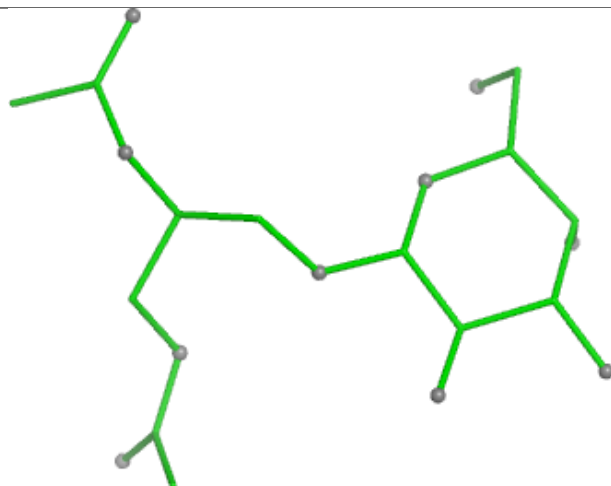




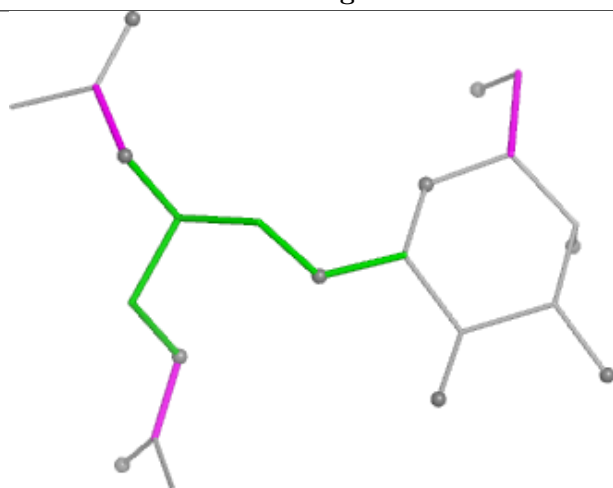
Ligand LMG YT 503



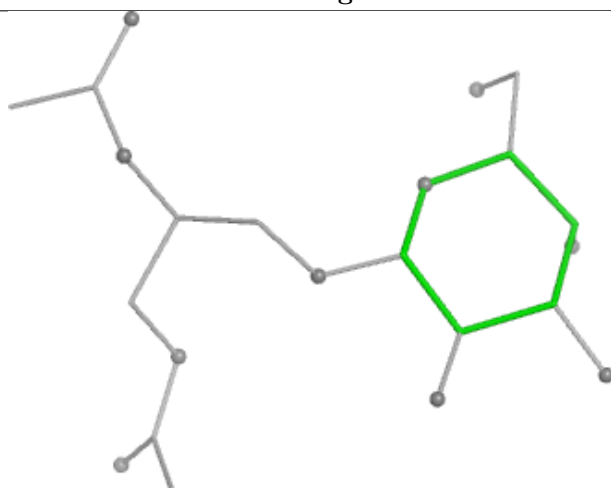
Bond lengths



Bond angles

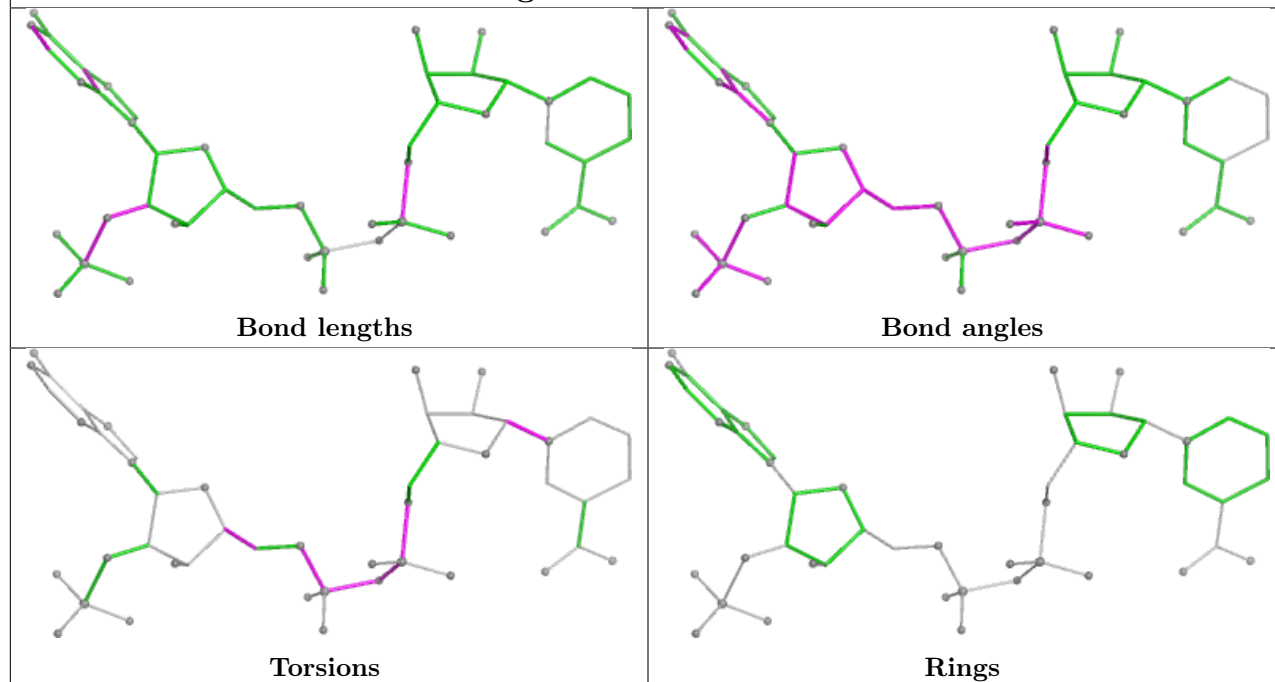


Torsions

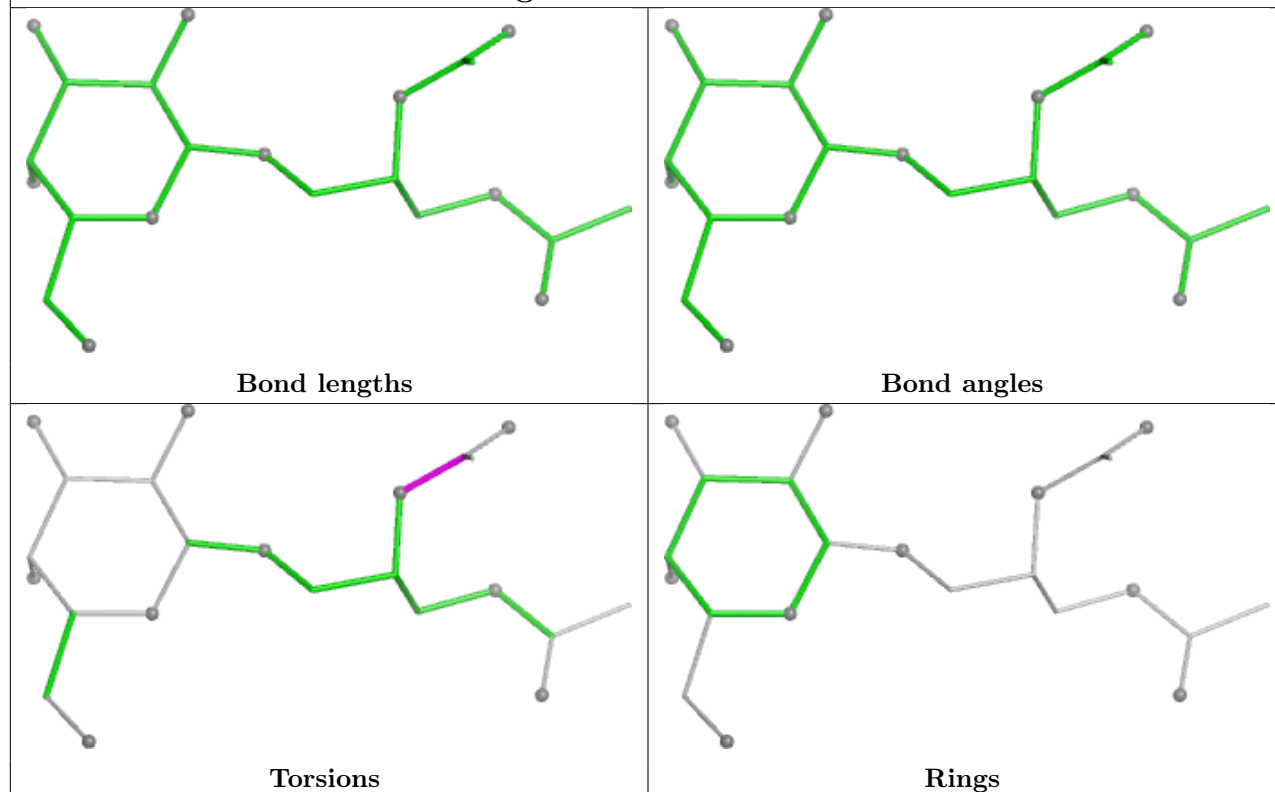


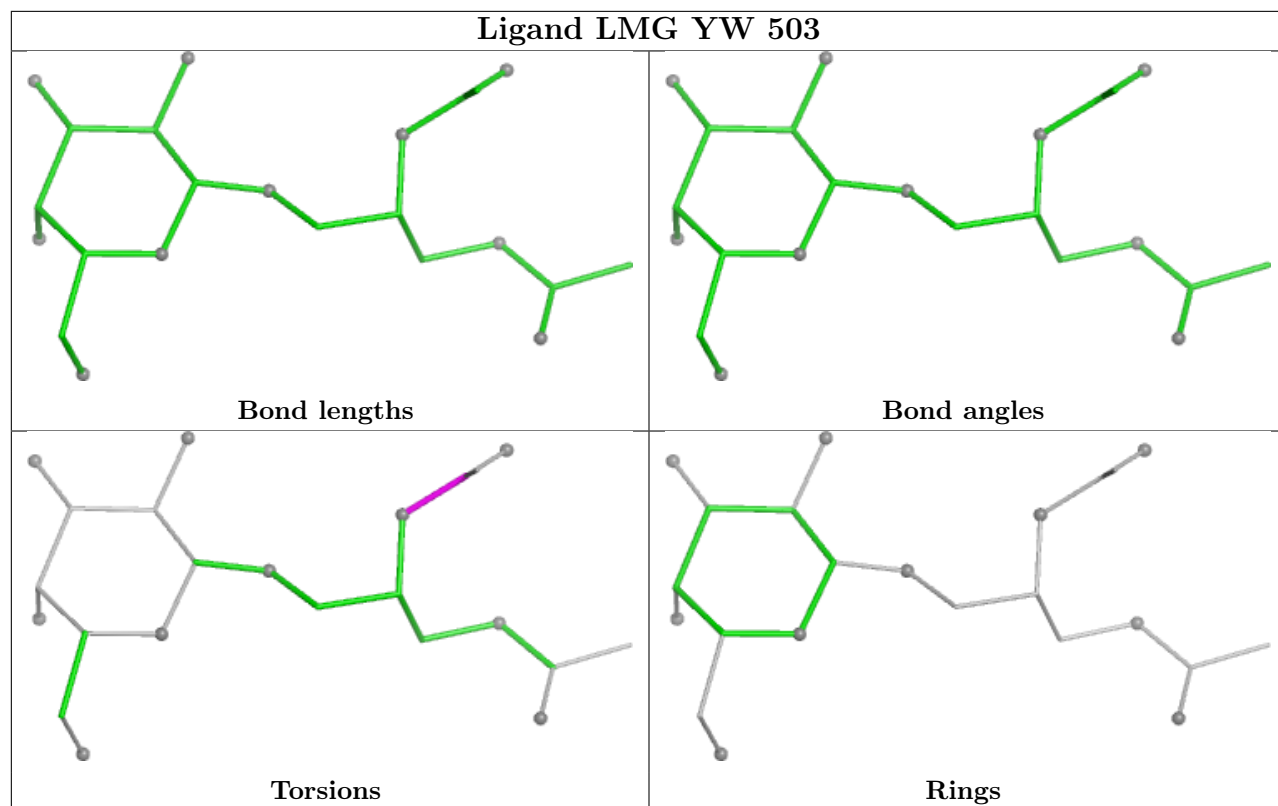
Rings

Ligand NDP ZA 501

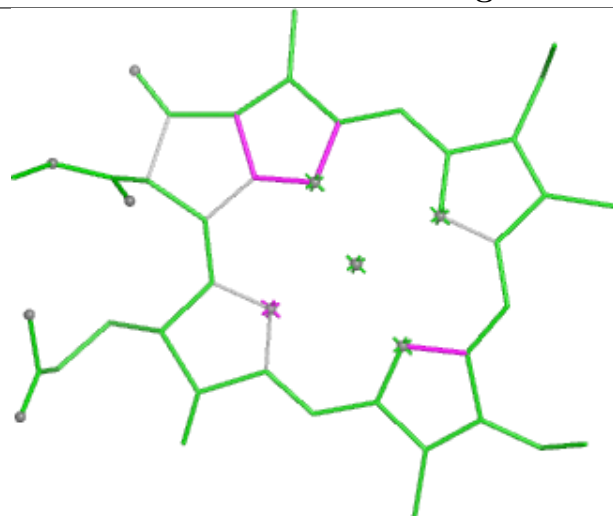


Ligand LMG YS 503

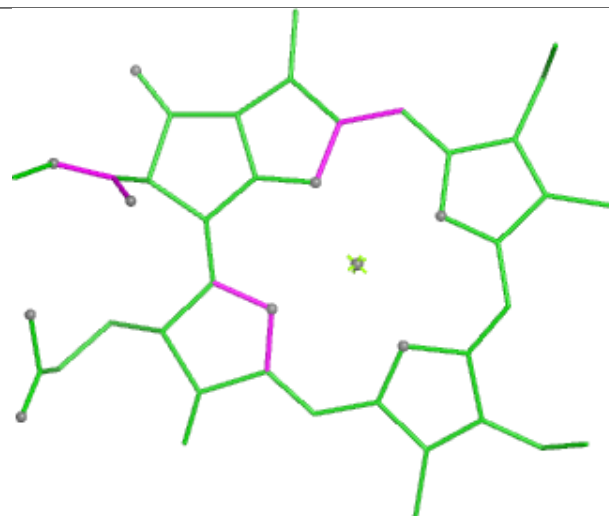




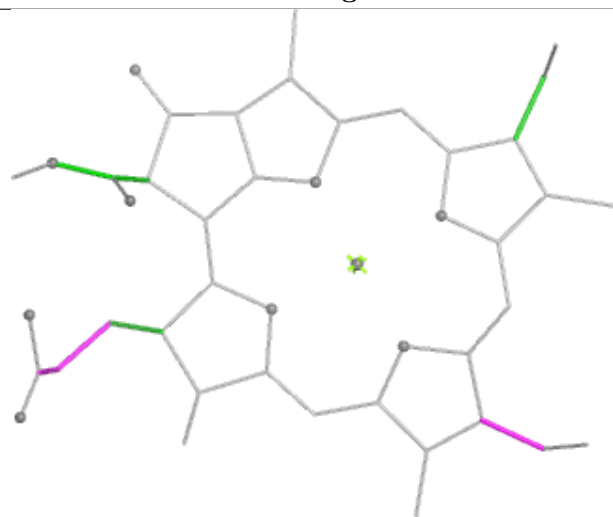
Ligand A1JWG YO 502



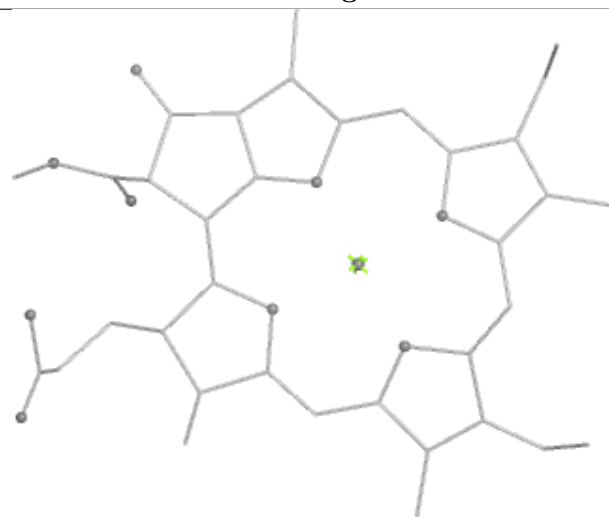
Bond lengths



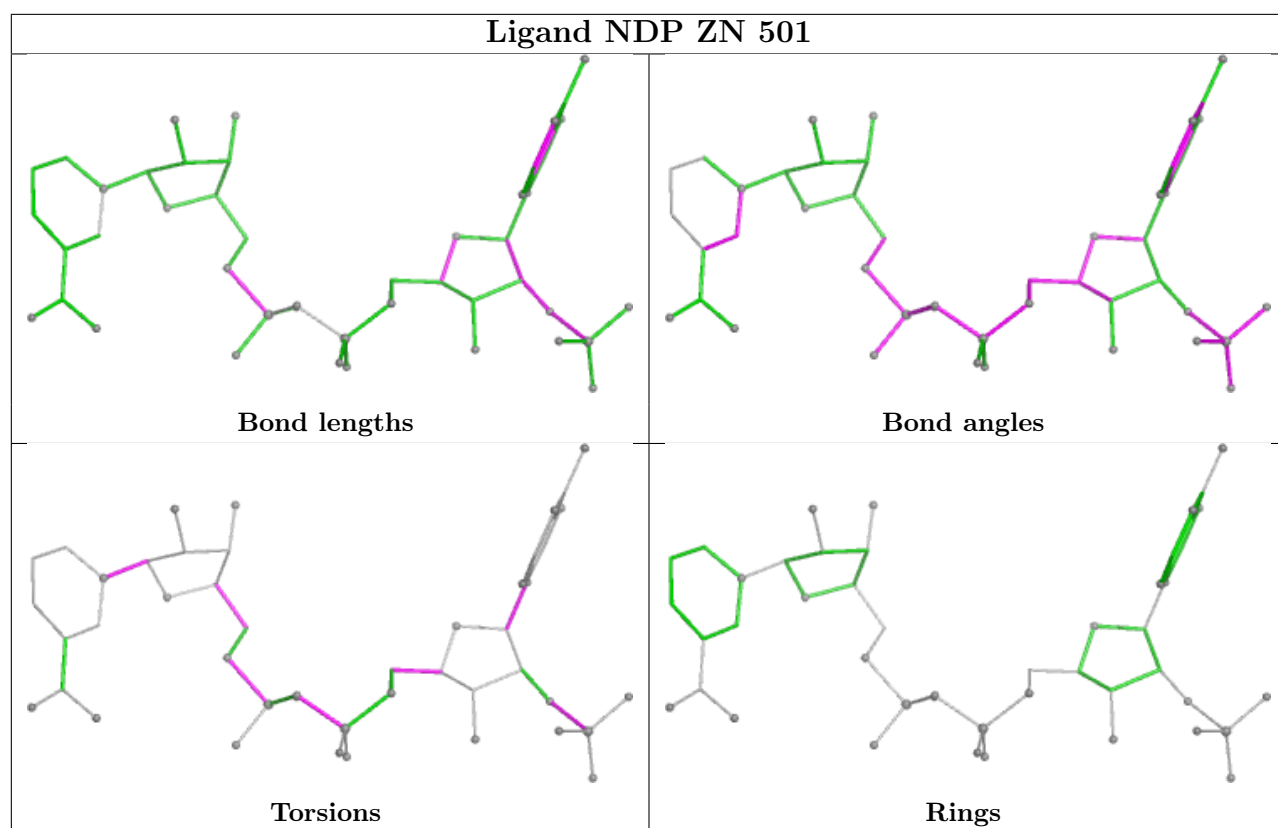
Bond angles

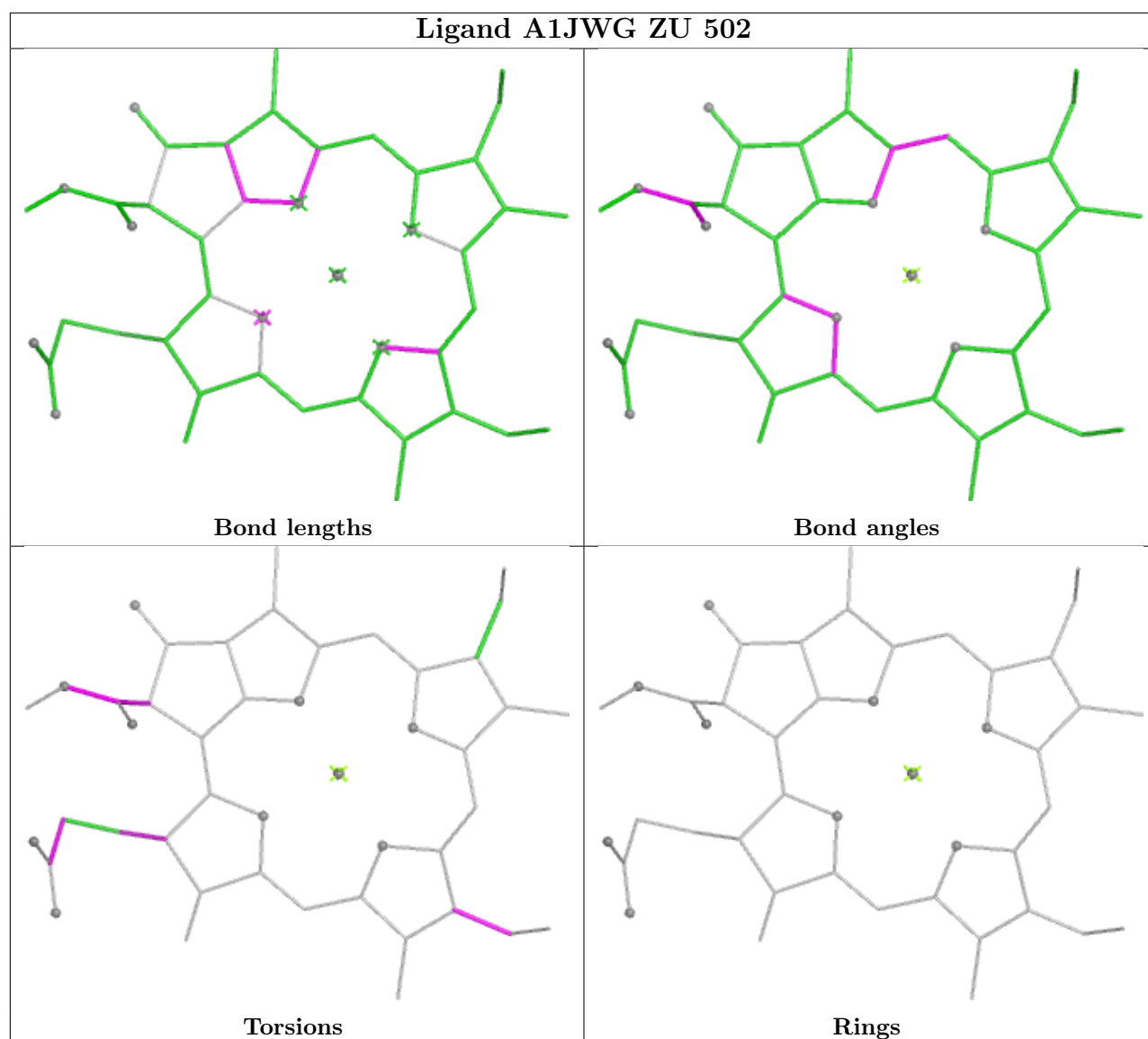


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

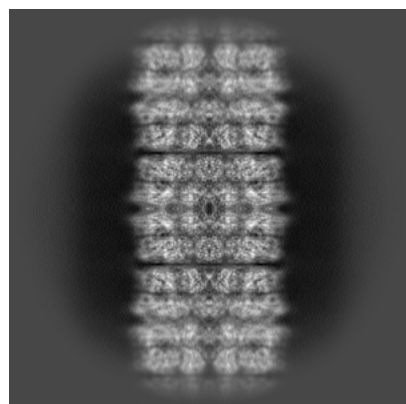
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56047. These allow visual inspection of the internal detail of the map and identification of artifacts.

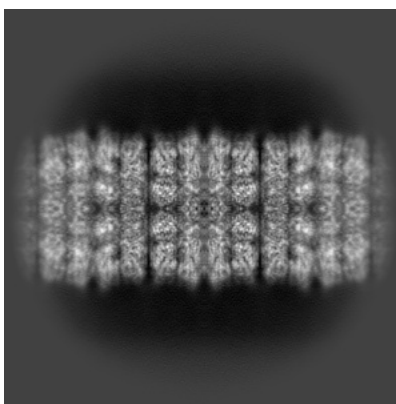
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

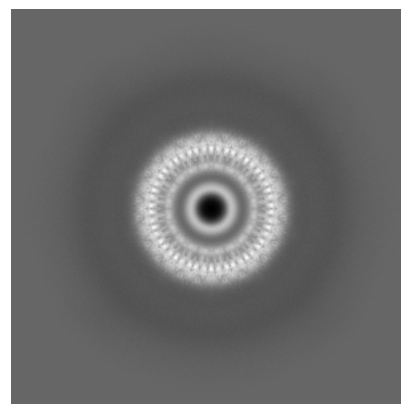
6.1.1 Primary map



X

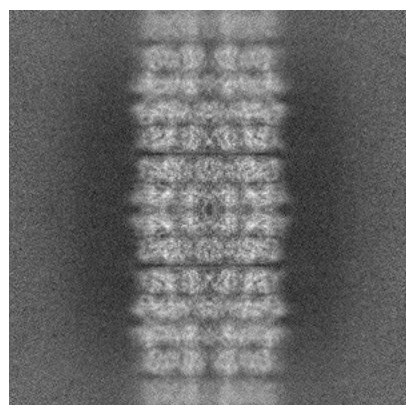


Y

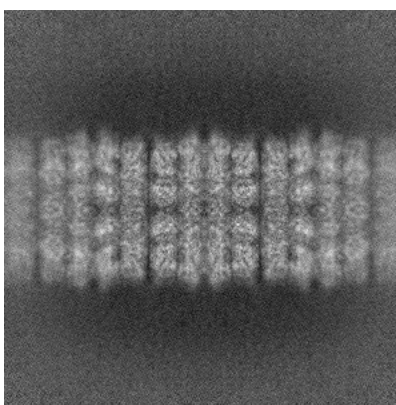


Z

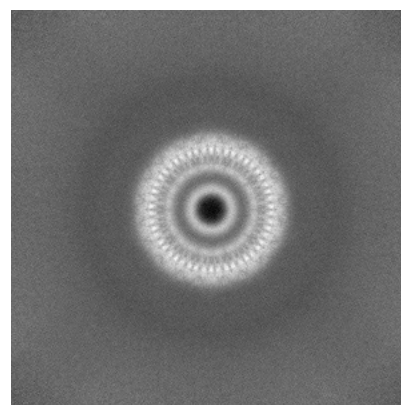
6.1.2 Raw map



X



Y

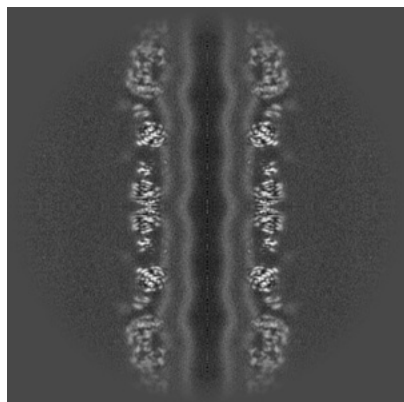


Z

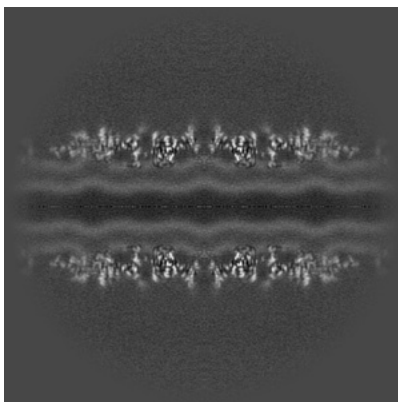
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

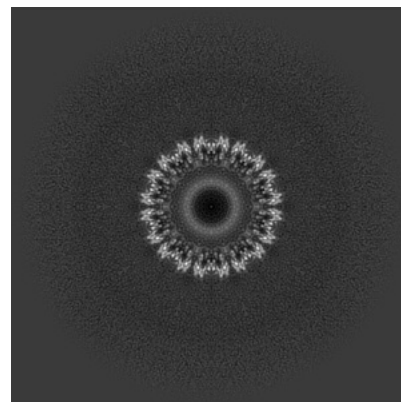
6.2.1 Primary map



X Index: 320

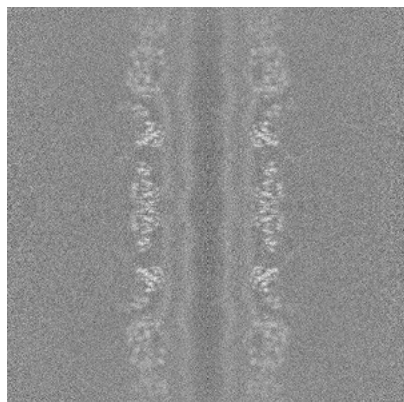


Y Index: 320

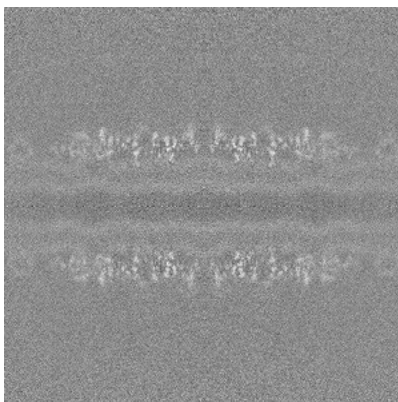


Z Index: 320

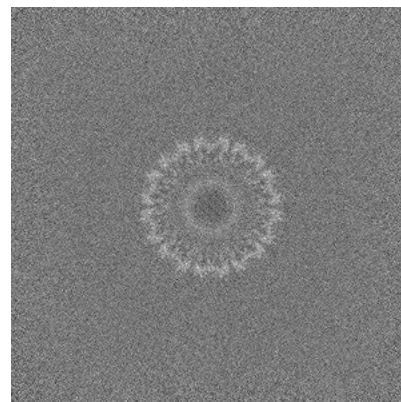
6.2.2 Raw map



X Index: 320



Y Index: 320

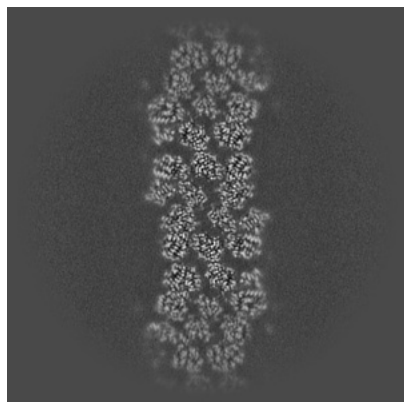


Z Index: 320

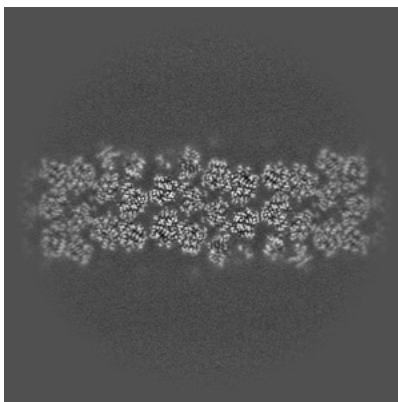
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

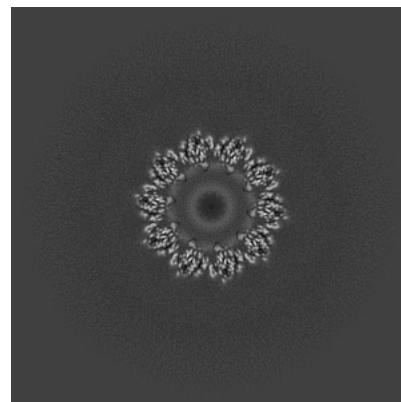
6.3.1 Primary map



X Index: 233

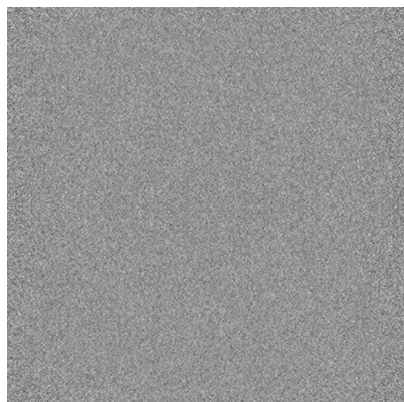


Y Index: 231

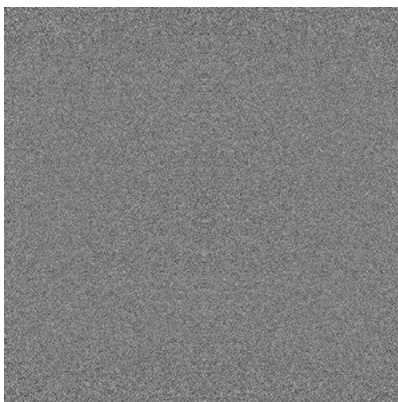


Z Index: 262

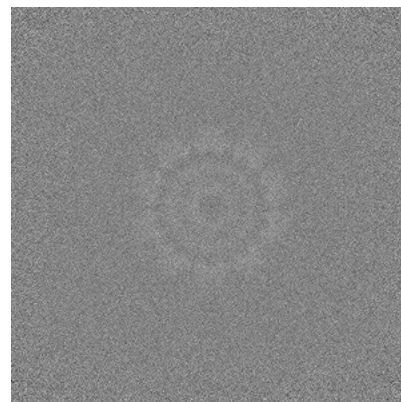
6.3.2 Raw map



X Index: 0



Y Index: 0

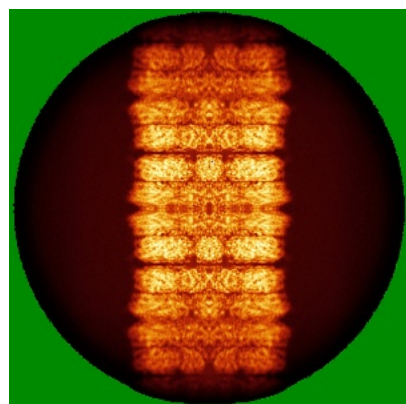


Z Index: 0

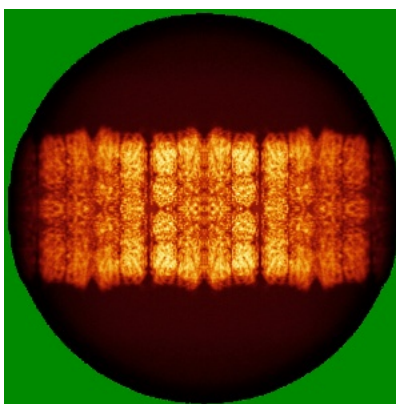
The images above show the largest variance slices of the map in three orthogonal directions.

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

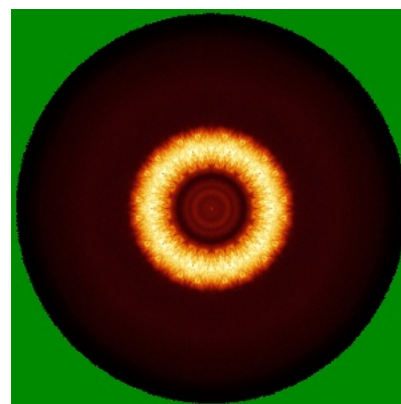
6.4.1 Primary map



X

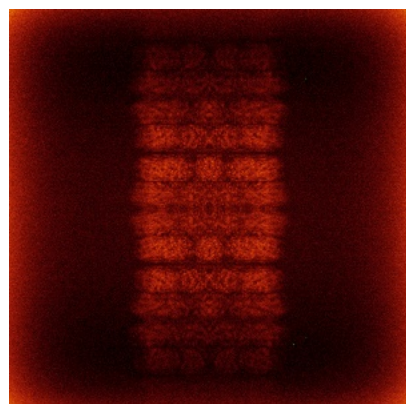


Y

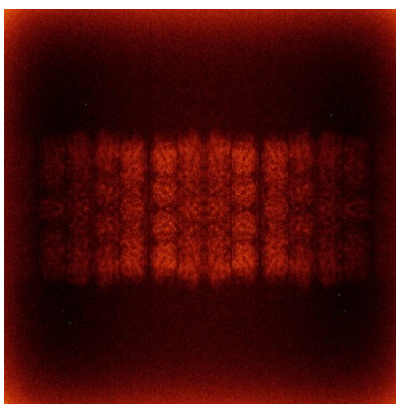


Z

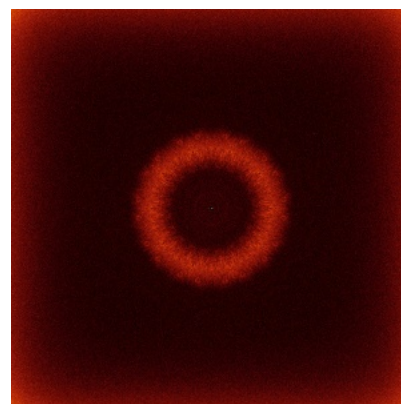
6.4.2 Raw map



X



Y

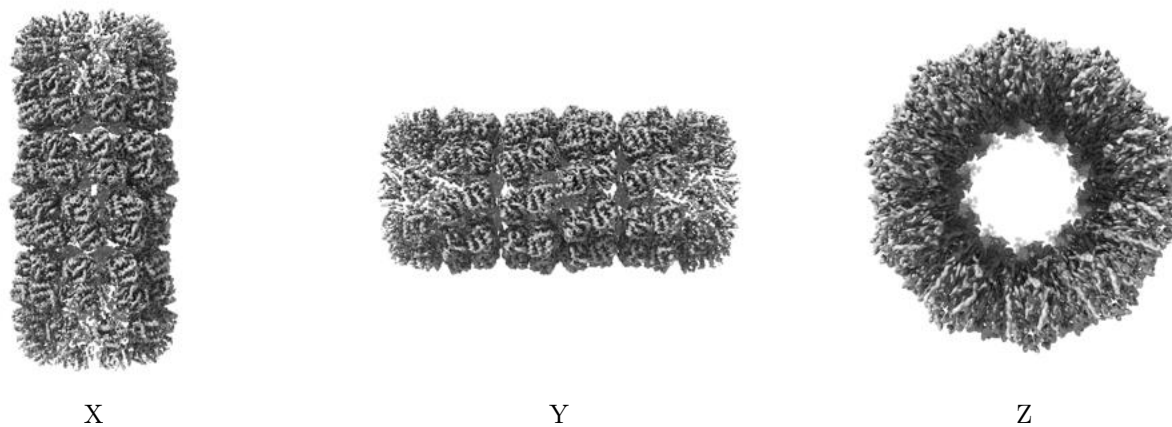


Z

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.

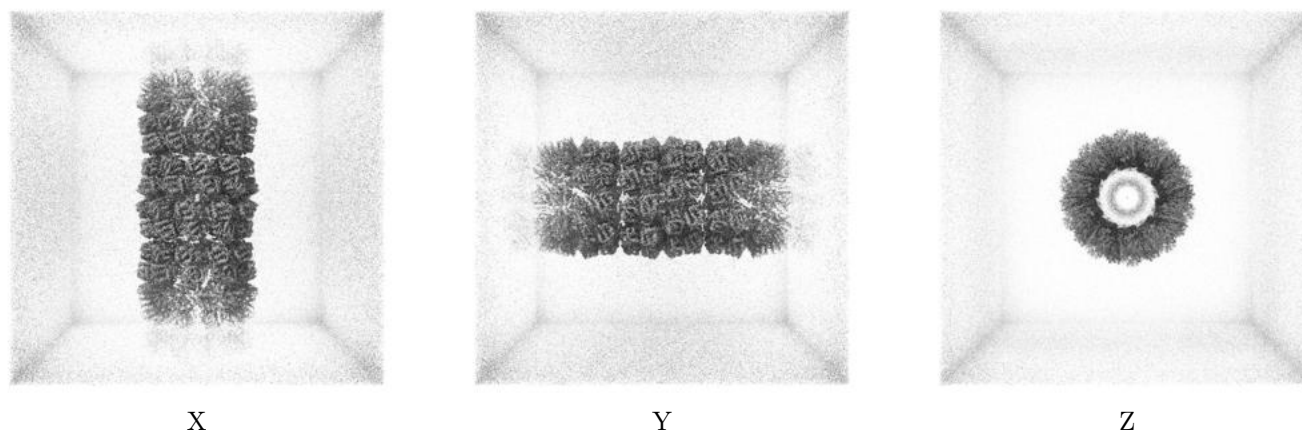
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

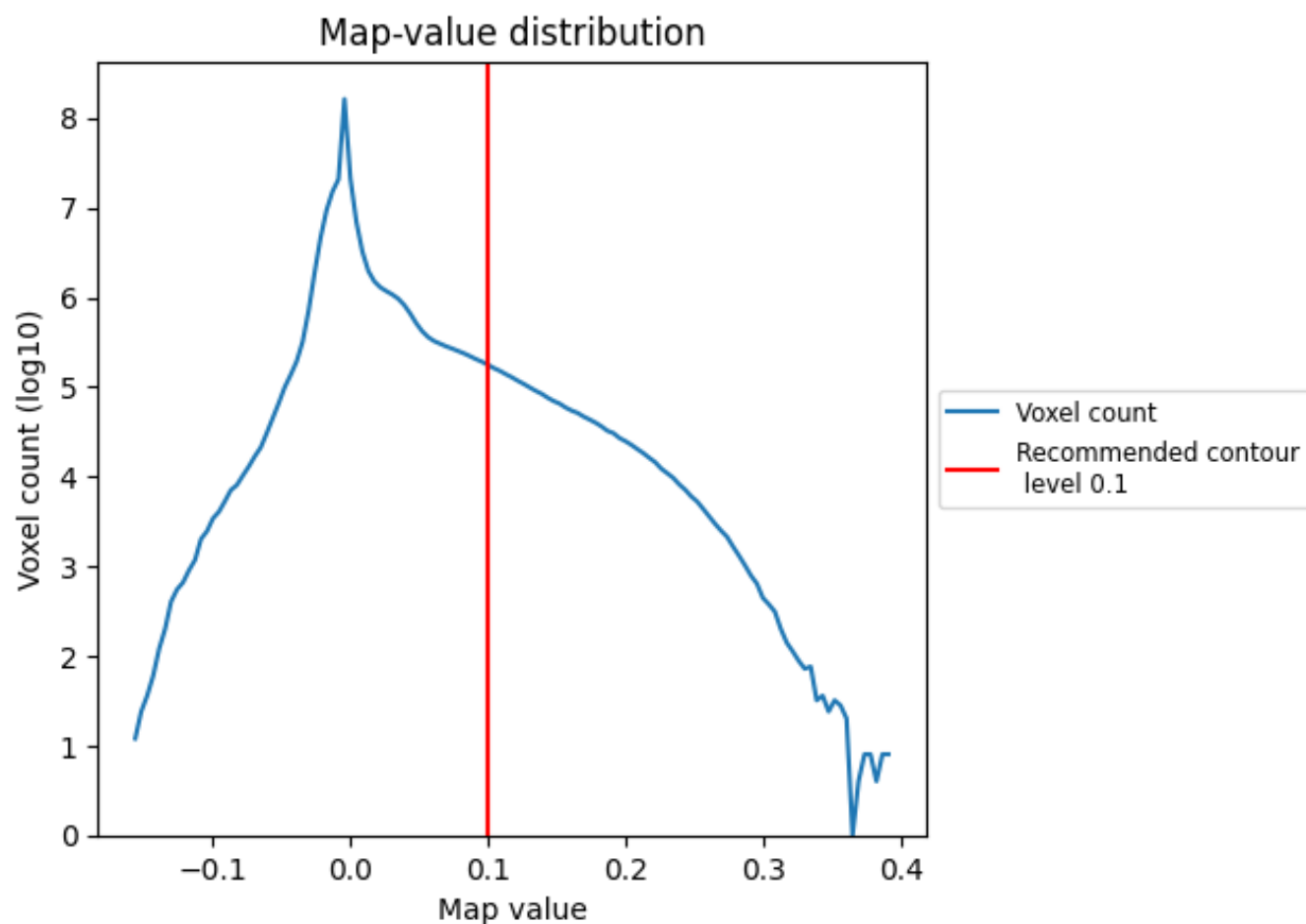
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

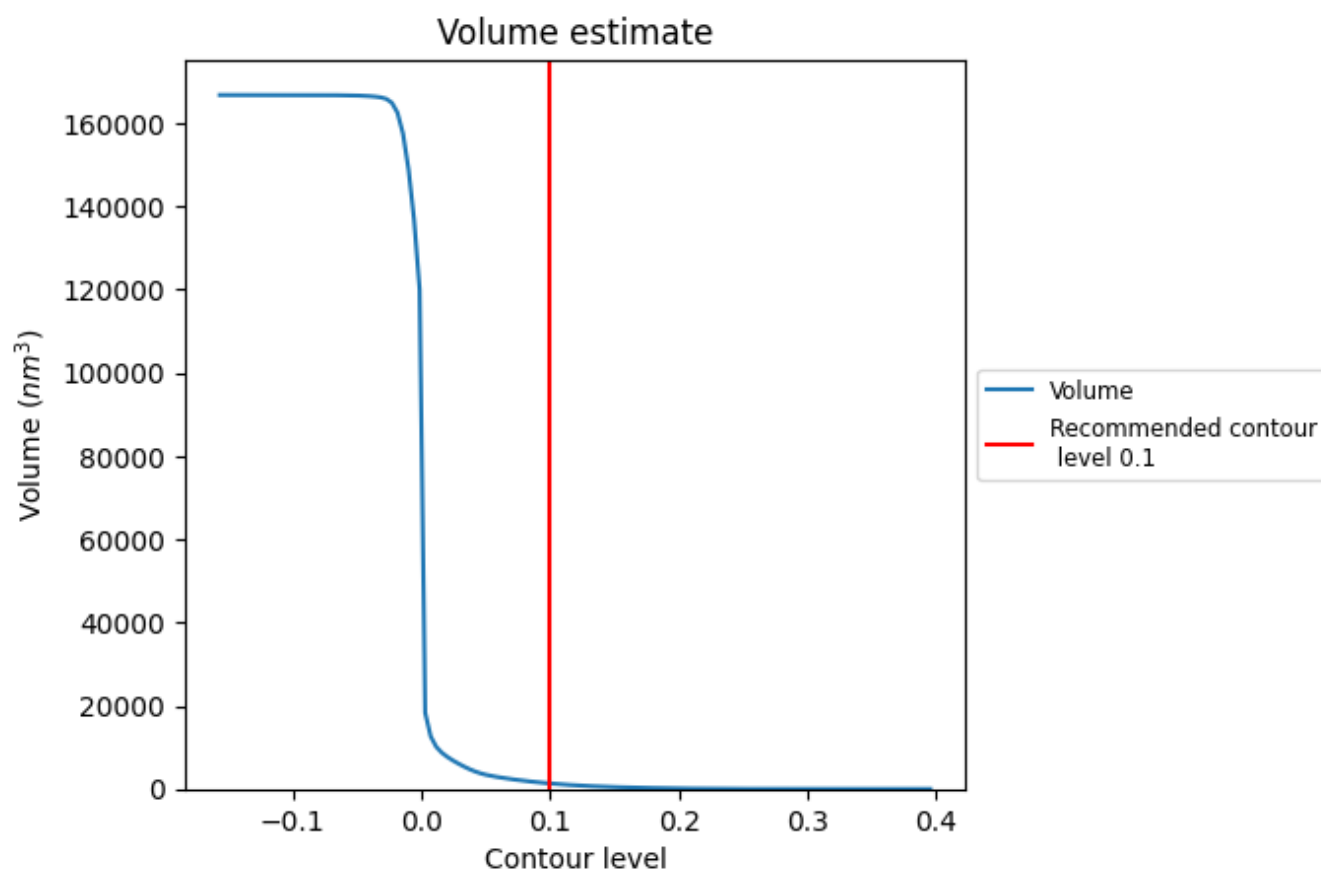
This section contains the results of statistical analysis of the map.

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.

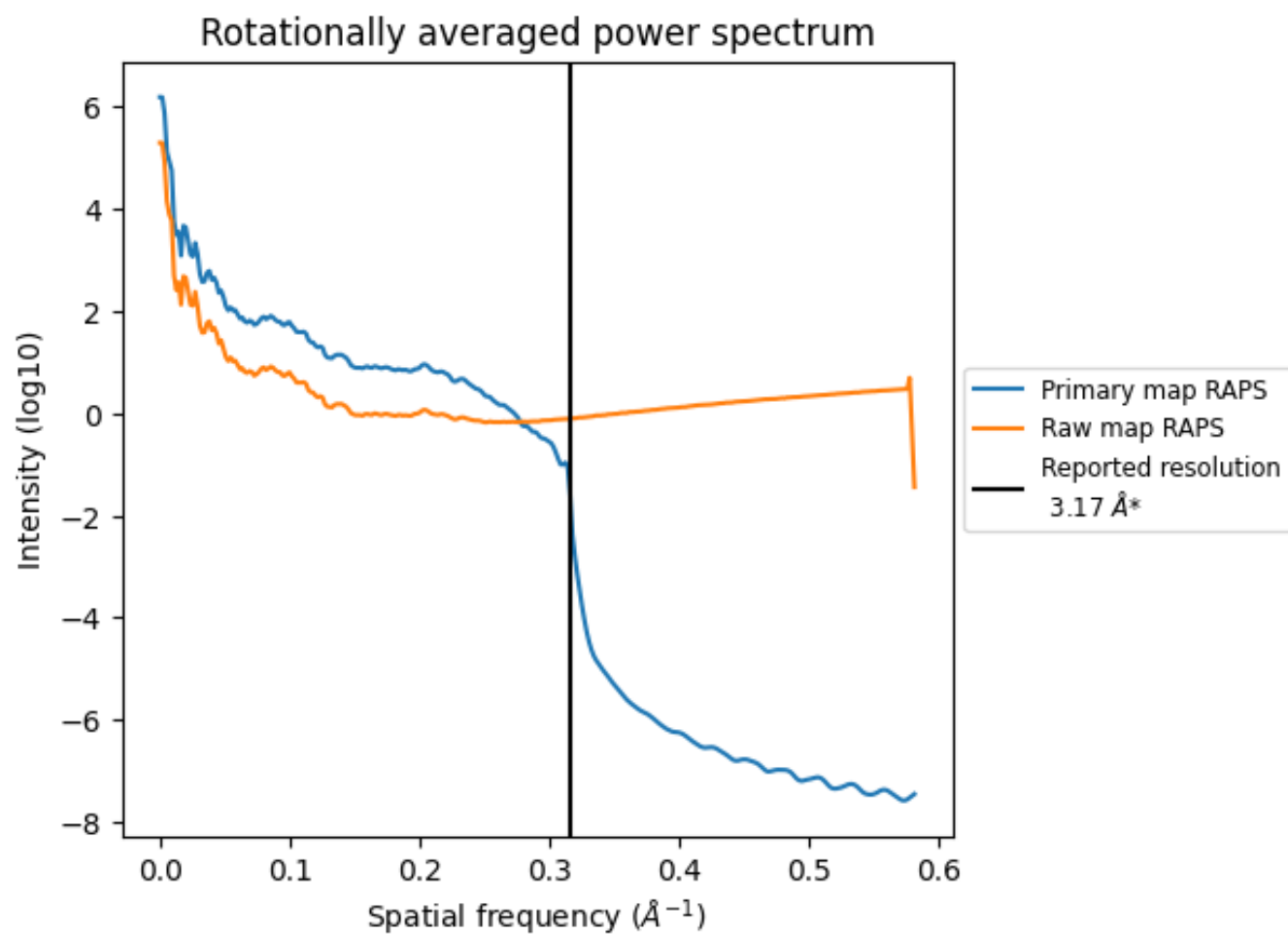
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1328 nm³; this corresponds to an approximate mass of 1200 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 ⓘ

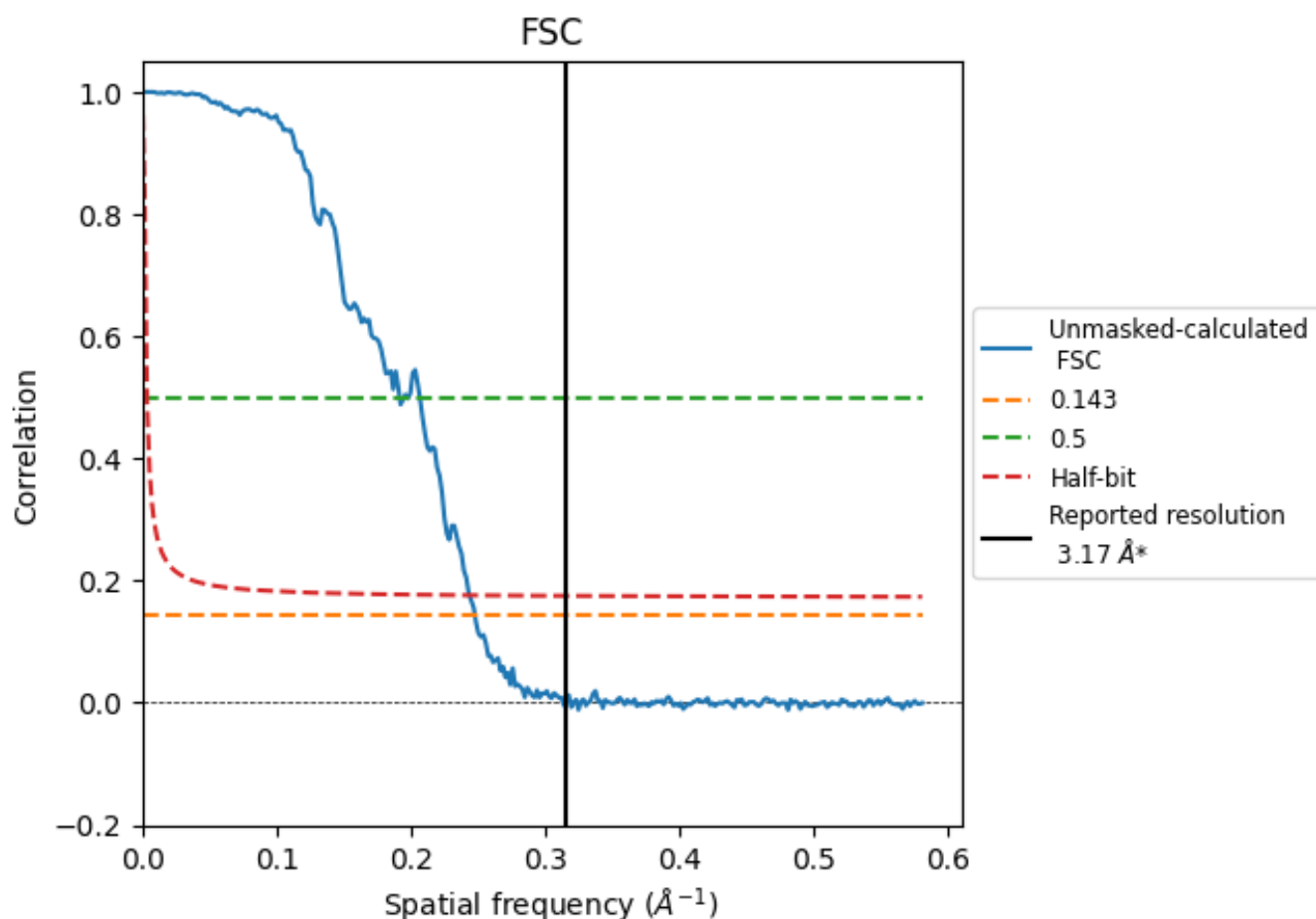


*Reported resolution corresponds to spatial frequency of 0.315 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.315 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

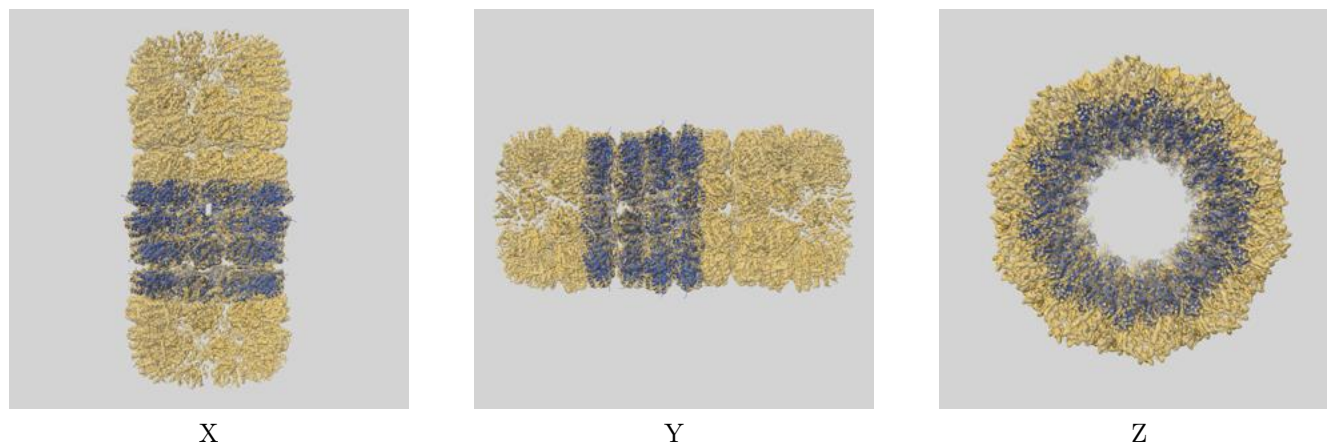
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	5.21	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 3.17 by more than 10 %

9 Map-model fit [i](#)

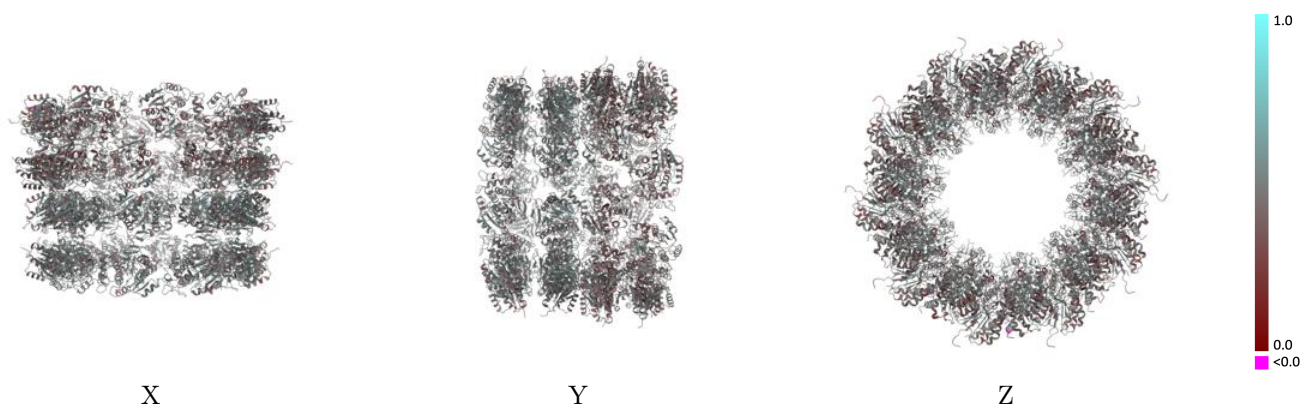
This section contains information regarding the fit between EMDB map EMD-56047 and PDB model 9TLA. Per-residue inclusion information can be found in section 3 on page 34.

9.1 Map-model overlay [i](#)



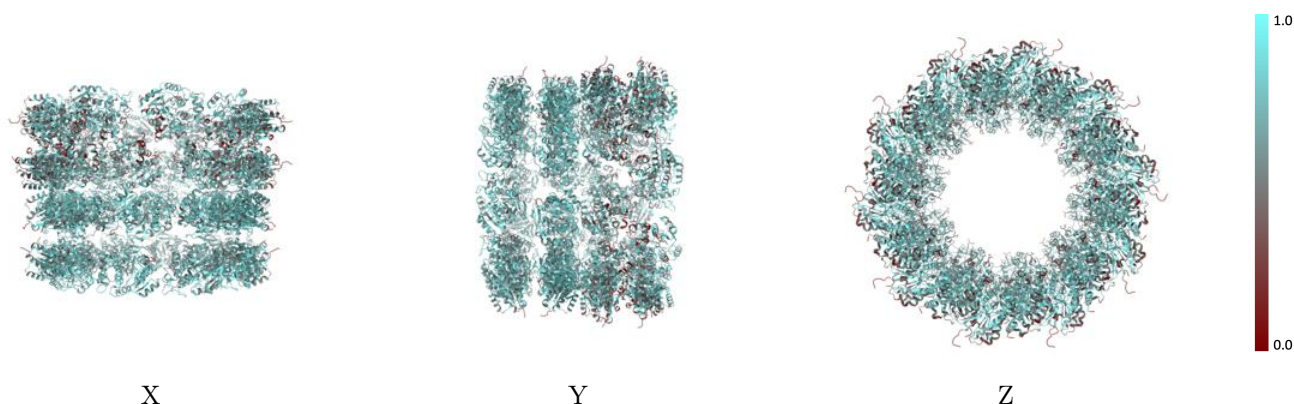
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



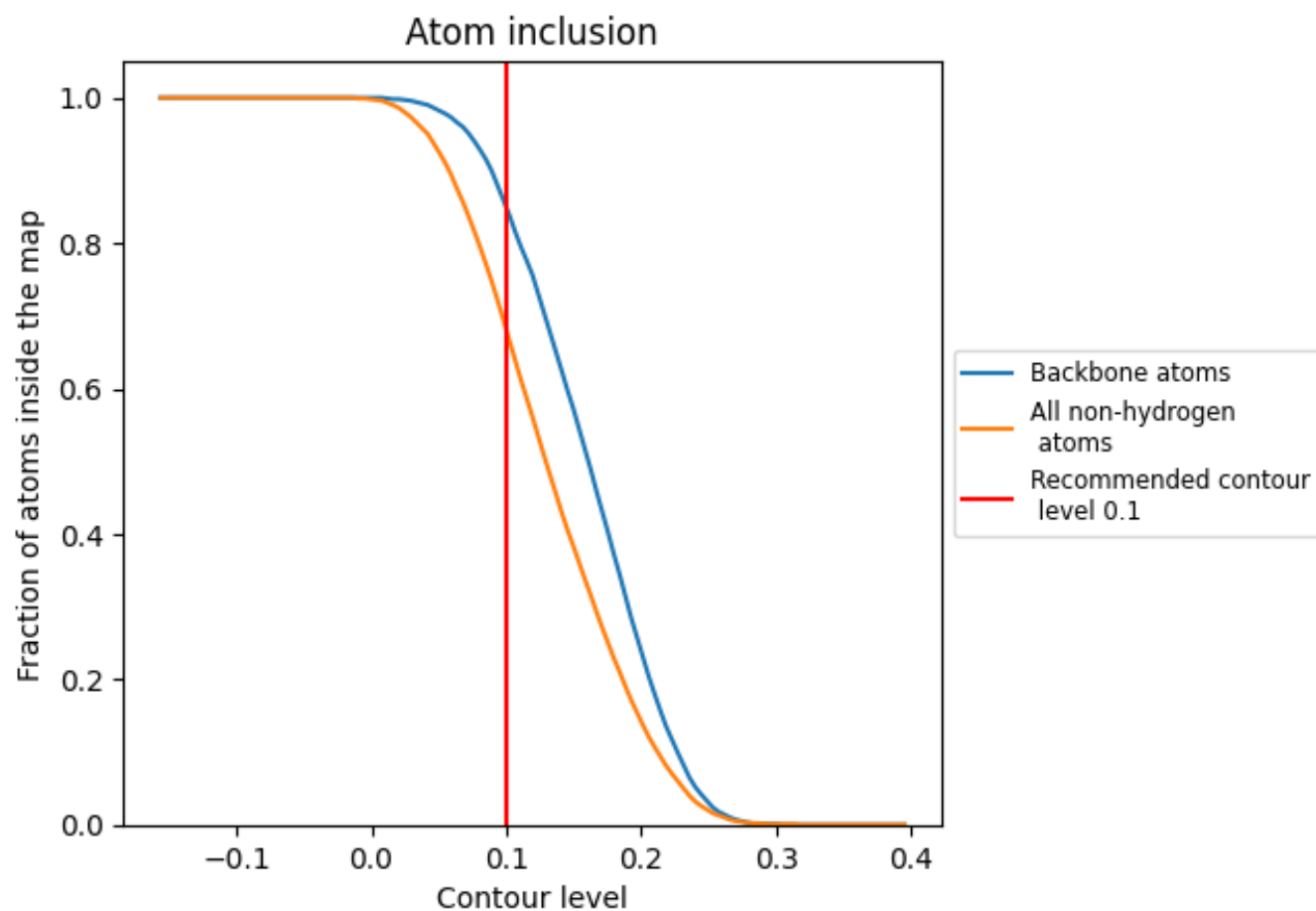
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6820	 0.4620
YM	 0.6270	 0.4330
YN	 0.7520	 0.4950
YO	 0.7080	 0.4790
YP	 0.6360	 0.4390
YQ	 0.6320	 0.4390
YR	 0.7510	 0.4920
YS	 0.7070	 0.4800
YT	 0.6380	 0.4410
YU	 0.6330	 0.4290
YV	 0.7510	 0.4960
YW	 0.7040	 0.4780
YX	 0.6420	 0.4480
YY	 0.6280	 0.4370
YZ	 0.7530	 0.4920
ZA	 0.7080	 0.4780
ZB	 0.6410	 0.4400
ZC	 0.6320	 0.4370
ZD	 0.7520	 0.4930
ZE	 0.7100	 0.4790
ZF	 0.6390	 0.4390
ZG	 0.6260	 0.4220
ZH	 0.7500	 0.4940
ZI	 0.7090	 0.4830
ZJ	 0.6380	 0.4430
ZK	 0.6260	 0.4370
ZL	 0.7470	 0.4920
ZM	 0.7100	 0.4810
ZN	 0.6400	 0.4380
ZO	 0.6240	 0.4230
ZP	 0.7500	 0.4930
ZQ	 0.7070	 0.4820
ZR	 0.6410	 0.4460
ZS	 0.6340	 0.4370
ZT	 0.7530	 0.4910



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
ZU	 0.7080	 0.4820
ZV	 0.6310	 0.4380
ZW	 0.6250	 0.4220
ZX	 0.7480	 0.4940
ZY	 0.7110	 0.4800
ZZ	 0.6400	 0.4470