



wwPDB EM Validation Summary Report ⓘ

Sep 5, 2026 – 11:53 am BST

PDB ID : 9TLK / pdb_00009tlk
EMDB ID : EMD-56056
Title : Cryo-EM Structure of the oligomeric LPOR:Chlide:NADPH Complexes HF-25
Authors : Gabruk, M.; Desfosses, A.; Estrozi, L.F.; Pintscher, S.; Rawski, M.
Deposited on : 2025-12-10
Resolution : 3.20 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:

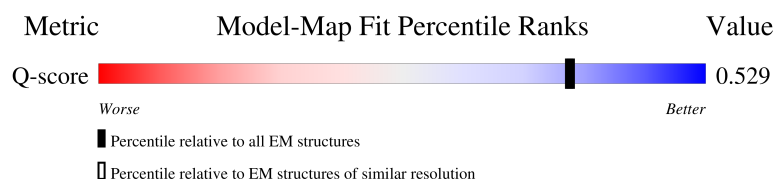
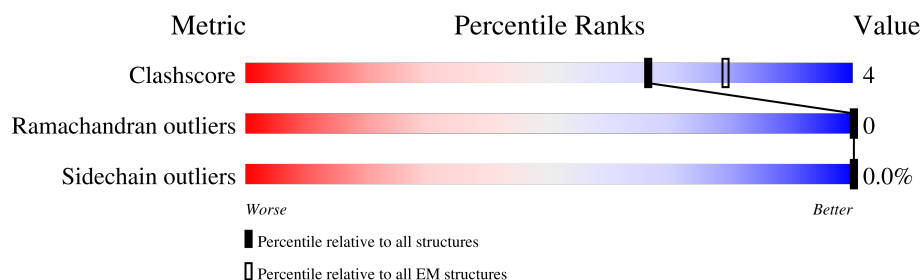
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.20 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.



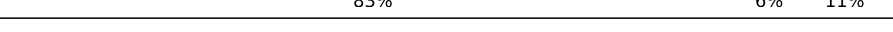
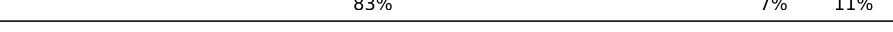
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	AA	353	
1	AB	353	
1	AC	353	
1	AD	353	

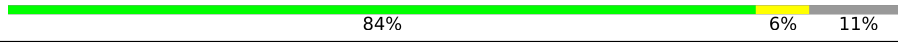
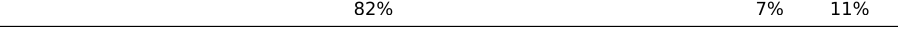
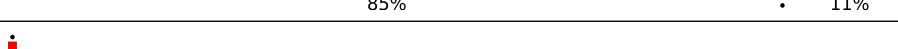
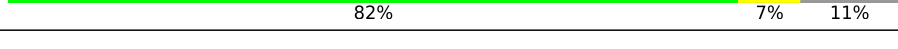
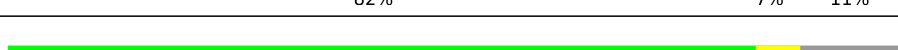
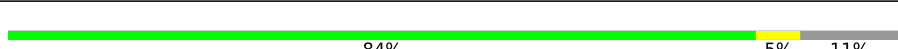
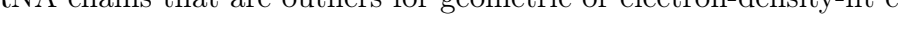
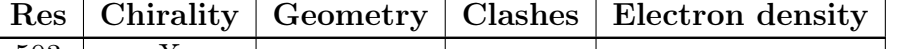
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Mol	Chain	Length	Quality of chain
1	AE	353	
1	AF	353	
1	AG	353	
1	AH	353	
1	AI	353	
1	AJ	353	
1	AK	353	
1	AL	353	
1	BA	353	
1	BB	353	
1	BC	353	
1	BD	353	
1	BE	353	
1	BF	353	
1	BG	353	
1	BH	353	
1	BI	353	
1	BJ	353	
1	BK	353	
1	BL	353	
1	CA	353	
1	CB	353	
1	CC	353	
1	CD	353	
1	CE	353	

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Mol	Chain	Length	Quality of chain
1	CF	353	
1	CG	353	
1	CH	353	
1	CI	353	
1	CJ	353	
1	CK	353	
1	CL	353	
1	DA	353	
1	DB	353	
1	DC	353	
1	DD	353	
1	DE	353	
1	DF	353	
1	DG	353	
1	DH	353	
1	DI	353	
1	DJ	353	
1	DK	353	
1	DL	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
4	A1JWG	AA	503	X	-	-	-
4	A1JWG	AB	503	X	-	-	-
4	A1JWG	AC	503	X	-	-	-
4	A1JWG	AD	503	X	-	-	-
4	A1JWG	AE	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	A1JWG	AF	503	X	-	-	-
4	A1JWG	AG	503	X	-	-	-
4	A1JWG	AH	503	X	-	-	-
4	A1JWG	AI	503	X	-	-	-
4	A1JWG	AJ	503	X	-	-	-
4	A1JWG	AK	503	X	-	-	-
4	A1JWG	AL	503	X	-	-	-
4	A1JWG	BA	503	X	-	-	-
4	A1JWG	BB	503	X	-	-	-
4	A1JWG	BC	503	X	-	-	-
4	A1JWG	BD	503	X	-	-	-
4	A1JWG	BE	503	X	-	-	-
4	A1JWG	BF	503	X	-	-	-
4	A1JWG	BG	503	X	-	-	-
4	A1JWG	BH	503	X	-	-	-
4	A1JWG	BI	503	X	-	-	-
4	A1JWG	BJ	503	X	-	-	-
4	A1JWG	BK	503	X	-	-	-
4	A1JWG	BL	503	X	-	-	-
4	A1JWG	CA	503	X	-	-	-
4	A1JWG	CB	503	X	-	-	-
4	A1JWG	CC	503	X	-	-	-
4	A1JWG	CD	503	X	-	-	-
4	A1JWG	CE	503	X	-	-	-
4	A1JWG	CF	503	X	-	-	-
4	A1JWG	CG	503	X	-	-	-
4	A1JWG	CH	503	X	-	-	-
4	A1JWG	CI	503	X	-	-	-
4	A1JWG	CJ	503	X	-	-	-
4	A1JWG	CK	503	X	-	-	-
4	A1JWG	CL	503	X	-	-	-
4	A1JWG	DA	503	X	-	-	-
4	A1JWG	DB	503	X	-	-	-
4	A1JWG	DC	503	X	-	-	-
4	A1JWG	DD	503	X	-	-	-
4	A1JWG	DE	503	X	-	-	-
4	A1JWG	DF	503	X	-	-	-
4	A1JWG	DG	503	X	-	-	-
4	A1JWG	DH	503	X	-	-	-
4	A1JWG	DI	503	X	-	-	-
4	A1JWG	DJ	503	X	-	-	-
4	A1JWG	DK	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	A1JWG	DL	503	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 237552 atoms, of which 116160 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	AA	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	AB	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	AC	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	AD	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	AE	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	AF	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	AG	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	AH	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	AI	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	AJ	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	AK	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	AL	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	BA	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	BB	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	BC	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	BD	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	BE	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	BF	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	BG	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	BH	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	BI	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	BJ	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	BK	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	BL	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CA	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CB	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CC	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CD	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CE	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CF	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CG	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CH	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CI	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CJ	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CK	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	CL	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	DA	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0
1	DB	315	Total 4800	C 1528	H 2387	N 417	O 458	S 10	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	DC	315	Total	C	H	N	O	S	0	0
			4800	1528	2387	417	458	10		
1	DD	315	Total	C	H	N	O	S	0	0
			4800	1528	2387	417	458	10		
1	DE	315	Total	C	H	N	O	S	0	0
			4800	1528	2387	417	458	10		
1	DF	315	Total	C	H	N	O	S	0	0
			4800	1528	2387	417	458	10		
1	DG	315	Total	C	H	N	O	S	0	0
			4800	1528	2387	417	458	10		
1	DH	315	Total	C	H	N	O	S	0	0
			4800	1528	2387	417	458	10		
1	DI	315	Total	C	H	N	O	S	0	0
			4800	1528	2387	417	458	10		
1	DJ	315	Total	C	H	N	O	S	0	0
			4800	1528	2387	417	458	10		
1	DK	315	Total	C	H	N	O	S	0	0
			4800	1528	2387	417	458	10		
1	DL	315	Total	C	H	N	O	S	0	0
			4800	1528	2387	417	458	10		

There are 912 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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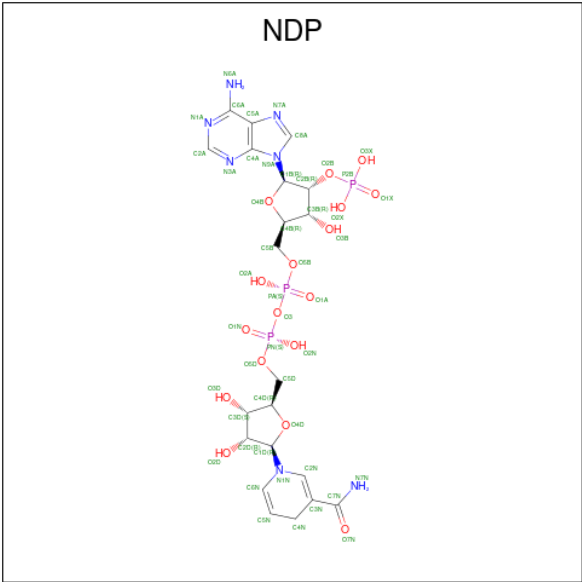
Chain	Residue	Modelled	Actual	Comment	Reference
DJ	53	HIS	-	expression tag	UNP P21218
DJ	54	HIS	-	expression tag	UNP P21218
DJ	55	HIS	-	expression tag	UNP P21218
DJ	56	HIS	-	expression tag	UNP P21218
DJ	57	HIS	-	expression tag	UNP P21218
DJ	58	HIS	-	expression tag	UNP P21218
DJ	59	SER	-	expression tag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

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Chain	Residue	Modelled	Actual	Comment	Reference
DL	57	HIS	-	expression tag	UNP P21218
DL	58	HIS	-	expression tag	UNP P21218
DL	59	SER	-	expression tag	UNP P21218
DL	60	SER	-	expression tag	UNP P21218
DL	61	GLY	-	expression tag	UNP P21218
DL	62	LEU	-	expression tag	UNP P21218
DL	63	VAL	-	expression tag	UNP P21218
DL	64	PRO	-	expression tag	UNP P21218
DL	65	ARG	-	expression tag	UNP P21218
DL	66	GLY	-	expression tag	UNP P21218
DL	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	AA	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	AB	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	AC	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	AD	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	AE	1	Total	C	N	O	P	0
			48	21	7	17	3	

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Mol	Chain	Residues	Atoms					AltConf
2	AF	1	Total 48	C 21	N 7	O 17	P 3	0
2	AG	1	Total 48	C 21	N 7	O 17	P 3	0
2	AH	1	Total 48	C 21	N 7	O 17	P 3	0
2	AI	1	Total 48	C 21	N 7	O 17	P 3	0
2	AJ	1	Total 48	C 21	N 7	O 17	P 3	0
2	AK	1	Total 48	C 21	N 7	O 17	P 3	0
2	AL	1	Total 48	C 21	N 7	O 17	P 3	0
2	BA	1	Total 48	C 21	N 7	O 17	P 3	0
2	BB	1	Total 48	C 21	N 7	O 17	P 3	0
2	BC	1	Total 48	C 21	N 7	O 17	P 3	0
2	BD	1	Total 48	C 21	N 7	O 17	P 3	0
2	BE	1	Total 48	C 21	N 7	O 17	P 3	0
2	BF	1	Total 48	C 21	N 7	O 17	P 3	0
2	BG	1	Total 48	C 21	N 7	O 17	P 3	0
2	BH	1	Total 48	C 21	N 7	O 17	P 3	0
2	BI	1	Total 48	C 21	N 7	O 17	P 3	0
2	BJ	1	Total 48	C 21	N 7	O 17	P 3	0
2	BK	1	Total 48	C 21	N 7	O 17	P 3	0
2	BL	1	Total 48	C 21	N 7	O 17	P 3	0
2	CA	1	Total 48	C 21	N 7	O 17	P 3	0
2	CB	1	Total 48	C 21	N 7	O 17	P 3	0

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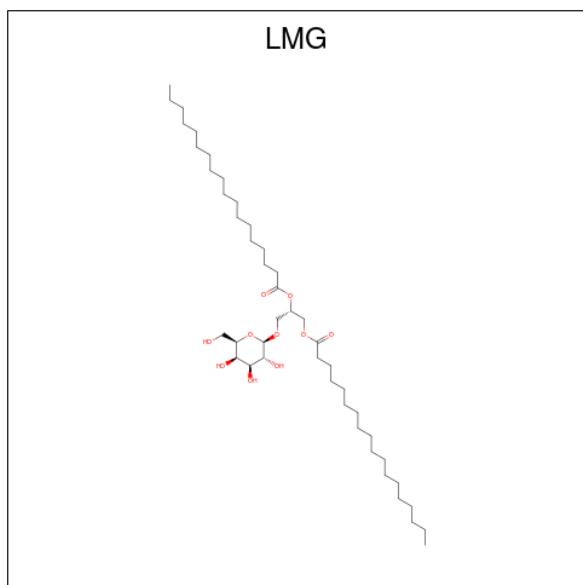
Mol	Chain	Residues	Atoms					AltConf
2	CC	1	Total 48	C 21	N 7	O 17	P 3	0
2	CD	1	Total 48	C 21	N 7	O 17	P 3	0
2	CE	1	Total 48	C 21	N 7	O 17	P 3	0
2	CF	1	Total 48	C 21	N 7	O 17	P 3	0
2	CG	1	Total 48	C 21	N 7	O 17	P 3	0
2	CH	1	Total 48	C 21	N 7	O 17	P 3	0
2	CI	1	Total 48	C 21	N 7	O 17	P 3	0
2	CJ	1	Total 48	C 21	N 7	O 17	P 3	0
2	CK	1	Total 48	C 21	N 7	O 17	P 3	0
2	CL	1	Total 48	C 21	N 7	O 17	P 3	0
2	DA	1	Total 48	C 21	N 7	O 17	P 3	0
2	DB	1	Total 48	C 21	N 7	O 17	P 3	0
2	DC	1	Total 48	C 21	N 7	O 17	P 3	0
2	DD	1	Total 48	C 21	N 7	O 17	P 3	0
2	DE	1	Total 48	C 21	N 7	O 17	P 3	0
2	DF	1	Total 48	C 21	N 7	O 17	P 3	0
2	DG	1	Total 48	C 21	N 7	O 17	P 3	0
2	DH	1	Total 48	C 21	N 7	O 17	P 3	0
2	DI	1	Total 48	C 21	N 7	O 17	P 3	0
2	DJ	1	Total 48	C 21	N 7	O 17	P 3	0
2	DK	1	Total 48	C 21	N 7	O 17	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
2	DL	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 3 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
3	AA	1	Total	C	O	0
			23	13	10	
3	AB	1	Total	C	O	0
			23	13	10	
3	AC	1	Total	C	O	0
			23	13	10	
3	AD	1	Total	C	O	0
			23	13	10	
3	AE	1	Total	C	O	0
			23	13	10	
3	AF	1	Total	C	O	0
			23	13	10	
3	AG	1	Total	C	O	0
			23	13	10	
3	AH	1	Total	C	O	0
			23	13	10	
3	AI	1	Total	C	O	0
			23	13	10	
3	AJ	1	Total	C	O	0
			23	13	10	

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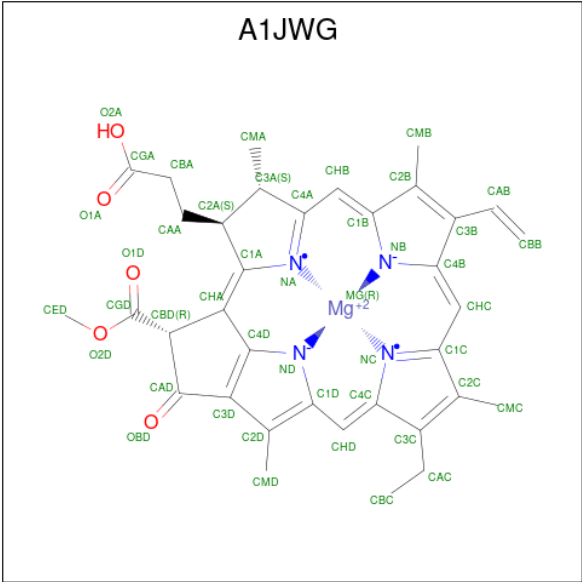
Mol	Chain	Residues	Atoms			AltConf
3	AK	1	Total 23	C 13	O 10	0
3	AL	1	Total 23	C 13	O 10	0
3	BA	1	Total 23	C 13	O 10	0
3	BB	1	Total 23	C 13	O 10	0
3	BC	1	Total 23	C 13	O 10	0
3	BD	1	Total 23	C 13	O 10	0
3	BE	1	Total 23	C 13	O 10	0
3	BF	1	Total 23	C 13	O 10	0
3	BG	1	Total 23	C 13	O 10	0
3	BH	1	Total 23	C 13	O 10	0
3	BI	1	Total 23	C 13	O 10	0
3	BJ	1	Total 23	C 13	O 10	0
3	BK	1	Total 23	C 13	O 10	0
3	BL	1	Total 23	C 13	O 10	0
3	CA	1	Total 23	C 13	O 10	0
3	CB	1	Total 23	C 13	O 10	0
3	CC	1	Total 23	C 13	O 10	0
3	CD	1	Total 23	C 13	O 10	0
3	CE	1	Total 23	C 13	O 10	0
3	CF	1	Total 23	C 13	O 10	0
3	CG	1	Total 23	C 13	O 10	0

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Mol	Chain	Residues	Atoms			AltConf
3	CH	1	Total	C	O	0
			23	13	10	
3	CI	1	Total	C	O	0
			23	13	10	
3	CJ	1	Total	C	O	0
			23	13	10	
3	CK	1	Total	C	O	0
			23	13	10	
3	CL	1	Total	C	O	0
			23	13	10	
3	DA	1	Total	C	O	0
			23	13	10	
3	DB	1	Total	C	O	0
			23	13	10	
3	DC	1	Total	C	O	0
			23	13	10	
3	DD	1	Total	C	O	0
			23	13	10	
3	DE	1	Total	C	O	0
			23	13	10	
3	DF	1	Total	C	O	0
			23	13	10	
3	DG	1	Total	C	O	0
			23	13	10	
3	DH	1	Total	C	O	0
			23	13	10	
3	DI	1	Total	C	O	0
			23	13	10	
3	DJ	1	Total	C	O	0
			23	13	10	
3	DK	1	Total	C	O	0
			23	13	10	
3	DL	1	Total	C	O	0
			23	13	10	

- Molecule 4 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
4	AA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	AB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	AC	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	AD	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	AE	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	AF	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	AG	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	AH	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	AI	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	AJ	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	AK	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	AL	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	BA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
4	BC	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	BD	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	BE	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	BF	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	BG	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	BH	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	BI	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	BJ	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	BK	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	BL	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	CA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	CB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	CC	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	CD	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	CE	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	CF	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	CG	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	CH	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	CI	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	CJ	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	CK	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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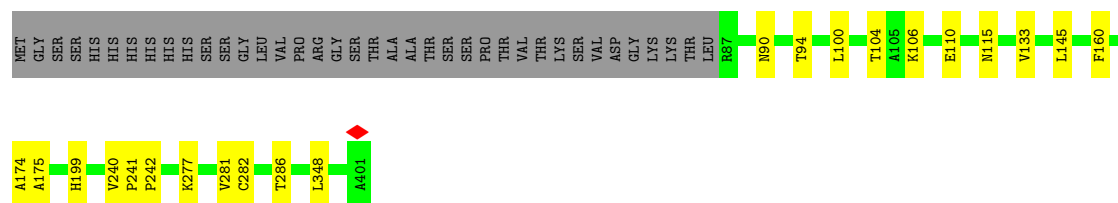
Mol	Chain	Residues	Atoms						AltConf
4	CL	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DC	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DD	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DE	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DF	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DG	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DH	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DI	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DJ	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DK	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
4	DL	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

3 Residue-property plots

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

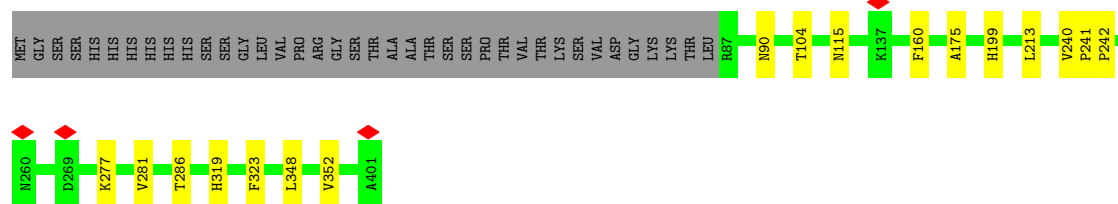
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AA: 



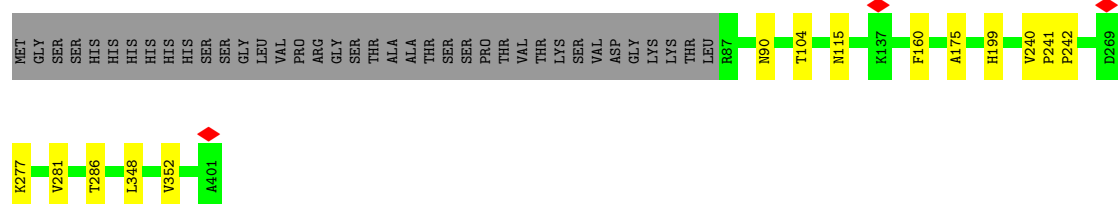
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AB: 



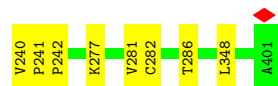
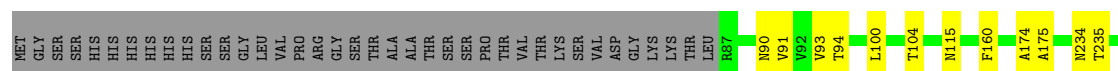
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AC: 

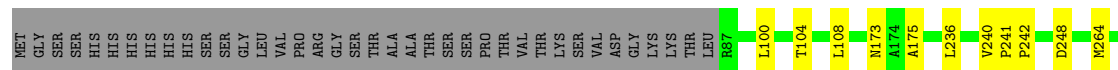
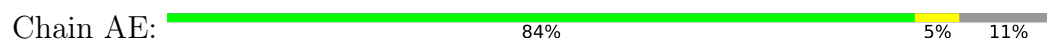


- Molecule 1: Protochlorophyllide reductase B, chloroplastic

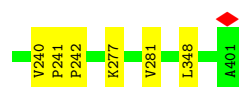
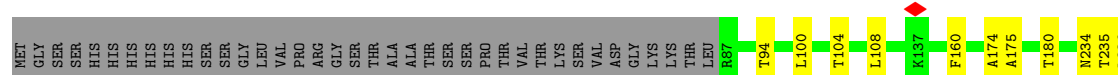
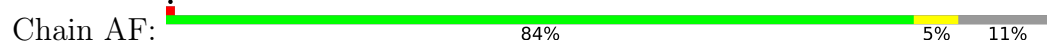
Chain AD: 



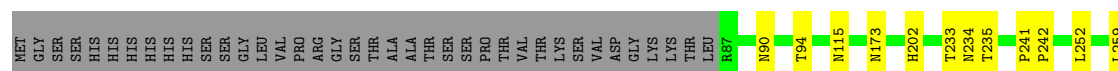
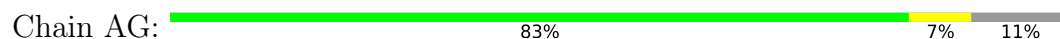
- Molecule 1: Protochlorophyllide reductase B, chloroplastic



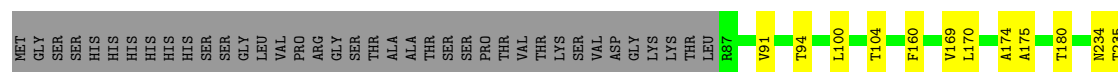
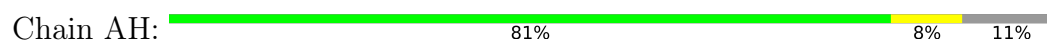
- Molecule 1: Protochlorophyllide reductase B, chloroplastic



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

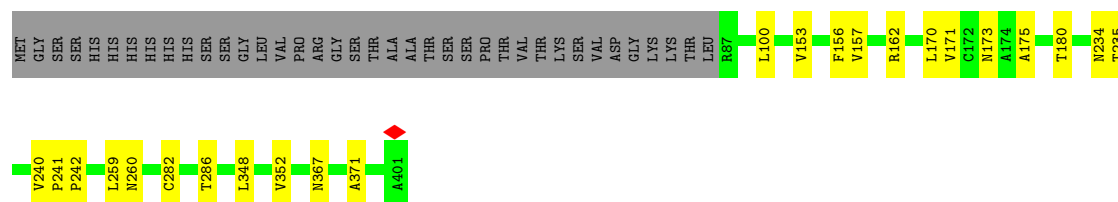


- Molecule 1: Protochlorophyllide reductase B, chloroplastic



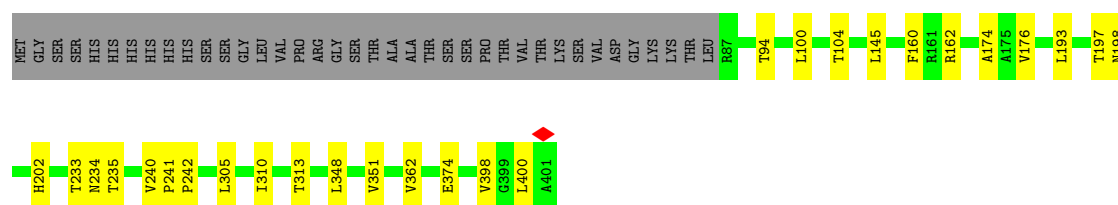
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AI:  83% 7% 11%



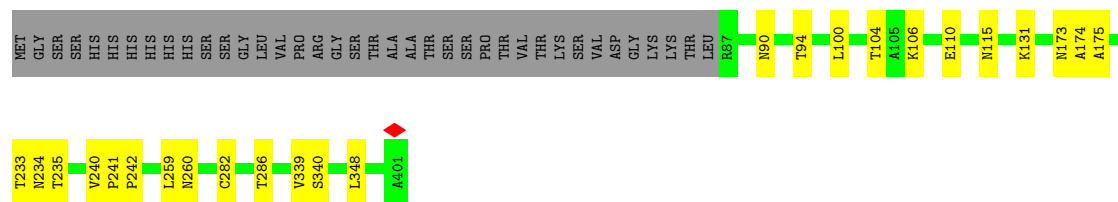
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AJ:  82% 8% 11%



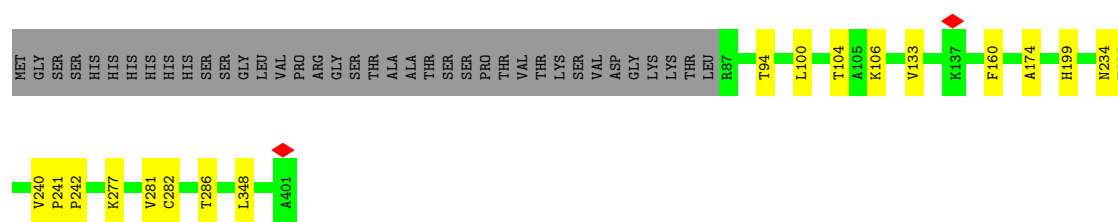
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AK:  82% 7% 11%



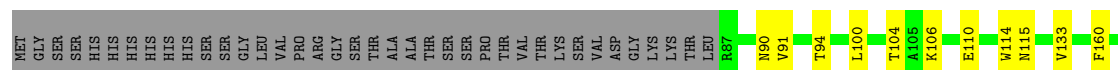
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

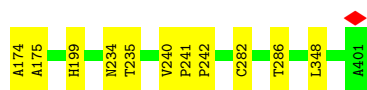
Chain AL:  84% 5% 11%



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

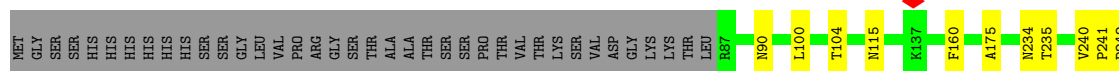
Chain BA:  83% 6% 11%





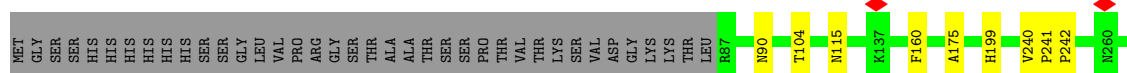
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BB: 85% 11%



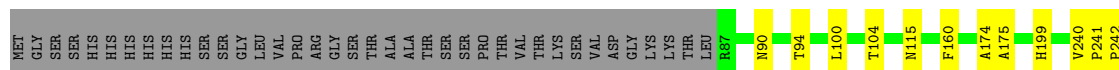
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BC: 85% 5% 11%



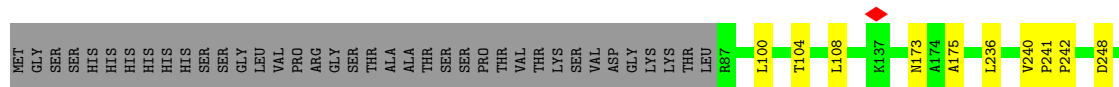
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BD: 84% 5% 11%



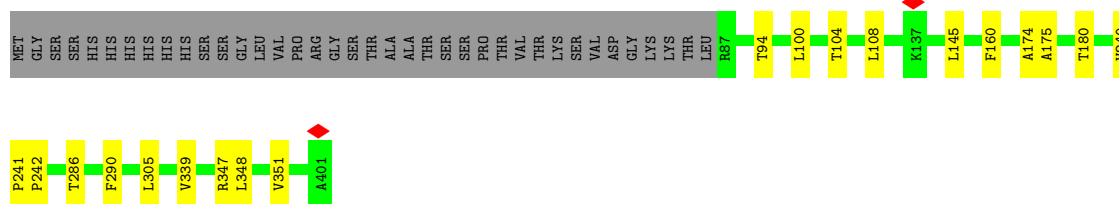
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BE: 84% 5% 11%



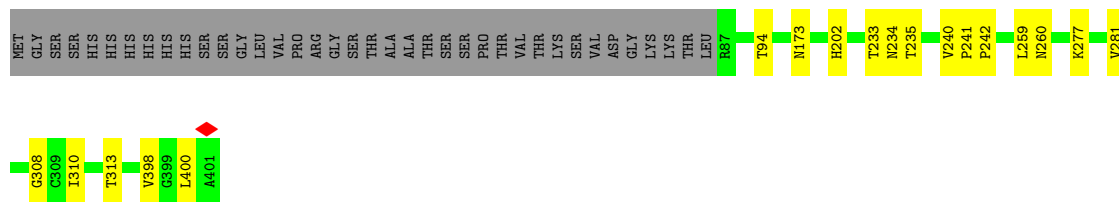
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BF:  84% 5% 11%



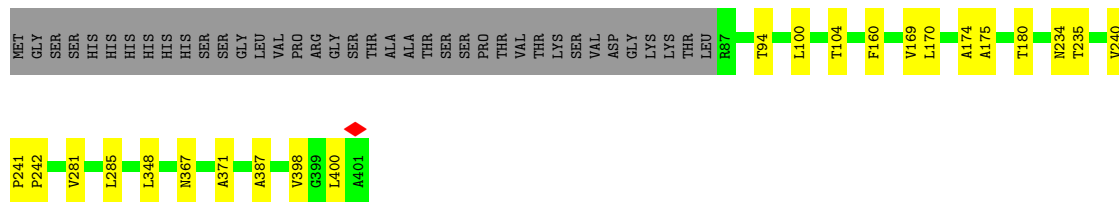
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BG:  84% 5% 11%



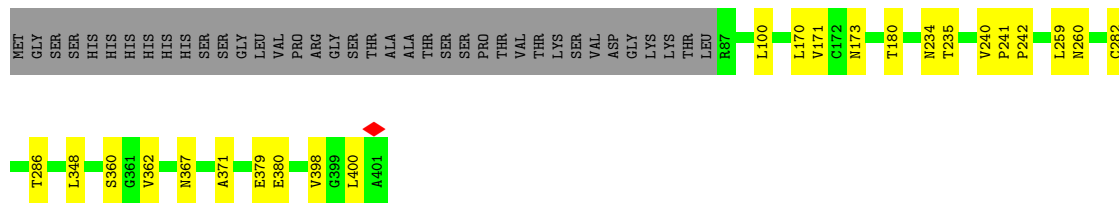
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BH:  83% 6% 11%



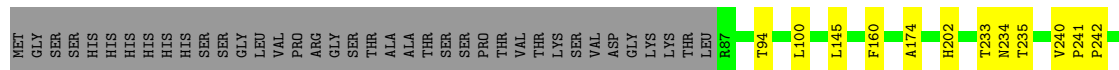
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BI:  83% 7% 11%



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

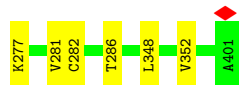
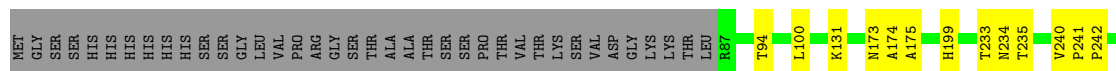
Chain BJ:  83% 6% 11%





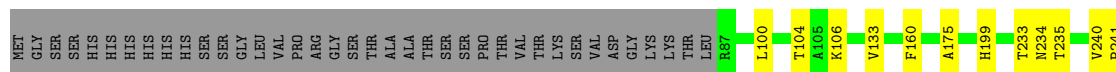
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BK: 84% 5% 11%



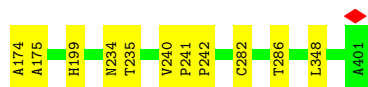
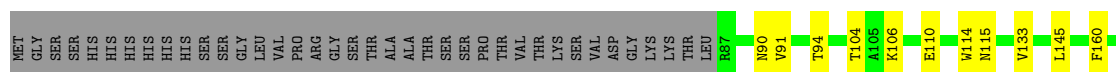
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BL: 84% 5% 11%



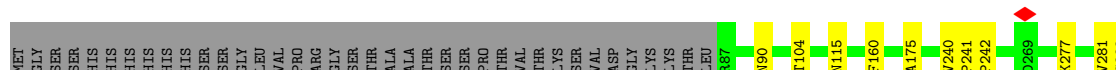
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CA: 83% 6% 11%



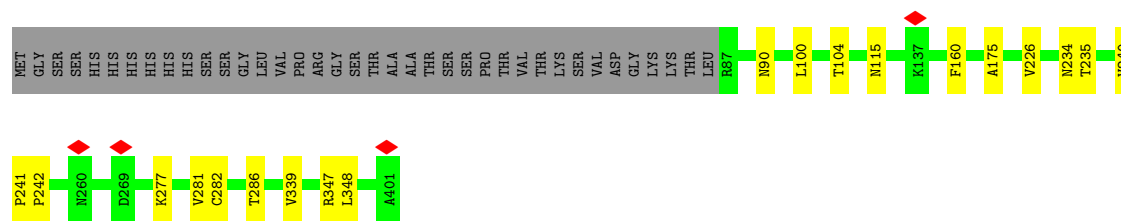
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CB: 84% 5% 11%



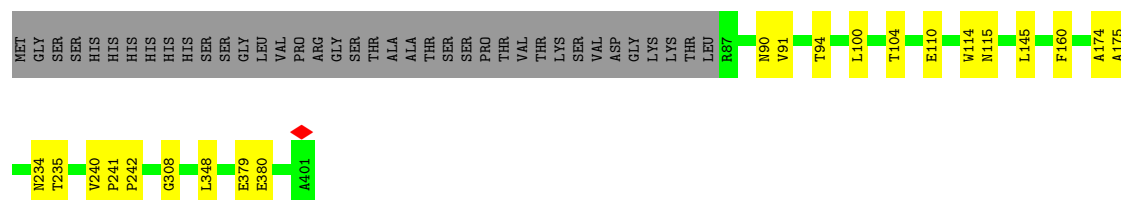
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CC: 84% 5% 11%



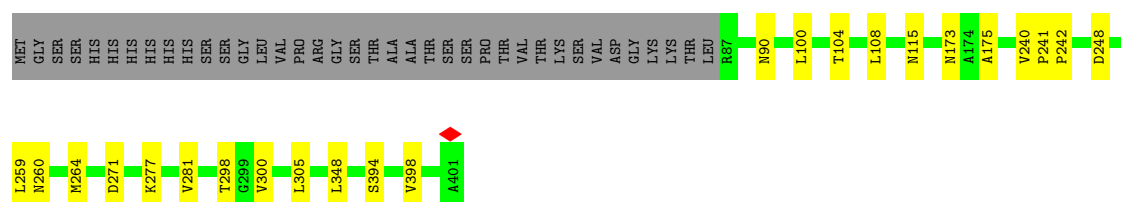
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CD: 83% 6% 11%



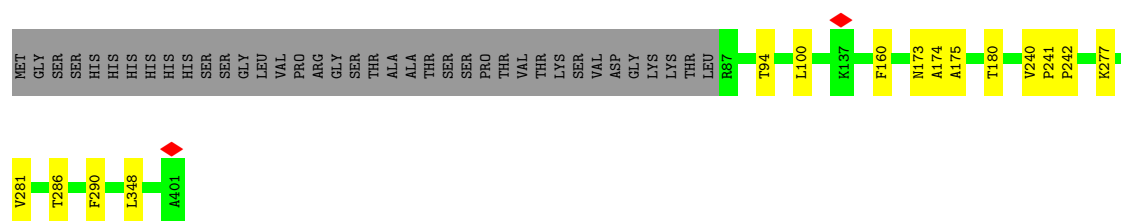
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CE: 83% 7% 11%



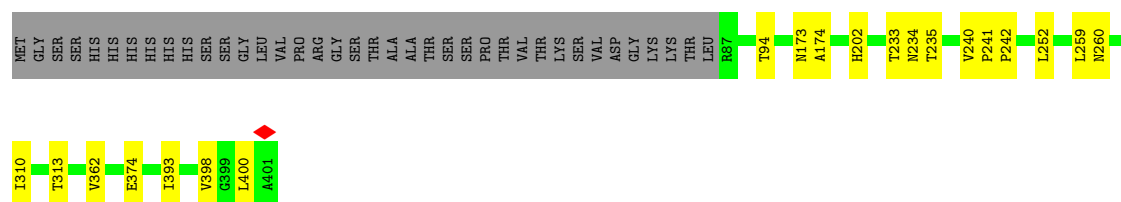
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CF: 85% 0% 11%



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CG: 84% 6% 11%

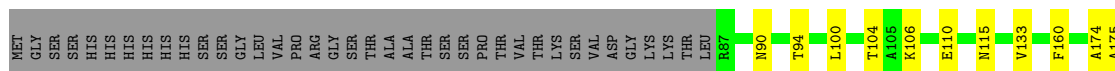


- | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|
| MET | GLY | SER | SER | SER | HIS | HIS | HIS | HIS | HIS | HIS | SER | SER | GLY | LEU | VAL | PRO | ARG | GLY | GLY | THR | ALA | ALA | ALA | ALA | THR | SER | SER | SER | PRO | PRO | THR | THR | THR | LYS | LYS | VAL | VAL | ASP | GLY | GLY | LYS | LYS | LYS | THR | THR | LEU | R87 | T94 | L100 | T104 | A105 | K106 | V133 | F160 | A174 | H199 | T233 | N234 | T235 |
|------|------|------|------|------|------|------|------|------|------|------|



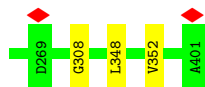
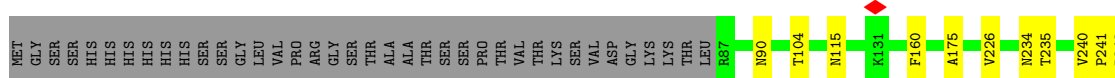
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DA: 83% 6% 11%



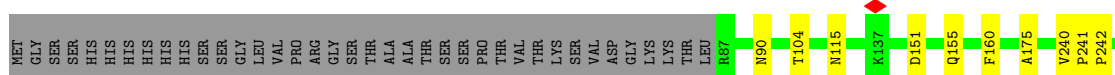
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DB: 85% • 11%



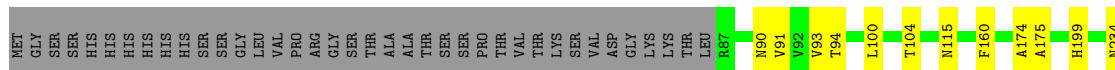
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DC: 84% 5% 11%



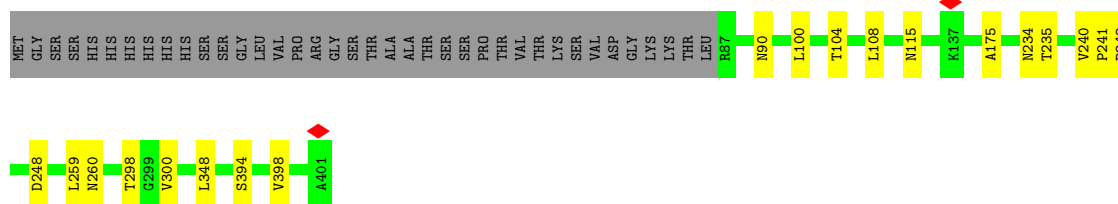
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DD: 83% 6% 11%



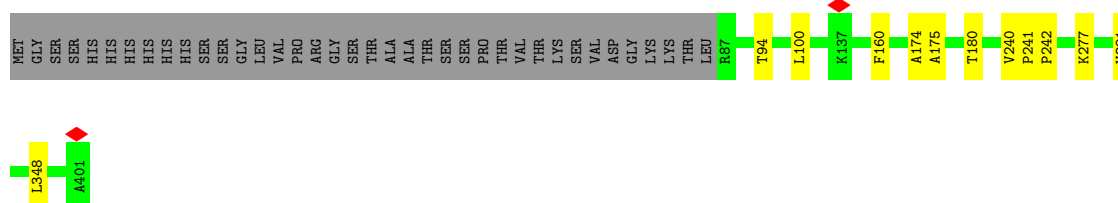
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DE:  84% 5% 11%



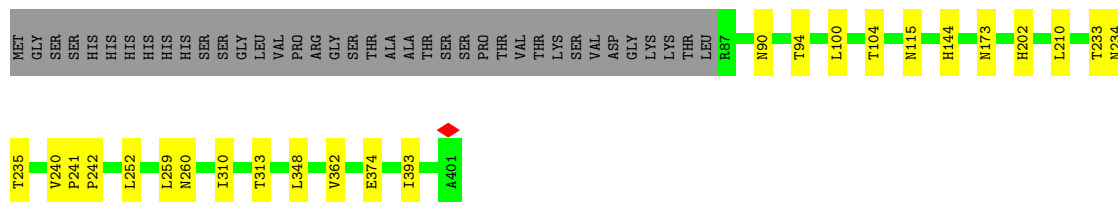
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DF:  86% 11%



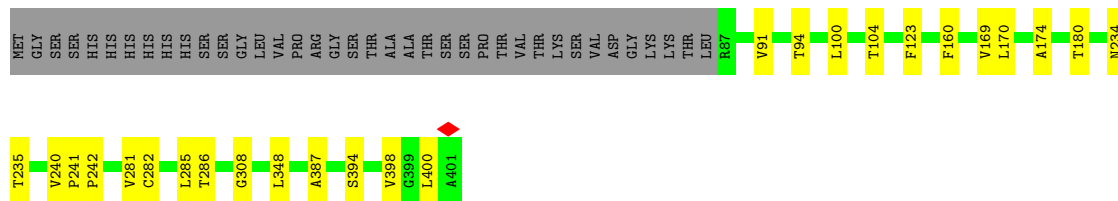
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DG:  82% 7% 11%



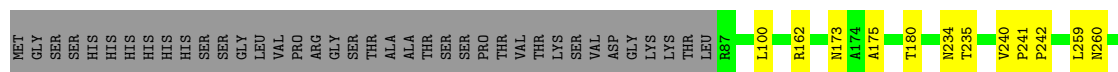
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

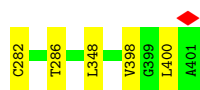
Chain DH:  82% 7% 11%



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

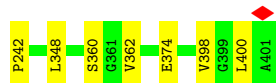
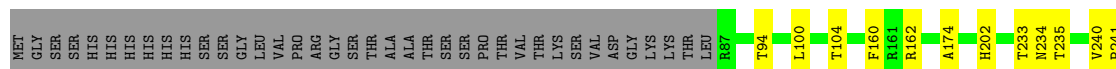
Chain DI:  84% 5% 11%





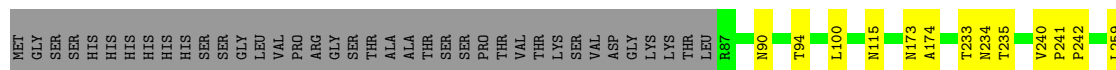
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DJ: 84% 5% 11%



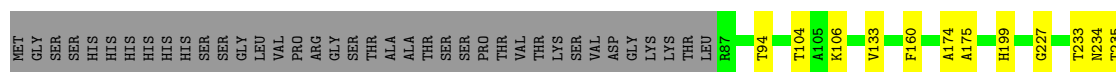
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DK: 84% 5% 11%



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DL: 84% 5% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-114.391°, rise=25.609 Å, axial sym=D4	Depositor
Number of segments used	23139	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	0.447	Depositor
Minimum map value	-0.210	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.105	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	AA	0.12	0/2462	0.36	2/3331 (0.1%)
1	AB	0.11	0/2462	0.37	2/3331 (0.1%)
1	AC	0.11	0/2462	0.37	2/3331 (0.1%)
1	AD	0.12	0/2462	0.36	2/3331 (0.1%)
1	AE	0.12	0/2462	0.31	0/3331
1	AF	0.12	0/2462	0.36	2/3331 (0.1%)
1	AG	0.13	0/2462	0.31	0/3331
1	AH	0.13	0/2462	0.37	2/3331 (0.1%)
1	AI	0.13	0/2462	0.32	0/3331
1	AJ	0.12	0/2462	0.38	2/3331 (0.1%)
1	AK	0.12	0/2462	0.31	0/3331
1	AL	0.12	0/2462	0.36	2/3331 (0.1%)
1	BA	0.12	0/2462	0.36	2/3331 (0.1%)
1	BB	0.12	0/2462	0.37	2/3331 (0.1%)
1	BC	0.11	0/2462	0.37	2/3331 (0.1%)
1	BD	0.12	0/2462	0.36	2/3331 (0.1%)
1	BE	0.12	0/2462	0.31	0/3331
1	BF	0.12	0/2462	0.37	2/3331 (0.1%)
1	BG	0.12	0/2462	0.31	0/3331
1	BH	0.13	0/2462	0.37	2/3331 (0.1%)
1	BI	0.13	0/2462	0.32	0/3331
1	BJ	0.12	0/2462	0.38	2/3331 (0.1%)
1	BK	0.12	0/2462	0.31	0/3331
1	BL	0.12	0/2462	0.35	2/3331 (0.1%)
1	CA	0.12	0/2462	0.36	2/3331 (0.1%)
1	CB	0.11	0/2462	0.37	2/3331 (0.1%)
1	CC	0.12	0/2462	0.37	2/3331 (0.1%)
1	CD	0.12	0/2462	0.36	2/3331 (0.1%)
1	CE	0.12	0/2462	0.31	0/3331
1	CF	0.12	0/2462	0.36	2/3331 (0.1%)
1	CG	0.12	0/2462	0.30	0/3331
1	CH	0.13	0/2462	0.37	2/3331 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CI	0.12	0/2462	0.31	0/3331
1	CJ	0.12	0/2462	0.38	2/3331 (0.1%)
1	CK	0.12	0/2462	0.31	0/3331
1	CL	0.12	0/2462	0.36	2/3331 (0.1%)
1	DA	0.12	0/2462	0.36	2/3331 (0.1%)
1	DB	0.12	0/2462	0.37	2/3331 (0.1%)
1	DC	0.12	0/2462	0.37	2/3331 (0.1%)
1	DD	0.12	0/2462	0.36	2/3331 (0.1%)
1	DE	0.12	0/2462	0.31	0/3331
1	DF	0.12	0/2462	0.36	2/3331 (0.1%)
1	DG	0.12	0/2462	0.30	0/3331
1	DH	0.13	0/2462	0.37	2/3331 (0.1%)
1	DI	0.12	0/2462	0.32	0/3331
1	DJ	0.12	0/2462	0.38	2/3331 (0.1%)
1	DK	0.12	0/2462	0.31	0/3331
1	DL	0.12	0/2462	0.36	2/3331 (0.1%)
All	All	0.12	0/118176	0.35	64/159888 (0.0%)

There are no bond length outliers.

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CJ	160	PHE	CA-C-N	9.08	133.36	120.28
1	CJ	160	PHE	C-N-CA	9.08	133.36	120.28
1	AJ	160	PHE	CA-C-N	9.01	133.25	120.28
1	AJ	160	PHE	C-N-CA	9.01	133.25	120.28
1	DJ	160	PHE	CA-C-N	8.97	133.20	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2413	2387	2406	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	2413	2387	2406	18	0
1	AC	2413	2387	2406	15	0
1	AD	2413	2387	2406	15	0
1	AE	2413	2387	2406	17	0
1	AF	2413	2387	2406	17	0
1	AG	2413	2387	2406	17	0
1	AH	2413	2387	2406	25	0
1	AI	2413	2387	2406	24	0
1	AJ	2413	2387	2406	22	0
1	AK	2413	2387	2406	21	0
1	AL	2413	2387	2406	17	0
1	BA	2413	2387	2406	18	0
1	BB	2413	2387	2406	14	0
1	BC	2413	2387	2406	16	0
1	BD	2413	2387	2406	16	0
1	BE	2413	2387	2406	17	0
1	BF	2413	2387	2406	16	0
1	BG	2413	2387	2406	17	0
1	BH	2413	2387	2406	17	0
1	BI	2413	2387	2406	22	0
1	BJ	2413	2387	2406	17	0
1	BK	2413	2387	2406	21	0
1	BL	2413	2387	2406	16	0
1	CA	2413	2387	2406	18	0
1	CB	2413	2387	2406	18	0
1	CC	2413	2387	2406	19	0
1	CD	2413	2387	2406	21	0
1	CE	2413	2387	2406	19	0
1	CF	2413	2387	2406	17	0
1	CG	2413	2387	2406	18	0
1	CH	2413	2387	2406	23	0
1	CI	2413	2387	2406	22	0
1	CJ	2413	2387	2406	16	0
1	CK	2413	2387	2406	19	0
1	CL	2413	2387	2406	18	0
1	DA	2413	2387	2406	19	0
1	DB	2413	2387	2406	16	0
1	DC	2413	2387	2406	15	0
1	DD	2413	2387	2406	20	0
1	DE	2413	2387	2406	17	0
1	DF	2413	2387	2406	15	0
1	DG	2413	2387	2406	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DH	2413	2387	2406	21	0
1	DI	2413	2387	2406	17	0
1	DJ	2413	2387	2406	19	0
1	DK	2413	2387	2406	16	0
1	DL	2413	2387	2406	19	0
2	AA	48	0	26	2	0
2	AB	48	0	26	2	0
2	AC	48	0	26	3	0
2	AD	48	0	26	1	0
2	AE	48	0	26	4	0
2	AF	48	0	26	1	0
2	AG	48	0	26	2	0
2	AH	48	0	26	3	0
2	AI	48	0	26	3	0
2	AJ	48	0	26	1	0
2	AK	48	0	26	3	0
2	AL	48	0	26	1	0
2	BA	48	0	26	3	0
2	BB	48	0	26	2	0
2	BC	48	0	26	2	0
2	BD	48	0	26	4	0
2	BE	48	0	26	2	0
2	BF	48	0	26	2	0
2	BG	48	0	26	4	0
2	BH	48	0	26	2	0
2	BI	48	0	26	3	0
2	BJ	48	0	26	1	0
2	BK	48	0	26	2	0
2	BL	48	0	26	2	0
2	CA	48	0	26	2	0
2	CB	48	0	26	4	0
2	CC	48	0	26	3	0
2	CD	48	0	26	3	0
2	CE	48	0	26	2	0
2	CF	48	0	26	1	0
2	CG	48	0	26	3	0
2	CH	48	0	26	2	0
2	CI	48	0	26	6	0
2	CJ	48	0	26	0	0
2	CK	48	0	26	3	0
2	CL	48	0	26	0	0
2	DA	48	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	DB	48	0	26	5	0
2	DC	48	0	26	3	0
2	DD	48	0	26	4	0
2	DE	48	0	26	5	0
2	DF	48	0	26	2	0
2	DG	48	0	26	3	0
2	DH	48	0	26	3	0
2	DI	48	0	26	2	0
2	DJ	48	0	26	1	0
2	DK	48	0	26	2	0
2	DL	48	0	26	4	0
3	AA	23	0	16	2	0
3	AB	23	0	16	3	0
3	AC	23	0	16	2	0
3	AD	23	0	16	0	0
3	AE	23	0	16	1	0
3	AF	23	0	16	3	0
3	AG	23	0	16	4	0
3	AH	23	0	16	2	0
3	AI	23	0	16	3	0
3	AJ	23	0	16	2	0
3	AK	23	0	16	2	0
3	AL	23	0	16	4	0
3	BA	23	0	16	1	0
3	BB	23	0	16	1	0
3	BC	23	0	16	2	0
3	BD	23	0	16	2	0
3	BE	23	0	16	4	0
3	BF	23	0	16	1	0
3	BG	23	0	16	3	0
3	BH	23	0	16	1	0
3	BI	23	0	16	2	0
3	BJ	23	0	16	1	0
3	BK	23	0	16	2	0
3	BL	23	0	16	2	0
3	CA	23	0	16	1	0
3	CB	23	0	16	4	0
3	CC	23	0	16	3	0
3	CD	23	0	16	4	0
3	CE	23	0	16	2	0
3	CF	23	0	16	4	0
3	CG	23	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CH	23	0	16	3	0
3	CI	23	0	16	3	0
3	CJ	23	0	16	2	0
3	CK	23	0	16	4	0
3	CL	23	0	16	2	0
3	DA	23	0	16	2	0
3	DB	23	0	16	1	0
3	DC	23	0	16	1	0
3	DD	23	0	16	3	0
3	DE	23	0	16	3	0
3	DF	23	0	16	4	0
3	DG	23	0	16	1	0
3	DH	23	0	16	1	0
3	DI	23	0	16	2	0
3	DJ	23	0	16	2	0
3	DK	23	0	16	3	0
3	DL	23	0	16	2	0
4	AA	45	33	0	1	0
4	AB	45	33	0	1	0
4	AC	45	33	0	1	0
4	AD	45	33	0	0	0
4	AE	45	33	0	2	0
4	AF	45	33	0	0	0
4	AG	45	33	0	1	0
4	AH	45	33	0	1	0
4	AI	45	33	0	1	0
4	AJ	45	33	0	1	0
4	AK	45	33	0	1	0
4	AL	45	33	0	1	0
4	BA	45	33	0	1	0
4	BB	45	33	0	1	0
4	BC	45	33	0	1	0
4	BD	45	33	0	1	0
4	BE	45	33	0	0	0
4	BF	45	33	0	1	0
4	BG	45	33	0	1	0
4	BH	45	33	0	1	0
4	BI	45	33	0	1	0
4	BJ	45	33	0	1	0
4	BK	45	33	0	0	0
4	BL	45	33	0	1	0
4	CA	45	33	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CB	45	33	0	3	0
4	CC	45	33	0	1	0
4	CD	45	33	0	1	0
4	CE	45	33	0	0	0
4	CF	45	33	0	0	0
4	CG	45	33	0	1	0
4	CH	45	33	0	1	0
4	CI	45	33	0	1	0
4	CJ	45	33	0	0	0
4	CK	45	33	0	1	0
4	CL	45	33	0	0	0
4	DA	45	33	0	1	0
4	DB	45	33	0	1	0
4	DC	45	33	0	1	0
4	DD	45	33	0	1	0
4	DE	45	33	0	2	0
4	DF	45	33	0	1	0
4	DG	45	33	0	1	0
4	DH	45	33	0	1	0
4	DI	45	33	0	0	0
4	DJ	45	33	0	1	0
4	DK	45	33	0	1	0
4	DL	45	33	0	1	0
All	All	121392	116160	117504	932	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 4.

The worst 5 of 932 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:CB:104:THR:HG21	1:CB:348:LEU:HD22	1.56	0.86
2:BI:501:NDP:H51N	2:BI:501:NDP:H2N	1.59	0.84
1:AL:241:PRO:HG2	1:AL:242:PRO:HD3	1.62	0.81
1:DK:241:PRO:HG2	1:DK:242:PRO:HD3	1.63	0.81
1:AG:298:THR:HG22	1:AG:300:VAL:HG13	1.62	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	AB	313/353 (89%)	306 (98%)	7 (2%)	0	100	100
1	AC	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	AD	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	AE	313/353 (89%)	306 (98%)	7 (2%)	0	100	100
1	AF	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	AG	313/353 (89%)	303 (97%)	10 (3%)	0	100	100
1	AH	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	AI	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	AJ	313/353 (89%)	303 (97%)	10 (3%)	0	100	100
1	AK	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	AL	313/353 (89%)	306 (98%)	7 (2%)	0	100	100
1	BA	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	BB	313/353 (89%)	307 (98%)	6 (2%)	0	100	100
1	BC	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	BD	313/353 (89%)	306 (98%)	7 (2%)	0	100	100
1	BE	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	BF	313/353 (89%)	303 (97%)	10 (3%)	0	100	100
1	BG	313/353 (89%)	302 (96%)	11 (4%)	0	100	100
1	BH	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	BI	313/353 (89%)	306 (98%)	7 (2%)	0	100	100
1	BJ	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	BK	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	BL	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	CA	313/353 (89%)	305 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CB	313/353 (89%)	308 (98%)	5 (2%)	0	100	100
1	CC	313/353 (89%)	307 (98%)	6 (2%)	0	100	100
1	CD	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	CE	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	CF	313/353 (89%)	303 (97%)	10 (3%)	0	100	100
1	CG	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	CH	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	CI	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	CJ	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	CK	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	CL	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	DA	313/353 (89%)	307 (98%)	6 (2%)	0	100	100
1	DB	313/353 (89%)	307 (98%)	6 (2%)	0	100	100
1	DC	313/353 (89%)	308 (98%)	5 (2%)	0	100	100
1	DD	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	DE	313/353 (89%)	306 (98%)	7 (2%)	0	100	100
1	DF	313/353 (89%)	303 (97%)	10 (3%)	0	100	100
1	DG	313/353 (89%)	302 (96%)	11 (4%)	0	100	100
1	DH	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	DI	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	DJ	313/353 (89%)	304 (97%)	9 (3%)	0	100	100
1	DK	313/353 (89%)	305 (97%)	8 (3%)	0	100	100
1	DL	313/353 (89%)	306 (98%)	7 (2%)	0	100	100
All	All	15024/16944 (89%)	14633 (97%)	391 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	258/290 (89%)	258 (100%)	0	100	100
1	AB	258/290 (89%)	258 (100%)	0	100	100
1	AC	258/290 (89%)	258 (100%)	0	100	100
1	AD	258/290 (89%)	258 (100%)	0	100	100
1	AE	258/290 (89%)	258 (100%)	0	100	100
1	AF	258/290 (89%)	258 (100%)	0	100	100
1	AG	258/290 (89%)	258 (100%)	0	100	100
1	AH	258/290 (89%)	257 (100%)	1 (0%)	84	86
1	AI	258/290 (89%)	258 (100%)	0	100	100
1	AJ	258/290 (89%)	258 (100%)	0	100	100
1	AK	258/290 (89%)	258 (100%)	0	100	100
1	AL	258/290 (89%)	258 (100%)	0	100	100
1	BA	258/290 (89%)	258 (100%)	0	100	100
1	BB	258/290 (89%)	258 (100%)	0	100	100
1	BC	258/290 (89%)	258 (100%)	0	100	100
1	BD	258/290 (89%)	258 (100%)	0	100	100
1	BE	258/290 (89%)	258 (100%)	0	100	100
1	BF	258/290 (89%)	258 (100%)	0	100	100
1	BG	258/290 (89%)	258 (100%)	0	100	100
1	BH	258/290 (89%)	258 (100%)	0	100	100
1	BI	258/290 (89%)	258 (100%)	0	100	100
1	BJ	258/290 (89%)	258 (100%)	0	100	100
1	BK	258/290 (89%)	258 (100%)	0	100	100
1	BL	258/290 (89%)	258 (100%)	0	100	100
1	CA	258/290 (89%)	258 (100%)	0	100	100
1	CB	258/290 (89%)	258 (100%)	0	100	100
1	CC	258/290 (89%)	258 (100%)	0	100	100
1	CD	258/290 (89%)	258 (100%)	0	100	100
1	CE	258/290 (89%)	258 (100%)	0	100	100
1	CF	258/290 (89%)	258 (100%)	0	100	100
1	CG	258/290 (89%)	258 (100%)	0	100	100
1	CH	258/290 (89%)	258 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CI	258/290 (89%)	258 (100%)	0	100	100
1	CJ	258/290 (89%)	258 (100%)	0	100	100
1	CK	258/290 (89%)	258 (100%)	0	100	100
1	CL	258/290 (89%)	258 (100%)	0	100	100
1	DA	258/290 (89%)	258 (100%)	0	100	100
1	DB	258/290 (89%)	258 (100%)	0	100	100
1	DC	258/290 (89%)	258 (100%)	0	100	100
1	DD	258/290 (89%)	258 (100%)	0	100	100
1	DE	258/290 (89%)	258 (100%)	0	100	100
1	DF	258/290 (89%)	258 (100%)	0	100	100
1	DG	258/290 (89%)	258 (100%)	0	100	100
1	DH	258/290 (89%)	258 (100%)	0	100	100
1	DI	258/290 (89%)	258 (100%)	0	100	100
1	DJ	258/290 (89%)	258 (100%)	0	100	100
1	DK	258/290 (89%)	258 (100%)	0	100	100
1	DL	258/290 (89%)	258 (100%)	0	100	100
All	All	12384/13920 (89%)	12383 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AH	288	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	CF	283	ASN
1	CL	291	HIS
1	CG	202	HIS
1	CI	288	GLN
1	DC	90	ASN

5.3.3 RNA ⓘ

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](#)

144 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	$\# Z > 2$
2	NDP	DC	501	-	49,52,52	2.24	6 (12%)	66,80,80	1.66	13 (19%)
3	LMG	AI	502	-	23,23,55	0.71	0	31,31,63	0.79	0
3	LMG	BG	502	-	23,23,55	0.68	0	31,31,63	0.78	0
2	NDP	DD	501	-	49,52,52	2.23	6 (12%)	66,80,80	1.66	13 (19%)
4	A1JWG	DI	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.08	2 (3%)
3	LMG	BE	502	-	23,23,55	0.69	0	31,31,63	0.74	0
3	LMG	CJ	502	-	23,23,55	0.70	0	31,31,63	0.74	0
2	NDP	BC	501	-	49,52,52	2.24	5 (10%)	66,80,80	1.65	12 (18%)
4	A1JWG	BJ	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.10	1 (1%)
2	NDP	CK	501	-	49,52,52	2.21	6 (12%)	66,80,80	1.65	14 (21%)
3	LMG	DF	502	-	23,23,55	0.70	0	31,31,63	0.78	0
4	A1JWG	CF	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.12	2 (3%)
3	LMG	DK	502	-	23,23,55	0.69	0	31,31,63	0.75	0
4	A1JWG	DC	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.11	1 (1%)
2	NDP	BE	501	-	49,52,52	2.22	6 (12%)	66,80,80	1.67	13 (19%)
4	A1JWG	DH	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.13	2 (3%)
3	LMG	BH	502	-	23,23,55	0.69	0	31,31,63	0.79	0
3	LMG	CB	502	-	23,23,55	0.69	0	31,31,63	0.74	0
3	LMG	BJ	502	-	23,23,55	0.69	0	31,31,63	0.75	0
2	NDP	BI	501	-	49,52,52	2.21	6 (12%)	66,80,80	1.66	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMG	BK	502	-	23,23,55	0.71	0	31,31,63	0.80	0
4	A1JWG	CL	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.10	3 (4%)
3	LMG	AE	502	-	23,23,55	0.68	0	31,31,63	0.75	0
4	A1JWG	AD	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.17	3 (4%)
3	LMG	AD	502	-	23,23,55	0.70	0	31,31,63	0.84	0
2	NDP	CF	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.66	13 (19%)
2	NDP	BD	501	-	49,52,52	2.23	6 (12%)	66,80,80	1.66	13 (19%)
2	NDP	DJ	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.64	12 (18%)
4	A1JWG	BL	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.07	2 (3%)
3	LMG	BF	502	-	23,23,55	0.69	0	31,31,63	0.77	0
3	LMG	DC	502	-	23,23,55	0.69	0	31,31,63	0.85	0
4	A1JWG	AC	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	2 (3%)
4	A1JWG	CB	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	1 (1%)
2	NDP	AC	501	-	49,52,52	2.25	5 (10%)	66,80,80	1.65	12 (18%)
3	LMG	DE	502	-	23,23,55	0.69	0	31,31,63	0.77	0
2	NDP	DE	501	-	49,52,52	2.24	6 (12%)	66,80,80	1.65	15 (22%)
3	LMG	DA	502	-	23,23,55	0.69	0	31,31,63	0.86	0
4	A1JWG	CK	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.06	2 (3%)
2	NDP	AD	501	-	49,52,52	2.21	6 (12%)	66,80,80	1.66	13 (19%)
4	A1JWG	DG	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.08	1 (1%)
4	A1JWG	AB	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.08	1 (1%)
4	A1JWG	CJ	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.10	1 (1%)
2	NDP	BA	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.65	13 (19%)
4	A1JWG	DD	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	2 (3%)
2	NDP	AG	501	-	49,52,52	2.21	5 (10%)	66,80,80	1.66	13 (19%)
3	LMG	CE	502	-	23,23,55	0.69	0	31,31,63	0.77	0
2	NDP	BF	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.66	13 (19%)
4	A1JWG	DK	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.08	2 (3%)
4	A1JWG	BK	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.10	3 (4%)
3	LMG	CC	502	-	23,23,55	0.69	0	31,31,63	0.84	0
2	NDP	BG	501	-	49,52,52	2.21	5 (10%)	66,80,80	1.65	12 (18%)
3	LMG	AF	502	-	23,23,55	0.69	0	31,31,63	0.77	0
2	NDP	CB	501	-	49,52,52	2.24	5 (10%)	66,80,80	1.65	13 (19%)
2	NDP	DG	501	-	49,52,52	2.21	6 (12%)	66,80,80	1.66	14 (21%)
4	A1JWG	AG	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.07	1 (1%)
2	NDP	AI	501	-	49,52,52	2.19	5 (10%)	66,80,80	1.66	13 (19%)
3	LMG	AJ	502	-	23,23,55	0.69	0	31,31,63	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1JWG	CC	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.06	1 (1%)
4	A1JWG	CD	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.11	2 (3%)
2	NDP	CD	501	-	49,52,52	2.23	5 (10%)	66,80,80	1.65	14 (21%)
3	LMG	AH	502	-	23,23,55	0.71	0	31,31,63	0.80	0
3	LMG	CD	502	-	23,23,55	0.70	0	31,31,63	0.78	0
4	A1JWG	AJ	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.08	1 (1%)
2	NDP	AA	501	-	49,52,52	2.21	6 (12%)	66,80,80	1.65	14 (21%)
3	LMG	BL	502	-	23,23,55	0.71	0	31,31,63	0.79	0
4	A1JWG	AL	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.10	1 (1%)
4	A1JWG	CI	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.09	2 (3%)
2	NDP	DK	501	-	49,52,52	2.20	5 (10%)	66,80,80	1.65	14 (21%)
3	LMG	BD	502	-	23,23,55	0.72	0	31,31,63	0.83	0
2	NDP	AJ	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.65	12 (18%)
3	LMG	DI	502	-	23,23,55	0.69	0	31,31,63	0.82	0
2	NDP	CA	501	-	49,52,52	2.21	6 (12%)	66,80,80	1.66	14 (21%)
3	LMG	BA	502	-	23,23,55	0.69	0	31,31,63	0.75	0
4	A1JWG	DB	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.04	2 (3%)
3	LMG	DJ	502	-	23,23,55	0.70	0	31,31,63	0.75	0
3	LMG	BC	502	-	23,23,55	0.70	0	31,31,63	0.80	0
3	LMG	AL	502	-	23,23,55	0.69	0	31,31,63	0.77	0
2	NDP	AL	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.65	14 (21%)
2	NDP	DH	501	-	49,52,52	2.21	6 (12%)	66,80,80	1.66	14 (21%)
2	NDP	BB	501	-	49,52,52	2.24	5 (10%)	66,80,80	1.65	13 (19%)
3	LMG	AG	502	-	23,23,55	0.69	0	31,31,63	0.82	0
2	NDP	DI	501	-	49,52,52	2.23	5 (10%)	66,80,80	1.66	13 (19%)
2	NDP	BK	501	-	49,52,52	2.21	5 (10%)	66,80,80	1.66	12 (18%)
4	A1JWG	DA	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.09	1 (1%)
4	A1JWG	DL	503	-	48,53,53	1.41	5 (10%)	62,89,89	1.13	4 (6%)
2	NDP	DA	501	-	49,52,52	2.23	6 (12%)	66,80,80	1.65	14 (21%)
3	LMG	BI	502	-	23,23,55	0.69	0	31,31,63	0.76	0
4	A1JWG	BG	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	2 (3%)
4	A1JWG	BE	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.10	2 (3%)
2	NDP	CL	501	-	49,52,52	2.20	5 (10%)	66,80,80	1.66	13 (19%)
4	A1JWG	AE	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.09	1 (1%)
4	A1JWG	DE	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.10	3 (4%)
2	NDP	DB	501	-	49,52,52	2.23	6 (12%)	66,80,80	1.66	12 (18%)
4	A1JWG	DJ	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.10	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1JWG	AF	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	2 (3%)
3	LMG	CK	502	-	23,23,55	0.71	0	31,31,63	0.82	0
3	LMG	DG	502	-	23,23,55	0.68	0	31,31,63	0.86	0
4	A1JWG	AK	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.07	2 (3%)
3	LMG	CG	502	-	23,23,55	0.67	0	31,31,63	0.88	0
3	LMG	AK	502	-	23,23,55	0.71	0	31,31,63	0.89	0
2	NDP	DL	501	-	49,52,52	2.19	5 (10%)	66,80,80	1.66	14 (21%)
4	A1JWG	DF	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.10	1 (1%)
3	LMG	CI	502	-	23,23,55	0.70	0	31,31,63	0.78	0
3	LMG	AB	502	-	23,23,55	0.70	0	31,31,63	0.76	0
4	A1JWG	AI	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.06	3 (4%)
2	NDP	AE	501	-	49,52,52	2.21	6 (12%)	66,80,80	1.66	13 (19%)
3	LMG	DL	502	-	23,23,55	0.70	0	31,31,63	0.78	0
2	NDP	CG	501	-	49,52,52	2.22	6 (12%)	66,80,80	1.66	13 (19%)
2	NDP	CC	501	-	49,52,52	2.24	5 (10%)	66,80,80	1.65	12 (18%)
3	LMG	CA	502	-	23,23,55	0.70	0	31,31,63	0.81	0
4	A1JWG	CE	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.13	3 (4%)
4	A1JWG	BC	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	1 (1%)
4	A1JWG	BD	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.09	2 (3%)
2	NDP	BH	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.66	14 (21%)
4	A1JWG	CG	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.10	1 (1%)
2	NDP	BJ	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.64	13 (19%)
2	NDP	CH	501	-	49,52,52	2.22	5 (10%)	66,80,80	1.65	14 (21%)
2	NDP	CI	501	-	49,52,52	2.22	7 (14%)	66,80,80	1.65	13 (19%)
3	LMG	CH	502	-	23,23,55	0.71	0	31,31,63	0.82	0
2	NDP	AH	501	-	49,52,52	2.23	5 (10%)	66,80,80	1.65	14 (21%)
4	A1JWG	BI	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.08	2 (3%)
3	LMG	DD	502	-	23,23,55	0.70	0	31,31,63	0.78	0
2	NDP	AB	501	-	49,52,52	2.24	5 (10%)	66,80,80	1.65	11 (16%)
3	LMG	CL	502	-	23,23,55	0.70	0	31,31,63	0.77	0
3	LMG	BB	502	-	23,23,55	0.70	0	31,31,63	0.81	0
3	LMG	DB	502	-	23,23,55	0.68	0	31,31,63	0.78	0
4	A1JWG	BF	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.08	2 (3%)
4	A1JWG	CH	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.09	3 (4%)
3	LMG	DH	502	-	23,23,55	0.71	0	31,31,63	0.85	0
3	LMG	AC	502	-	23,23,55	0.69	0	31,31,63	0.89	1 (3%)
4	A1JWG	BH	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.07	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1JWG	BB	503	-	48,53,53	1.39	5 (10%)	62,89,89	1.12	3 (4%)
3	LMG	CF	502	-	23,23,55	0.69	0	31,31,63	0.76	0
2	NDP	AF	501	-	49,52,52	2.21	5 (10%)	66,80,80	1.66	13 (19%)
2	NDP	BL	501	-	49,52,52	2.20	5 (10%)	66,80,80	1.65	12 (18%)
3	LMG	AA	502	-	23,23,55	0.70	0	31,31,63	0.80	0
4	A1JWG	AH	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.10	2 (3%)
4	A1JWG	AA	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.07	1 (1%)
2	NDP	CE	501	-	49,52,52	2.21	6 (12%)	66,80,80	1.66	12 (18%)
2	NDP	DF	501	-	49,52,52	2.21	5 (10%)	66,80,80	1.66	13 (19%)
4	A1JWG	BA	503	-	48,53,53	1.40	5 (10%)	62,89,89	1.10	2 (3%)
2	NDP	AK	501	-	49,52,52	2.21	5 (10%)	66,80,80	1.65	13 (19%)
2	NDP	CJ	501	-	49,52,52	2.21	5 (10%)	66,80,80	1.66	14 (21%)
4	A1JWG	CA	503	-	48,53,53	1.38	5 (10%)	62,89,89	1.09	1 (1%)

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
2	NDP	DC	501	-	-	13/34/77/77	0/5/5/5
3	LMG	AI	502	-	-	6/16/36/70	0/1/1/1
3	LMG	BG	502	-	-	3/16/36/70	0/1/1/1
2	NDP	DD	501	-	-	13/34/77/77	0/5/5/5
4	A1JWG	DI	503	-	2/2/15/15	5/15/91/91	-
3	LMG	BE	502	-	-	4/16/36/70	0/1/1/1
3	LMG	CJ	502	-	-	2/16/36/70	0/1/1/1
2	NDP	BC	501	-	-	10/34/77/77	0/5/5/5
4	A1JWG	BJ	503	-	3/3/15/15	5/15/91/91	-
2	NDP	CK	501	-	-	13/34/77/77	0/5/5/5
3	LMG	DF	502	-	-	8/16/36/70	0/1/1/1
4	A1JWG	CF	503	-	3/3/15/15	6/15/91/91	-
3	LMG	DK	502	-	-	1/16/36/70	0/1/1/1
4	A1JWG	DC	503	-	3/3/15/15	5/15/91/91	-
2	NDP	BE	501	-	-	10/34/77/77	0/5/5/5
4	A1JWG	DH	503	-	3/3/15/15	6/15/91/91	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMG	BH	502	-	-	6/16/36/70	0/1/1/1
3	LMG	CB	502	-	-	3/16/36/70	0/1/1/1
3	LMG	BJ	502	-	-	4/16/36/70	0/1/1/1
2	NDP	BI	501	-	-	14/34/77/77	0/5/5/5
3	LMG	BK	502	-	-	4/16/36/70	0/1/1/1
4	A1JWG	CL	503	-	2/2/15/15	6/15/91/91	-
4	A1JWG	AD	503	-	3/3/15/15	8/15/91/91	-
3	LMG	AE	502	-	-	7/16/36/70	0/1/1/1
3	LMG	AD	502	-	-	4/16/36/70	0/1/1/1
2	NDP	CF	501	-	-	10/34/77/77	0/5/5/5
2	NDP	BD	501	-	-	13/34/77/77	0/5/5/5
2	NDP	DJ	501	-	-	14/34/77/77	0/5/5/5
4	A1JWG	BL	503	-	3/3/15/15	6/15/91/91	-
3	LMG	BF	502	-	-	6/16/36/70	0/1/1/1
4	A1JWG	AC	503	-	3/3/15/15	5/15/91/91	-
4	A1JWG	CB	503	-	3/3/15/15	6/15/91/91	-
3	LMG	DC	502	-	-	9/16/36/70	0/1/1/1
2	NDP	AC	501	-	-	7/34/77/77	0/5/5/5
3	LMG	DE	502	-	-	4/16/36/70	0/1/1/1
2	NDP	DE	501	-	-	11/34/77/77	0/5/5/5
3	LMG	DA	502	-	-	5/16/36/70	0/1/1/1
4	A1JWG	CK	503	-	3/3/15/15	5/15/91/91	-
4	A1JWG	DG	503	-	3/3/15/15	4/15/91/91	-
2	NDP	AD	501	-	-	10/34/77/77	0/5/5/5
4	A1JWG	AB	503	-	3/3/15/15	3/15/91/91	-
4	A1JWG	CJ	503	-	3/3/15/15	7/15/91/91	-
2	NDP	BA	501	-	-	8/34/77/77	0/5/5/5
4	A1JWG	DD	503	-	3/3/15/15	6/15/91/91	-
2	NDP	AG	501	-	-	10/34/77/77	0/5/5/5
3	LMG	CE	502	-	-	4/16/36/70	0/1/1/1
2	NDP	BF	501	-	-	5/34/77/77	0/5/5/5
4	A1JWG	DK	503	-	3/3/15/15	3/15/91/91	-
4	A1JWG	BK	503	-	2/2/15/15	6/15/91/91	-
3	LMG	CC	502	-	-	7/16/36/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	BG	501	-	-	11/34/77/77	0/5/5/5
3	LMG	AF	502	-	-	4/16/36/70	0/1/1/1
4	A1JWG	AG	503	-	3/3/15/15	4/15/91/91	-
2	NDP	CB	501	-	-	11/34/77/77	0/5/5/5
2	NDP	DG	501	-	-	15/34/77/77	0/5/5/5
2	NDP	AI	501	-	-	6/34/77/77	0/5/5/5
4	A1JWG	CC	503	-	3/3/15/15	4/15/91/91	-
3	LMG	AJ	502	-	-	10/16/36/70	0/1/1/1
4	A1JWG	CD	503	-	3/3/15/15	3/15/91/91	-
2	NDP	CD	501	-	-	11/34/77/77	0/5/5/5
3	LMG	AH	502	-	-	2/16/36/70	0/1/1/1
3	LMG	CD	502	-	-	4/16/36/70	0/1/1/1
4	A1JWG	AJ	503	-	3/3/15/15	3/15/91/91	-
2	NDP	AA	501	-	-	10/34/77/77	0/5/5/5
3	LMG	BL	502	-	-	3/16/36/70	0/1/1/1
4	A1JWG	AL	503	-	3/3/15/15	3/15/91/91	-
4	A1JWG	CI	503	-	3/3/15/15	6/15/91/91	-
2	NDP	DK	501	-	-	10/34/77/77	0/5/5/5
3	LMG	BD	502	-	-	7/16/36/70	0/1/1/1
2	NDP	AJ	501	-	-	11/34/77/77	0/5/5/5
4	A1JWG	DB	503	-	3/3/15/15	7/15/91/91	-
2	NDP	CA	501	-	-	13/34/77/77	0/5/5/5
3	LMG	BA	502	-	-	6/16/36/70	0/1/1/1
3	LMG	DI	502	-	-	5/16/36/70	0/1/1/1
3	LMG	DJ	502	-	-	4/16/36/70	0/1/1/1
3	LMG	BC	502	-	-	4/16/36/70	0/1/1/1
3	LMG	AL	502	-	-	4/16/36/70	0/1/1/1
2	NDP	AL	501	-	-	8/34/77/77	0/5/5/5
2	NDP	DH	501	-	-	14/34/77/77	0/5/5/5
2	NDP	BB	501	-	-	10/34/77/77	0/5/5/5
3	LMG	AG	502	-	-	8/16/36/70	0/1/1/1
2	NDP	DI	501	-	-	13/34/77/77	0/5/5/5
2	NDP	BK	501	-	-	11/34/77/77	0/5/5/5
4	A1JWG	DA	503	-	3/3/15/15	6/15/91/91	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1JWG	DL	503	-	3/3/15/15	10/15/91/91	-
2	NDP	DA	501	-	-	10/34/77/77	0/5/5/5
4	A1JWG	BG	503	-	3/3/15/15	6/15/91/91	-
3	LMG	BI	502	-	-	3/16/36/70	0/1/1/1
4	A1JWG	BE	503	-	2/2/15/15	5/15/91/91	-
2	NDP	CL	501	-	-	9/34/77/77	0/5/5/5
4	A1JWG	AE	503	-	3/3/15/15	7/15/91/91	-
4	A1JWG	DE	503	-	3/3/15/15	2/15/91/91	-
2	NDP	DB	501	-	-	7/34/77/77	0/5/5/5
4	A1JWG	DJ	503	-	3/3/15/15	3/15/91/91	-
4	A1JWG	AF	503	-	3/3/15/15	6/15/91/91	-
3	LMG	CK	502	-	-	6/16/36/70	0/1/1/1
3	LMG	DG	502	-	-	6/16/36/70	0/1/1/1
4	A1JWG	AK	503	-	3/3/15/15	3/15/91/91	-
3	LMG	CG	502	-	-	5/16/36/70	0/1/1/1
3	LMG	AK	502	-	-	8/16/36/70	0/1/1/1
2	NDP	DL	501	-	-	9/34/77/77	0/5/5/5
4	A1JWG	DF	503	-	3/3/15/15	7/15/91/91	-
3	LMG	CI	502	-	-	4/16/36/70	0/1/1/1
3	LMG	AB	502	-	-	5/16/36/70	0/1/1/1
4	A1JWG	AI	503	-	3/3/15/15	1/15/91/91	-
2	NDP	AE	501	-	-	5/34/77/77	0/5/5/5
3	LMG	DL	502	-	-	6/16/36/70	0/1/1/1
2	NDP	CG	501	-	-	15/34/77/77	0/5/5/5
2	NDP	CC	501	-	-	10/34/77/77	0/5/5/5
4	A1JWG	CE	503	-	3/3/15/15	10/15/91/91	-
3	LMG	CA	502	-	-	7/16/36/70	0/1/1/1
4	A1JWG	BC	503	-	3/3/15/15	6/15/91/91	-
4	A1JWG	CG	503	-	3/3/15/15	3/15/91/91	-
4	A1JWG	BD	503	-	3/3/15/15	4/15/91/91	-
2	NDP	BH	501	-	-	13/34/77/77	0/5/5/5
4	A1JWG	BI	503	-	2/2/15/15	4/15/91/91	-
2	NDP	BJ	501	-	-	7/34/77/77	0/5/5/5
2	NDP	CH	501	-	-	15/34/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	CI	501	-	-	13/34/77/77	0/5/5/5
2	NDP	AH	501	-	-	12/34/77/77	0/5/5/5
3	LMG	CH	502	-	-	6/16/36/70	0/1/1/1
3	LMG	DD	502	-	-	6/16/36/70	0/1/1/1
2	NDP	AB	501	-	-	8/34/77/77	0/5/5/5
3	LMG	CL	502	-	-	2/16/36/70	0/1/1/1
3	LMG	BB	502	-	-	2/16/36/70	0/1/1/1
3	LMG	DB	502	-	-	8/16/36/70	0/1/1/1
4	A1JWG	BF	503	-	2/2/15/15	1/15/91/91	-
4	A1JWG	CH	503	-	3/3/15/15	6/15/91/91	-
3	LMG	DH	502	-	-	6/16/36/70	0/1/1/1
3	LMG	AC	502	-	-	5/16/36/70	0/1/1/1
4	A1JWG	BH	503	-	3/3/15/15	6/15/91/91	-
4	A1JWG	BB	503	-	3/3/15/15	5/15/91/91	-
3	LMG	CF	502	-	-	2/16/36/70	0/1/1/1
2	NDP	AF	501	-	-	11/34/77/77	0/5/5/5
2	NDP	BL	501	-	-	9/34/77/77	0/5/5/5
3	LMG	AA	502	-	-	4/16/36/70	0/1/1/1
4	A1JWG	AH	503	-	3/3/15/15	6/15/91/91	-
4	A1JWG	AA	503	-	3/3/15/15	2/15/91/91	-
2	NDP	CE	501	-	-	11/34/77/77	0/5/5/5
2	NDP	DF	501	-	-	11/34/77/77	0/5/5/5
4	A1JWG	BA	503	-	3/3/15/15	3/15/91/91	-
2	NDP	AK	501	-	-	9/34/77/77	0/5/5/5
2	NDP	CJ	501	-	-	11/34/77/77	0/5/5/5
4	A1JWG	CA	503	-	3/3/15/15	3/15/91/91	-

The worst 5 of 499 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BB	501	NDP	P2B-O2B	12.76	1.83	1.59
2	CB	501	NDP	P2B-O2B	12.76	1.83	1.59
2	DB	501	NDP	P2B-O2B	12.73	1.83	1.59
2	DE	501	NDP	P2B-O2B	12.73	1.83	1.59
2	DD	501	NDP	P2B-O2B	12.72	1.83	1.59

The worst 5 of 717 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	DD	501	NDP	PN-O3-PA	-7.29	107.81	132.83
2	DC	501	NDP	PN-O3-PA	-7.28	107.84	132.83
2	BD	501	NDP	PN-O3-PA	-7.28	107.85	132.83
2	DG	501	NDP	PN-O3-PA	-7.27	107.89	132.83
2	CG	501	NDP	PN-O3-PA	-7.26	107.91	132.83

5 of 138 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	AA	503	A1JWG	NB
4	AA	503	A1JWG	NA
4	AA	503	A1JWG	NC
4	AB	503	A1JWG	NB
4	AB	503	A1JWG	NA

5 of 986 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AA	501	NDP	C5B-O5B-PA-O1A
2	AA	501	NDP	PN-O3-PA-O5B
2	AA	501	NDP	C5D-O5D-PN-O1N
2	AA	501	NDP	C5D-O5D-PN-O2N
2	AB	501	NDP	C5D-O5D-PN-O1N

There are no ring outliers.

132 monomers are involved in 230 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DC	501	NDP	3	0
3	AI	502	LMG	3	0
3	BG	502	LMG	3	0
2	DD	501	NDP	4	0
3	BE	502	LMG	4	0
3	CJ	502	LMG	2	0
2	BC	501	NDP	2	0
4	BJ	503	A1JWG	1	0
2	CK	501	NDP	3	0
3	DF	502	LMG	4	0
3	DK	502	LMG	3	0
4	DC	503	A1JWG	1	0
2	BE	501	NDP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	DH	503	A1JWG	1	0
3	BH	502	LMG	1	0
3	CB	502	LMG	4	0
3	BJ	502	LMG	1	0
2	BI	501	NDP	3	0
3	BK	502	LMG	2	0
3	AE	502	LMG	1	0
2	CF	501	NDP	1	0
2	BD	501	NDP	4	0
2	DJ	501	NDP	1	0
4	BL	503	A1JWG	1	0
3	BF	502	LMG	1	0
3	DC	502	LMG	1	0
4	AC	503	A1JWG	1	0
4	CB	503	A1JWG	3	0
2	AC	501	NDP	3	0
3	DE	502	LMG	3	0
2	DE	501	NDP	5	0
3	DA	502	LMG	2	0
4	CK	503	A1JWG	1	0
2	AD	501	NDP	1	0
4	DG	503	A1JWG	1	0
4	AB	503	A1JWG	1	0
2	BA	501	NDP	3	0
4	DD	503	A1JWG	1	0
2	AG	501	NDP	2	0
3	CE	502	LMG	2	0
2	BF	501	NDP	2	0
4	DK	503	A1JWG	1	0
3	CC	502	LMG	3	0
2	BG	501	NDP	4	0
3	AF	502	LMG	3	0
2	CB	501	NDP	4	0
2	DG	501	NDP	3	0
4	AG	503	A1JWG	1	0
2	AI	501	NDP	3	0
3	AJ	502	LMG	2	0
4	CC	503	A1JWG	1	0
4	CD	503	A1JWG	1	0
2	CD	501	NDP	3	0
3	AH	502	LMG	2	0
3	CD	502	LMG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AJ	503	A1JWG	1	0
2	AA	501	NDP	2	0
3	BL	502	LMG	2	0
4	AL	503	A1JWG	1	0
4	CI	503	A1JWG	1	0
2	DK	501	NDP	2	0
3	BD	502	LMG	2	0
2	AJ	501	NDP	1	0
3	DI	502	LMG	2	0
2	CA	501	NDP	2	0
3	BA	502	LMG	1	0
4	DB	503	A1JWG	1	0
3	DJ	502	LMG	2	0
3	BC	502	LMG	2	0
3	AL	502	LMG	4	0
2	AL	501	NDP	1	0
2	DH	501	NDP	3	0
2	BB	501	NDP	2	0
3	AG	502	LMG	4	0
2	DI	501	NDP	2	0
2	BK	501	NDP	2	0
4	DA	503	A1JWG	1	0
4	DL	503	A1JWG	1	0
2	DA	501	NDP	2	0
3	BI	502	LMG	2	0
4	BG	503	A1JWG	1	0
4	AE	503	A1JWG	2	0
4	DE	503	A1JWG	2	0
2	DB	501	NDP	5	0
4	DJ	503	A1JWG	1	0
3	CK	502	LMG	4	0
3	DG	502	LMG	1	0
4	AK	503	A1JWG	1	0
3	CG	502	LMG	3	0
3	AK	502	LMG	2	0
2	DL	501	NDP	4	0
4	DF	503	A1JWG	1	0
3	CI	502	LMG	3	0
3	AB	502	LMG	3	0
4	AI	503	A1JWG	1	0
2	AE	501	NDP	4	0
3	DL	502	LMG	2	0

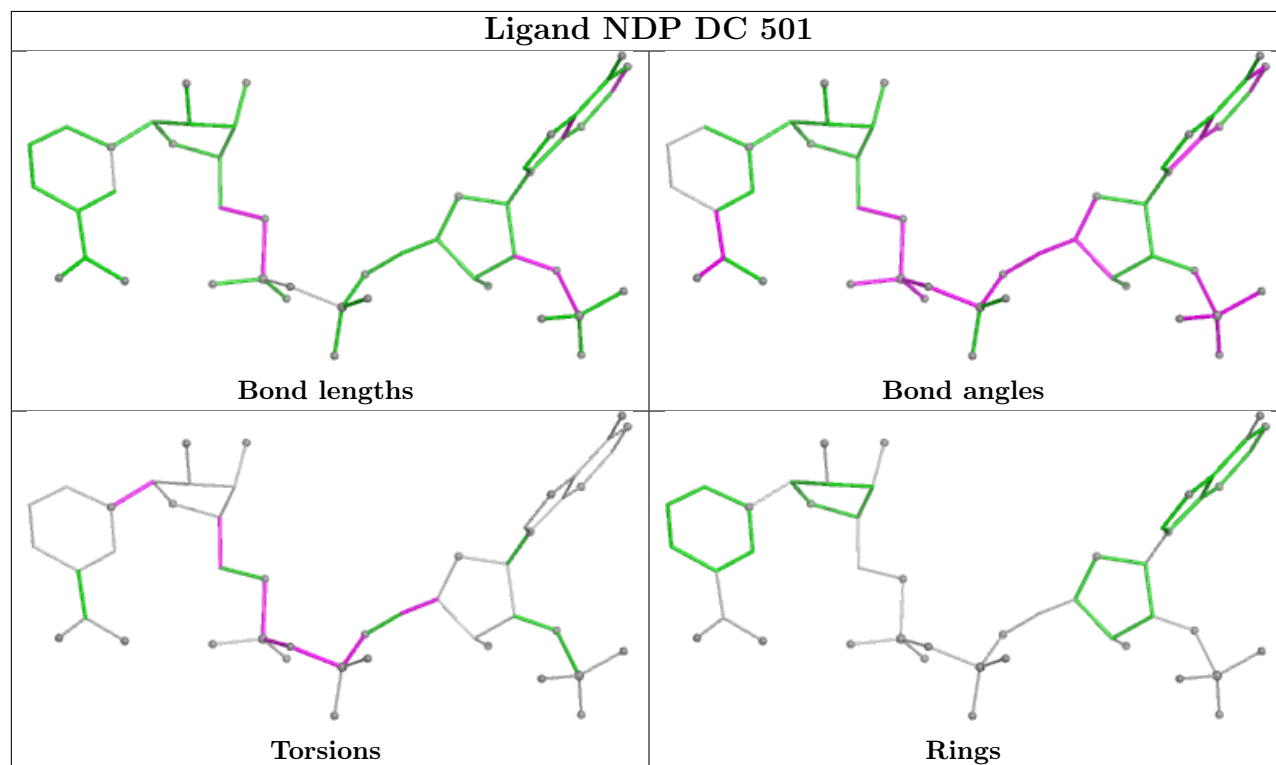
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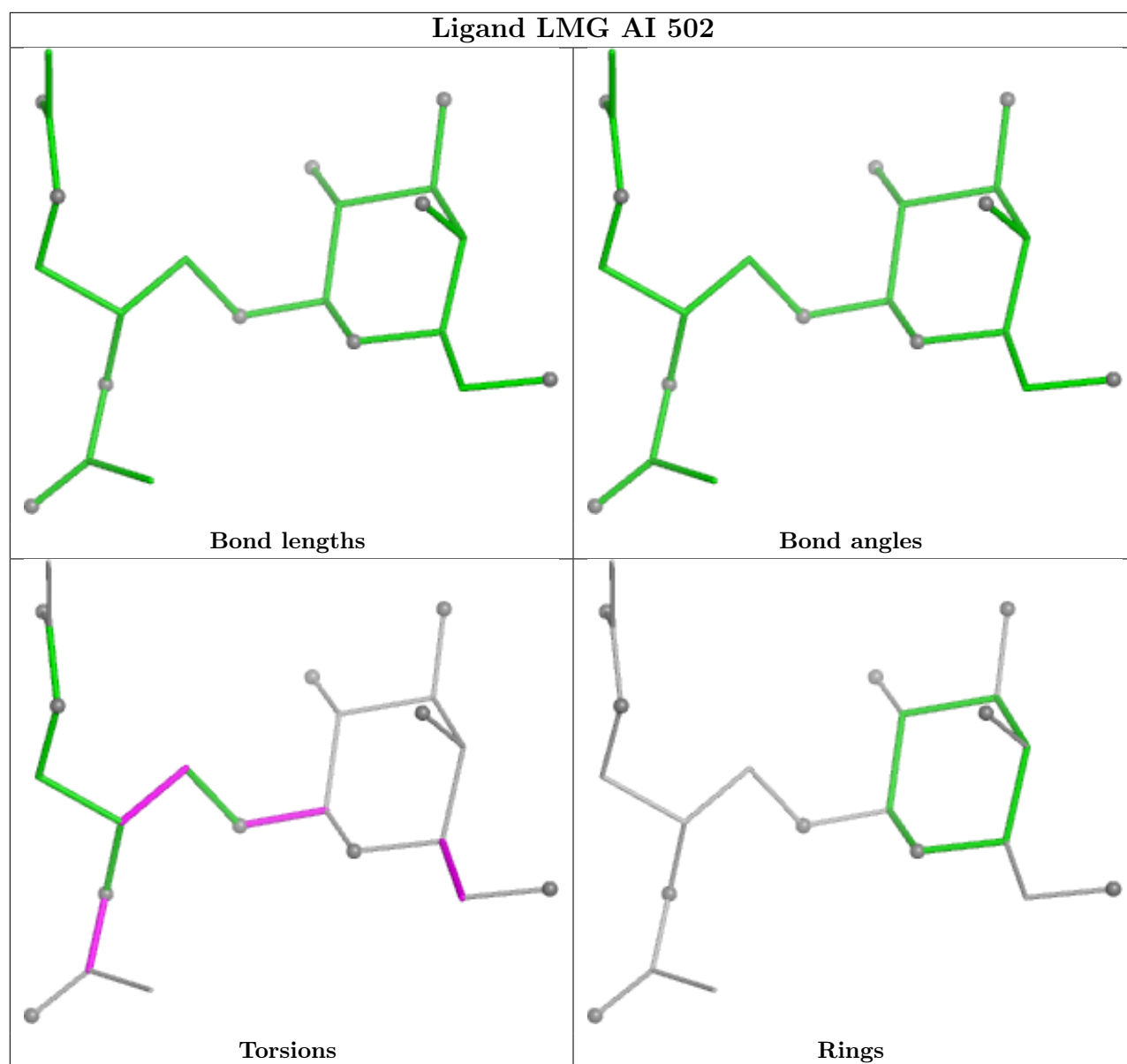
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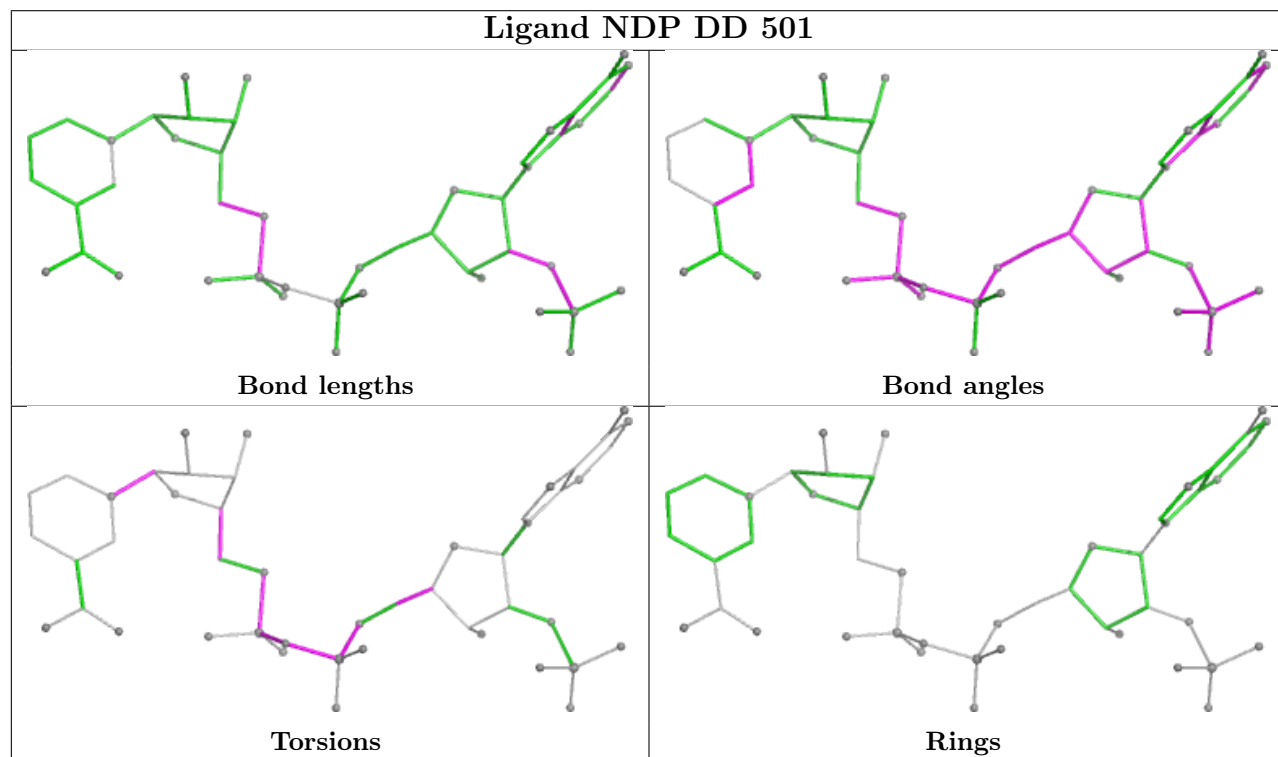
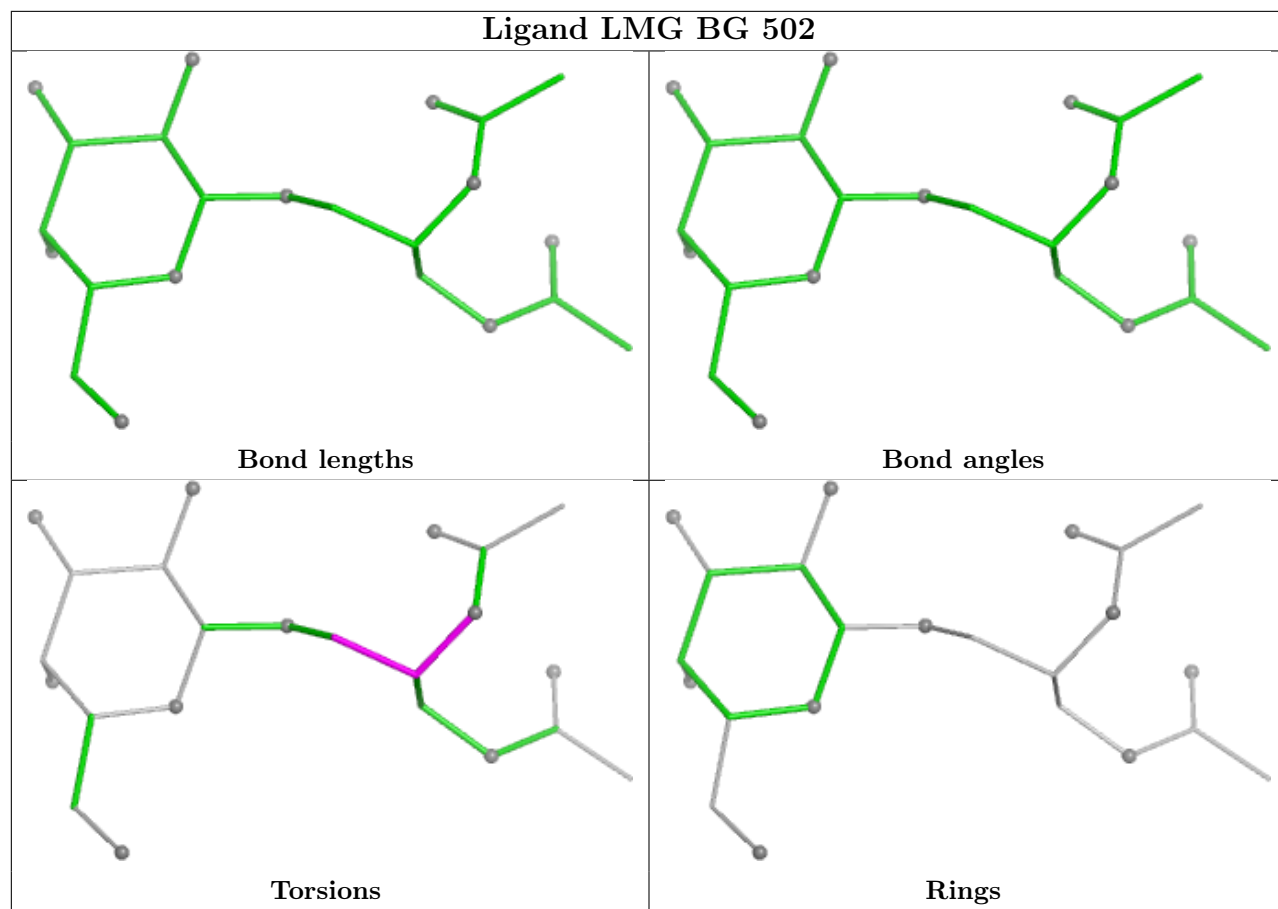
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CG	501	NDP	3	0
2	CC	501	NDP	3	0
3	CA	502	LMG	1	0
4	BC	503	A1JWG	1	0
4	BD	503	A1JWG	1	0
2	BH	501	NDP	2	0
4	CG	503	A1JWG	1	0
2	BJ	501	NDP	1	0
2	CH	501	NDP	2	0
2	CI	501	NDP	6	0
3	CH	502	LMG	3	0
2	AH	501	NDP	3	0
4	BI	503	A1JWG	1	0
3	DD	502	LMG	3	0
2	AB	501	NDP	2	0
3	CL	502	LMG	2	0
3	BB	502	LMG	1	0
3	DB	502	LMG	1	0
4	BF	503	A1JWG	1	0
4	CH	503	A1JWG	1	0
3	DH	502	LMG	1	0
3	AC	502	LMG	2	0
4	BH	503	A1JWG	1	0
4	BB	503	A1JWG	1	0
3	CF	502	LMG	4	0
2	AF	501	NDP	1	0
2	BL	501	NDP	2	0
3	AA	502	LMG	2	0
4	AH	503	A1JWG	1	0
4	AA	503	A1JWG	1	0
2	CE	501	NDP	2	0
2	DF	501	NDP	2	0
4	BA	503	A1JWG	1	0
2	AK	501	NDP	3	0
4	CA	503	A1JWG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

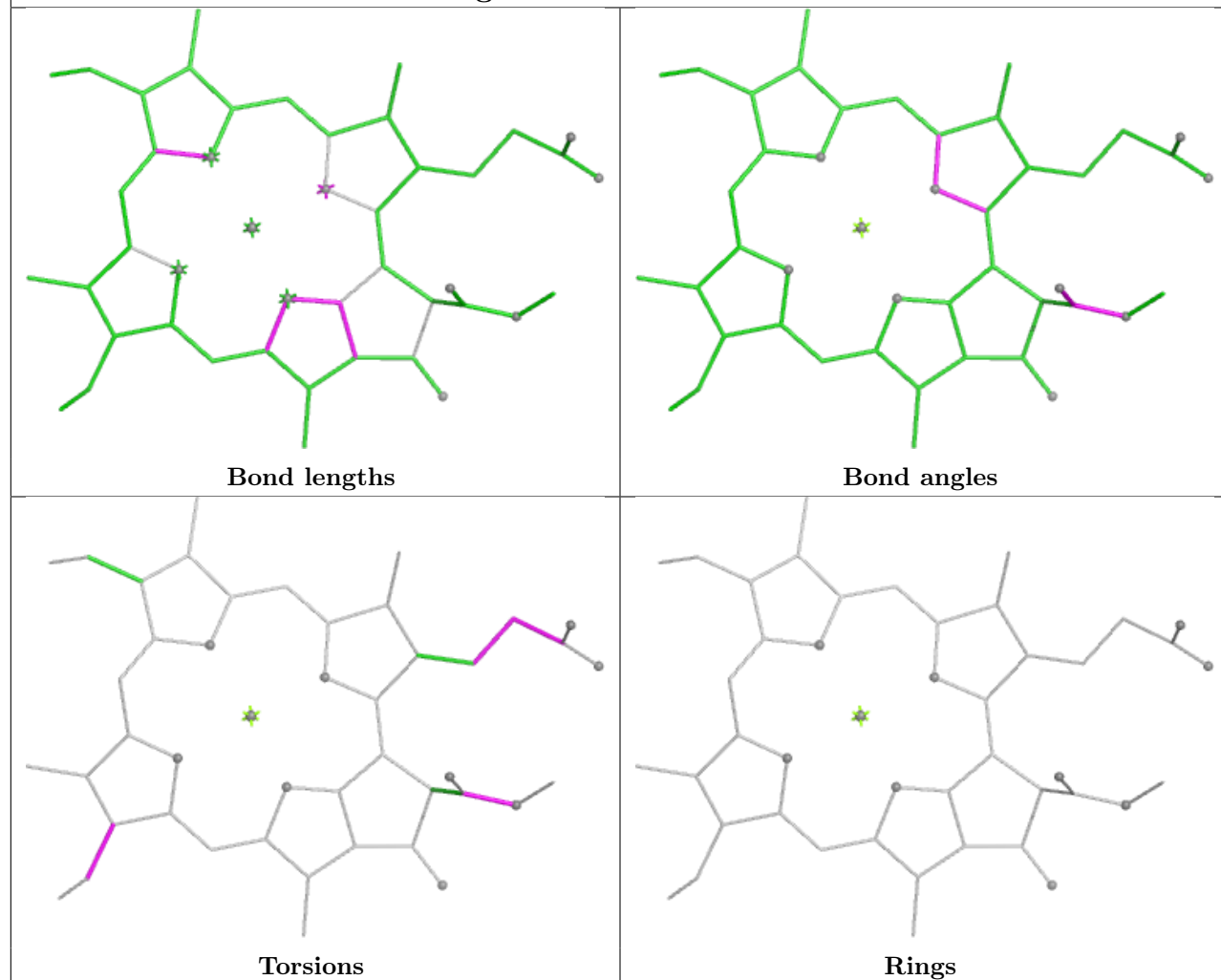
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

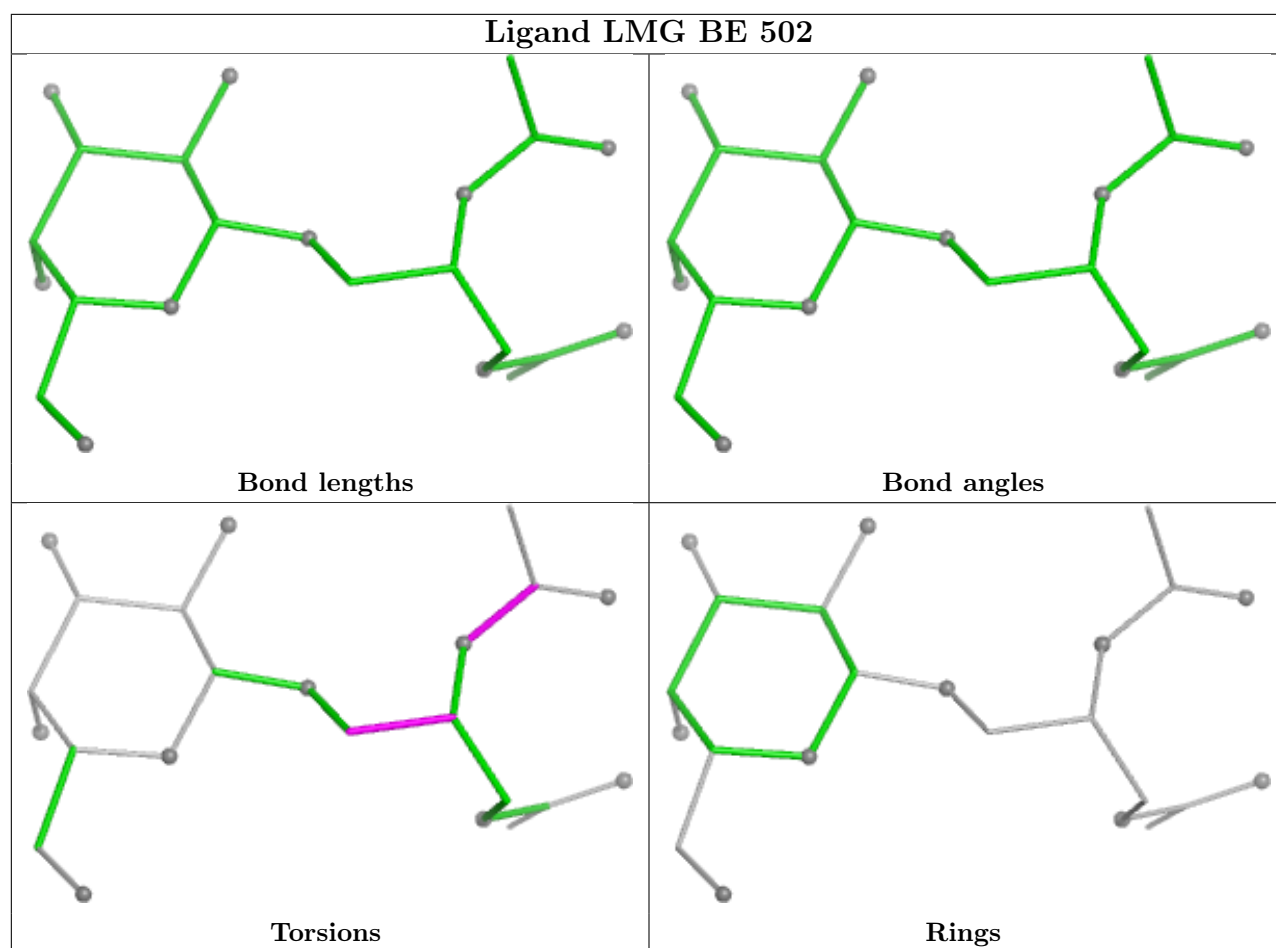


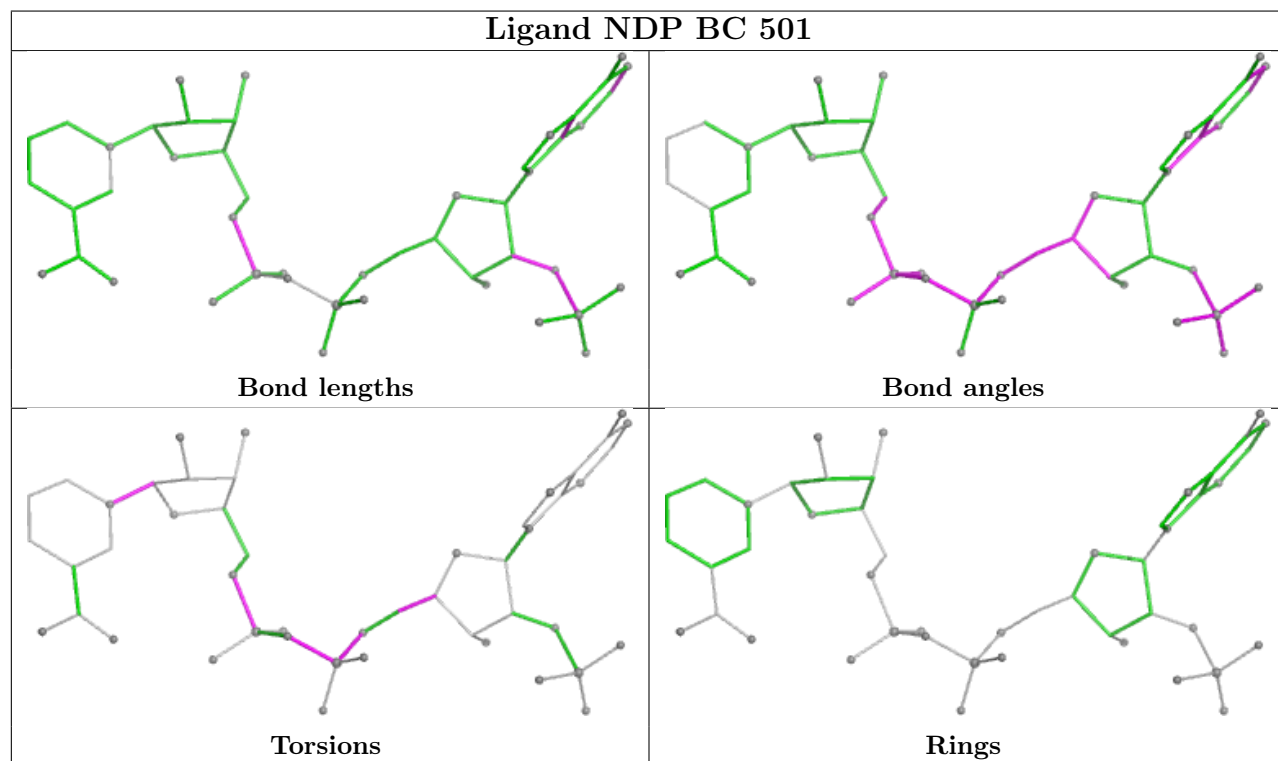
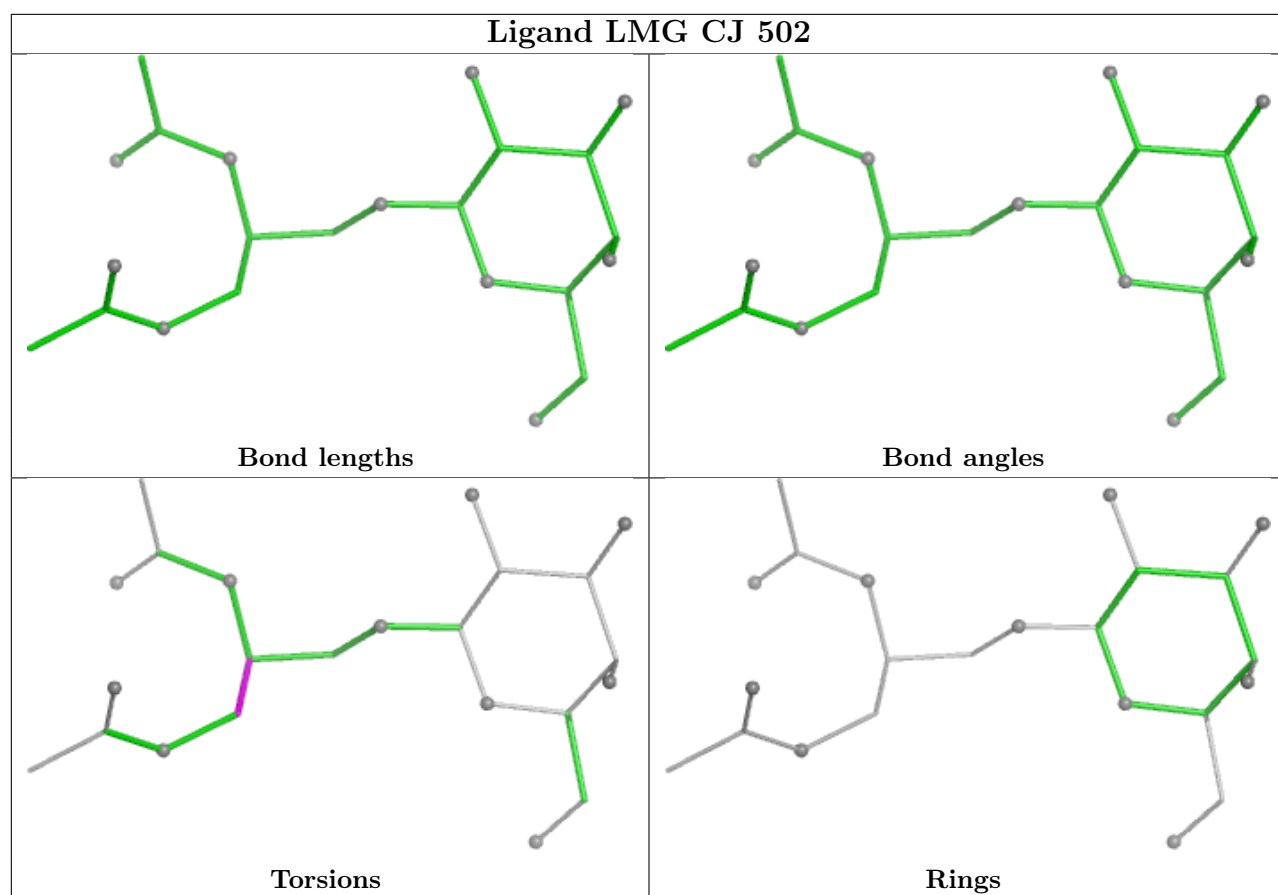




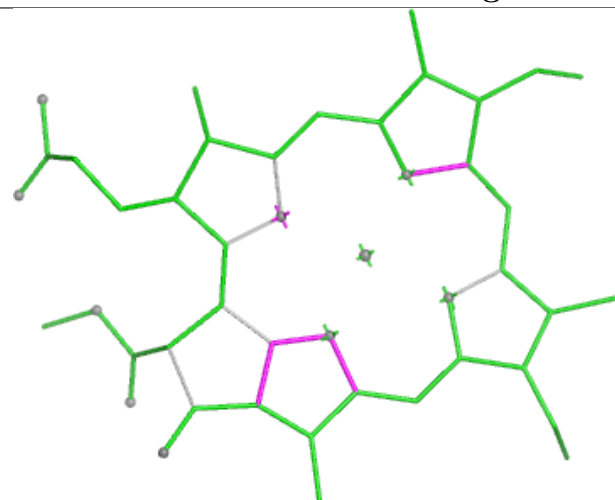
Ligand A1JWG DI 503



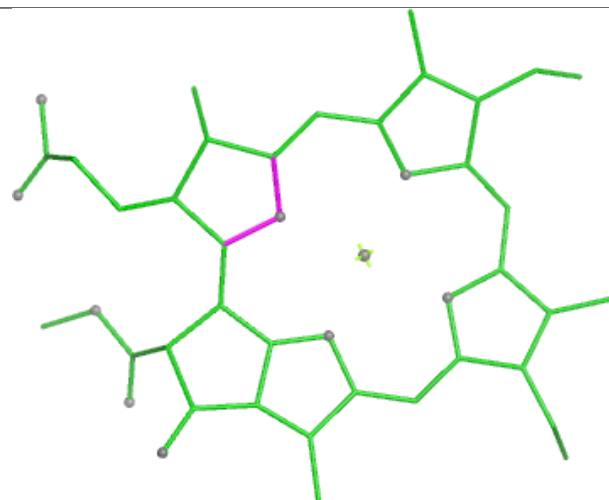




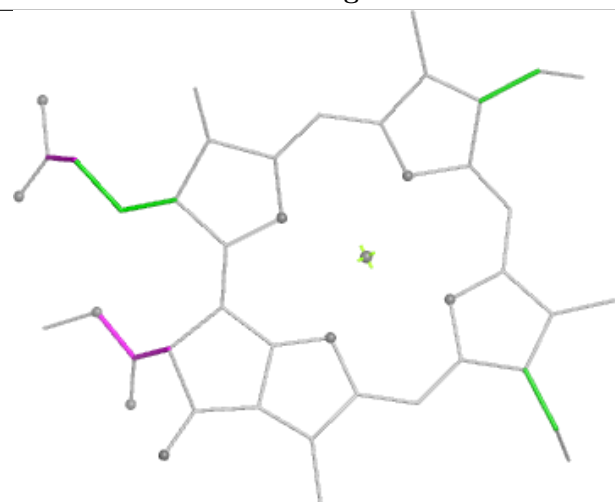
Ligand A1JWG BJ 503



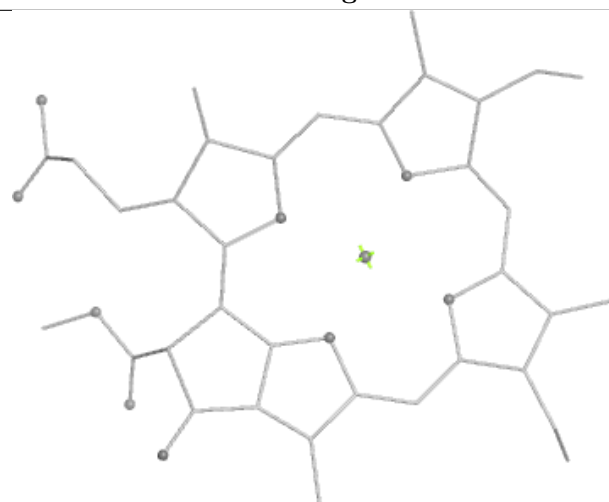
Bond lengths



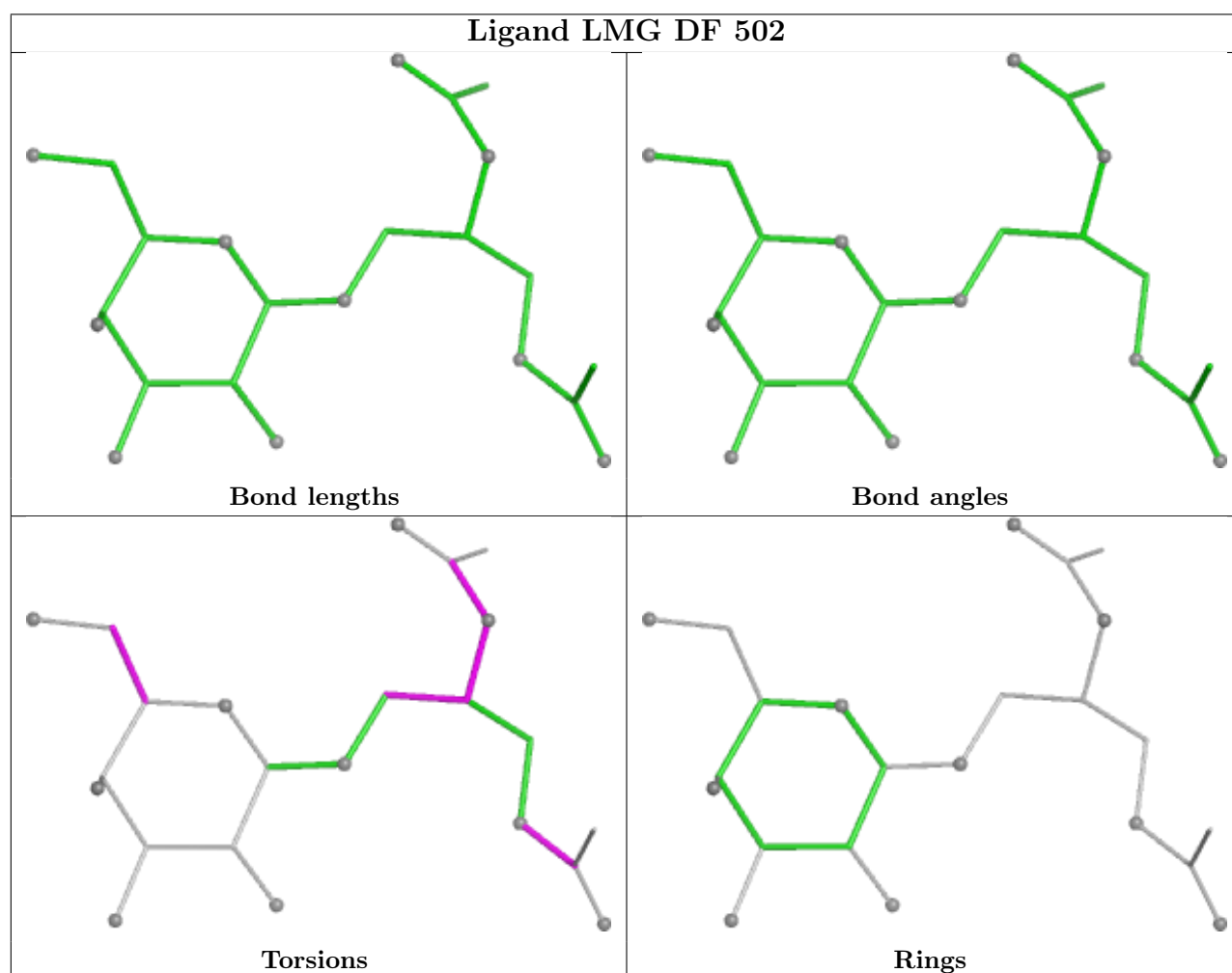
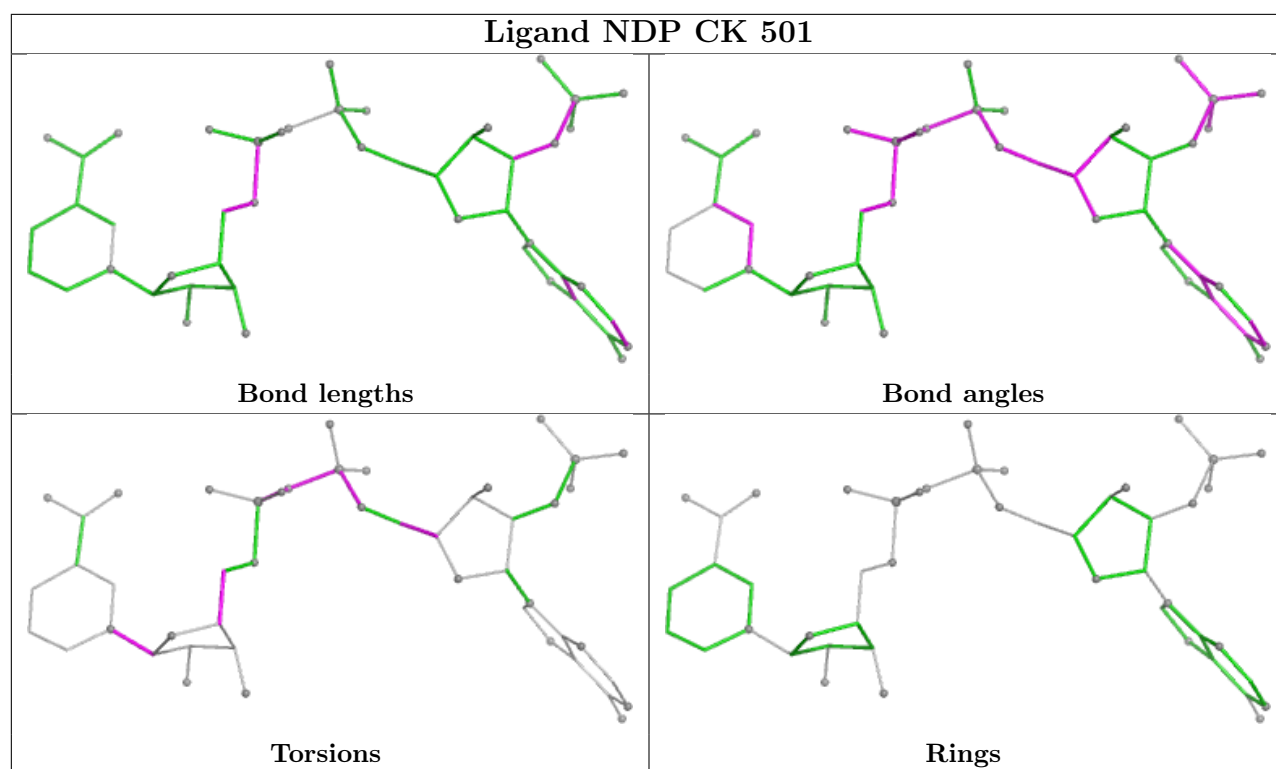
Bond angles



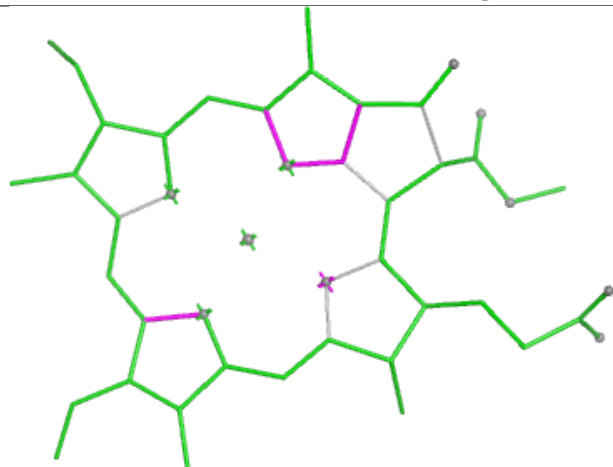
Torsions



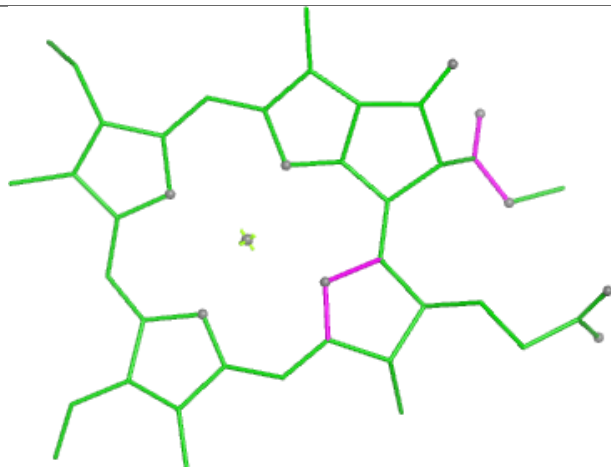
Rings



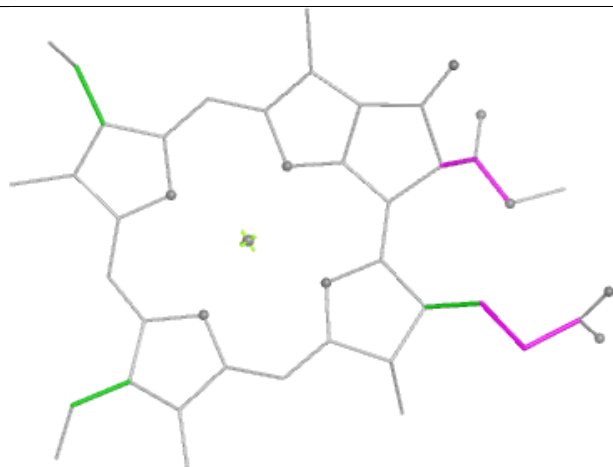
Ligand A1JWG CF 503



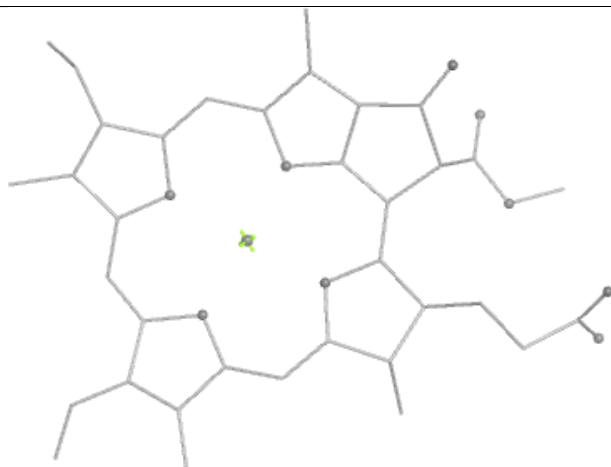
Bond lengths



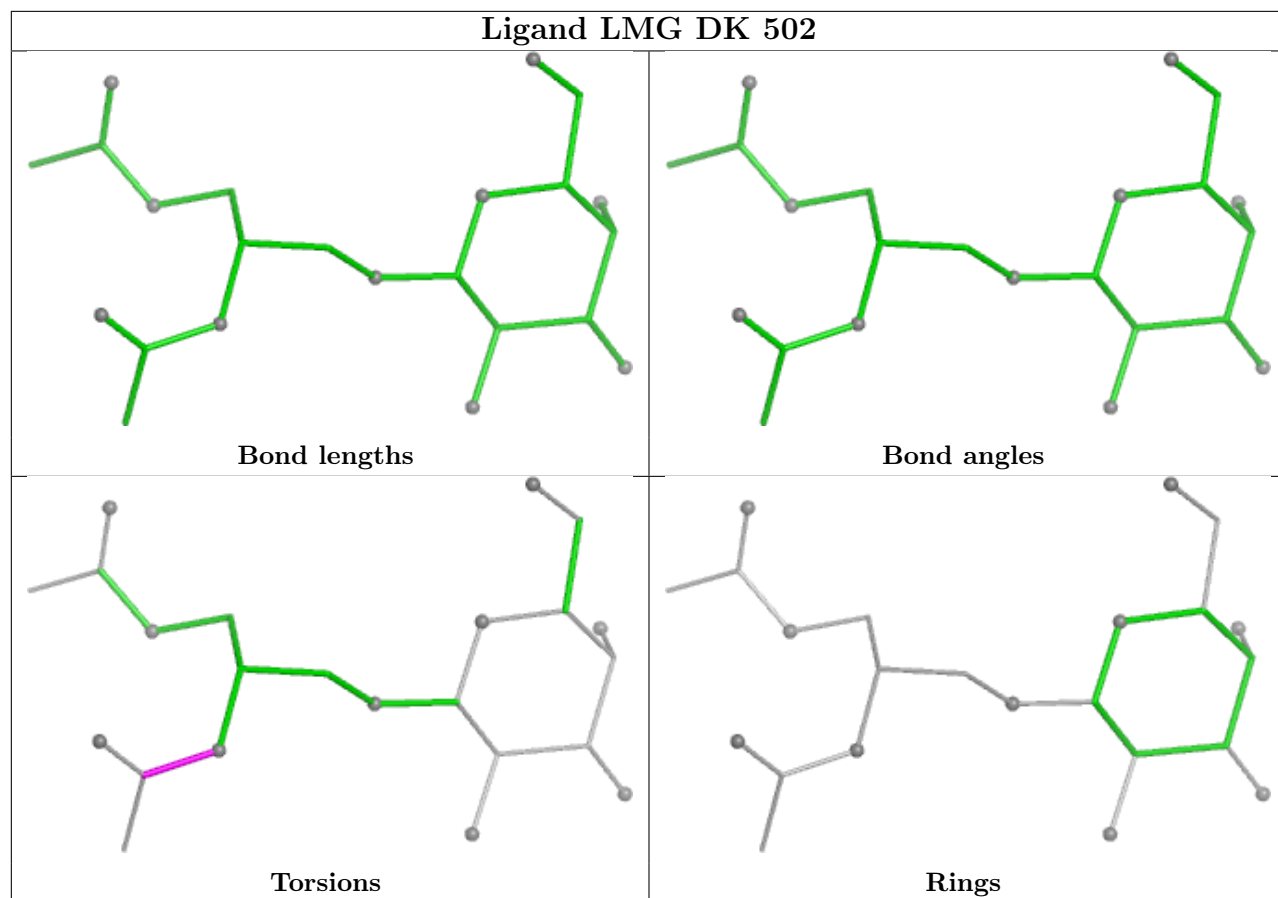
Bond angles



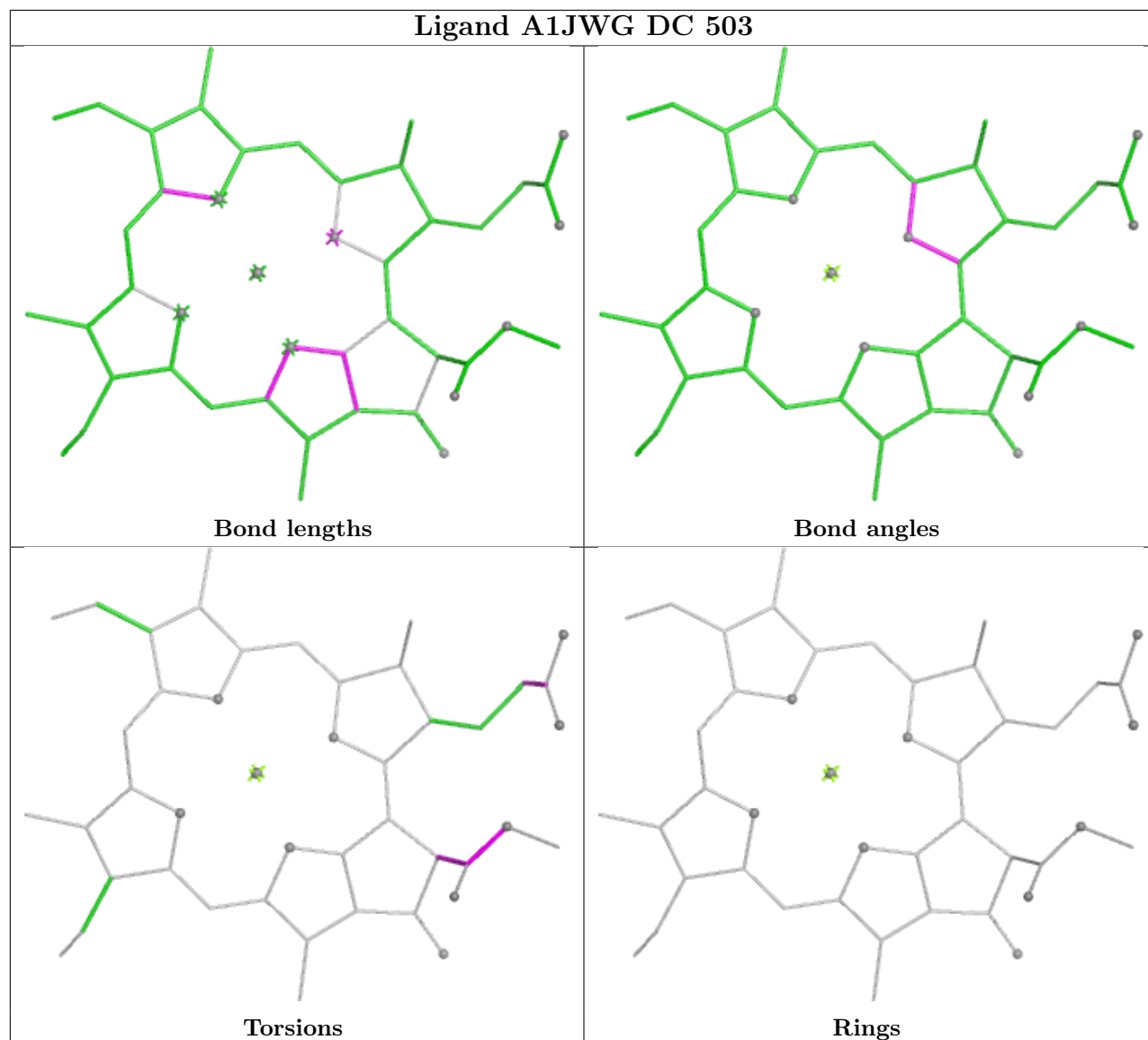
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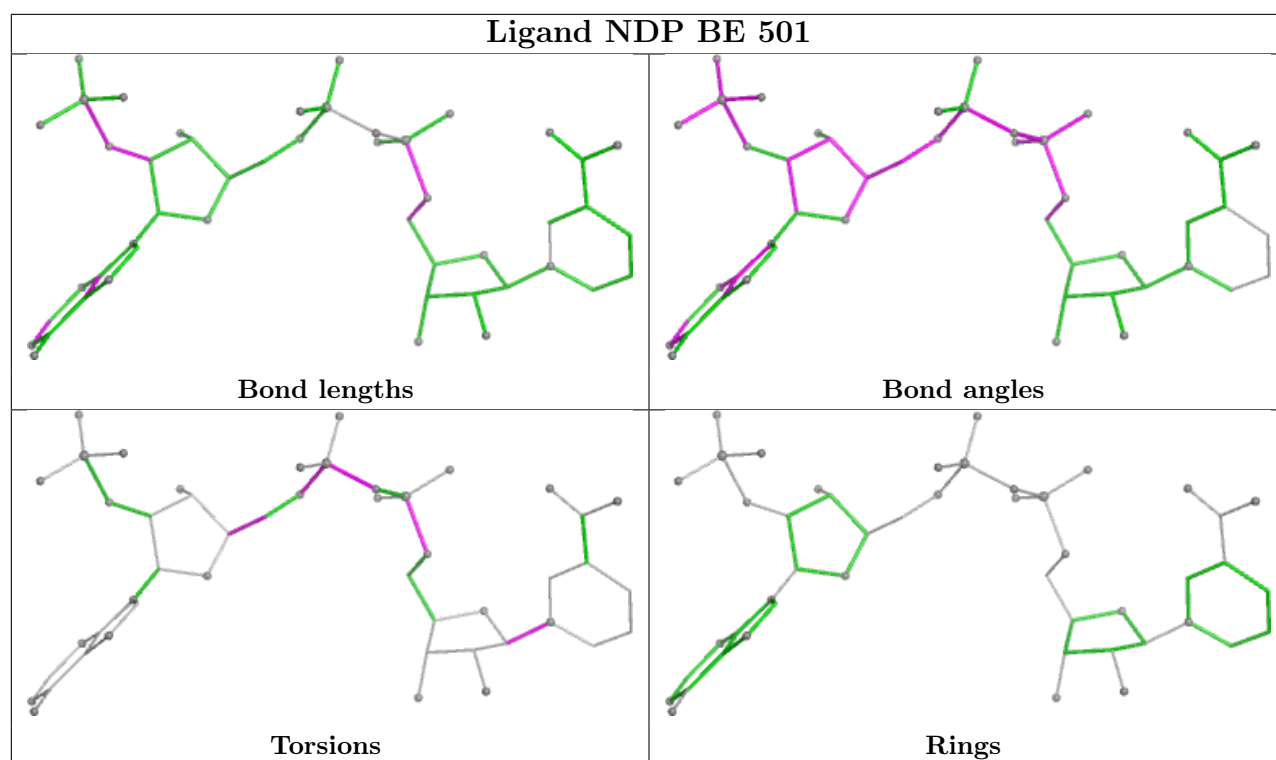


Rings

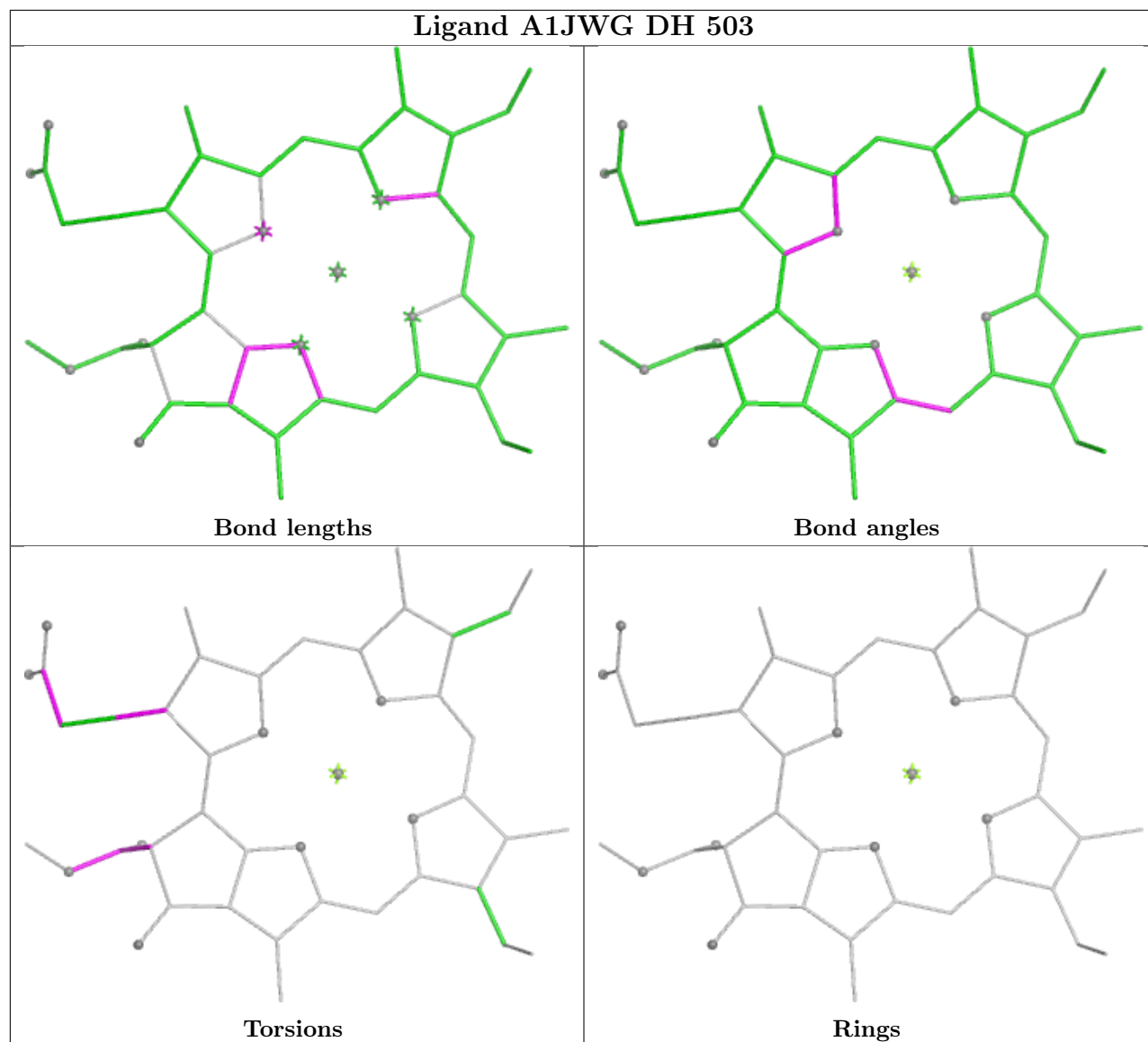


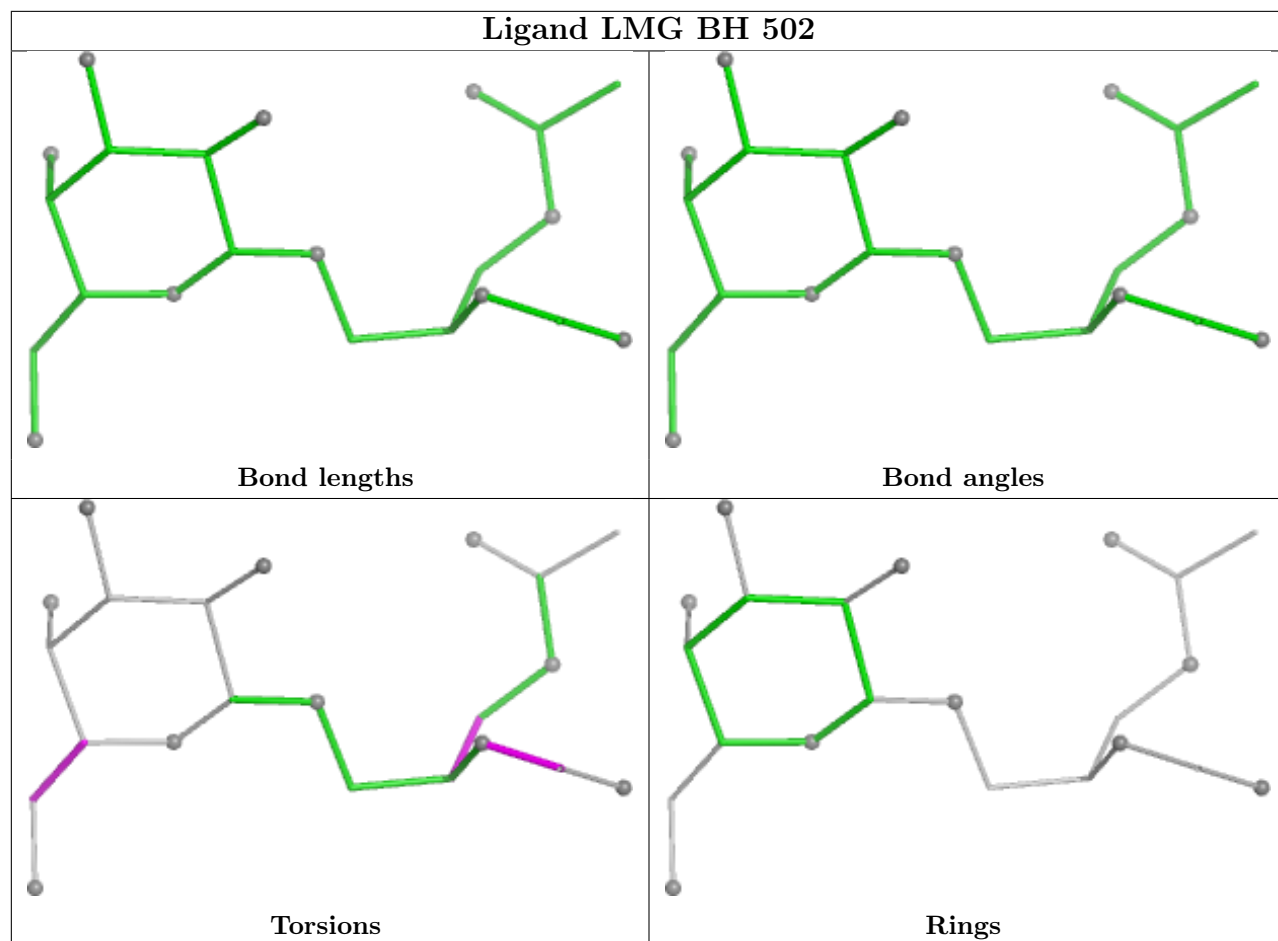
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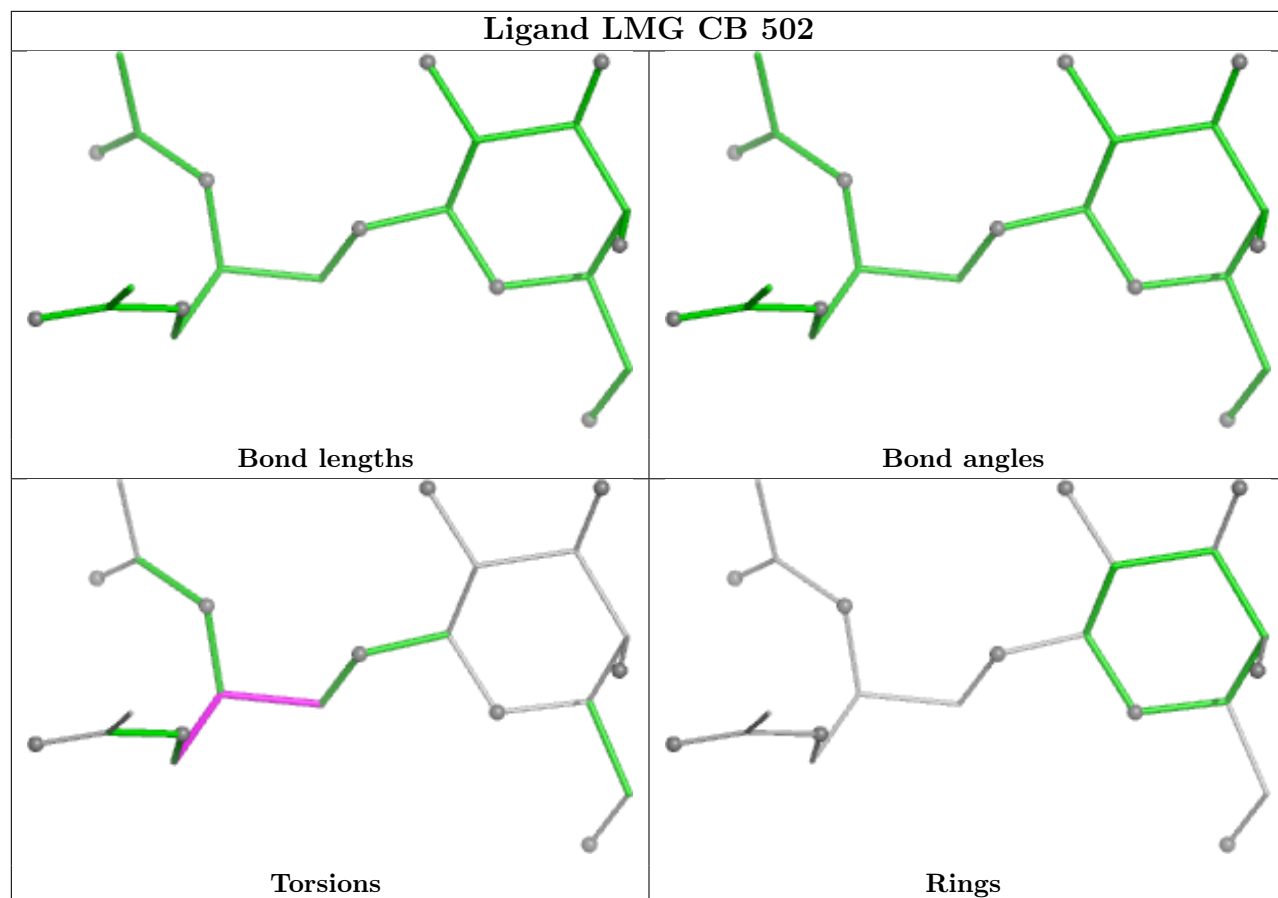




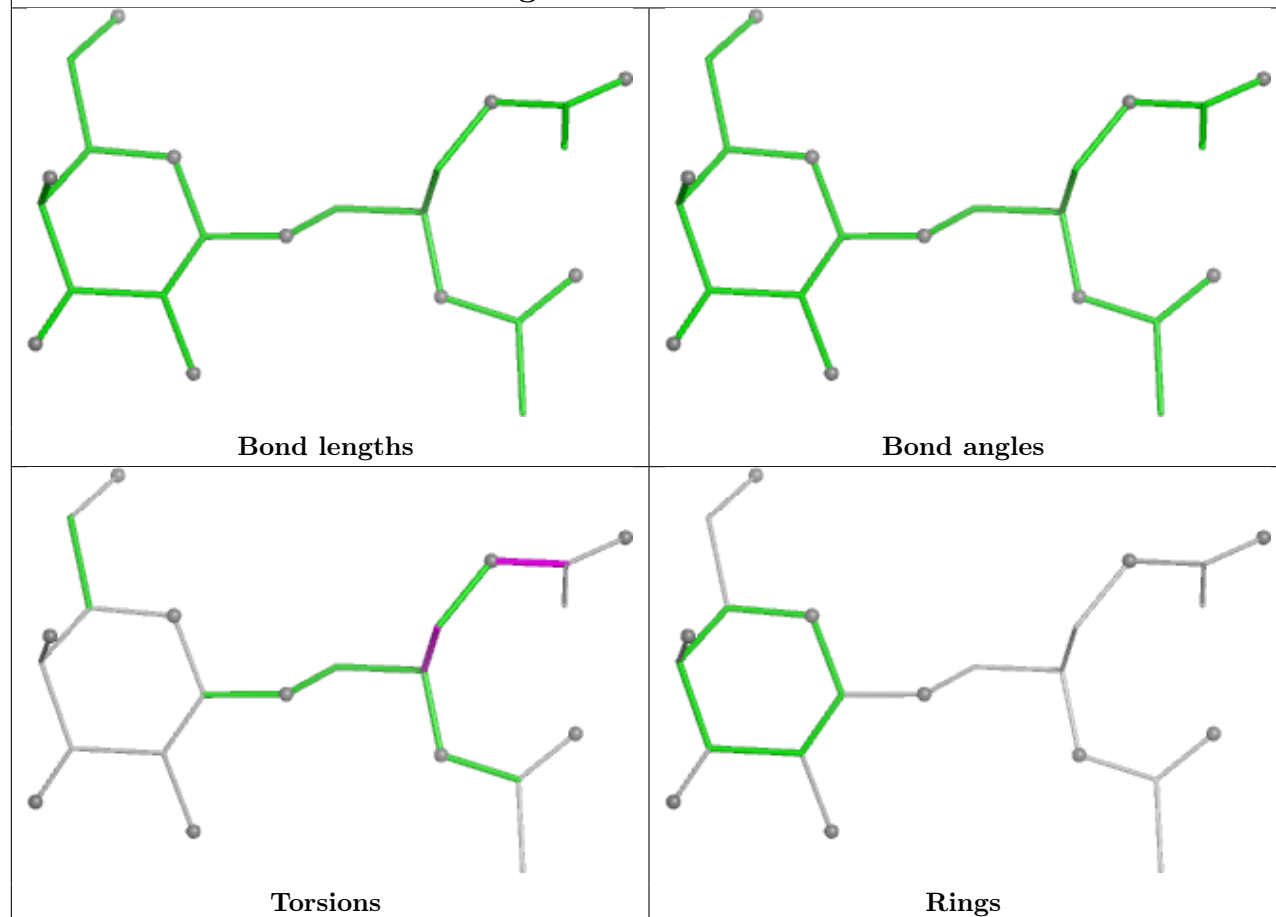
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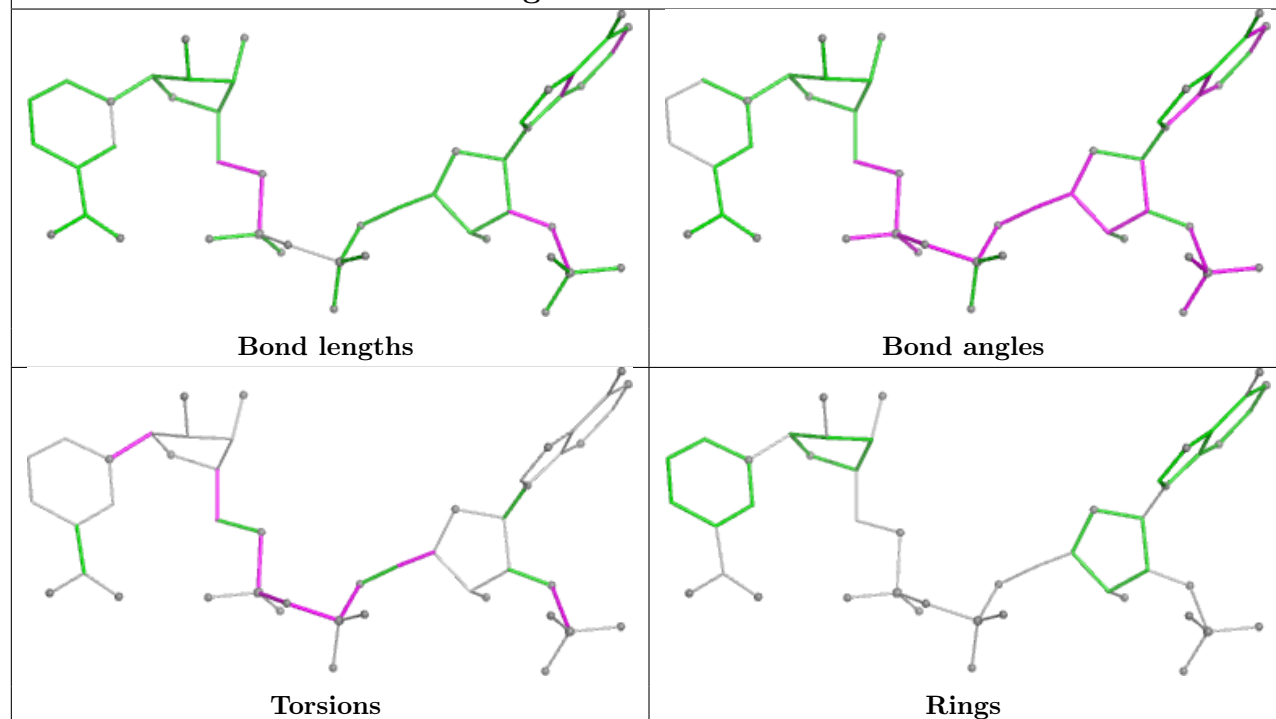


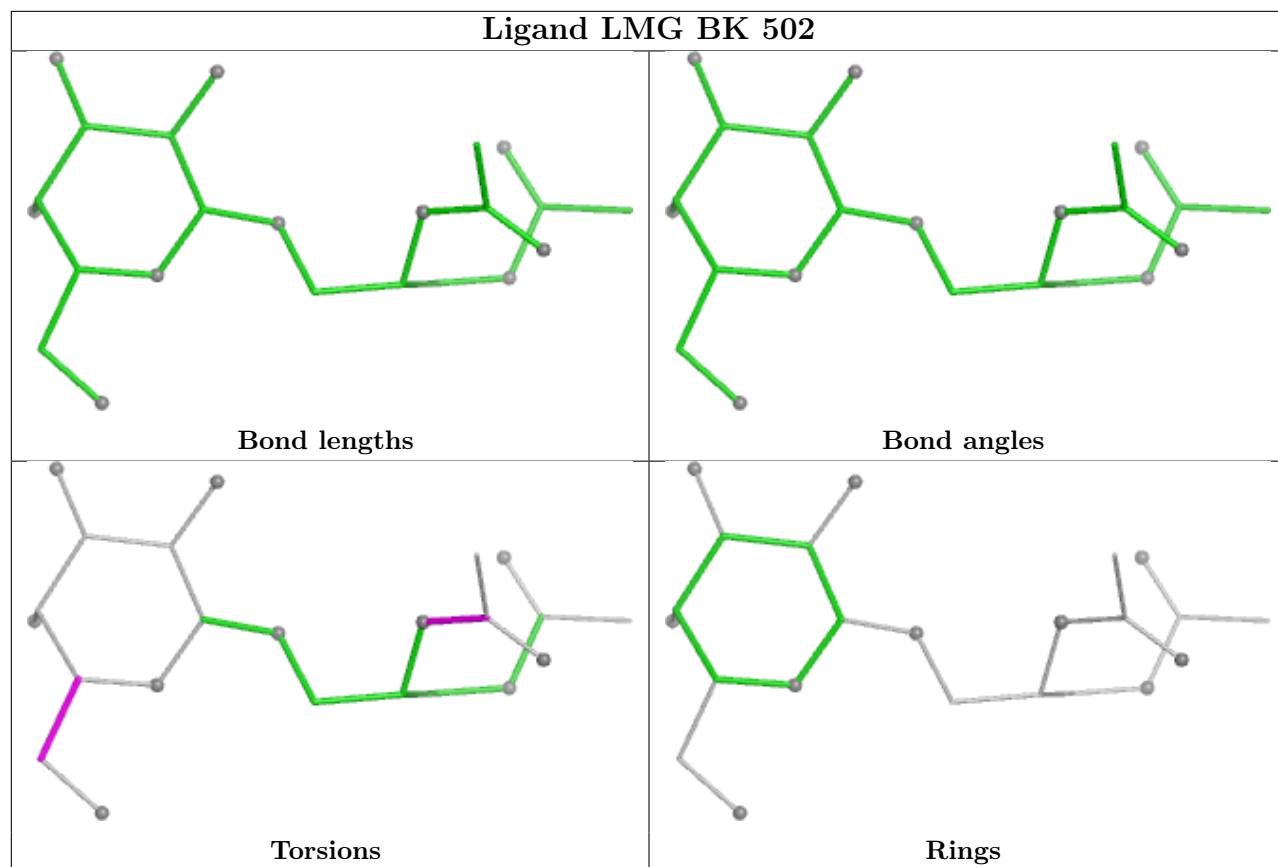


Ligand LMG BJ 502

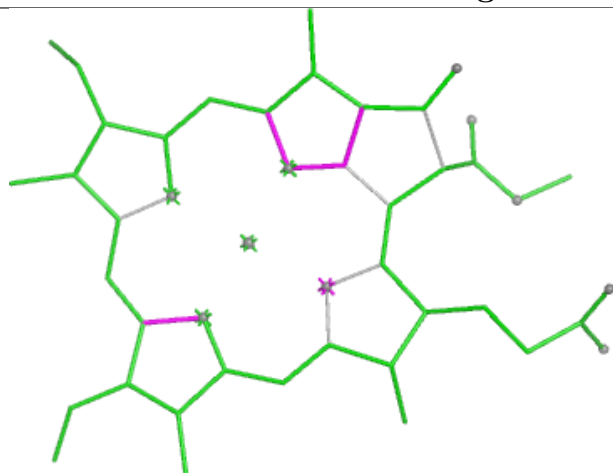


Ligand NDP BI 501

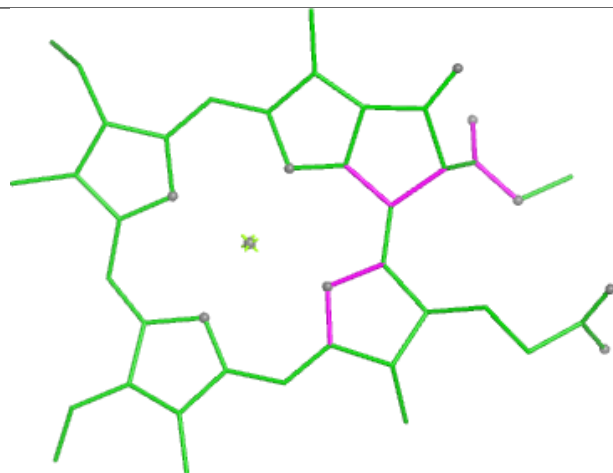




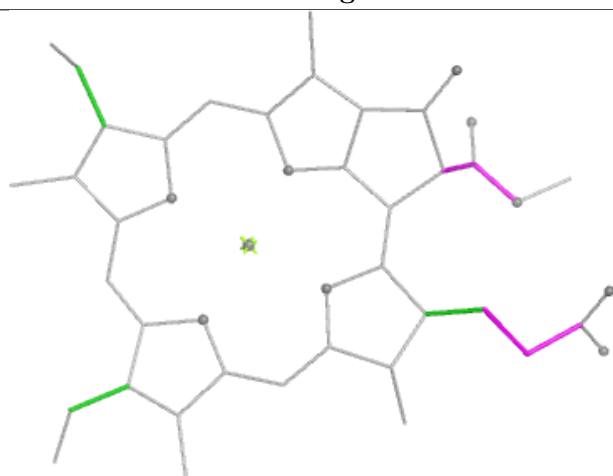
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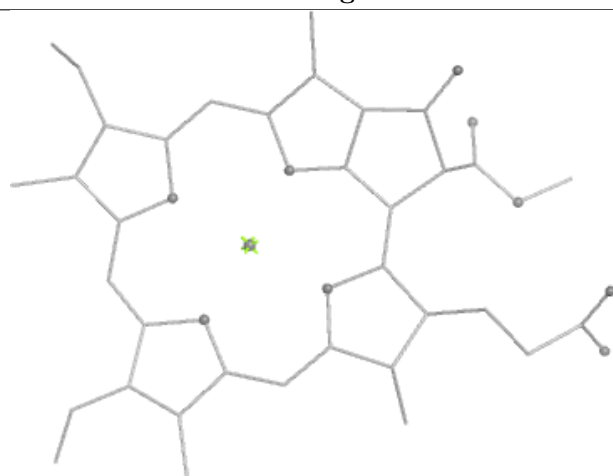
Bond lengths



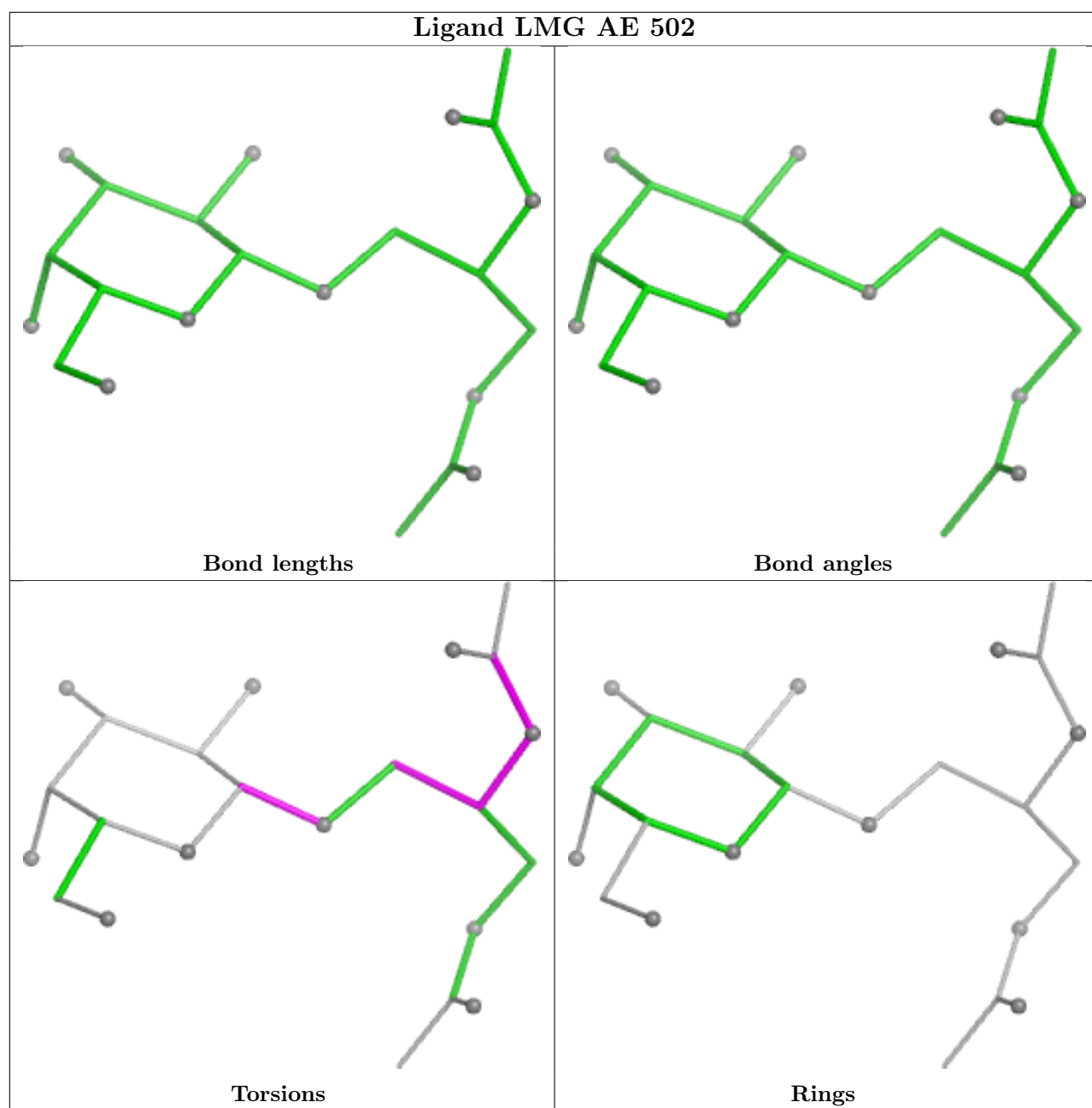
Bond angles



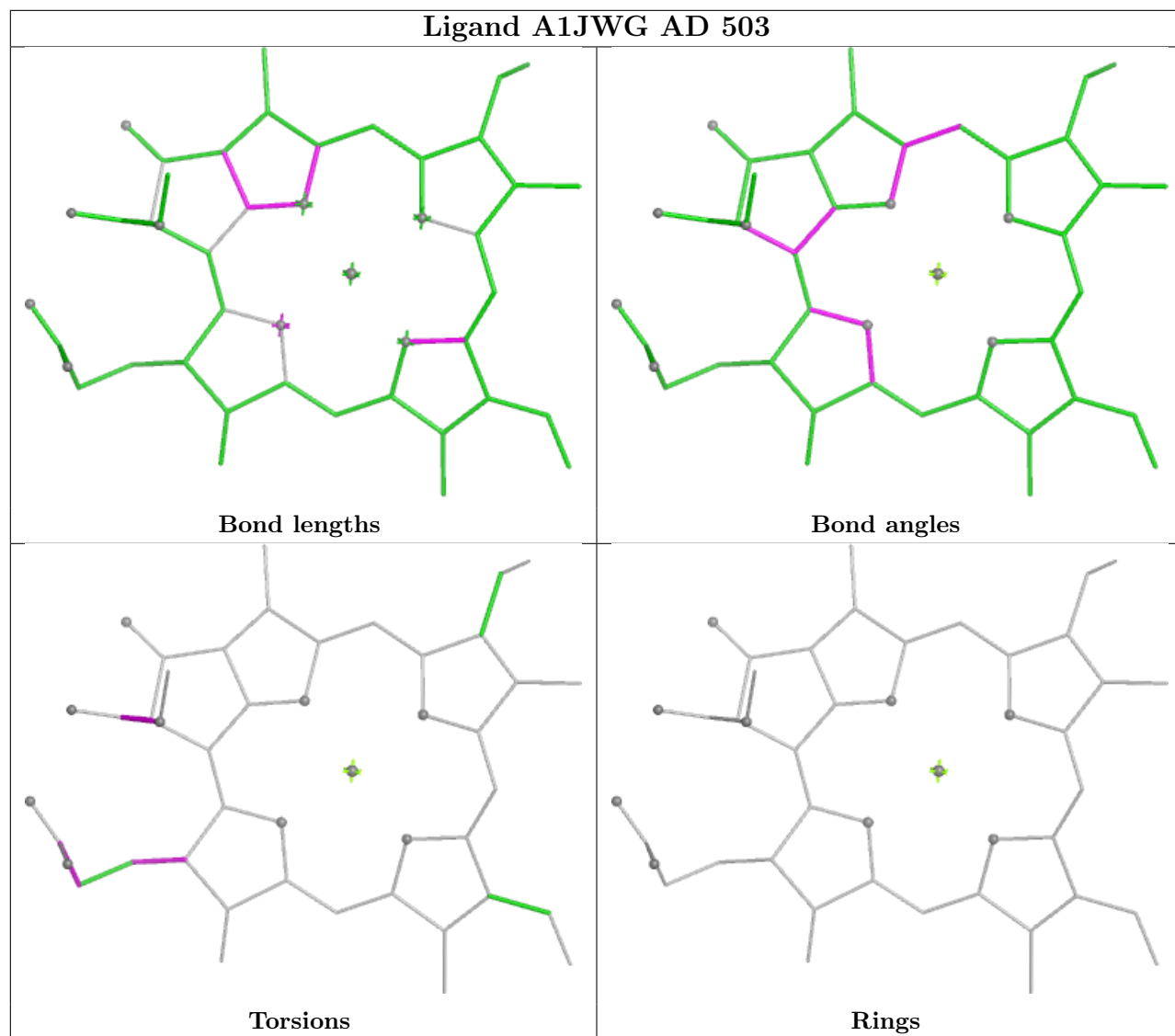
Torsions

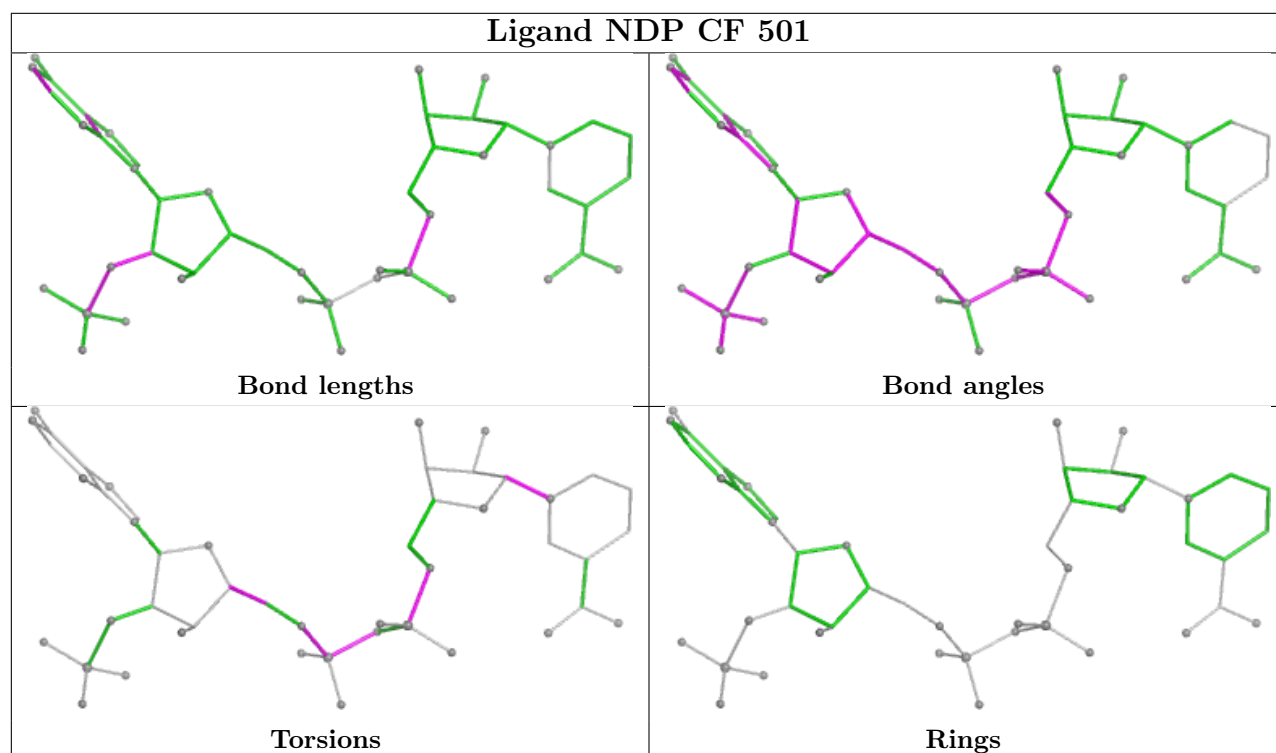
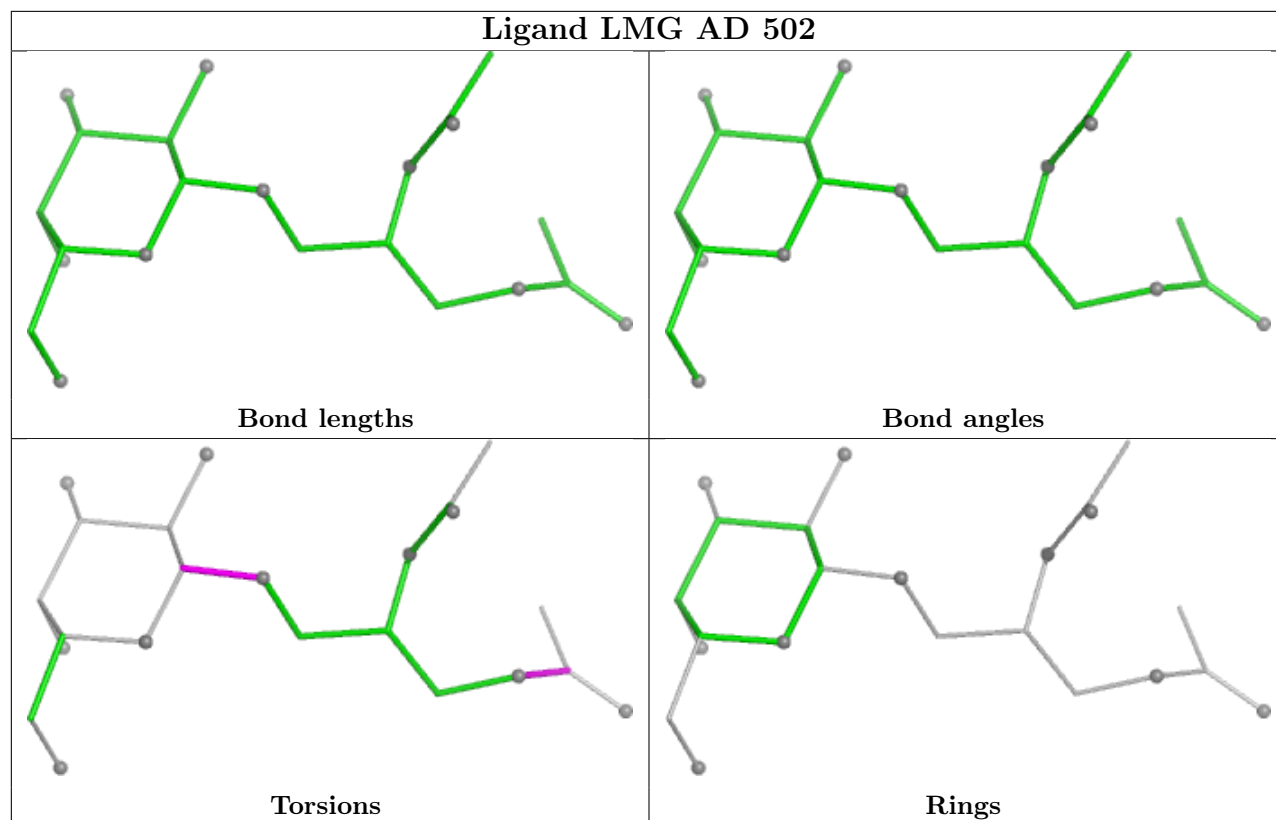


Rings

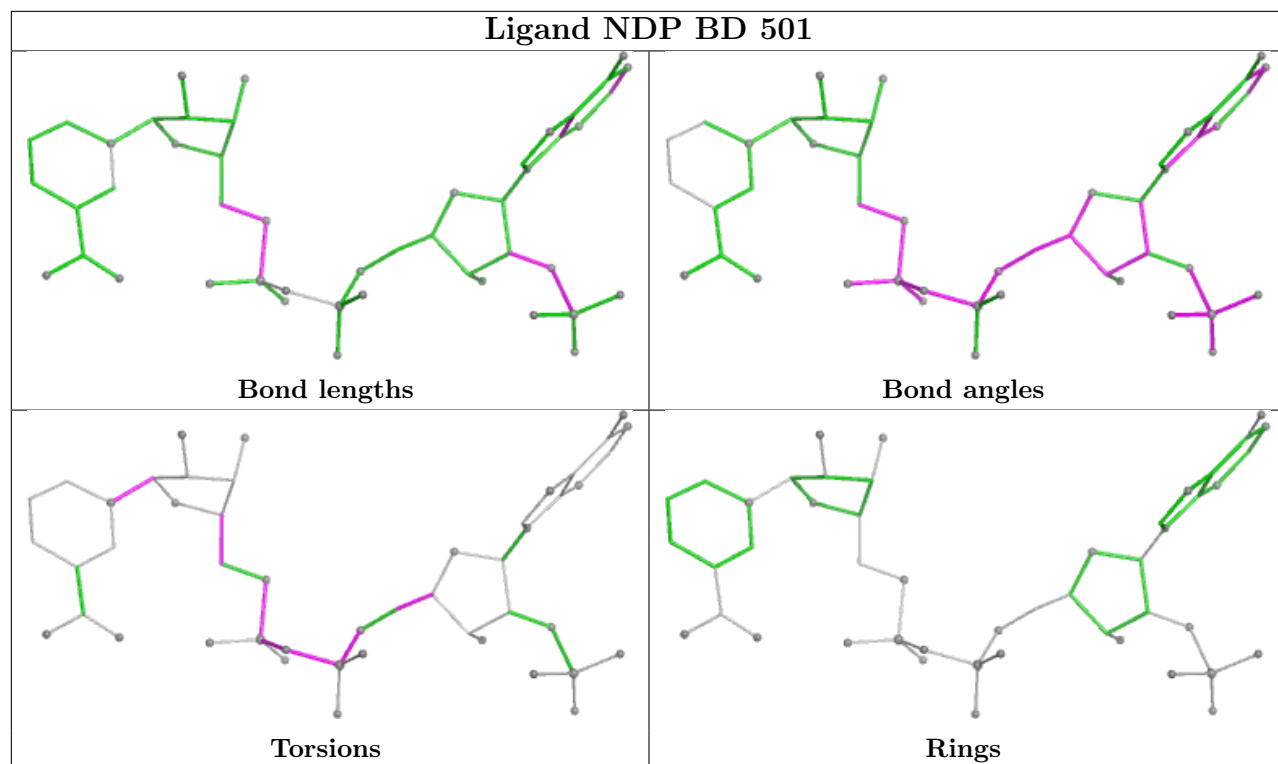


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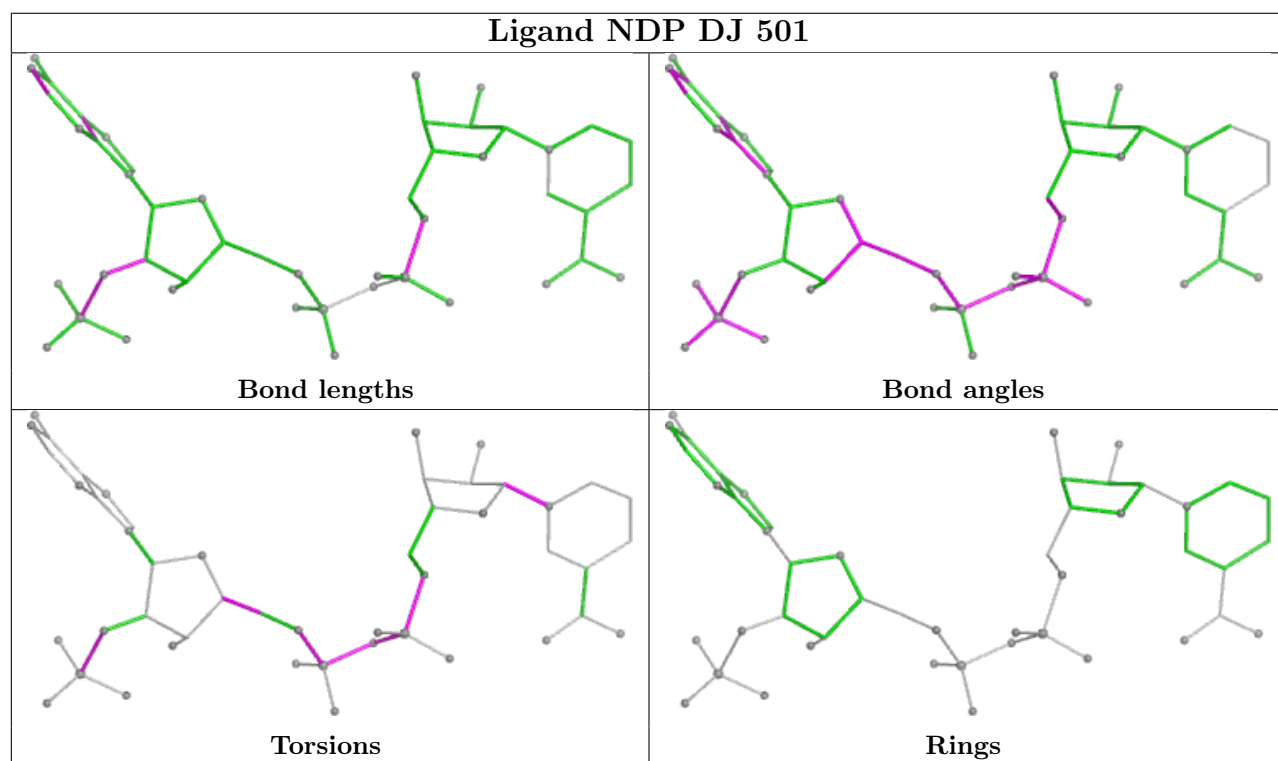




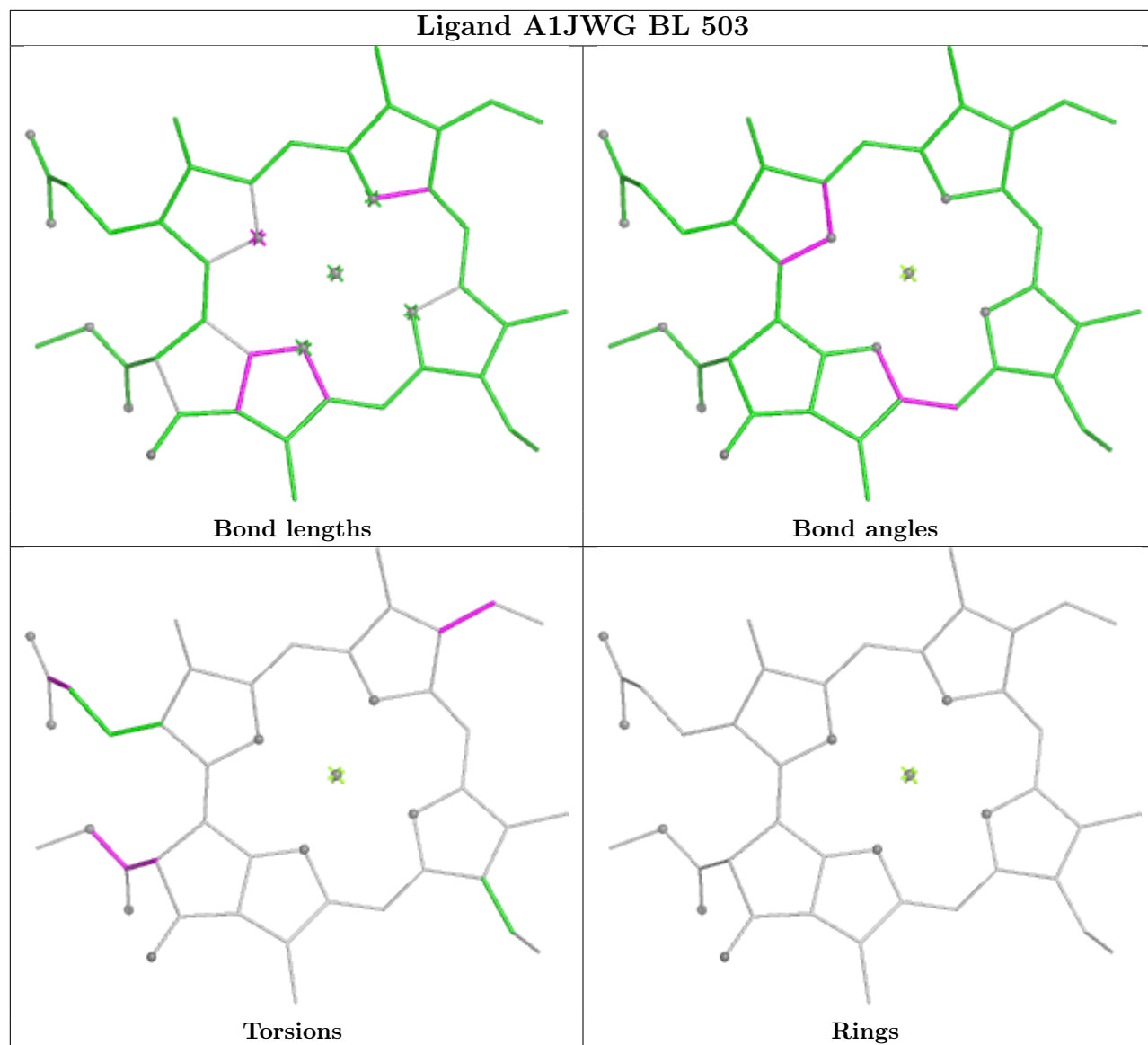
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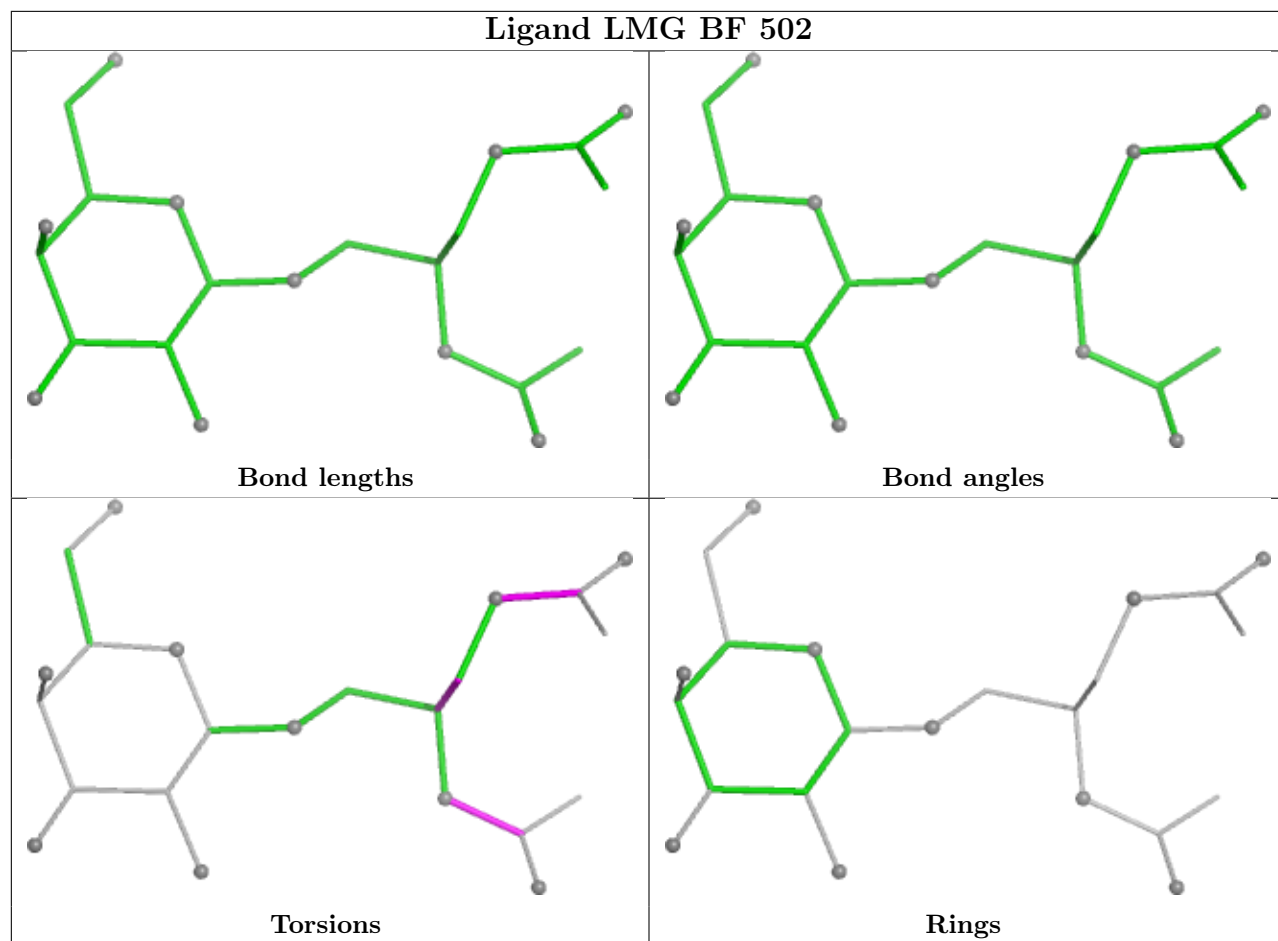
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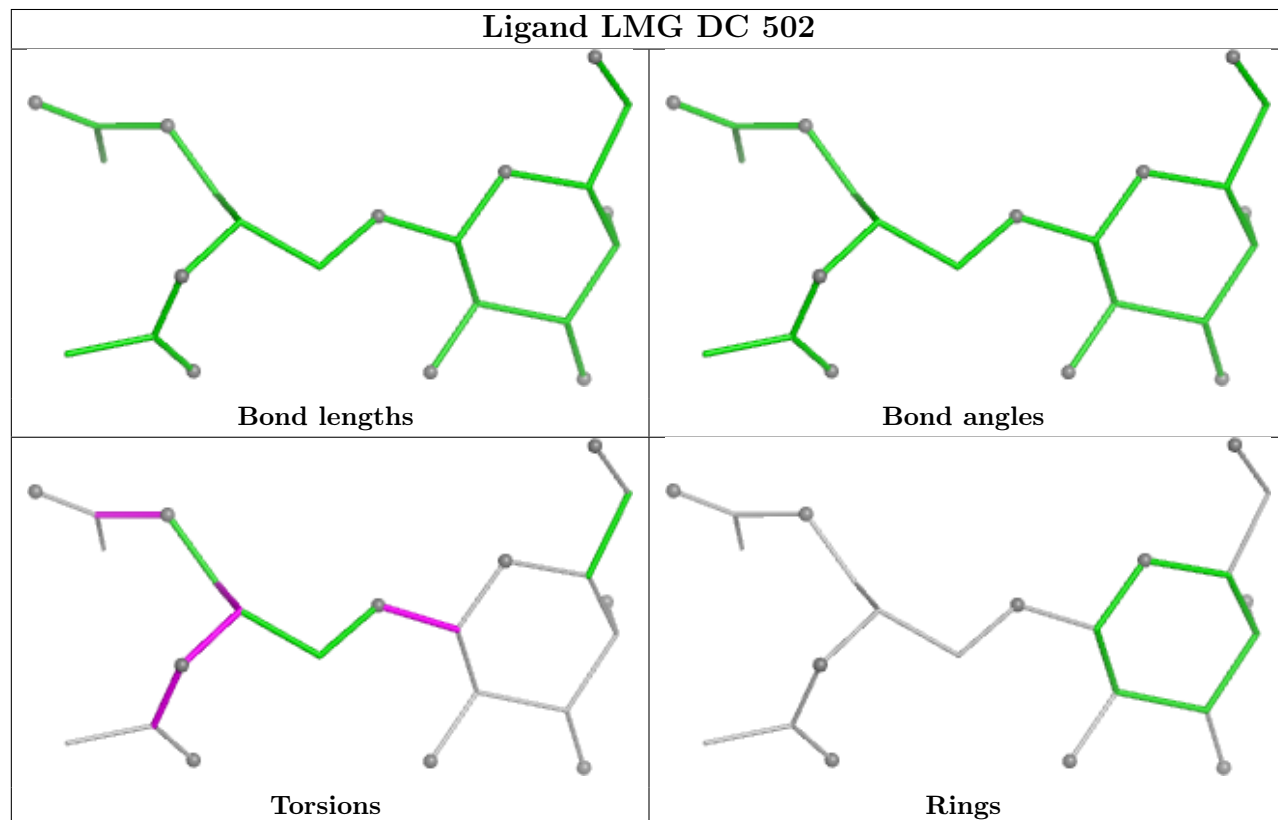
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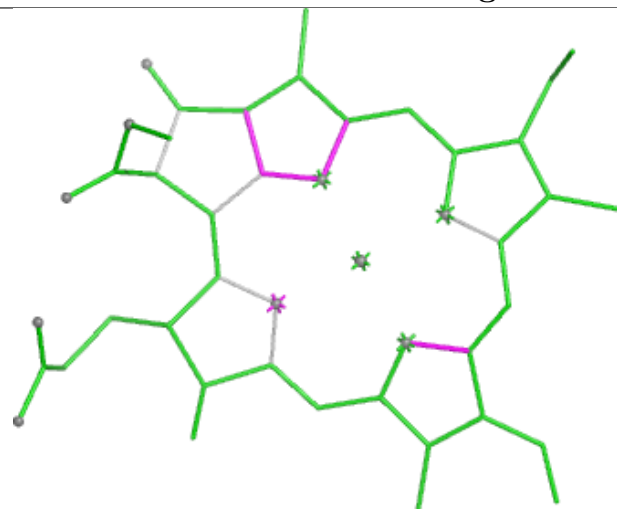
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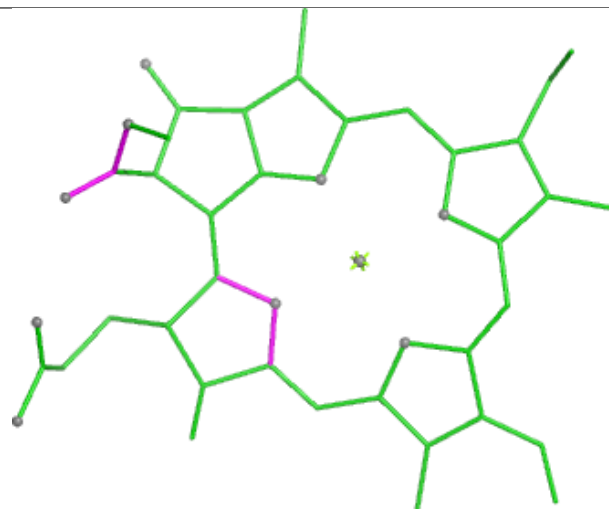
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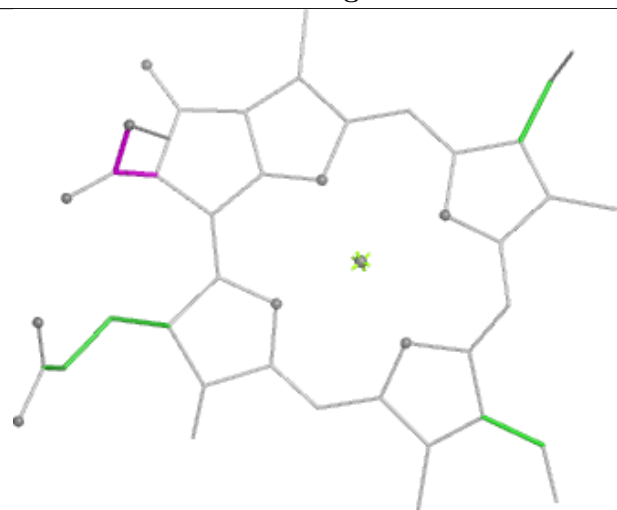
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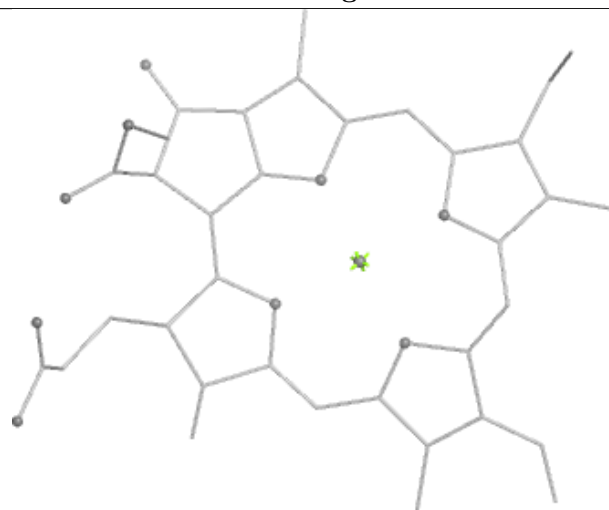
Bond lengths



Bond angles

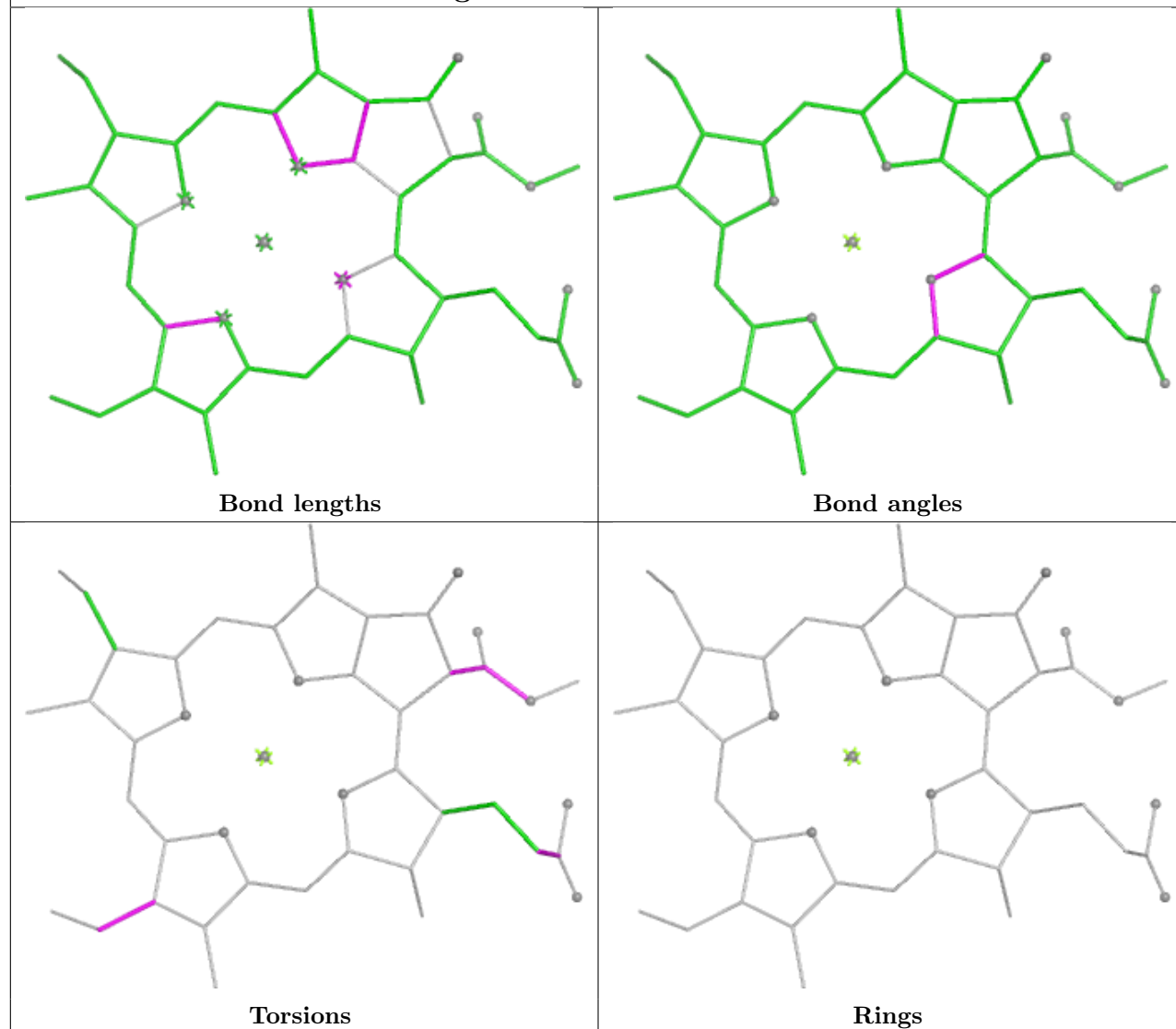


Torsions

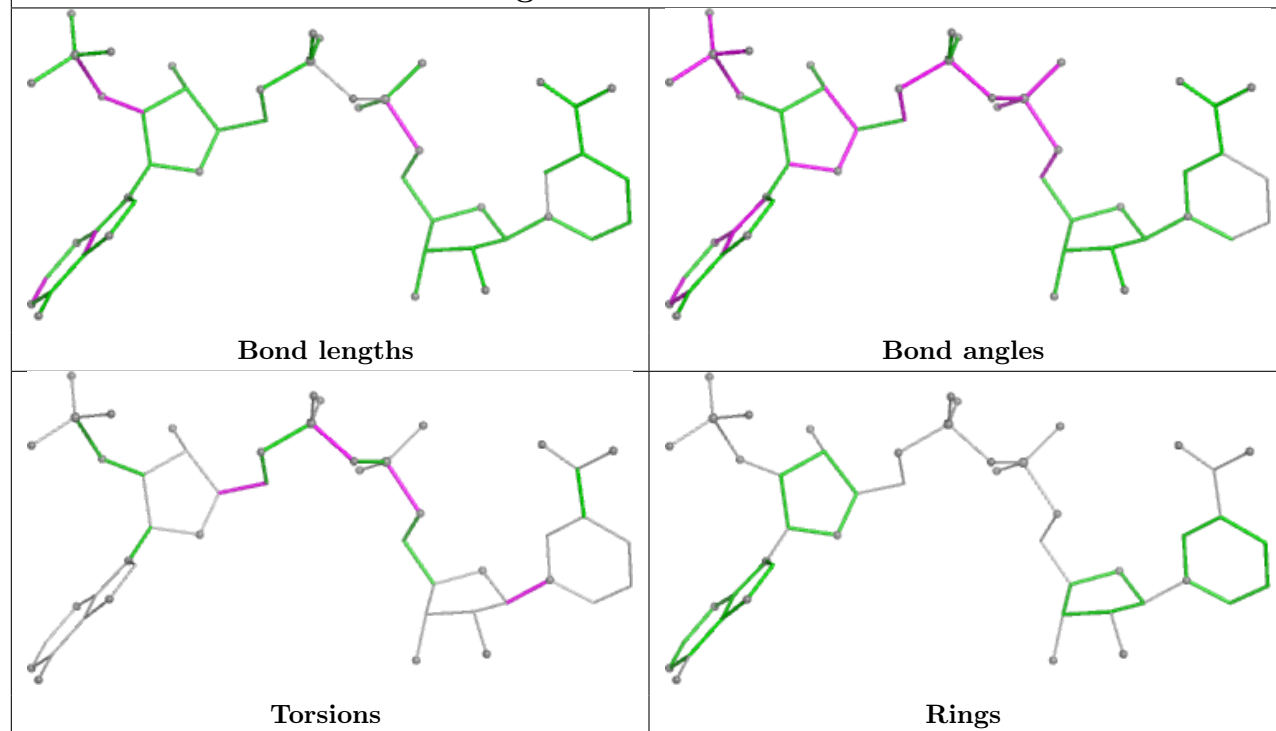


Rings

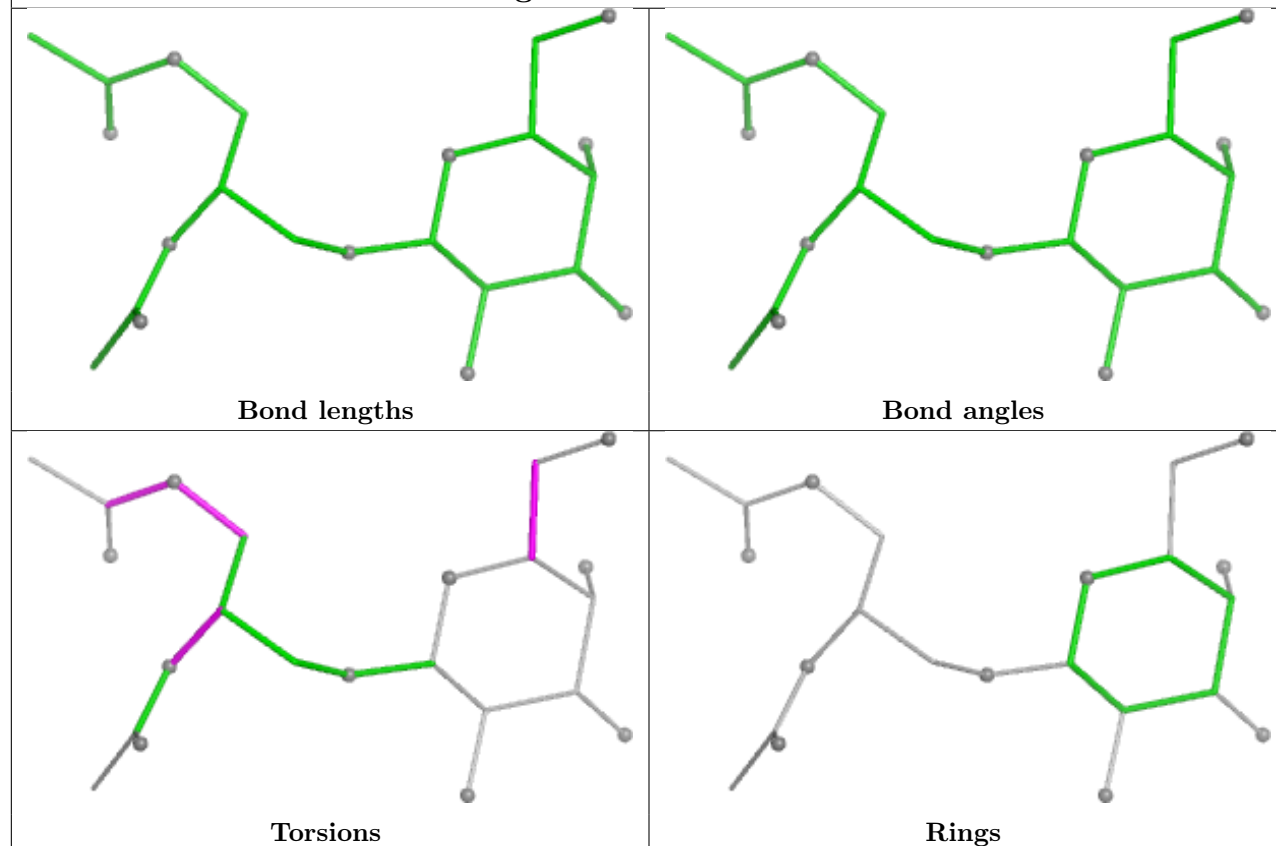
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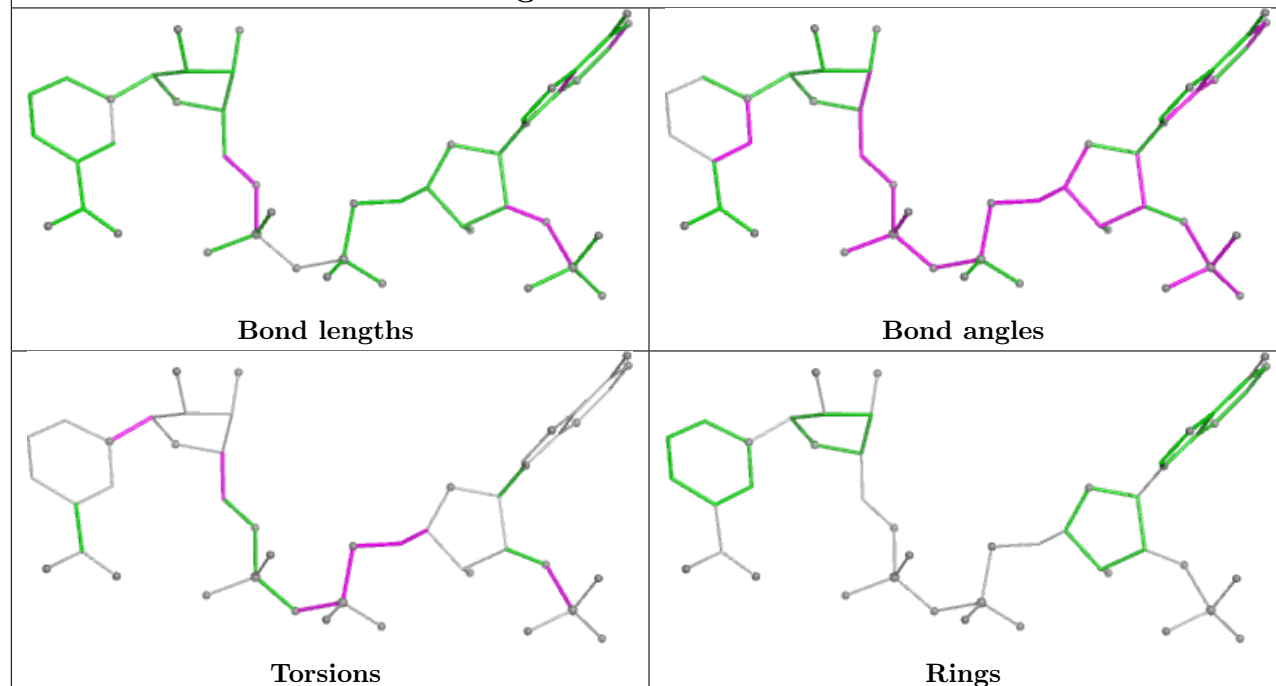
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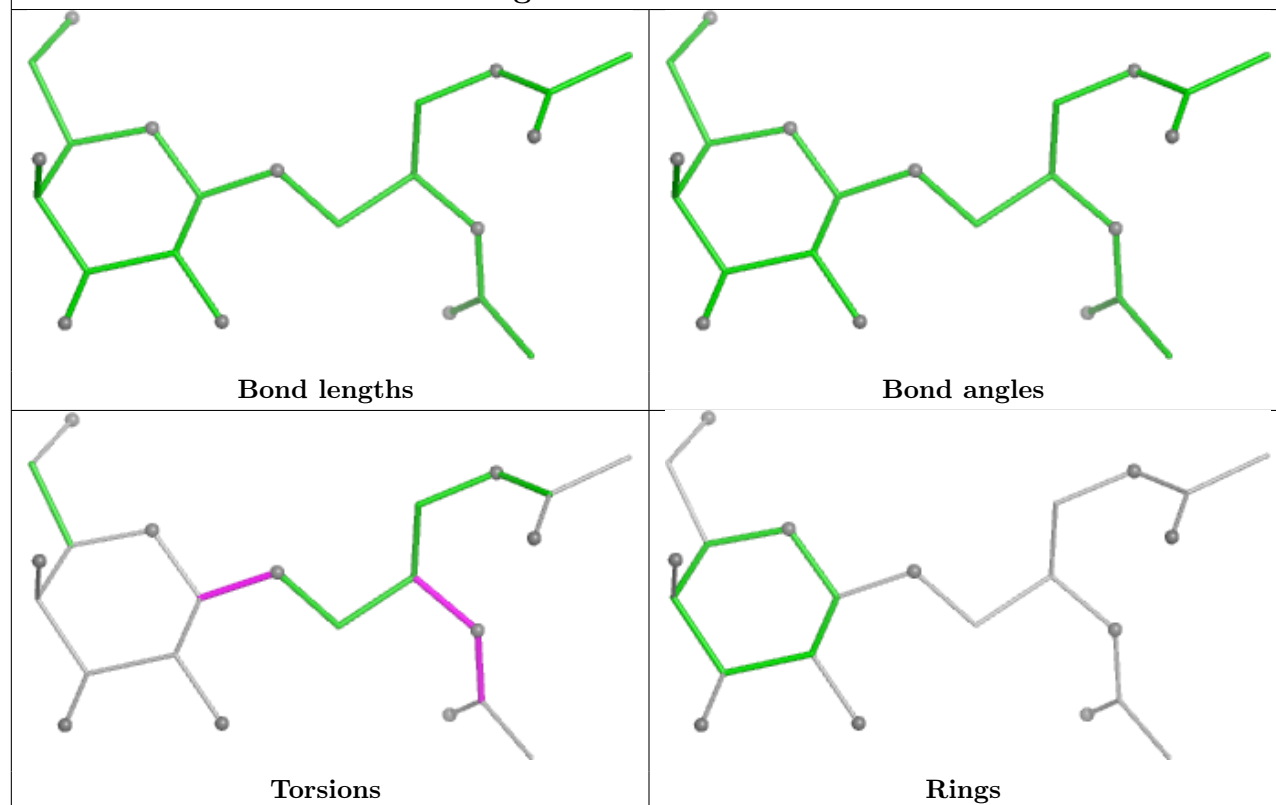
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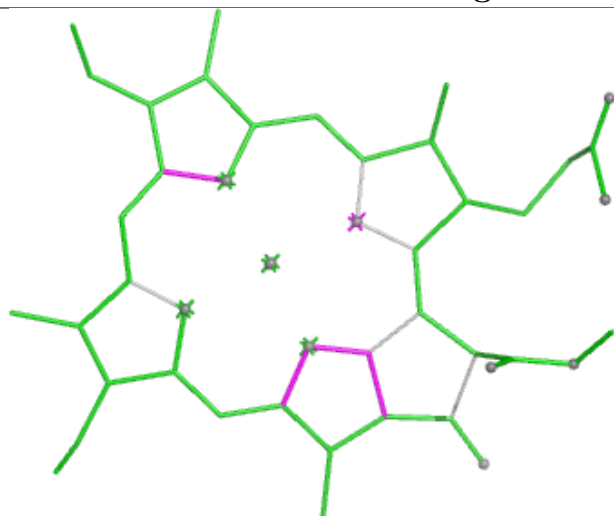
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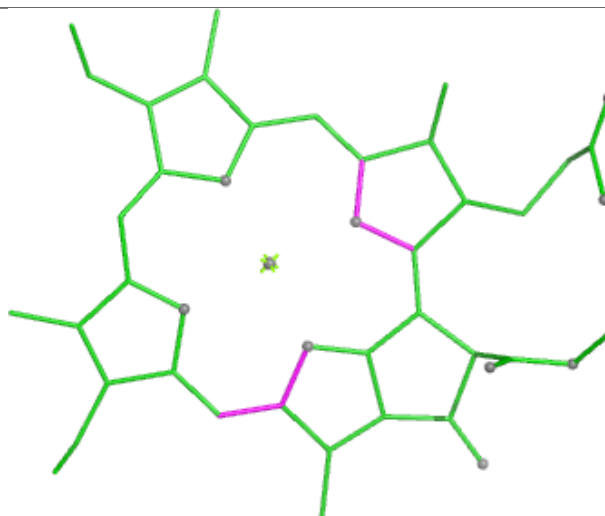
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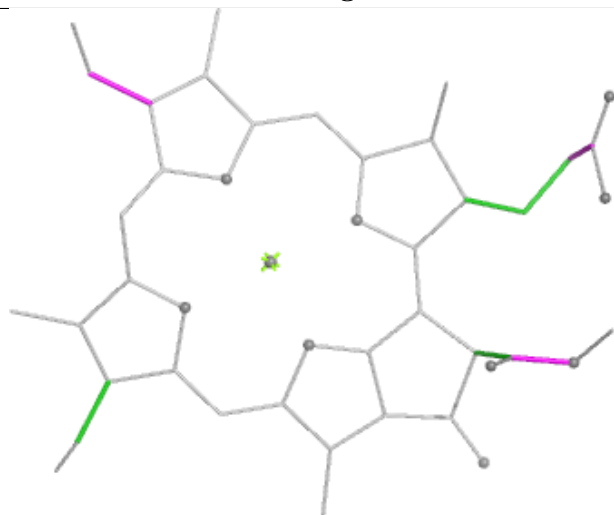
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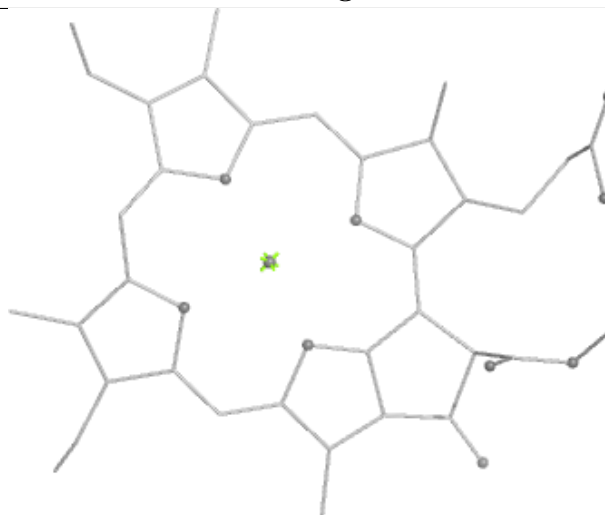
Bond lengths



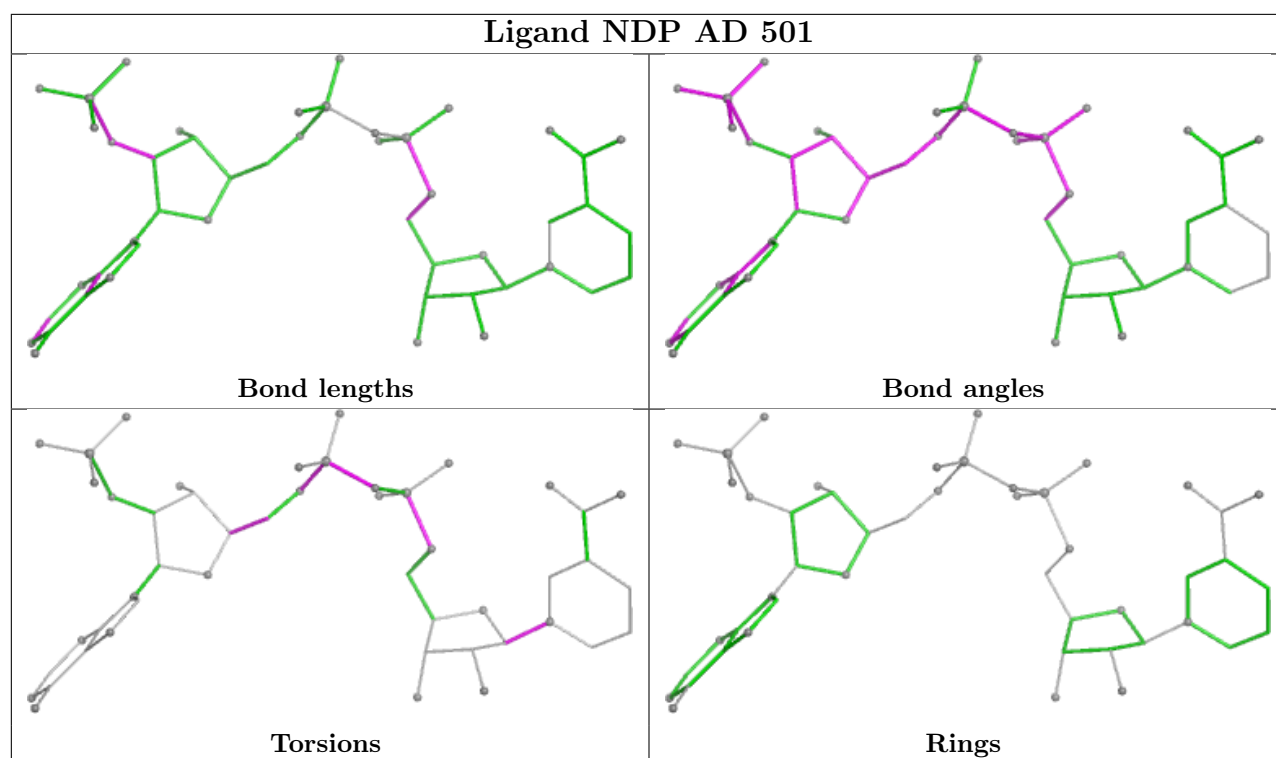
Bond angles



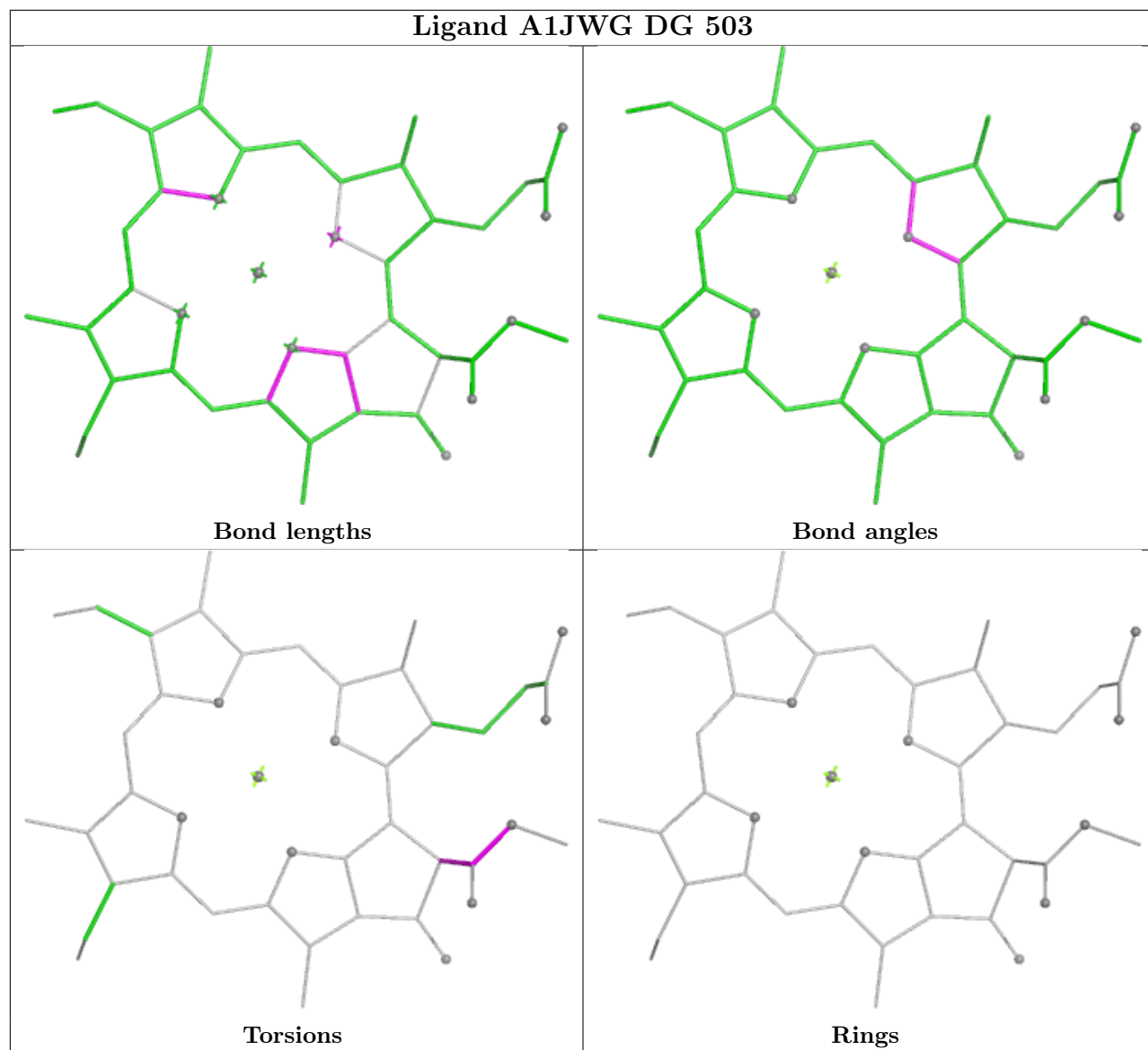
Torsions



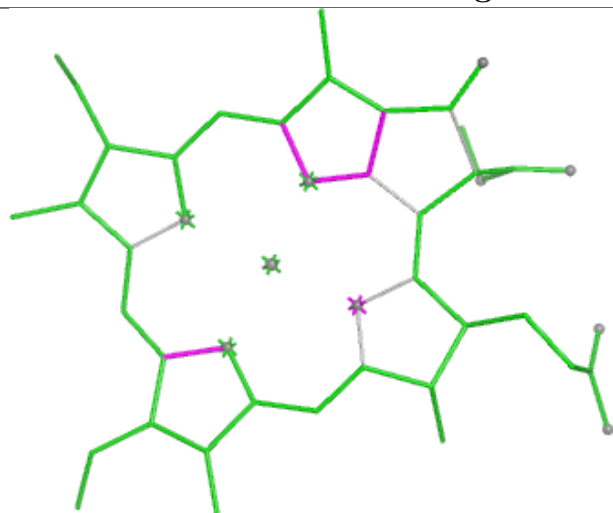
Rings



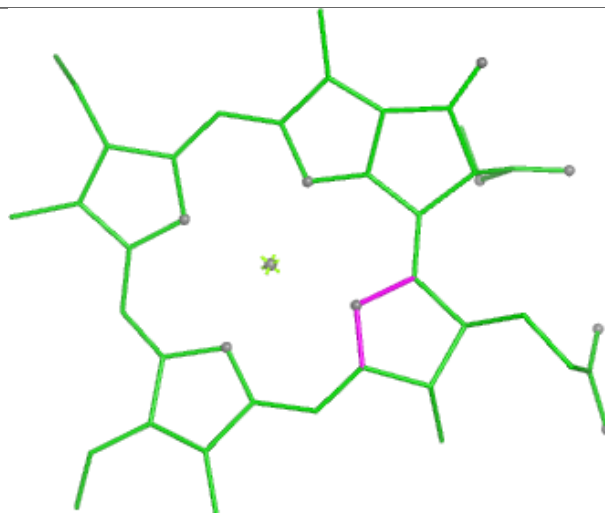
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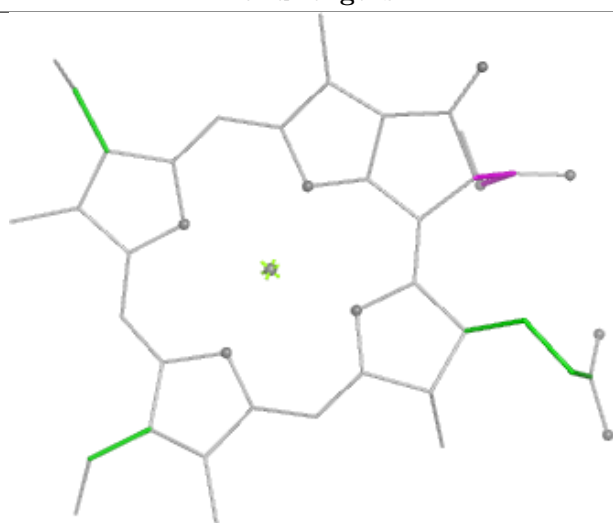
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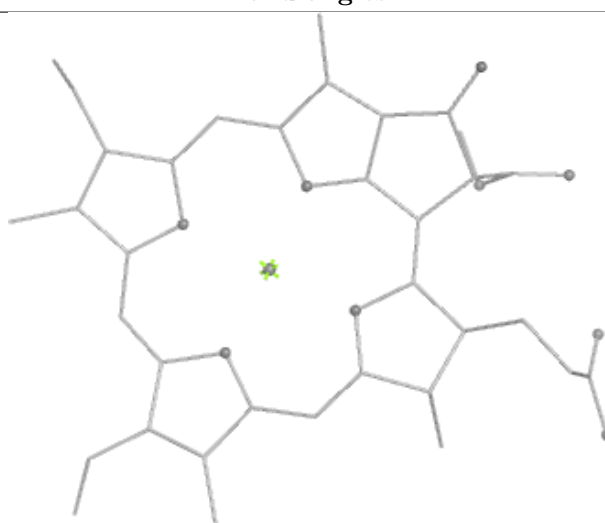
Bond lengths



Bond angles

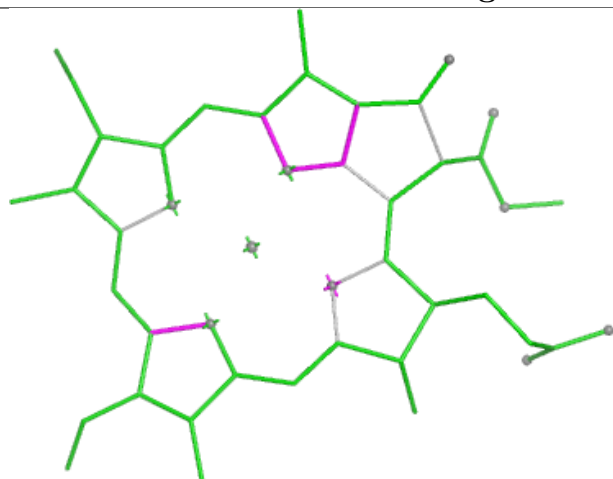


Torsions

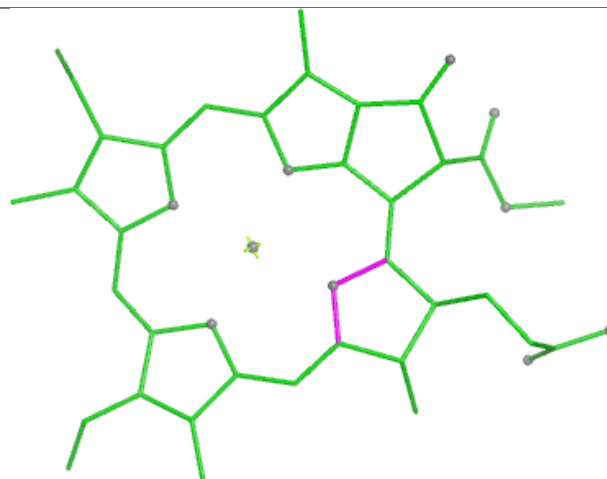


Rings

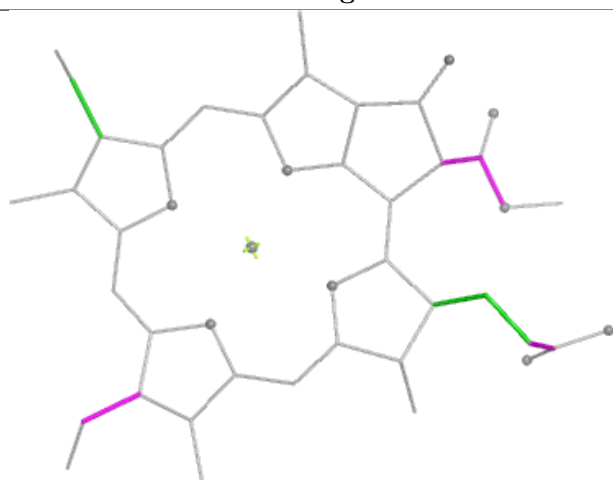
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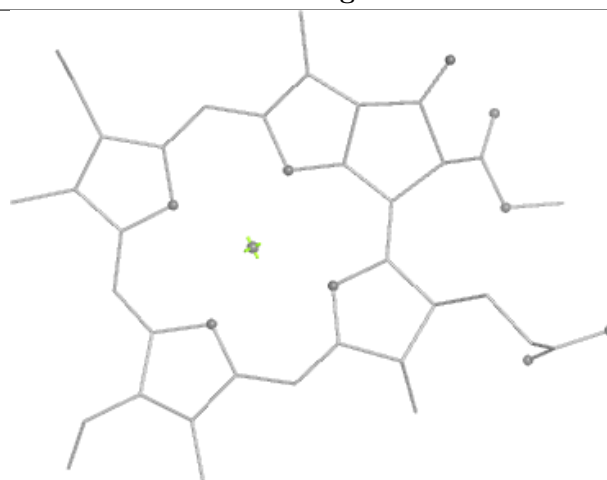
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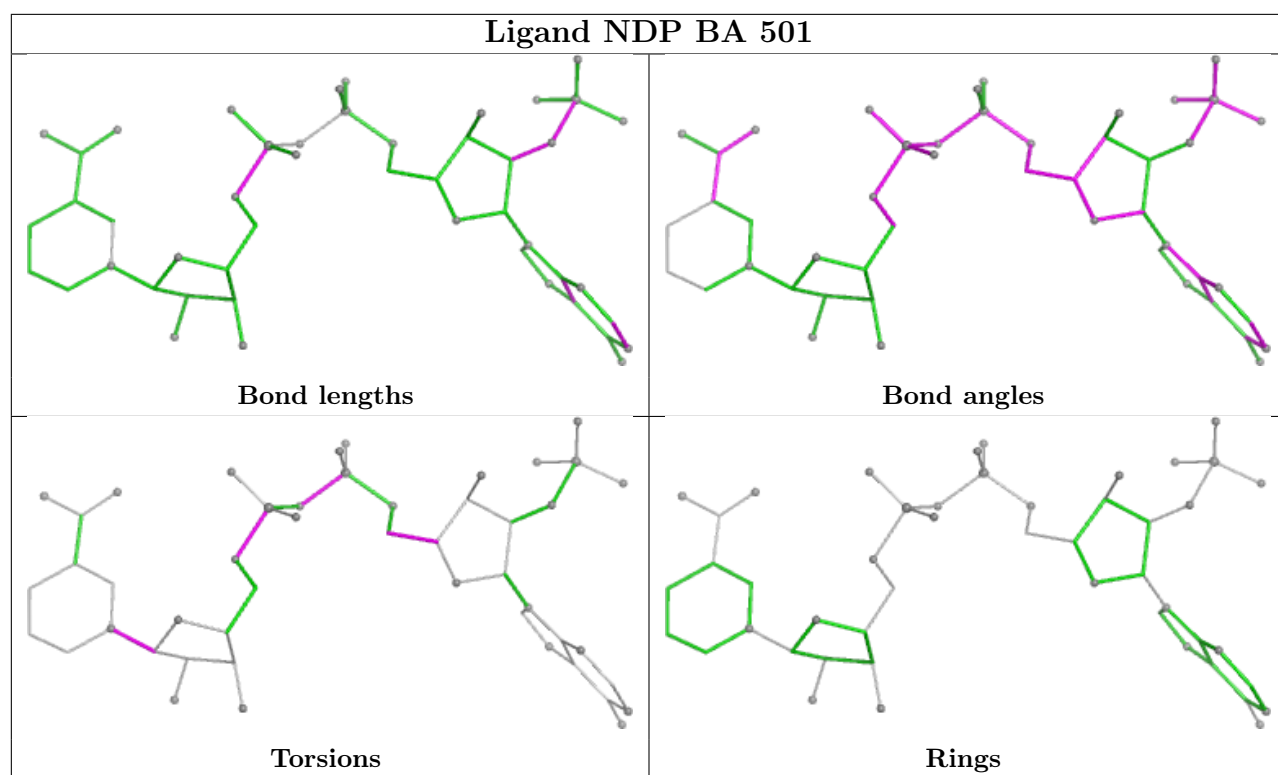
Bond angles



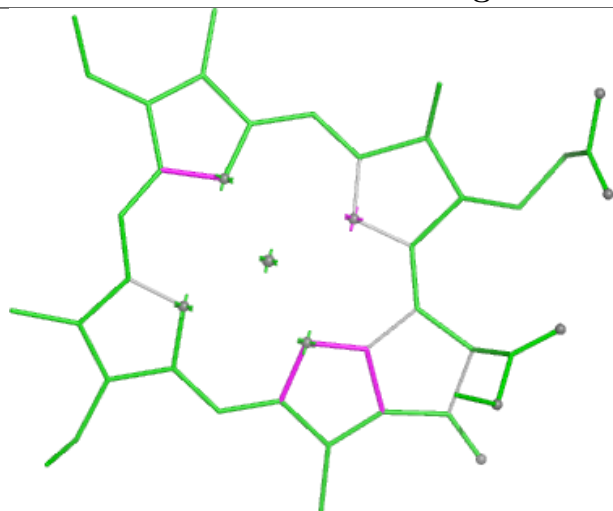
Torsions



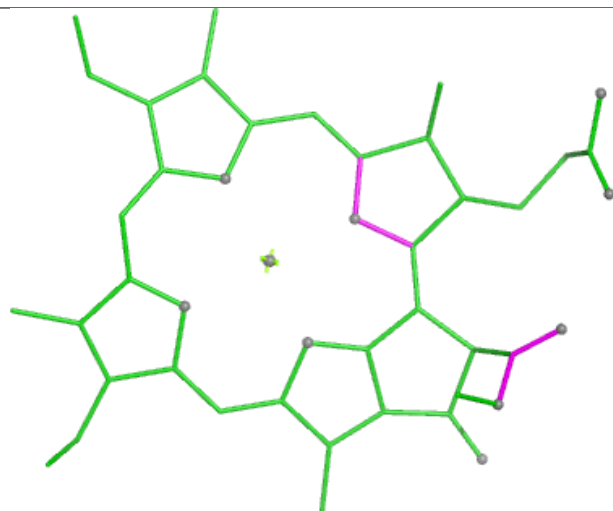
Rings



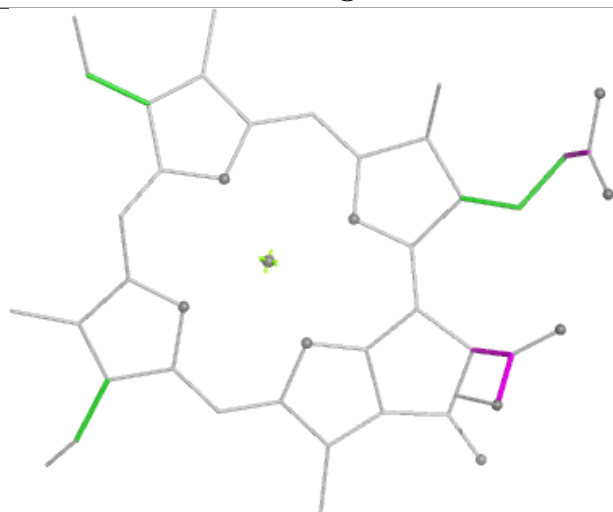
Ligand A1JWG DD 503



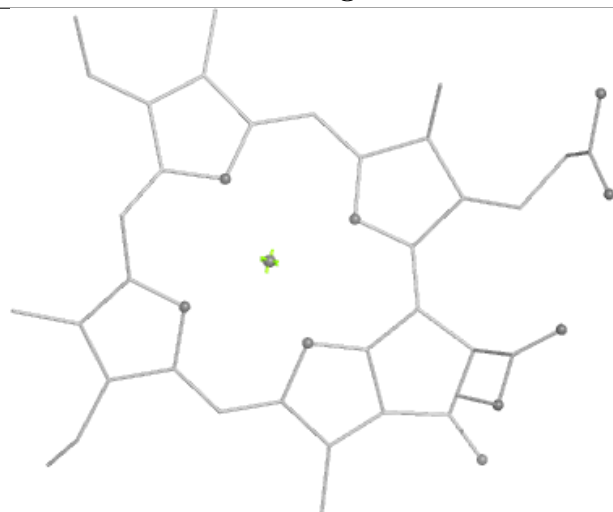
Bond lengths



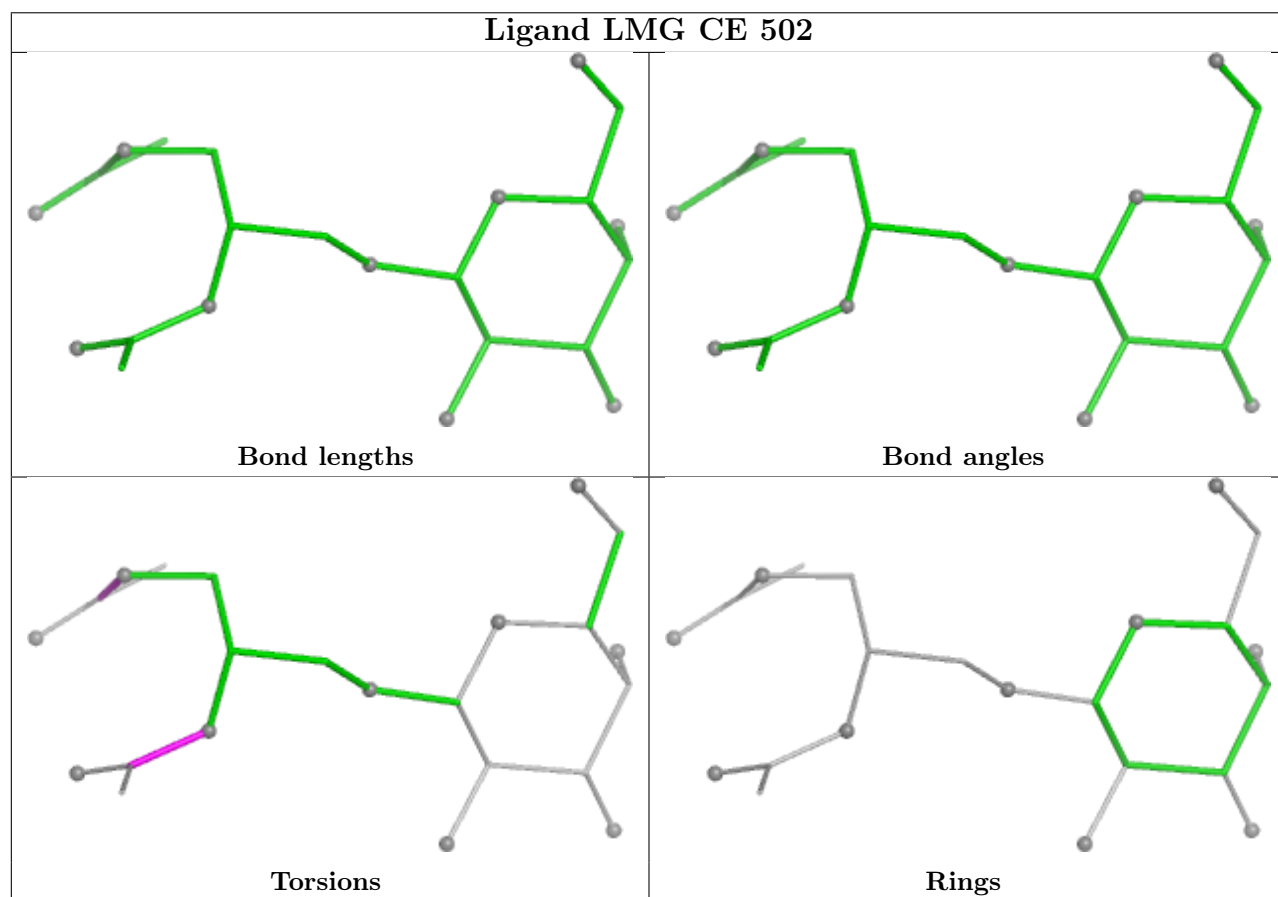
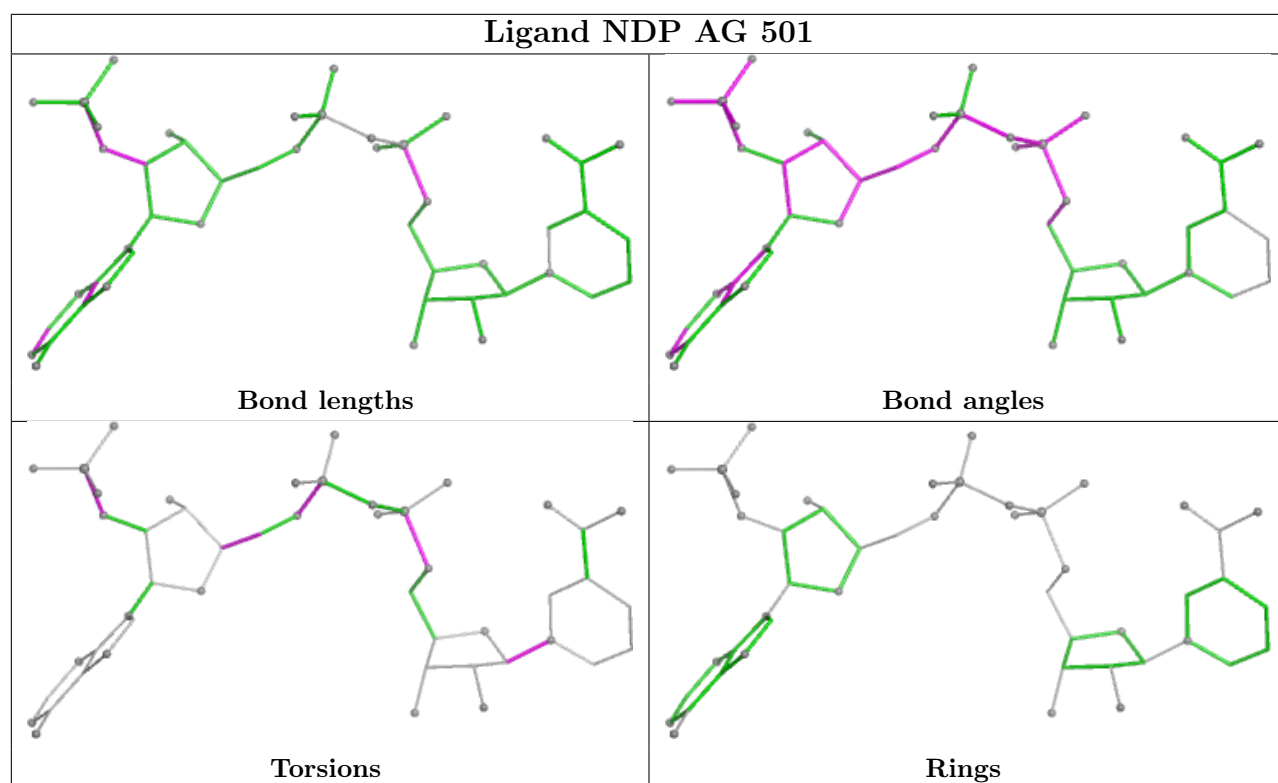
Bond angles

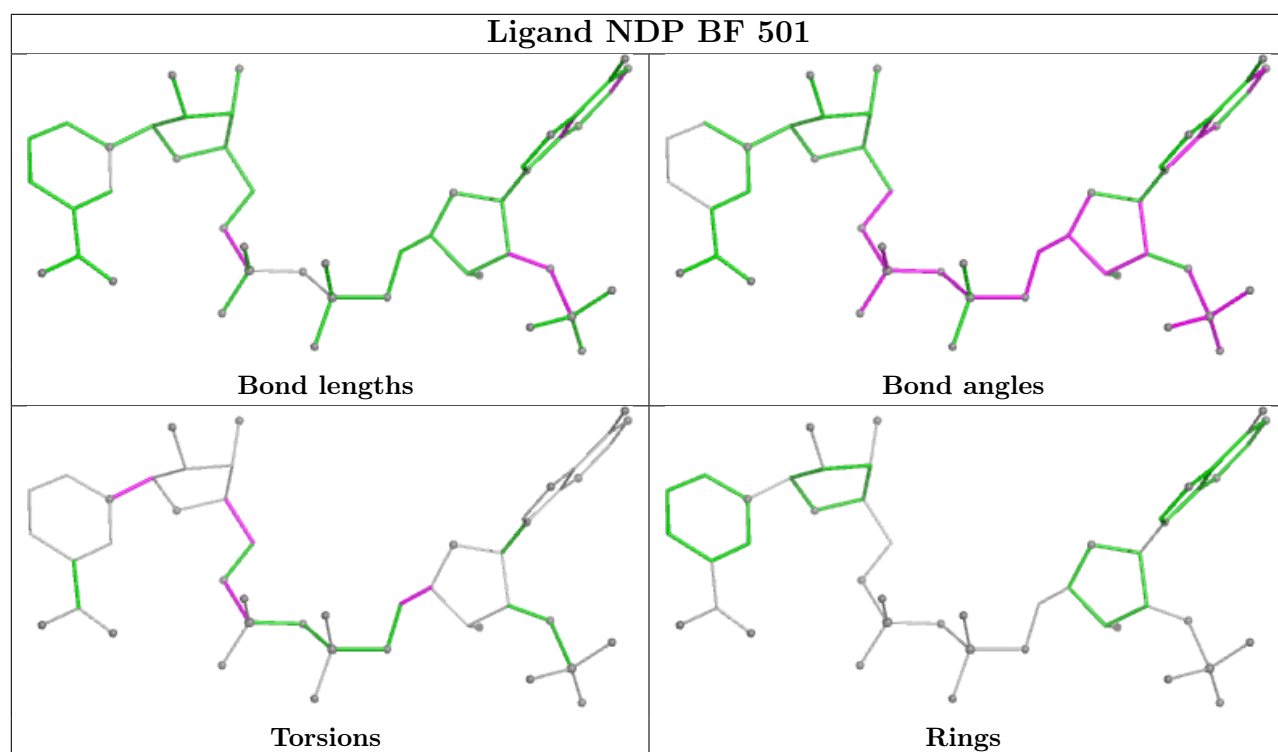


Torsions

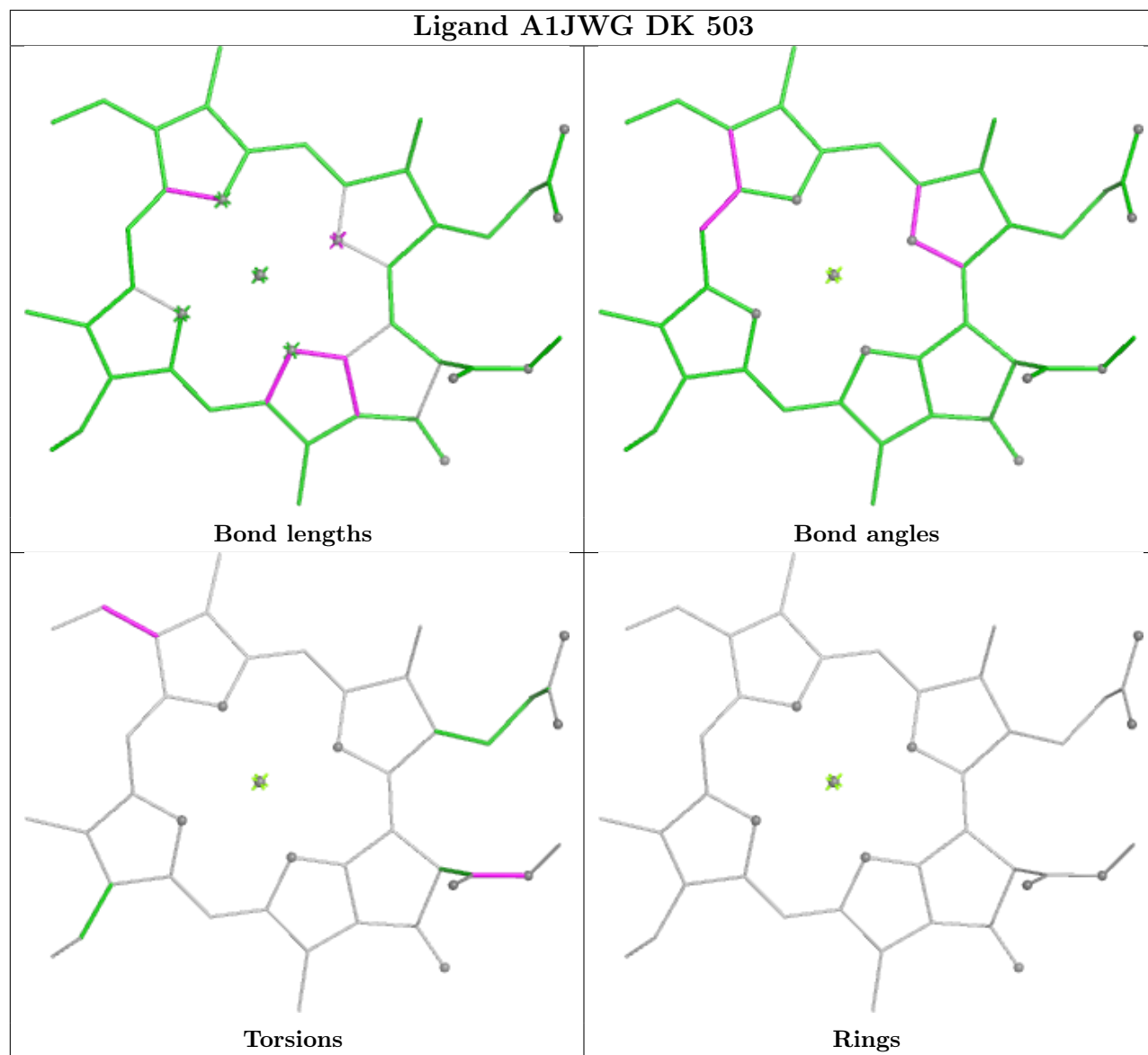


Rings

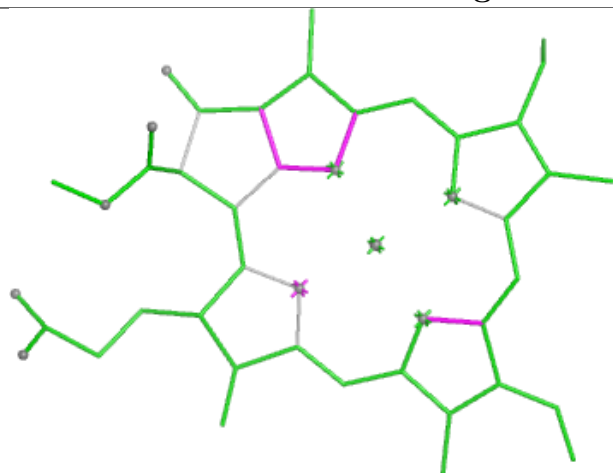




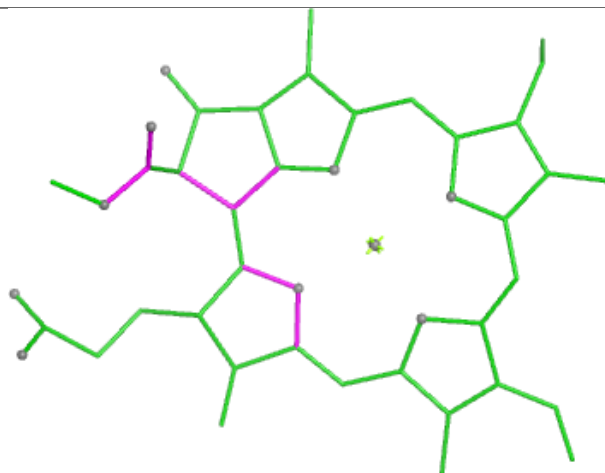
Ligand A1JWG DK 503



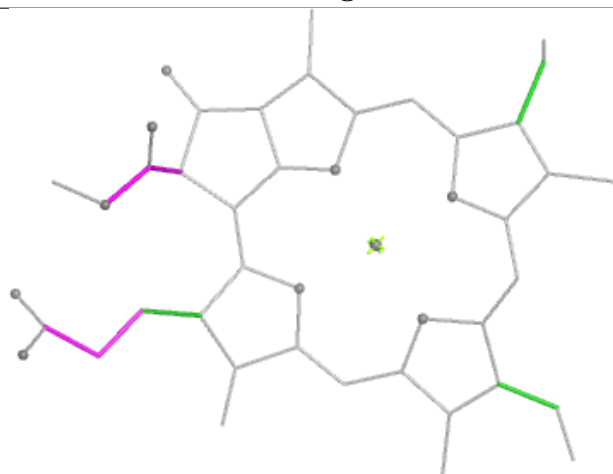
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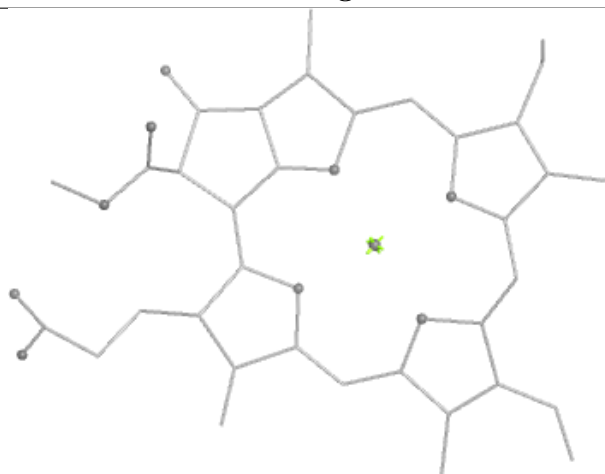
Bond lengths



Bond angles

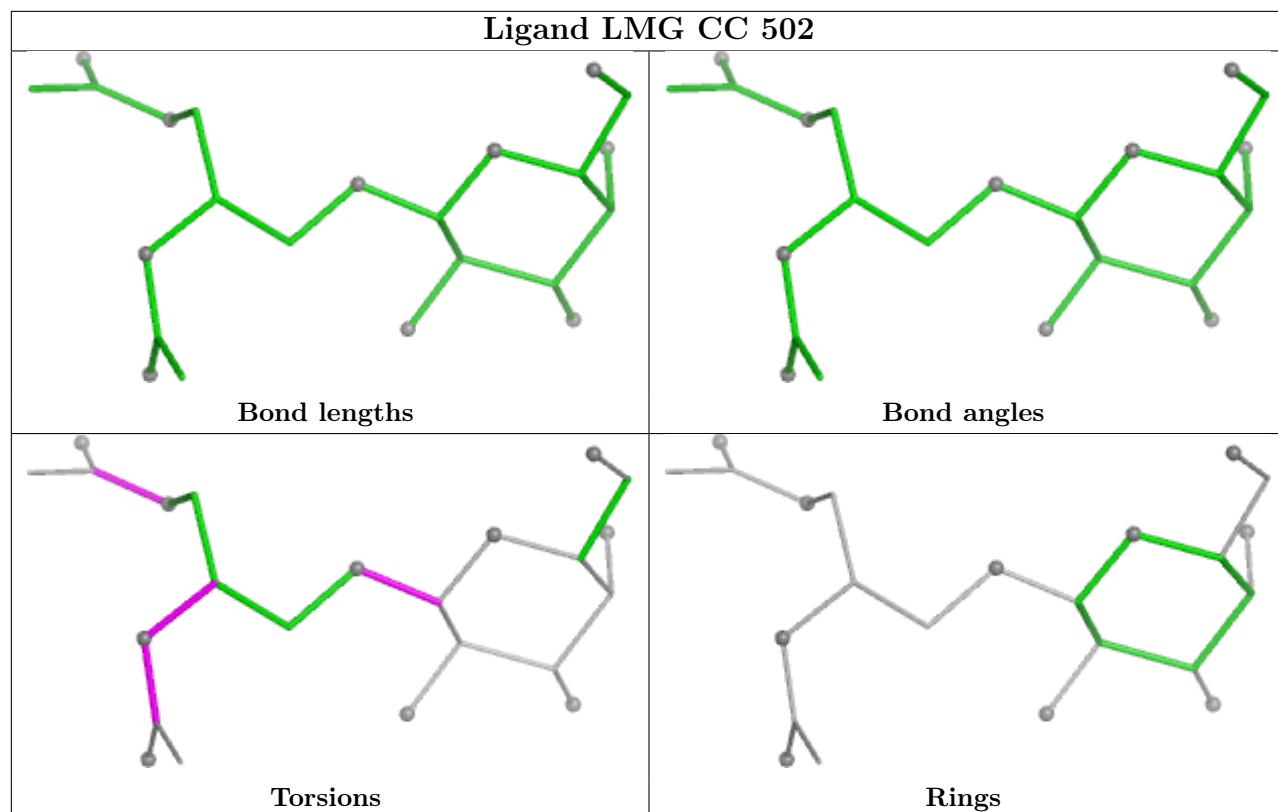


Torsions

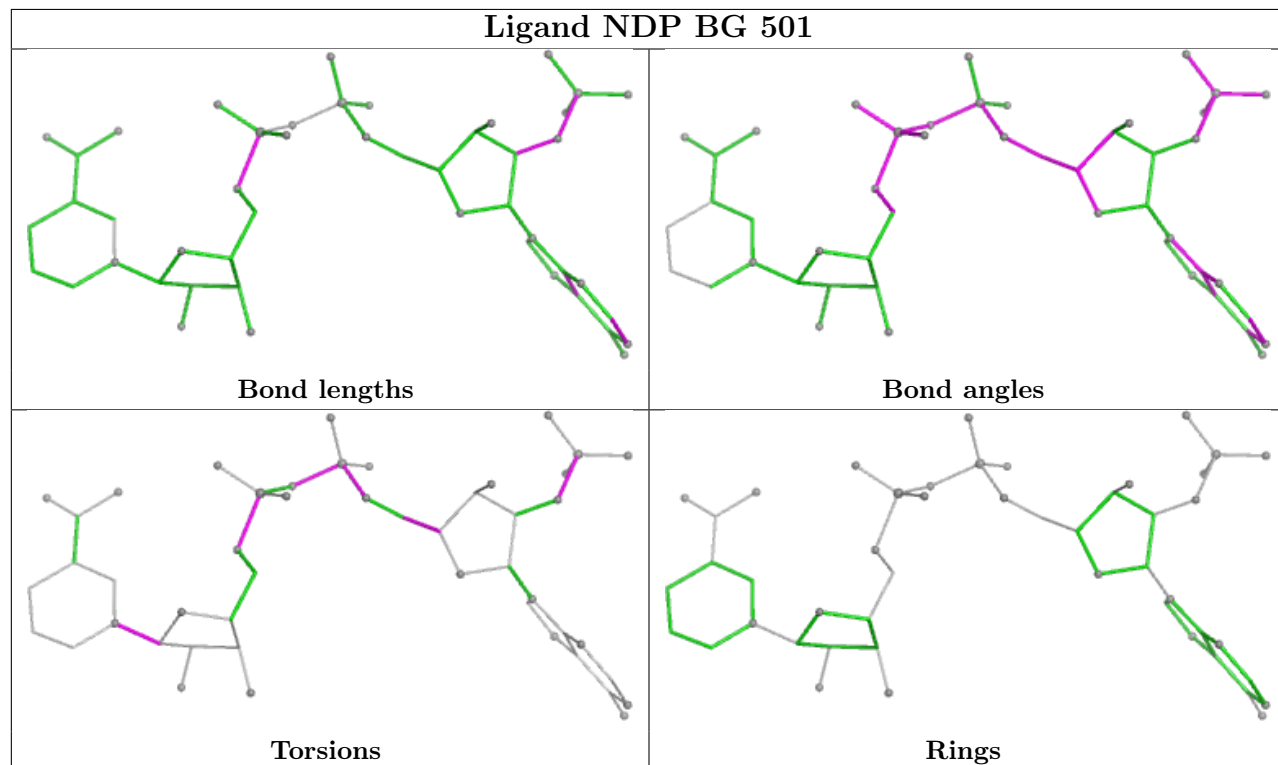


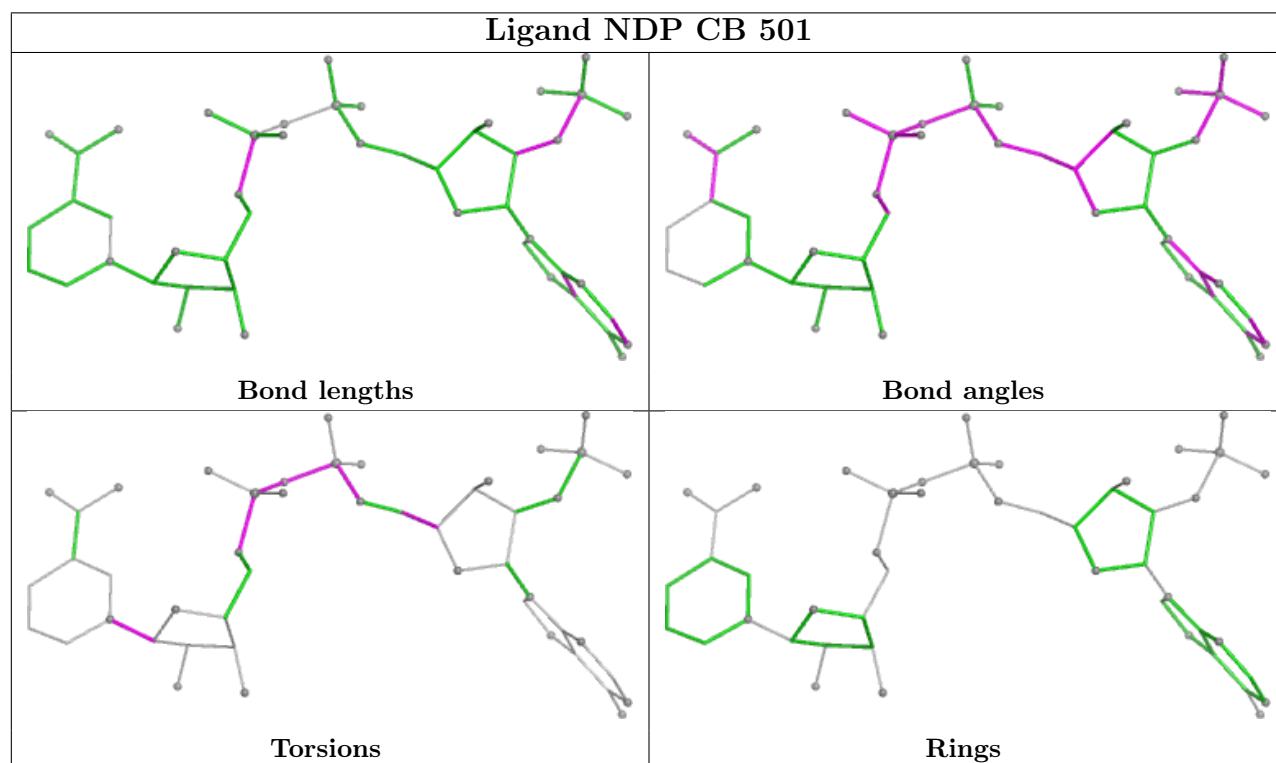
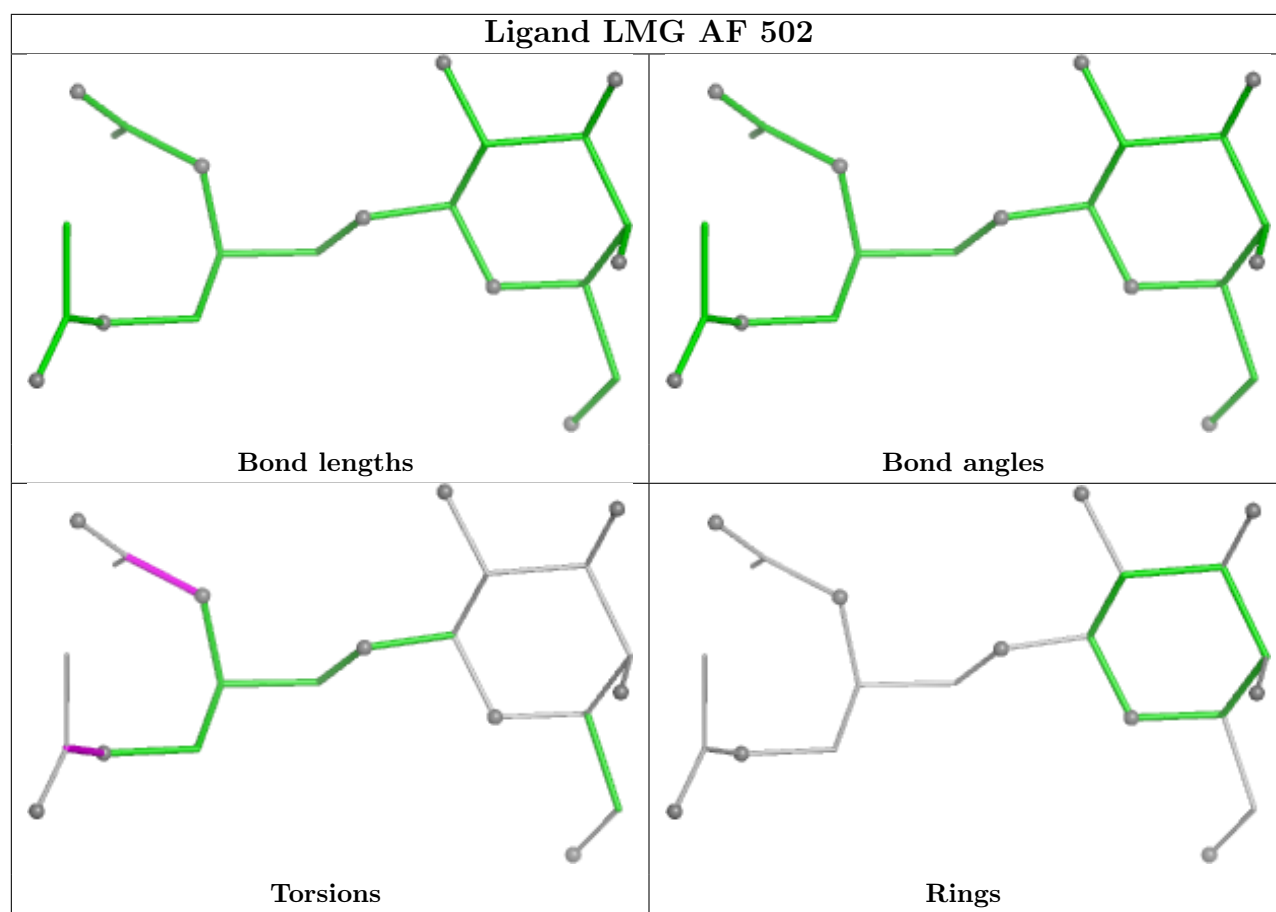
Rings

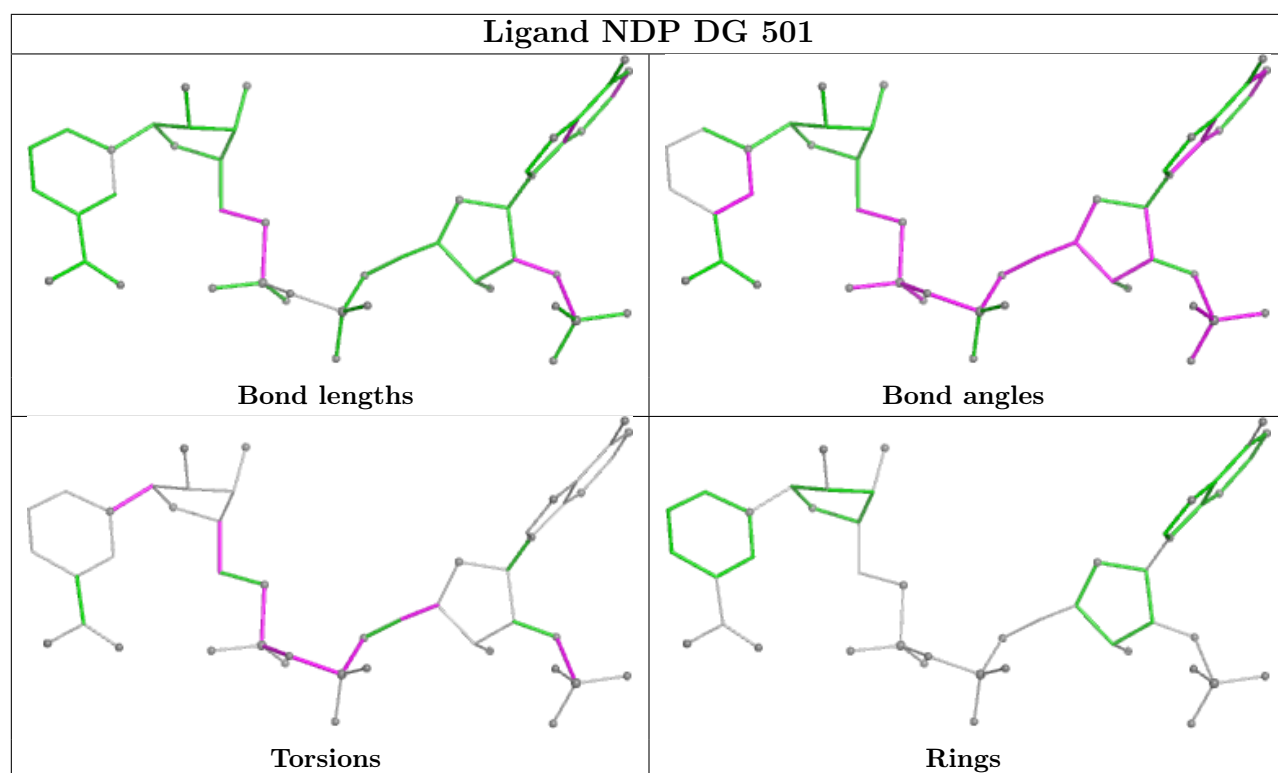
Ligand LMG CC 502



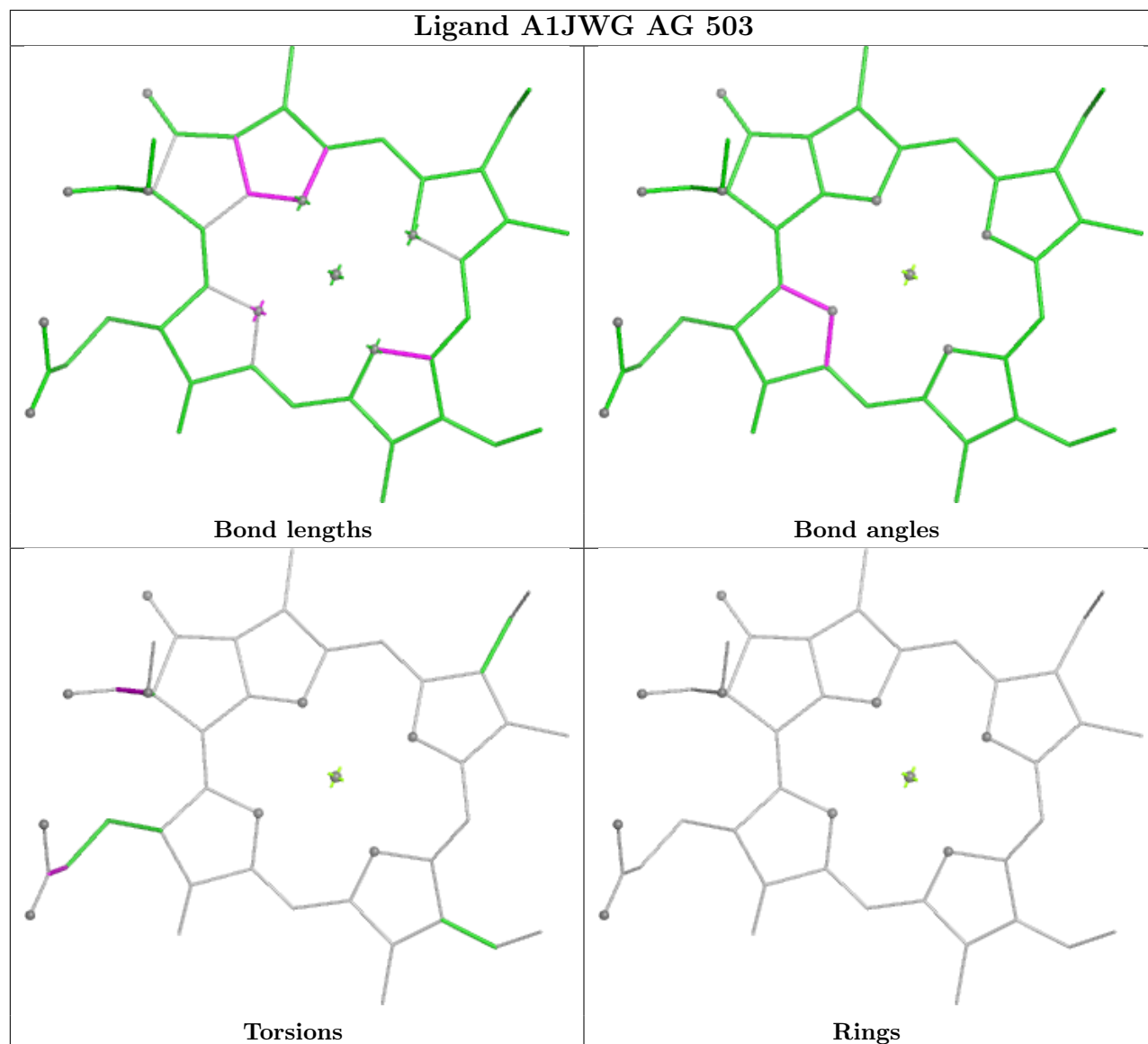
Ligand NDP BG 501

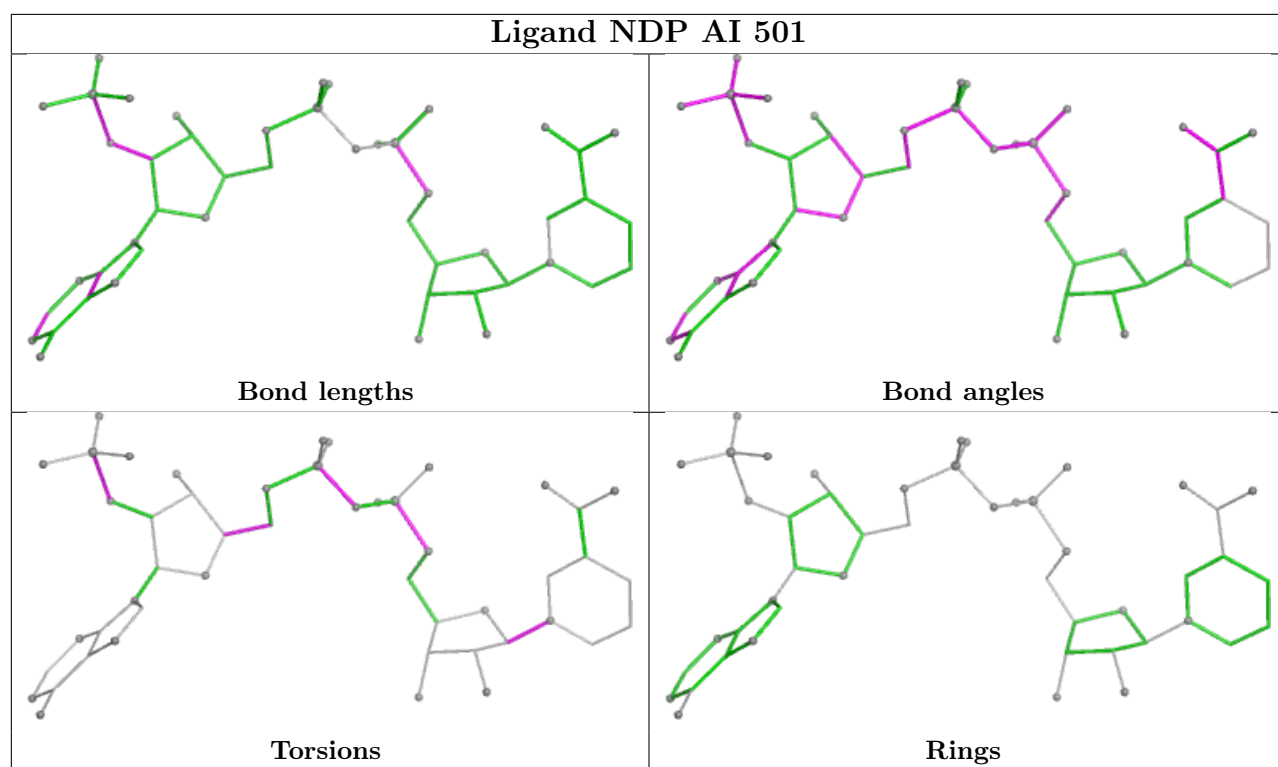


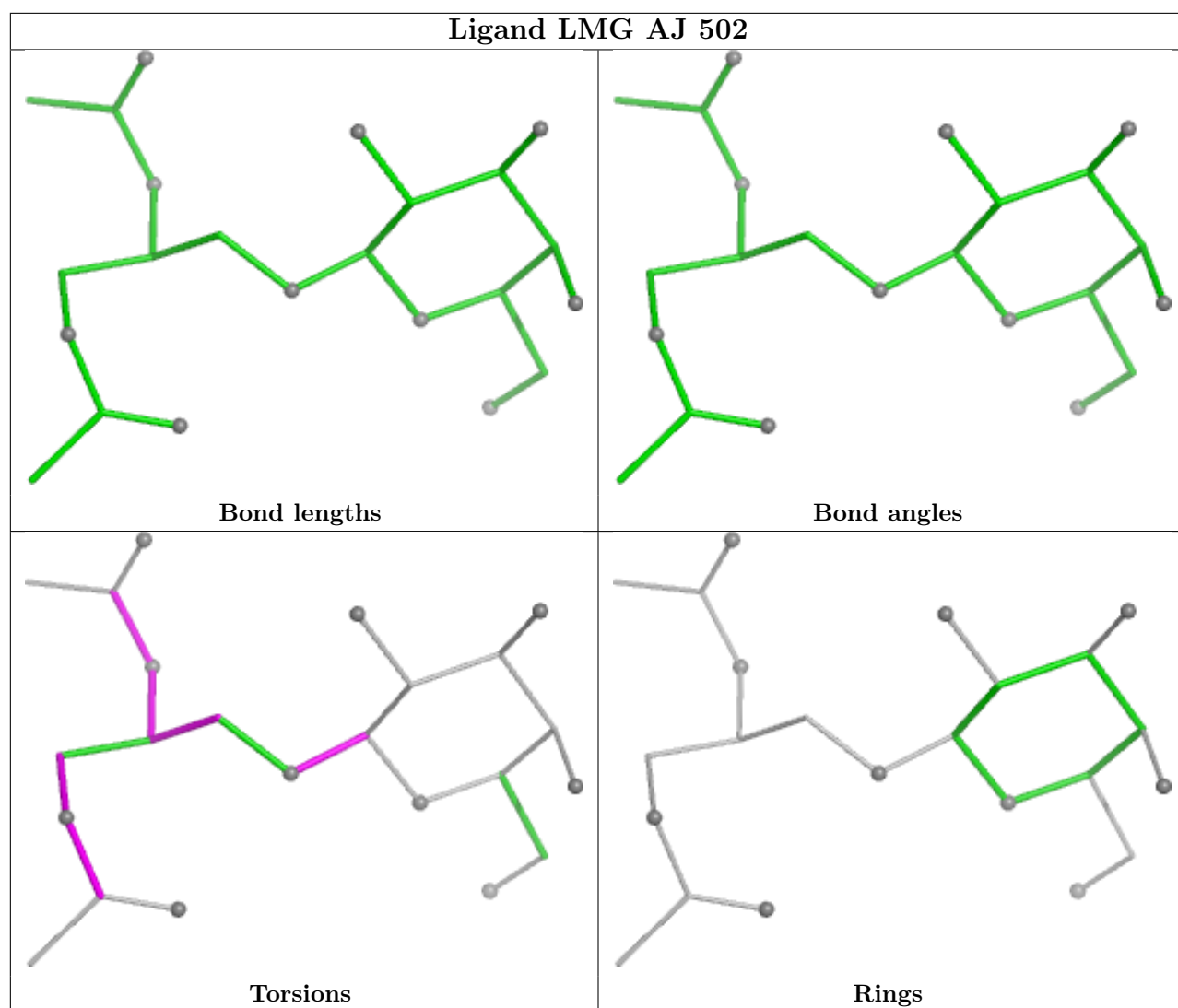




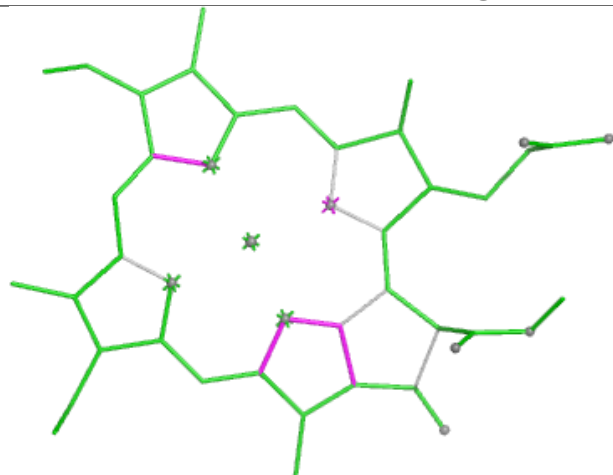
Ligand A1JWG AG 503



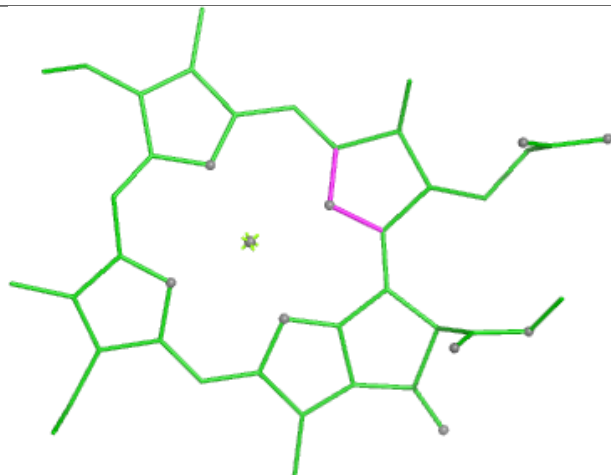




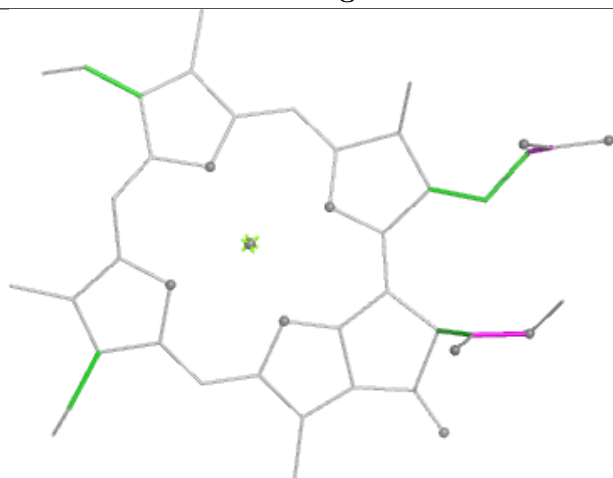
Ligand A1JWG CC 503



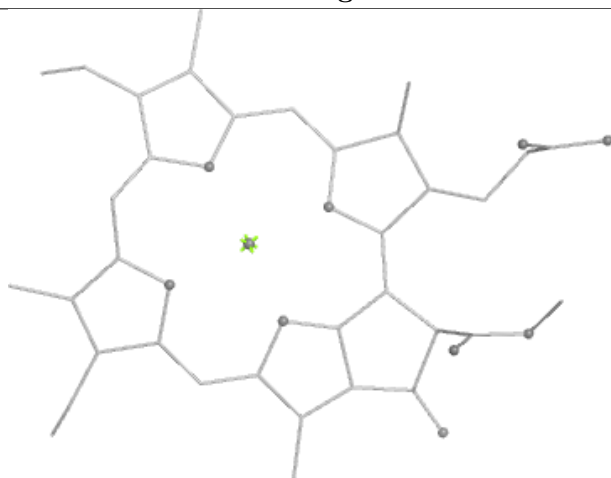
Bond lengths



Bond angles

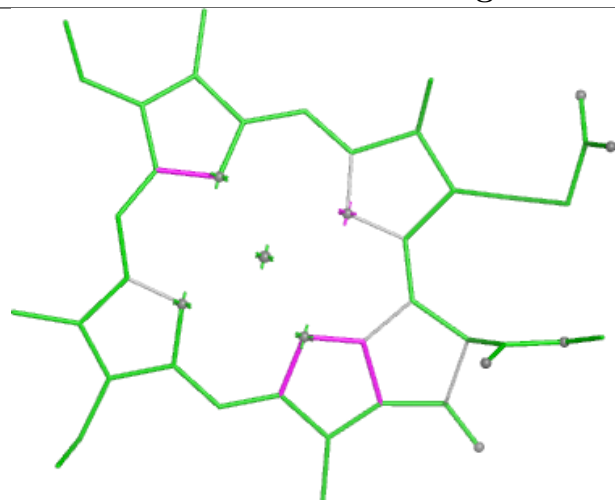


Torsions

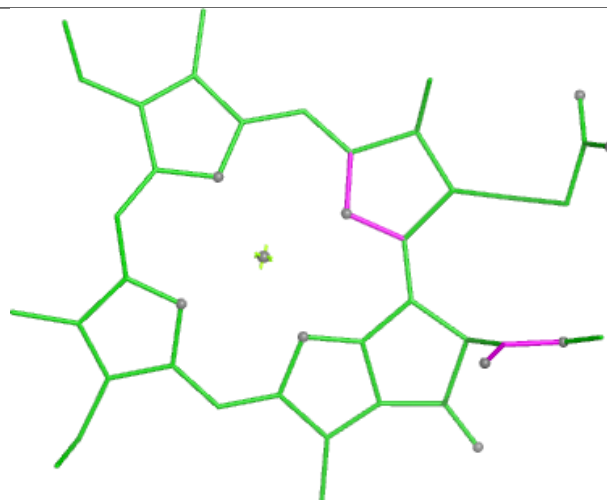


Rings

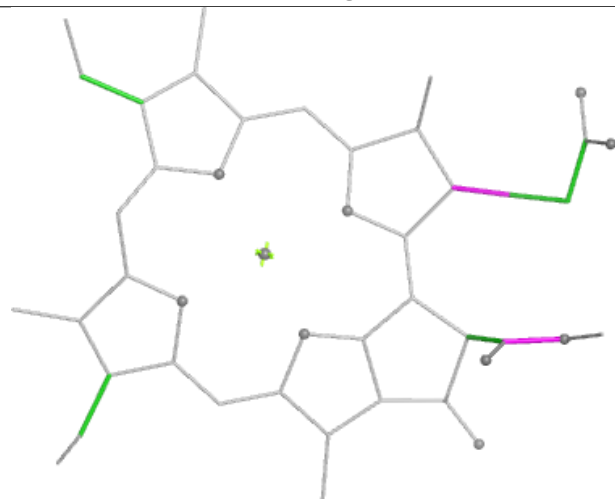
Ligand A1JWG CD 503



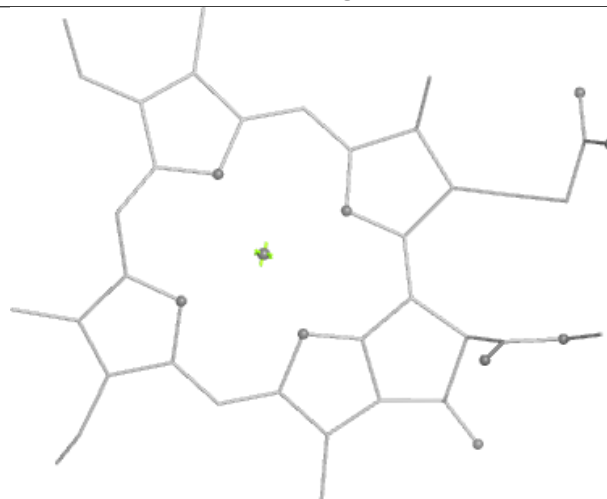
Bond lengths



Bond angles

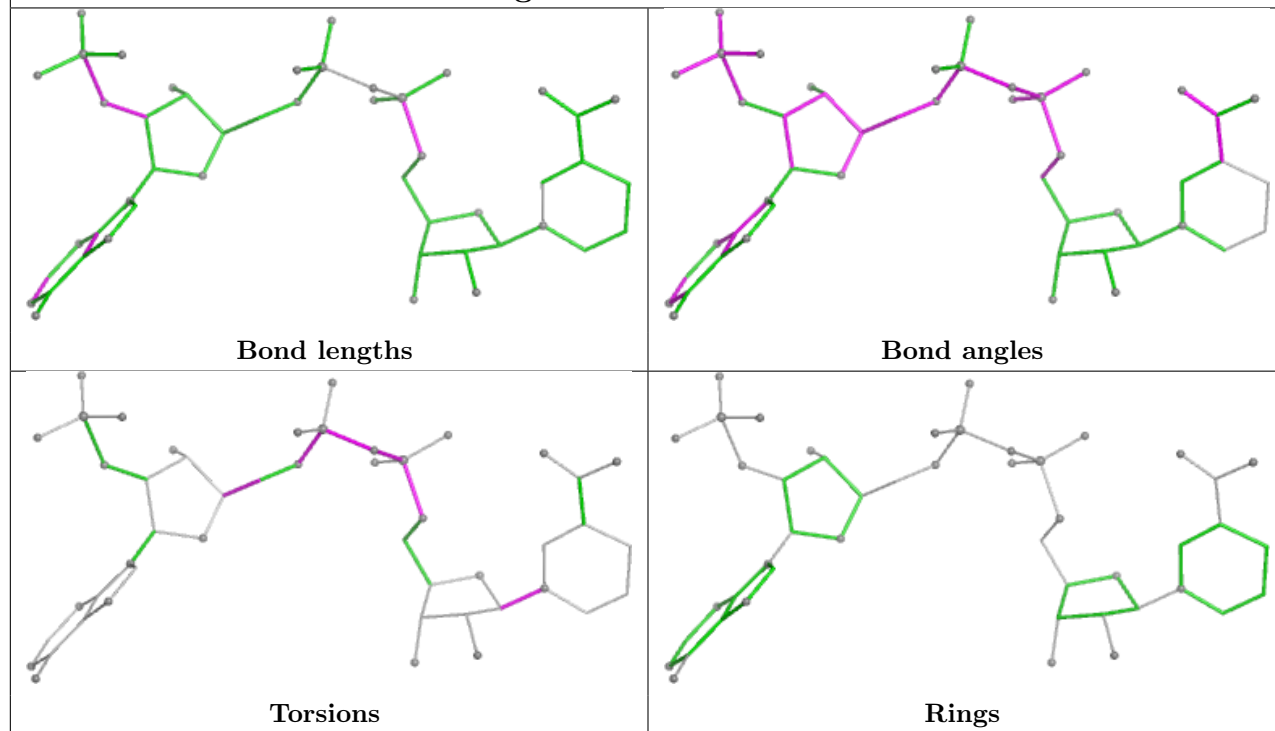


Torsions

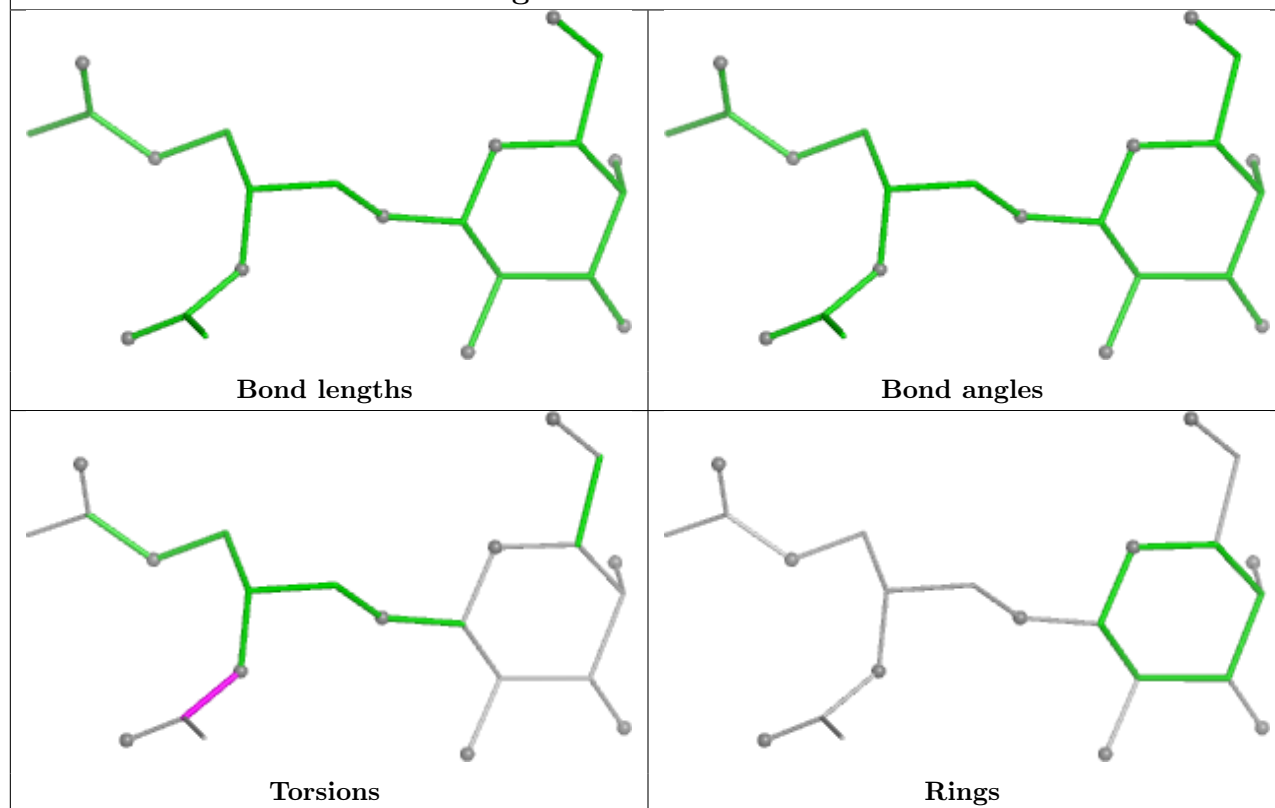


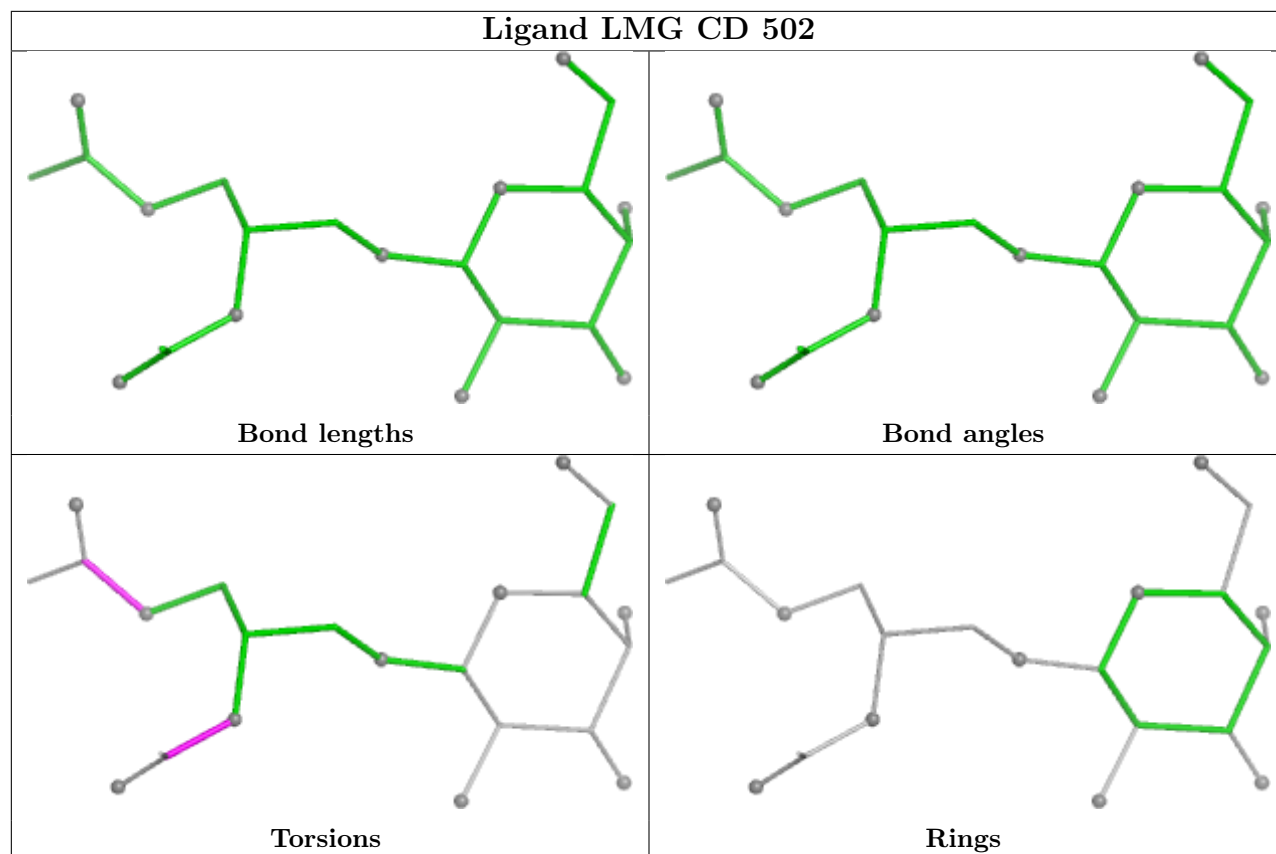
Rings

Ligand NDP CD 501

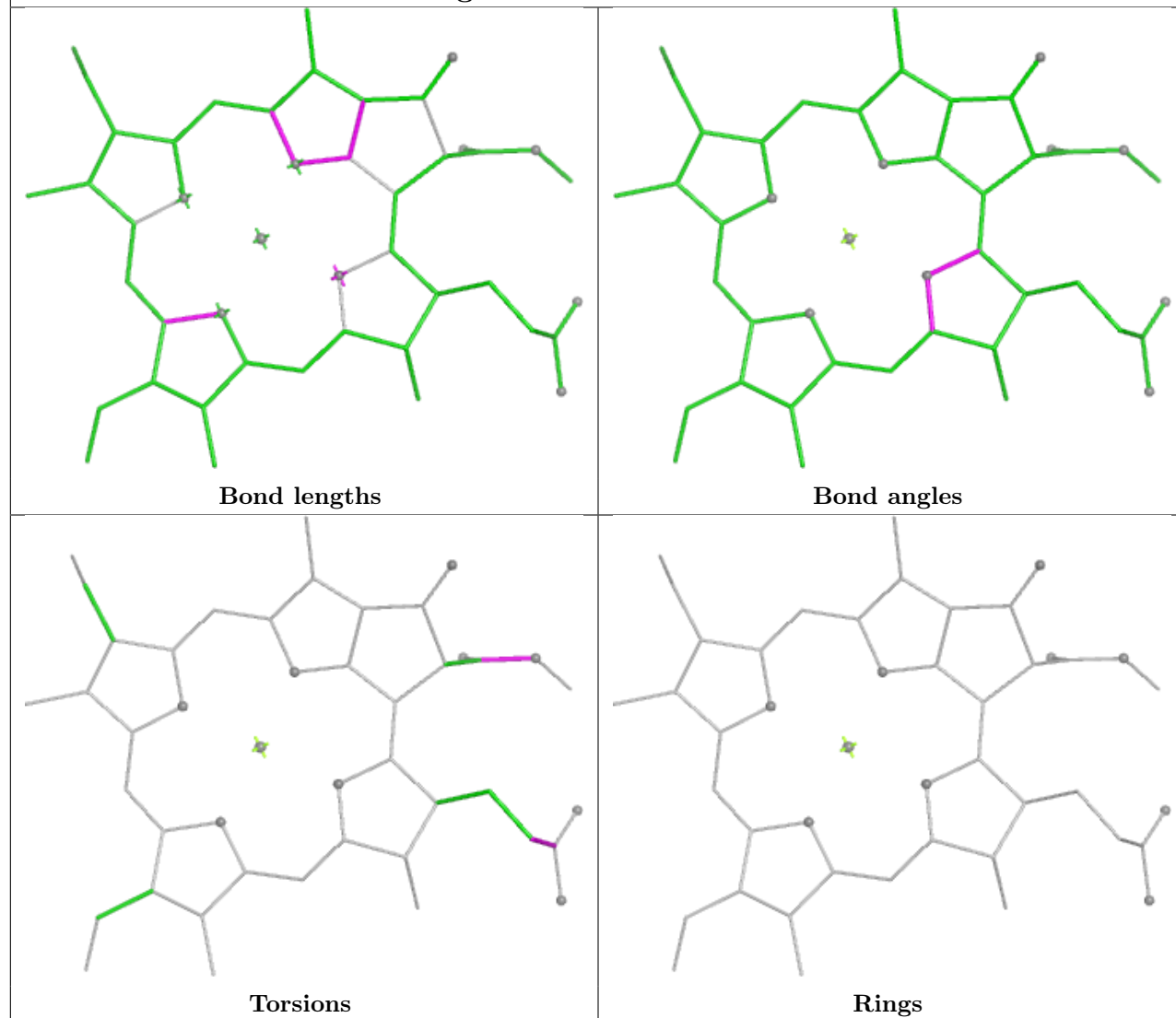


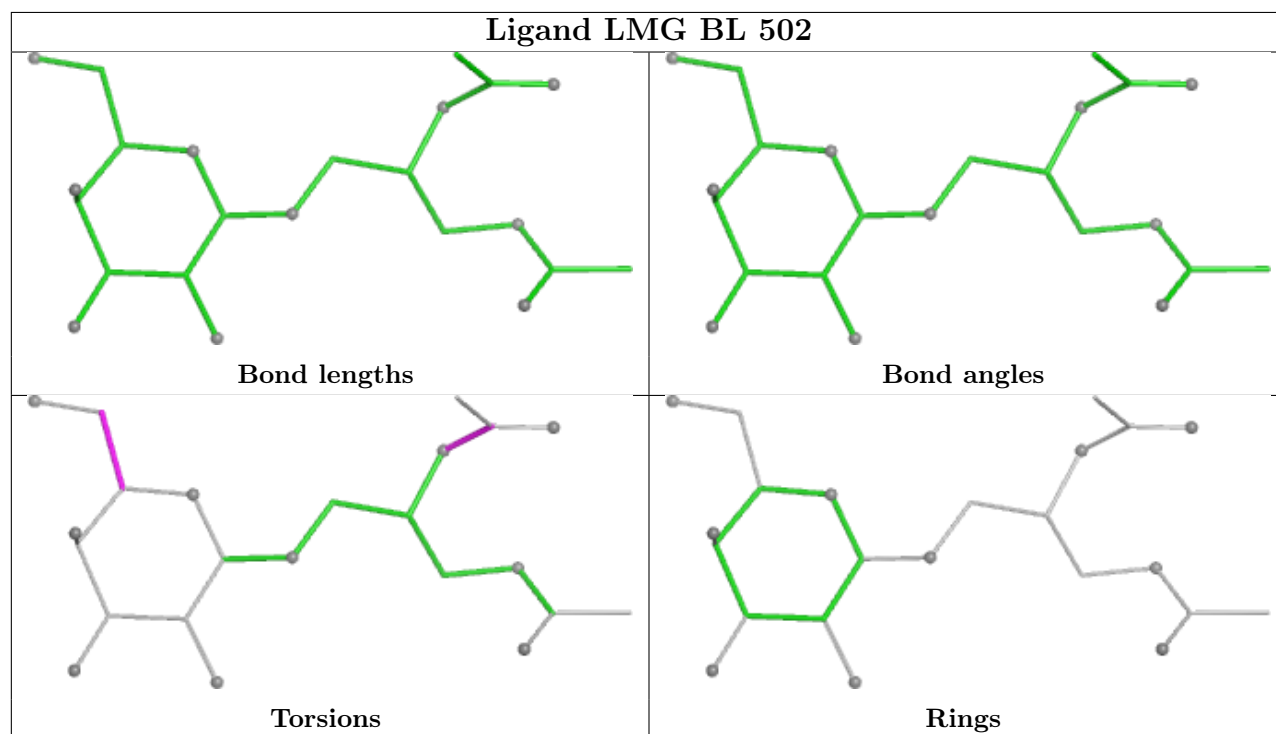
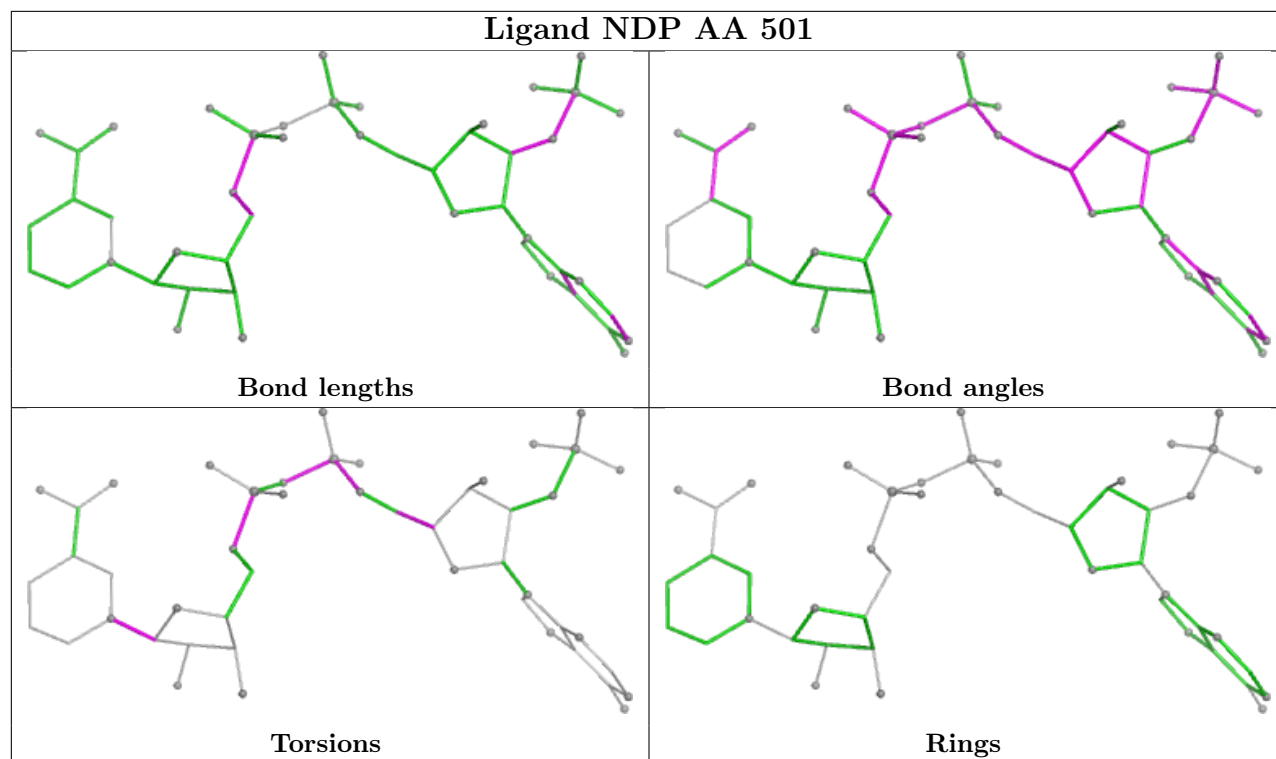
Ligand LMG AH 502



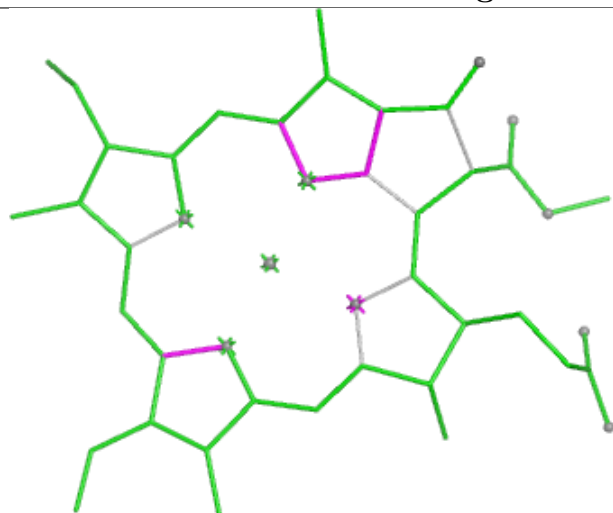


Ligand A1JWG AJ 503

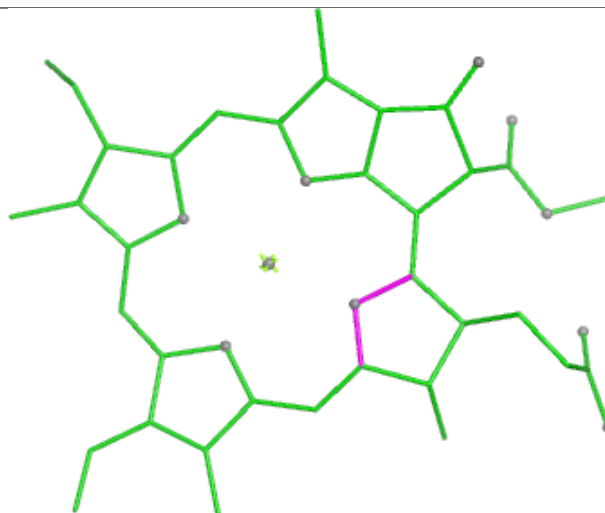




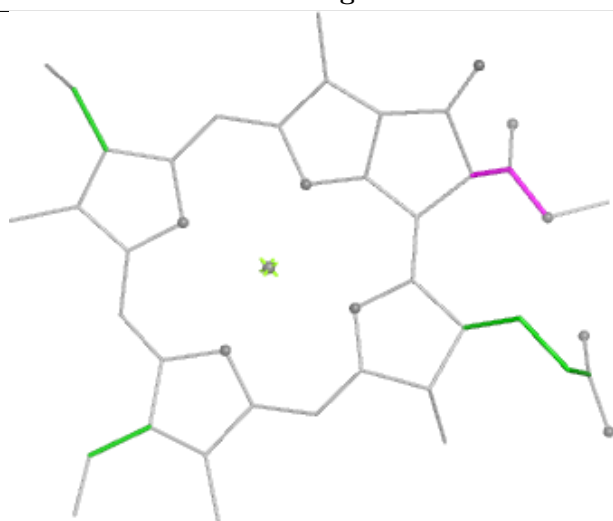
Ligand A1JWG AL 503



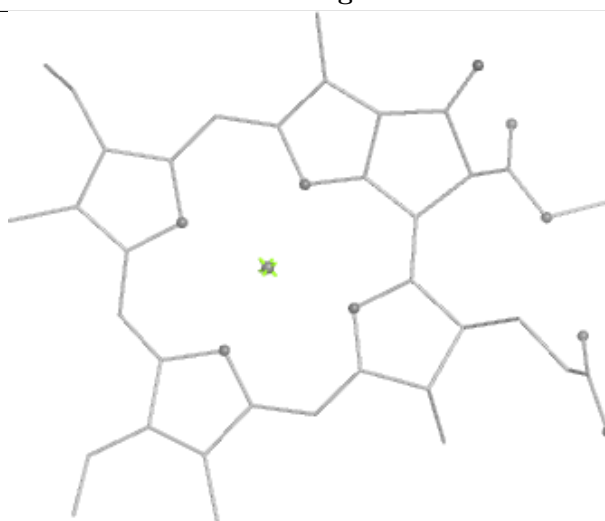
Bond lengths



Bond angles

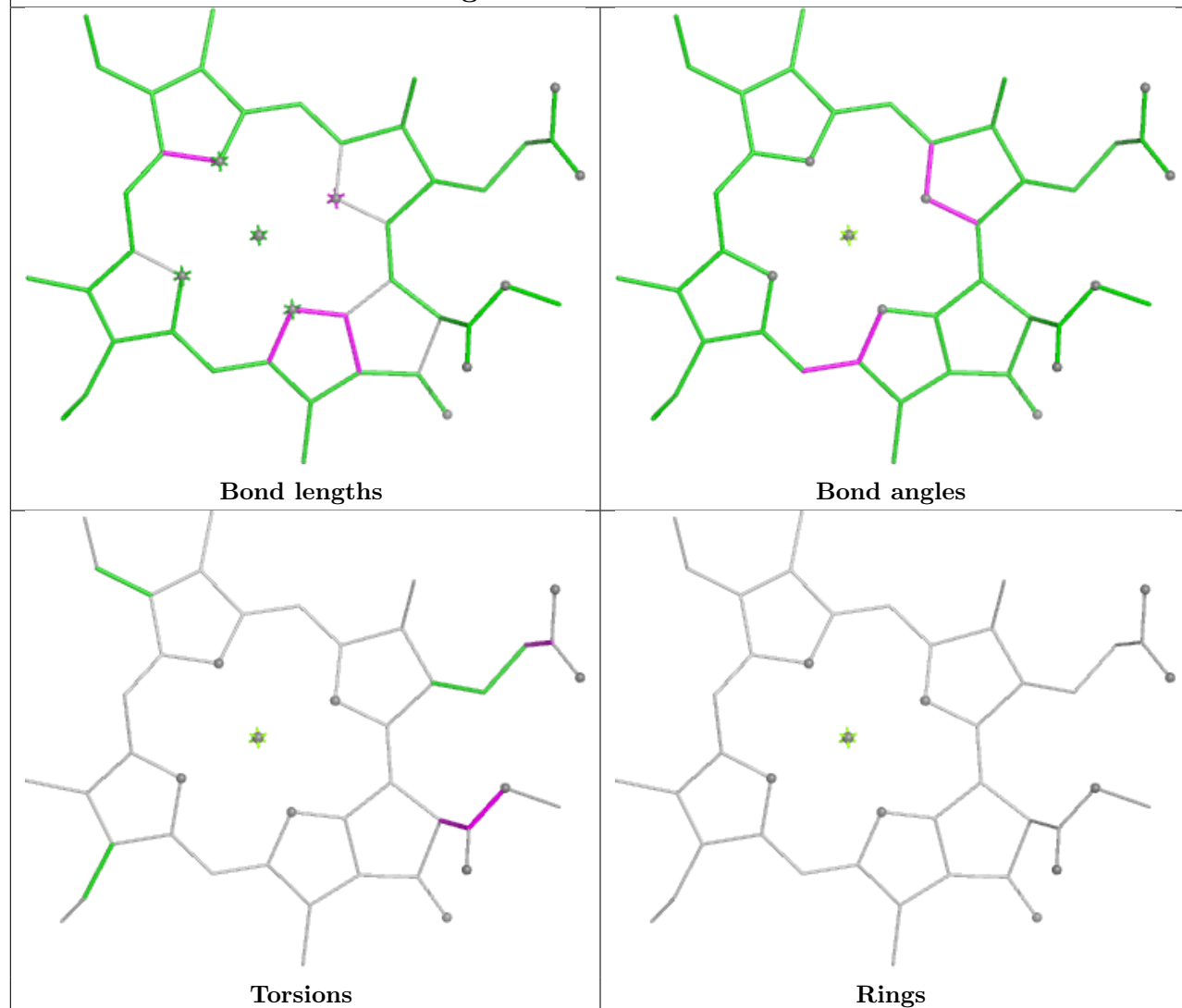


Torsions

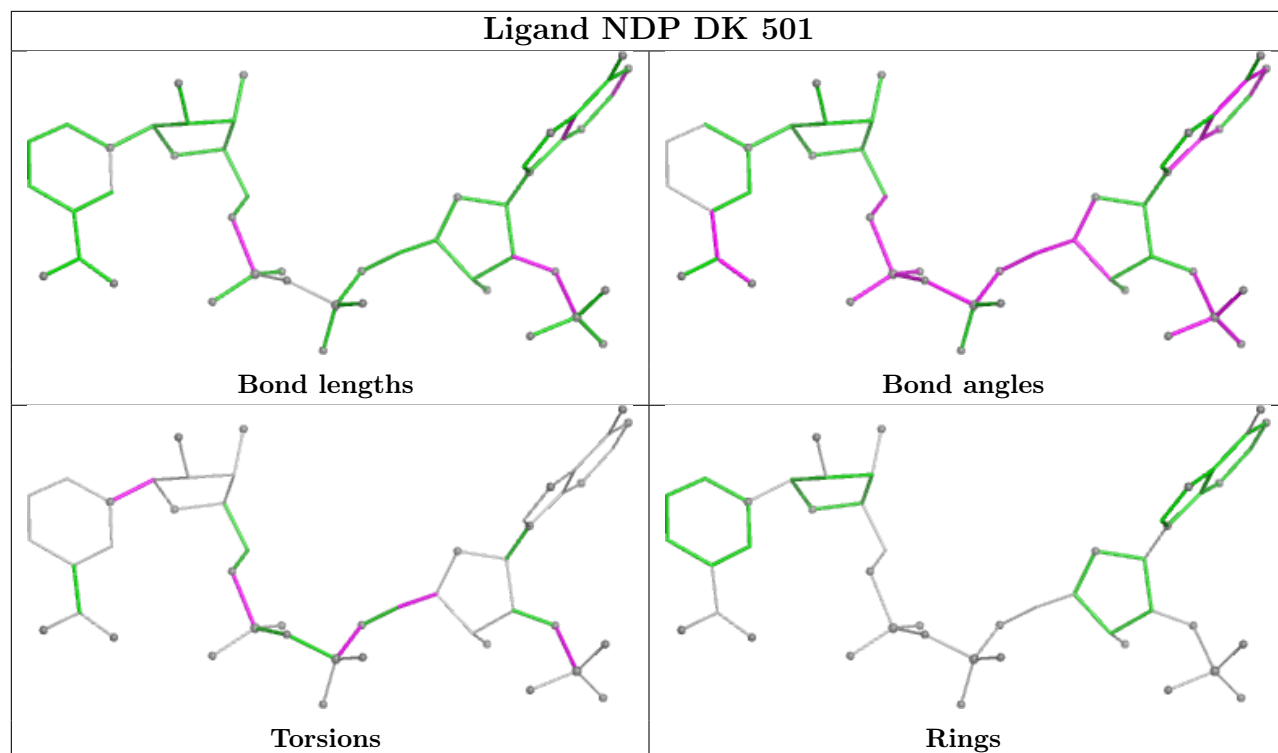


Rings

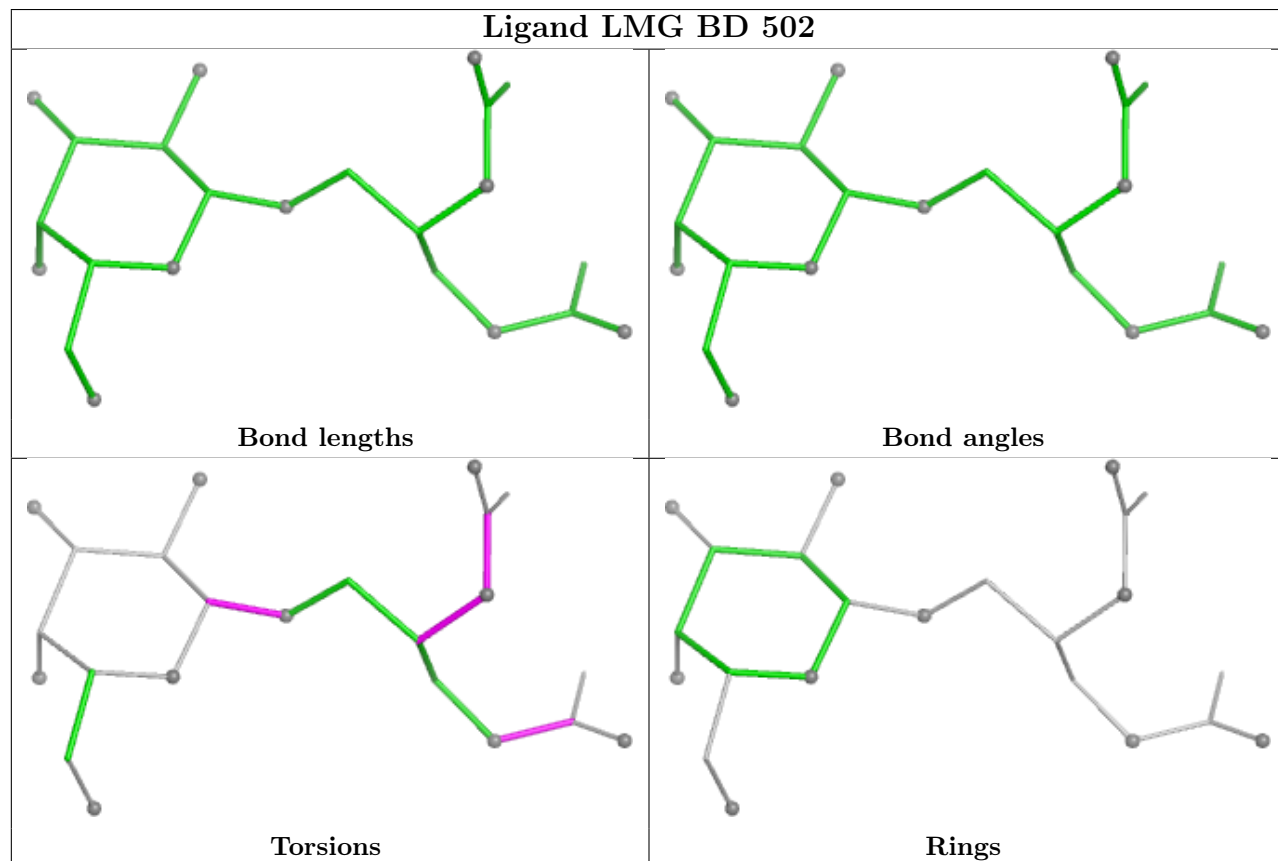
Ligand A1JWG CI 503

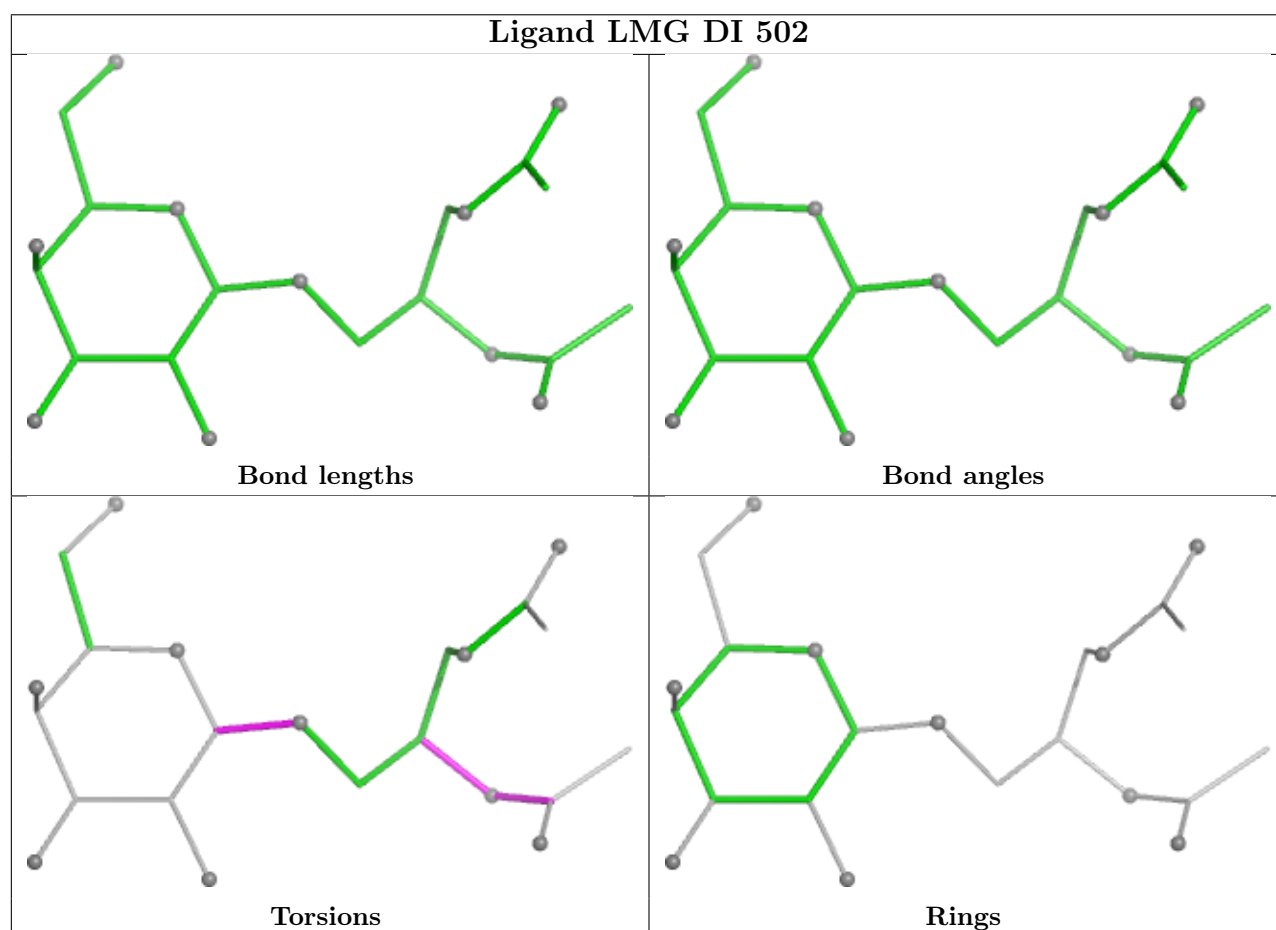
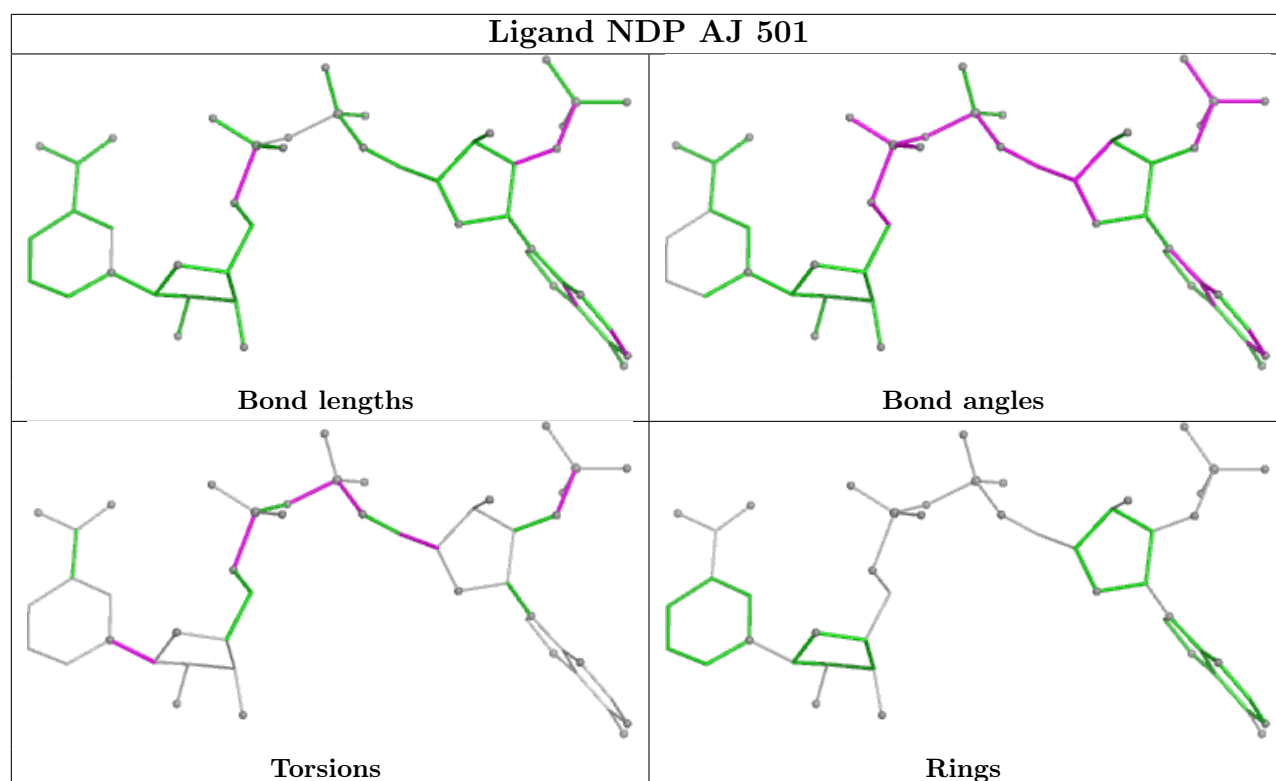


Ligand NDP DK 501

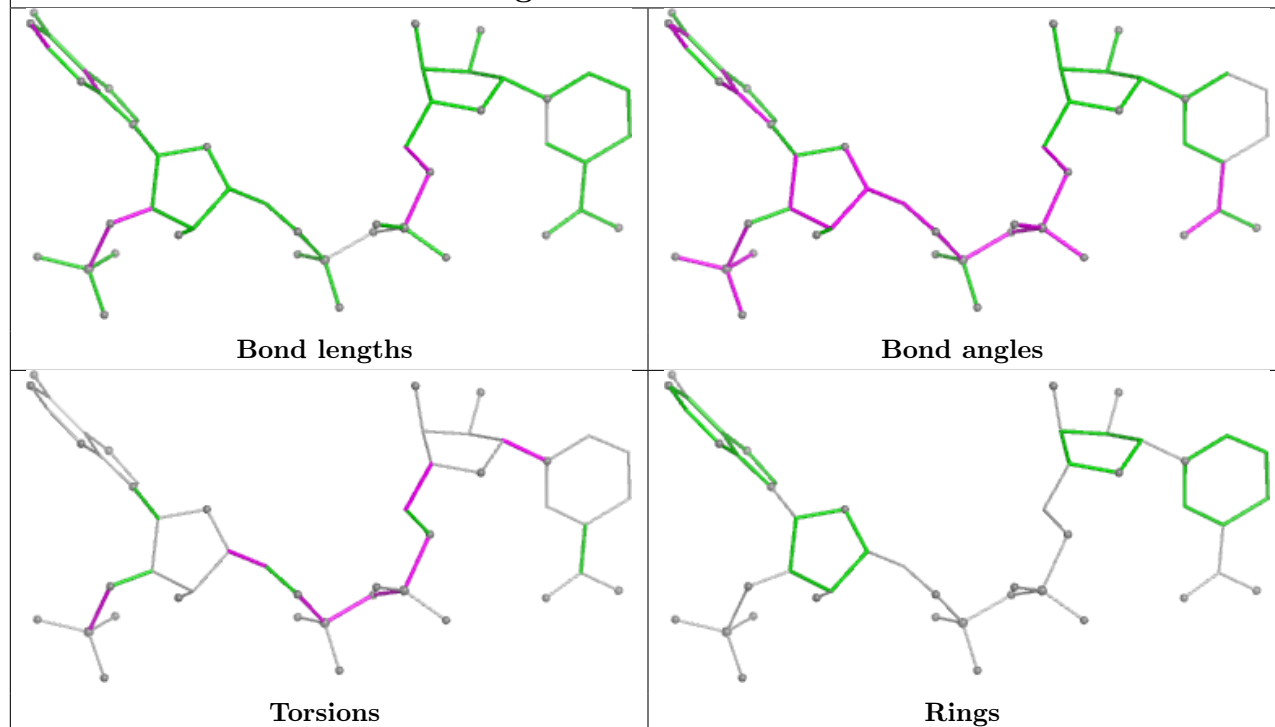


Ligand LMG BD 502

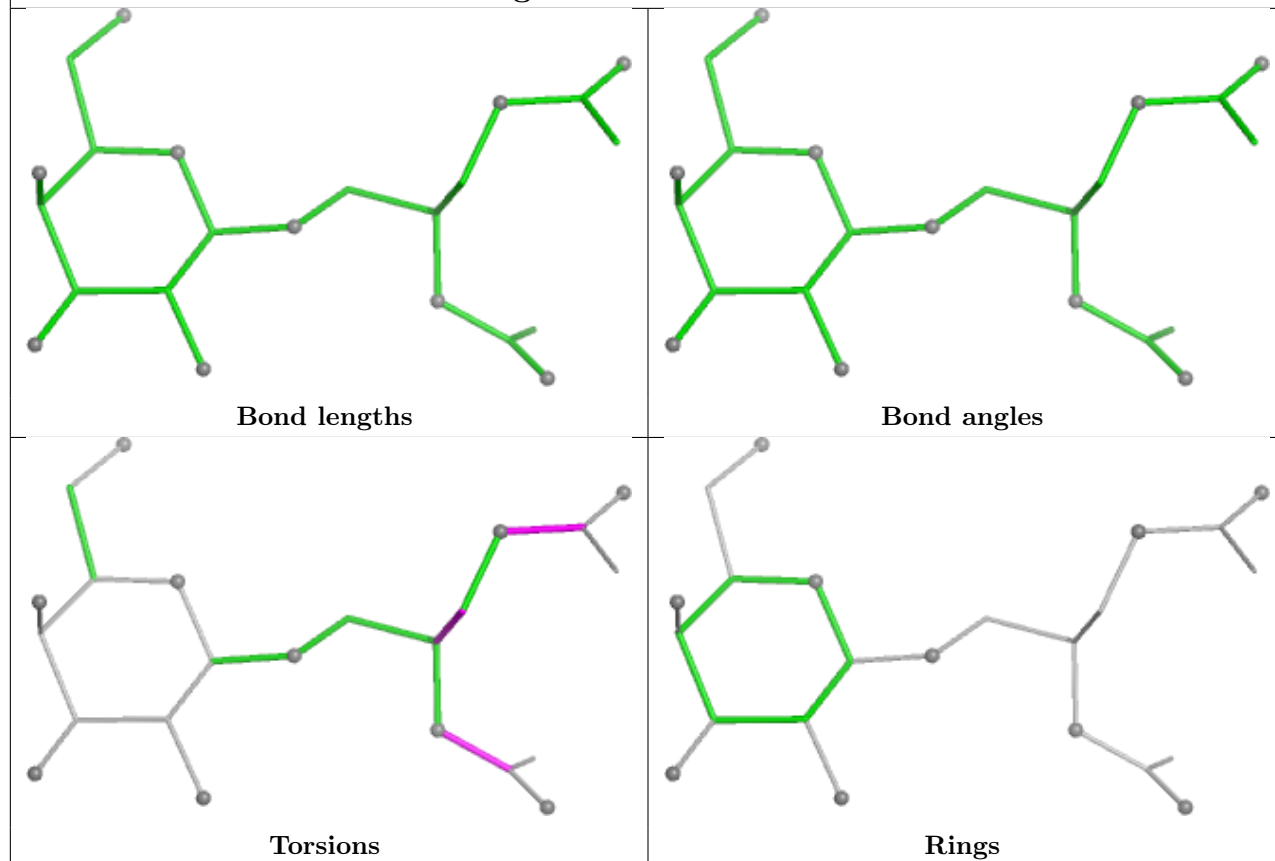




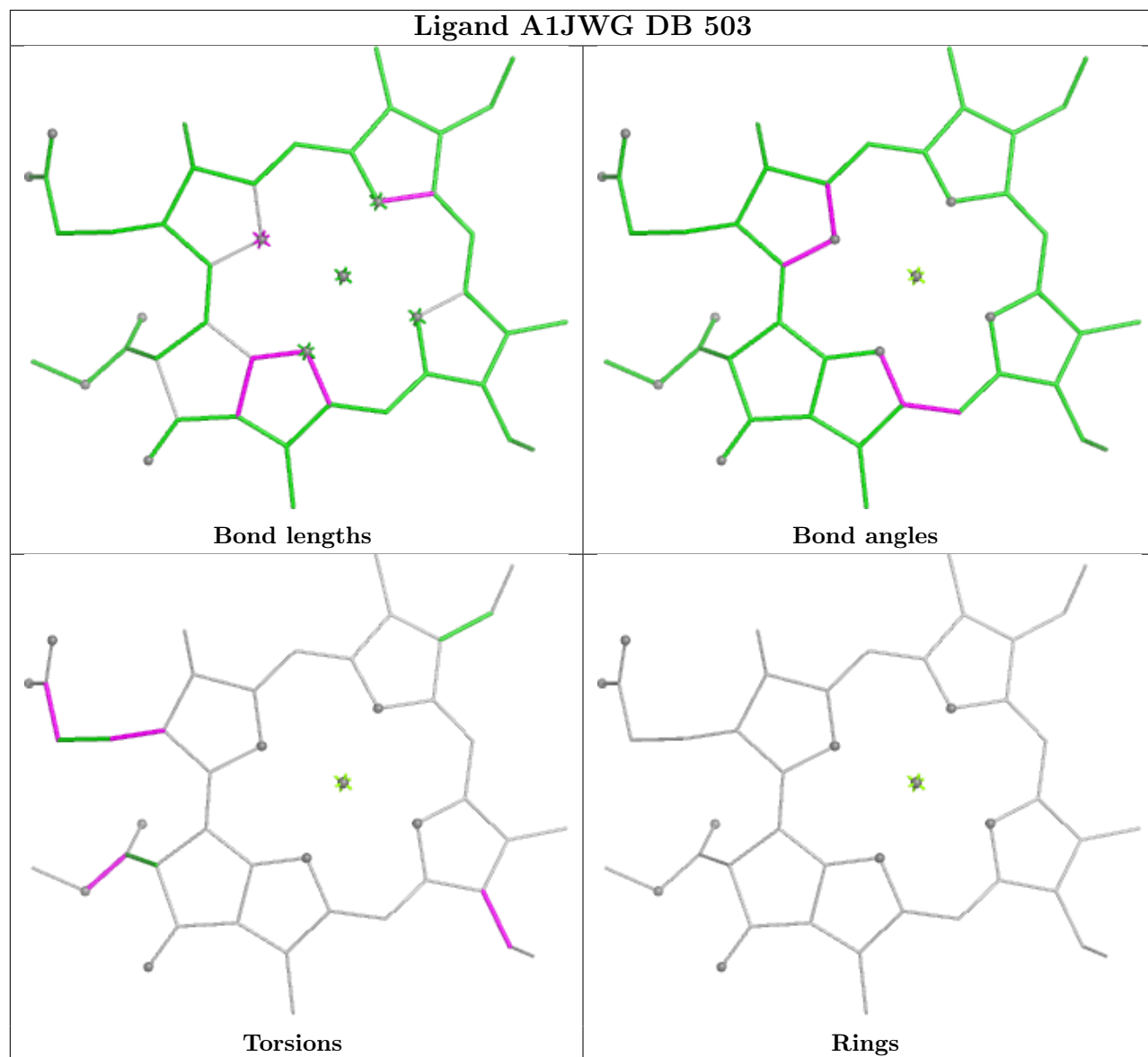
Ligand NDP CA 501



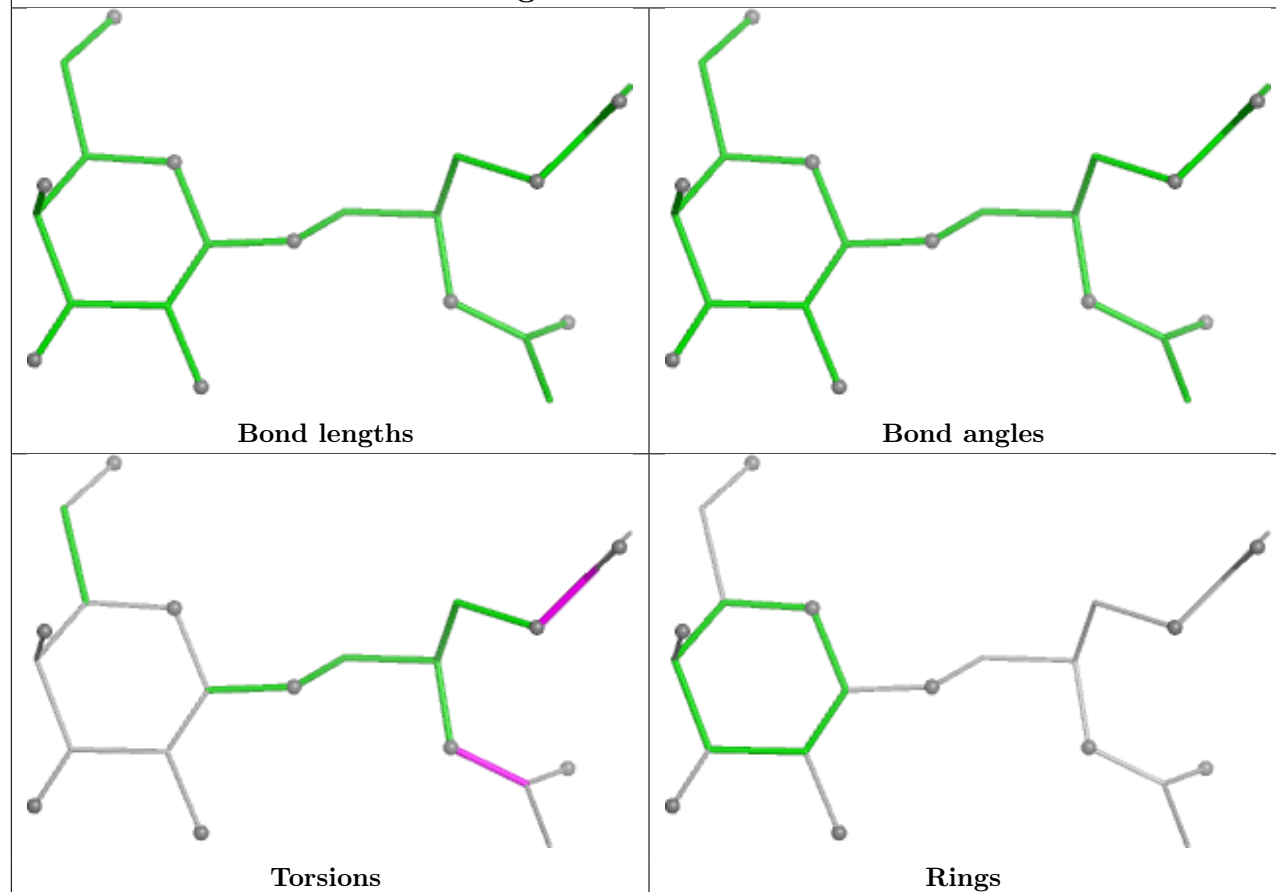
Ligand LMG BA 502



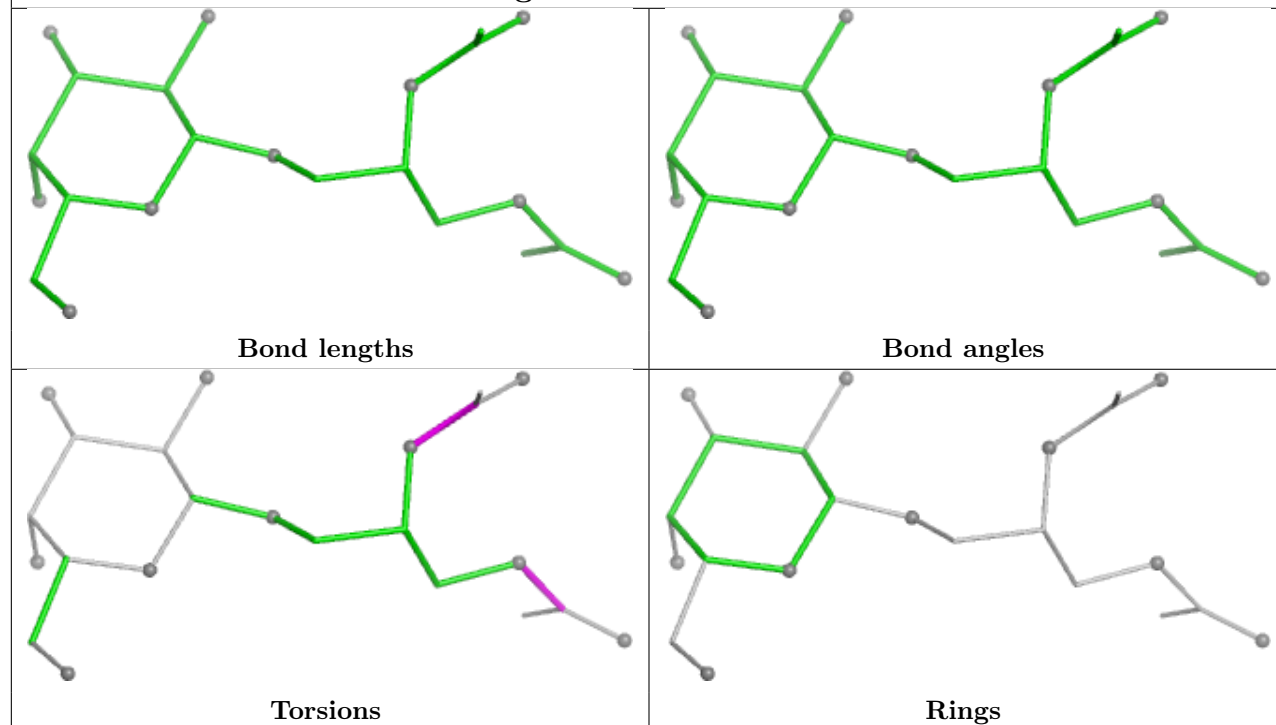
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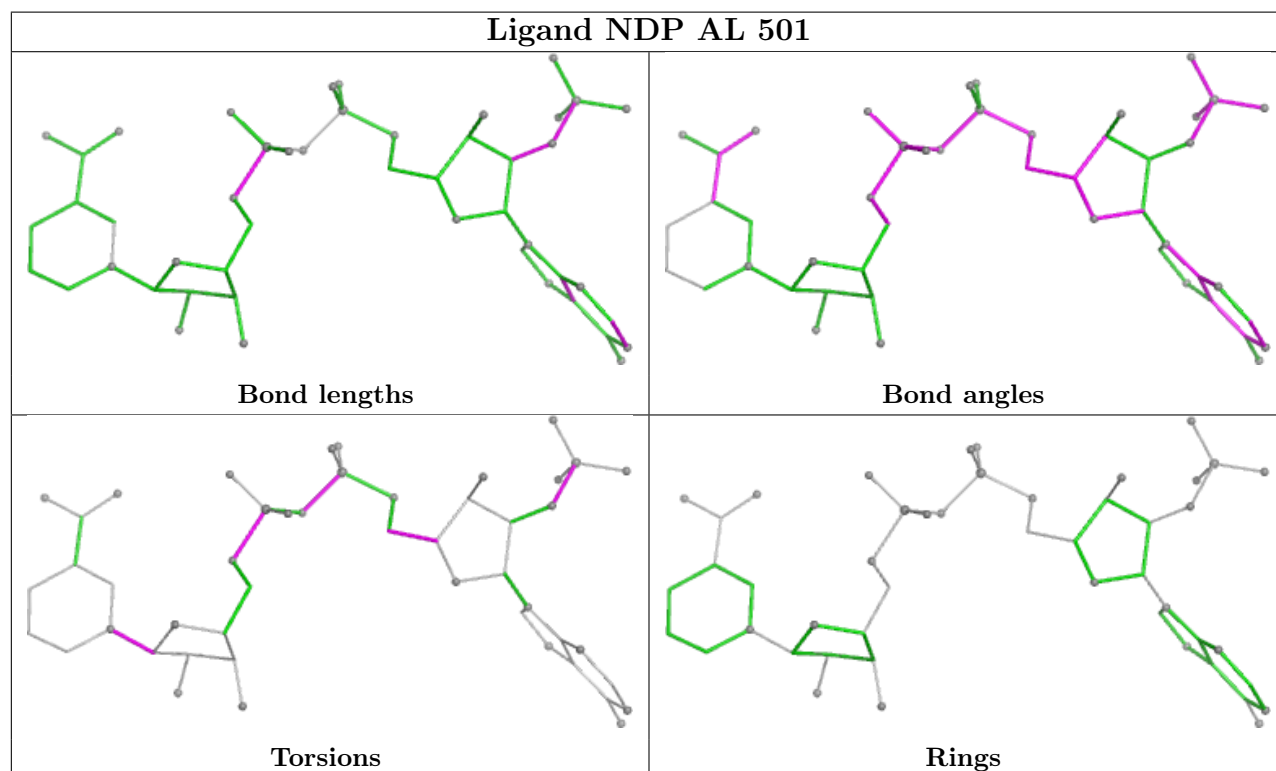
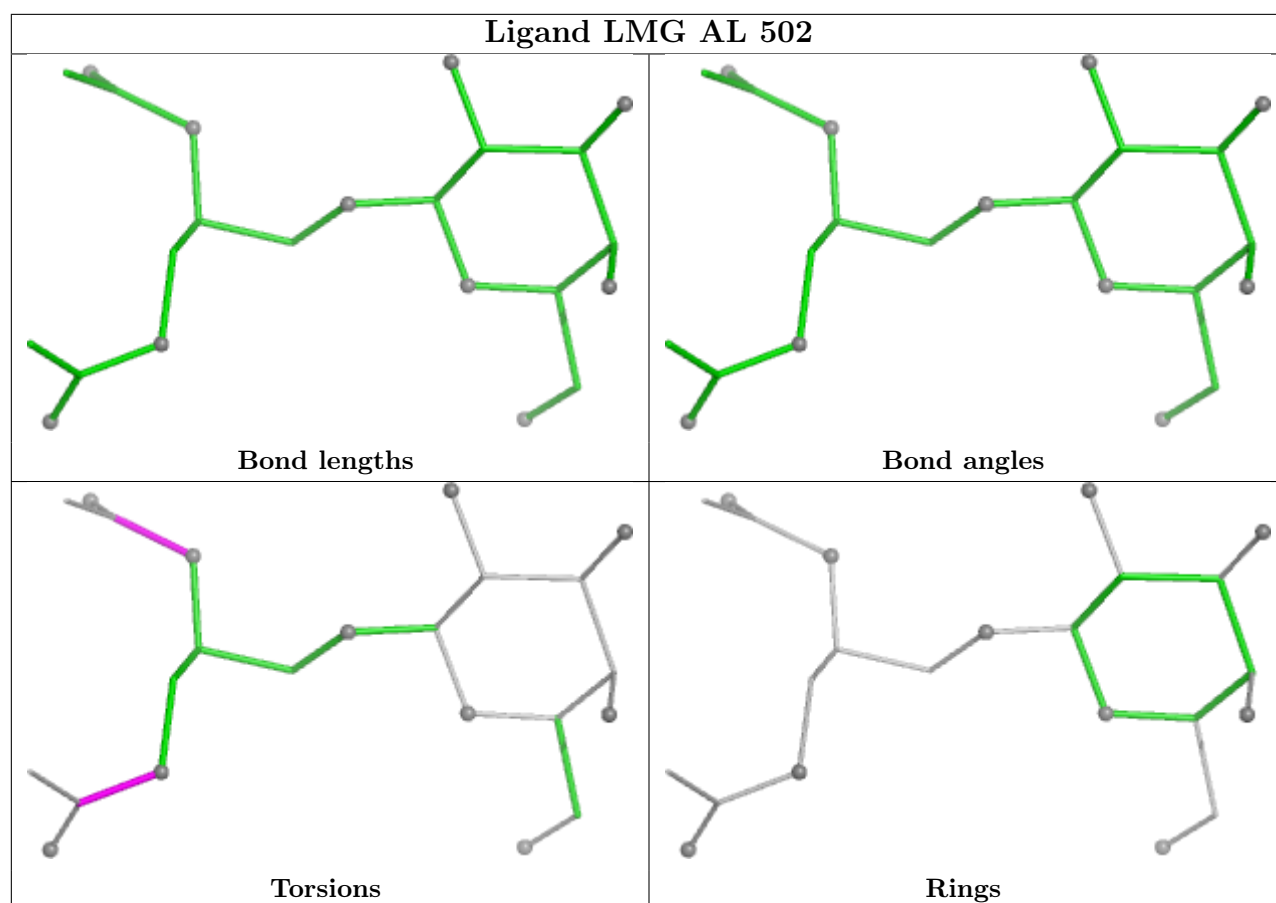


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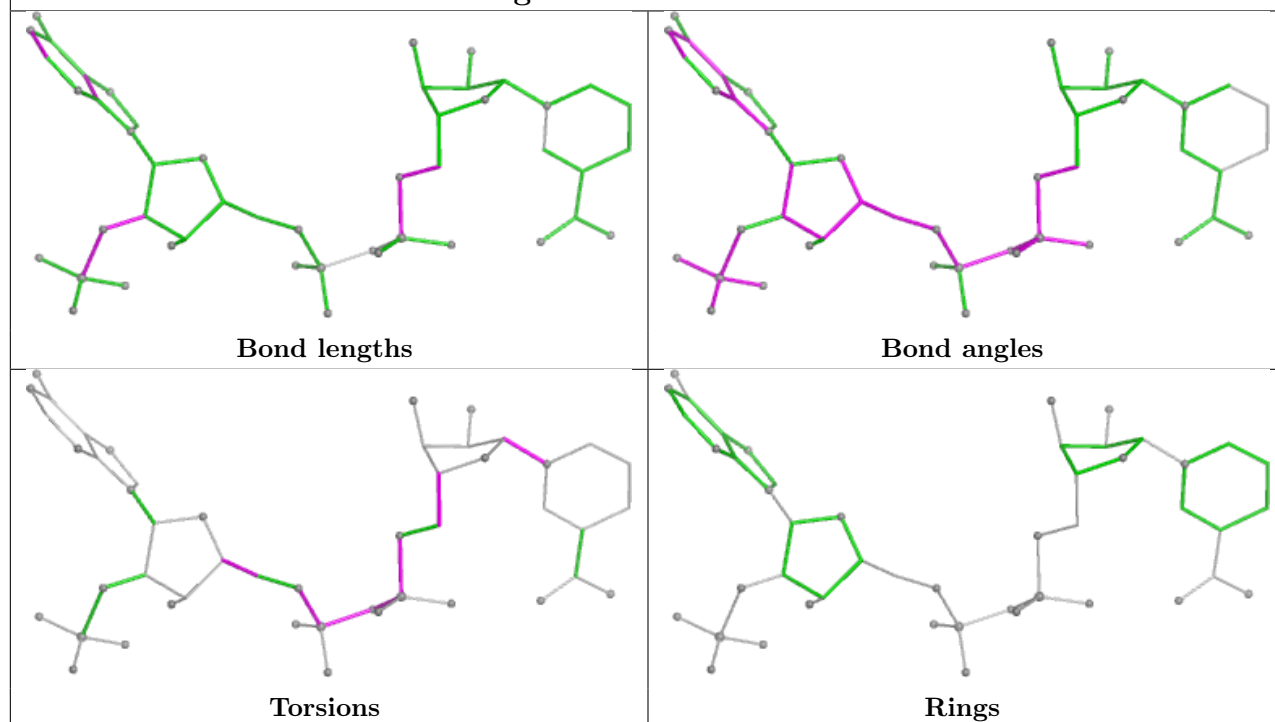


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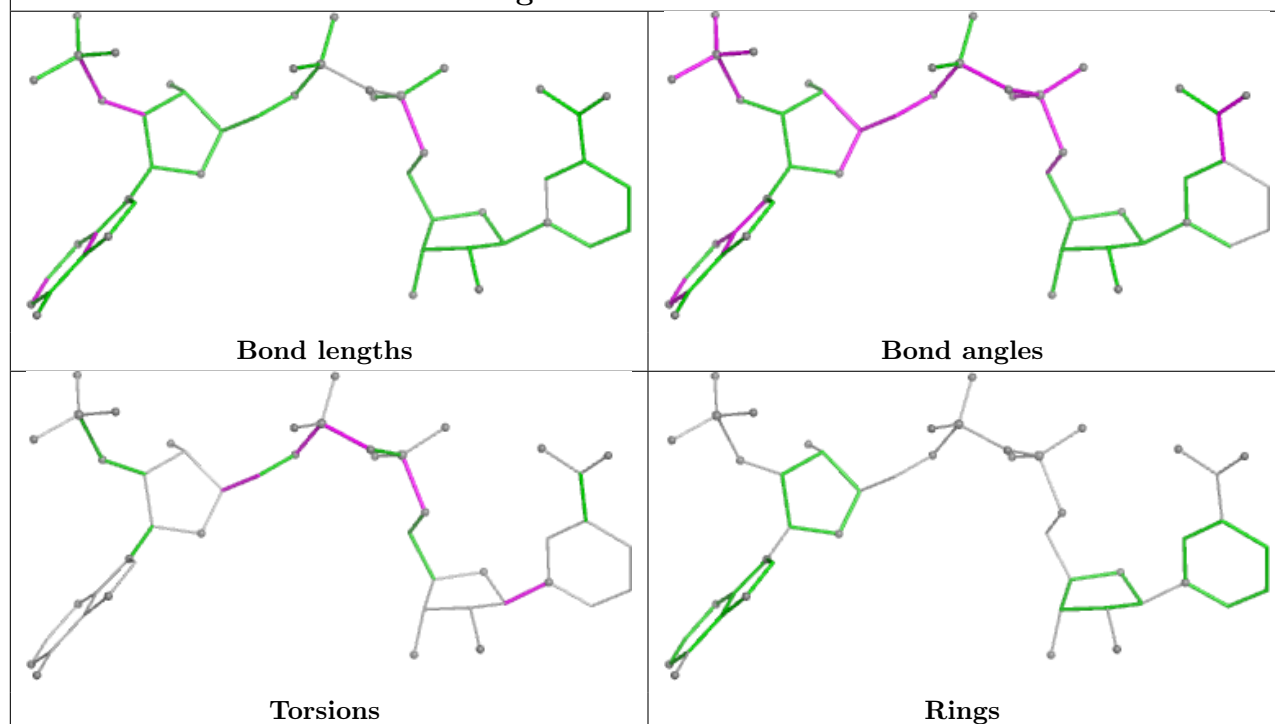




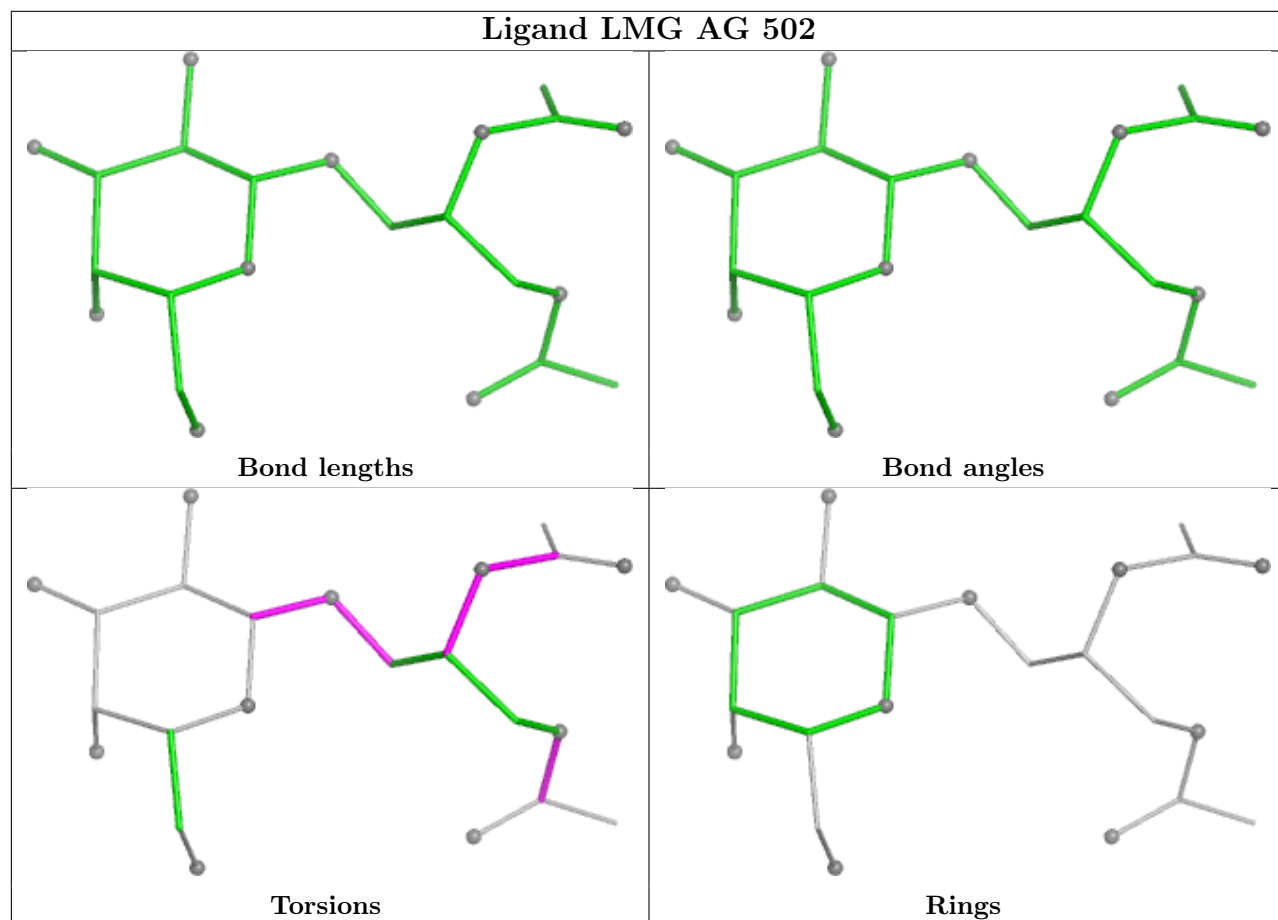
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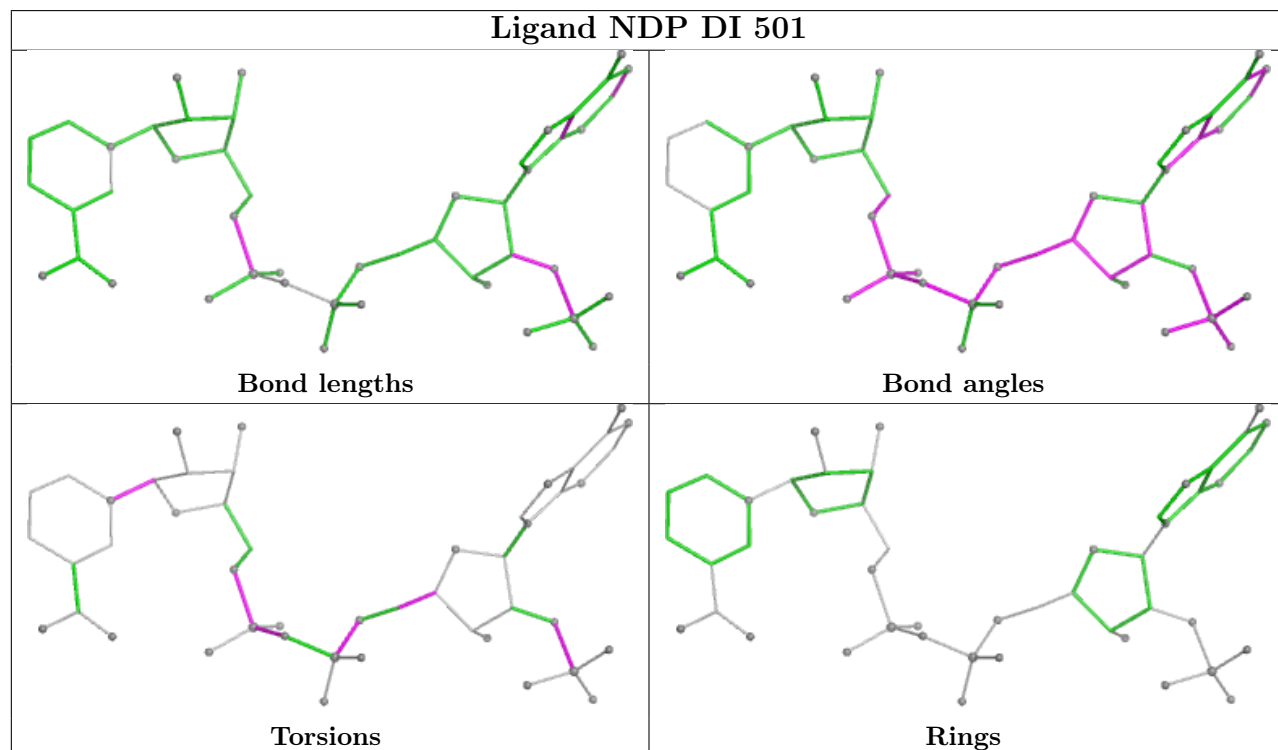
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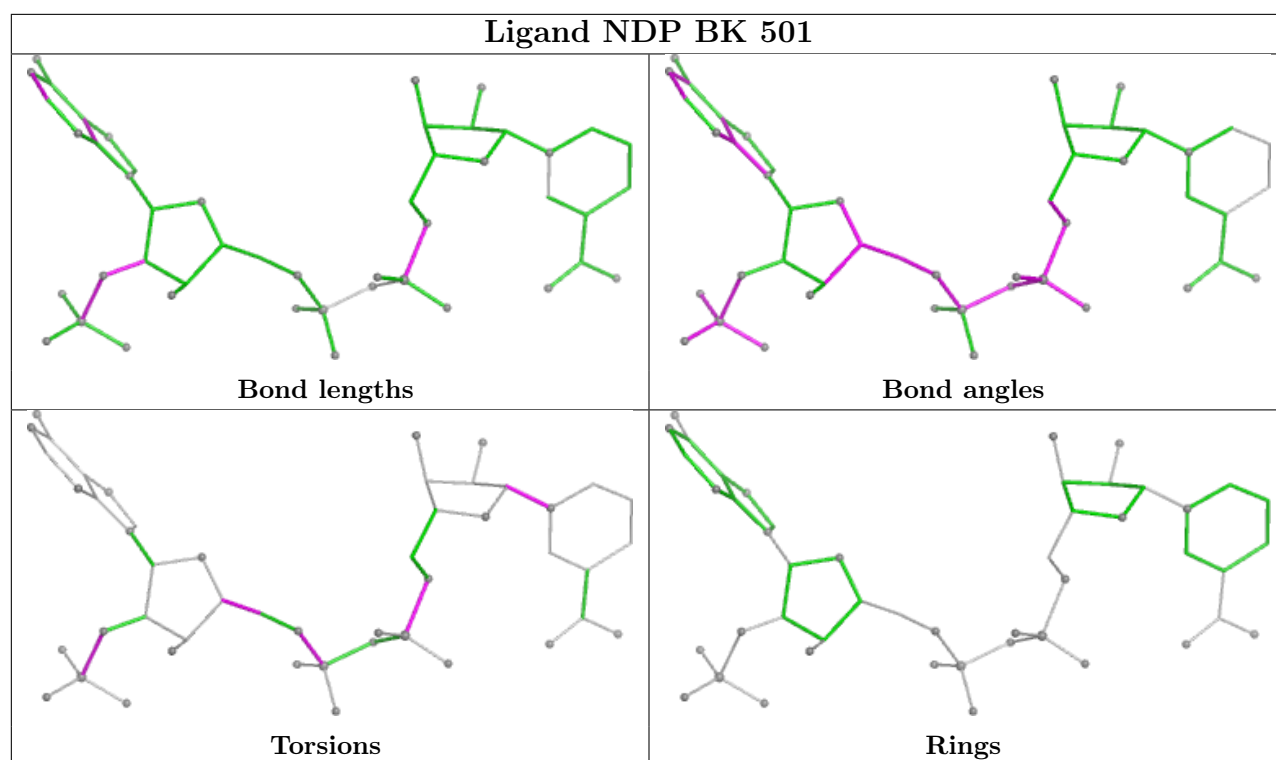


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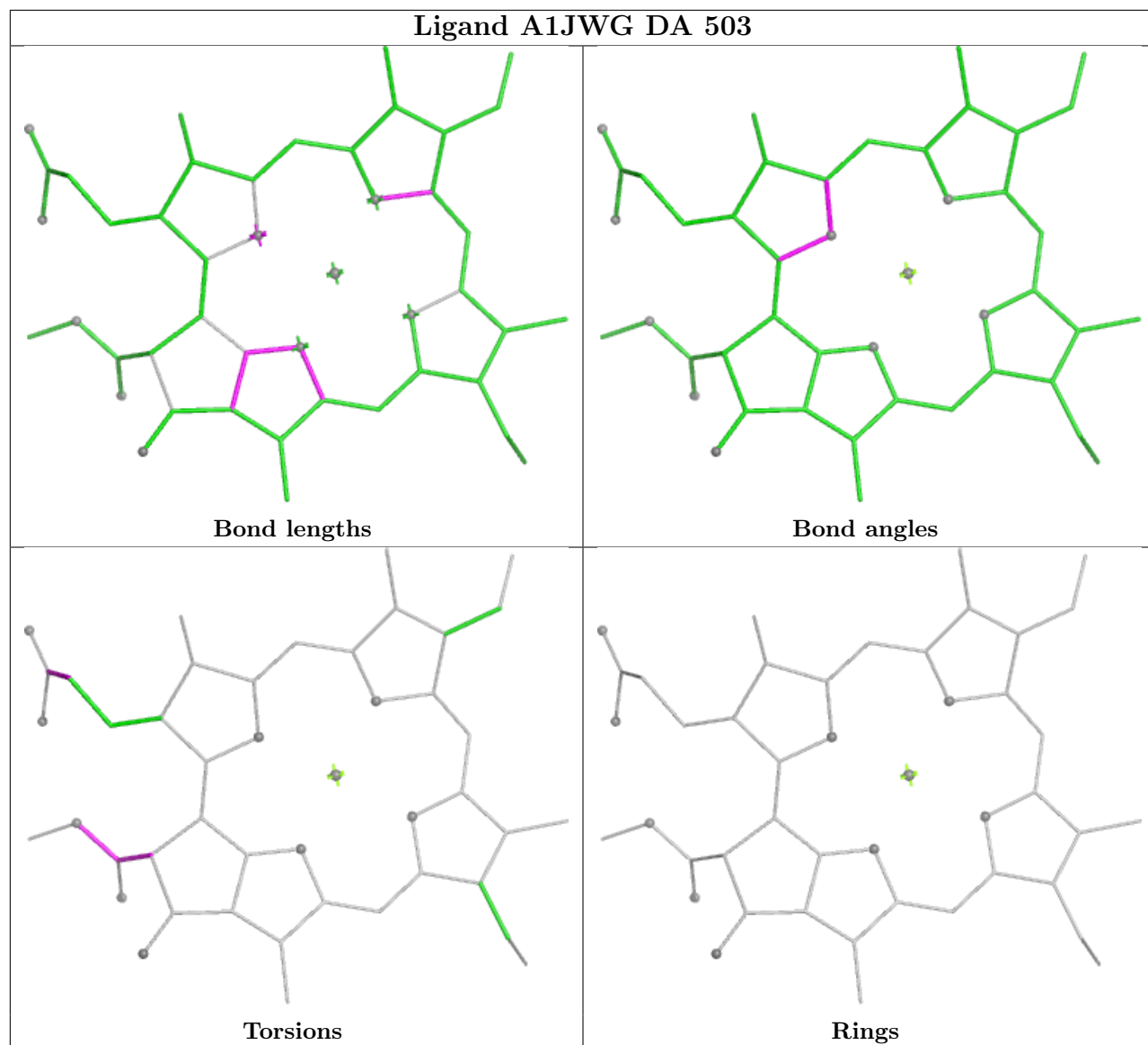


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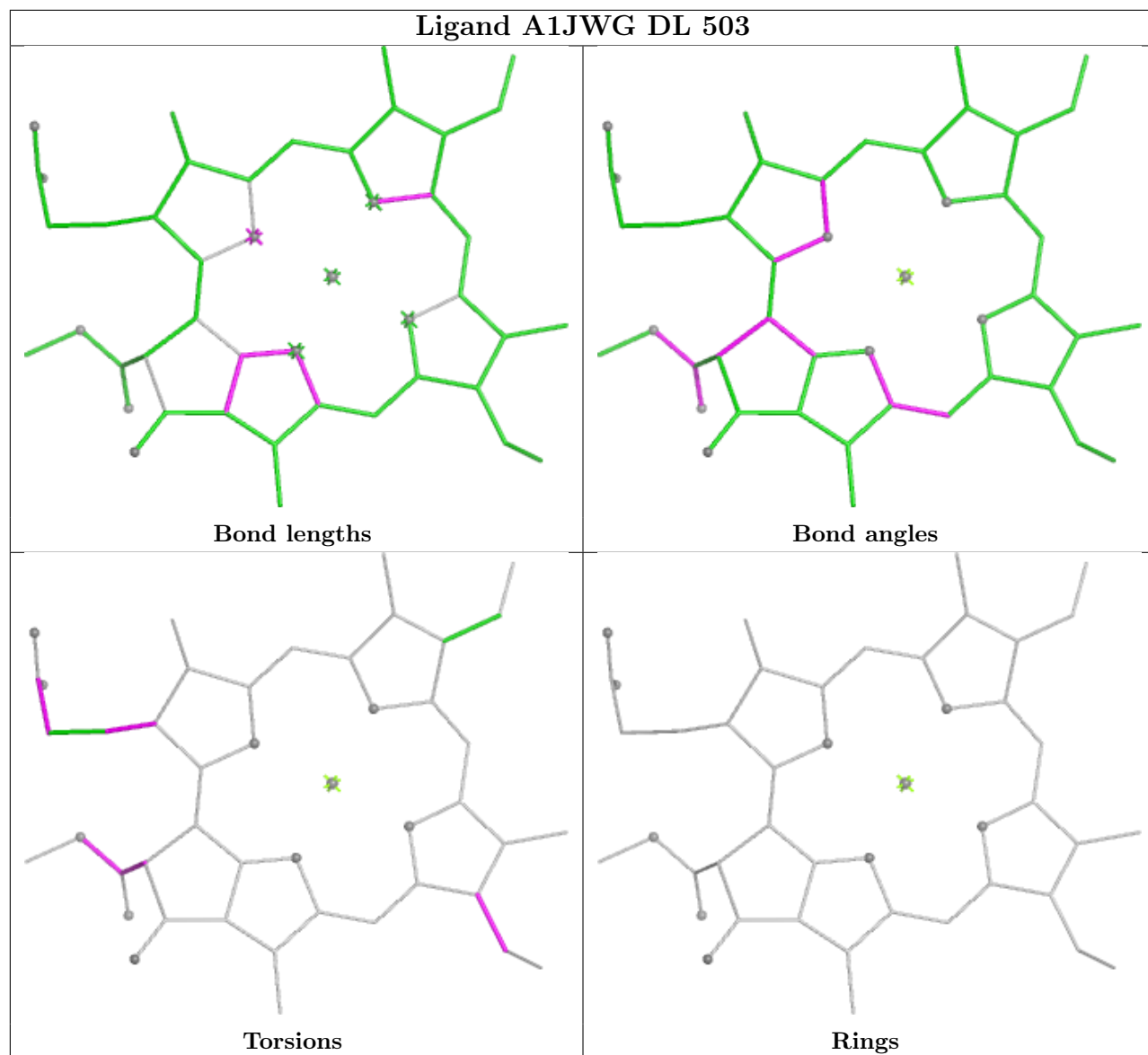




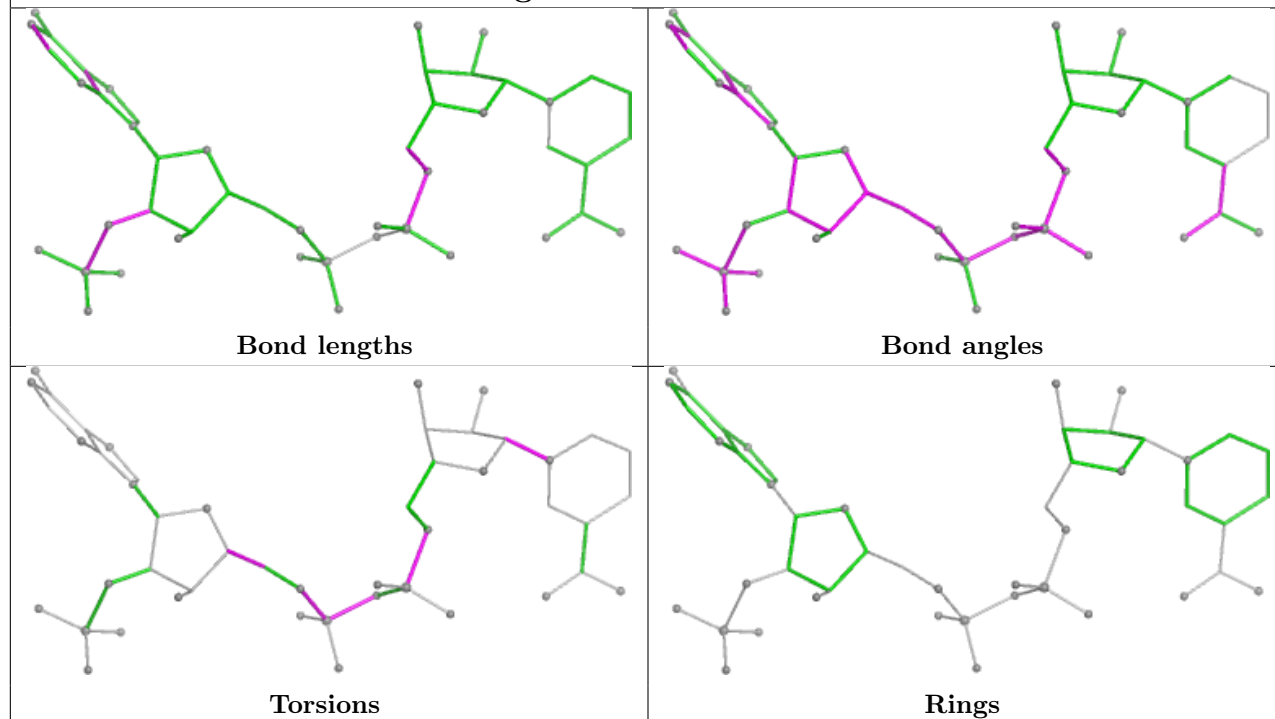
Ligand A1JWG DA 503



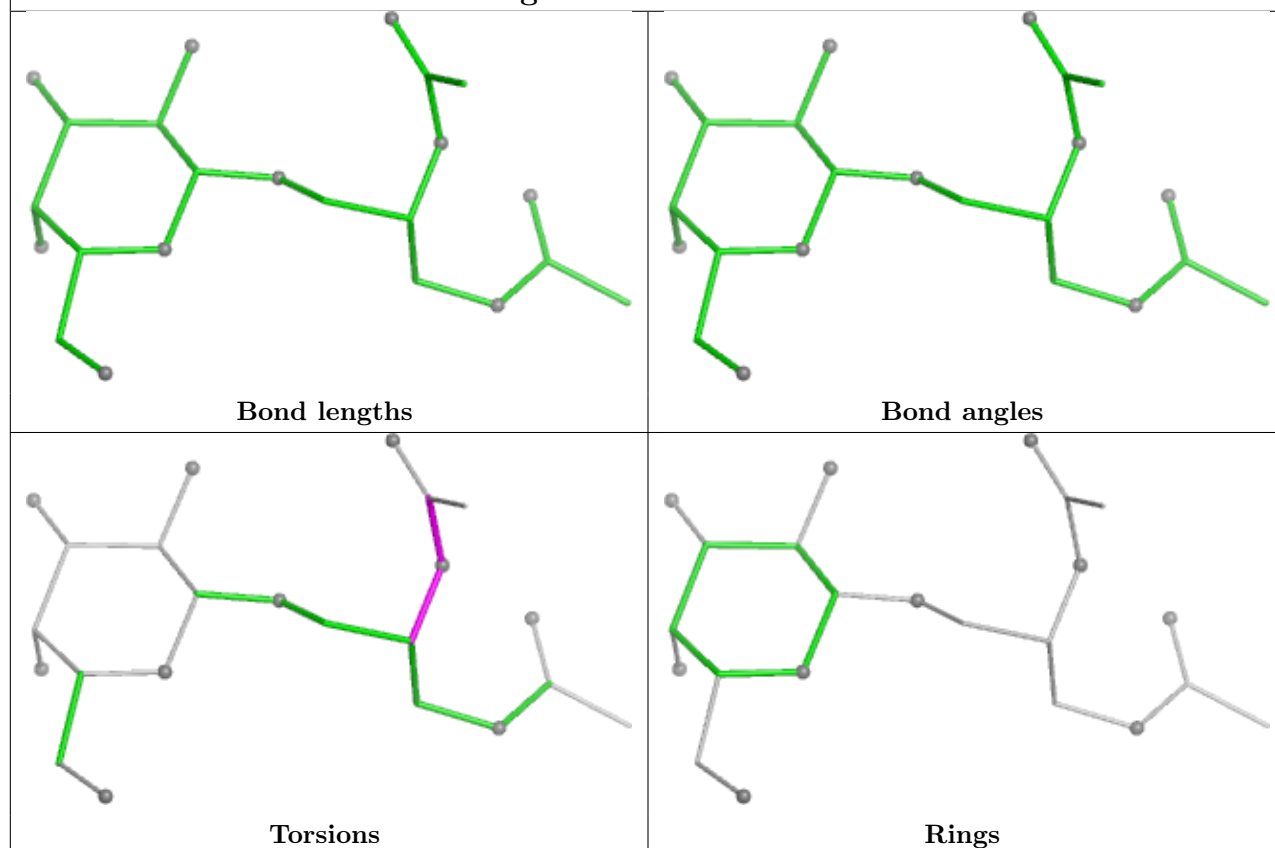
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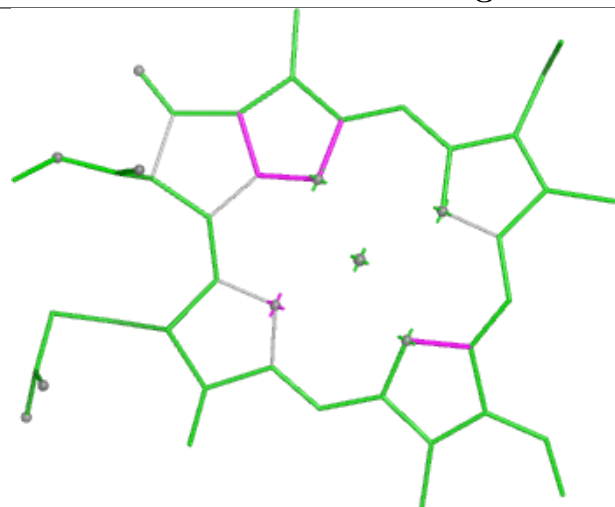
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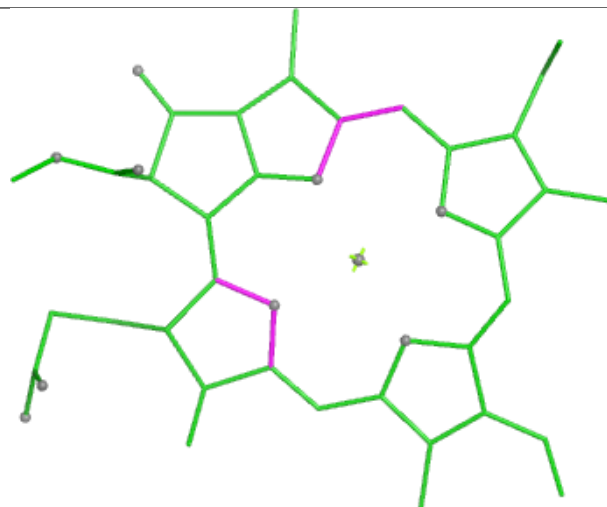
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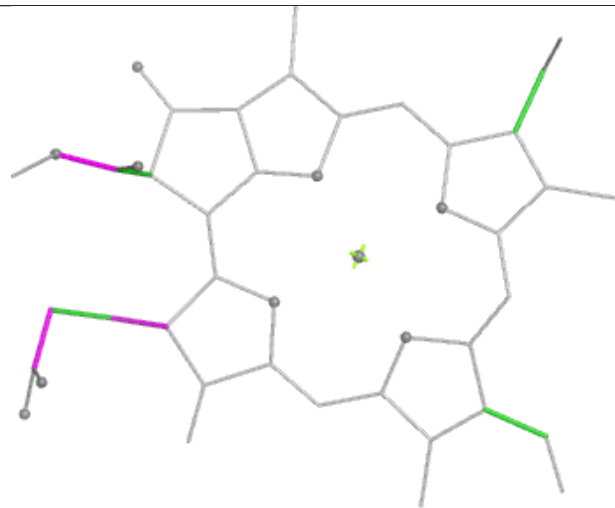
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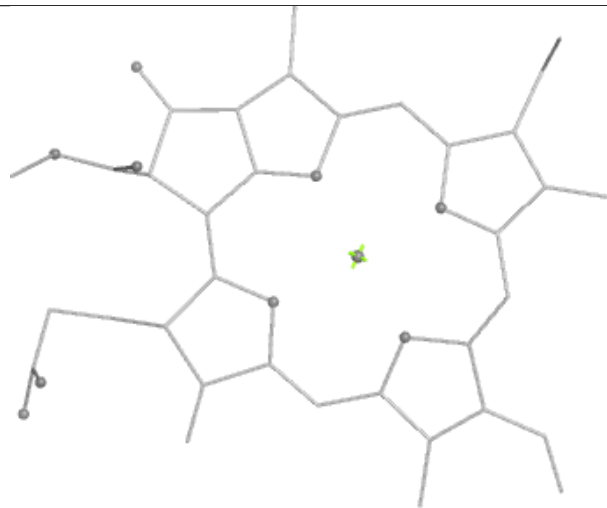
Bond lengths



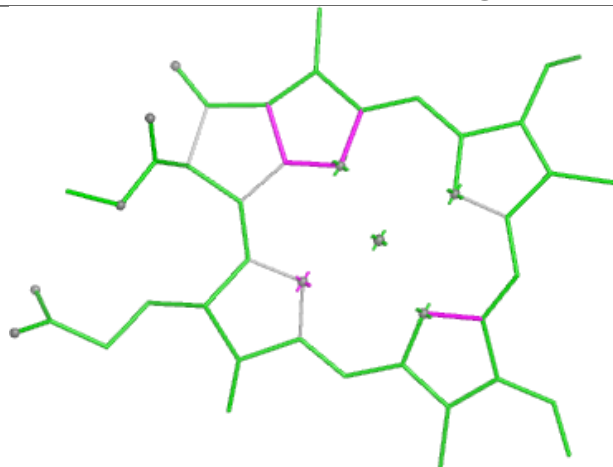
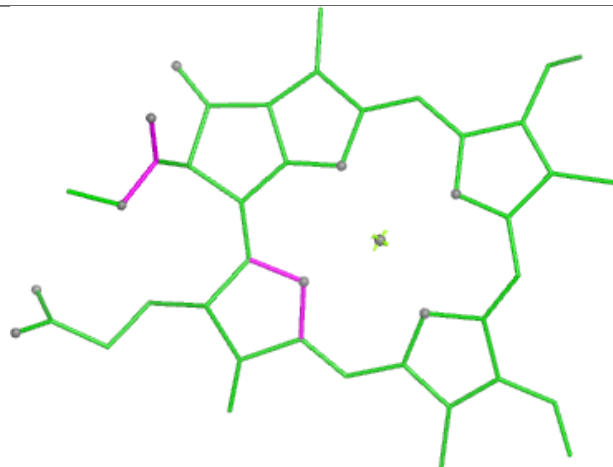
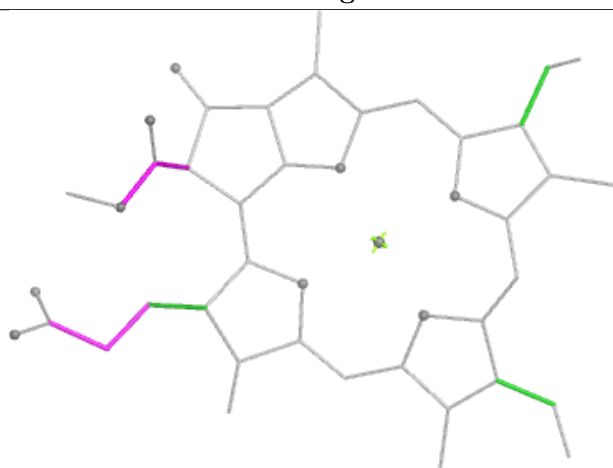
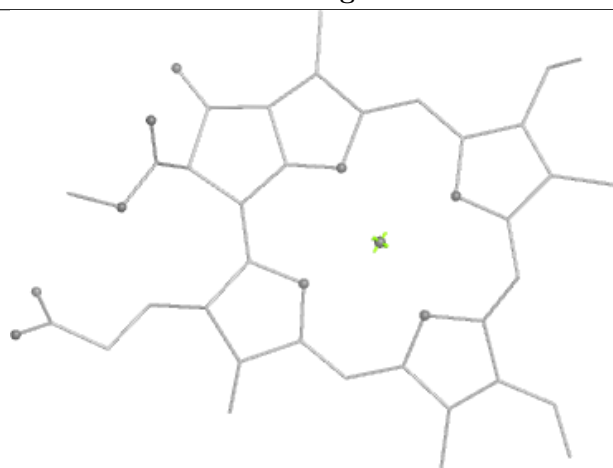
Bond angles

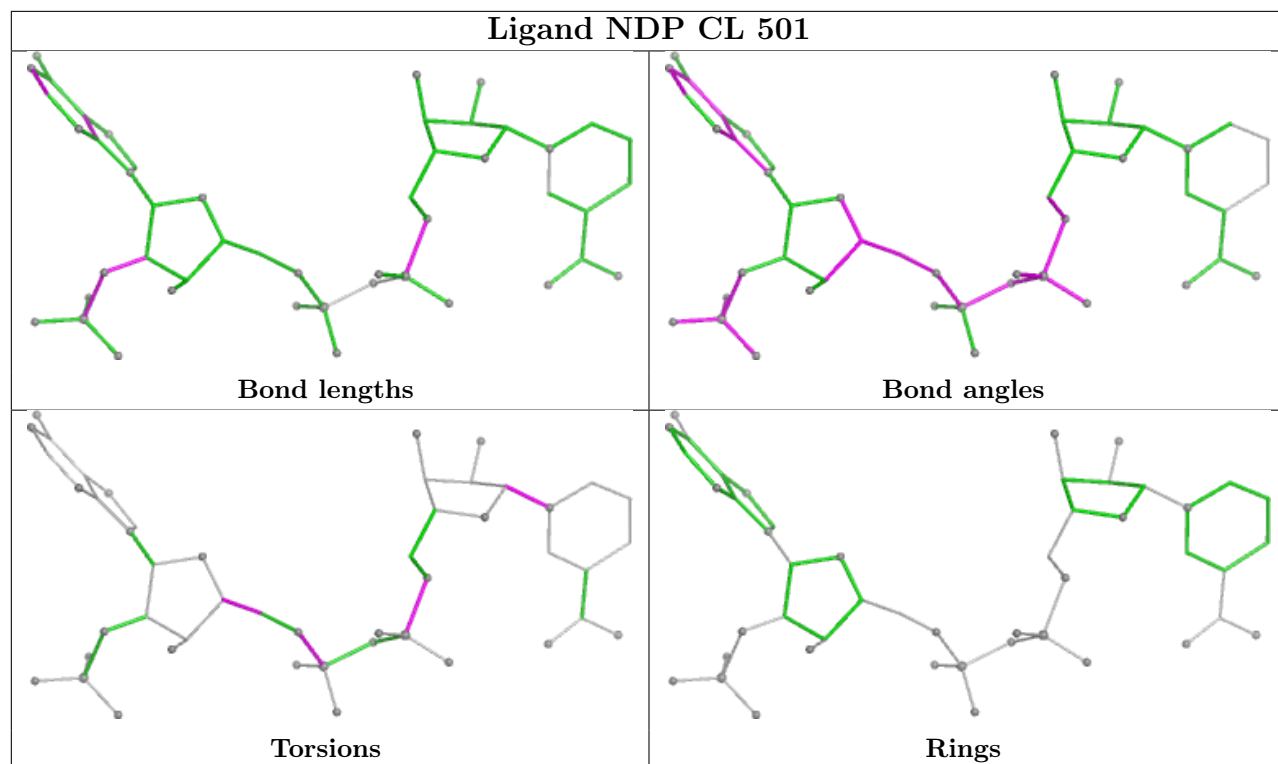


Torsions

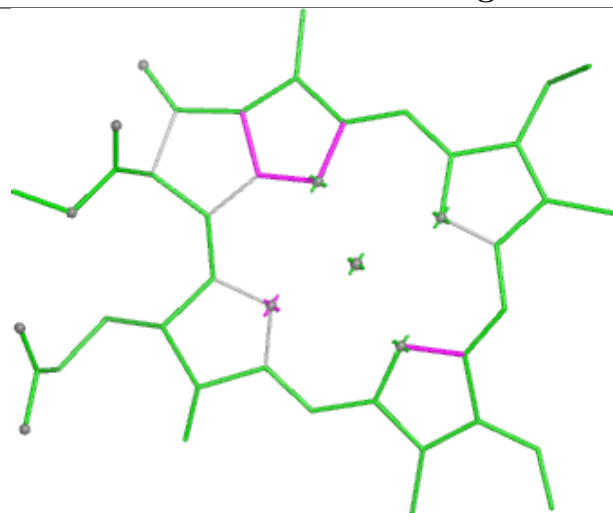


Rings

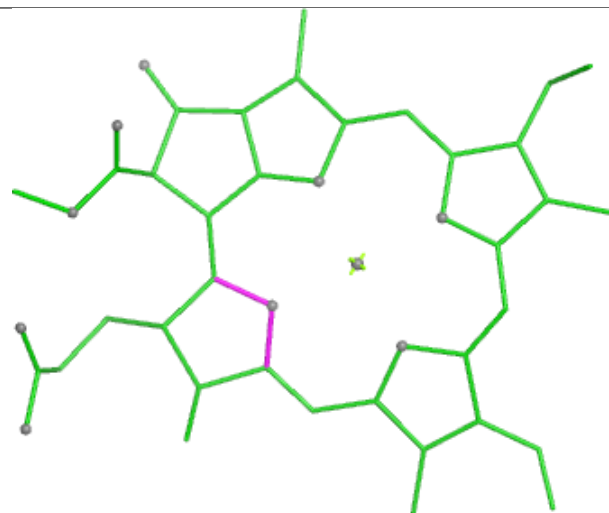
Ligand A1JWG BE 503**Bond lengths****Bond angles****Torsions****Rings**



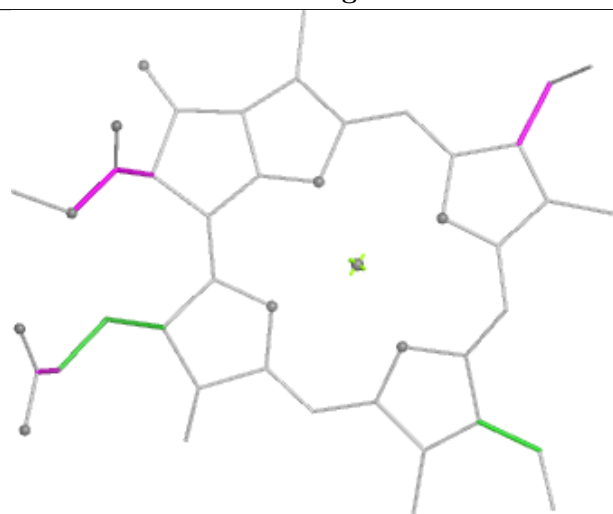
Ligand A1JWG AE 503



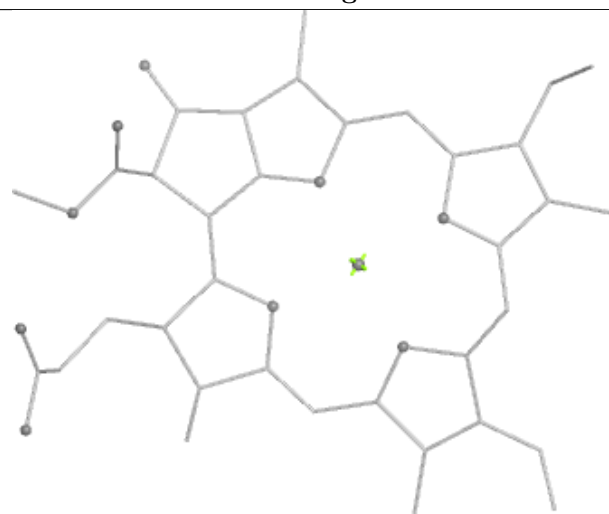
Bond lengths



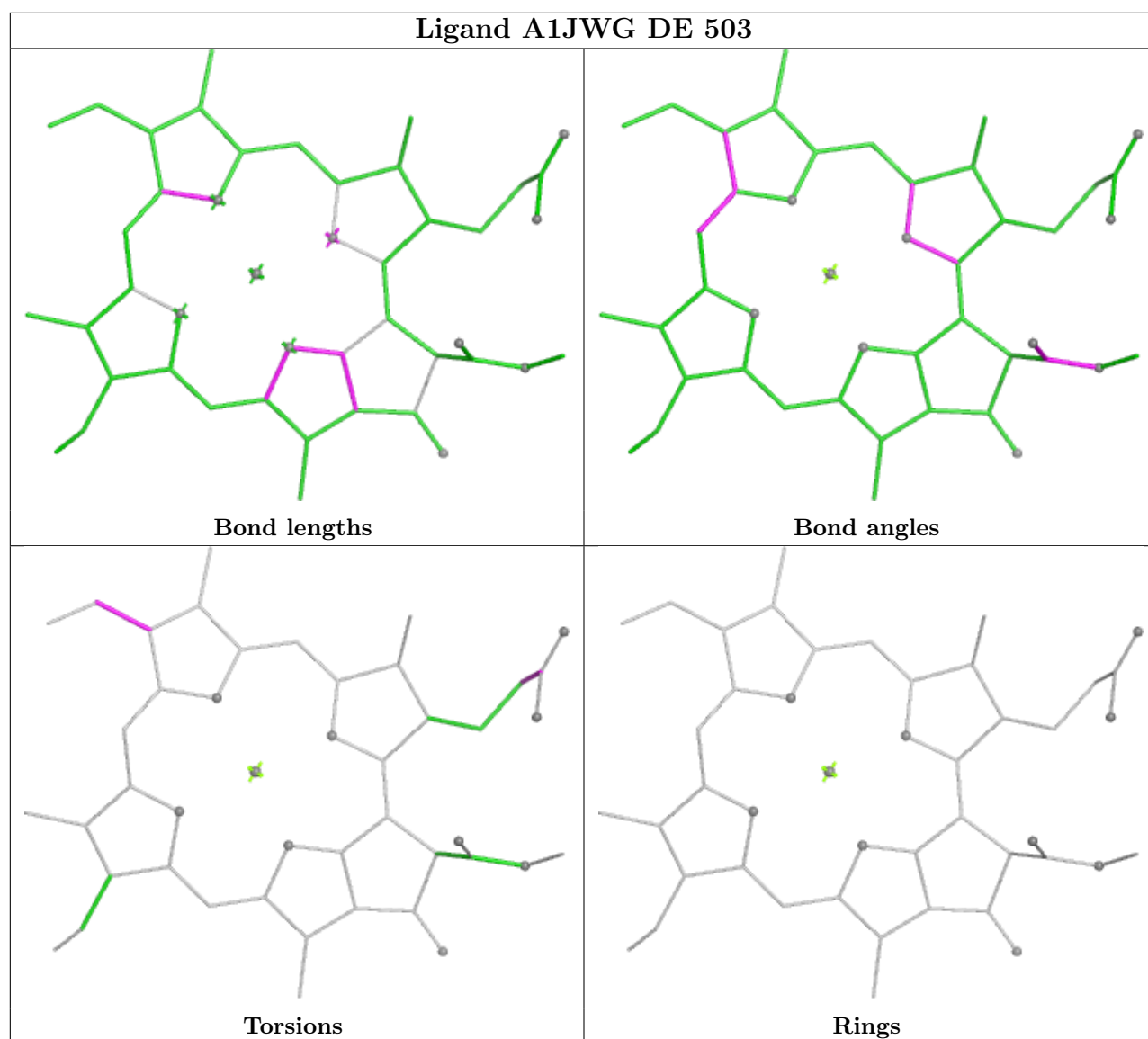
Bond angles

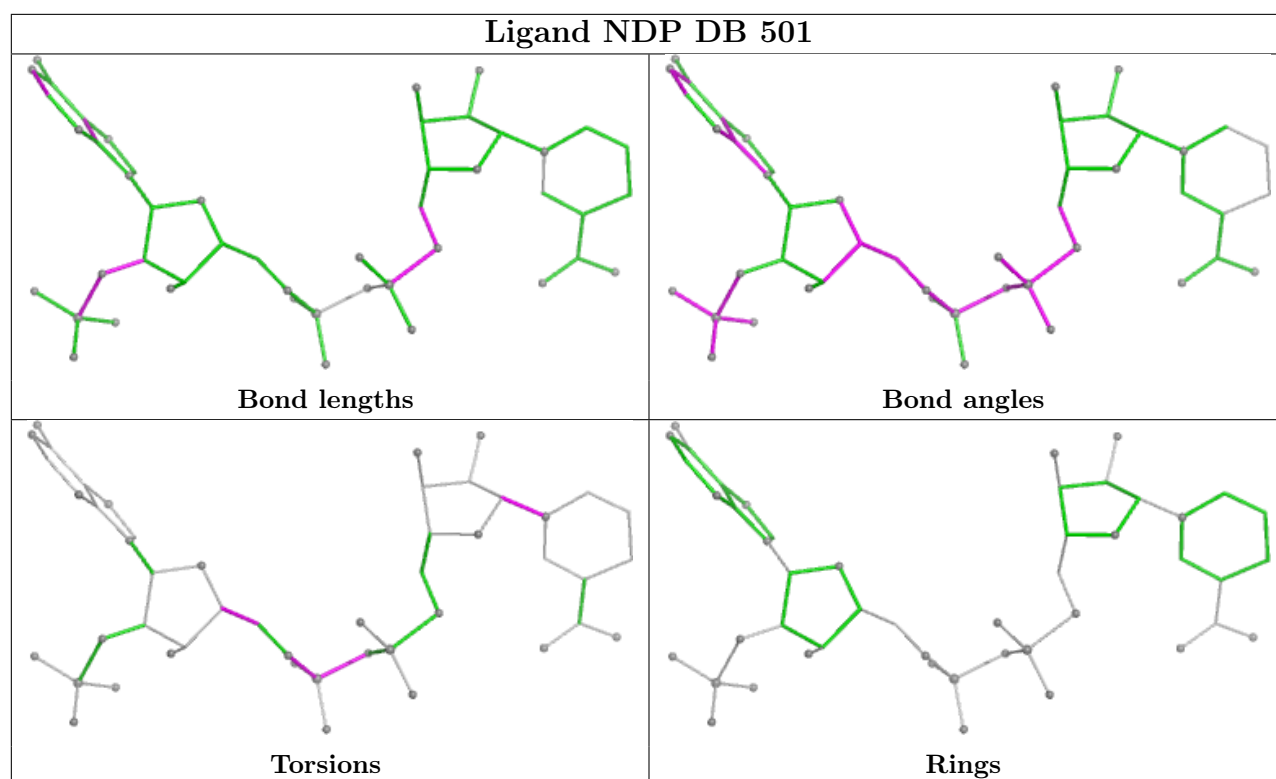


Torsions

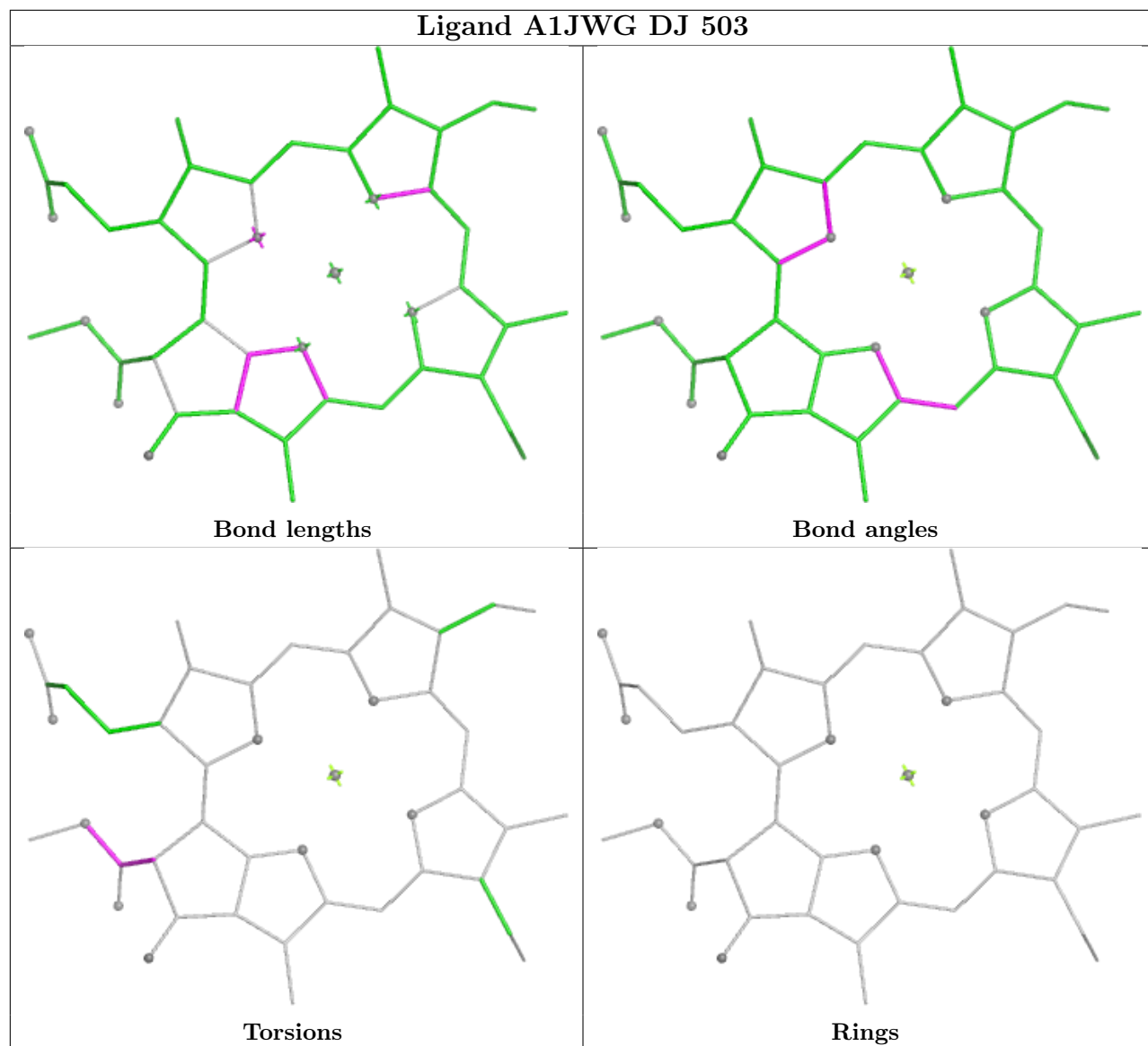


Rings

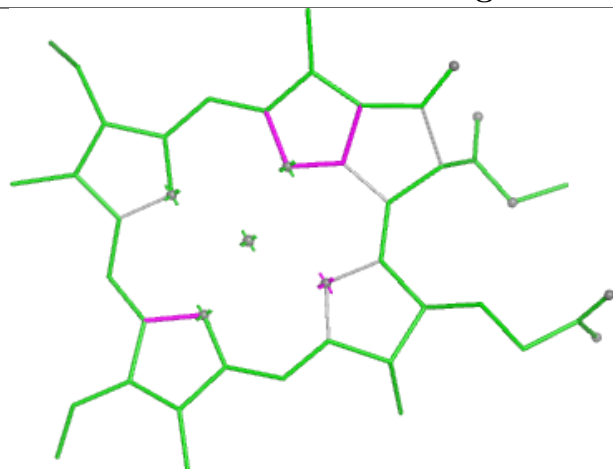




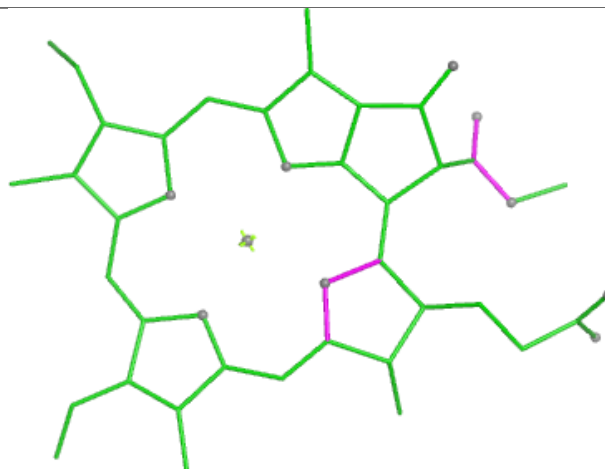
Ligand A1JWG DJ 503



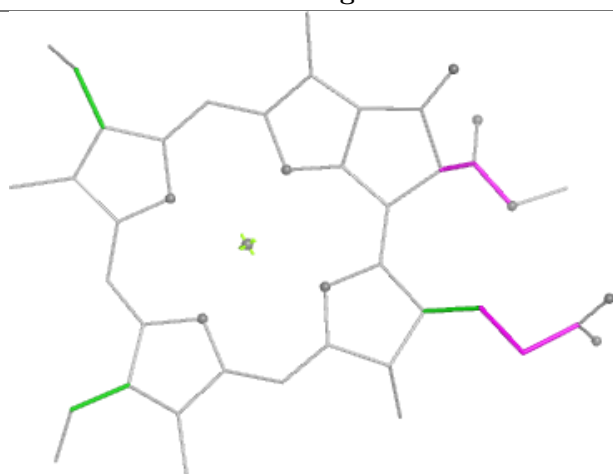
Ligand A1JWG AF 503



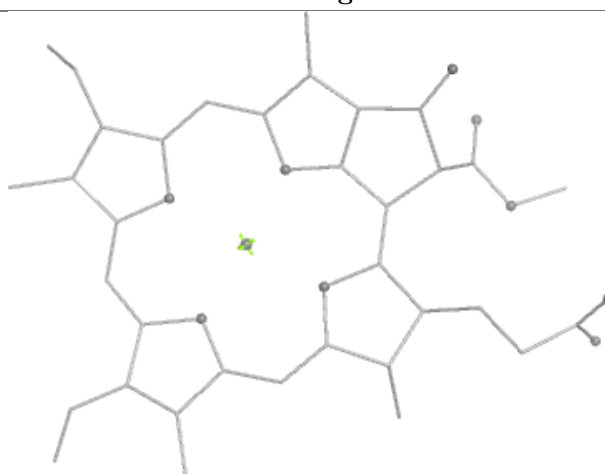
Bond lengths



Bond angles

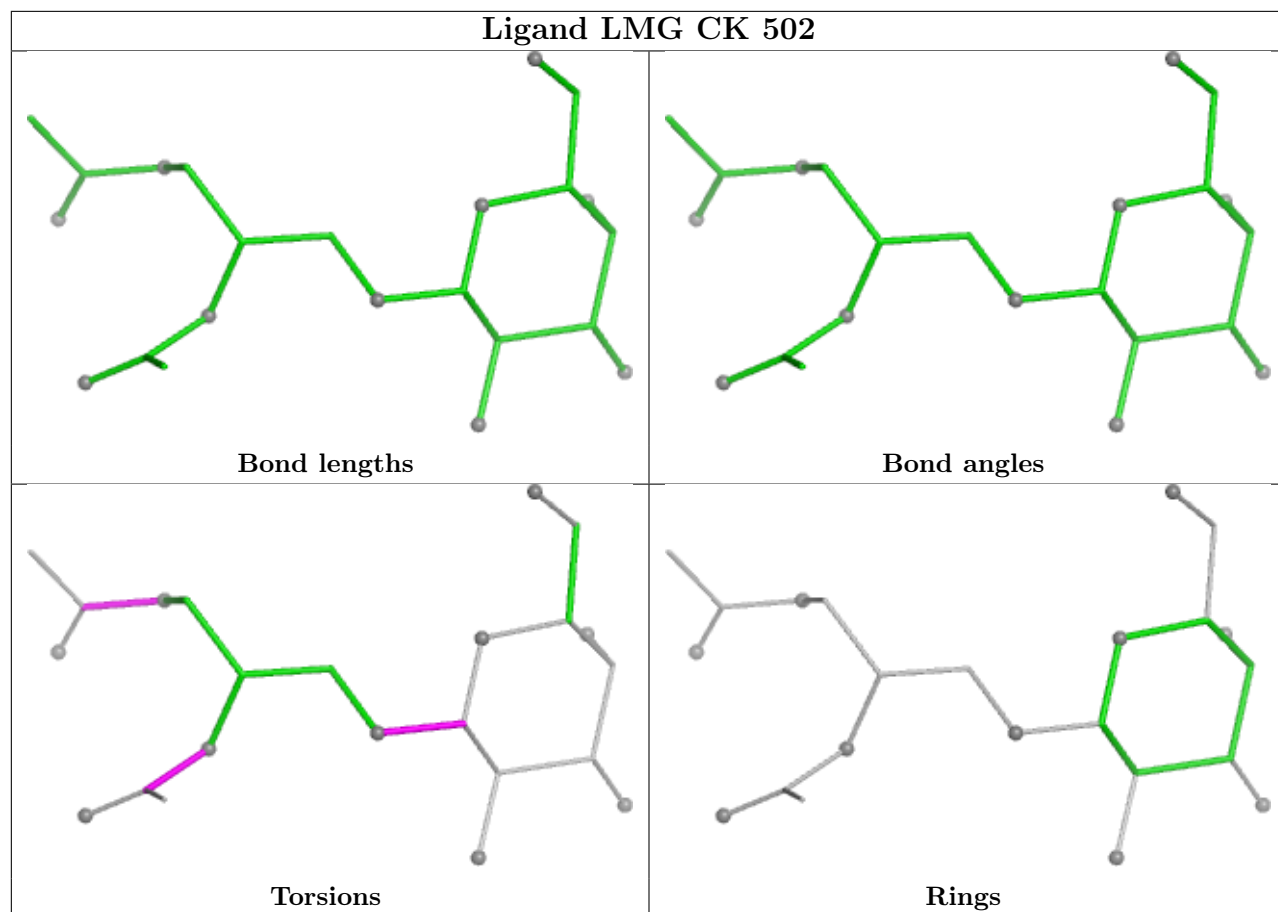


Torsions

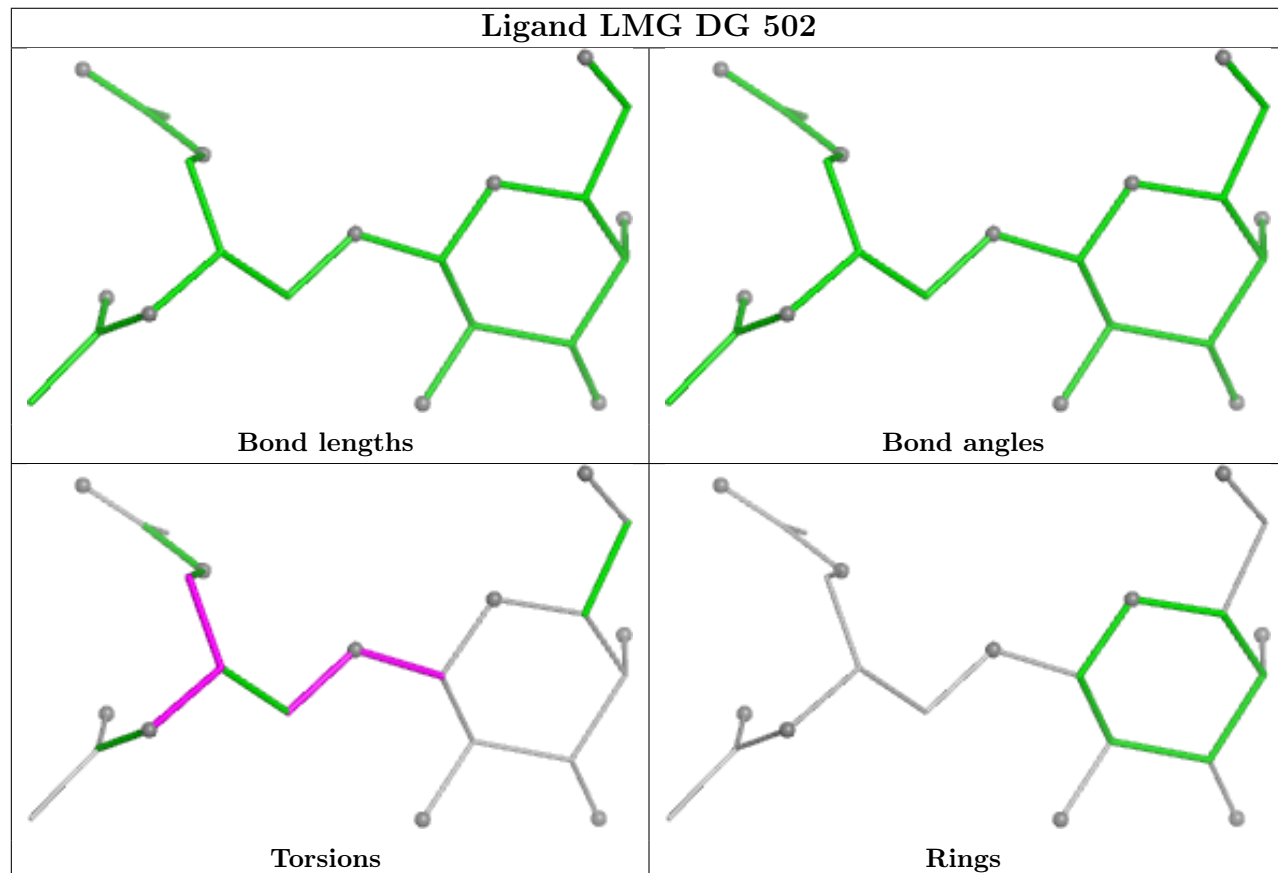


Rings

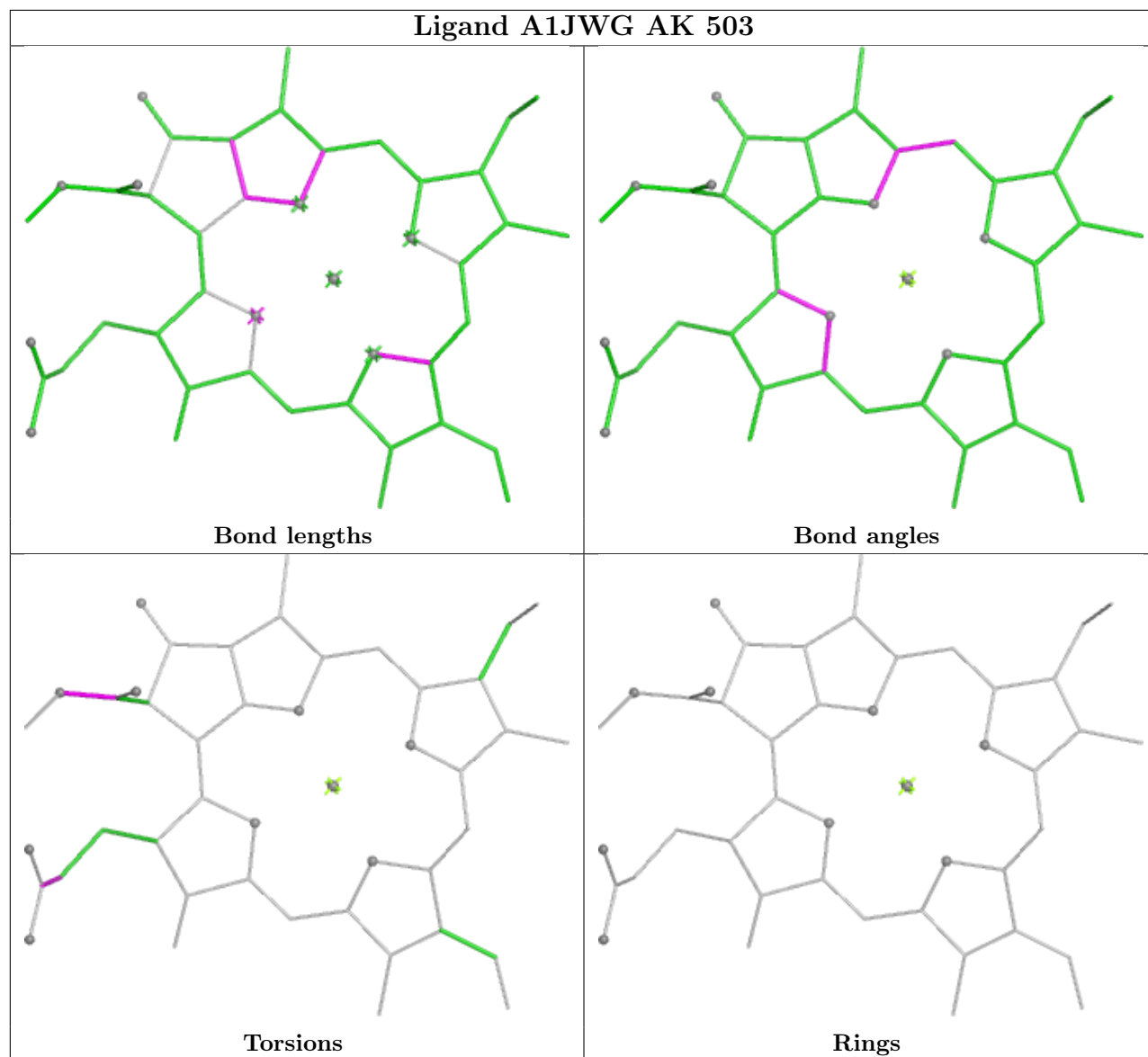
Ligand LMG CK 502



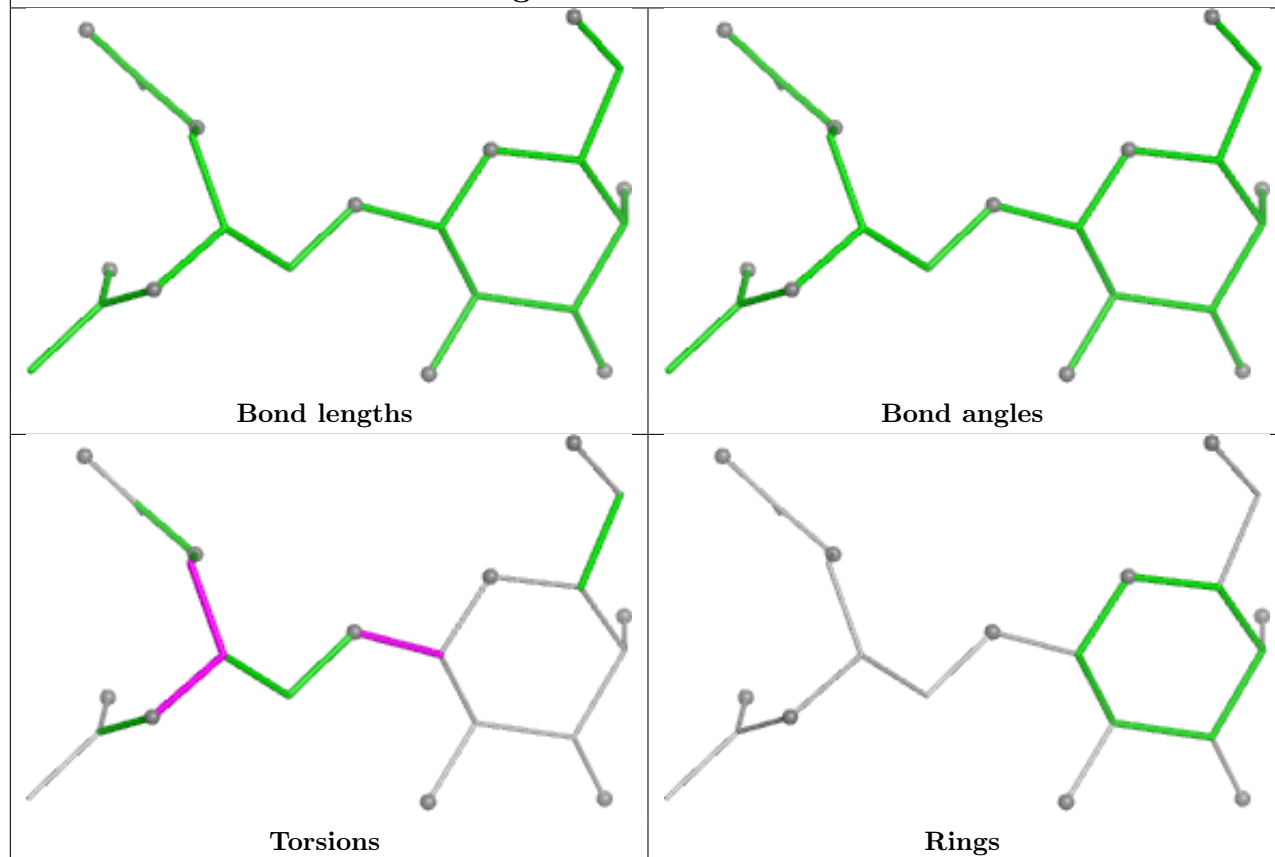
Ligand LMG DG 502



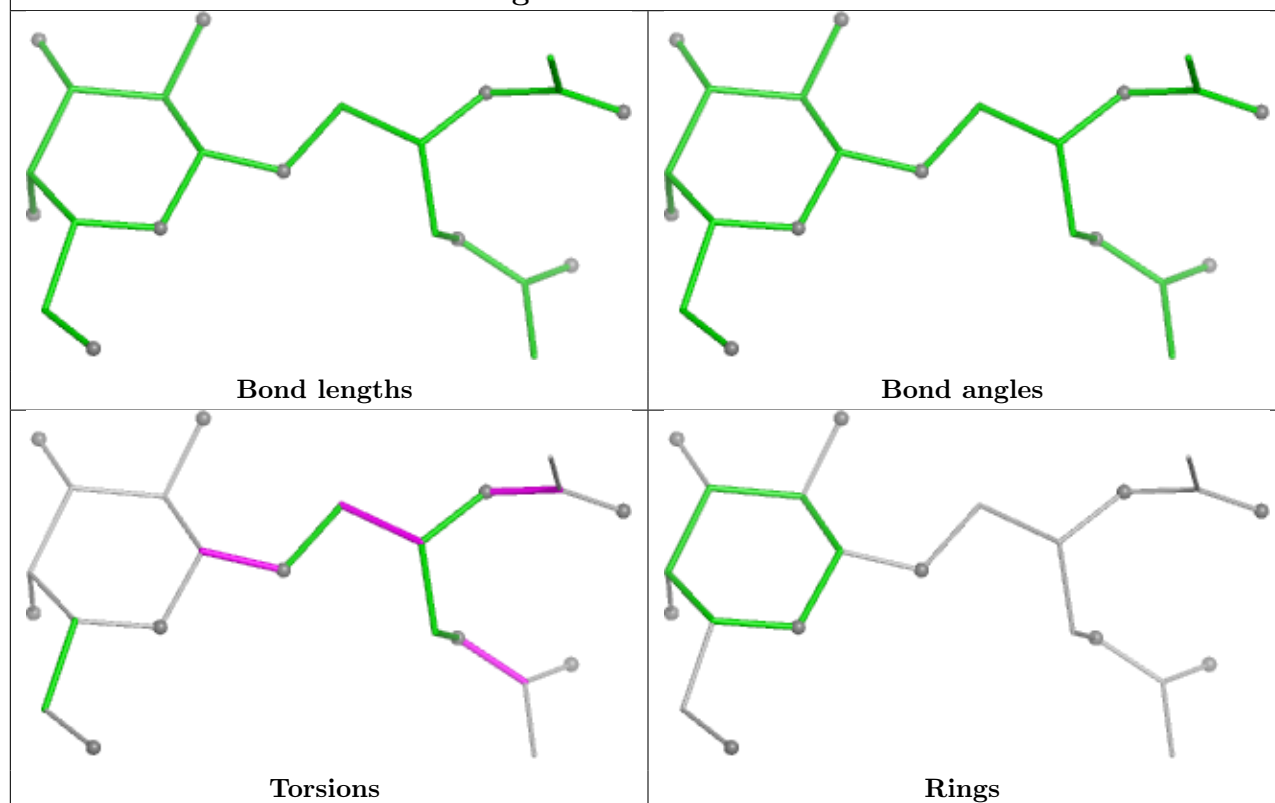
Ligand A1JWG AK 503

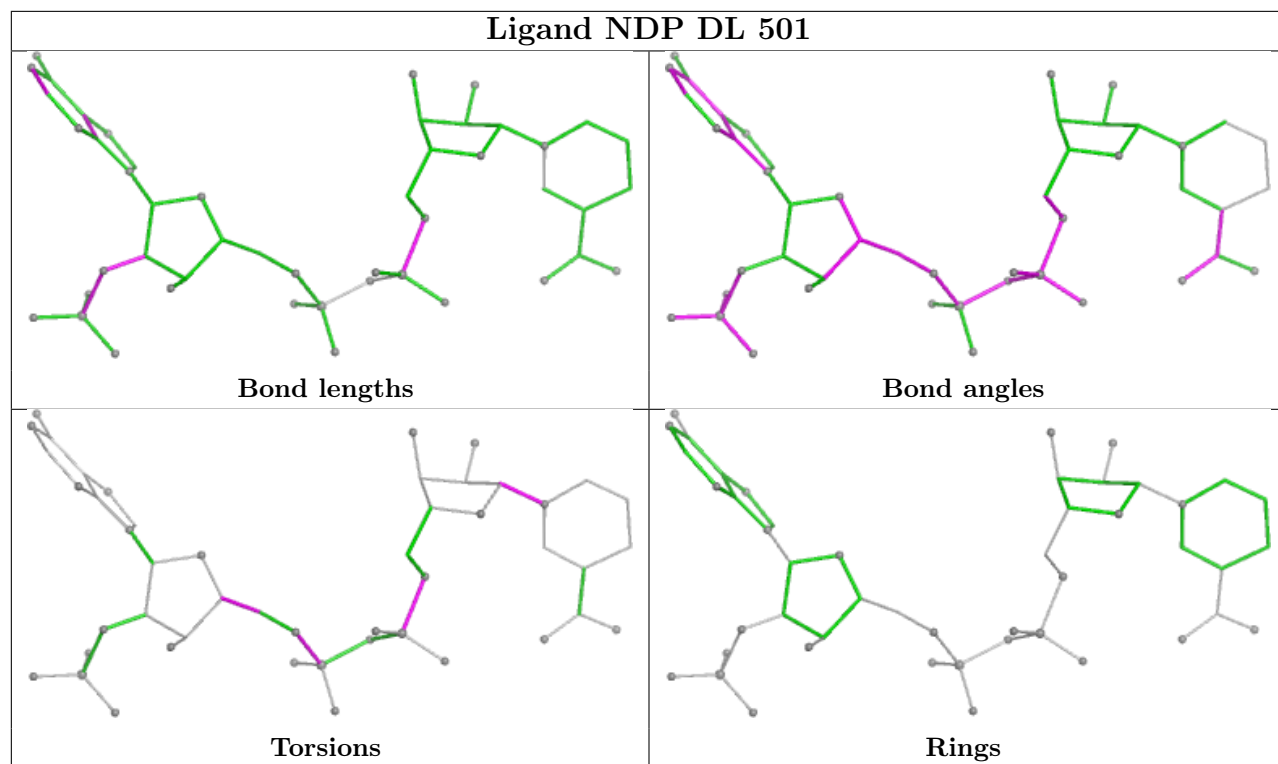


Ligand LMG CG 502

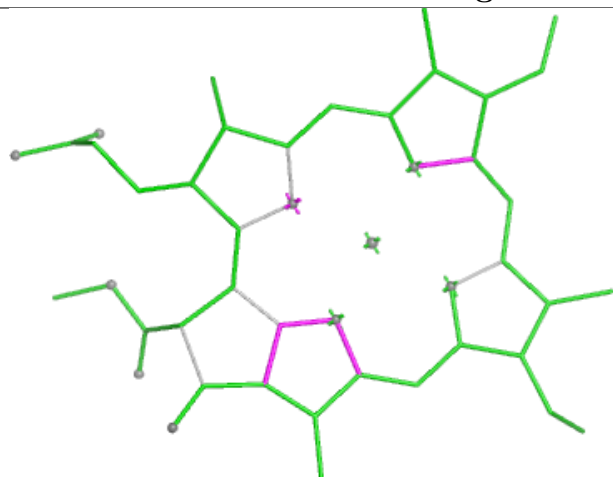


Ligand LMG AK 502

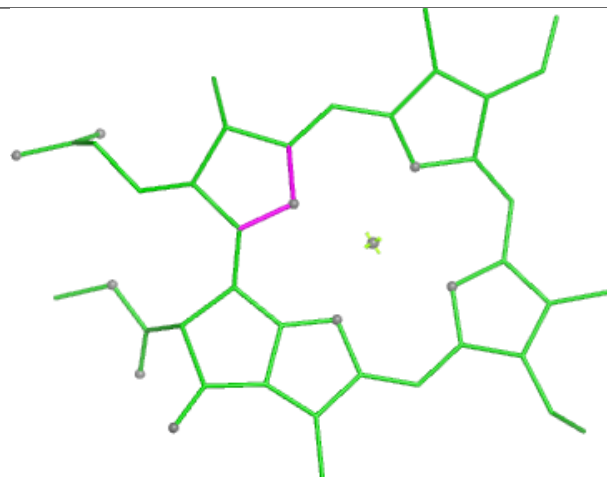




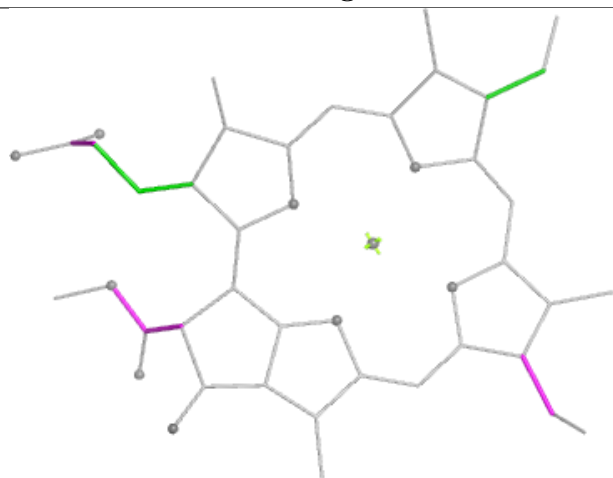
Ligand A1JWG DF 503



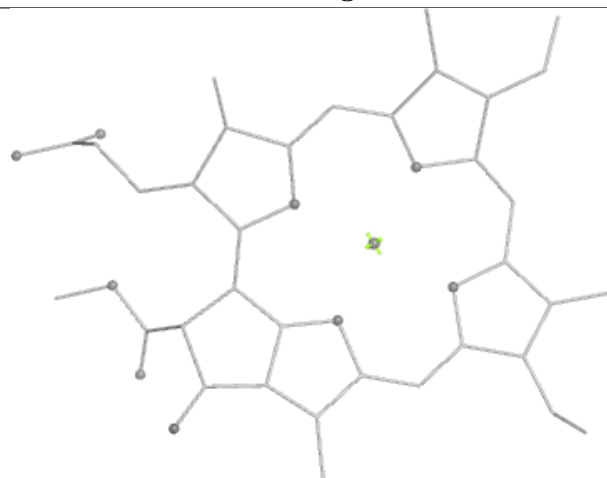
Bond lengths



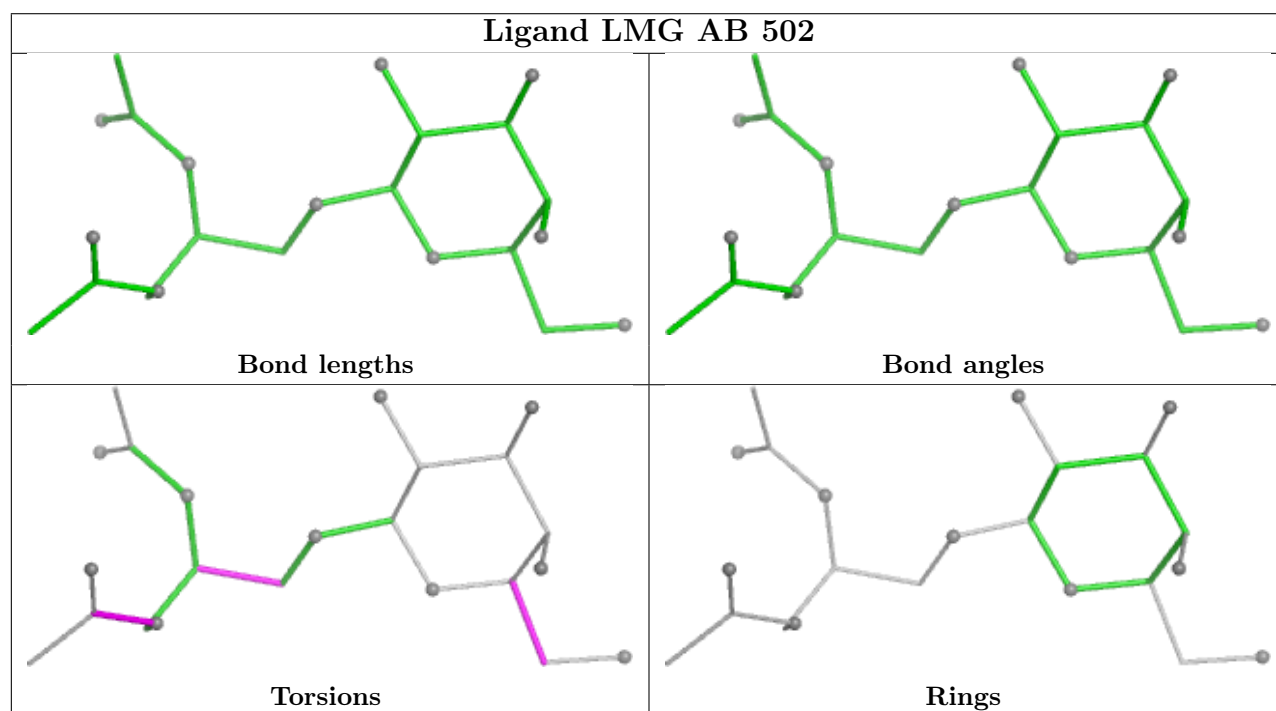
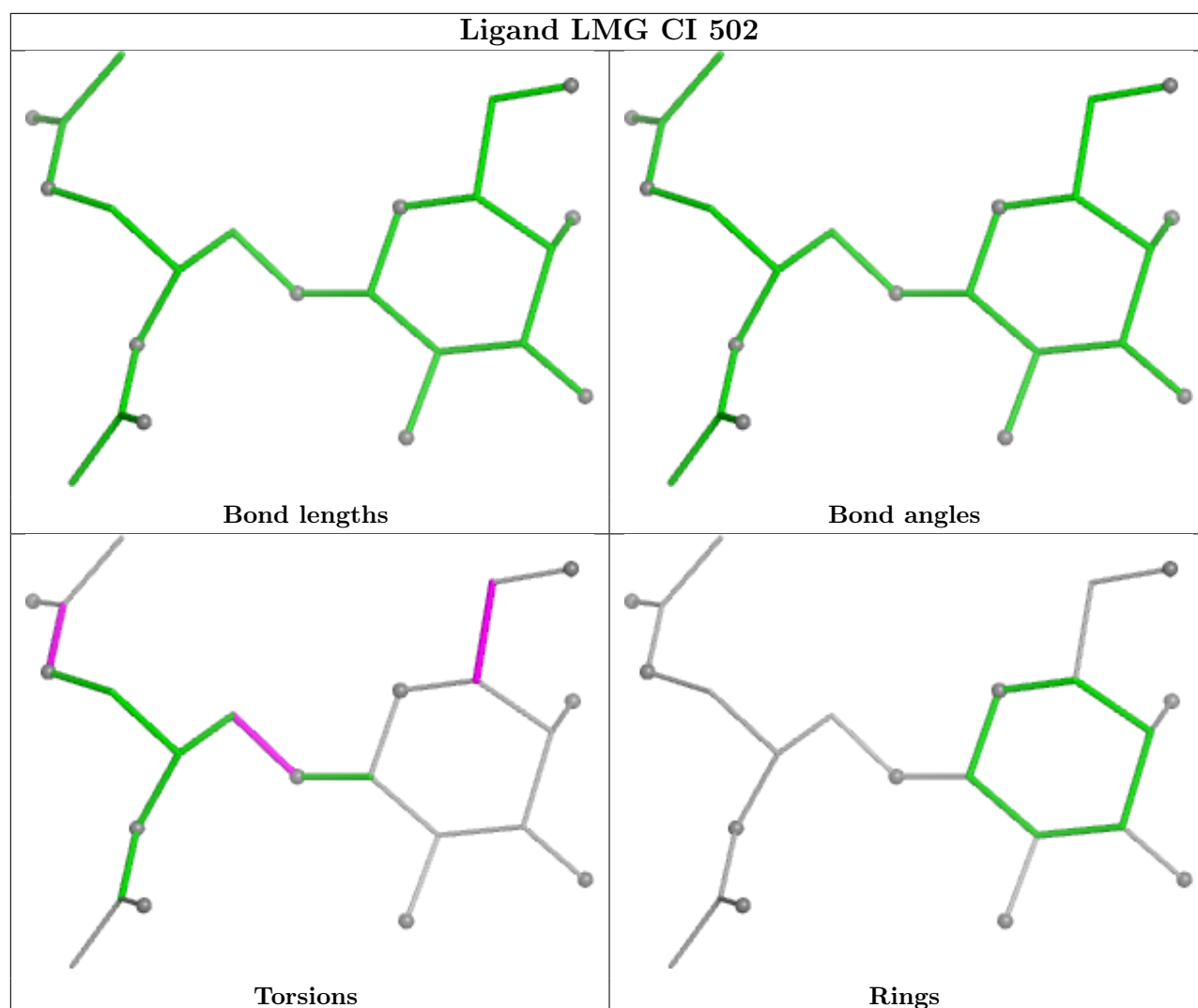
Bond angles



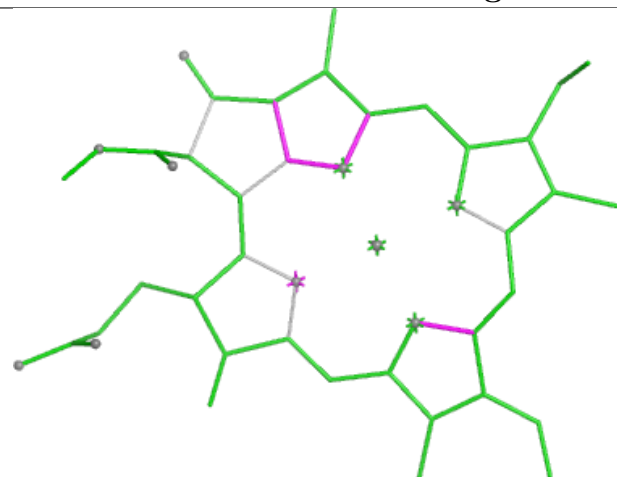
Torsions



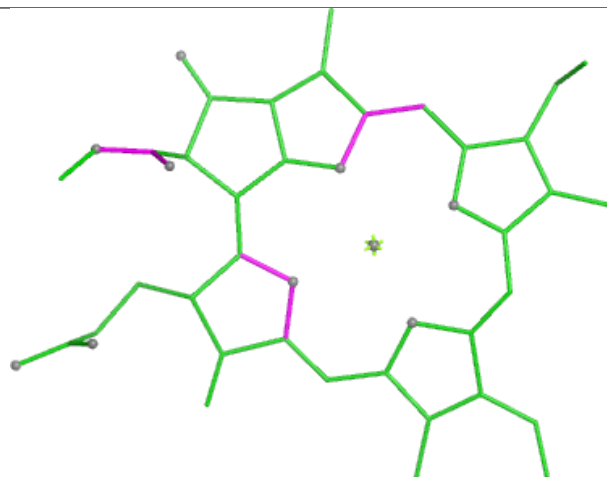
Rings



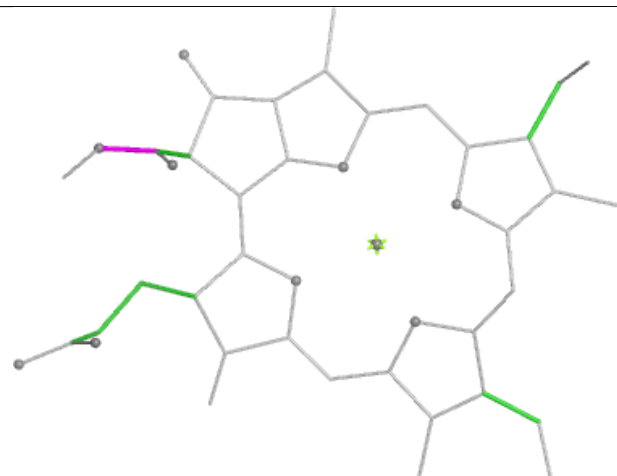
Ligand A1JWG AI 503



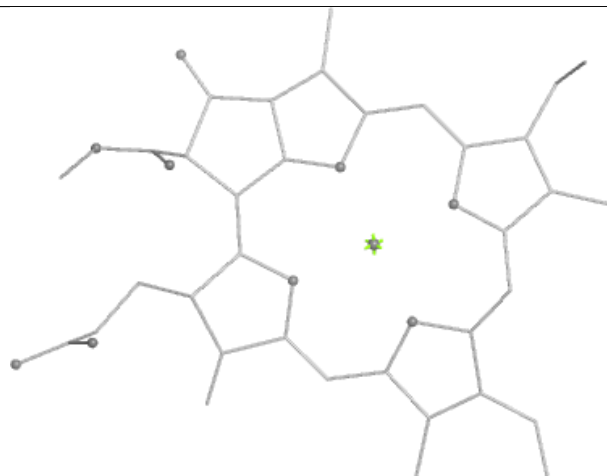
Bond lengths



Bond angles

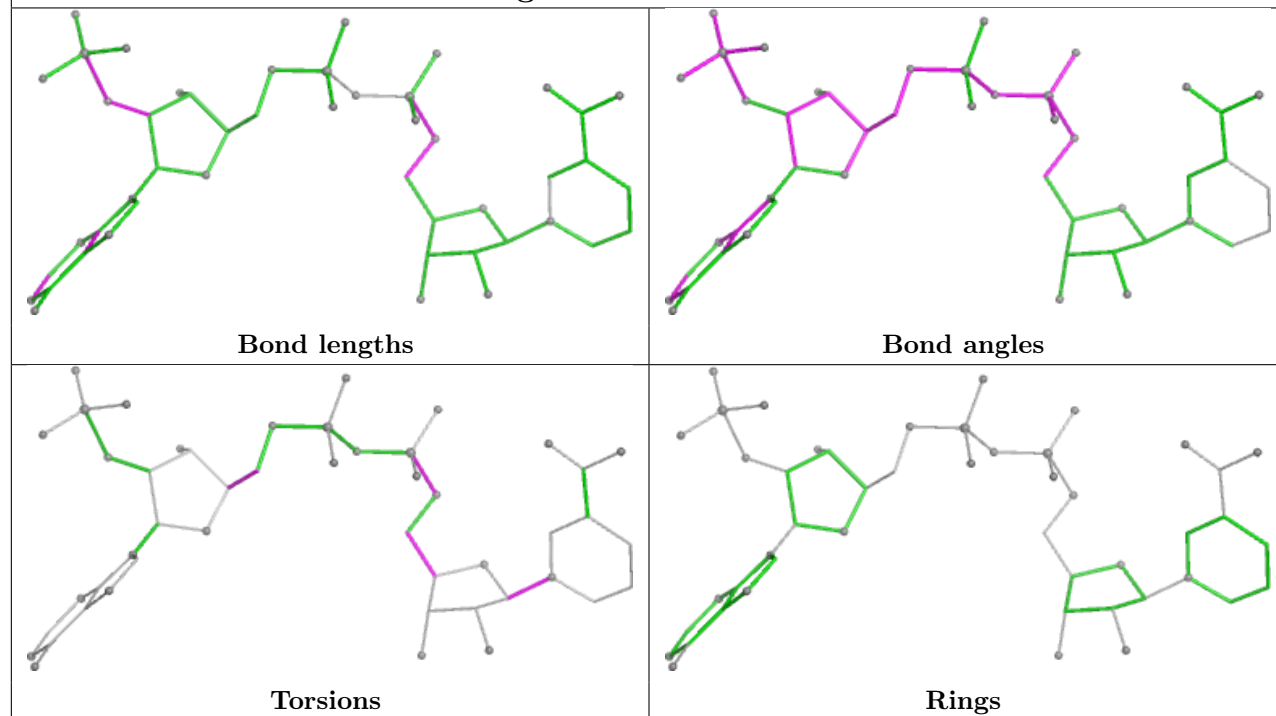


Torsions

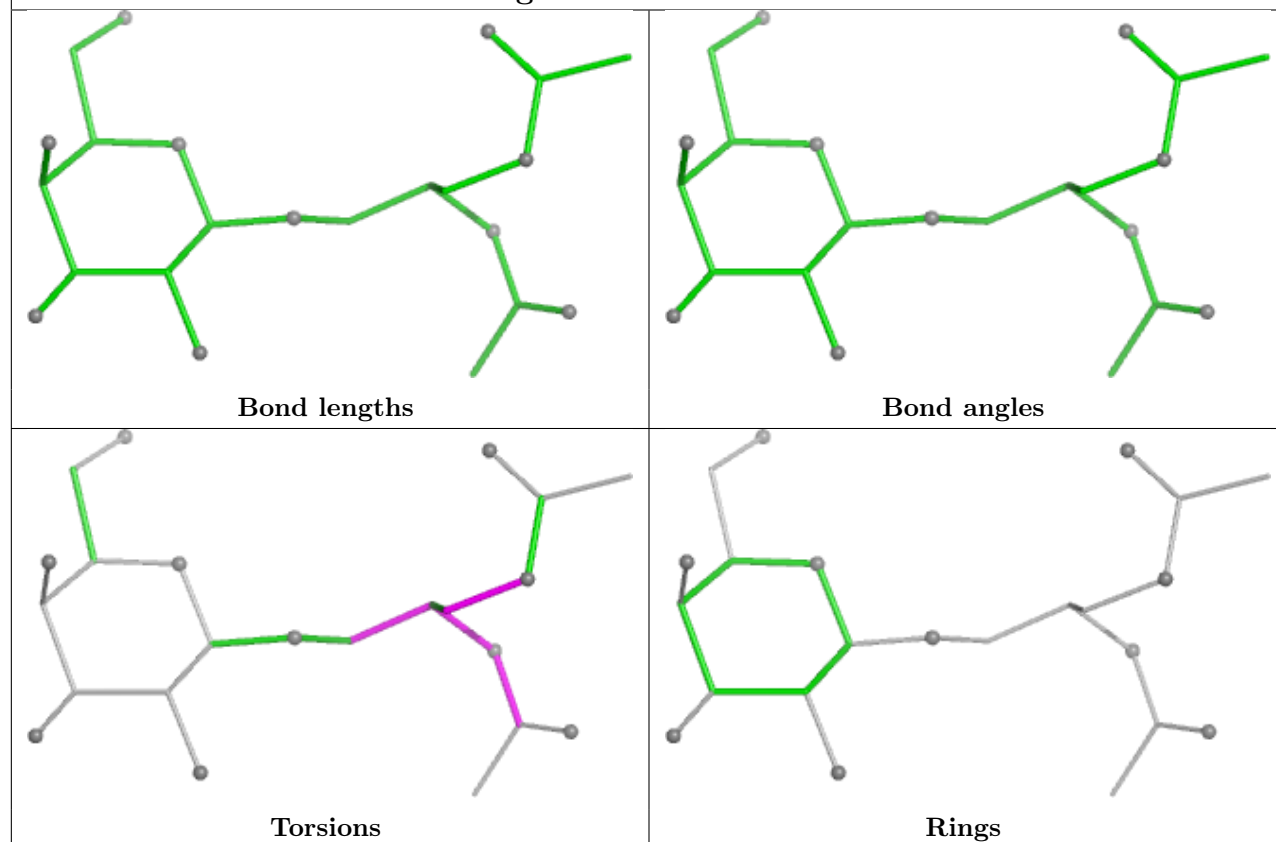


Rings

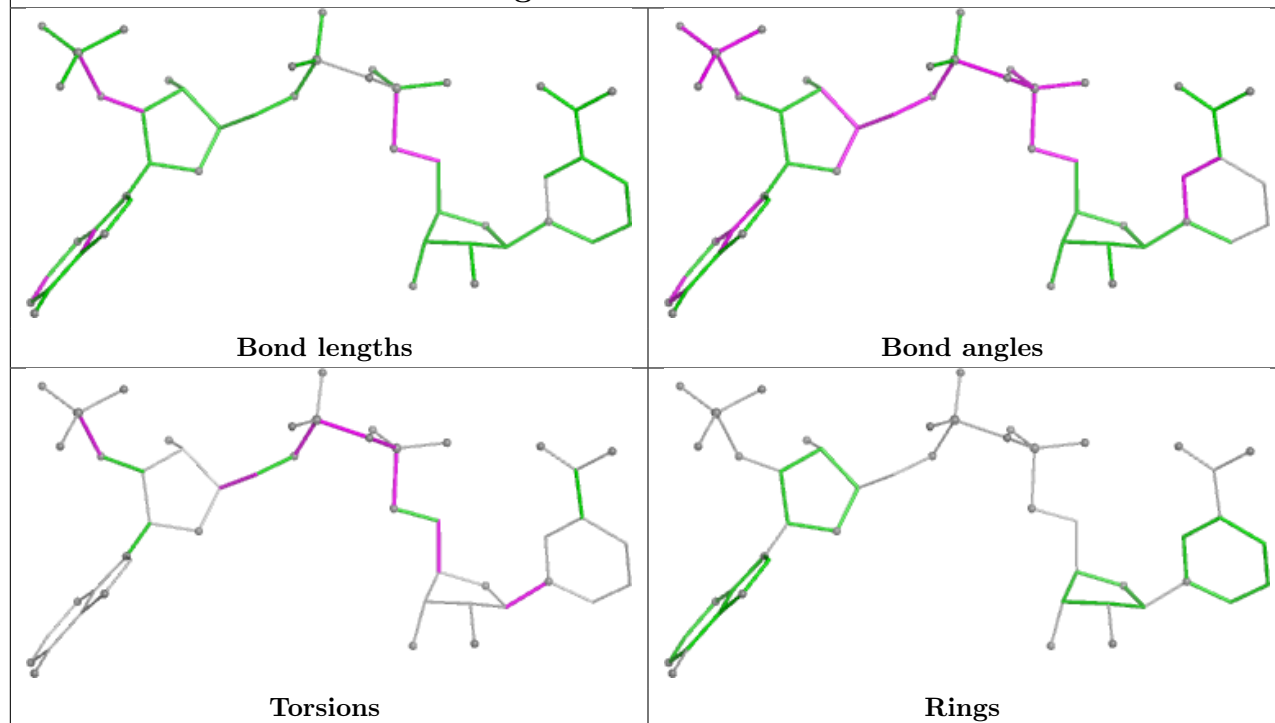
Ligand NDP AE 501



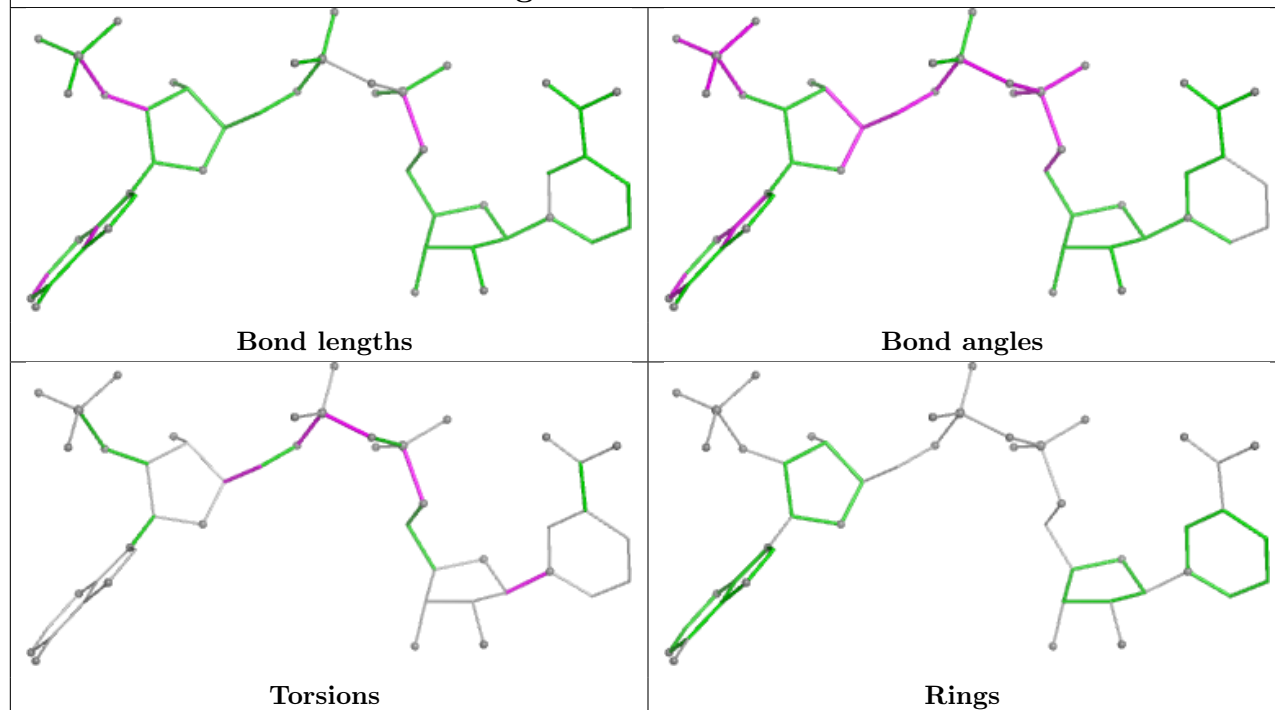
Ligand LMG DL 502

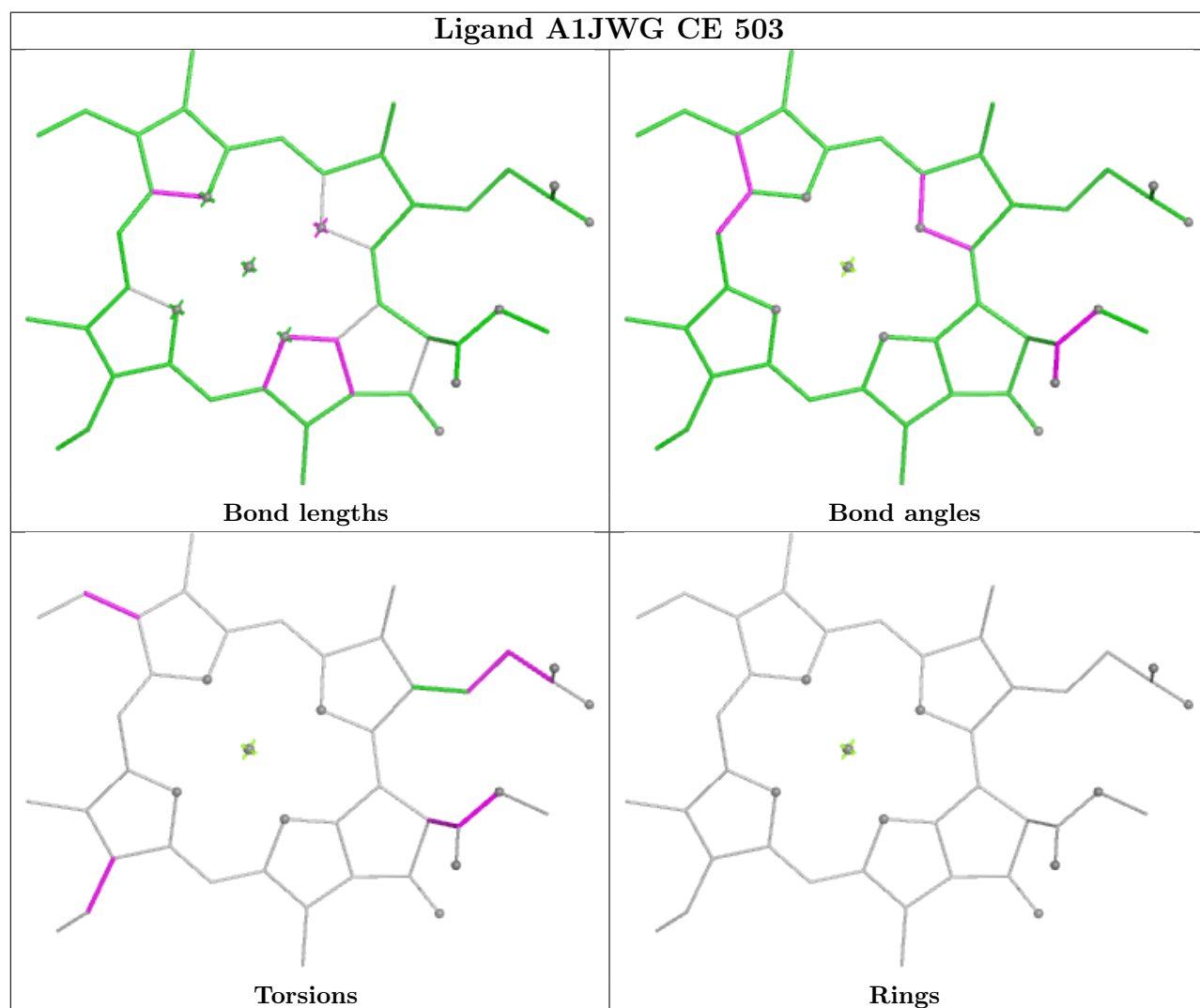
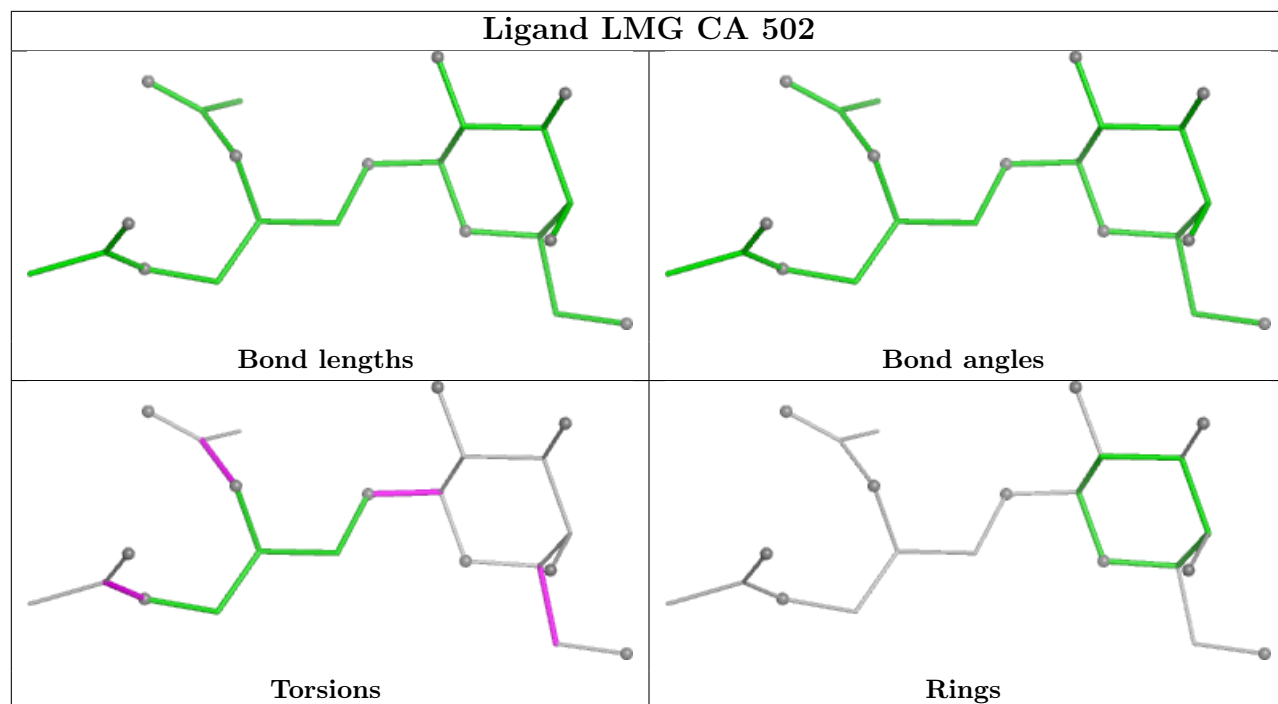


Ligand NDP CG 501

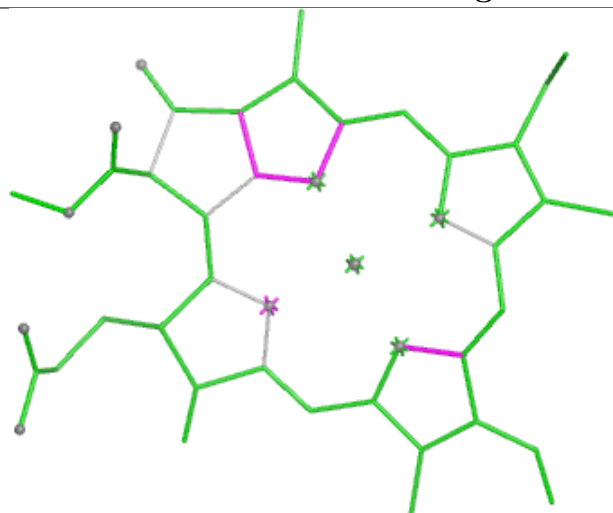


Ligand NDP CC 501

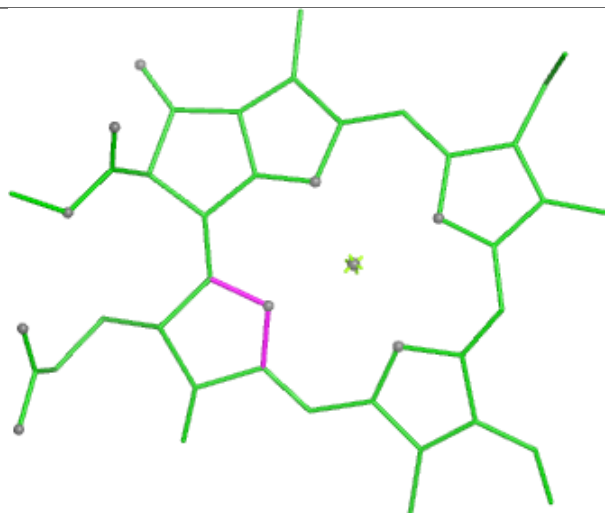




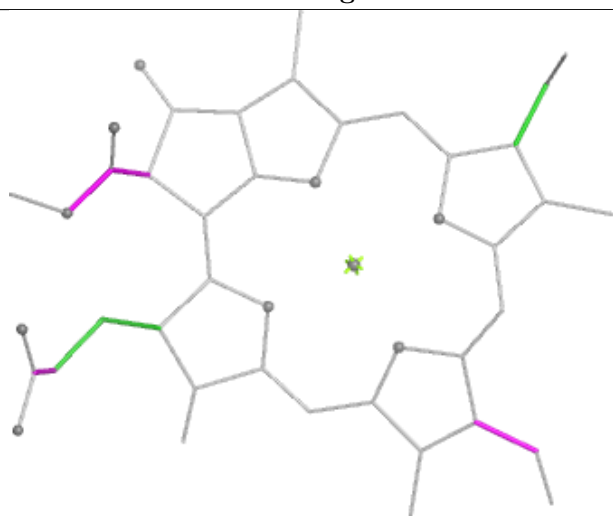
Ligand A1JWG BC 503



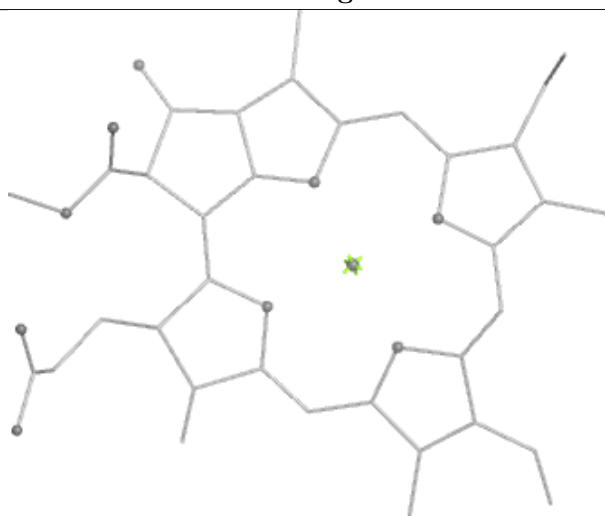
Bond lengths



Bond angles

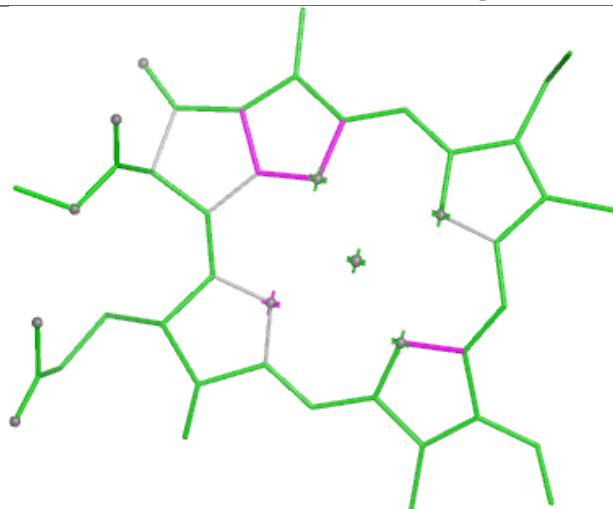


Torsions

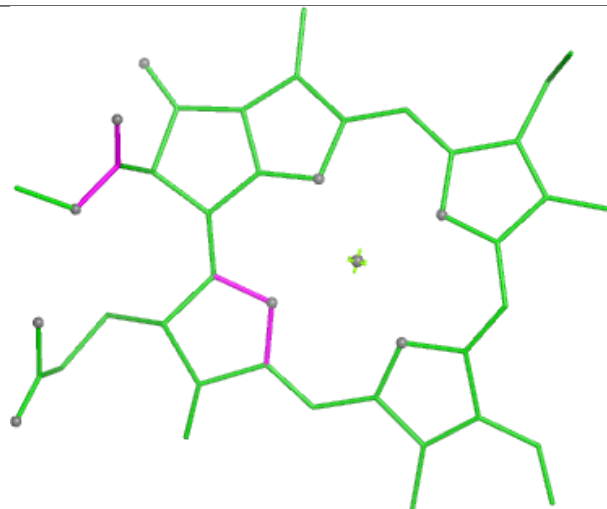


Rings

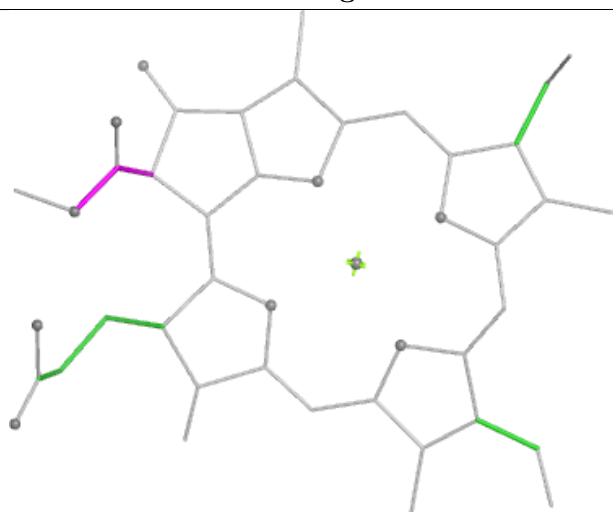
Ligand A1JWG BD 503



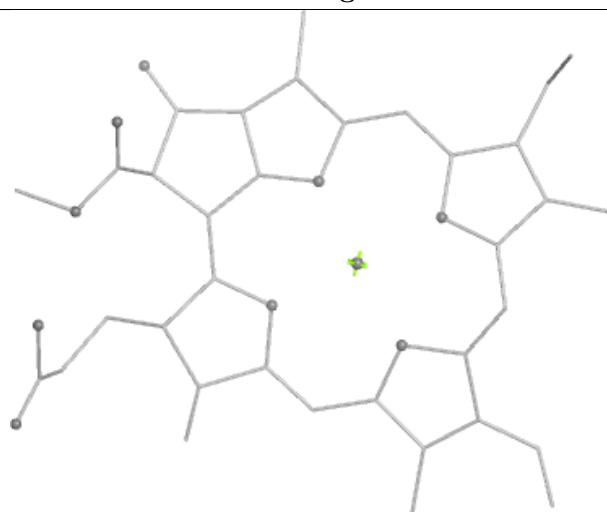
Bond lengths



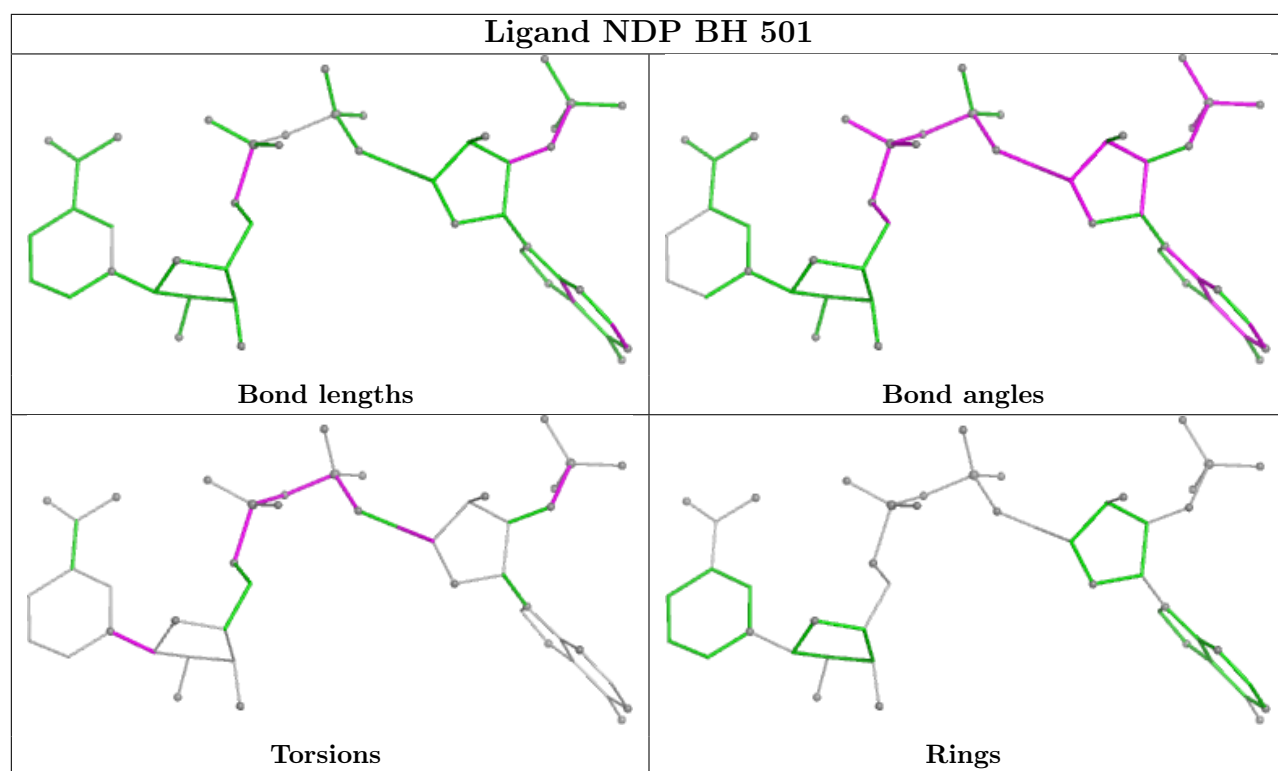
Bond angles



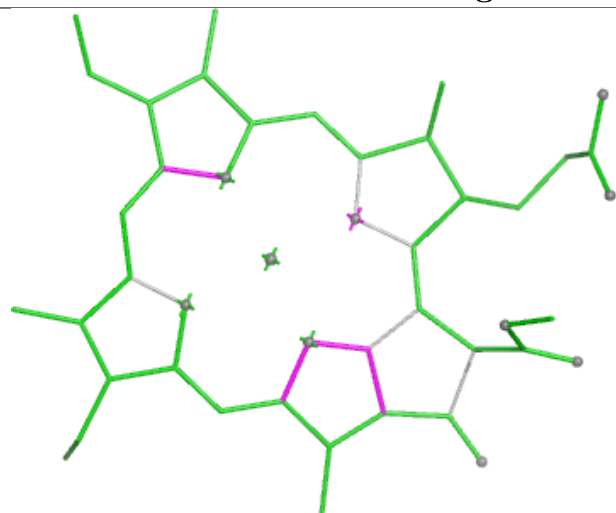
Torsions



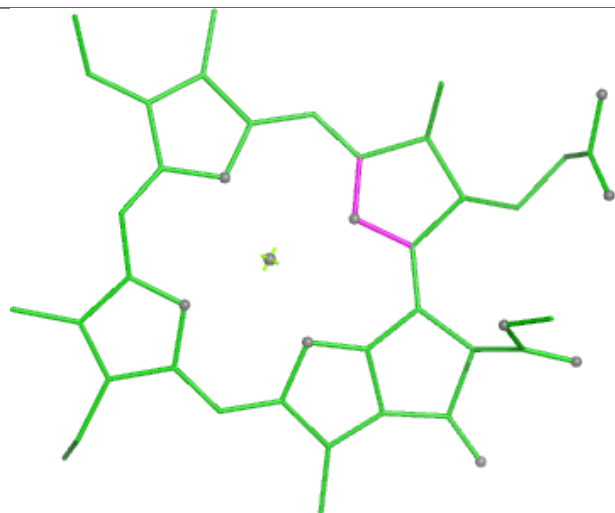
Rings



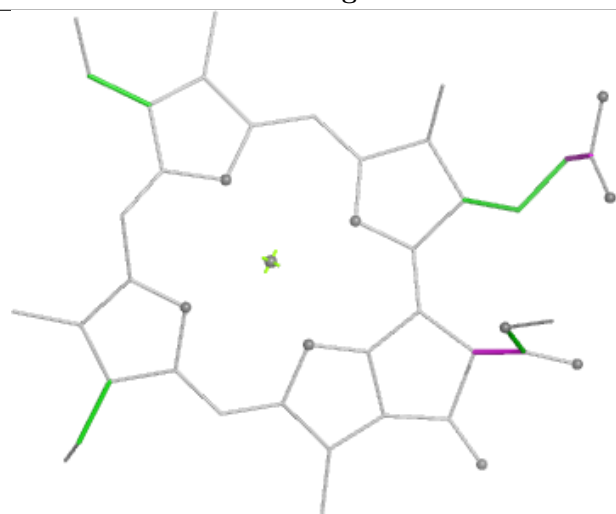
Ligand A1JWG CG 503



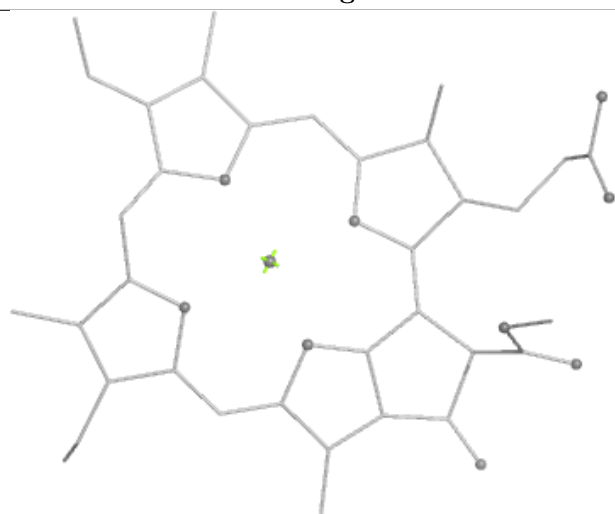
Bond lengths



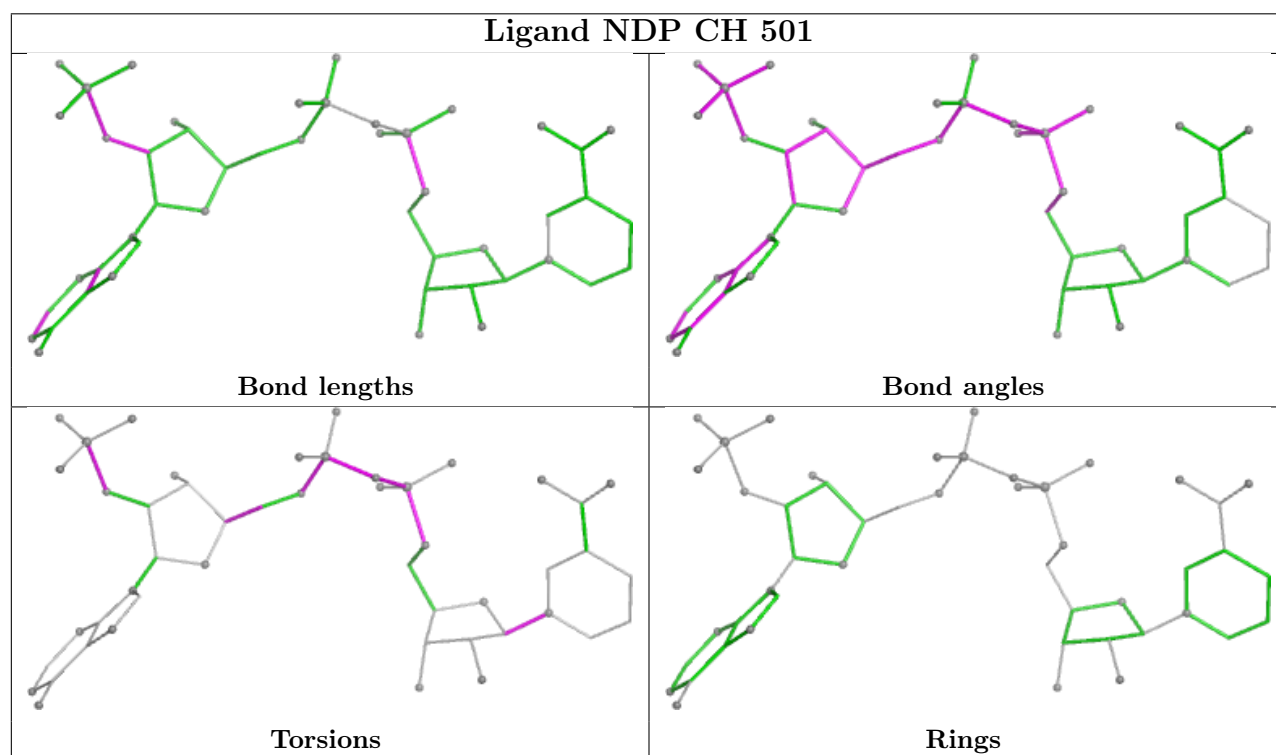
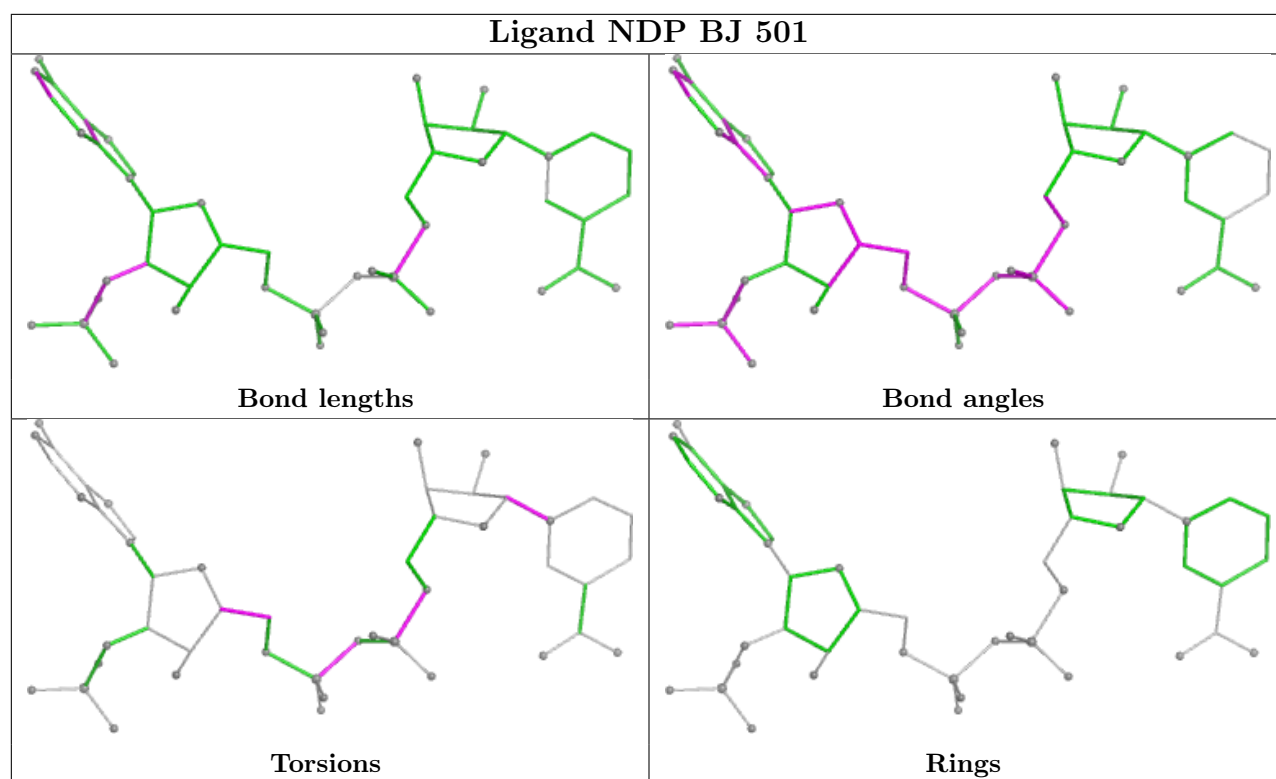
Bond angles



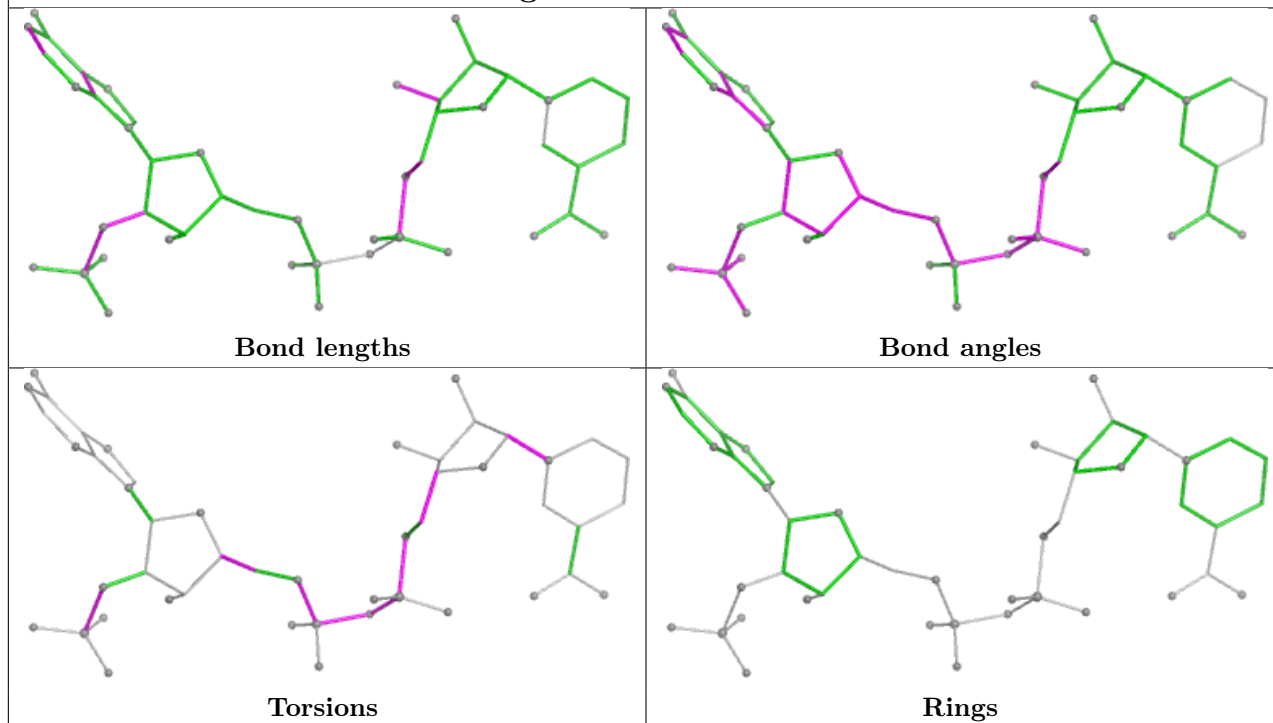
Torsions



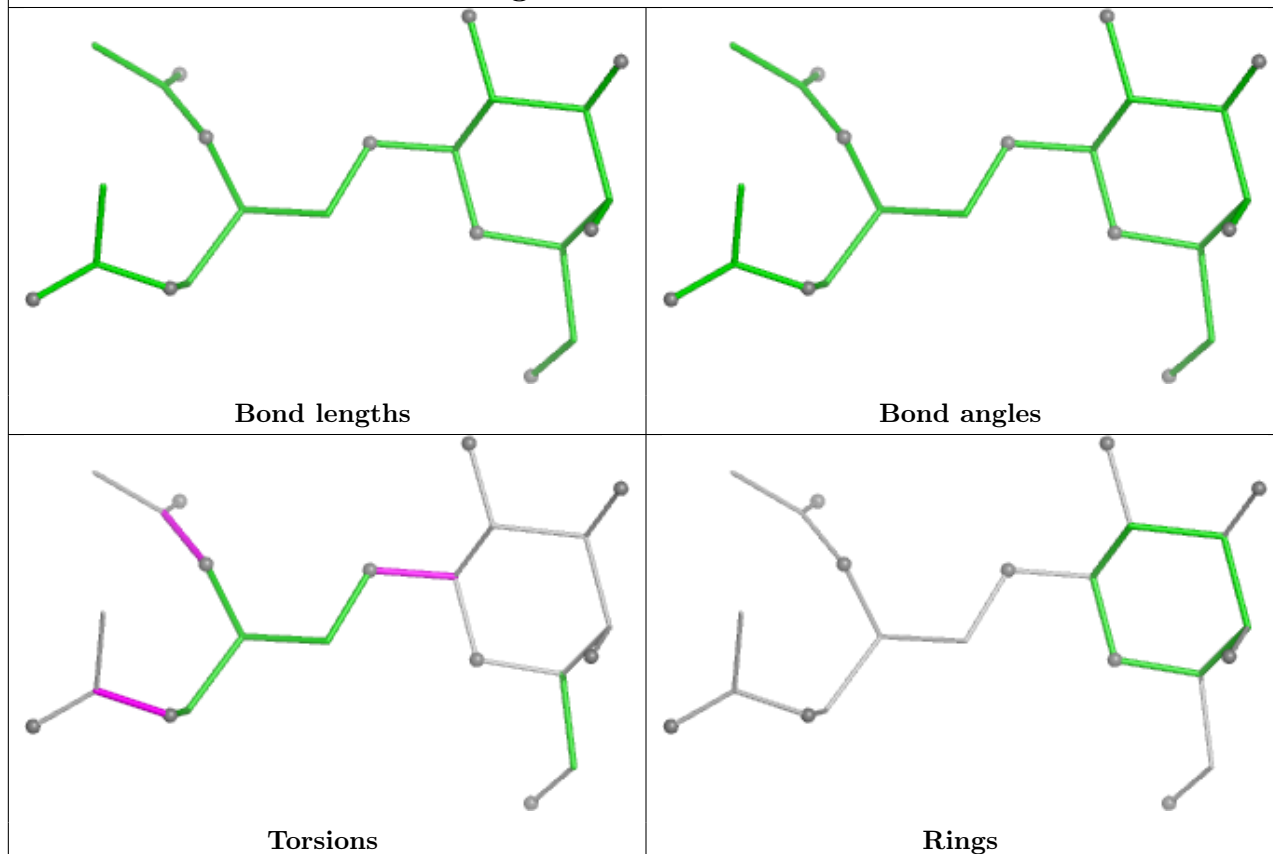
Rings

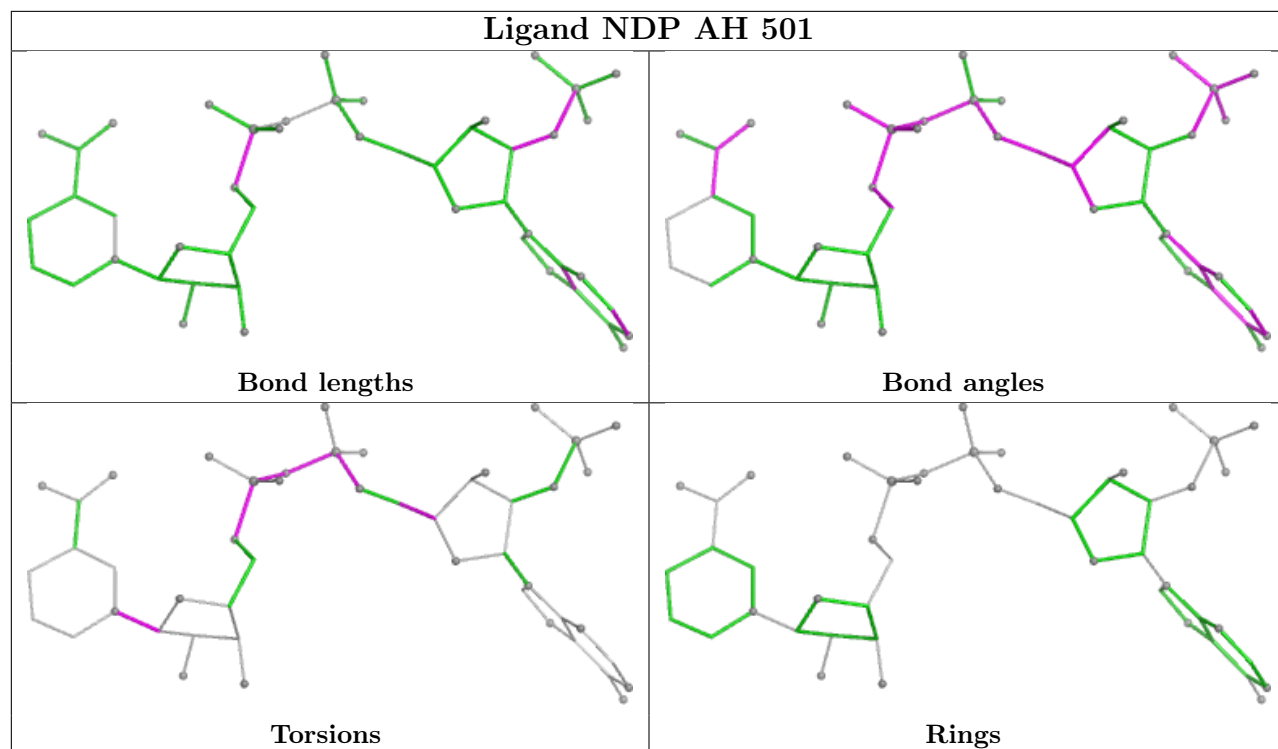


Ligand NDP CI 501

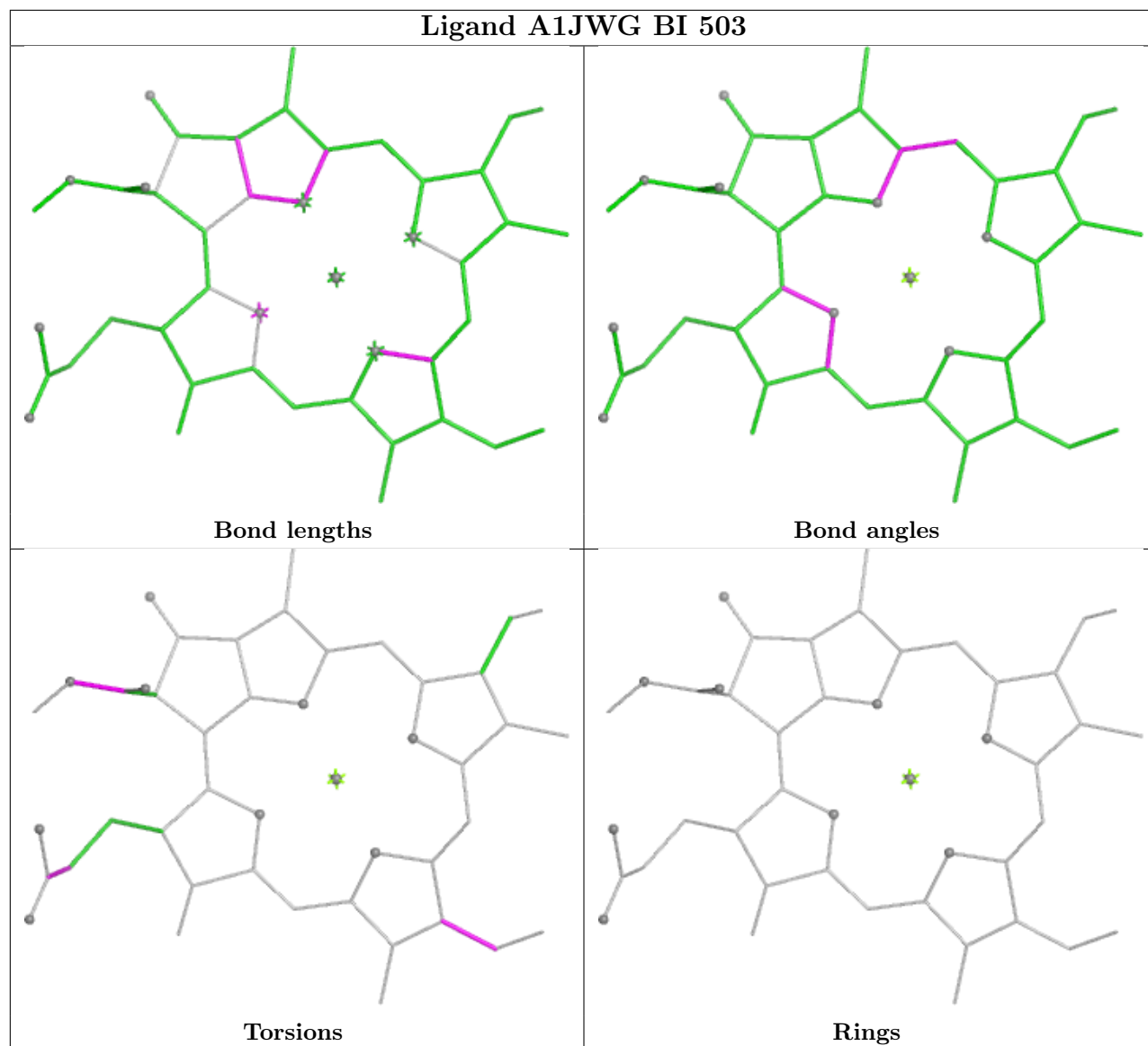


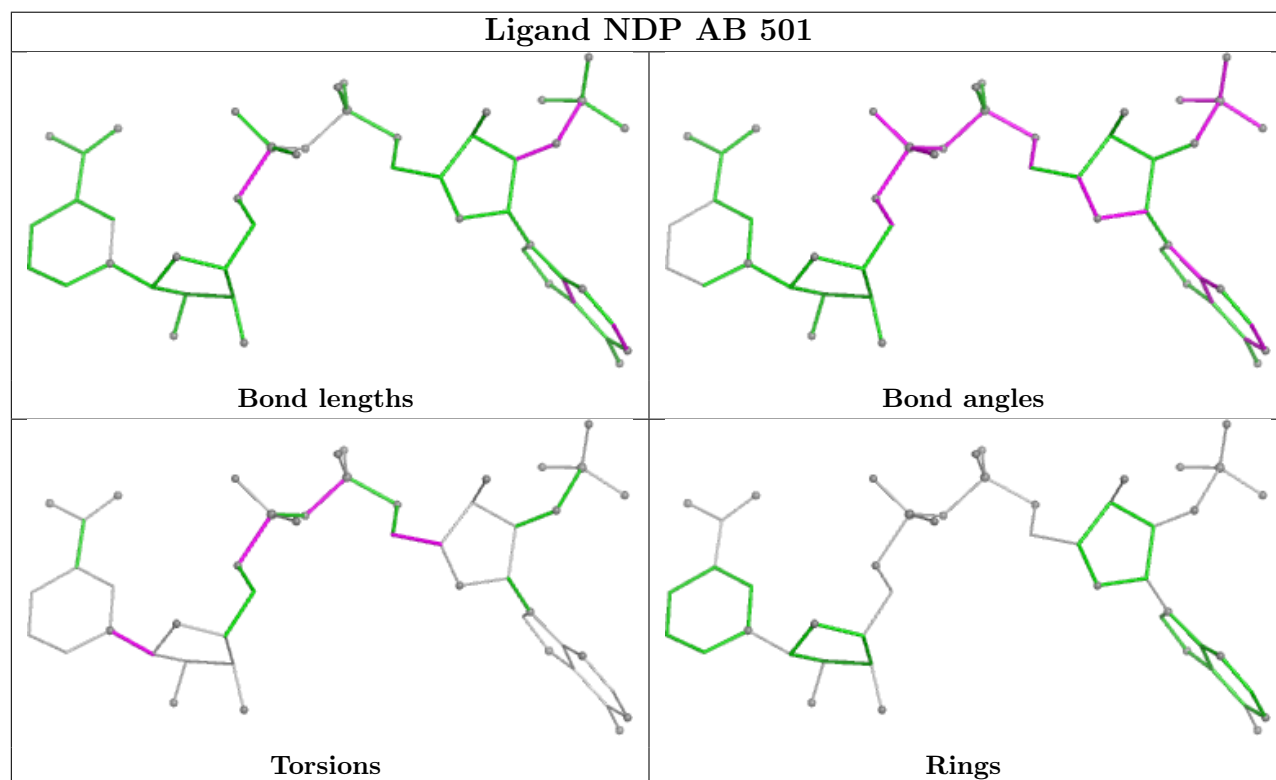
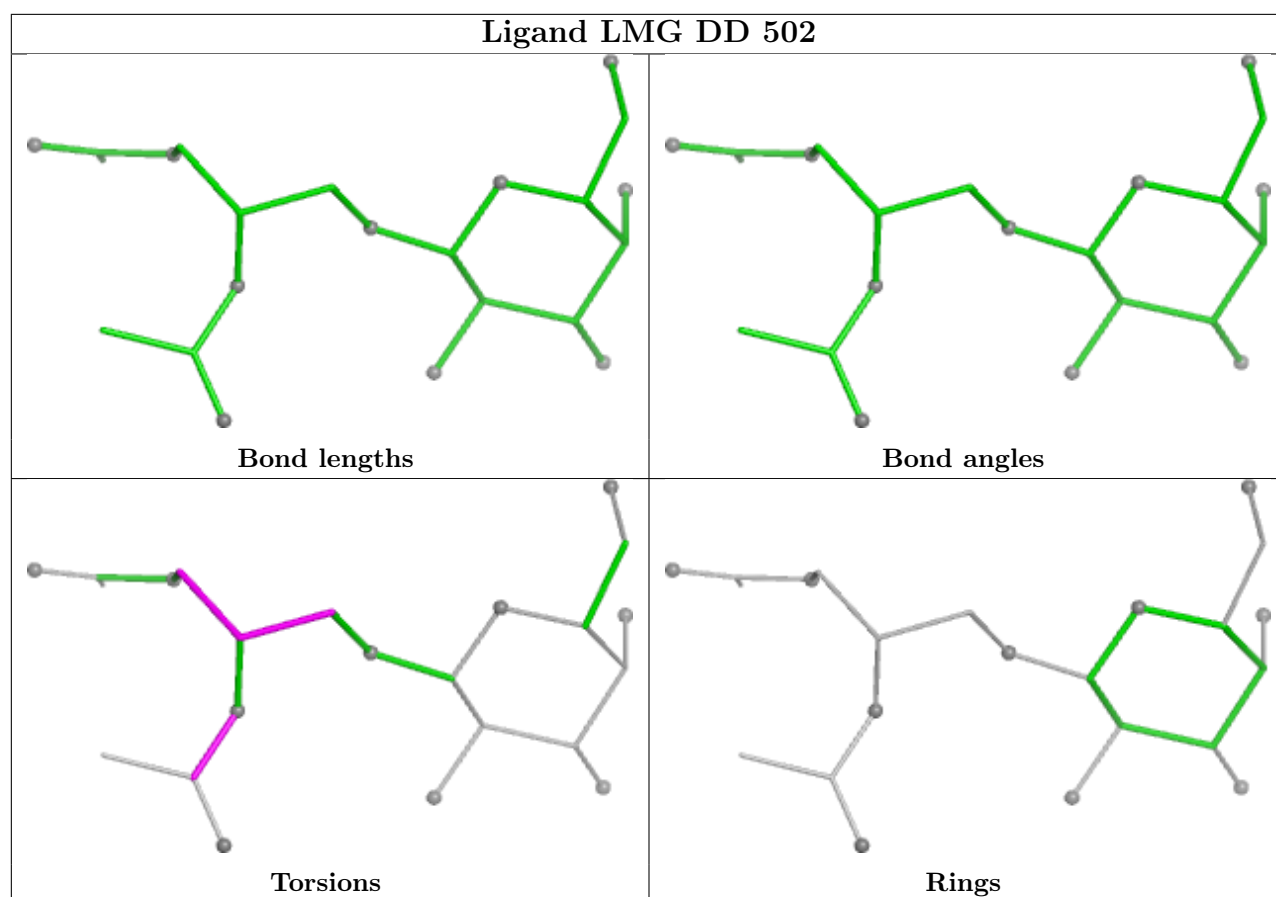
Ligand LMG CH 502



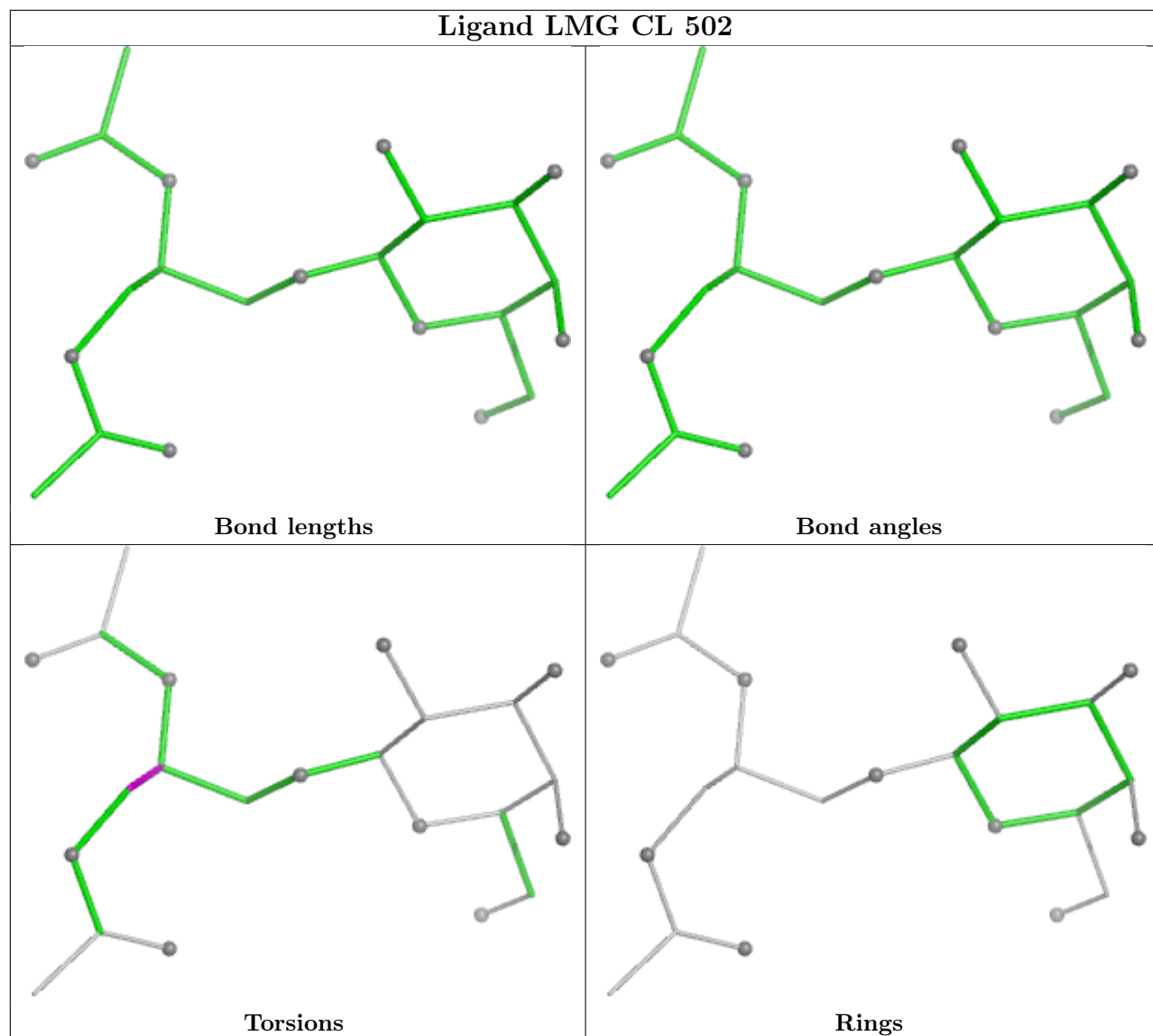


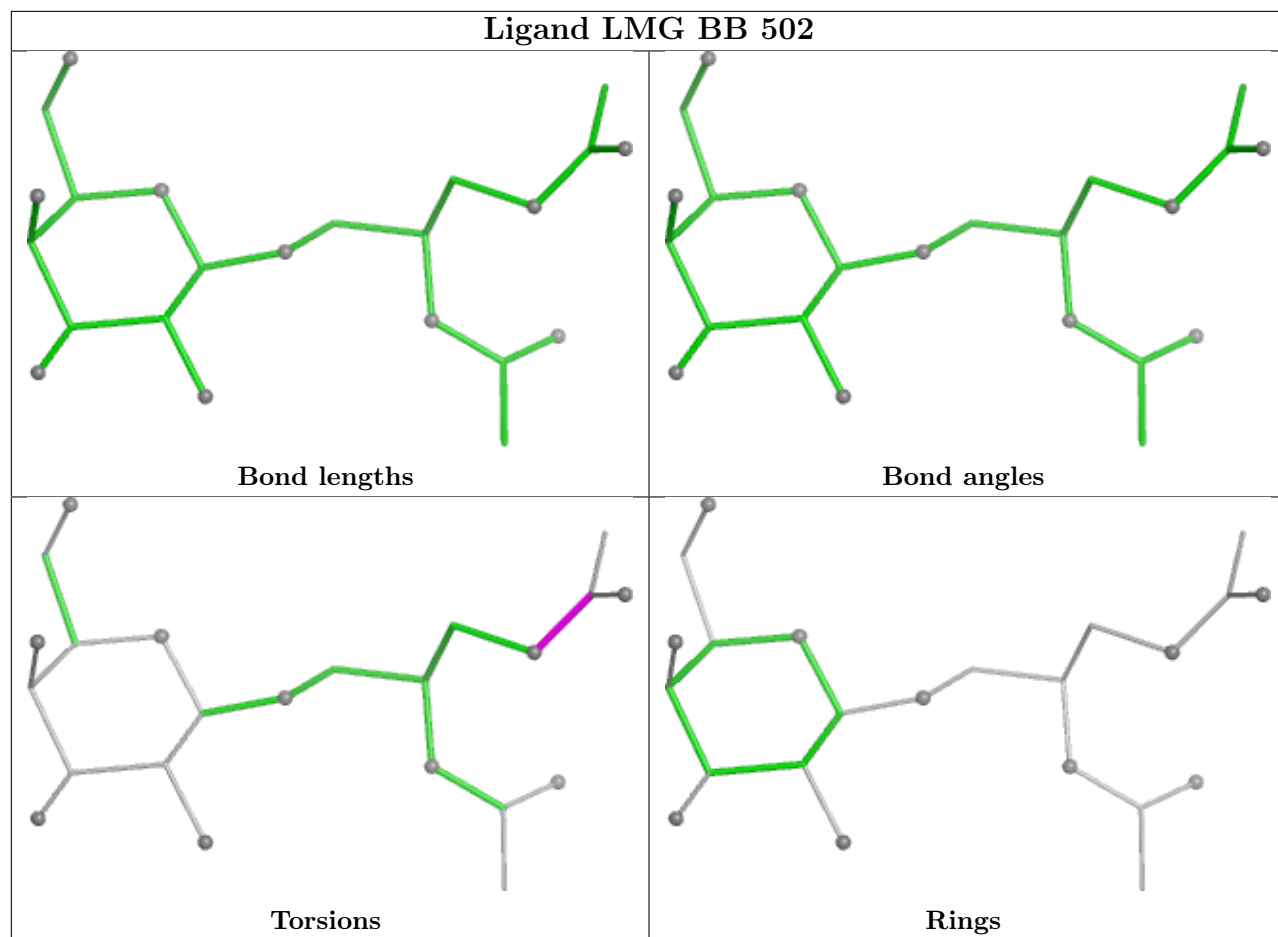
Ligand A1JWG BI 503

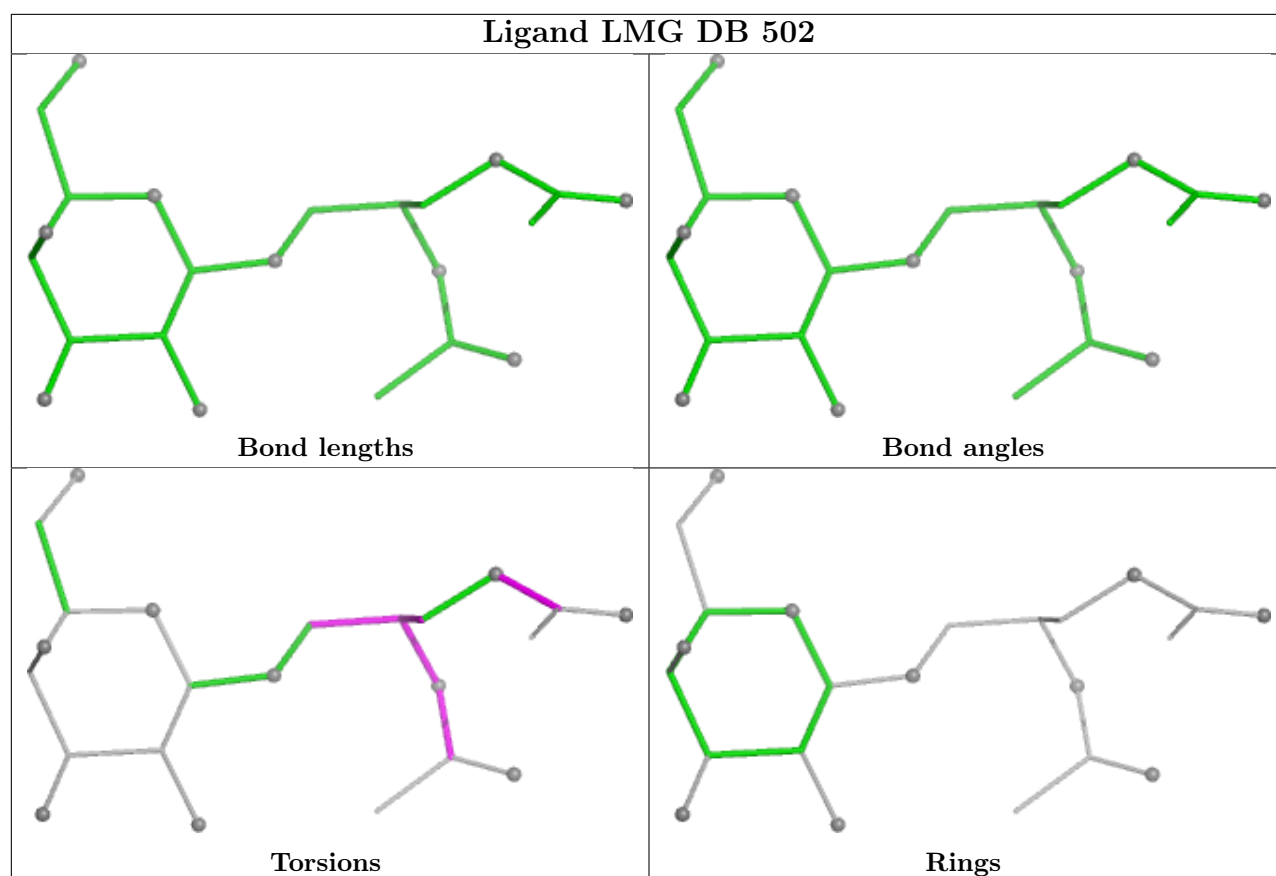




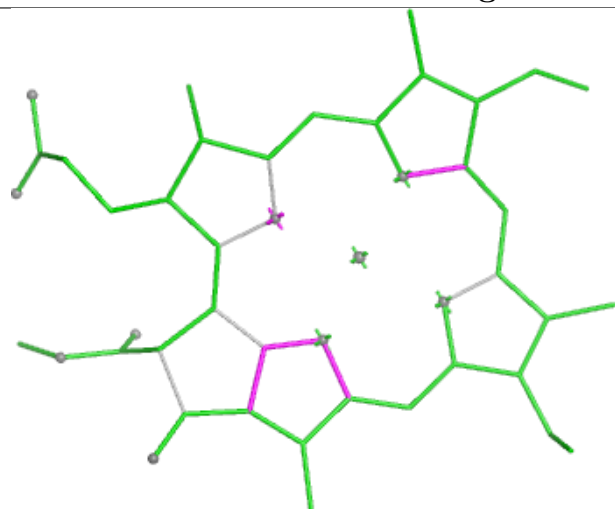
Ligand LMG CL 502



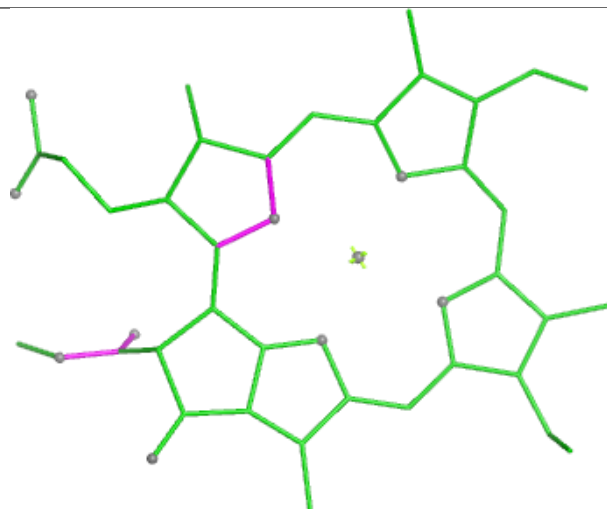




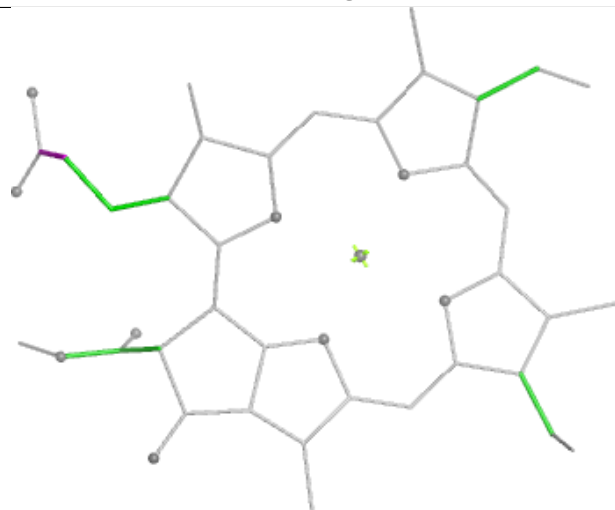
Ligand A1JWG BF 503



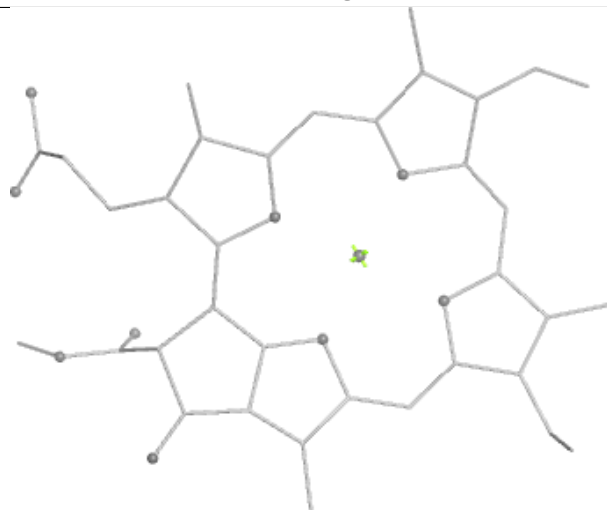
Bond lengths



Bond angles

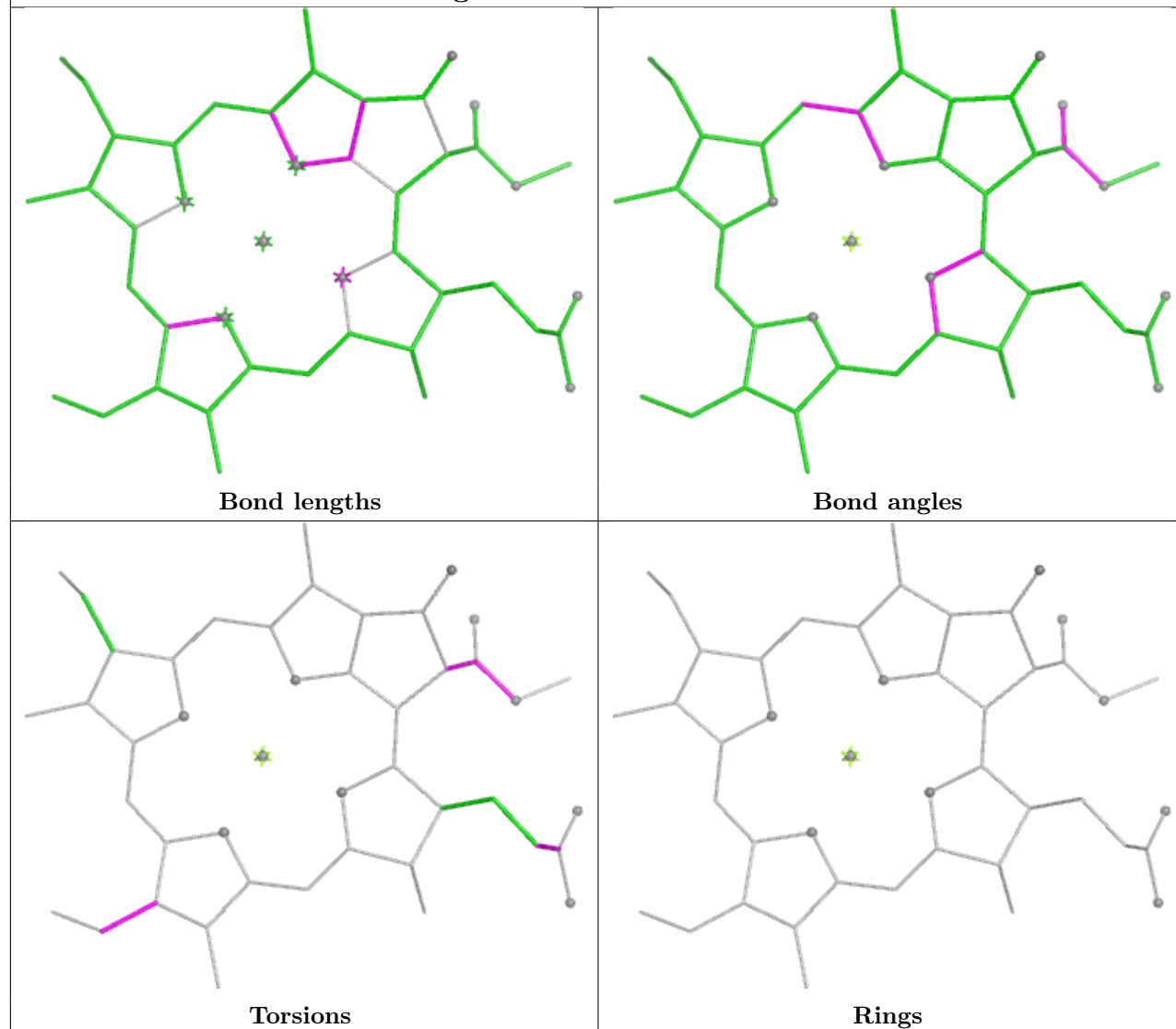


Torsions

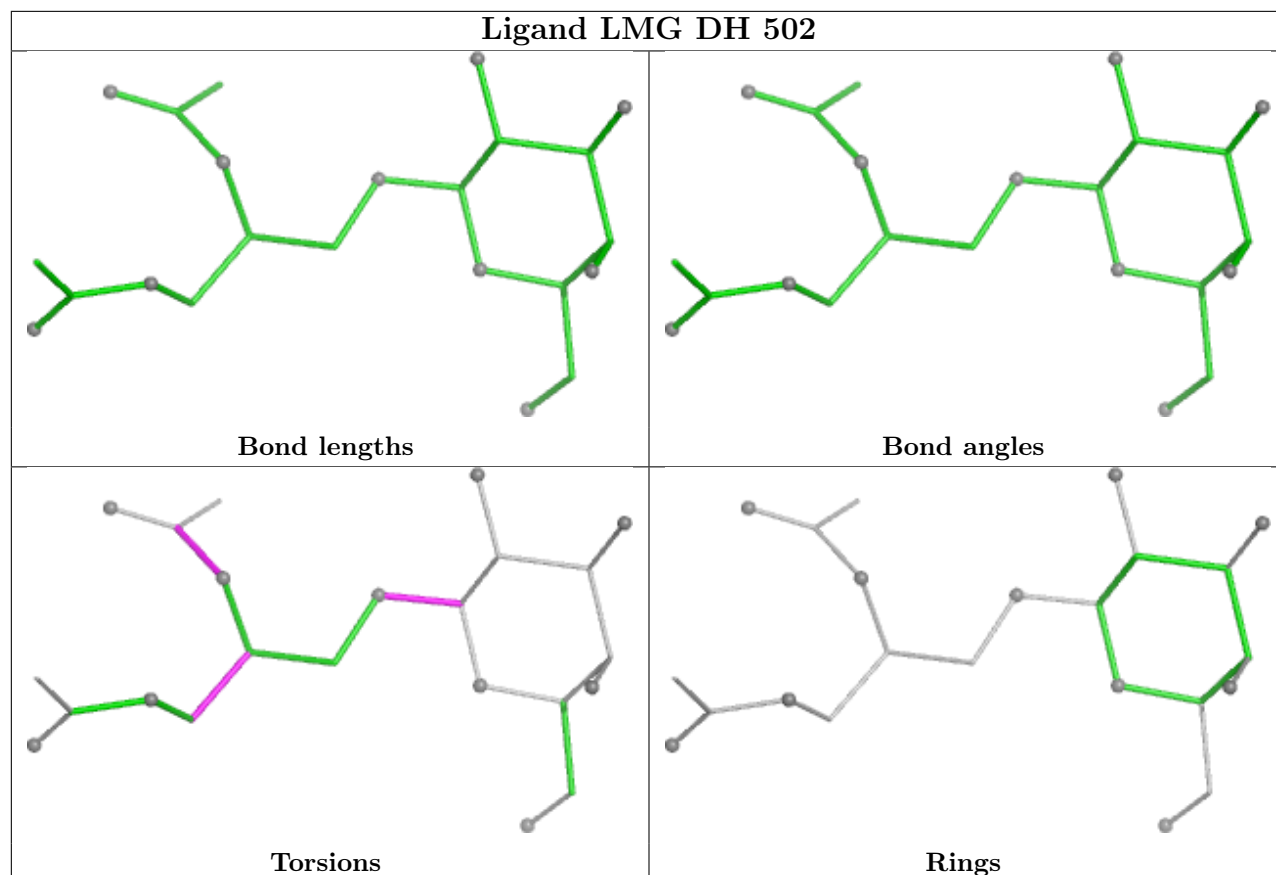


Rings

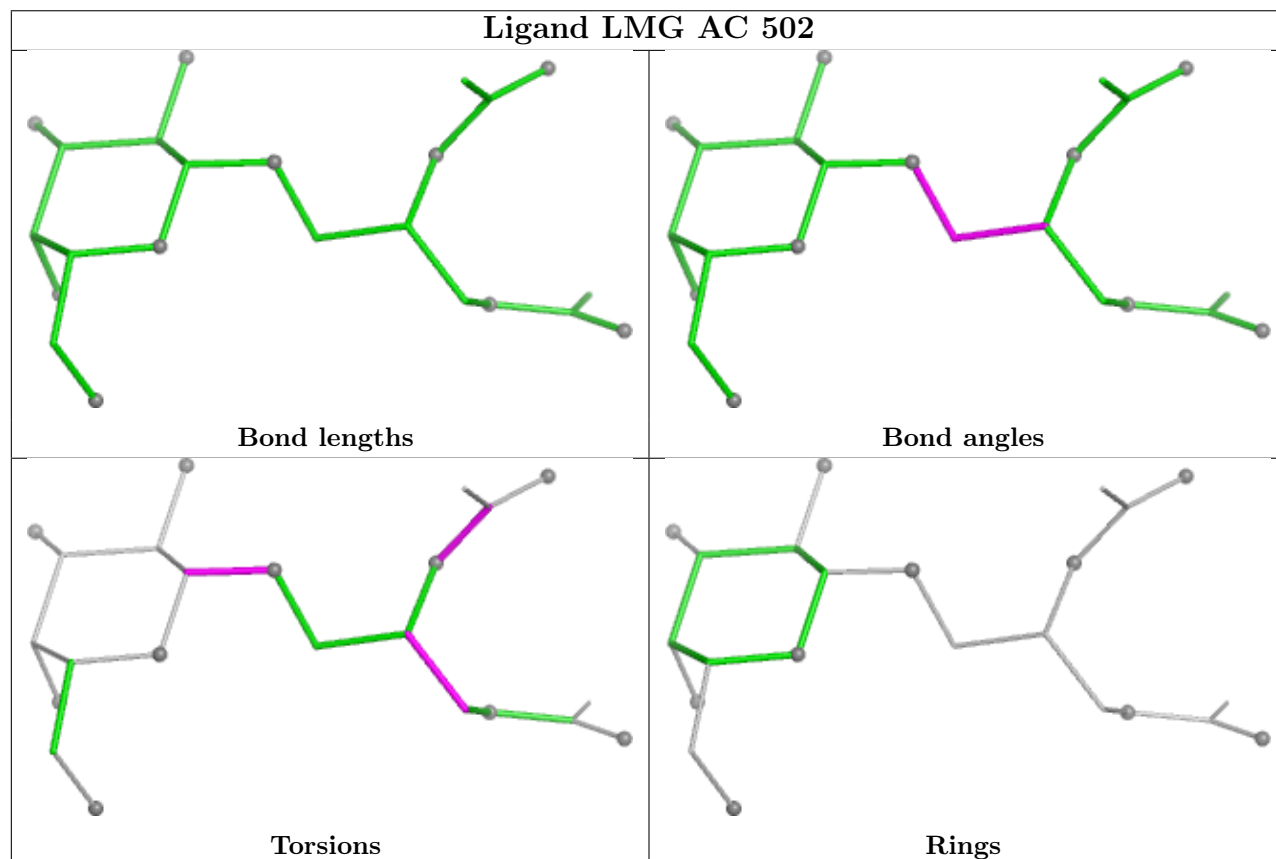
Ligand A1JWG CH 503



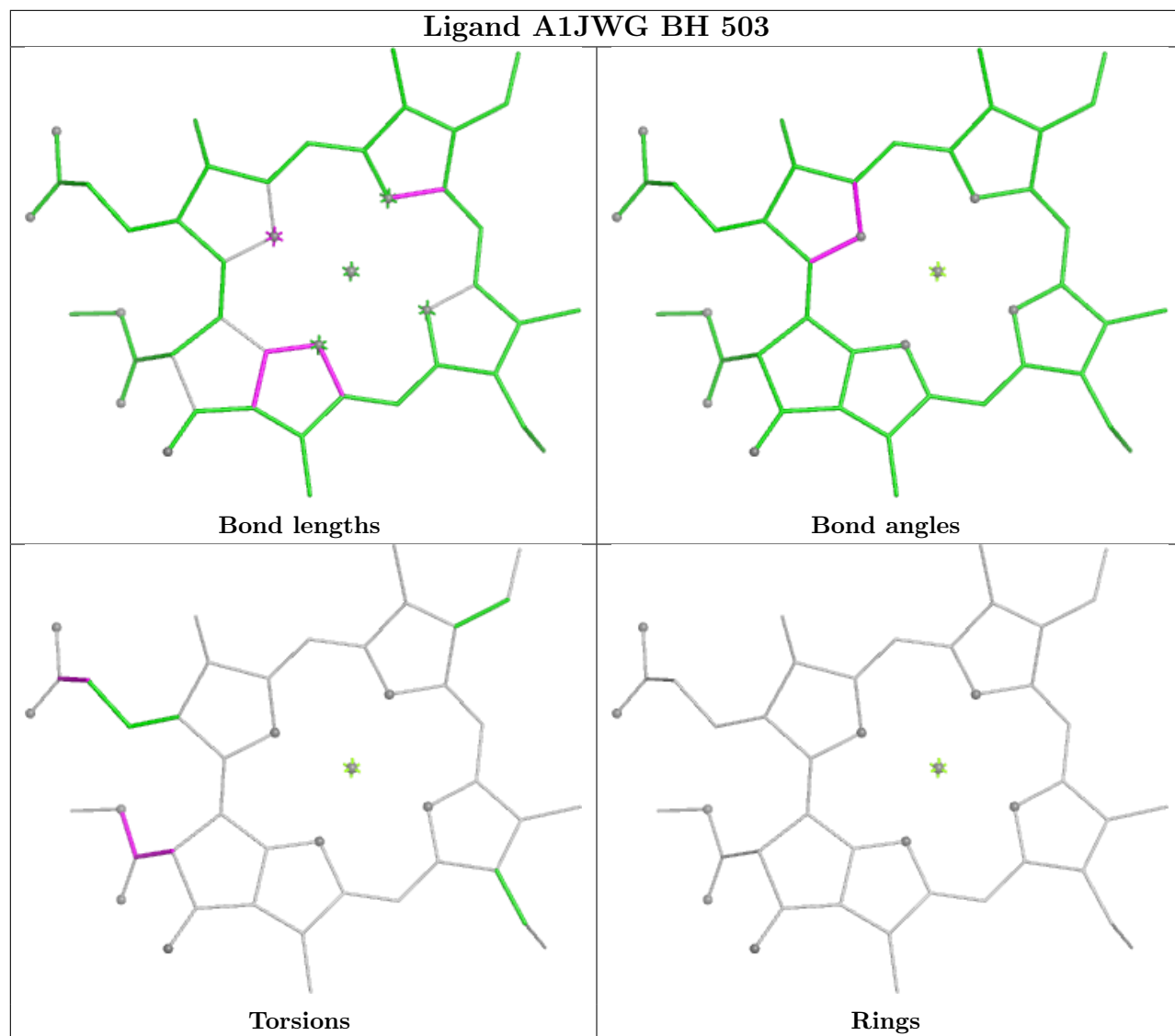
Ligand LMG DH 502



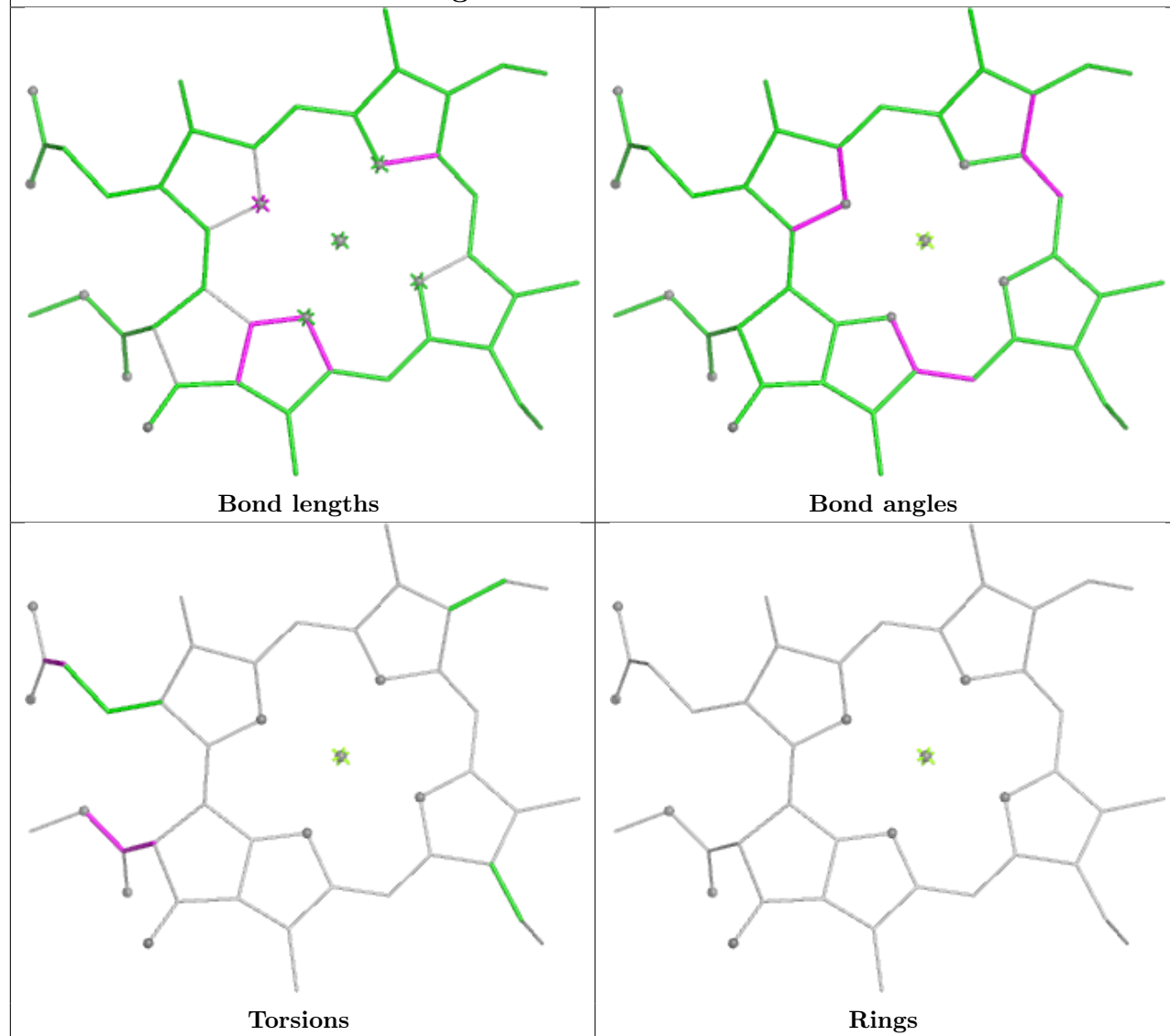
Ligand LMG AC 502

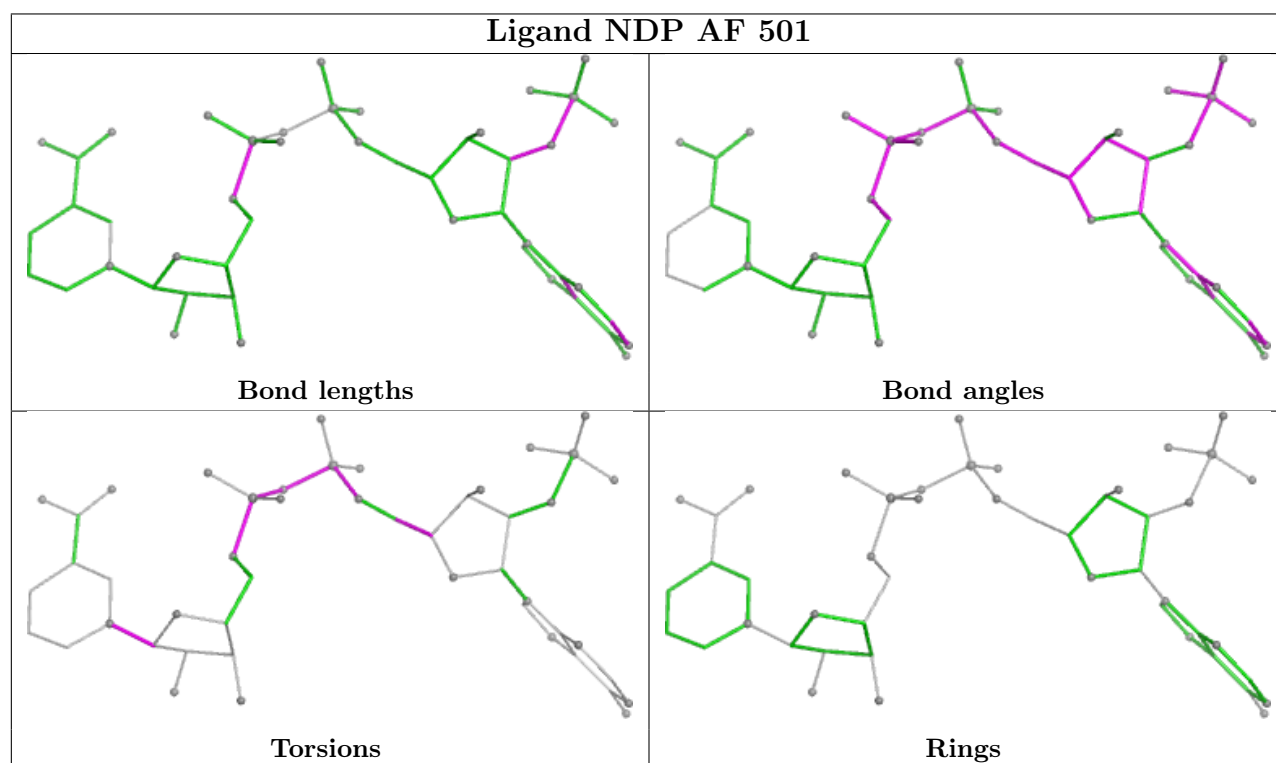
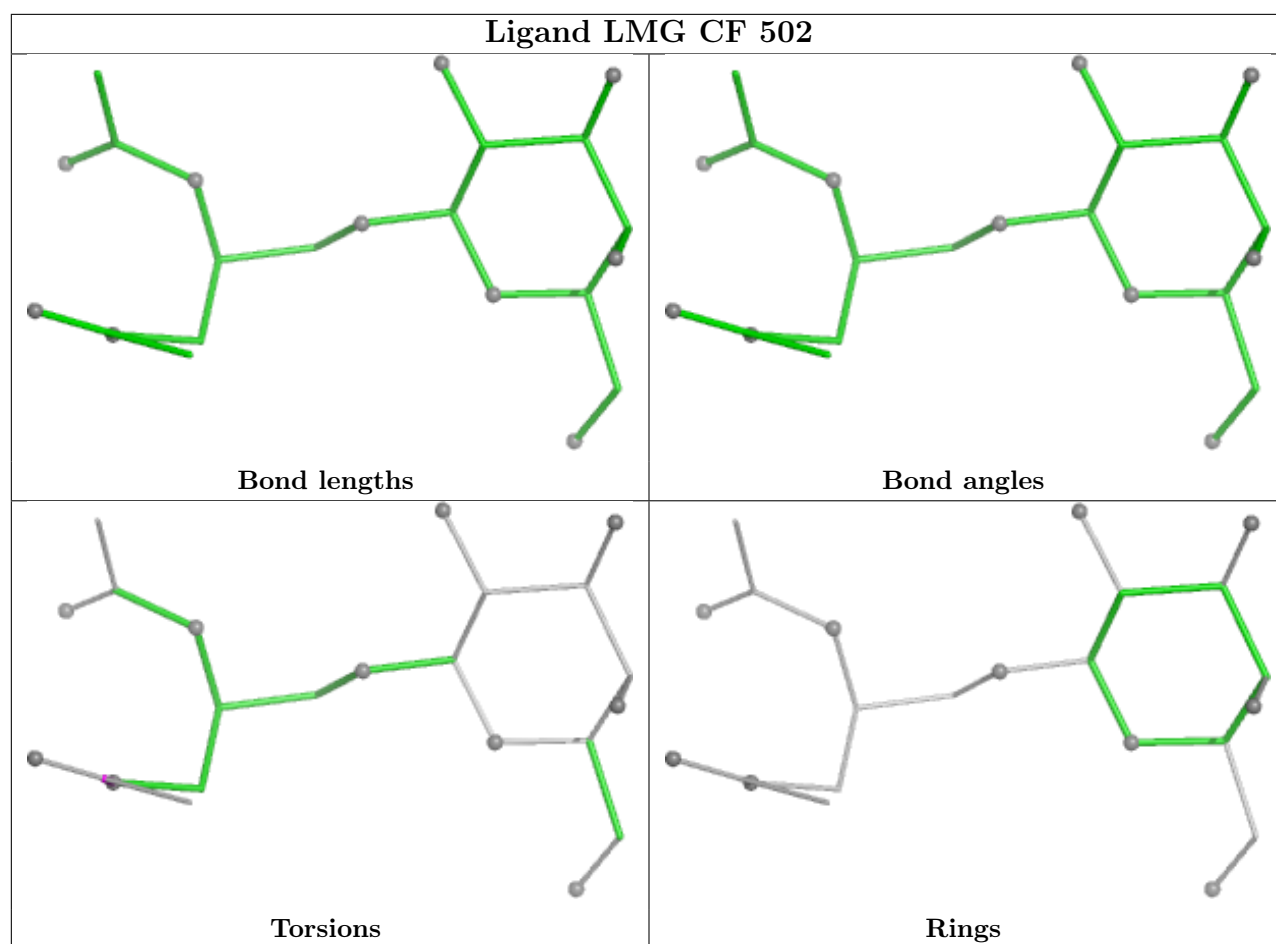


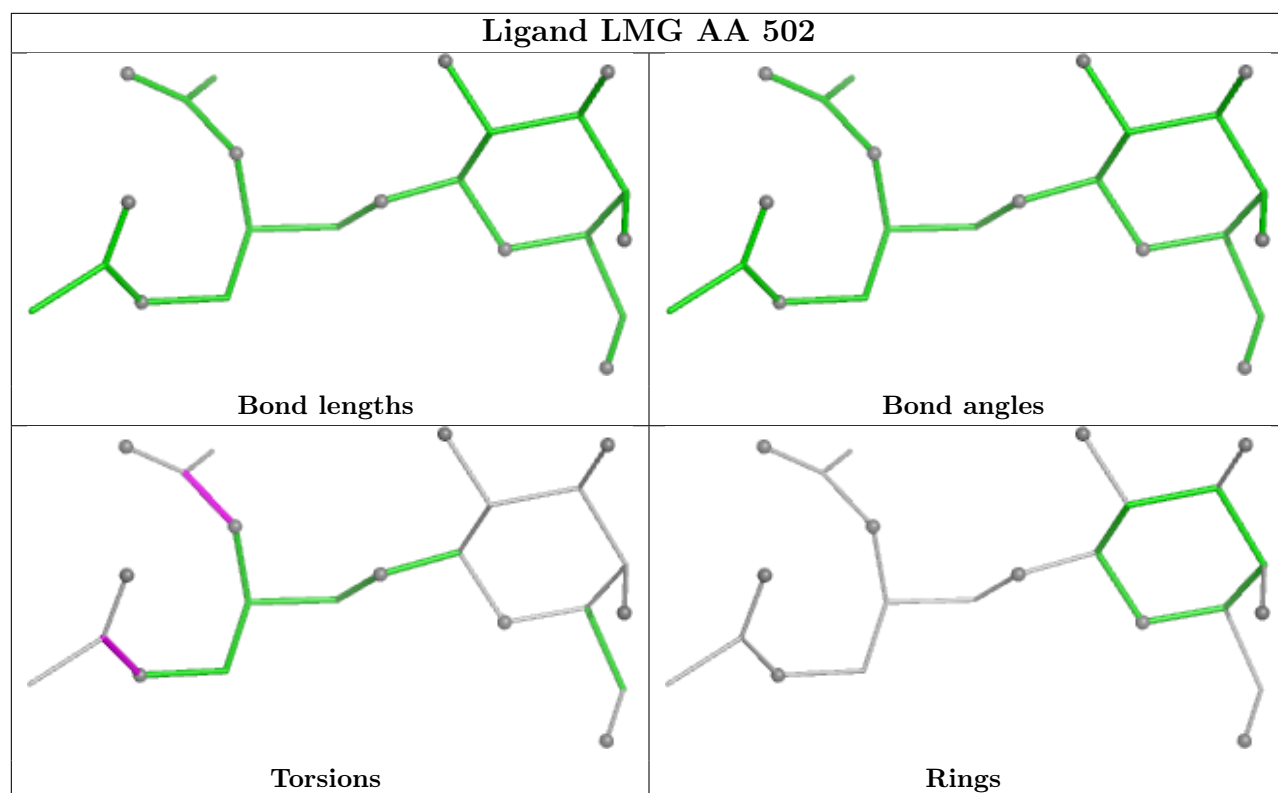
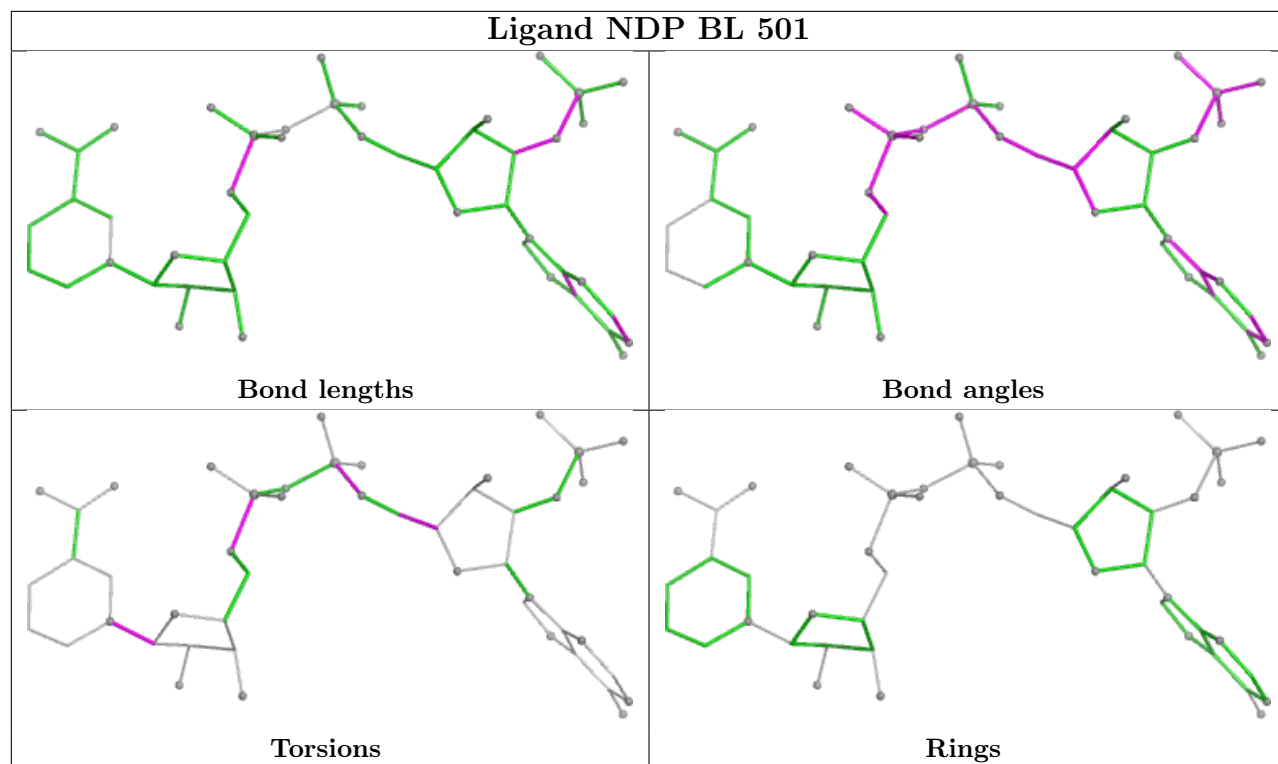
Ligand A1JWG BH 503



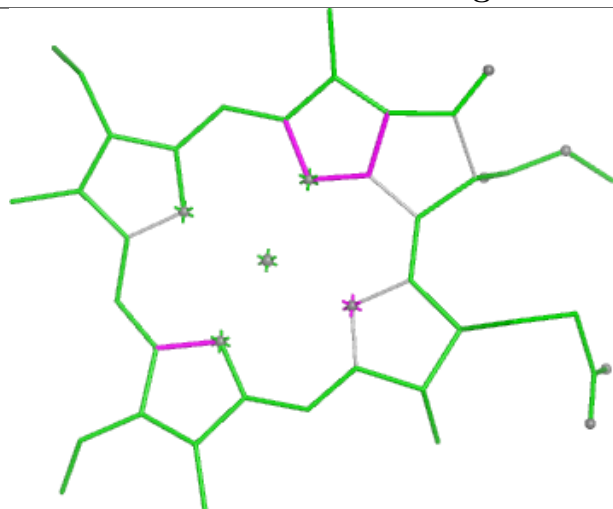
Ligand A1JWG BB 503



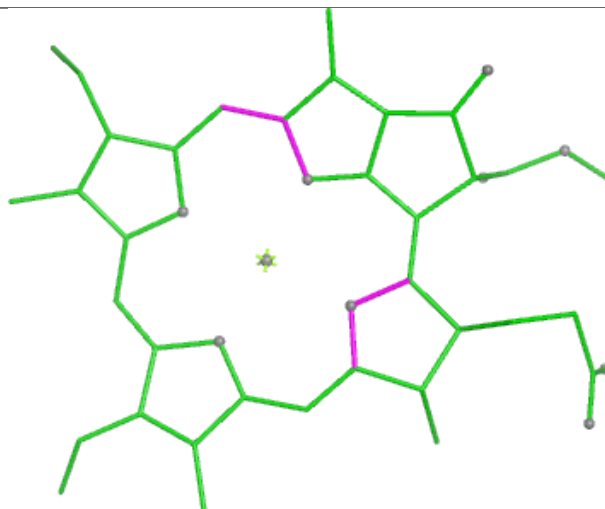




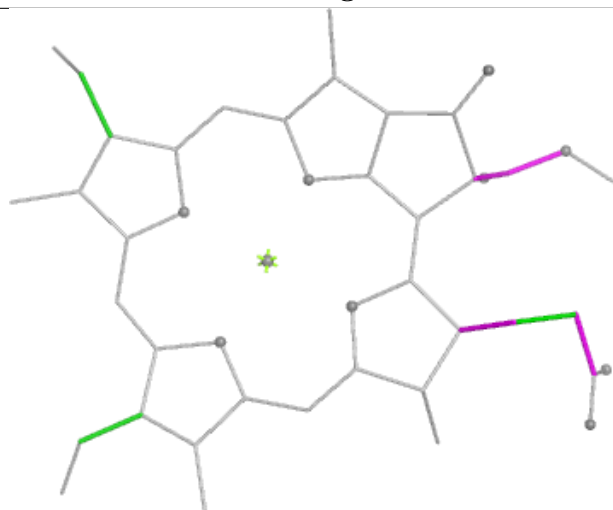
Ligand A1JWG AH 503



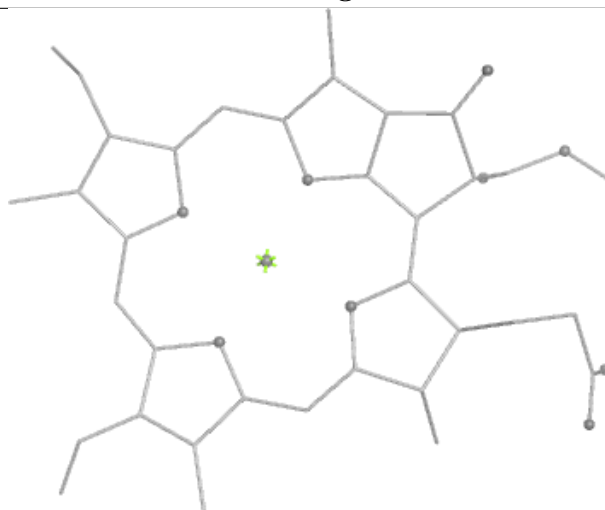
Bond lengths



Bond angles

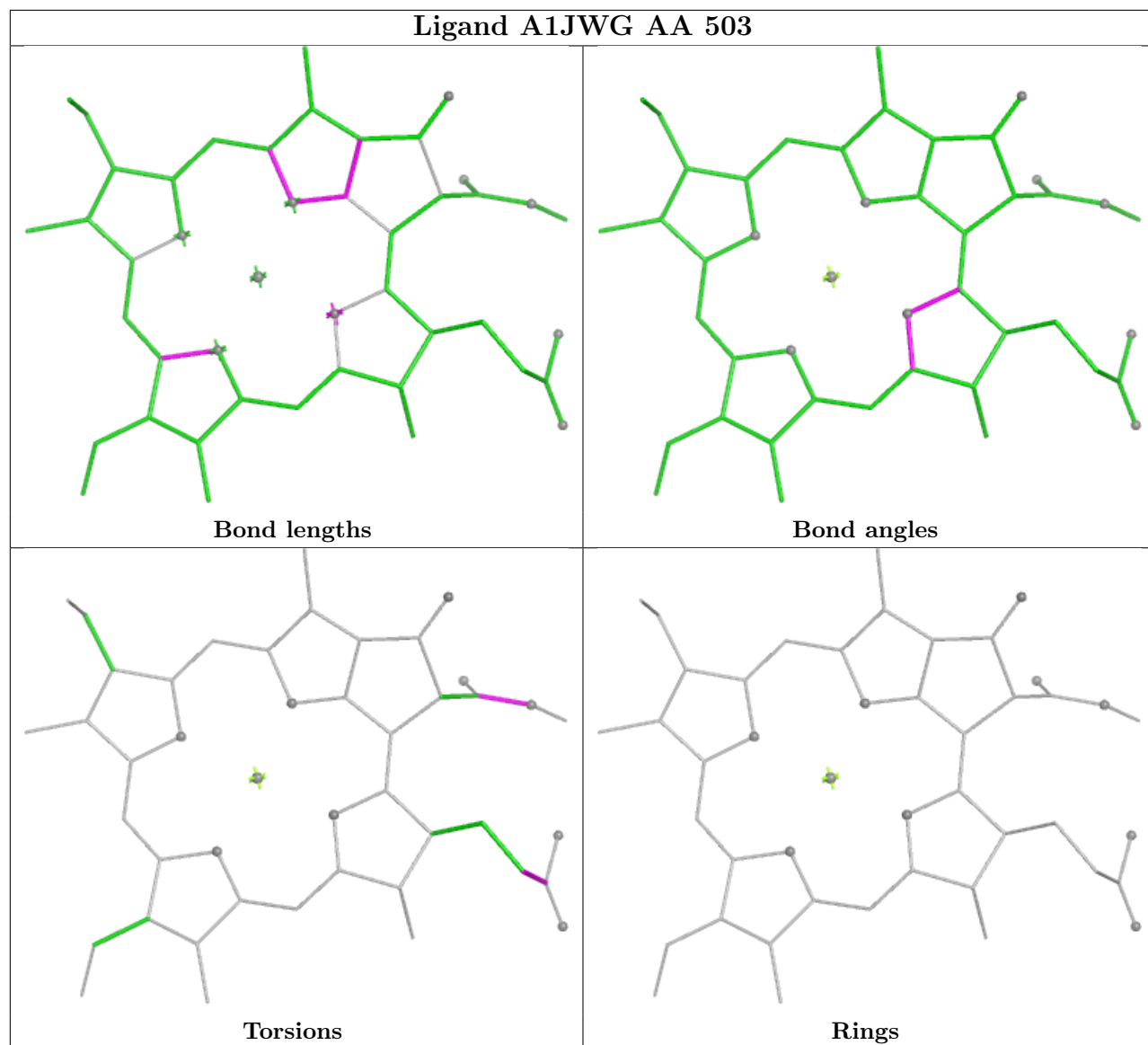


Torsions

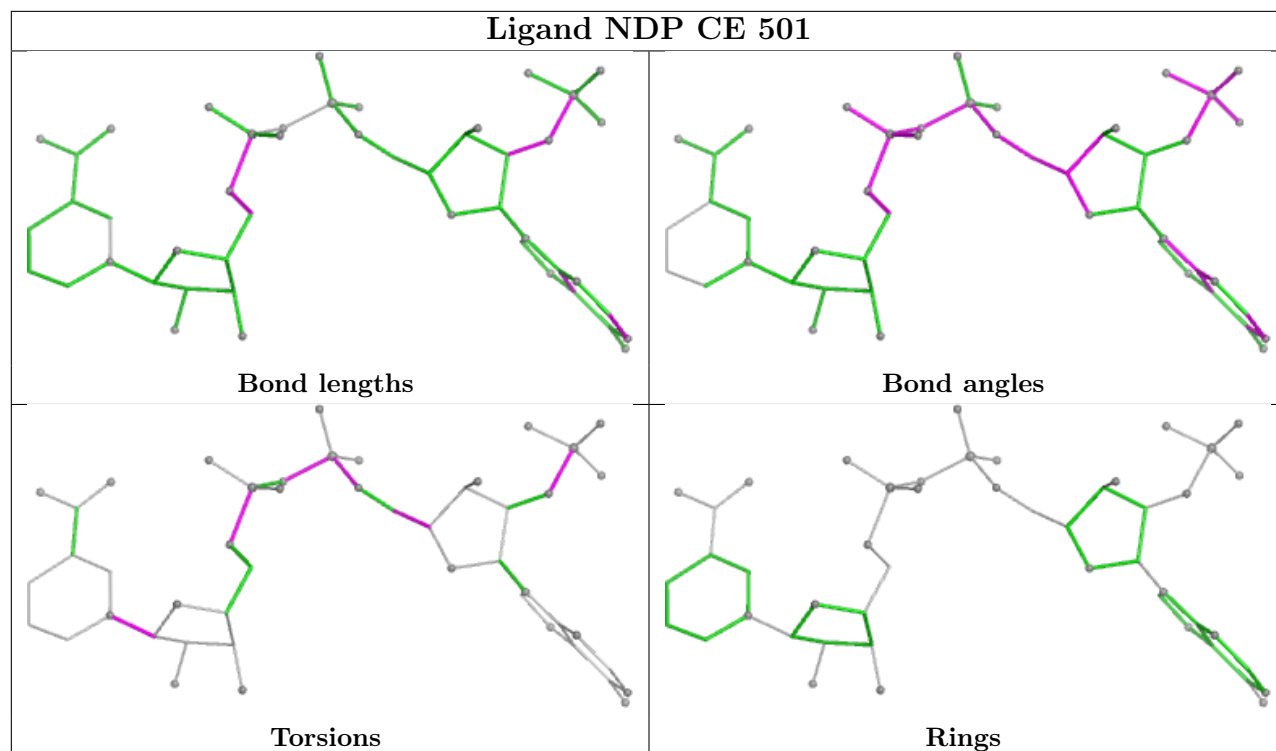


Rings

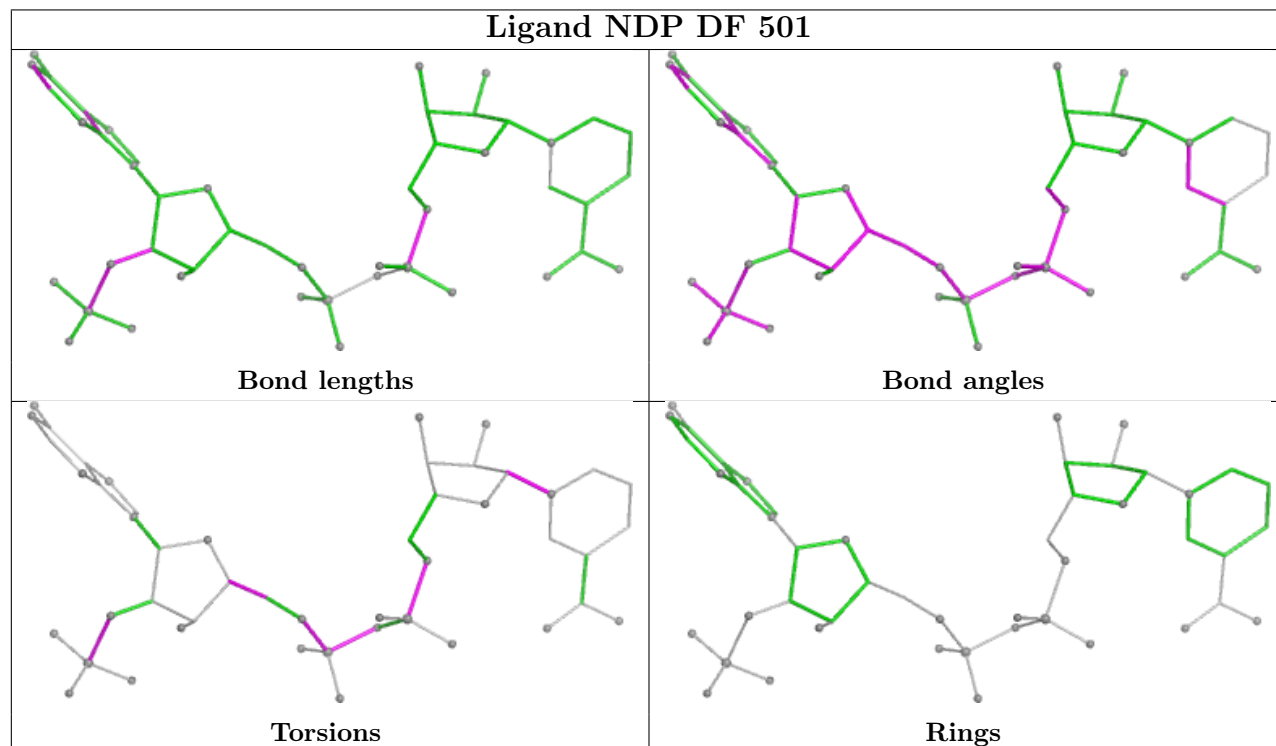
Ligand A1JWG AA 503



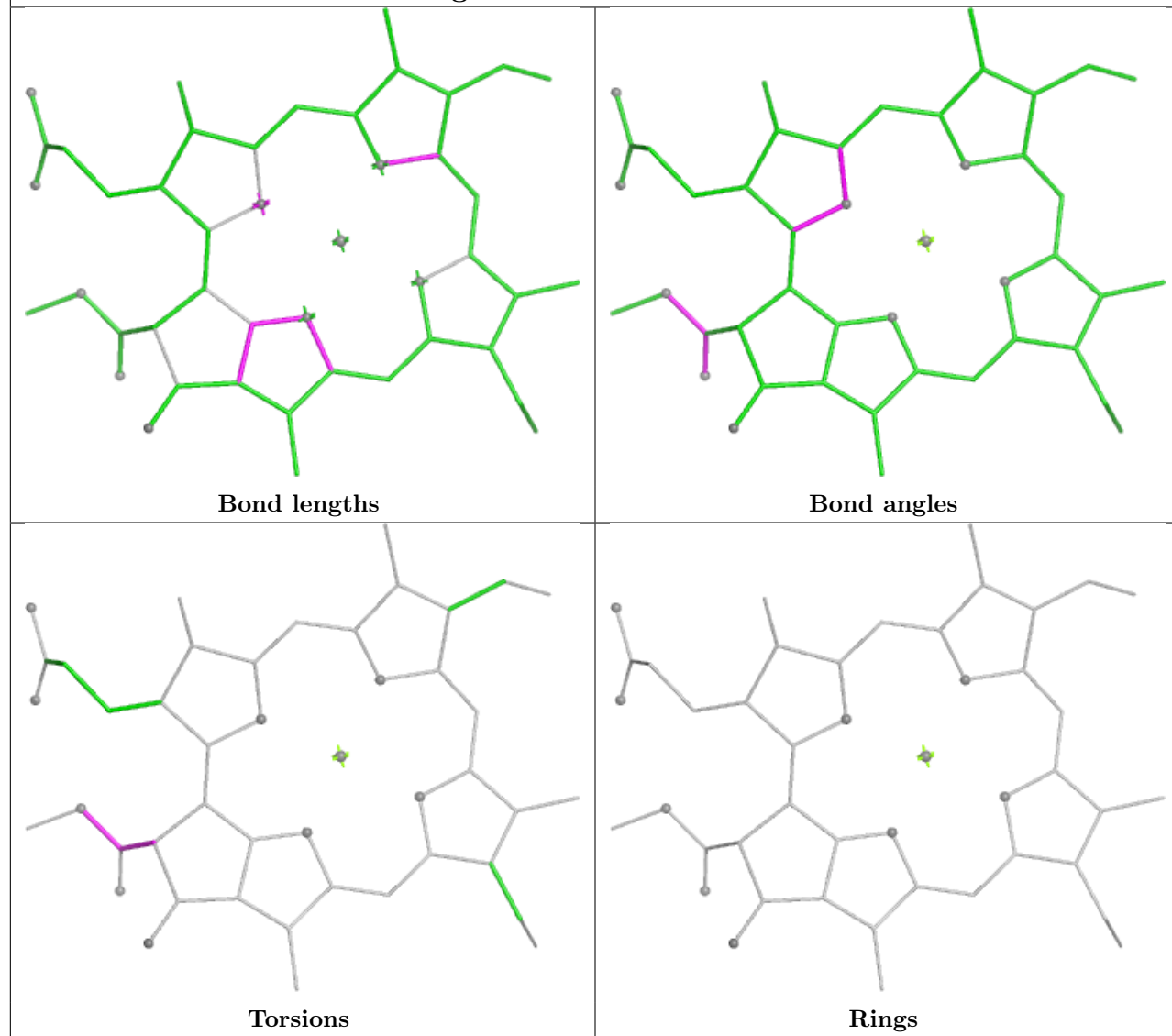
Ligand NDP CE 501



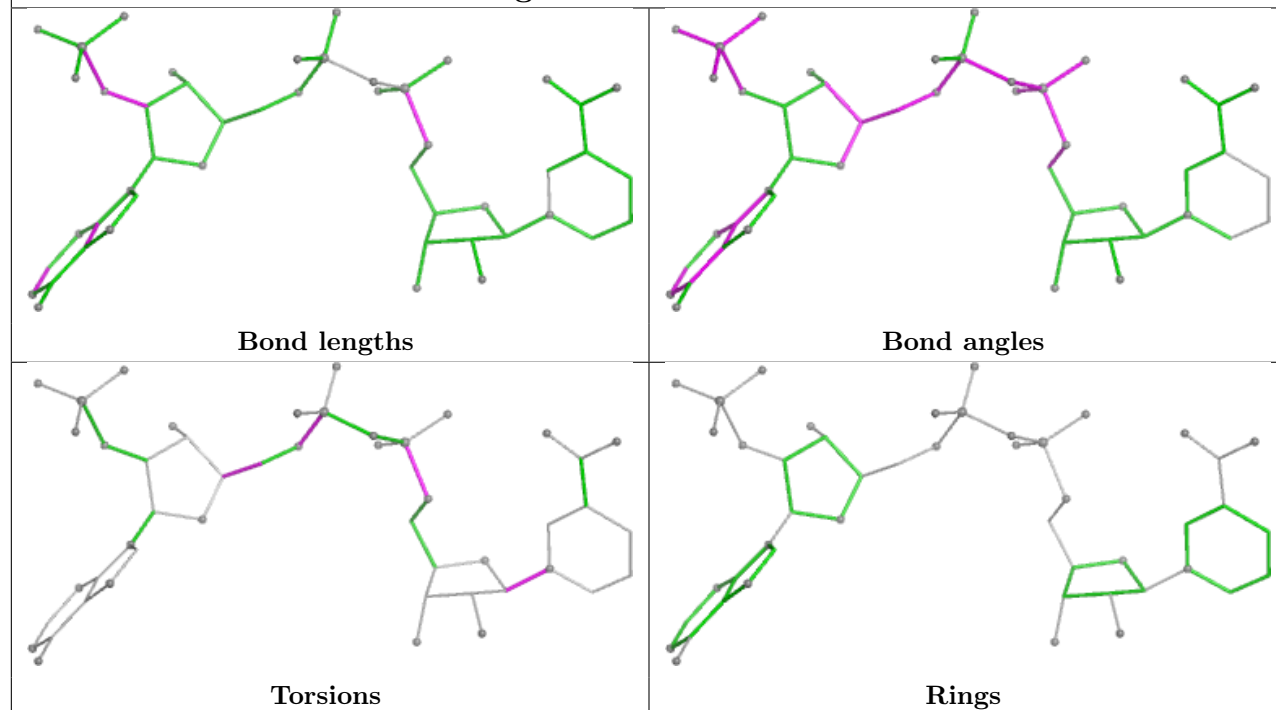
Ligand NDP DF 501



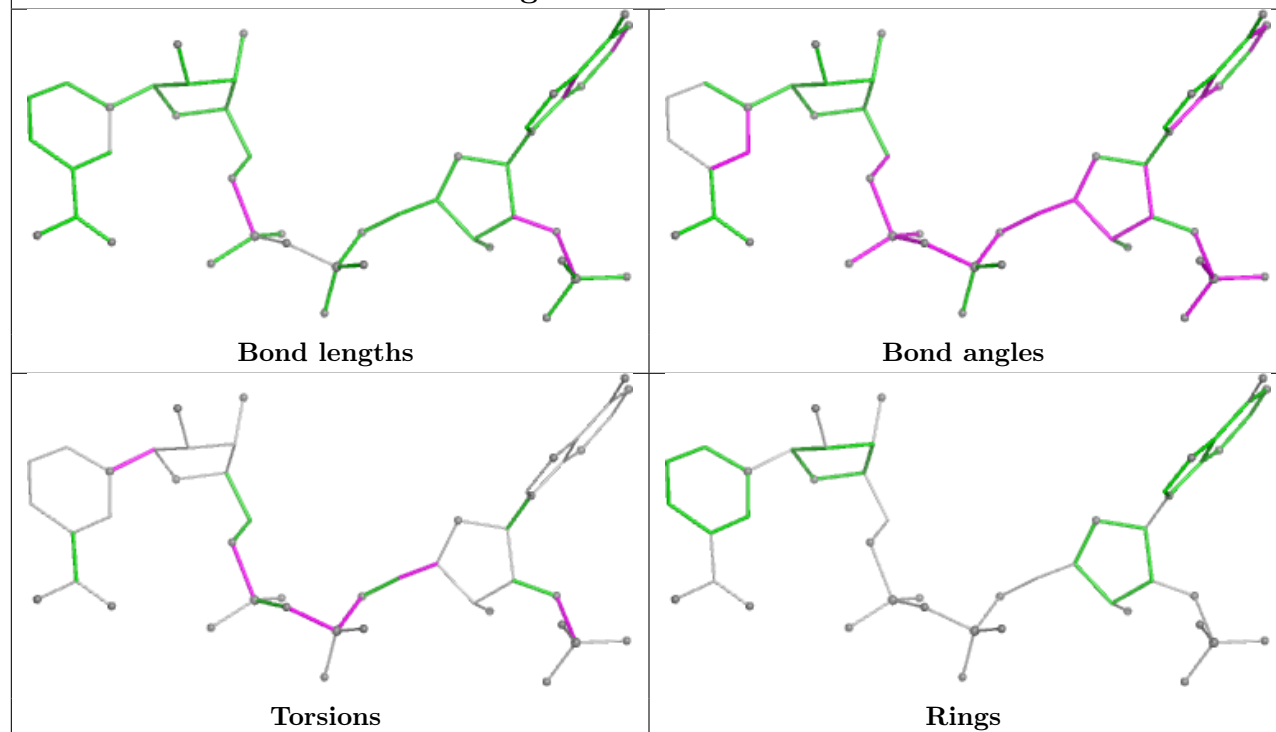
Ligand A1JWG BA 503

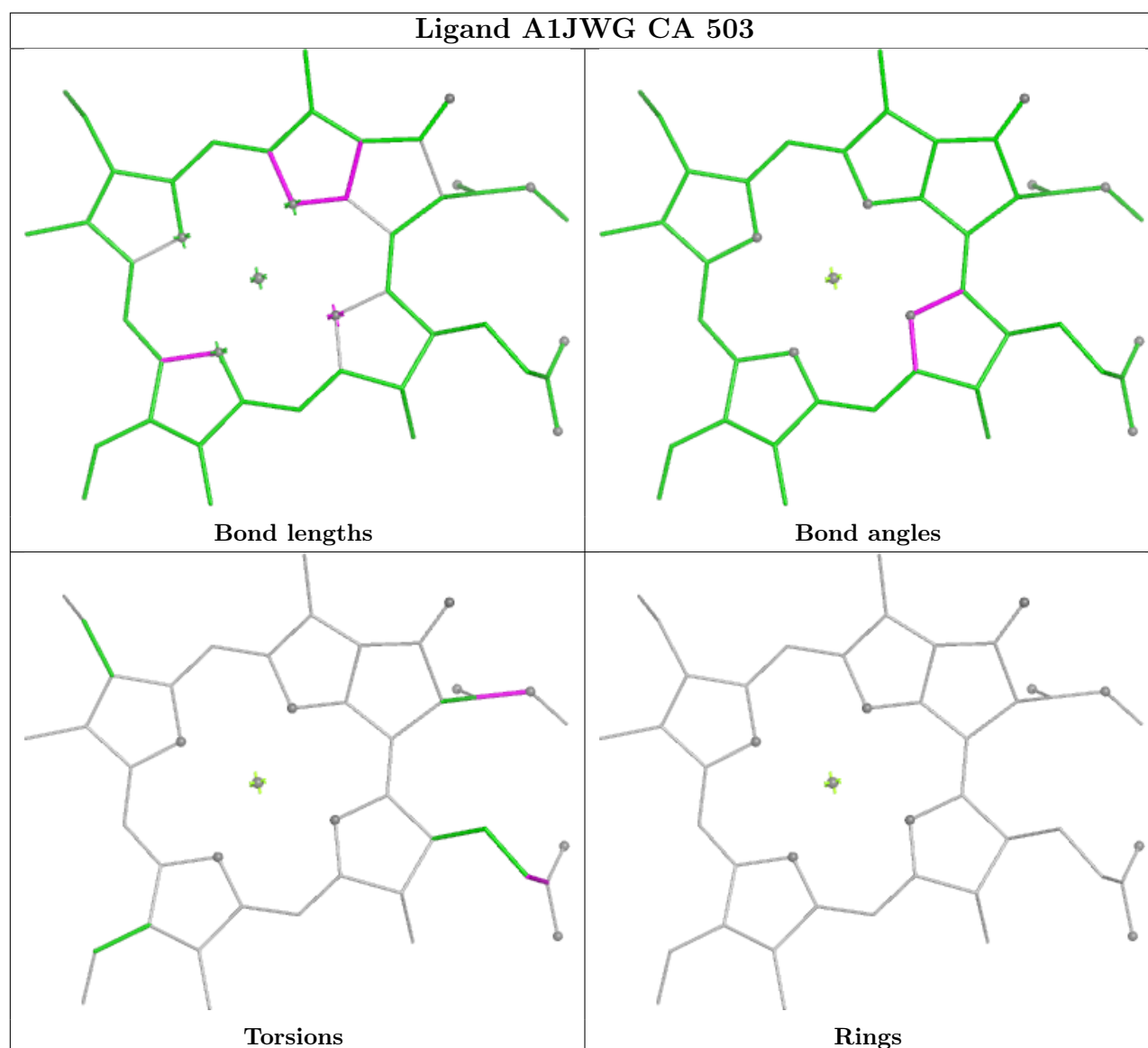


Ligand NDP AK 501



Ligand NDP CJ 501





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.

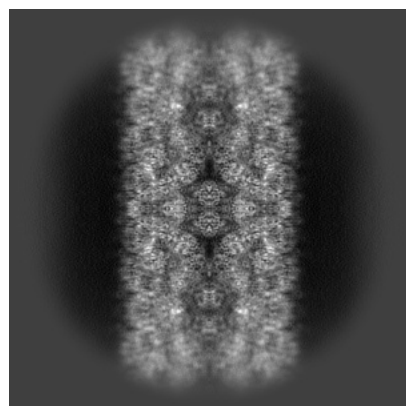
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56056. These allow visual inspection of the internal detail of the map and identification of artifacts.

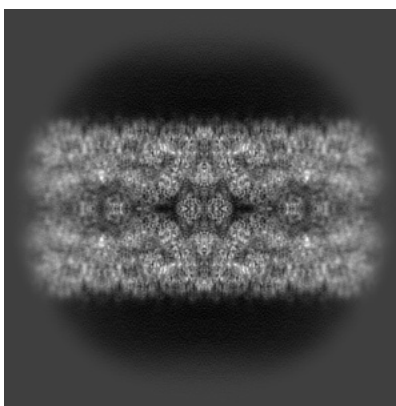
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

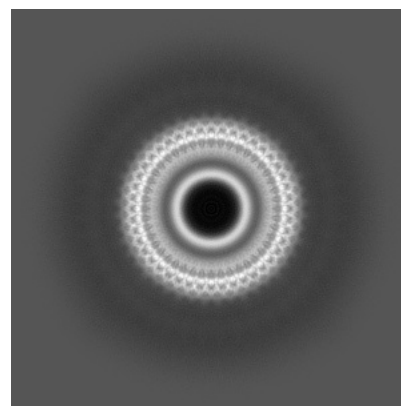
6.1.1 Primary map



X

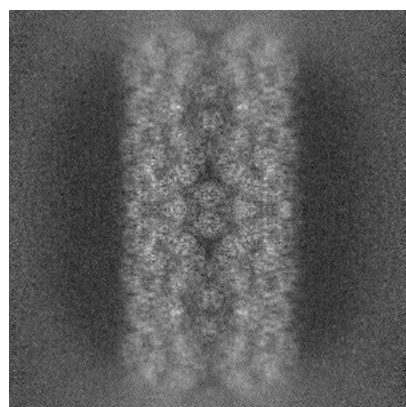


Y

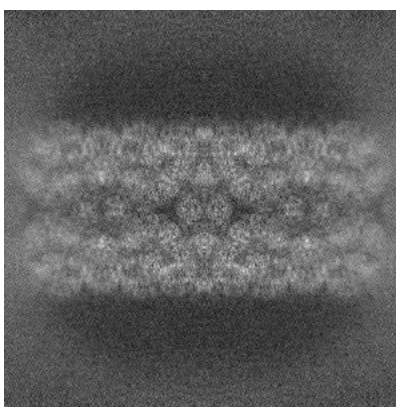


Z

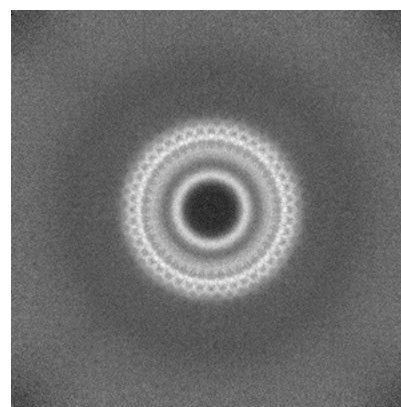
6.1.2 Raw map



X



Y

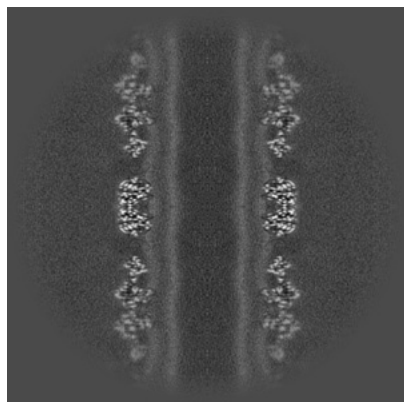


Z

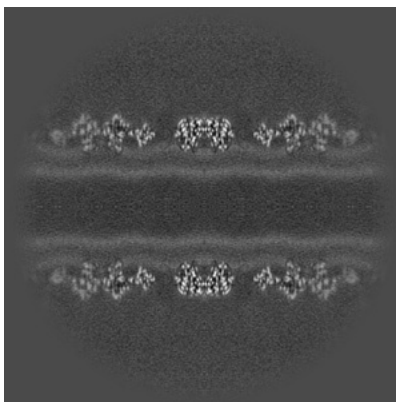
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

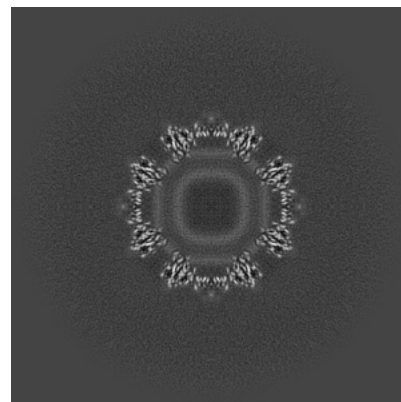
6.2.1 Primary map



X Index: 320

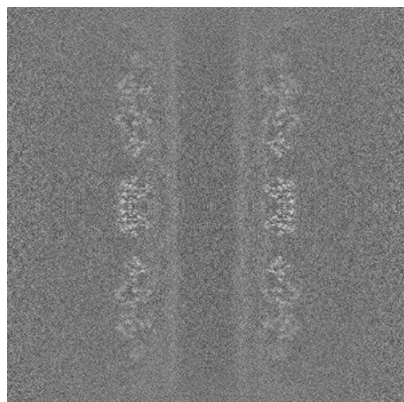


Y Index: 320

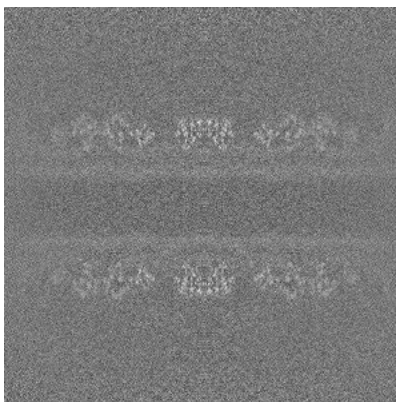


Z Index: 320

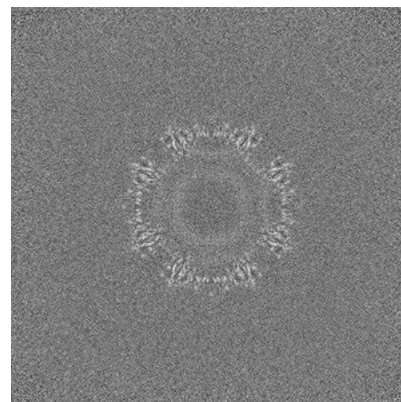
6.2.2 Raw map



X Index: 320



Y Index: 320

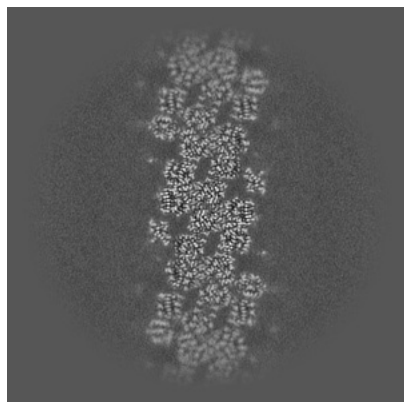


Z Index: 320

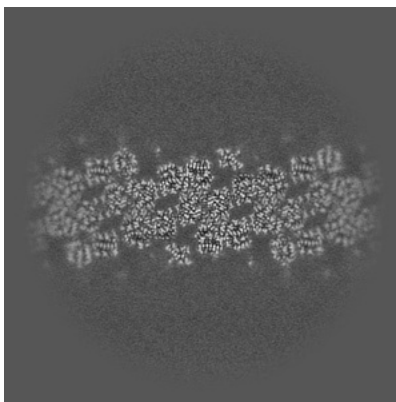
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

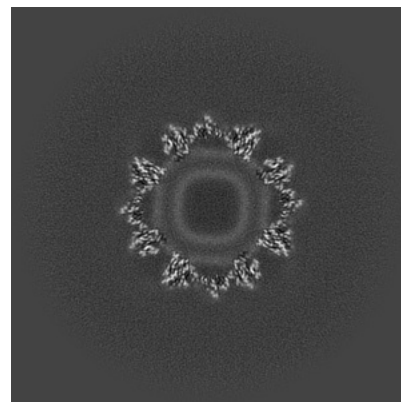
6.3.1 Primary map



X Index: 433

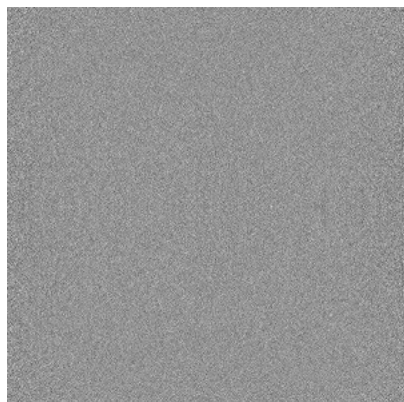


Y Index: 207

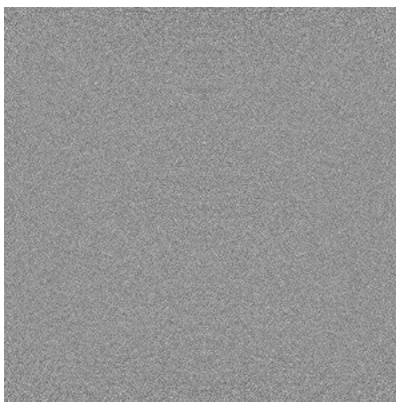


Z Index: 324

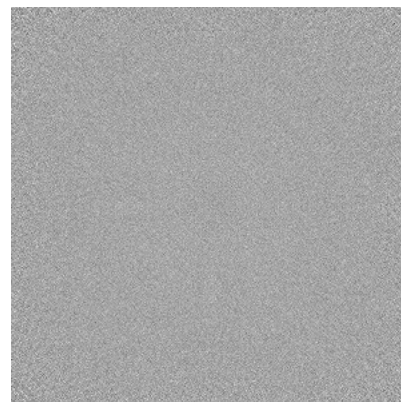
6.3.2 Raw map



X Index: 0



Y Index: 0

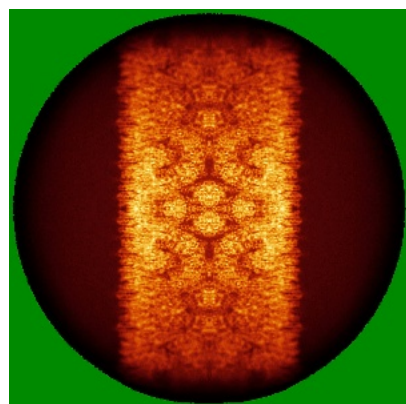


Z Index: 0

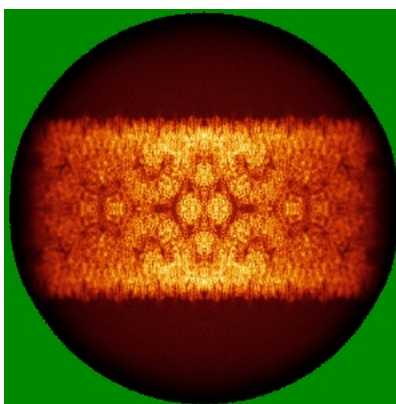
The images above show the largest variance slices of the map in three orthogonal directions.

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

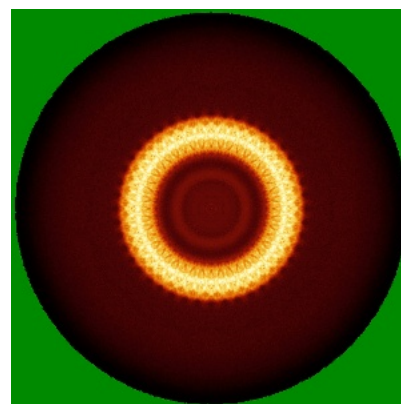
6.4.1 Primary map



X

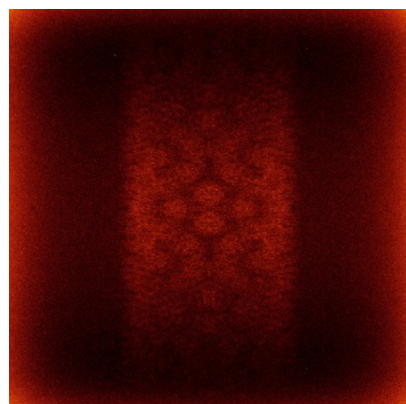


Y

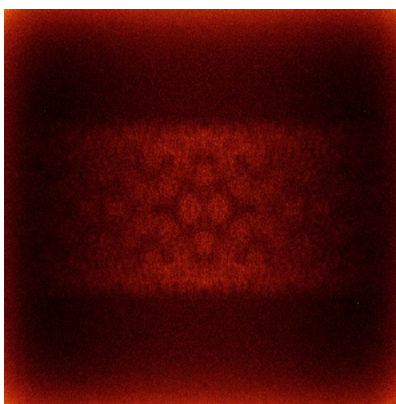


Z

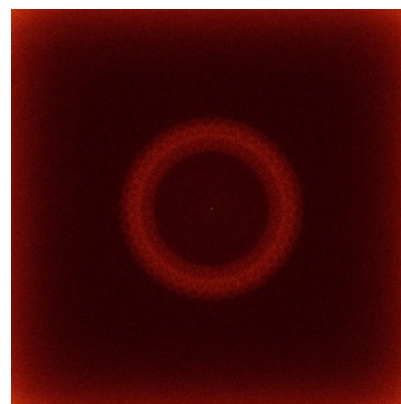
6.4.2 Raw map



X



Y

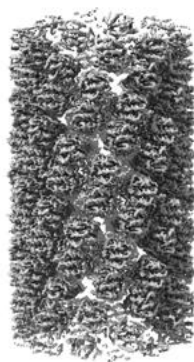


Z

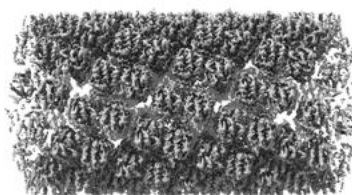
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

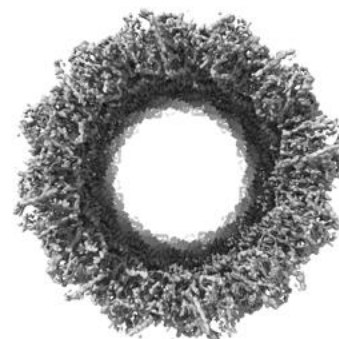
6.5.1 Primary map



X



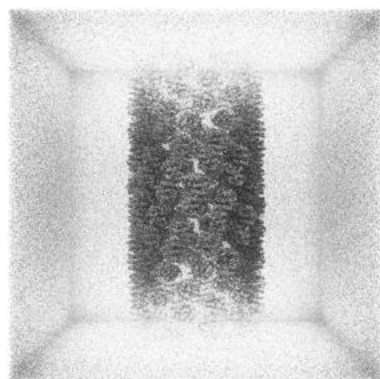
Y



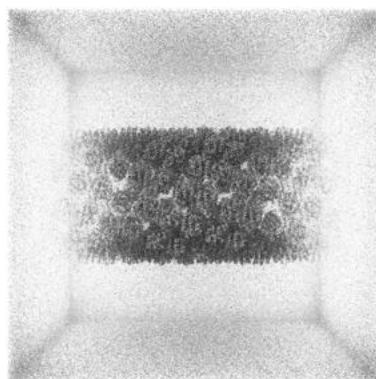
Z

The images above show the 3D surface view of the map at the recommended contour level 0.105. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

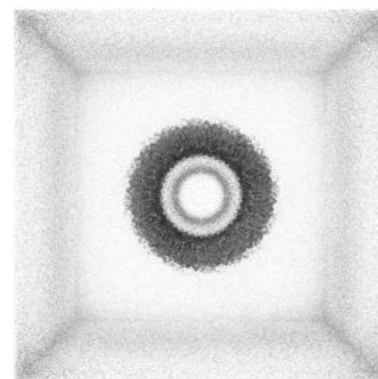
6.5.2 Raw map



X



Y



Z

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.

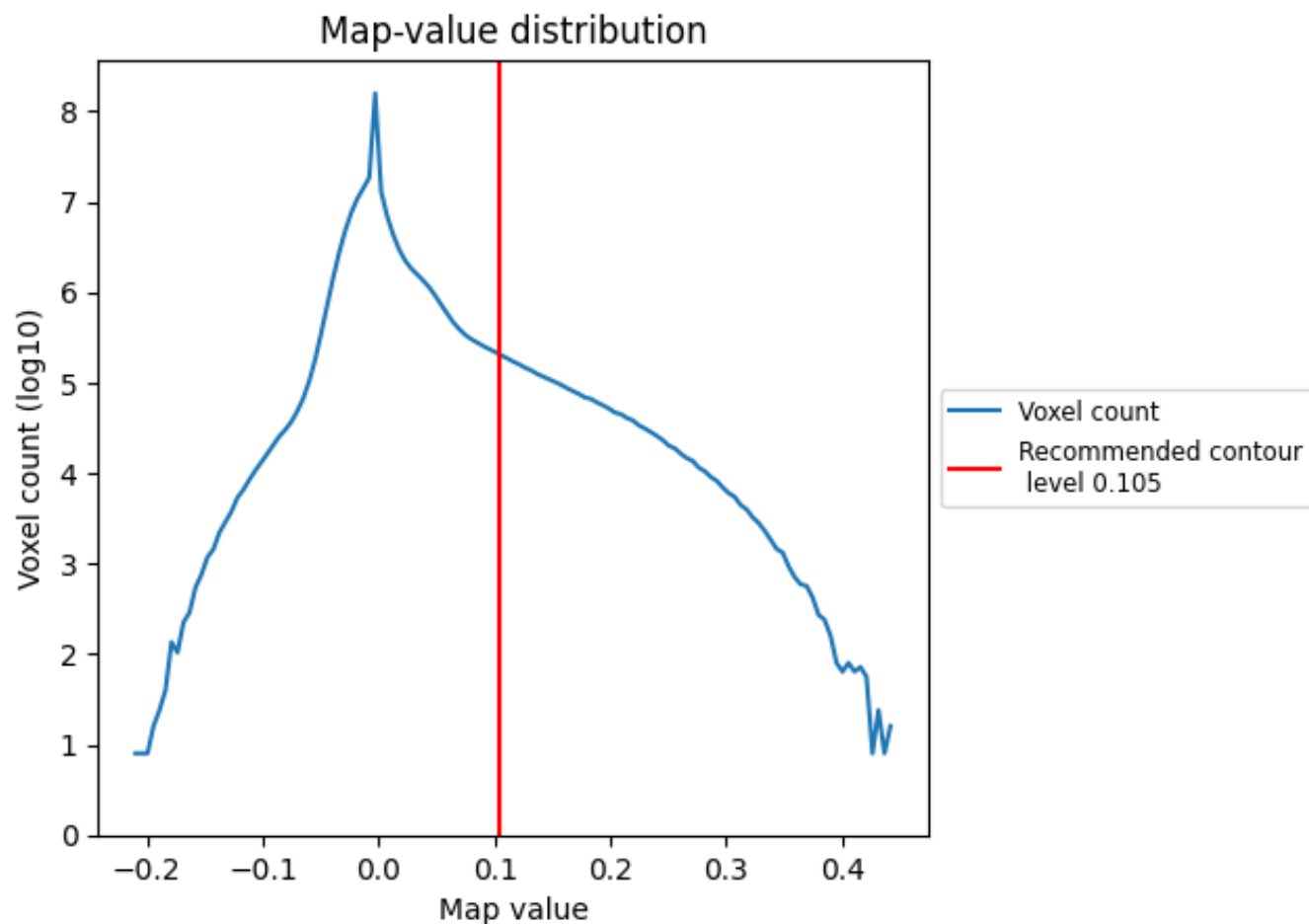
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

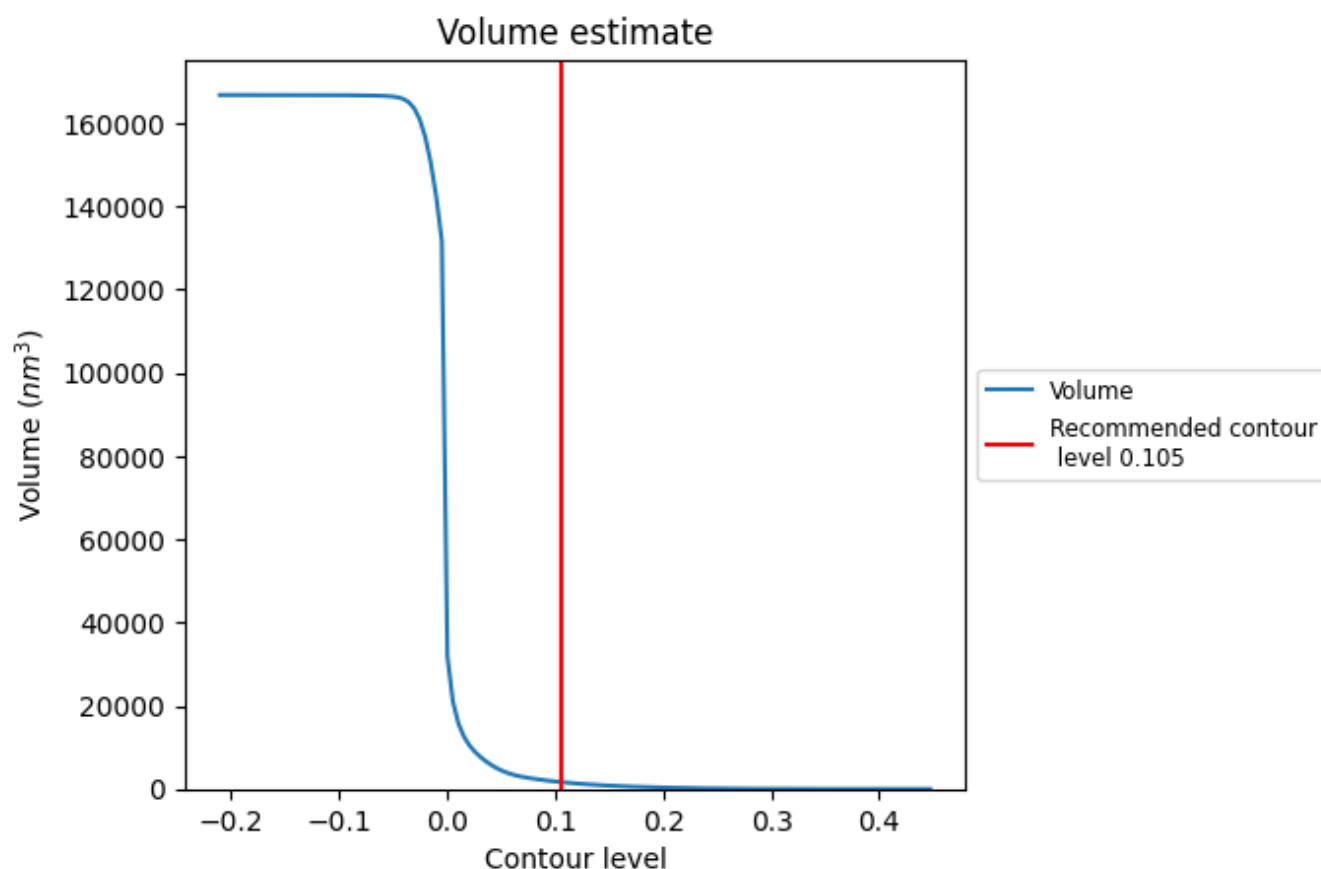
This section contains the results of statistical analysis of the map.

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.

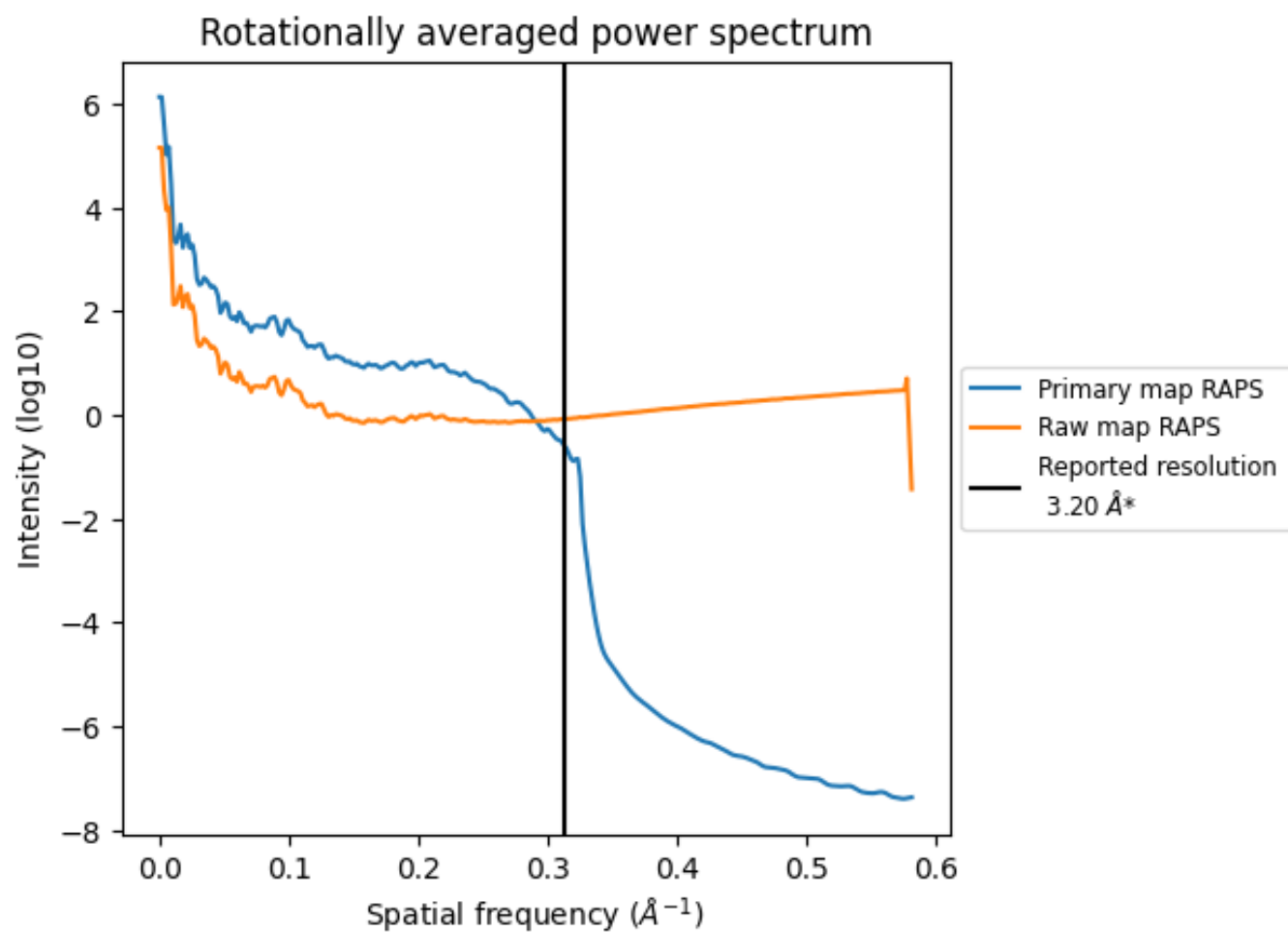
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1663 nm^3 ; this corresponds to an approximate mass of 1502 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 ⓘ

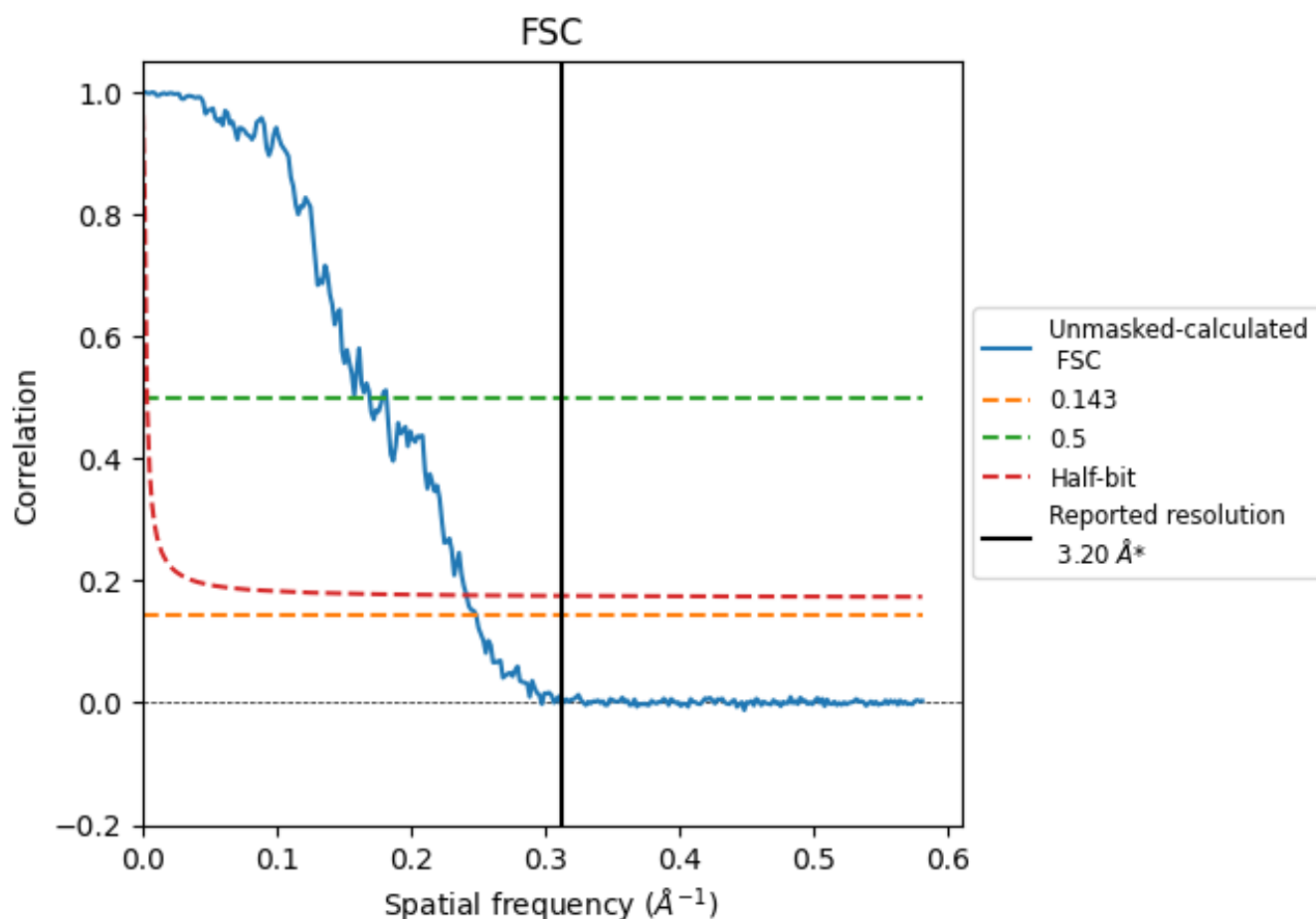


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

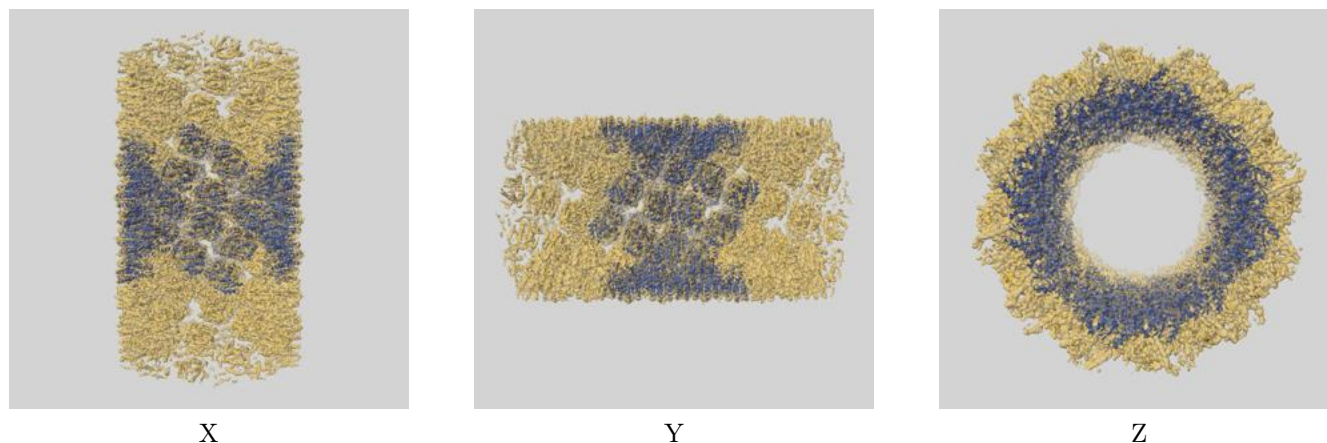
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	5.90	4.14

*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 4.02 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

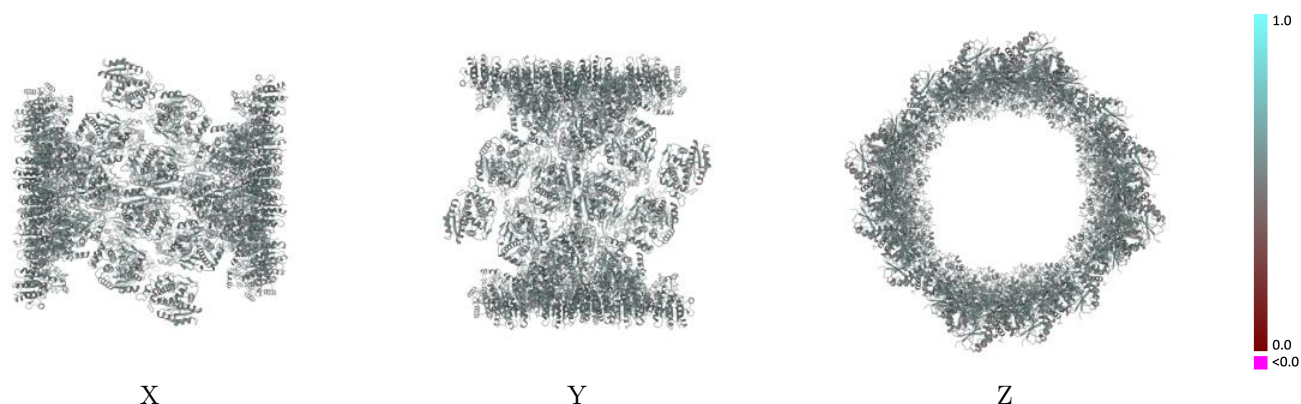
This section contains information regarding the fit between EMDB map EMD-56056 and PDB model 9TLK. Per-residue inclusion information can be found in section [3](#) on page [40](#).

9.1 Map-model overlay [i](#)



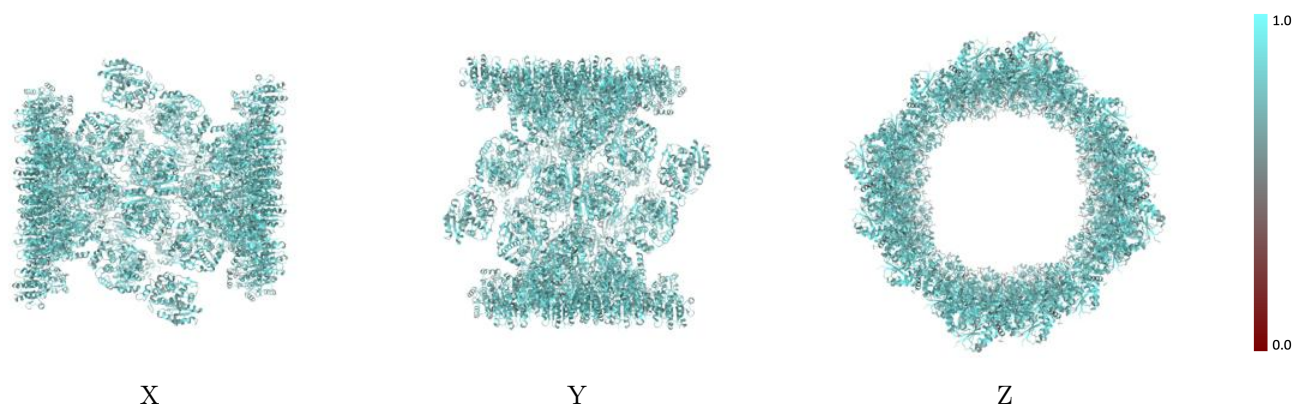
The images above show the 3D surface view of the map at the recommended contour level 0.105 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



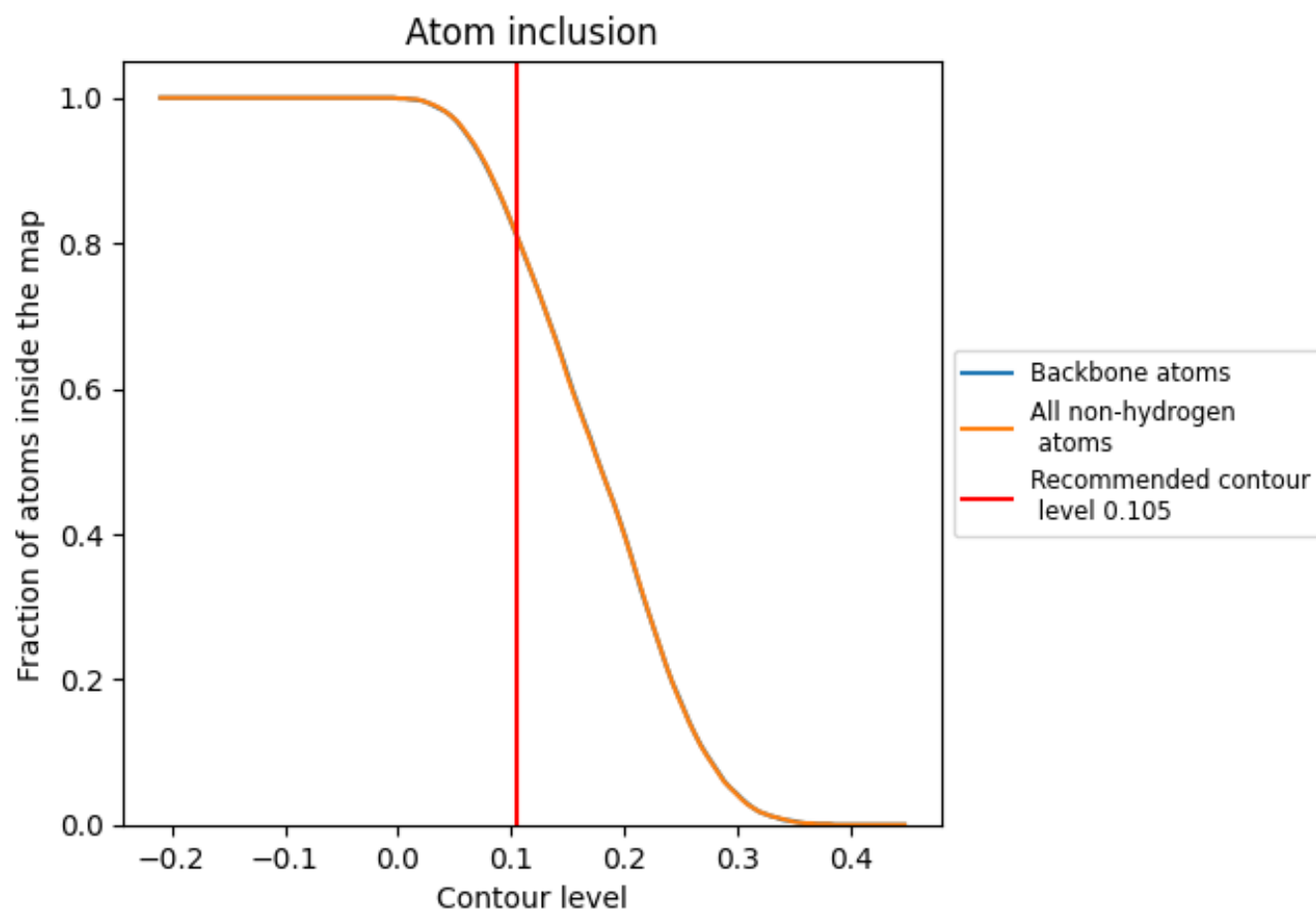
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.105).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.105) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8100	 0.5290
AA	 0.8290	 0.5330
AB	 0.7660	 0.5120
AC	 0.7650	 0.5110
AD	 0.8280	 0.5330
AE	 0.8010	 0.5270
AF	 0.8020	 0.5270
AG	 0.8240	 0.5310
AH	 0.8380	 0.5350
AI	 0.8340	 0.5340
AJ	 0.8280	 0.5330
AK	 0.8340	 0.5330
AL	 0.8340	 0.5360
BA	 0.8270	 0.5350
BB	 0.7620	 0.5120
BC	 0.7660	 0.5140
BD	 0.8280	 0.5340
BE	 0.8000	 0.5260
BF	 0.7990	 0.5260
BG	 0.8280	 0.5330
BH	 0.8370	 0.5350
BI	 0.8390	 0.5350
BJ	 0.8290	 0.5340
BK	 0.8400	 0.5360
BL	 0.8380	 0.5360
CA	 0.8320	 0.5340
CB	 0.7650	 0.5120
CC	 0.7650	 0.5120
CD	 0.8330	 0.5360
CE	 0.8020	 0.5280
CF	 0.7980	 0.5270
CG	 0.8260	 0.5320
CH	 0.8370	 0.5350
CI	 0.8370	 0.5340
CJ	 0.8280	 0.5330



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Chain	Atom inclusion	Q-score
CK	 0.8380	 0.5360
CL	 0.8380	 0.5350
DA	 0.8320	 0.5360
DB	 0.7650	 0.5100
DC	 0.7640	 0.5130
DD	 0.8300	 0.5340
DE	 0.8000	 0.5280
DF	 0.8000	 0.5260
DG	 0.8260	 0.5320
DH	 0.8370	 0.5340
DI	 0.8370	 0.5350
DJ	 0.8300	 0.5340
DK	 0.8380	 0.5360
DL	 0.8380	 0.5350