



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:39 AM UTC

PDB ID : 6M31 / pdb_00006m31
Title : Structural and Functional Insights into an Archaeal Lipid Synthase
Authors : Ren, S.; Cheng, W.
Deposited on : 2020-03-02
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

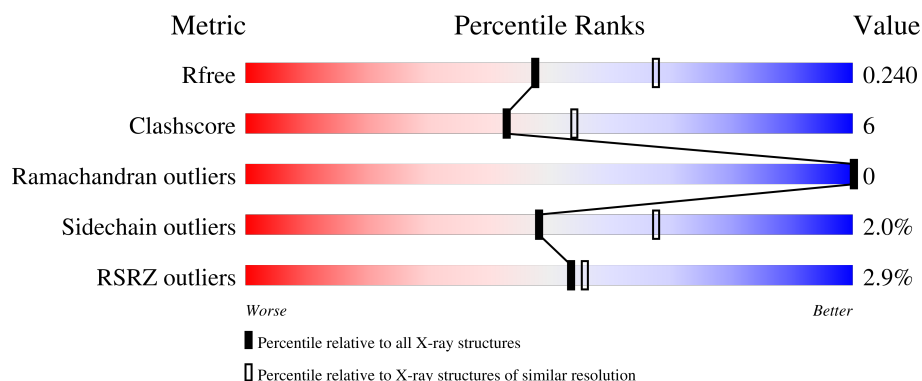
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	283	 2% 88% 10% ..
1	B	283	 3% 88% 11% .

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
2	LDA	A	308	-	-	X	-
2	LDA	A	311	-	-	X	-
3	PO4	A	312	-	-	X	-
3	PO4	A	314	-	-	X	-
3	PO4	B	313	-	X	-	-

2 Entry composition [i](#)

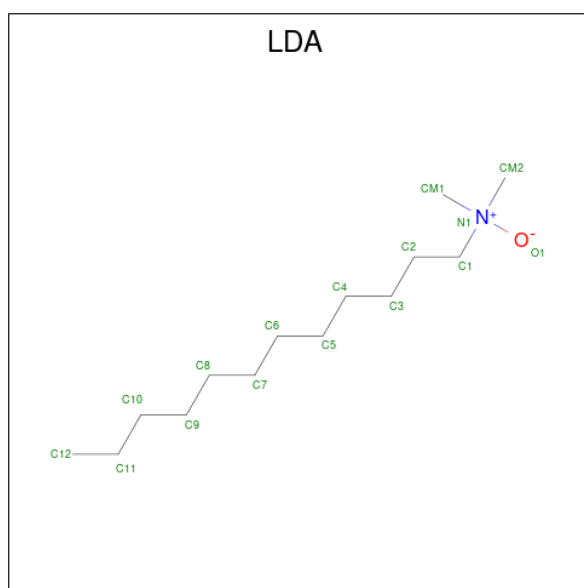
There are 6 unique types of molecules in this entry. The entry contains 5336 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Digeranylgeranyl glyceryl phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2224	1516	334	365	9			
1	B	280	Total	C	N	O	S	0	0	0
			2224	1516	334	365	9			

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO) (labeled as "Ligand of Interest" by depositor).



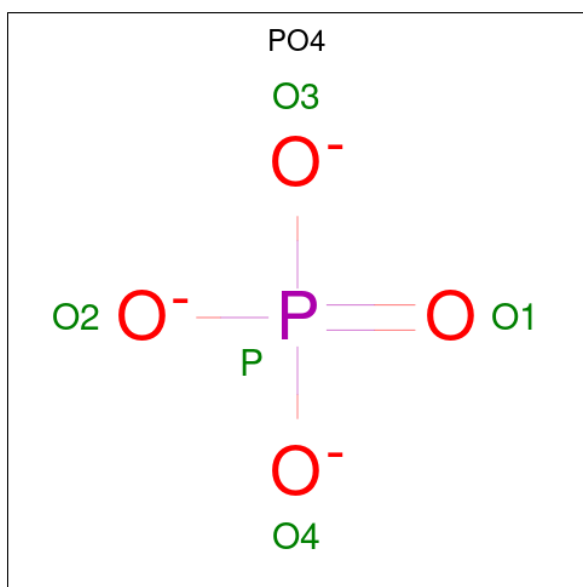
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).

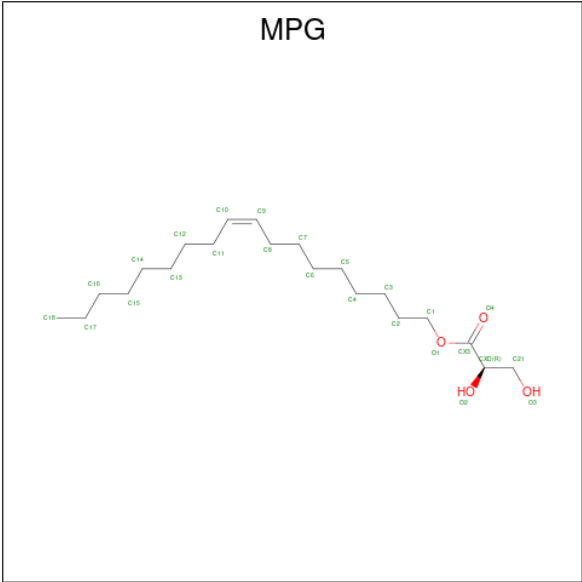


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (CCD ID: MPG) (formula: C₂₁H₄₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		

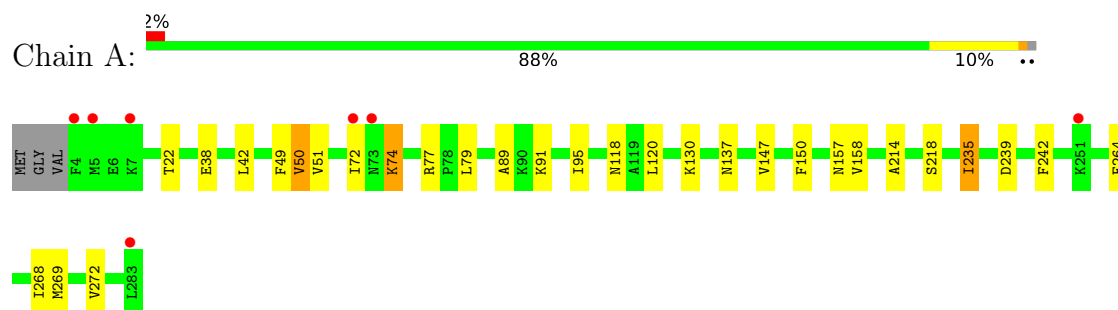
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total	O	0	0
			25	25		
6	B	18	Total	O	0	0
			18	18		

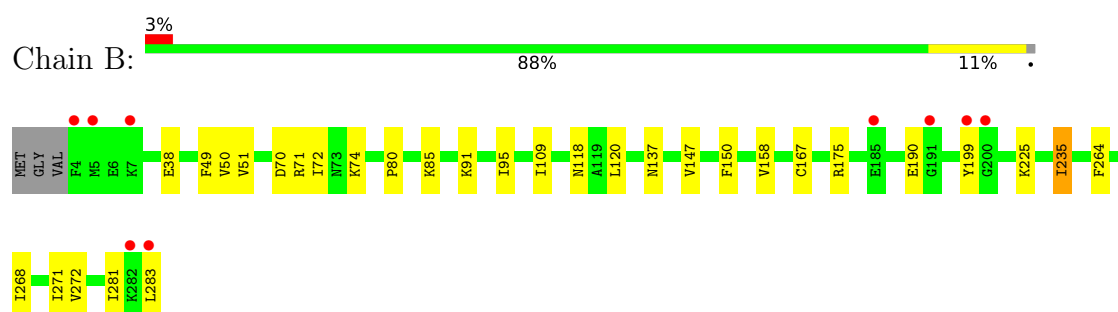
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Digeranylgeranylglyceryl phosphate synthase



- Molecule 1: Digeranylgeranylglyceryl phosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	70.00Å 133.49Å 79.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 2.30 48.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.89-2.30) 99.8 (48.89-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.29Å)	Xtriage
Refinement program	SHELX	Depositor
R, R_{free}	0.201 , 0.230 0.208 , 0.240	Depositor DCC
R_{free} test set	1689 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5336	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8172e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, LDA, MPG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.93	1/2271 (0.0%)	1.36	4/3069 (0.1%)
1	B	0.91	0/2271	1.37	5/3069 (0.2%)
All	All	0.92	1/4542 (0.0%)	1.36	9/6138 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	VAL	C-N	-8.45	1.23	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ASN	CA-CB-CG	6.19	118.79	112.60
1	B	137	ASN	CA-CB-CG	5.97	118.57	112.60
1	A	49	PHE	CA-CB-CG	-5.55	108.25	113.80
1	B	38	GLU	CA-C-N	5.30	128.98	121.66
1	B	38	GLU	C-N-CA	5.30	128.98	121.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2224	0	2426	32	0
1	B	2224	0	2426	21	0
2	A	176	0	341	20	0
2	B	192	0	372	10	0
3	A	15	0	0	4	0
3	B	10	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	325	0	520	21	0
5	B	125	0	200	7	0
6	A	25	0	0	0	0
6	B	18	0	0	0	0
All	All	5336	0	6285	72	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 6.

The worst 5 of 72 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:308:LDA:H102	2:A:311:LDA:H112	1.30	1.12
2:A:308:LDA:H101	5:A:328:MPG:H112	1.46	0.95
1:A:158:VAL:HG12	2:A:311:LDA:HM13	1.54	0.88
2:A:308:LDA:H123	2:A:311:LDA:H121	1.53	0.87
2:A:308:LDA:H102	2:A:311:LDA:C11	2.08	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	278/283 (98%)	266 (96%)	12 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	278/283 (98%)	271 (98%)	7 (2%)	0	100	100
All	All	556/566 (98%)	537 (97%)	19 (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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/247 (99%)	241 (98%)	4 (2%)	55	73
1	B	245/247 (99%)	239 (98%)	6 (2%)	43	62
All	All	490/494 (99%)	480 (98%)	10 (2%)	48	67

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	235	ILE
1	B	281	ILE
1	B	283	LEU
1	A	235	ILE
1	B	85	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	B	118	ASN
1	B	254	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 48 ligands modelled in this entry, 2 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	MPG	A	327	-	24,24,24	0.30	0	24,25,25	0.60	1 (4%)
5	MPG	B	318	-	24,24,24	0.20	0	24,25,25	0.36	0
5	MPG	A	320	-	24,24,24	0.20	0	24,25,25	0.40	0
2	LDA	B	306	-	13,15,15	0.12	0	14,17,17	0.25	0
5	MPG	B	319	-	24,24,24	0.21	0	24,25,25	0.33	0
5	MPG	B	316	-	24,24,24	0.21	0	24,25,25	0.42	0
2	LDA	A	310	-	13,15,15	0.13	0	14,17,17	0.15	0
2	LDA	B	310	-	13,15,15	0.12	0	14,17,17	0.16	0
2	LDA	A	302	-	13,15,15	0.14	0	14,17,17	0.21	0
3	PO4	B	314	-	4,4,4	2.58	3 (75%)	6,6,6	0.49	0
2	LDA	B	304	-	13,15,15	0.13	0	14,17,17	0.31	0
3	PO4	A	312	-	4,4,4	0.93	0	6,6,6	0.45	0
2	LDA	B	308	-	13,15,15	0.11	0	14,17,17	0.23	0
5	MPG	A	319	-	24,24,24	0.19	0	24,25,25	0.44	0
5	MPG	A	324	-	24,24,24	0.22	0	24,25,25	0.38	0
5	MPG	A	325	-	24,24,24	0.37	0	24,25,25	0.33	0
5	MPG	A	322	-	24,24,24	0.20	0	24,25,25	0.34	0
2	LDA	B	303	-	13,15,15	0.19	0	14,17,17	0.26	0
2	LDA	B	307	-	13,15,15	0.12	0	14,17,17	0.22	0
2	LDA	A	309	-	13,15,15	0.17	0	14,17,17	0.33	0
3	PO4	A	313	-	4,4,4	2.55	2 (50%)	6,6,6	0.47	0
3	PO4	A	314	-	4,4,4	0.70	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LDA	B	302	-	13,15,15	0.13	0	14,17,17	0.17	0
5	MPG	A	317	-	24,24,24	0.24	0	24,25,25	0.36	0
2	LDA	A	305	-	13,15,15	0.12	0	14,17,17	0.22	0
2	LDA	A	308	-	13,15,15	0.28	0	14,17,17	0.16	0
2	LDA	B	311	-	13,15,15	0.19	0	14,17,17	0.15	0
5	MPG	A	318	-	24,24,24	0.24	0	24,25,25	0.37	0
3	PO4	B	313	-	4,4,4	2.09	4 (100%)	6,6,6	0.37	0
2	LDA	A	301	-	13,15,15	0.09	0	14,17,17	0.18	0
2	LDA	B	301	-	13,15,15	0.18	0	14,17,17	0.25	0
2	LDA	A	303	-	13,15,15	0.16	0	14,17,17	0.11	0
5	MPG	B	320	-	24,24,24	0.21	0	24,25,25	0.37	0
2	LDA	B	305	-	13,15,15	0.12	0	14,17,17	0.26	0
5	MPG	B	317	-	24,24,24	0.21	0	24,25,25	0.46	0
5	MPG	A	321	-	24,24,24	0.19	0	24,25,25	0.44	0
5	MPG	A	326	-	24,24,24	0.24	0	24,25,25	0.42	0
5	MPG	A	323	-	24,24,24	0.29	0	24,25,25	0.43	0
2	LDA	A	306	-	13,15,15	0.22	0	14,17,17	0.17	0
2	LDA	A	311	-	13,15,15	0.51	0	14,17,17	0.14	0
2	LDA	A	304	-	13,15,15	0.13	0	14,17,17	0.28	0
2	LDA	B	312	-	13,15,15	0.46	0	14,17,17	0.34	0
2	LDA	A	307	-	13,15,15	0.14	0	14,17,17	0.30	0
5	MPG	A	328	-	24,24,24	0.45	0	24,25,25	0.38	0
5	MPG	A	316	-	24,24,24	0.23	0	24,25,25	0.35	0
2	LDA	B	309	-	13,15,15	0.12	0	14,17,17	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPG	A	327	-	-	15/25/25/25	-
5	MPG	B	318	-	-	16/25/25/25	-
5	MPG	A	320	-	-	16/25/25/25	-
2	LDA	B	306	-	-	8/13/13/13	-
5	MPG	B	319	-	-	15/25/25/25	-
5	MPG	B	316	-	-	14/25/25/25	-
2	LDA	A	310	-	-	9/13/13/13	-
2	LDA	B	310	-	-	12/13/13/13	-
2	LDA	A	302	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	B	304	-	-	11/13/13/13	-
2	LDA	B	308	-	-	8/13/13/13	-
5	MPG	A	319	-	-	16/25/25/25	-
5	MPG	A	324	-	-	16/25/25/25	-
5	MPG	A	325	-	-	19/25/25/25	-
5	MPG	A	322	-	-	11/25/25/25	-
2	LDA	B	303	-	-	8/13/13/13	-
2	LDA	B	307	-	-	5/13/13/13	-
2	LDA	A	309	-	-	7/13/13/13	-
2	LDA	B	302	-	-	4/13/13/13	-
5	MPG	A	317	-	-	11/25/25/25	-
2	LDA	A	305	-	-	9/13/13/13	-
2	LDA	A	308	-	-	8/13/13/13	-
2	LDA	B	311	-	-	10/13/13/13	-
5	MPG	A	318	-	-	13/25/25/25	-
2	LDA	A	301	-	-	10/13/13/13	-
2	LDA	B	301	-	-	9/13/13/13	-
2	LDA	A	303	-	-	3/13/13/13	-
5	MPG	B	320	-	-	15/25/25/25	-
2	LDA	B	305	-	-	5/13/13/13	-
5	MPG	B	317	-	-	18/25/25/25	-
5	MPG	A	321	-	-	12/25/25/25	-
5	MPG	A	326	-	-	11/25/25/25	-
5	MPG	A	323	-	-	19/25/25/25	-
2	LDA	A	306	-	-	10/13/13/13	-
2	LDA	A	311	-	-	10/13/13/13	-
2	LDA	A	304	-	-	4/13/13/13	-
2	LDA	B	312	-	-	9/13/13/13	-
2	LDA	A	307	-	-	9/13/13/13	-
5	MPG	A	328	-	-	14/25/25/25	-
5	MPG	A	316	-	-	10/25/25/25	-
2	LDA	B	309	-	-	6/13/13/13	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	314	PO4	P-O1	4.27	1.60	1.50
3	A	313	PO4	P-O1	4.23	1.60	1.50
3	B	313	PO4	P-O1	2.31	1.56	1.50
3	B	313	PO4	P-O2	2.03	1.60	1.54
3	B	314	PO4	P-O3	2.02	1.60	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	327	MPG	O3-C21-CXD	-2.16	106.61	111.95

There are no chirality outliers.

5 of 441 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	LDA	C2-C1-N1-CM1
2	A	301	LDA	N1-C1-C2-C3
2	A	302	LDA	C2-C1-N1-CM2
2	A	305	LDA	N1-C1-C2-C3
2	A	306	LDA	C2-C1-N1-CM1

There are no ring outliers.

25 monomers are involved in 53 short contacts:

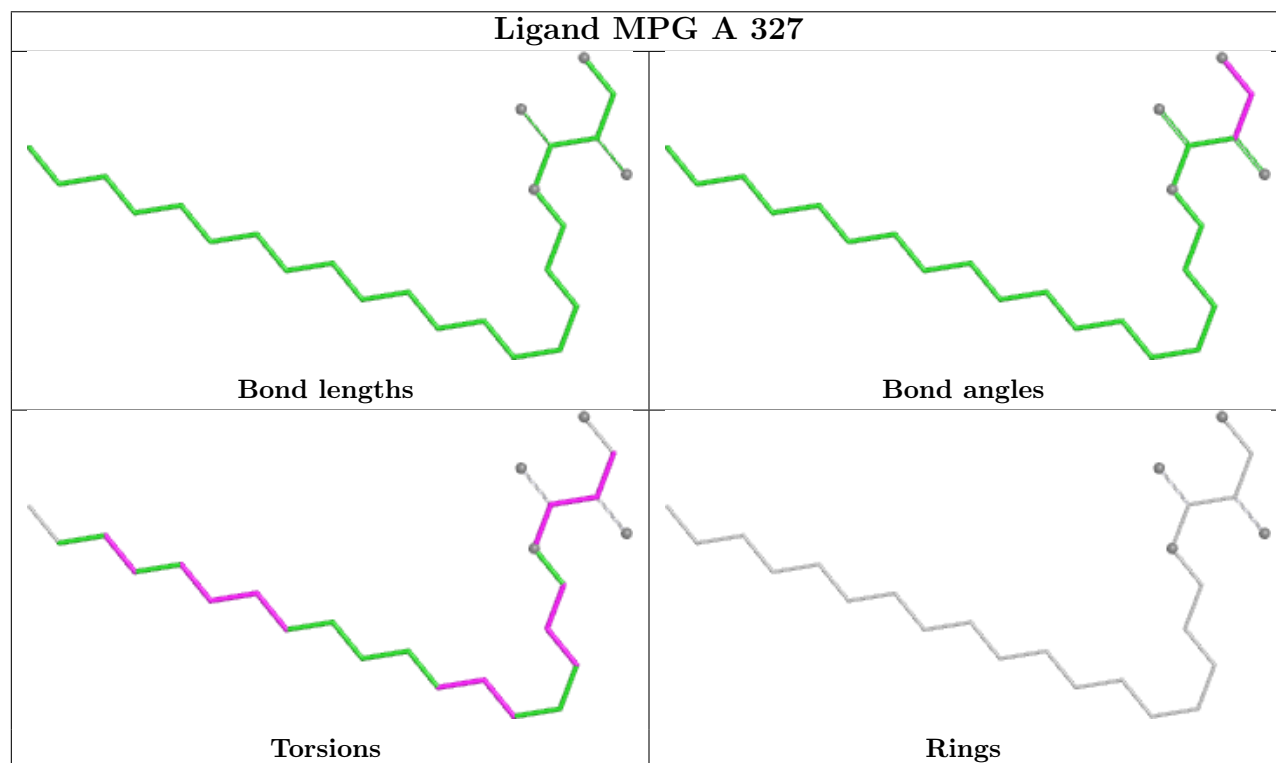
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	327	MPG	4	0
5	B	318	MPG	3	0
5	B	316	MPG	1	0
2	B	310	LDA	5	0
2	A	302	LDA	1	0
3	A	312	PO4	2	0
2	B	308	LDA	2	0
5	A	319	MPG	1	0
5	A	324	MPG	4	0
2	B	303	LDA	1	0
2	A	309	LDA	1	0
3	A	314	PO4	2	0
2	A	305	LDA	2	0
2	A	308	LDA	11	0
2	B	311	LDA	1	0
3	B	313	PO4	1	0
2	A	301	LDA	1	0

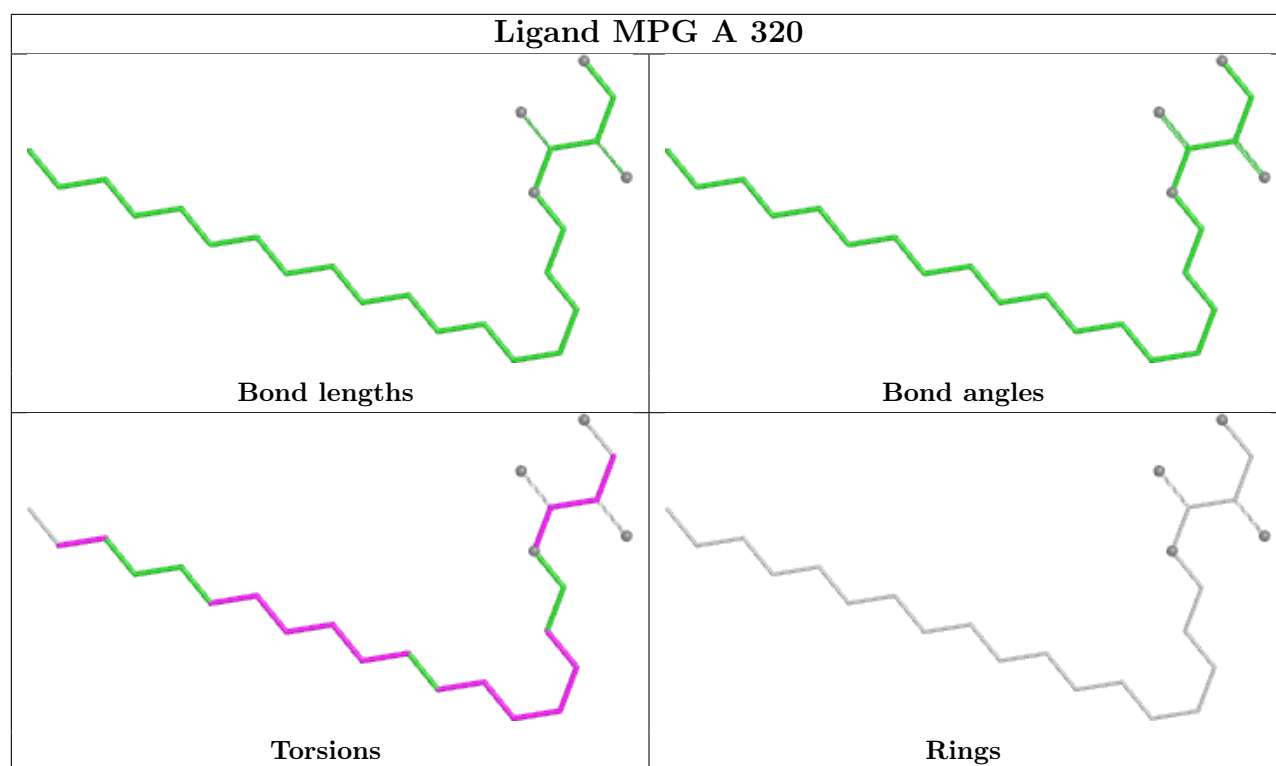
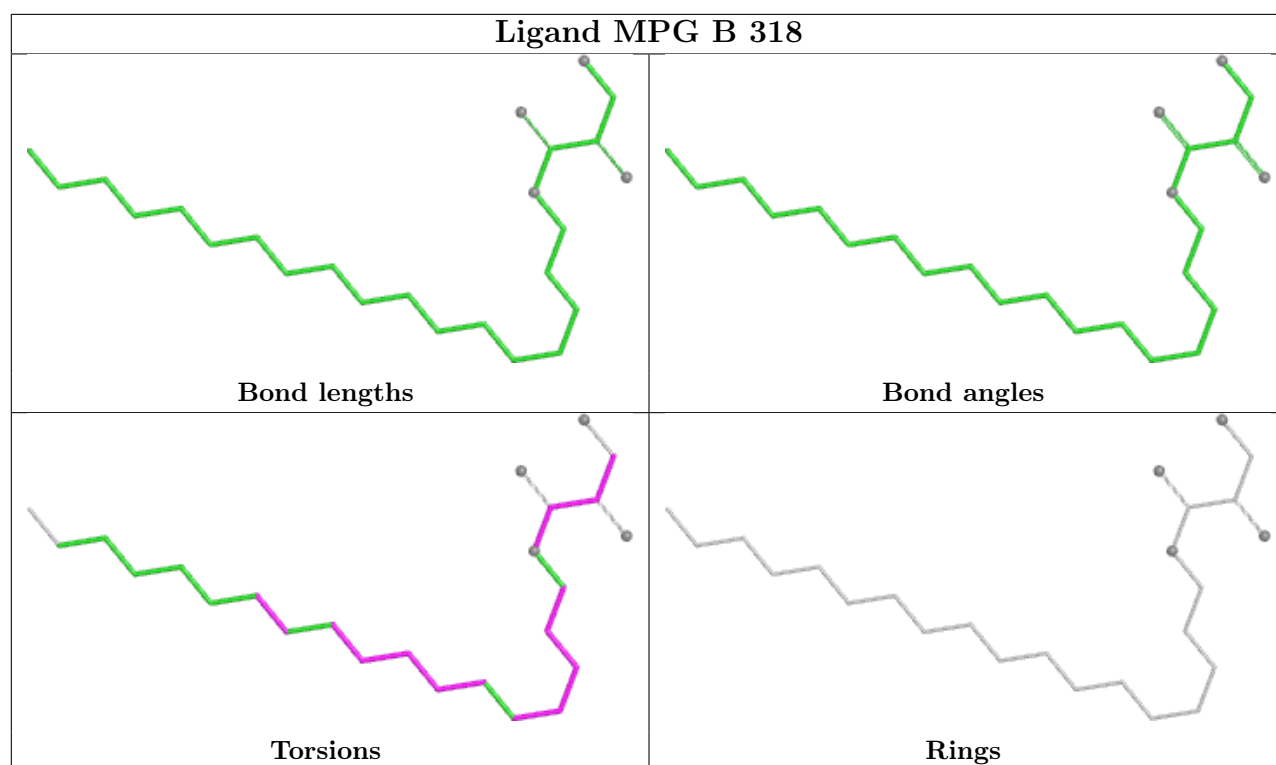
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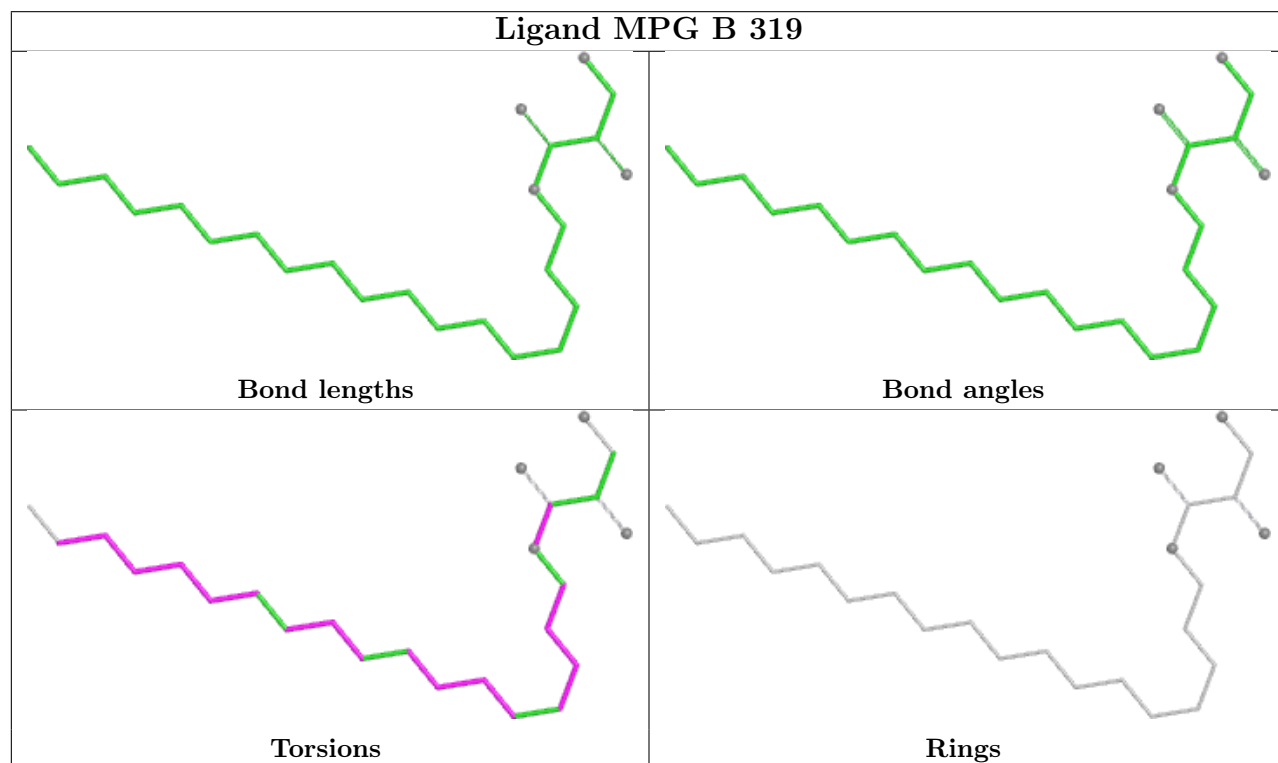
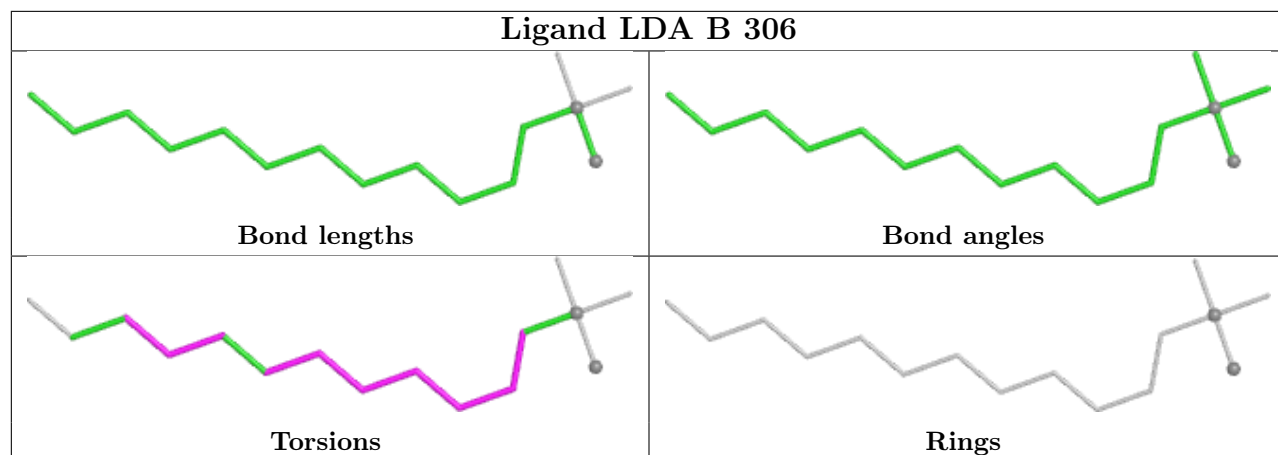
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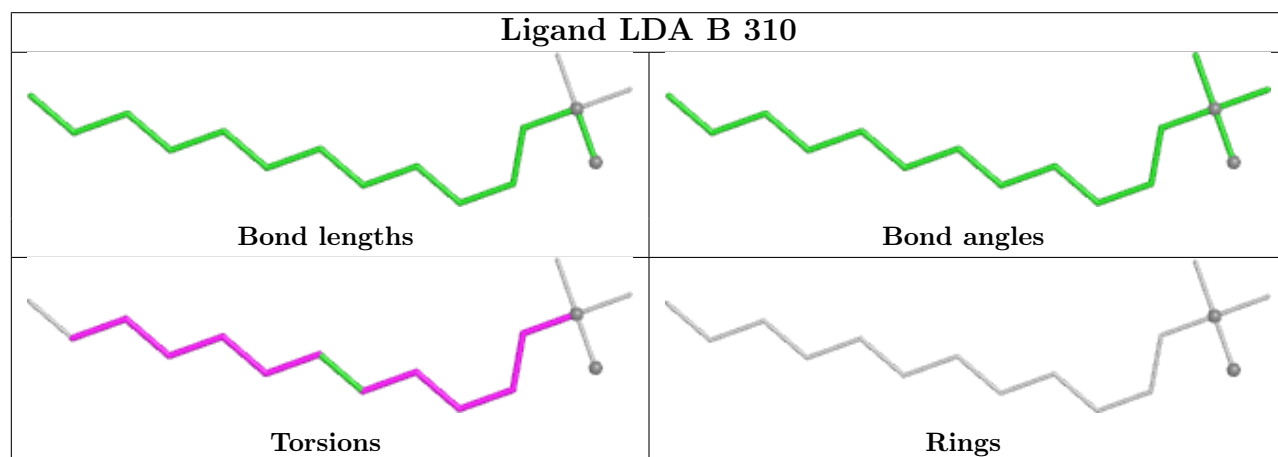
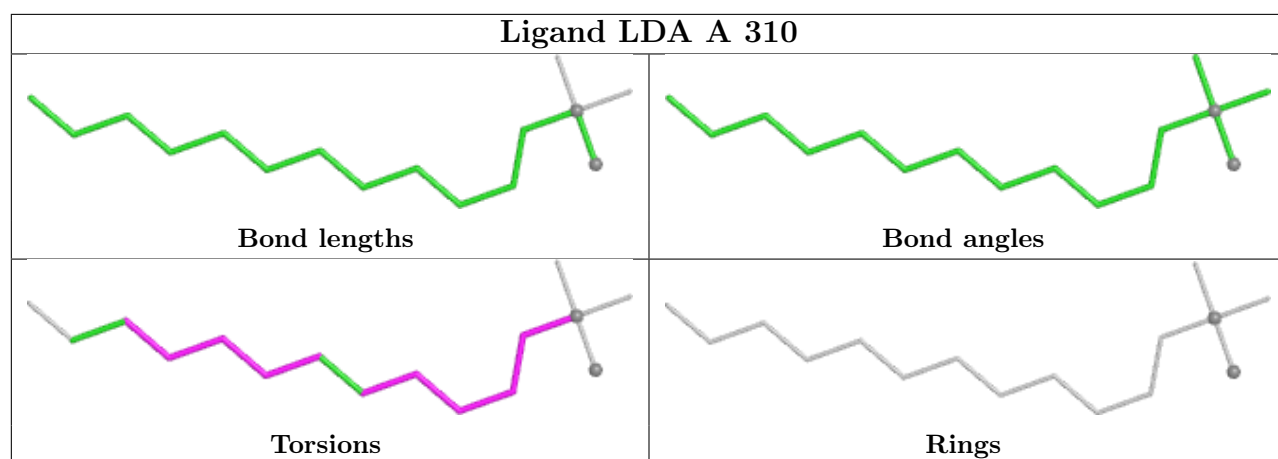
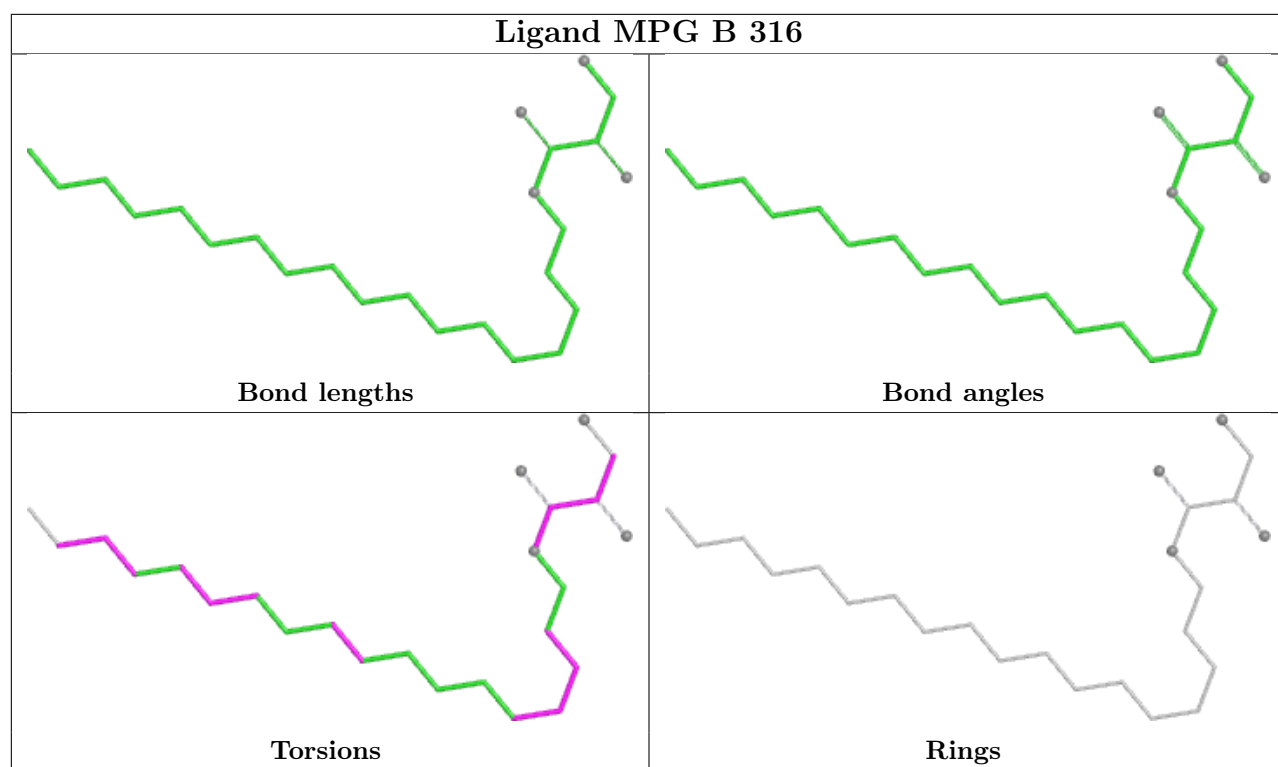
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	LDA	1	0
5	B	320	MPG	3	0
5	A	326	MPG	1	0
5	A	323	MPG	8	0
2	A	311	LDA	11	0
2	A	304	LDA	1	0
2	A	307	LDA	1	0
5	A	328	MPG	3	0

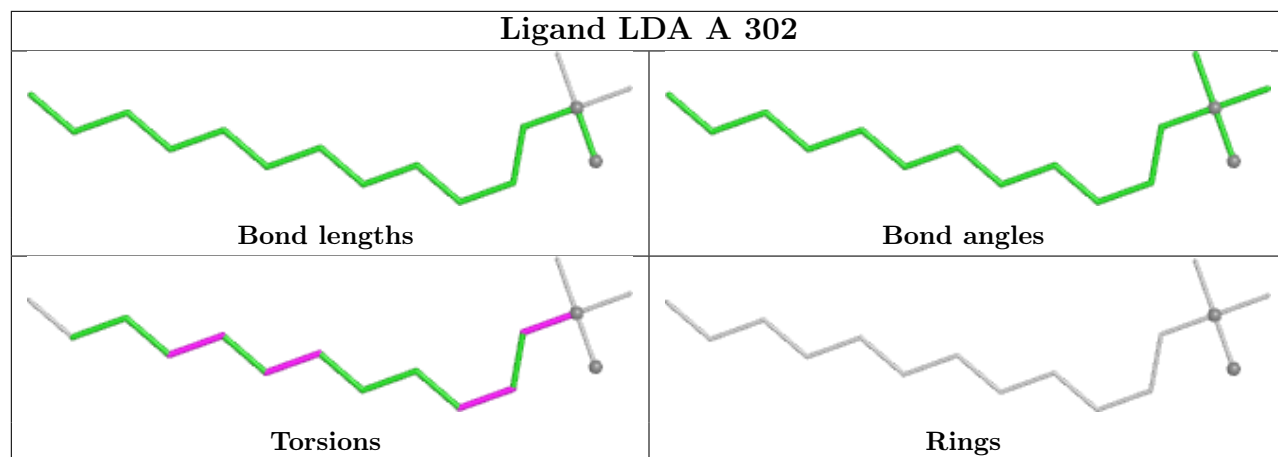
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

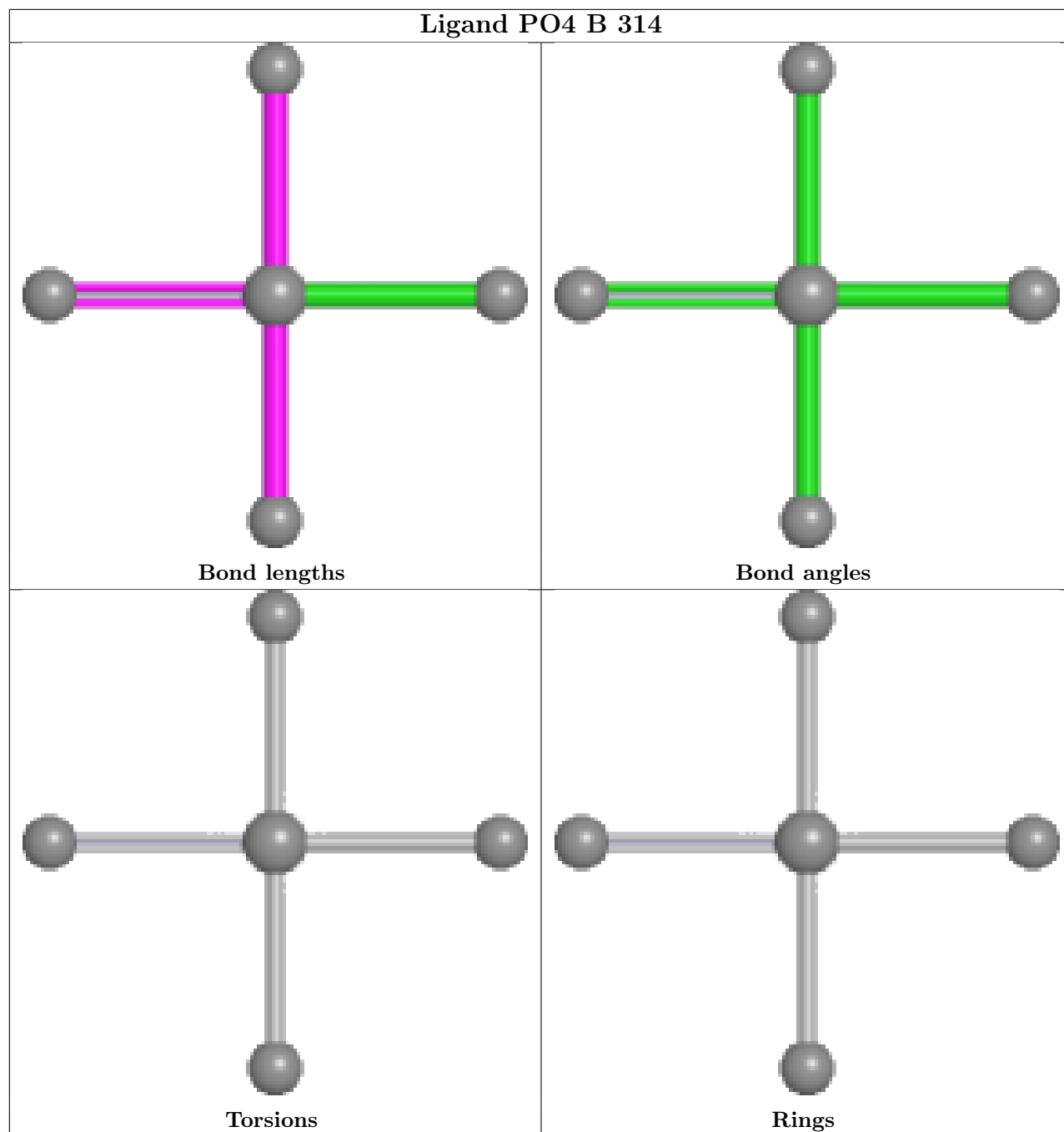


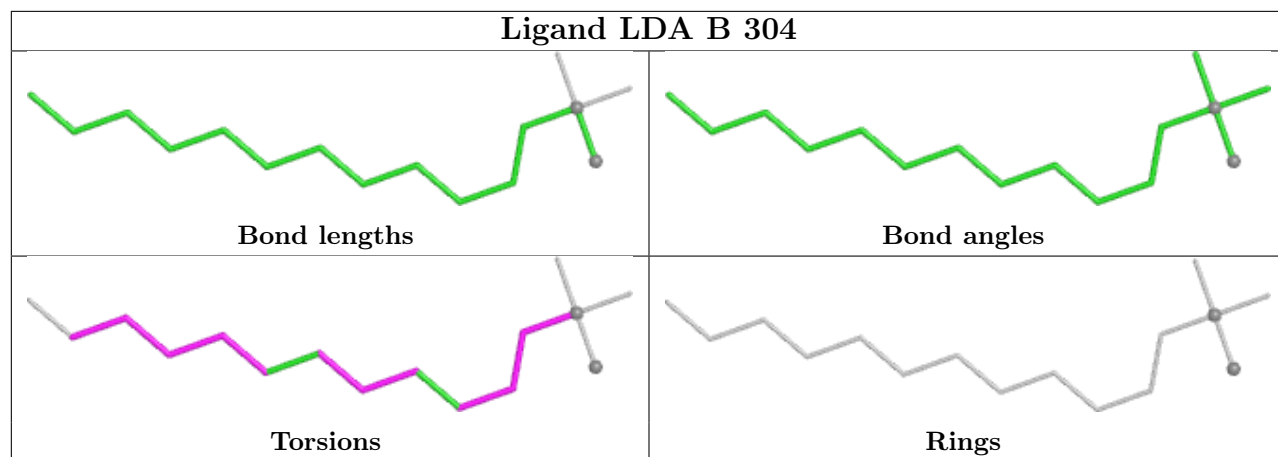


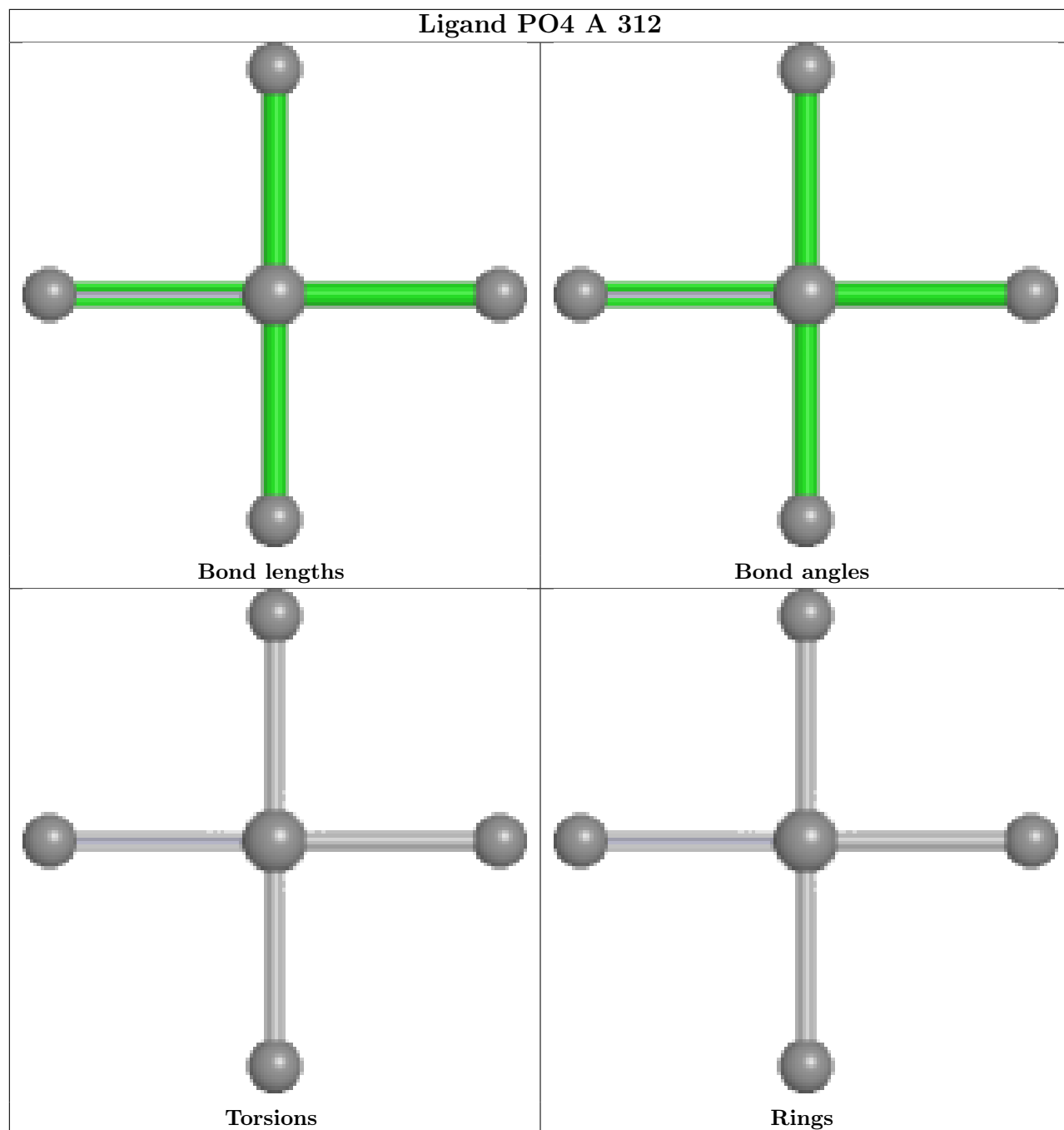


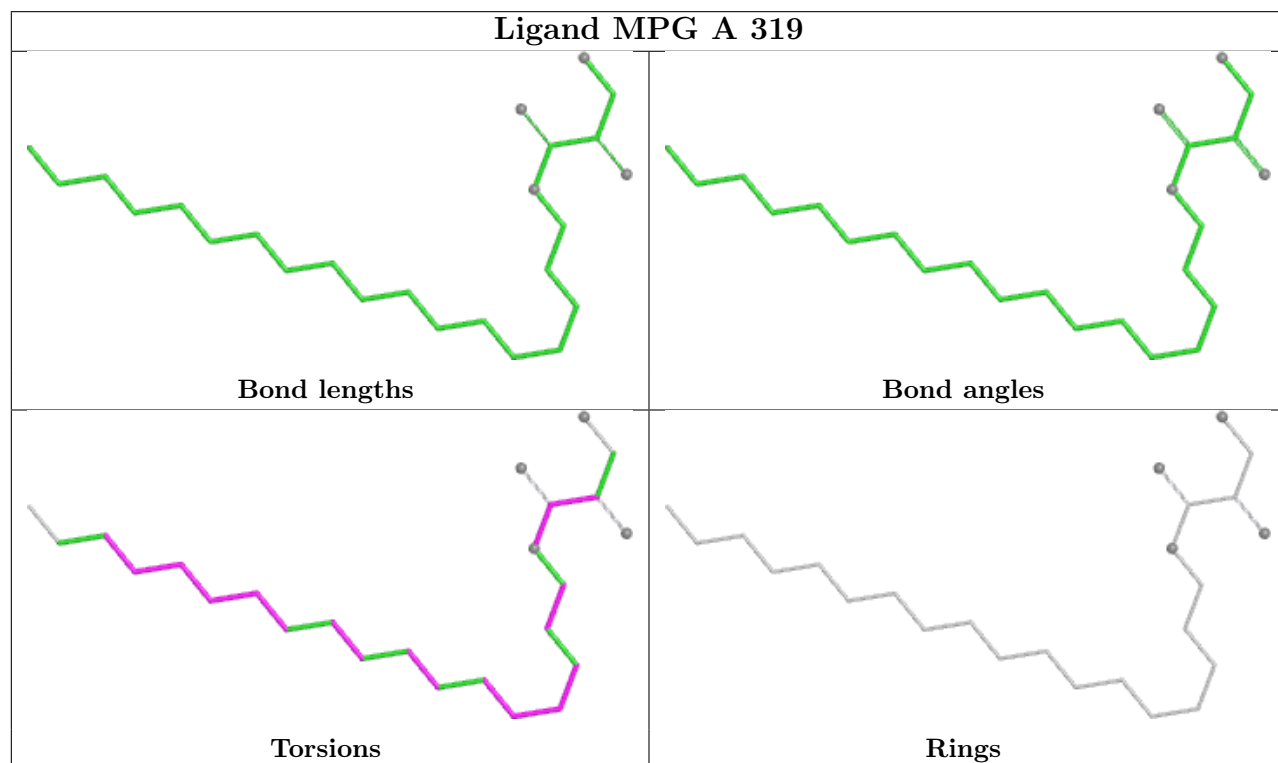
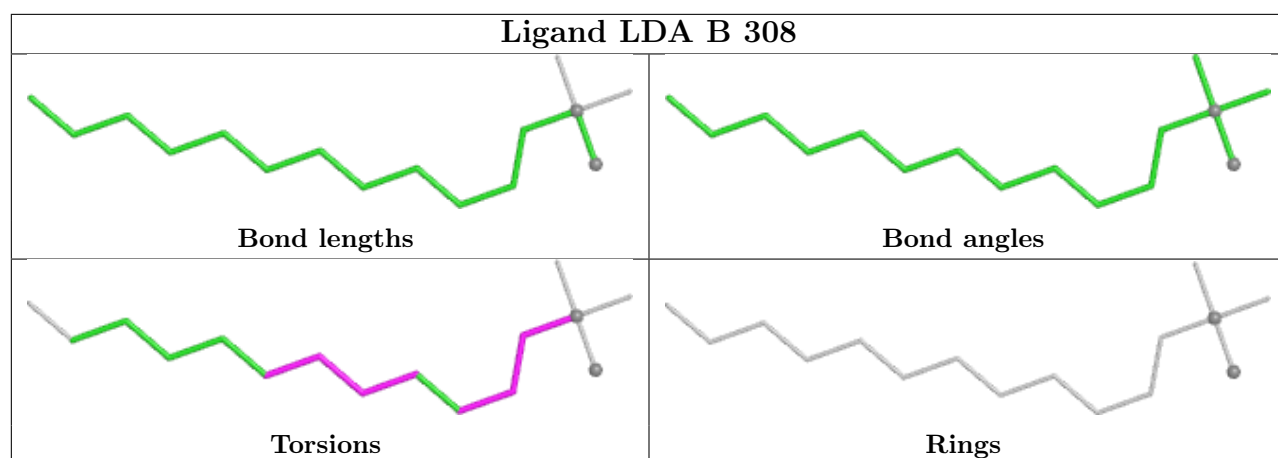


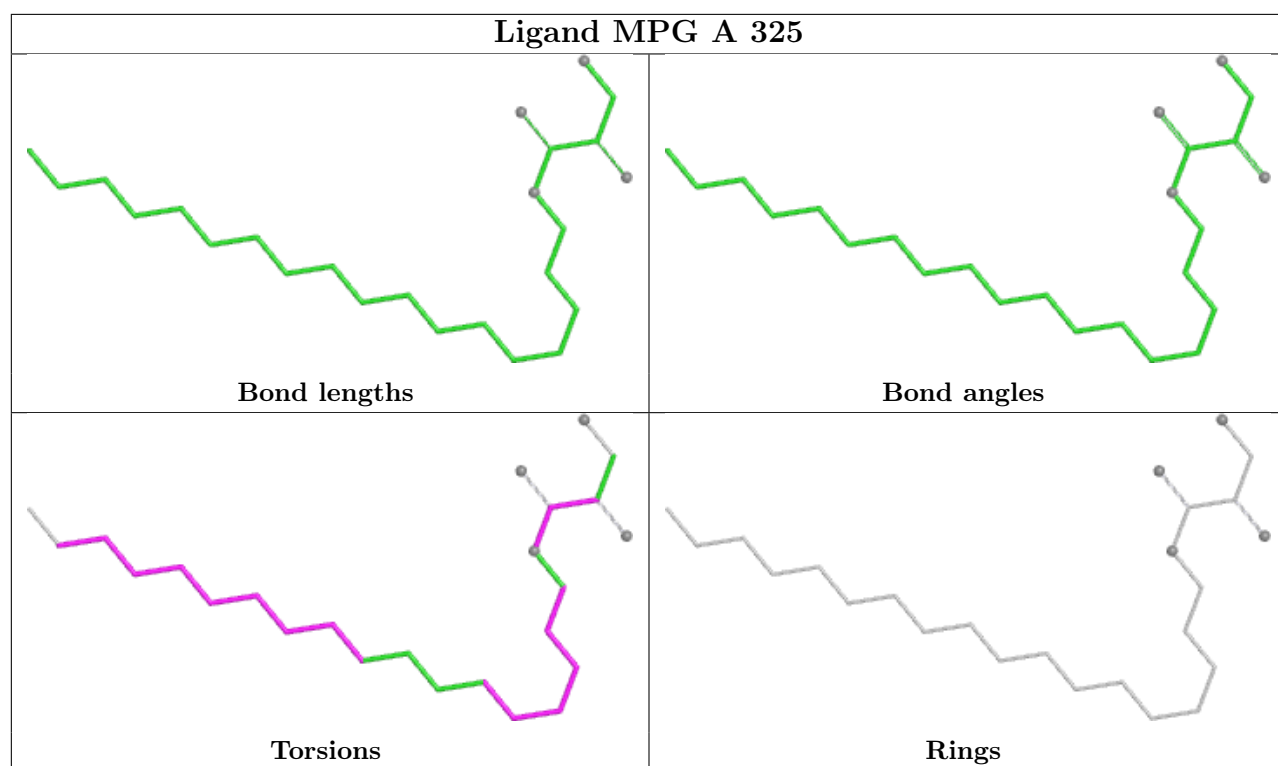
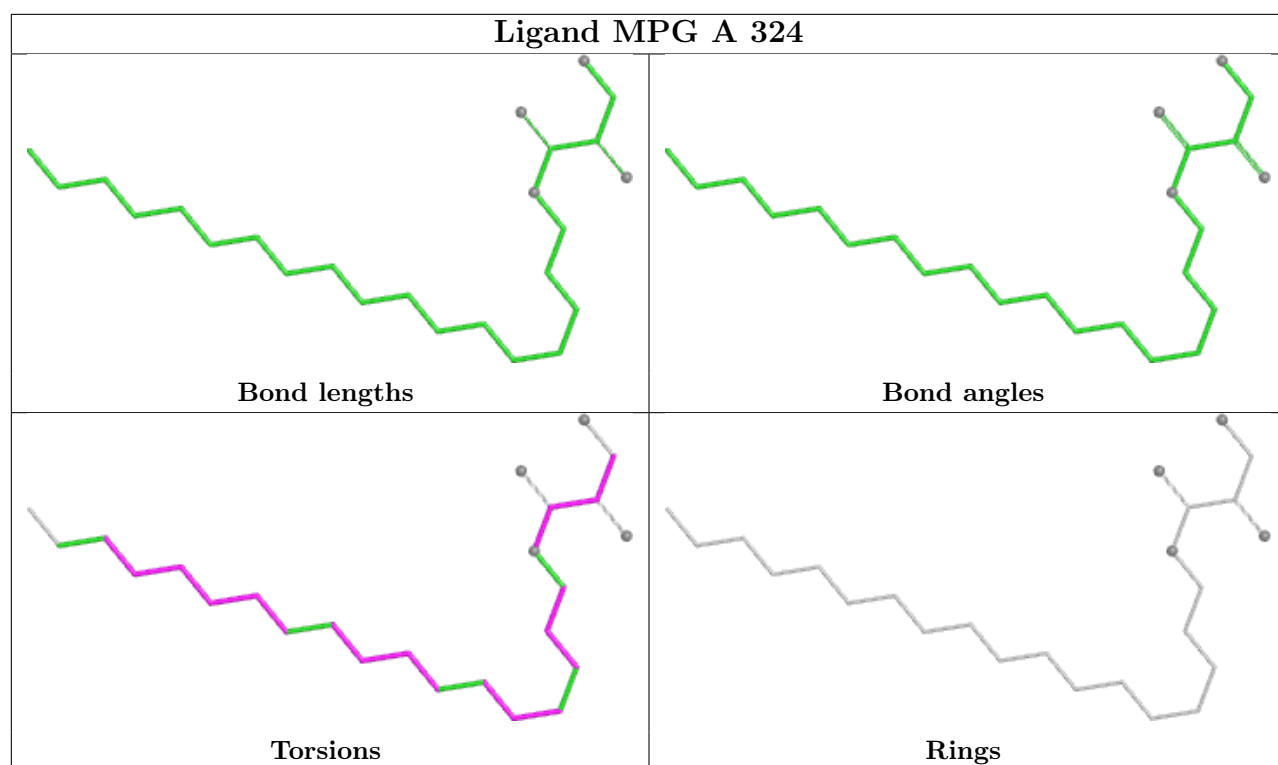


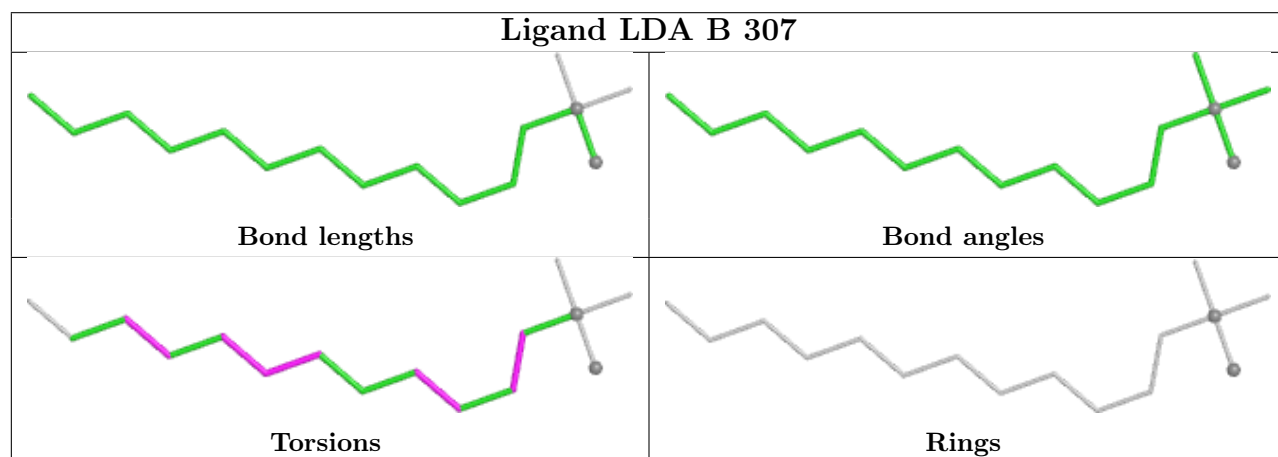
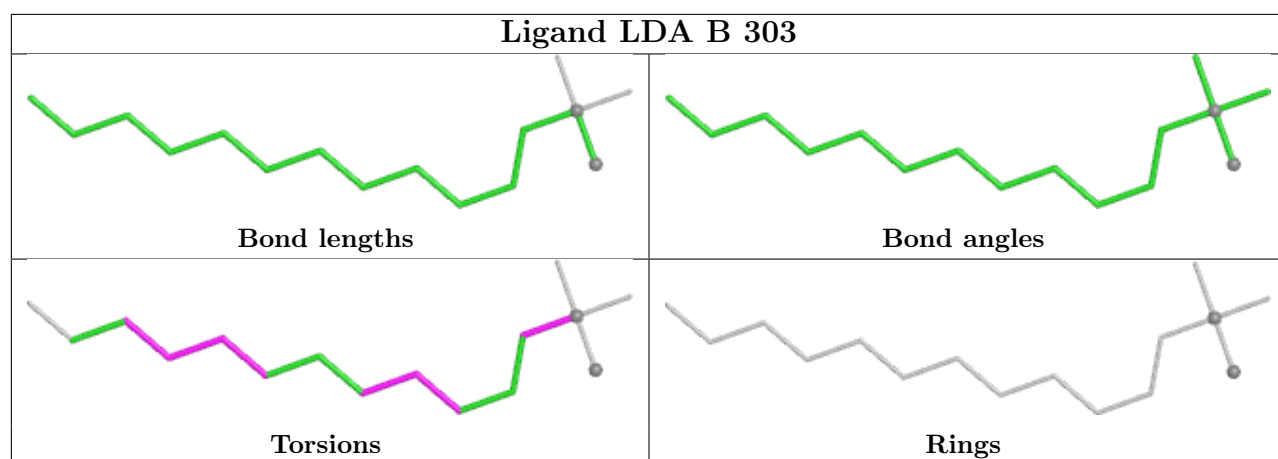
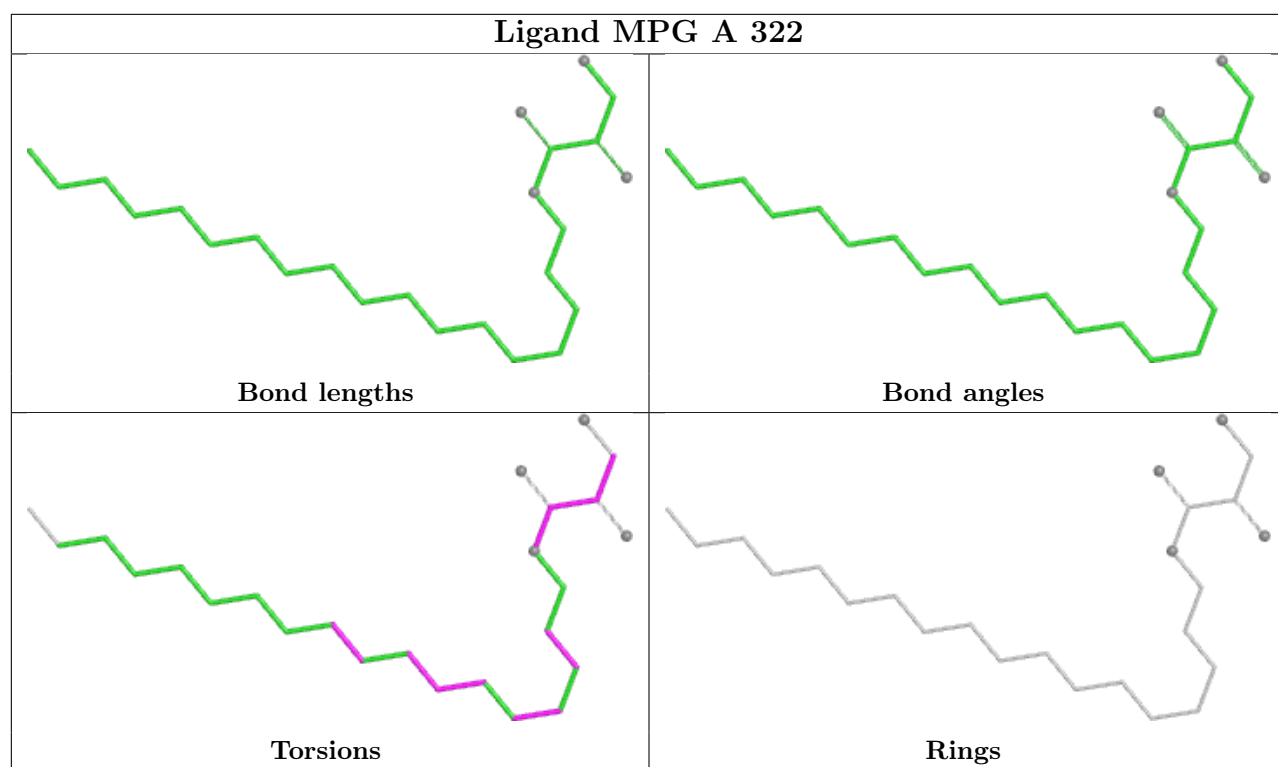


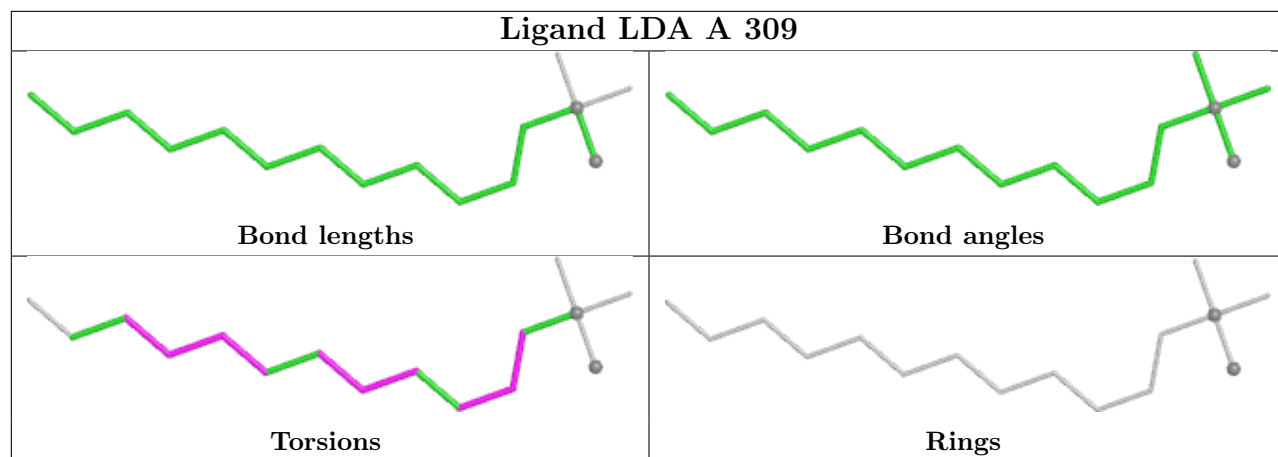


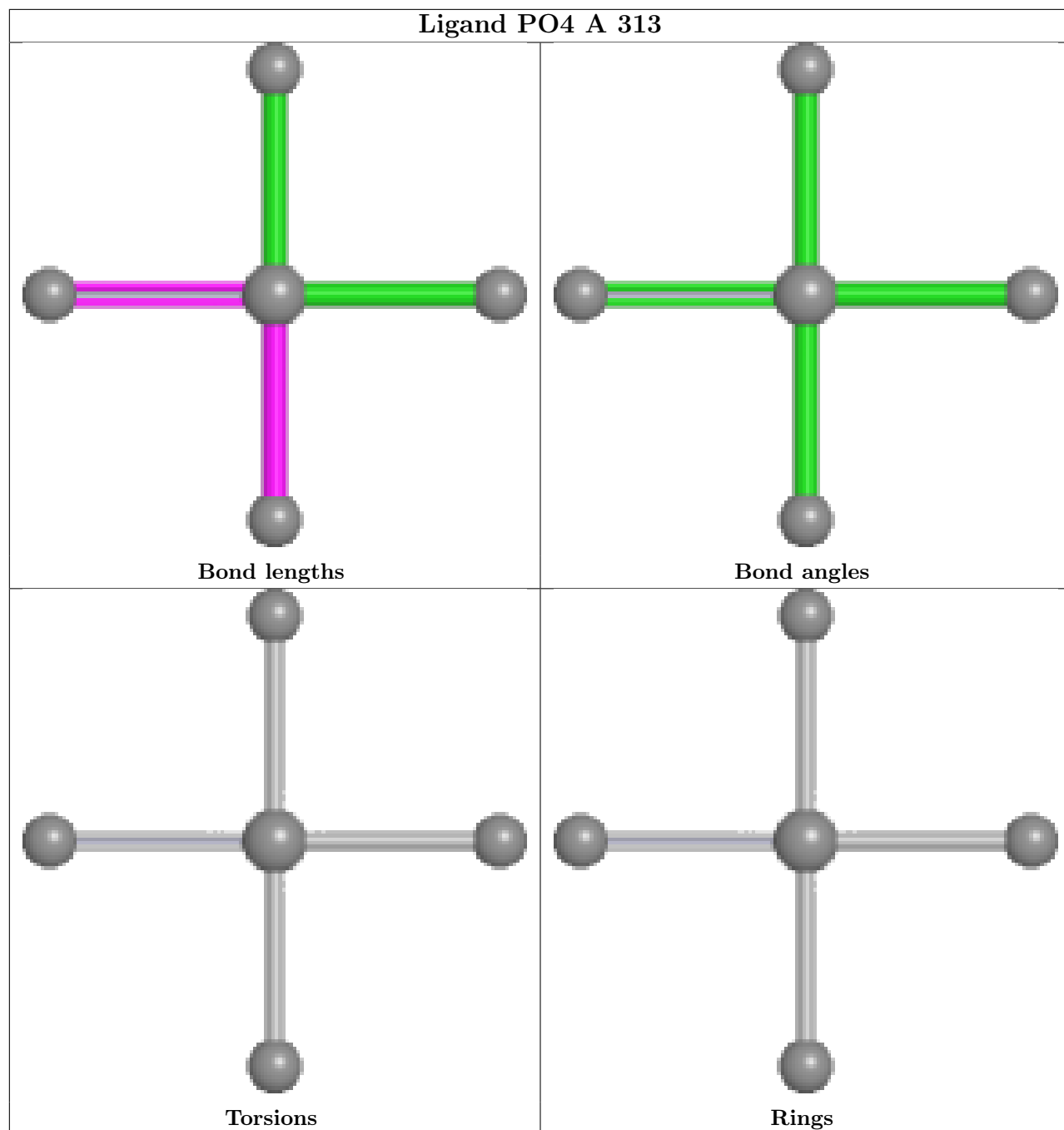


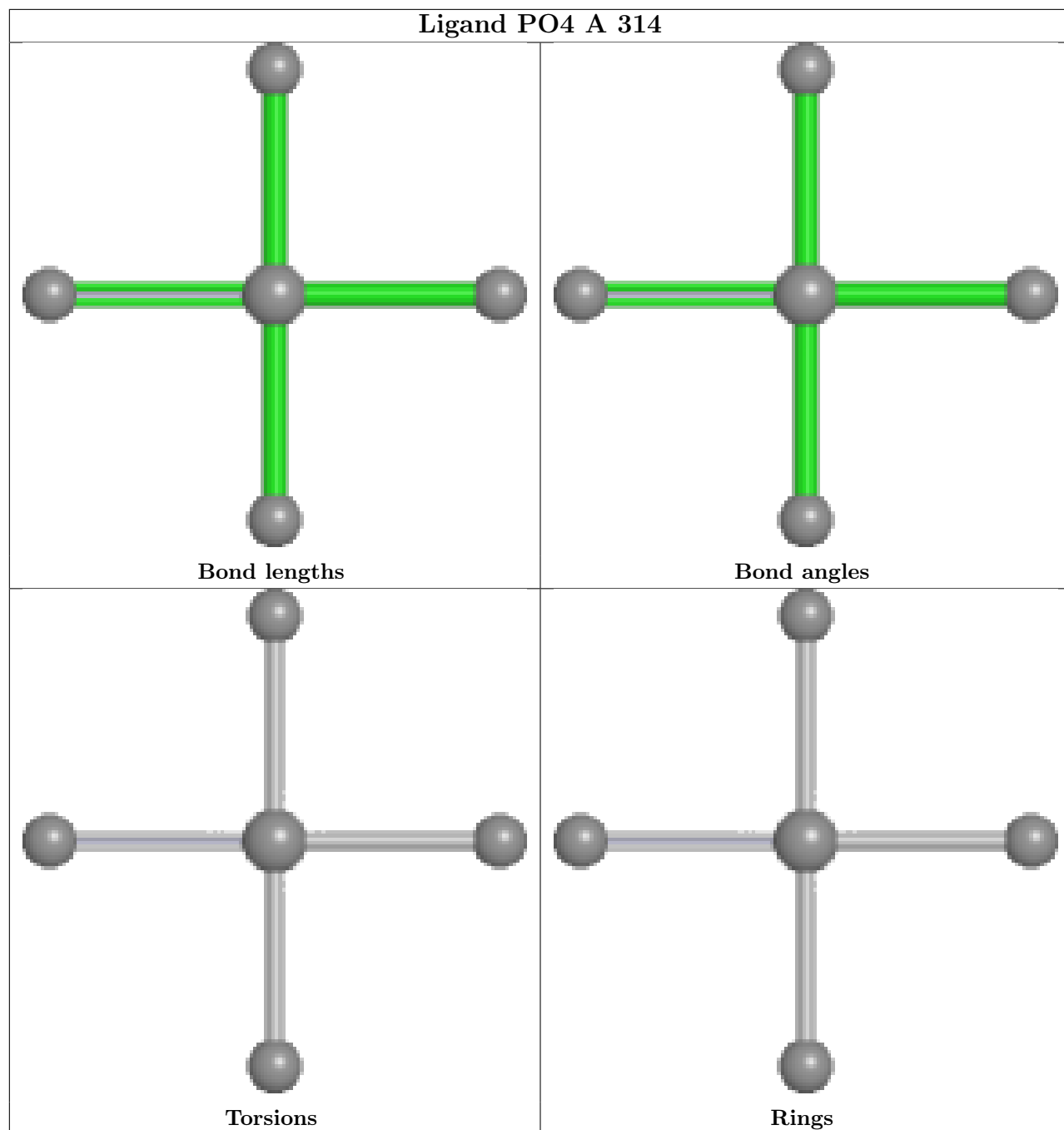


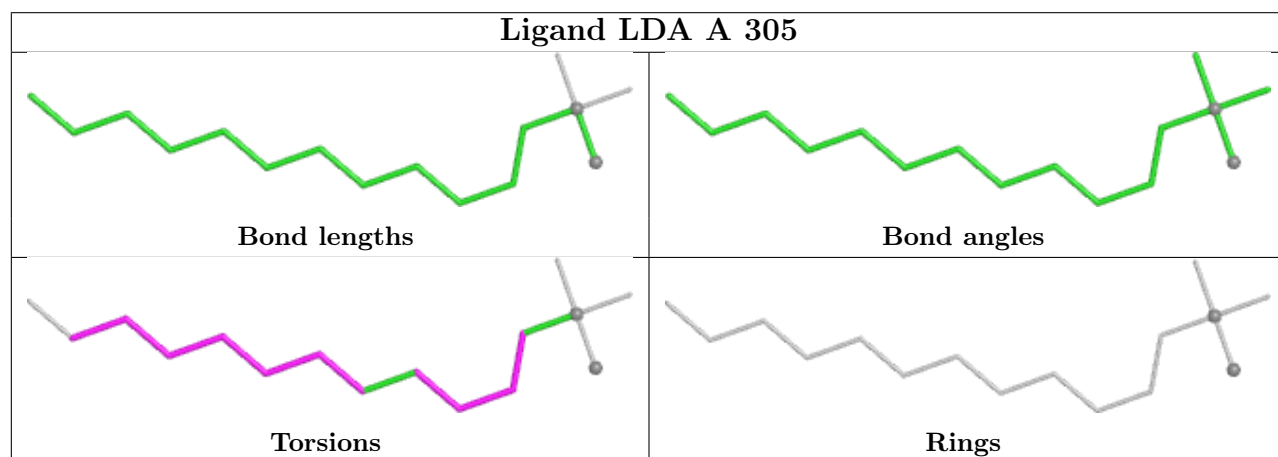
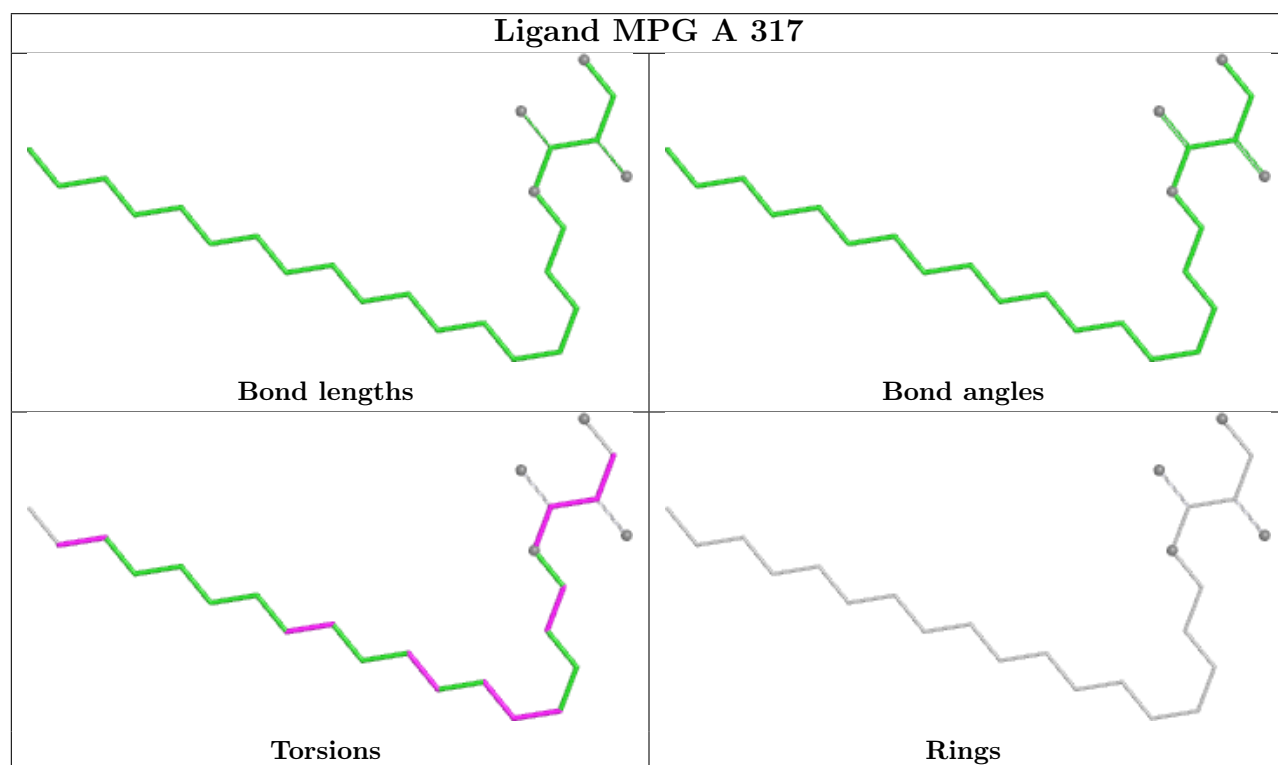
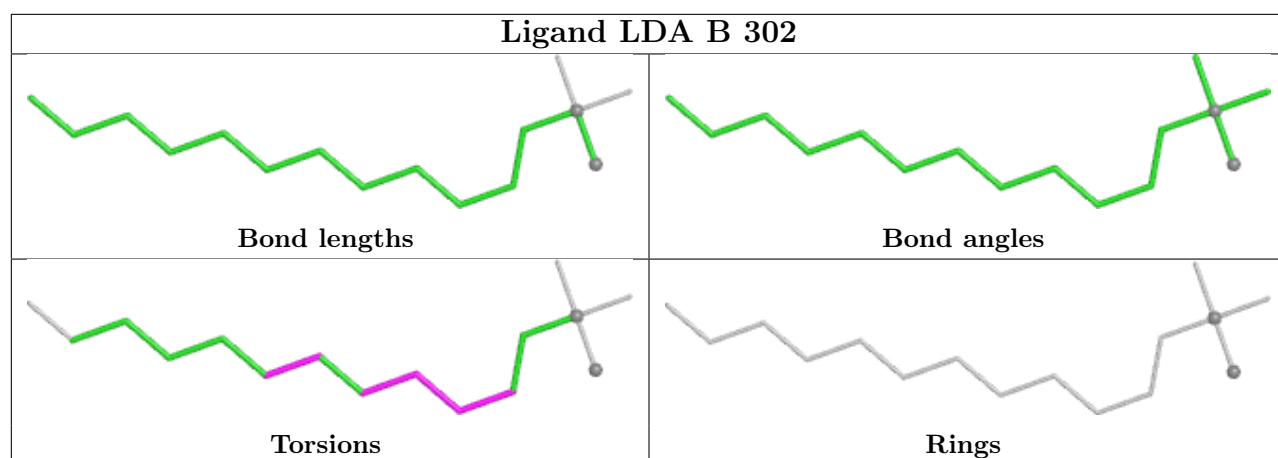


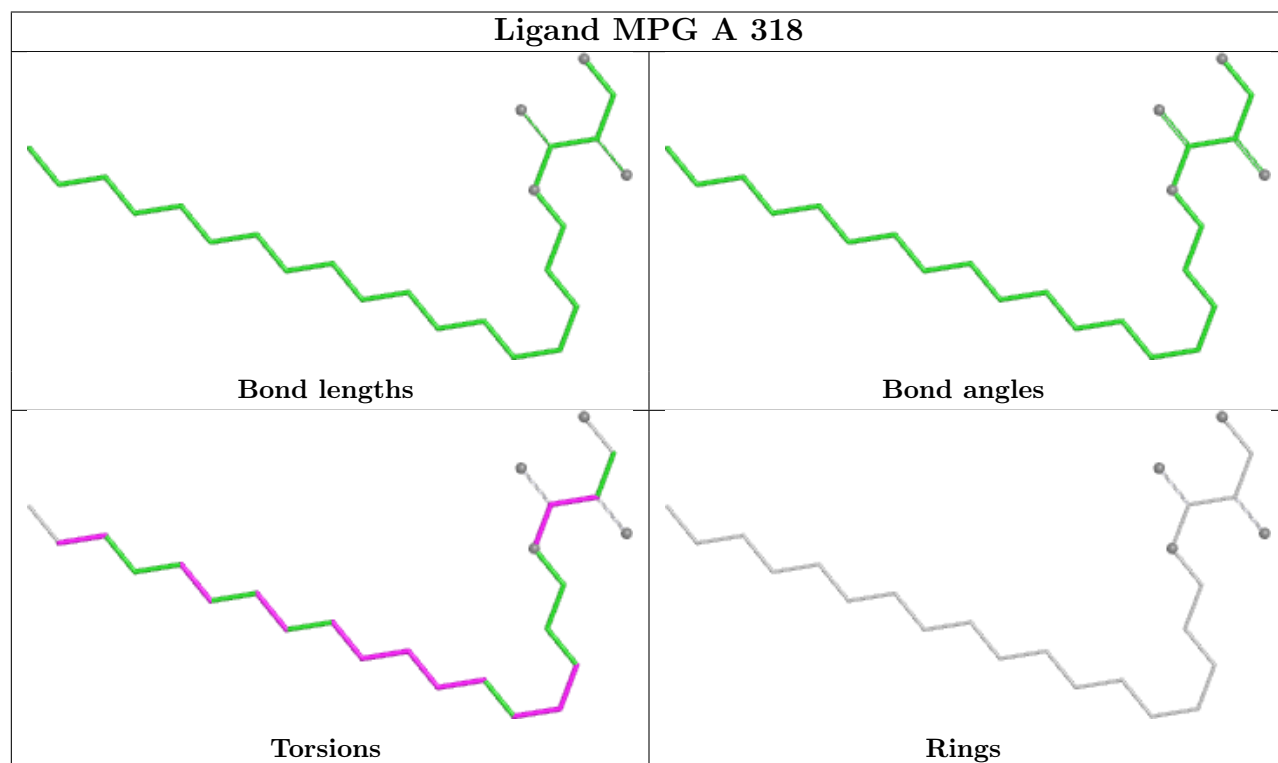
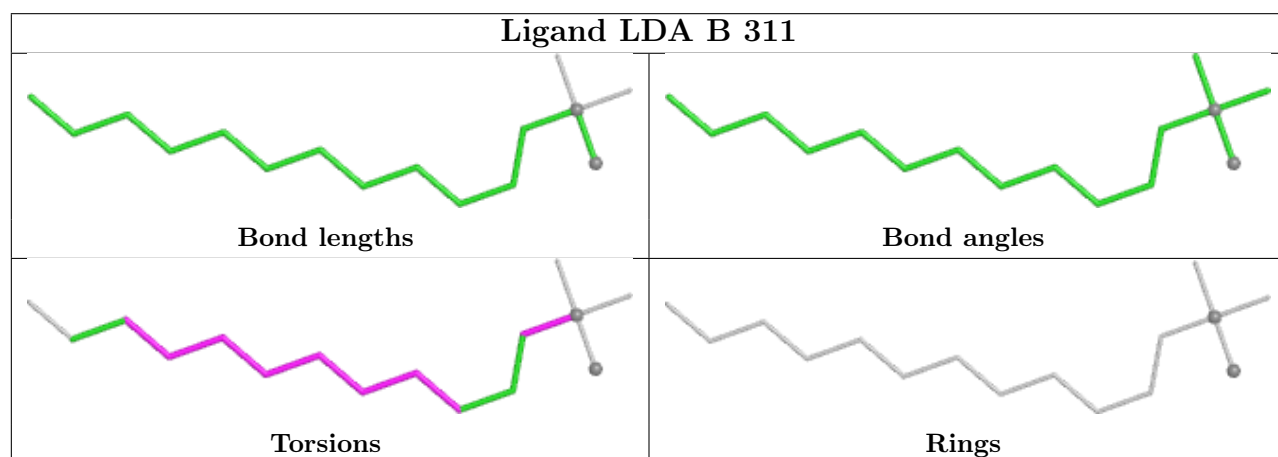
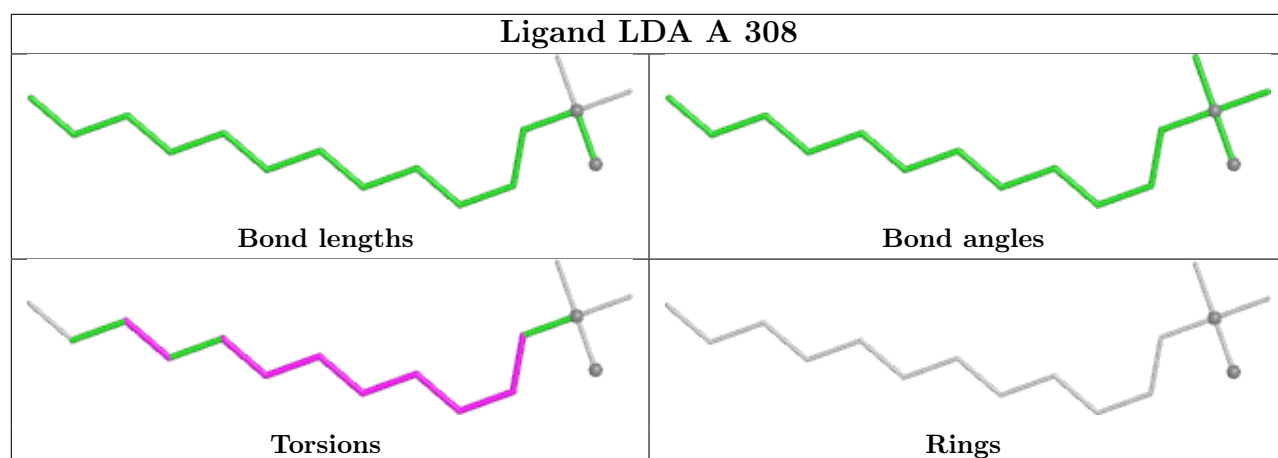


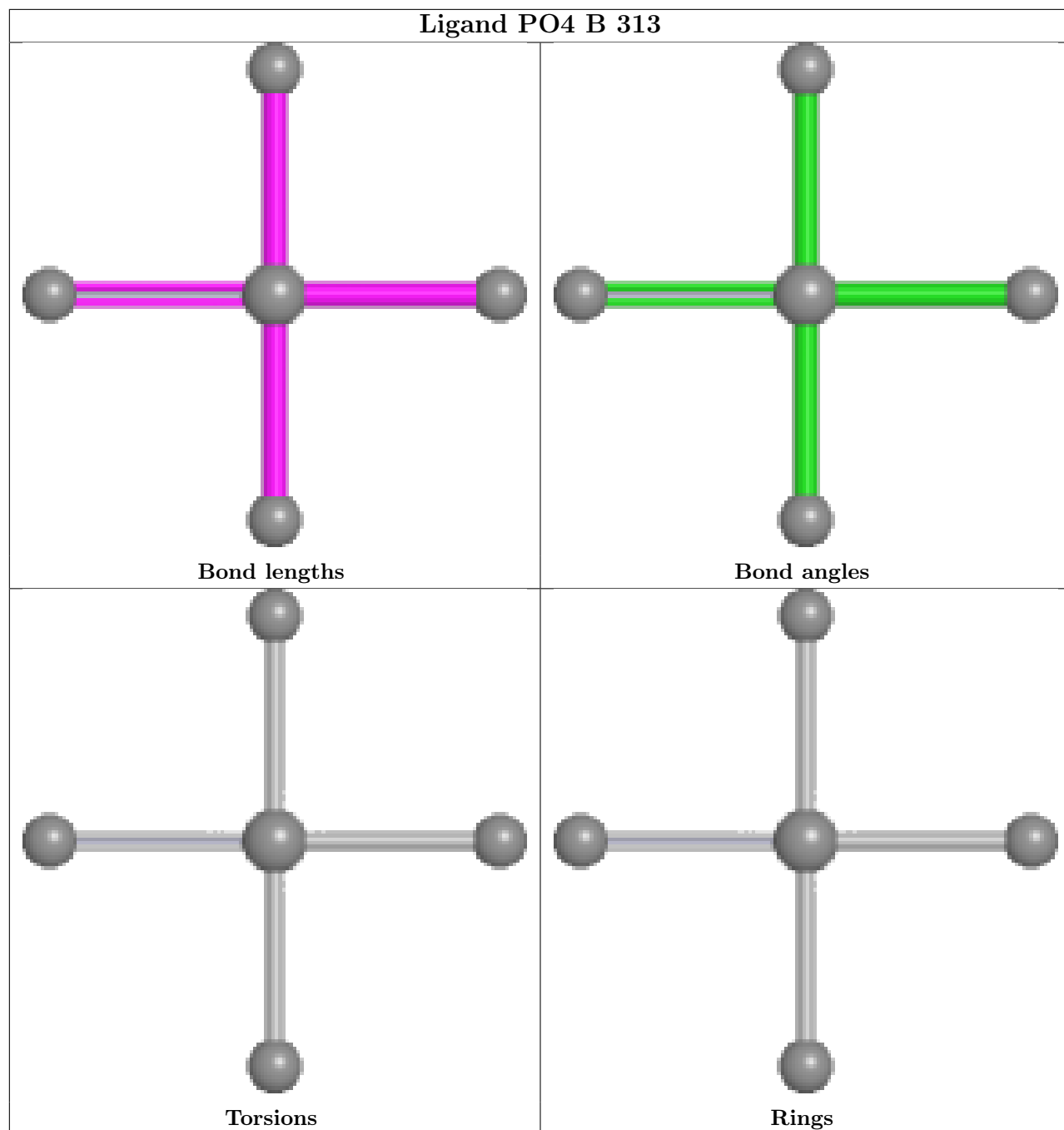


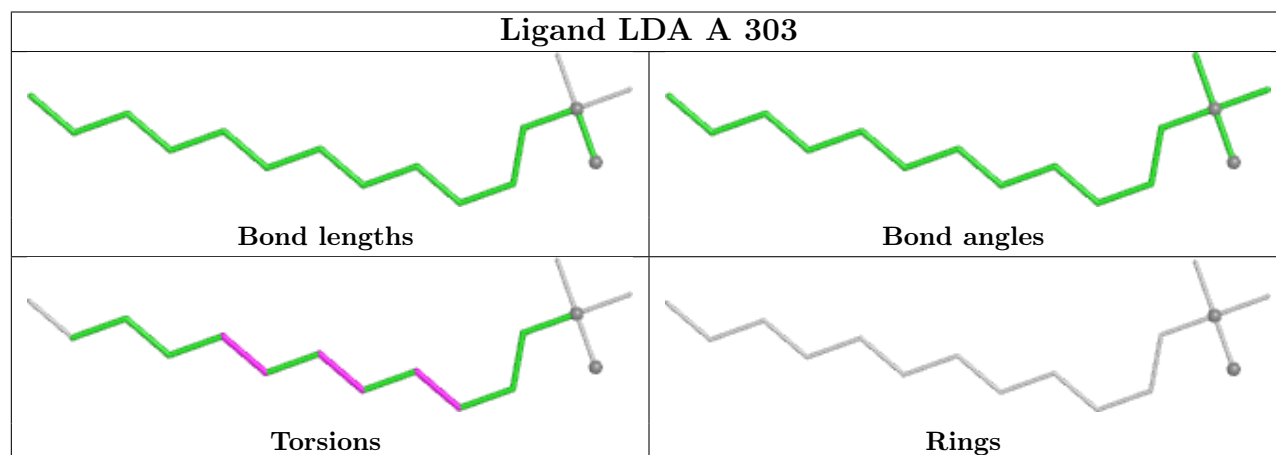
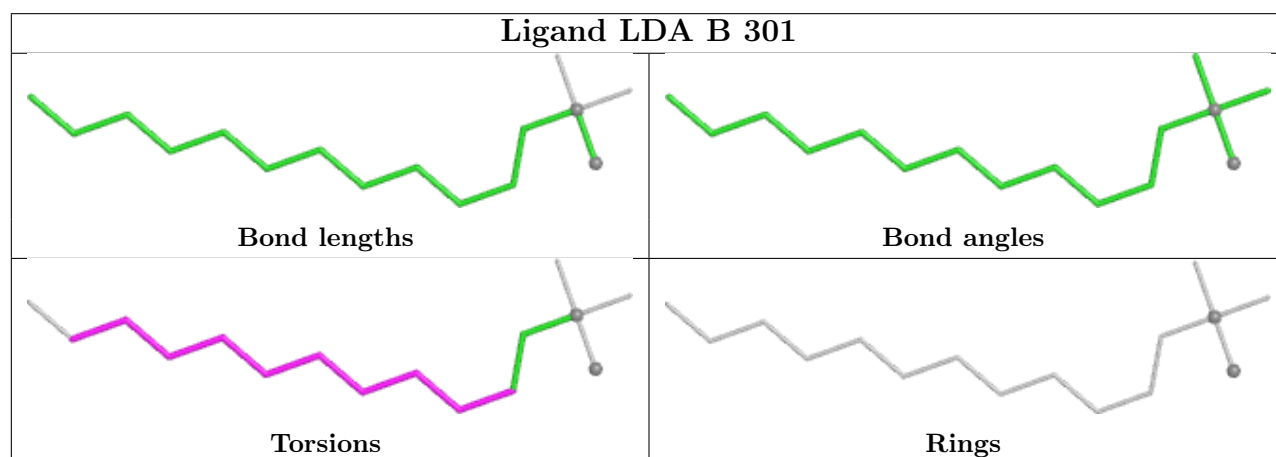
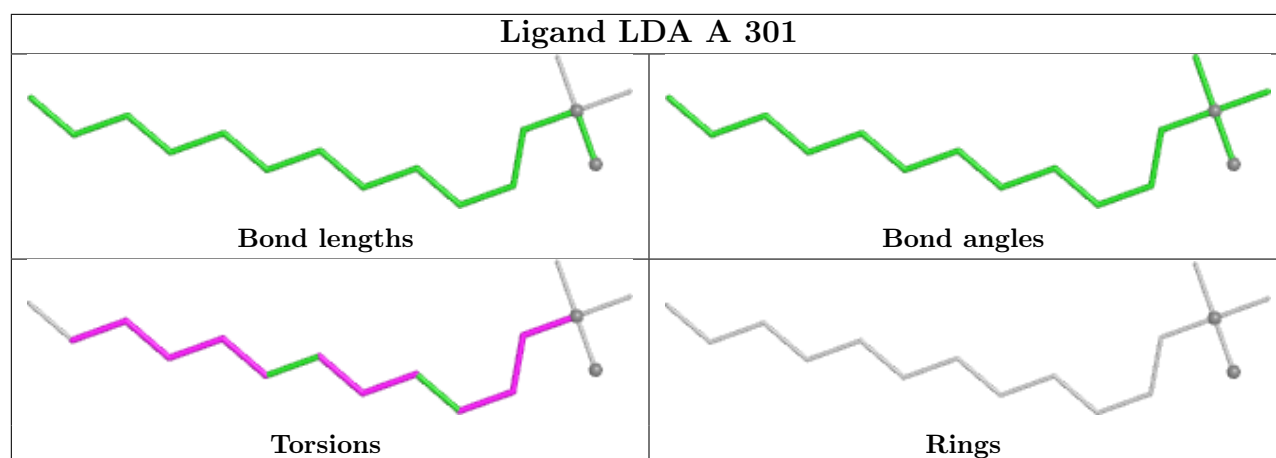


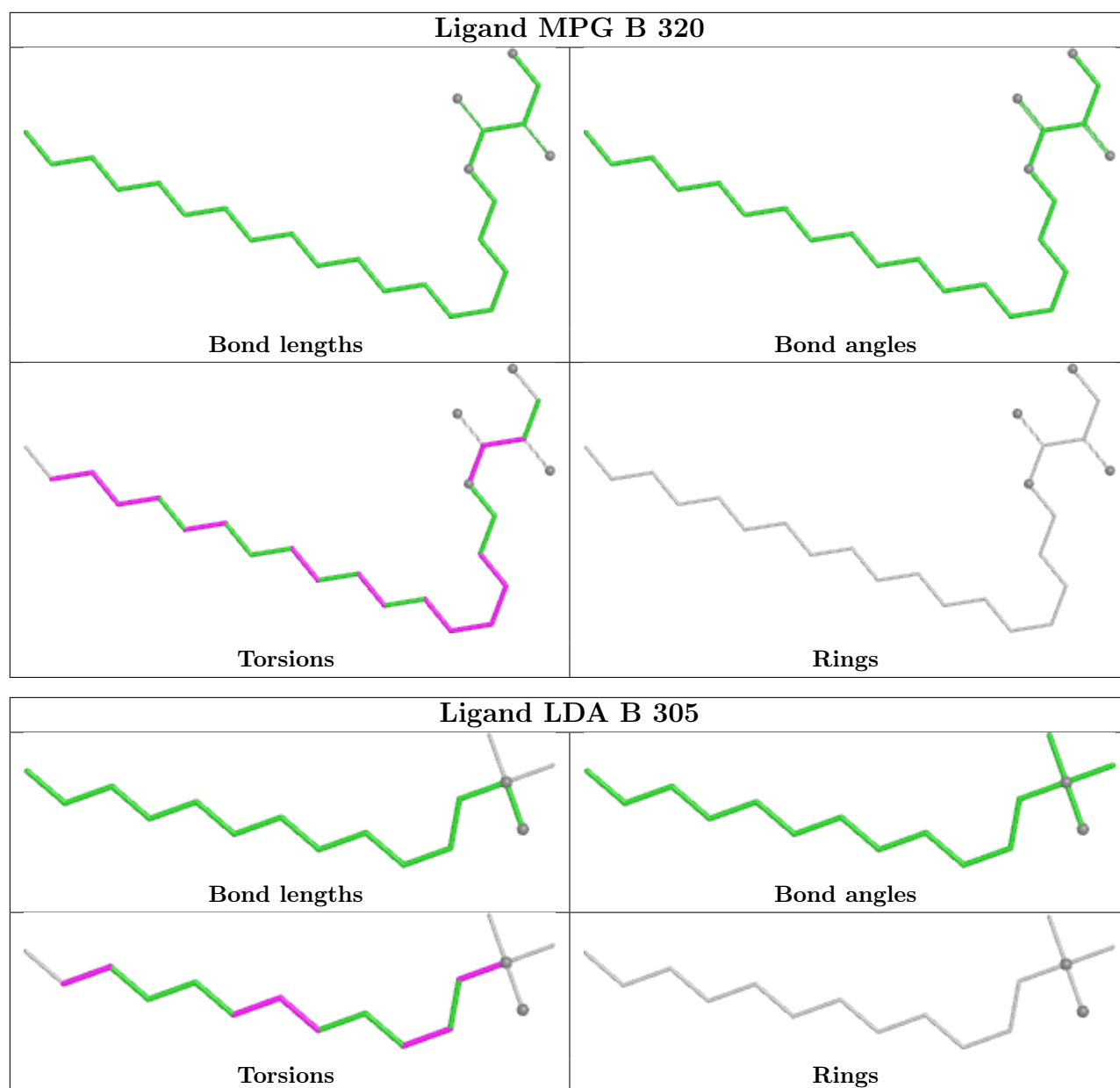


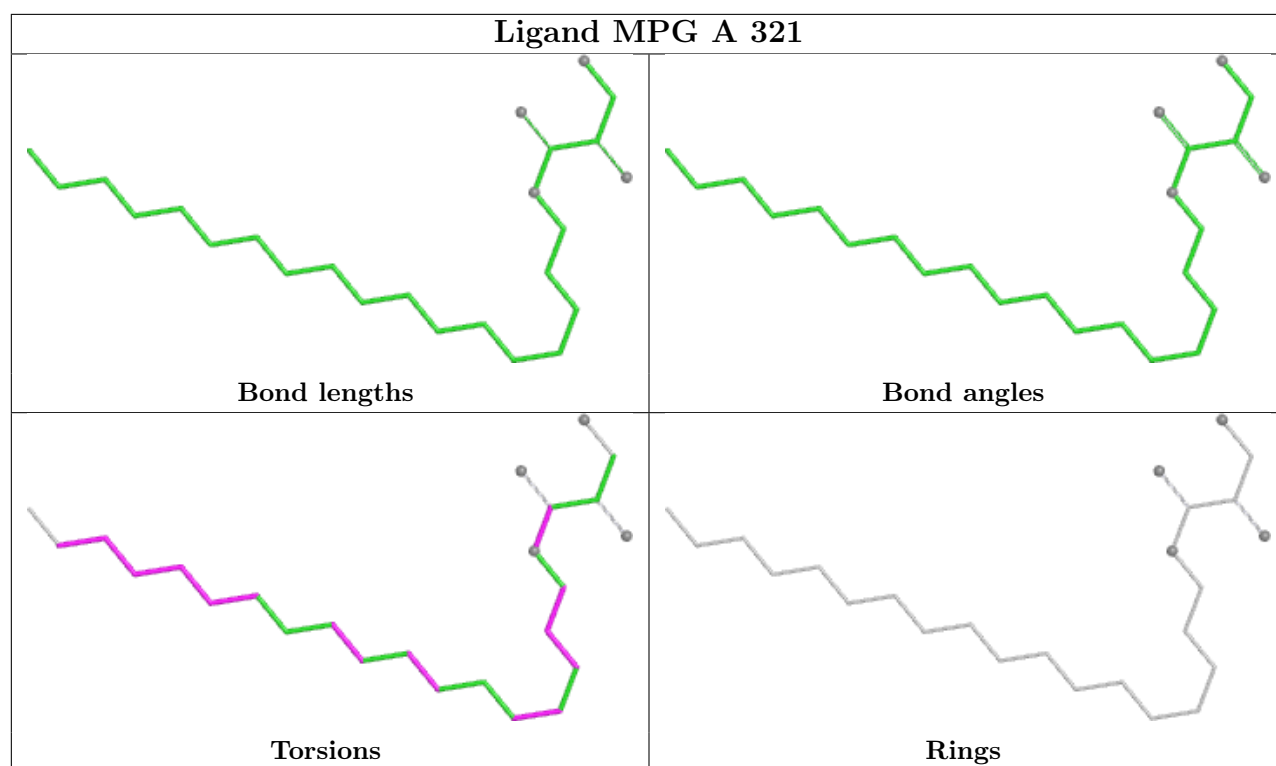
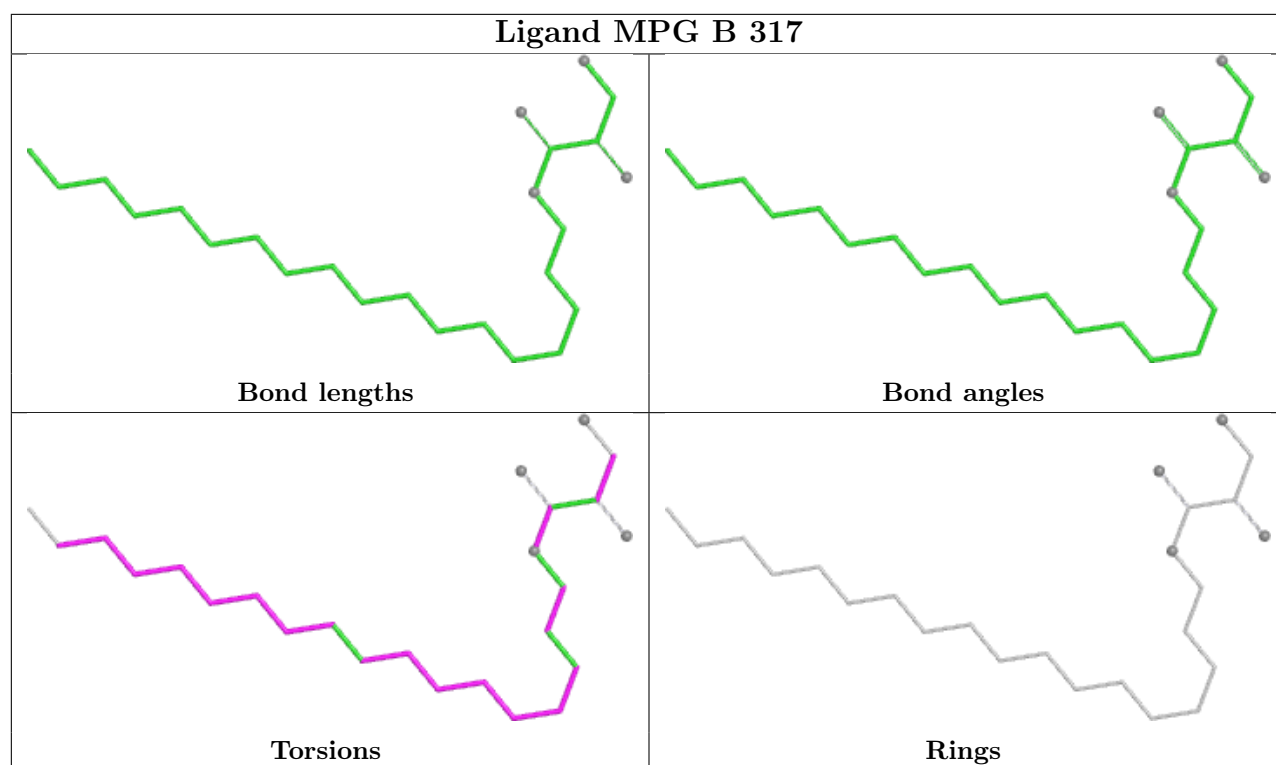


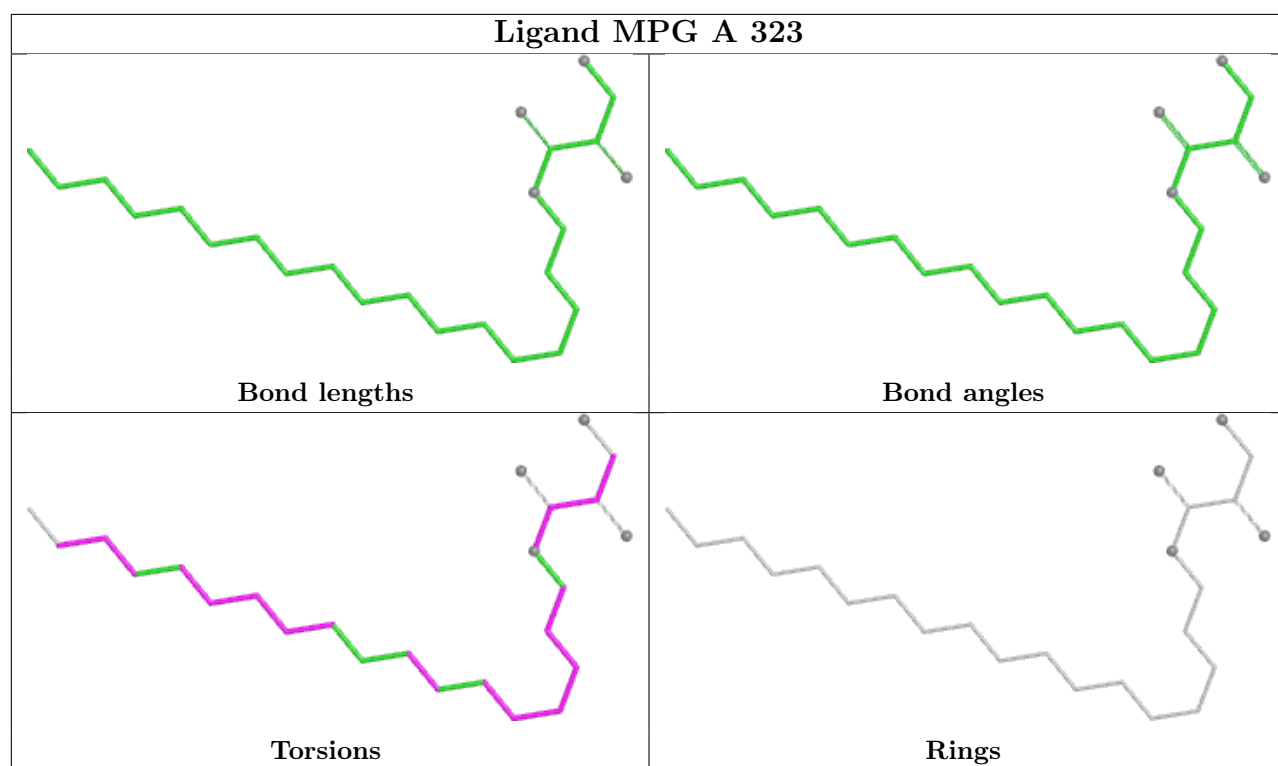
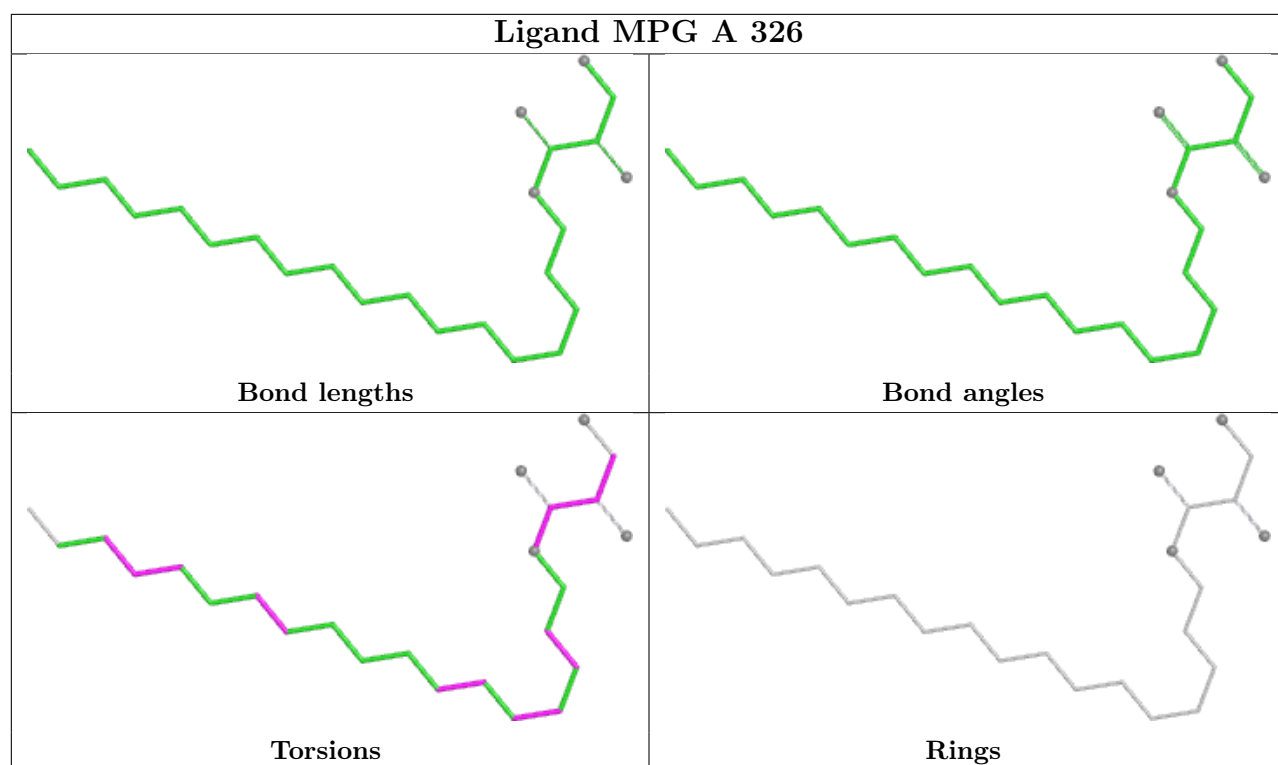


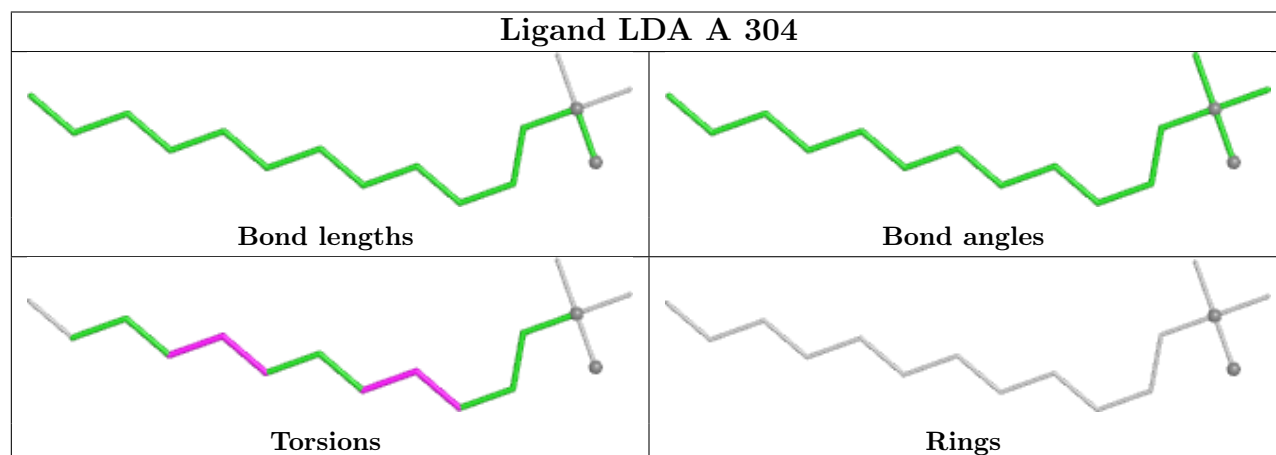
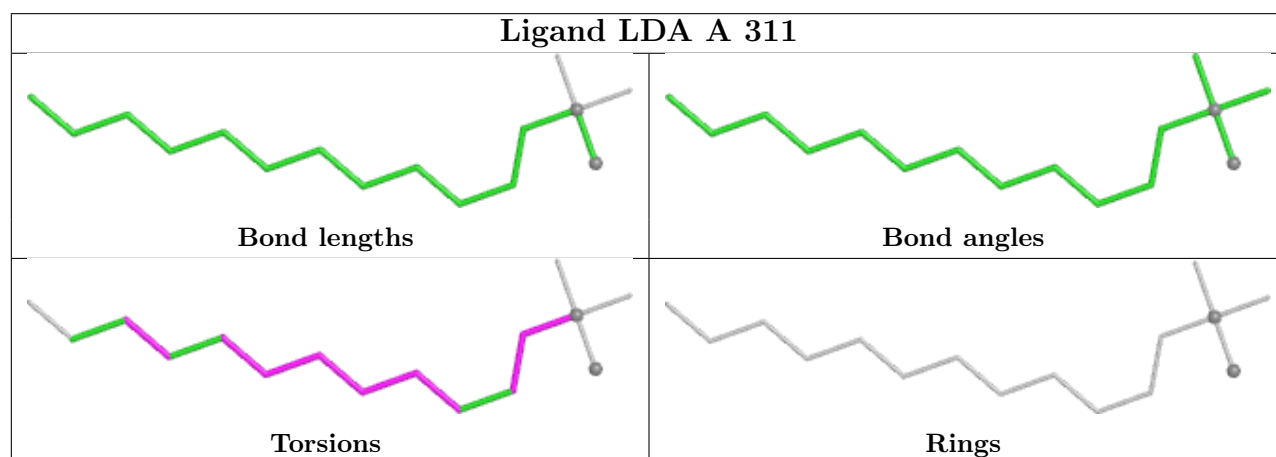
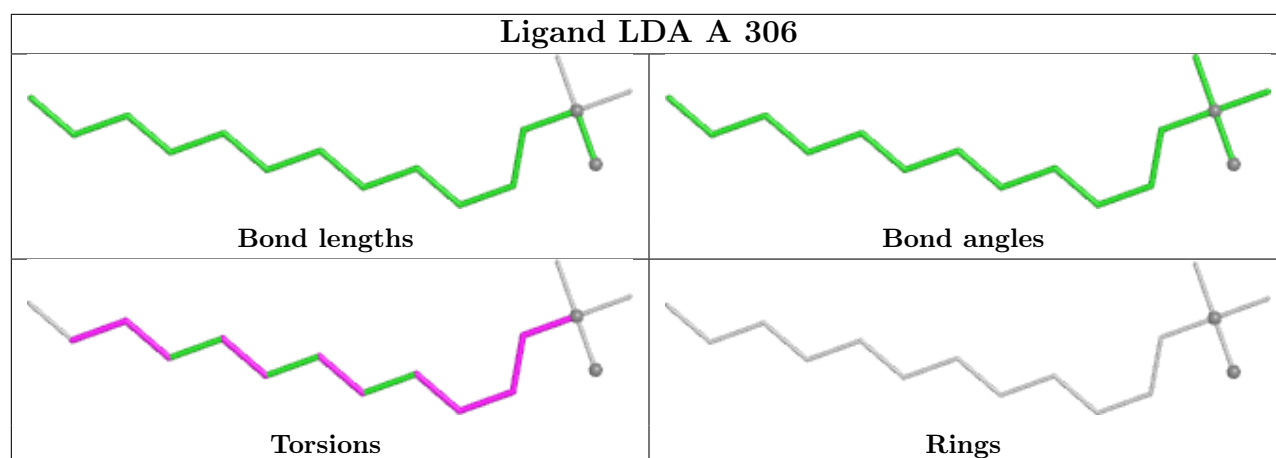


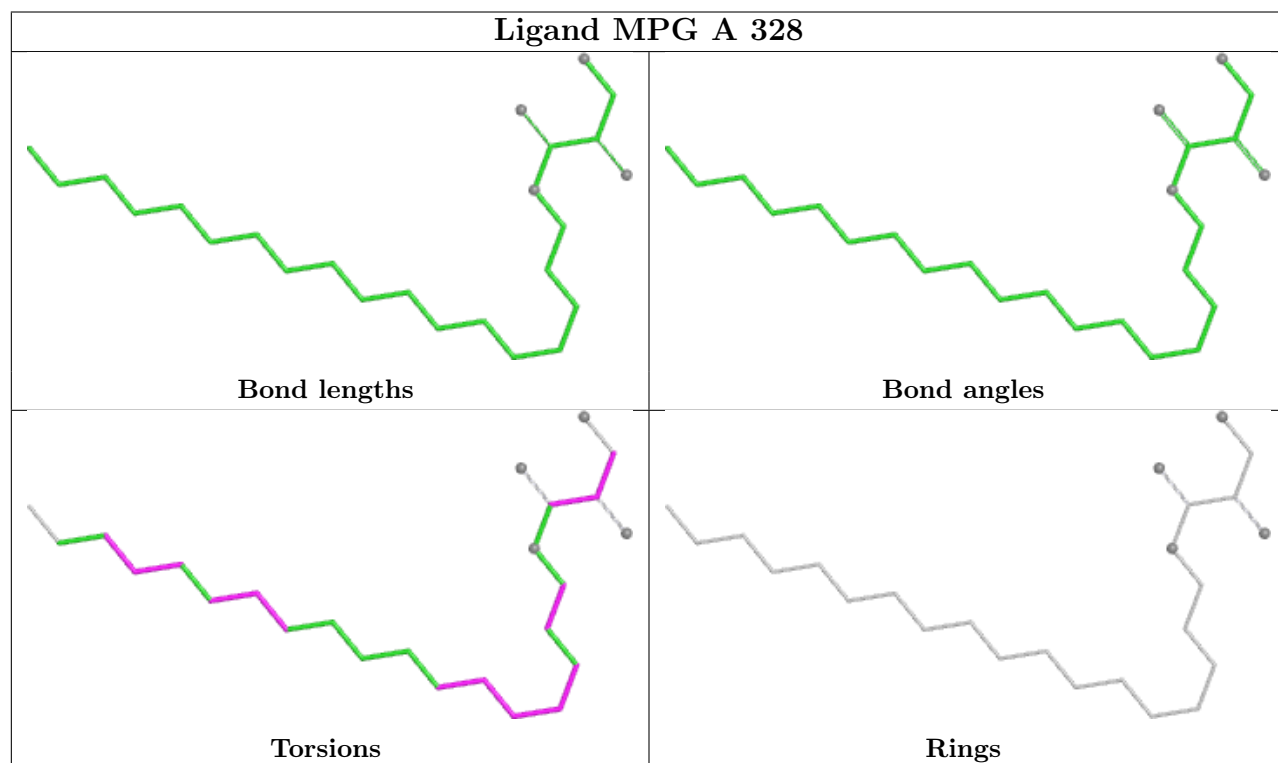
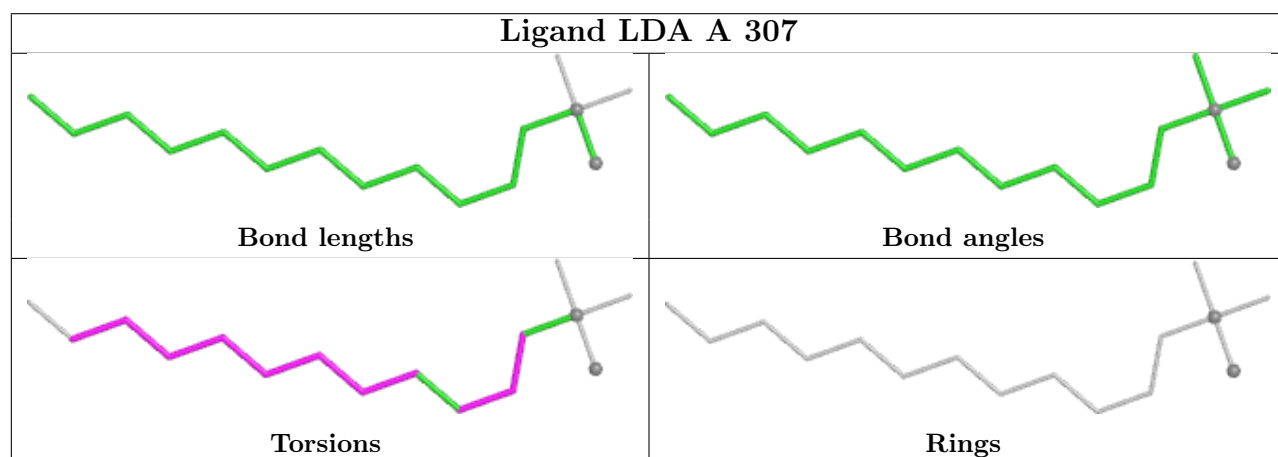
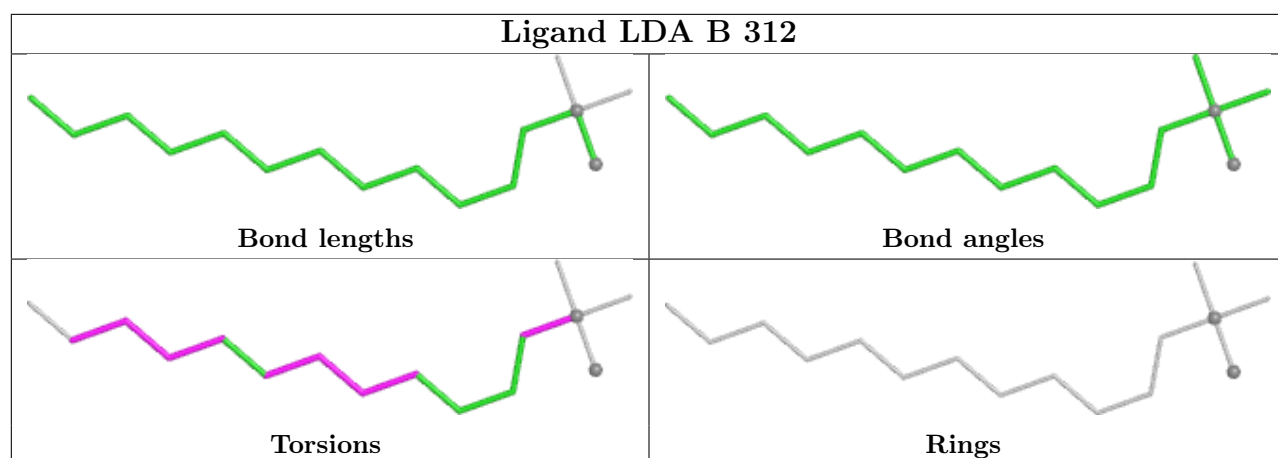


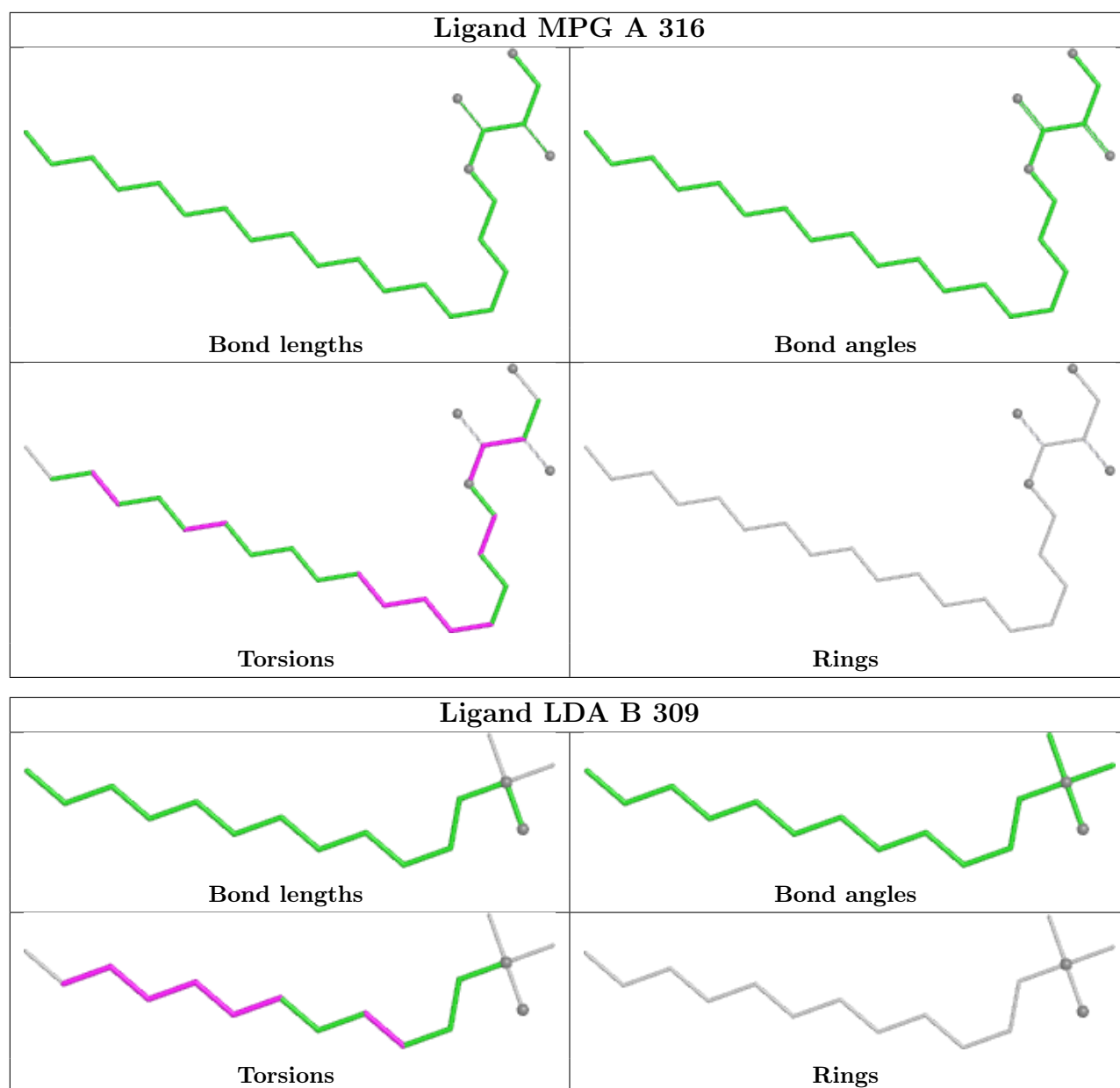












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	280/283 (98%)	0.07	7 (2%) 58 60	32, 43, 76, 104	0
1	B	280/283 (98%)	0.08	9 (3%) 50 52	33, 43, 79, 101	0
All	All	560/566 (98%)	0.07	16 (2%) 53 56	32, 43, 79, 104	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	283	LEU	4.2
1	B	4	PHE	4.2
1	A	283	LEU	3.9
1	A	5	MET	3.9
1	A	4	PHE	3.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LDA	B	312	16/16	0.35	0.20	20,20,20,20	0
3	PO4	A	312	5/5	0.62	0.11	129,130,130,130	0
2	LDA	B	308	16/16	0.63	0.24	68,77,90,91	0
3	PO4	B	313	5/5	0.64	0.13	125,126,126,127	0
2	LDA	A	311	16/16	0.66	0.25	75,81,90,90	0
3	PO4	B	314	5/5	0.67	0.11	109,110,110,110	0
2	LDA	A	308	16/16	0.69	0.23	114,116,125,125	0
5	MPG	A	325	25/25	0.70	0.21	77,81,89,90	0
3	PO4	A	314	5/5	0.71	0.13	144,145,145,145	0
5	MPG	A	327	25/25	0.71	0.20	77,83,94,95	0
2	LDA	B	311	16/16	0.72	0.29	102,112,116,117	0
5	MPG	A	328	25/25	0.75	0.21	66,74,84,84	0
5	MPG	A	322	25/25	0.76	0.20	65,80,97,100	0
2	LDA	B	307	16/16	0.76	0.22	77,83,97,97	0
2	LDA	A	309	16/16	0.76	0.28	86,100,111,111	0
5	MPG	A	319	25/25	0.76	0.20	74,90,99,102	0
2	LDA	B	309	16/16	0.77	0.21	70,80,86,86	0
2	LDA	B	305	16/16	0.77	0.23	70,77,83,83	0
5	MPG	A	326	25/25	0.77	0.21	79,84,86,89	0
2	LDA	A	304	16/16	0.77	0.24	72,75,78,78	0
2	LDA	B	302	16/16	0.77	0.25	71,76,81,83	0
3	PO4	A	313	5/5	0.78	0.10	98,98,99,100	0
2	LDA	B	310	16/16	0.78	0.25	106,109,116,116	0
5	MPG	A	316	25/25	0.78	0.18	65,71,90,93	0
5	MPG	B	318	25/25	0.78	0.18	54,78,92,92	0
5	MPG	B	319	25/25	0.78	0.20	69,85,105,107	0
2	LDA	B	301	16/16	0.79	0.21	71,74,78,80	0
5	MPG	B	320	25/25	0.79	0.20	63,71,86,89	0
2	LDA	B	303	16/16	0.80	0.18	66,71,73,75	0
2	LDA	B	304	16/16	0.80	0.21	77,80,87,87	0
2	LDA	A	301	16/16	0.80	0.24	73,80,86,87	0
2	LDA	B	306	16/16	0.81	0.23	73,76,80,81	0
5	MPG	A	323	25/25	0.81	0.17	54,67,92,93	0
5	MPG	B	316	25/25	0.81	0.17	61,67,79,81	0
5	MPG	B	317	25/25	0.82	0.20	79,89,95,97	0
5	MPG	A	324	25/25	0.82	0.20	61,70,82,85	0
2	LDA	A	306	16/16	0.82	0.22	67,70,86,88	0
5	MPG	A	321	25/25	0.82	0.16	72,79,91,94	0
5	MPG	A	318	25/25	0.83	0.18	54,65,100,104	0
2	LDA	A	310	16/16	0.83	0.21	81,88,99,100	0
2	LDA	A	303	16/16	0.83	0.18	53,61,69,74	0
5	MPG	A	320	25/25	0.85	0.17	62,71,88,90	0
5	MPG	A	317	25/25	0.85	0.16	51,70,84,85	0

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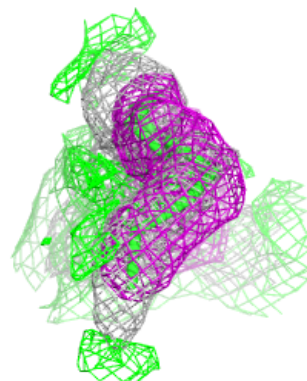
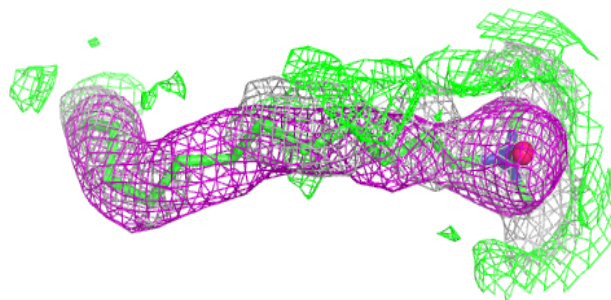
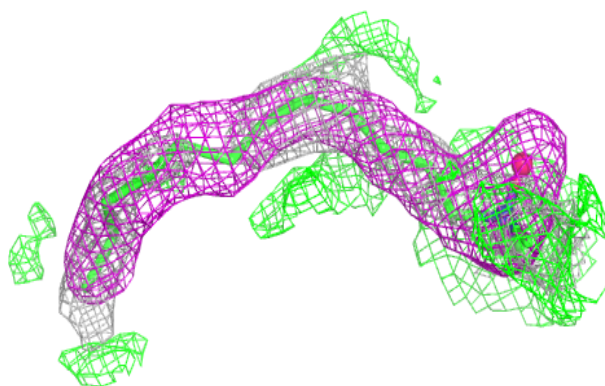
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LDA	A	302	16/16	0.86	0.15	52,56,72,73	0
2	LDA	A	305	16/16	0.86	0.18	82,86,91,91	0
2	LDA	A	307	16/16	0.87	0.16	62,68,71,72	0
4	MG	B	315	1/1	0.93	0.31	64,64,64,64	0
4	MG	A	315	1/1	0.96	0.24	55,55,55,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

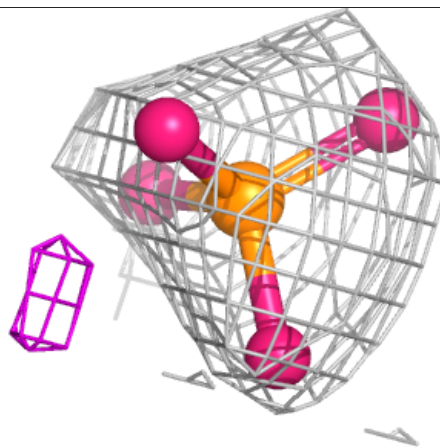
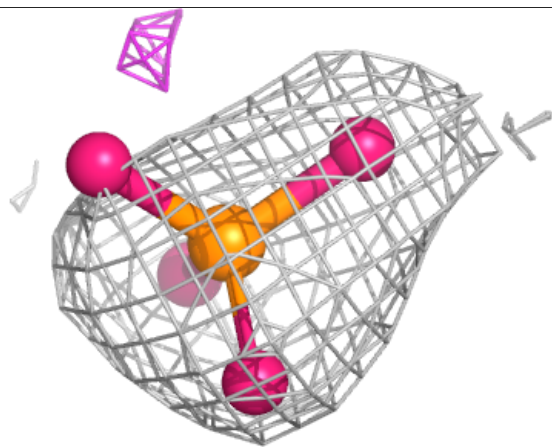
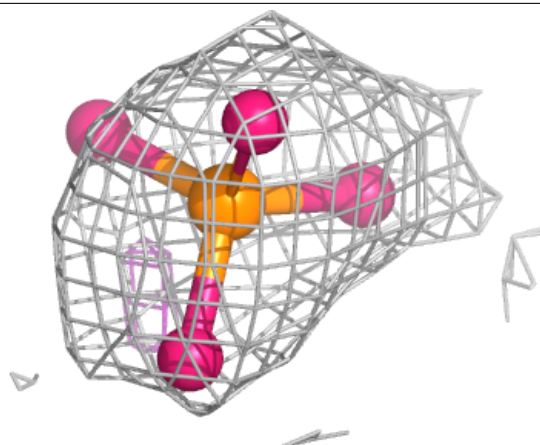
Electron density around LDA B 312:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



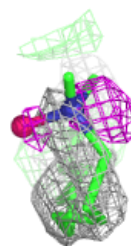
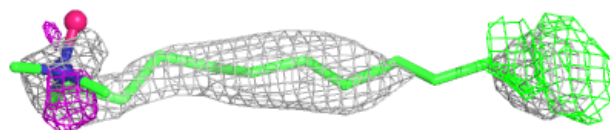
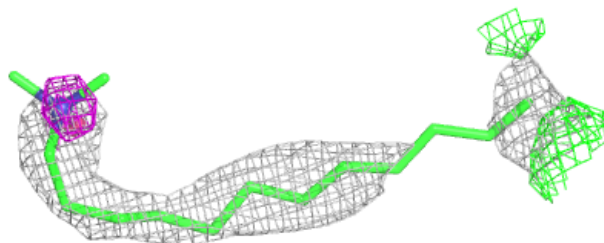
Electron density around PO4 A 312:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



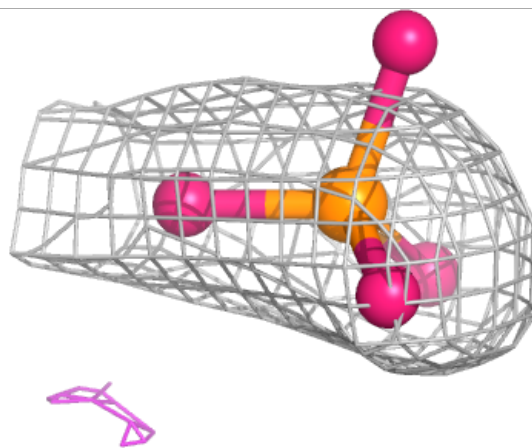
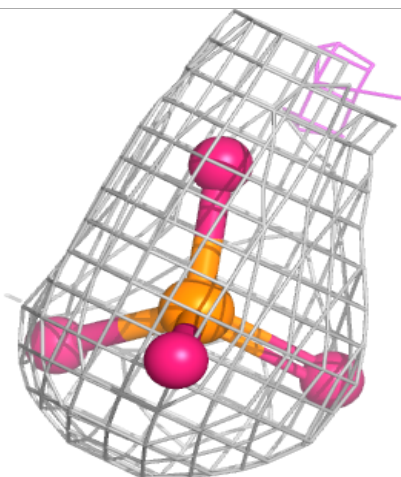
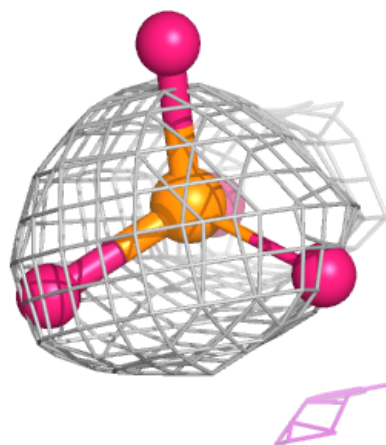
Electron density around LDA B 308:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



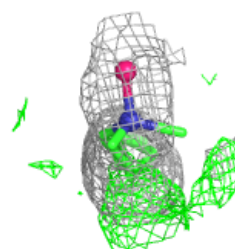
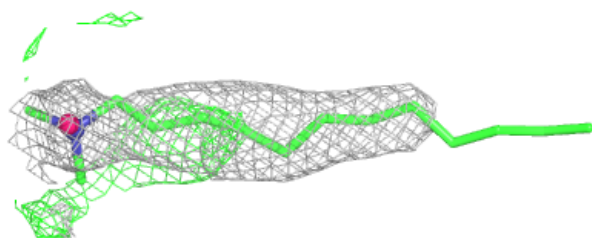
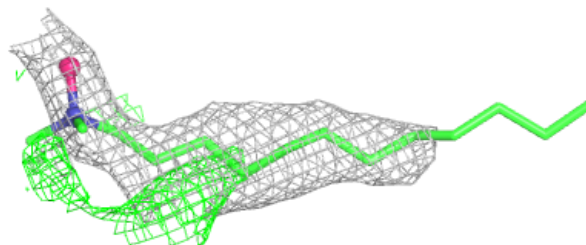
Electron density around PO4 B 313:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



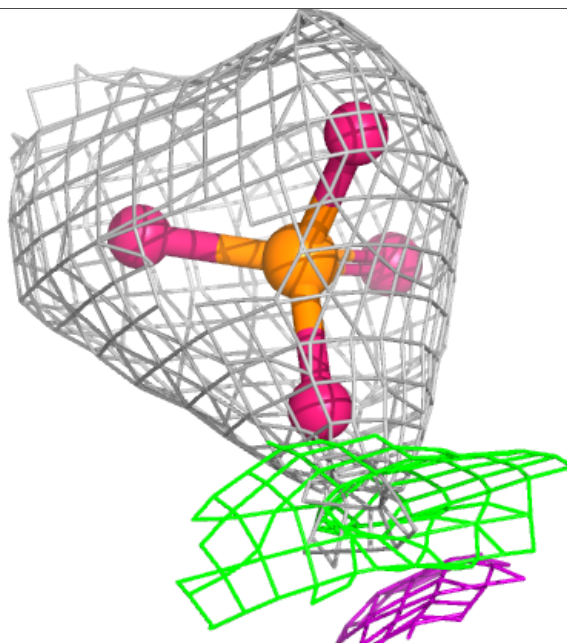
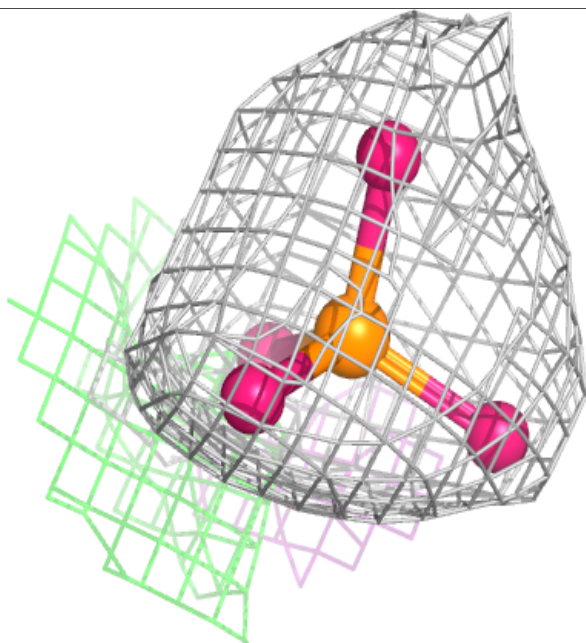
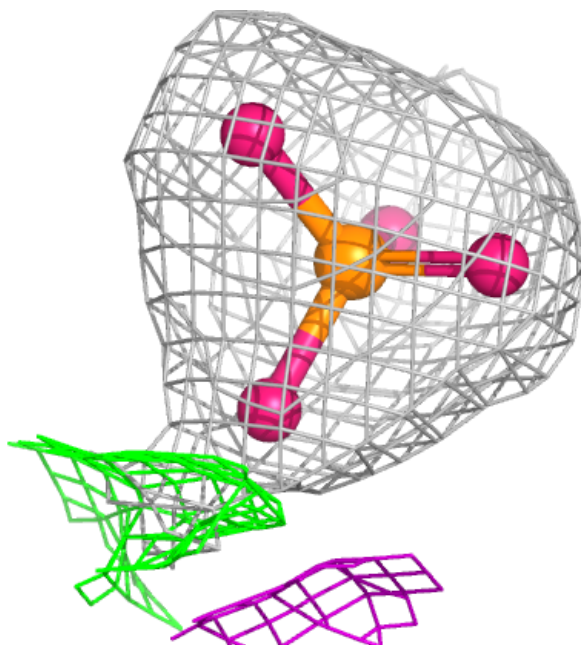
Electron density around LDA A 311:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



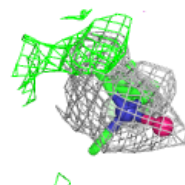
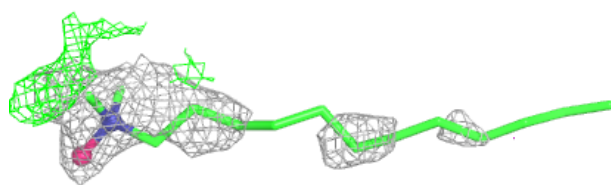
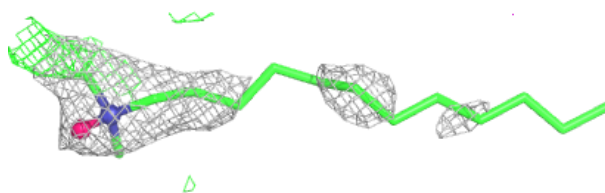
Electron density around PO4 B 314:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

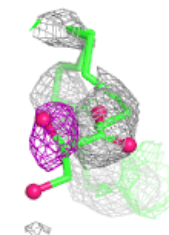
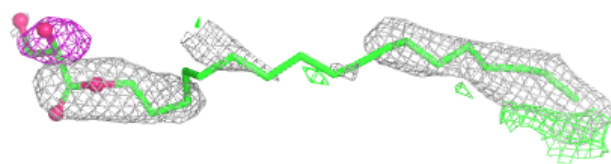
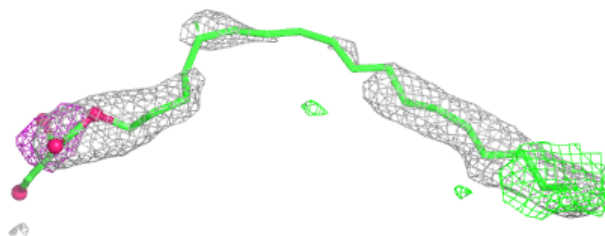


Electron density around LDA A 308:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

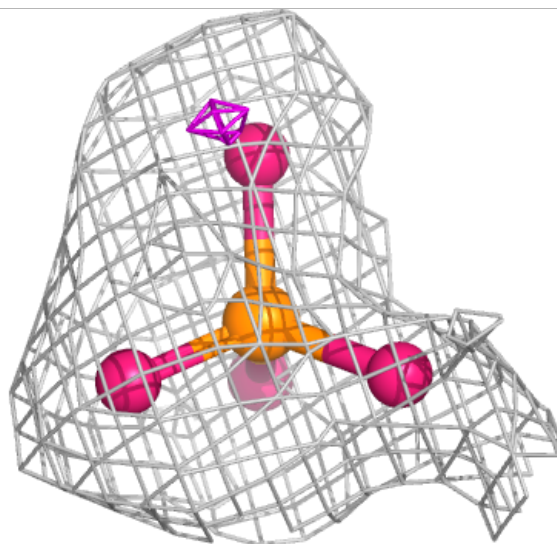
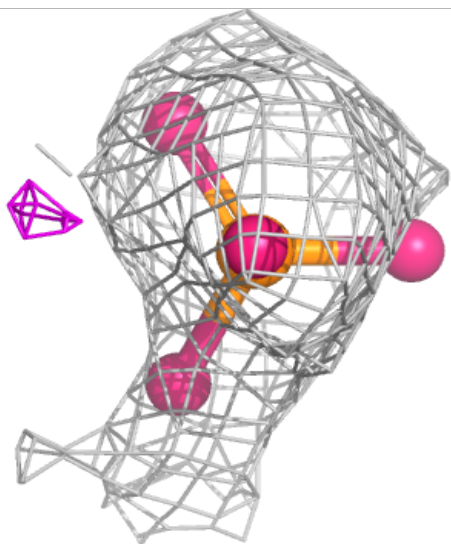
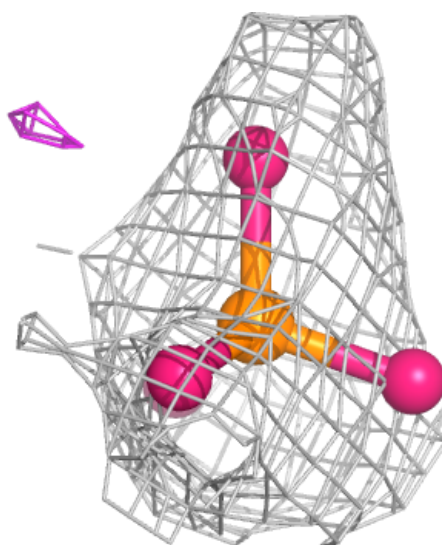
**Electron density around MPG A 325:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



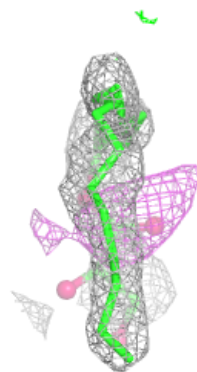
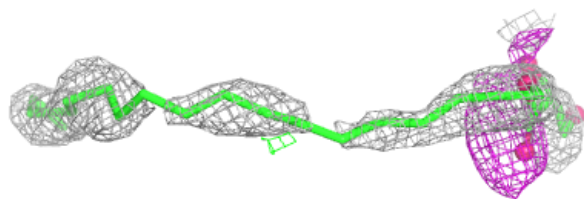
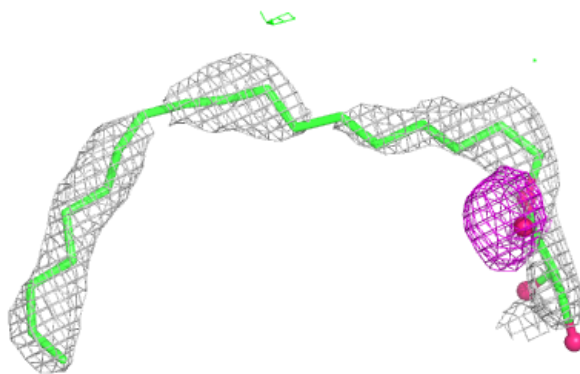
Electron density around PO4 A 314:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

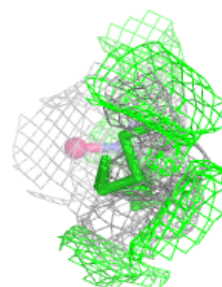
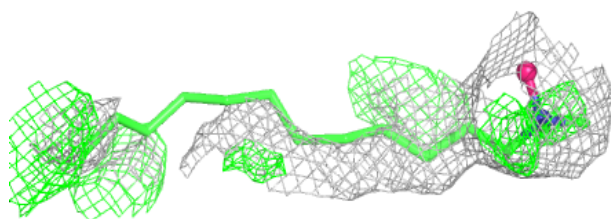
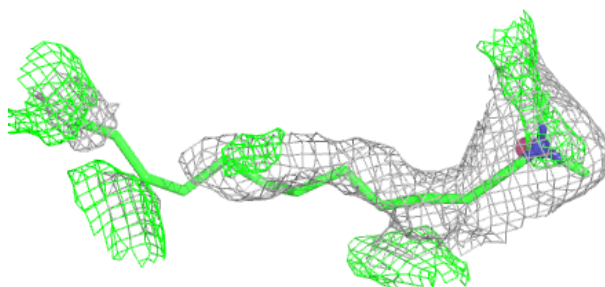


Electron density around MPG A 327:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

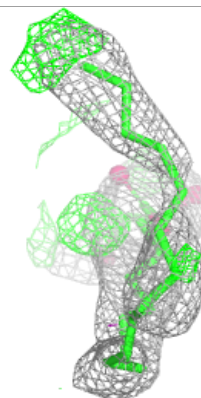
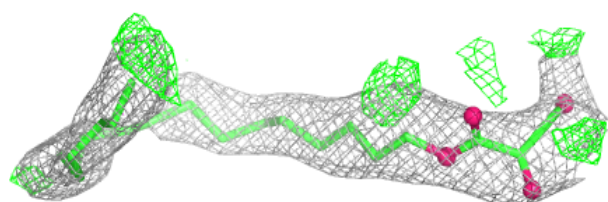
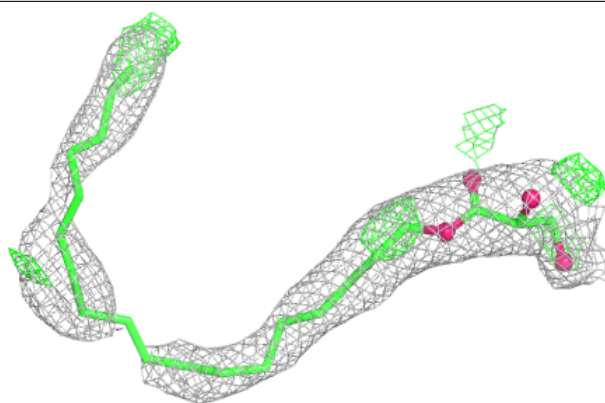
**Electron density around LDA B 311:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

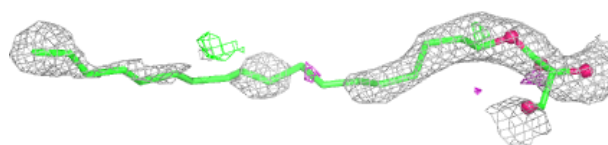
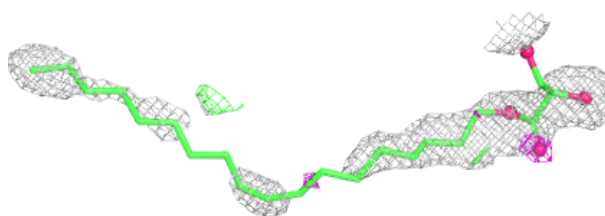


Electron density around MPG A 328:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

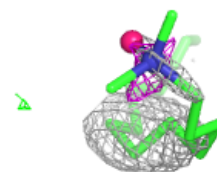
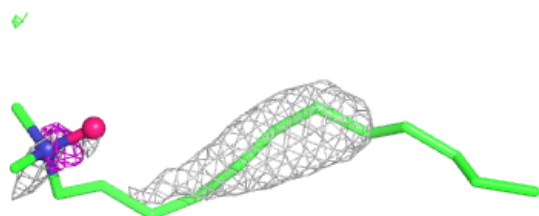
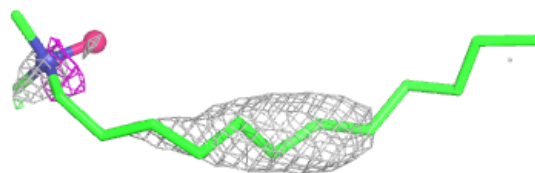
**Electron density around MPG A 322:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

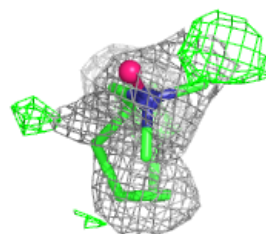
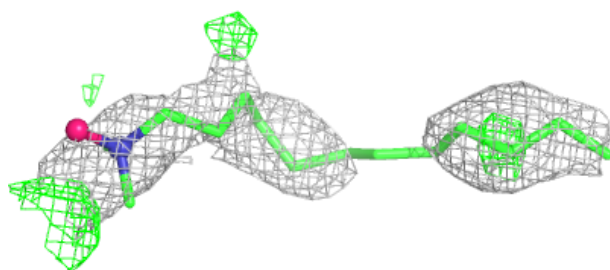
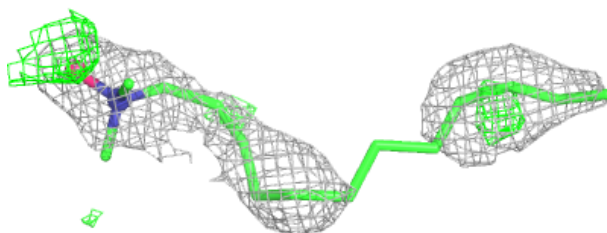


Electron density around LDA B 307:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

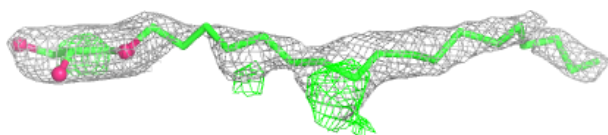
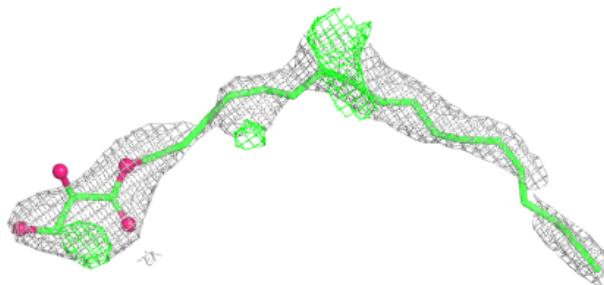
**Electron density around LDA A 309:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

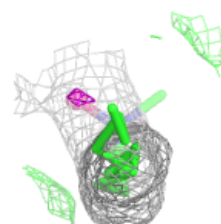
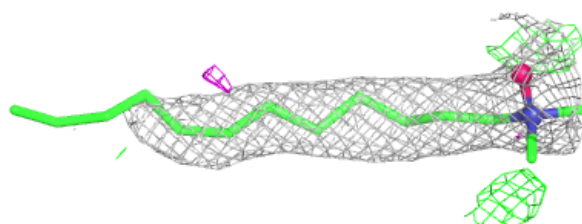
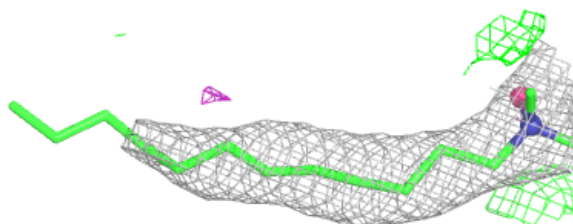


Electron density around MPG A 319:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

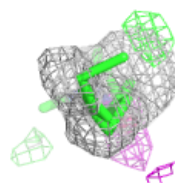
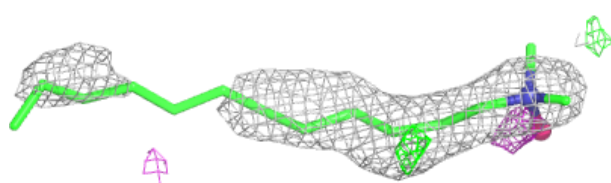
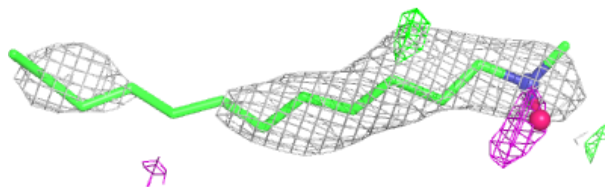
**Electron density around LDA B 309:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

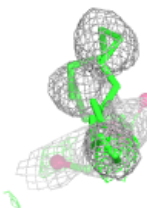
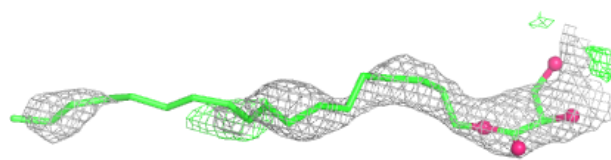
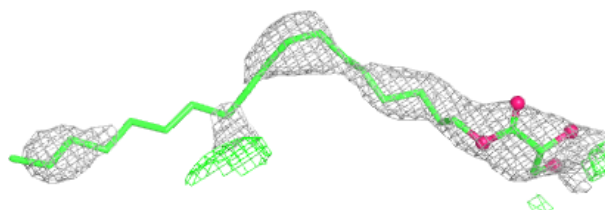


Electron density around LDA B 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

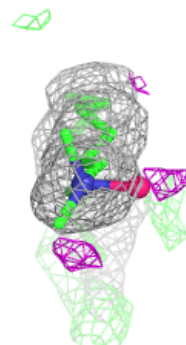
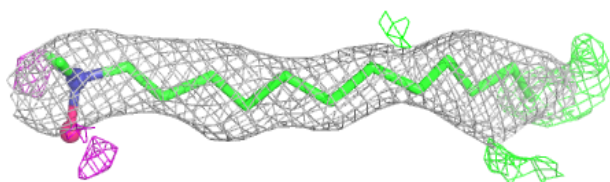
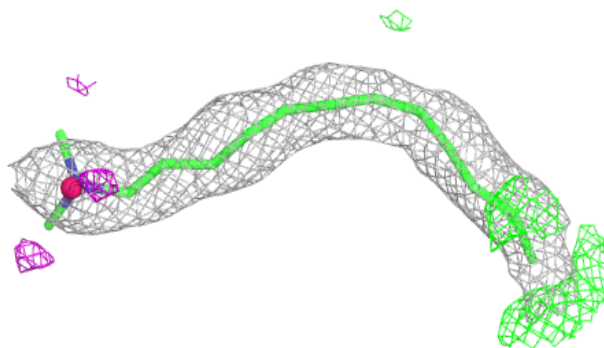
**Electron density around MPG A 326:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

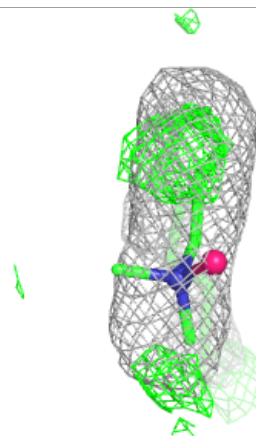
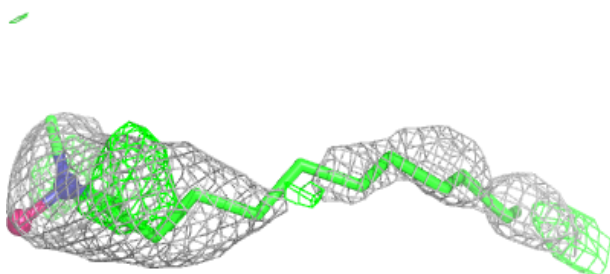
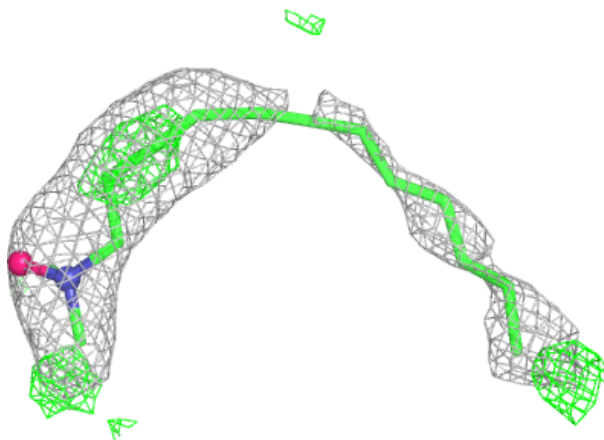


Electron density around LDA A 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

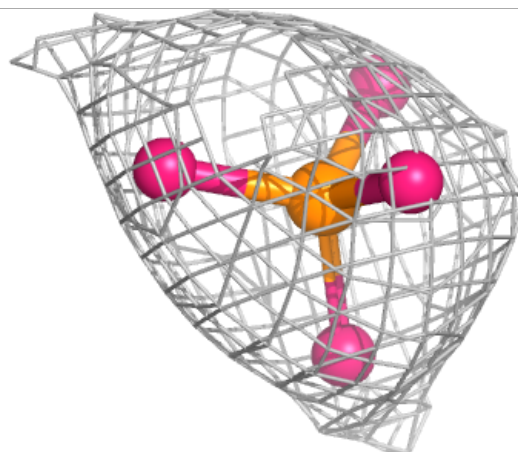
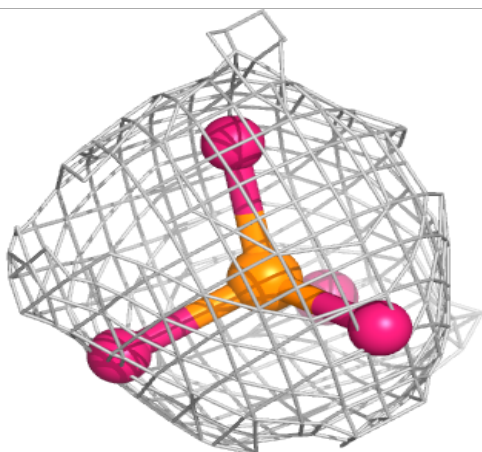
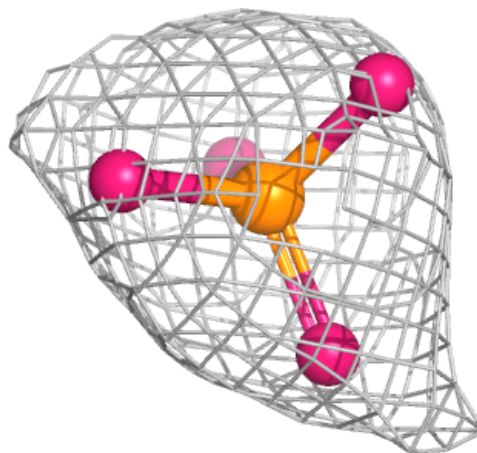
**Electron density around LDA B 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



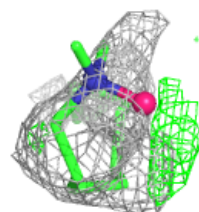
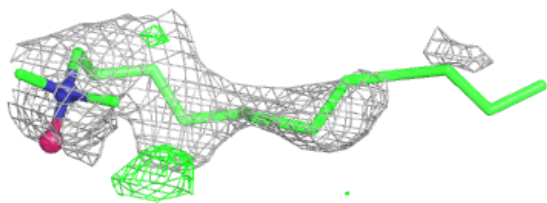
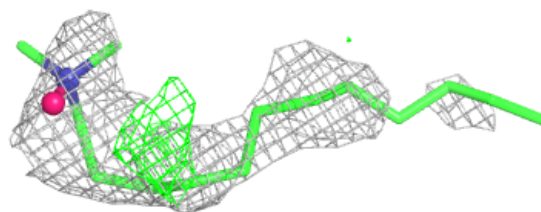
Electron density around PO4 A 313:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

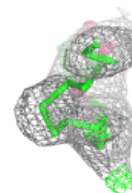
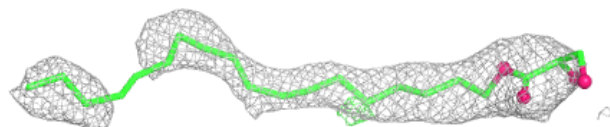
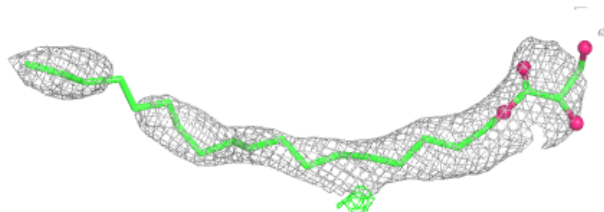


Electron density around LDA B 310:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

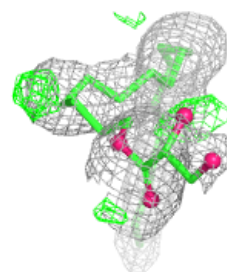
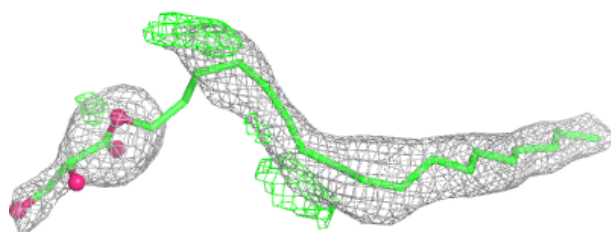
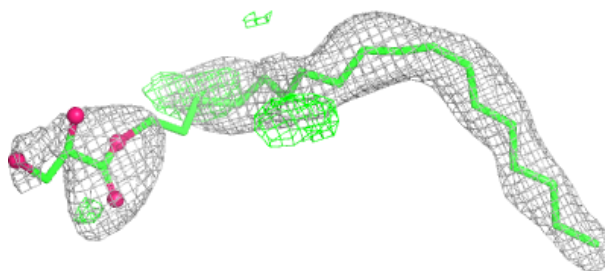
**Electron density around MPG A 316:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

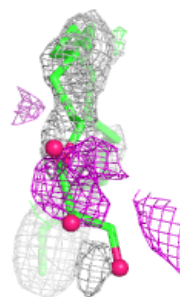
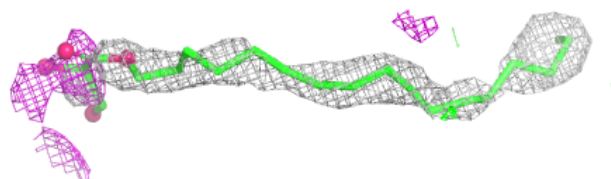
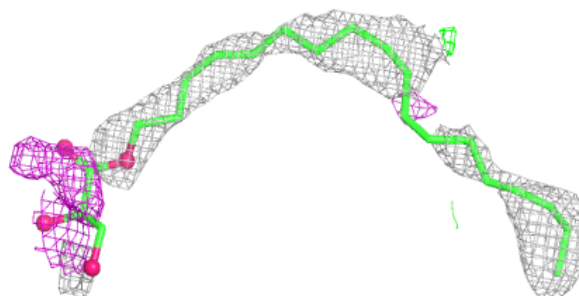


Electron density around MPG B 318:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

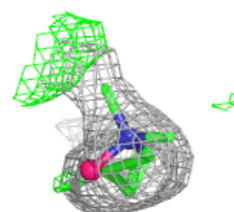
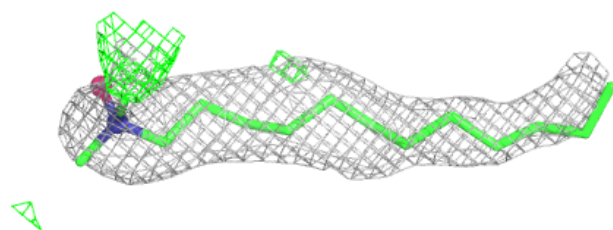
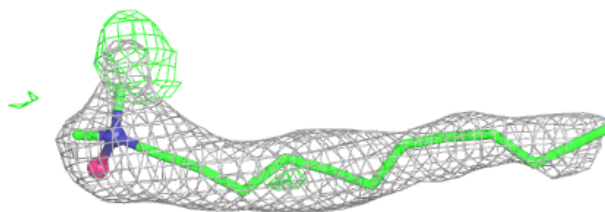
**Electron density around MPG B 319:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

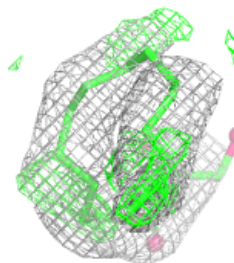
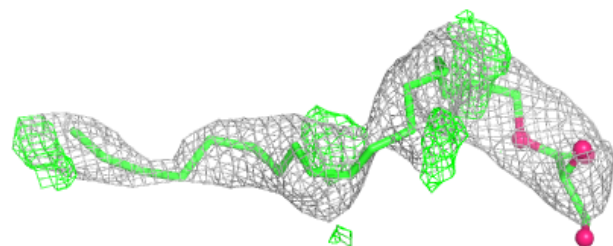
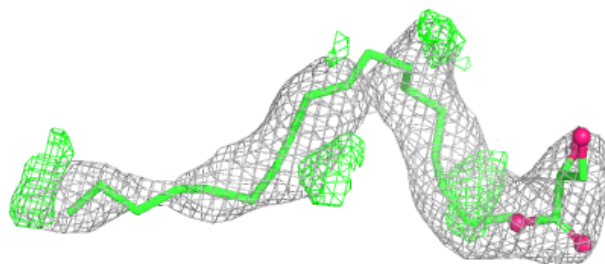


Electron density around LDA B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

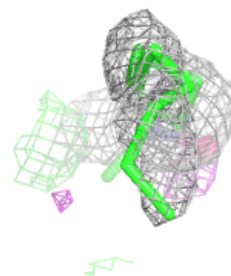
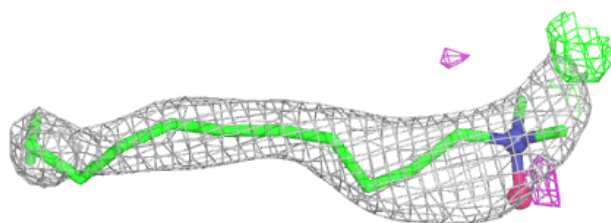
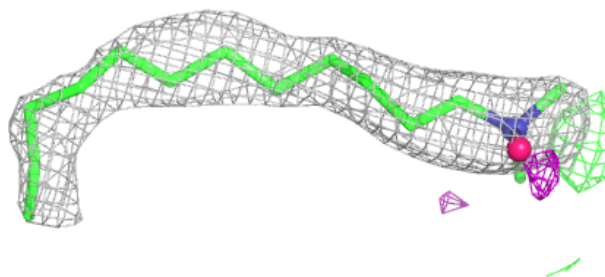
**Electron density around MPG B 320:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

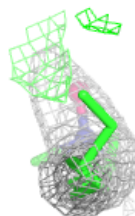
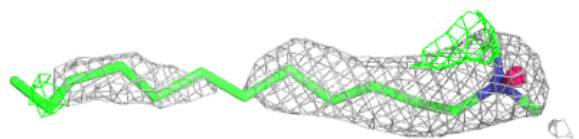
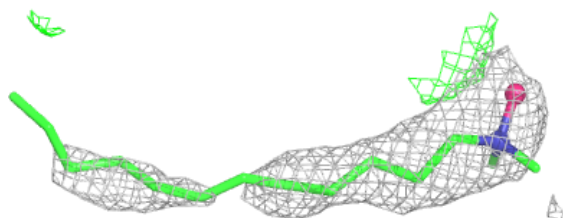


Electron density around LDA B 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

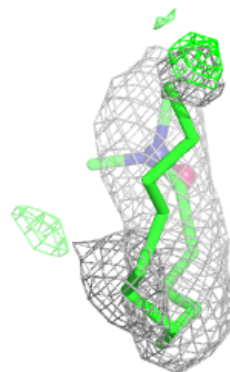
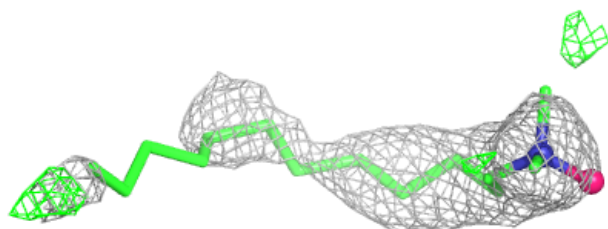
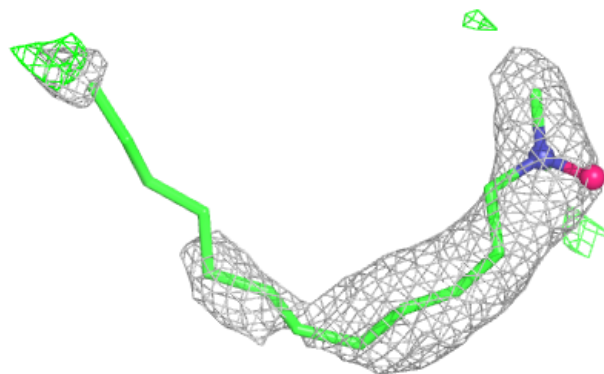
**Electron density around LDA B 304:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

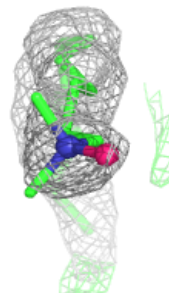
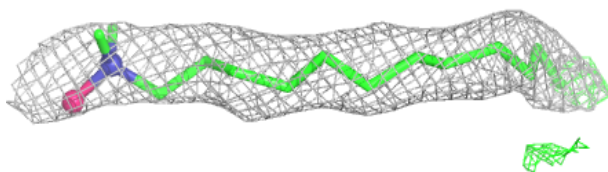
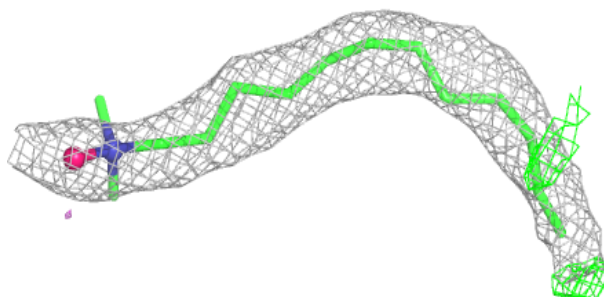


Electron density around LDA A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

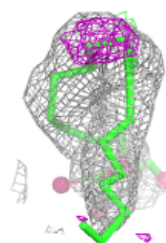
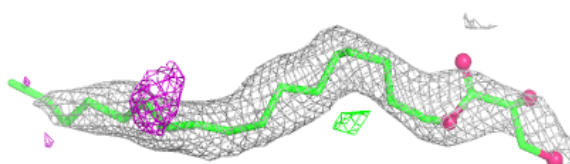
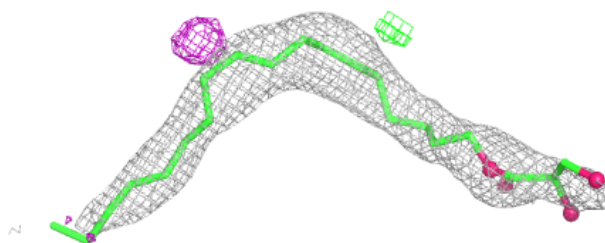
**Electron density around LDA B 306:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

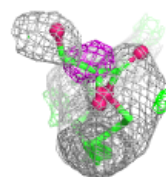
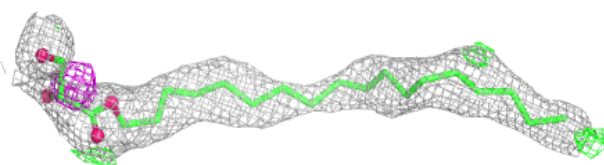
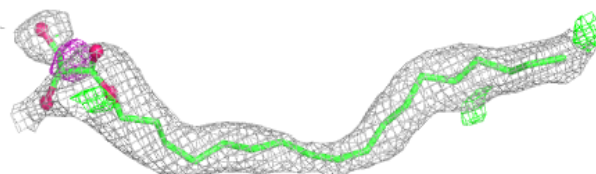


Electron density around MPG A 323:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

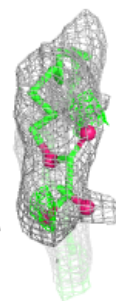
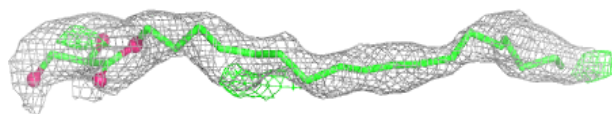
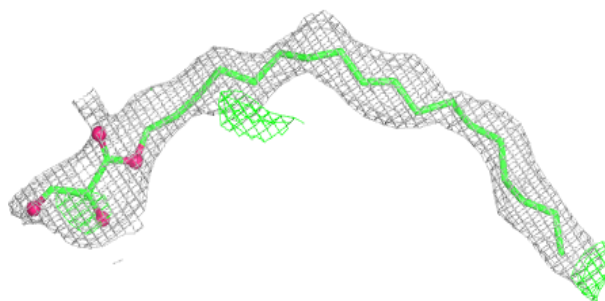
**Electron density around MPG B 316:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

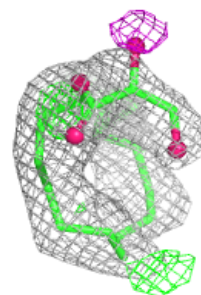
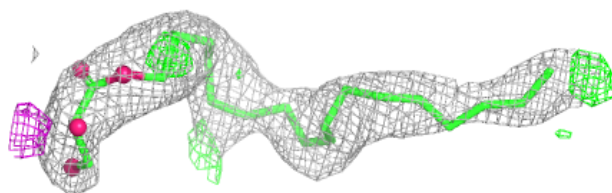
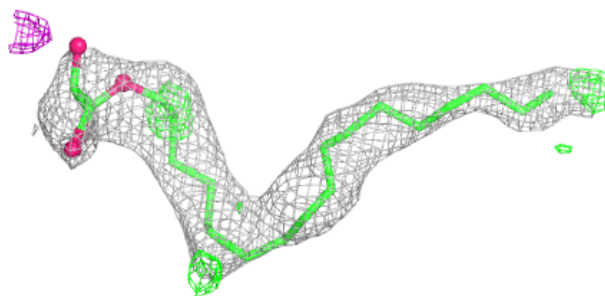


Electron density around MPG B 317:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

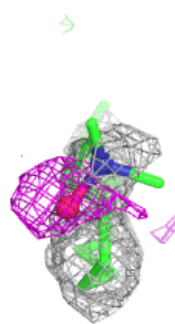
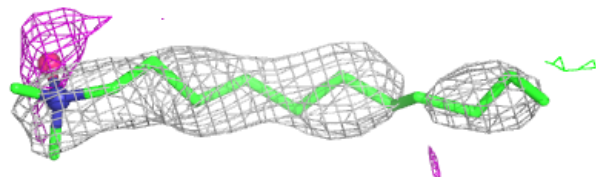
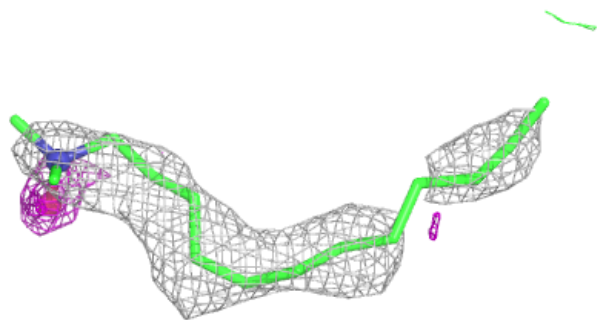
**Electron density around MPG A 324:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

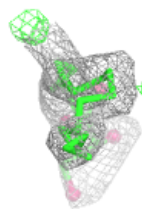
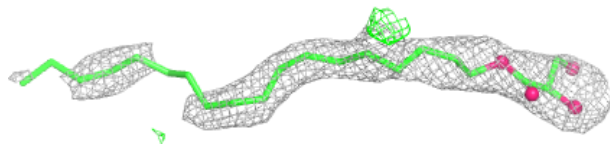
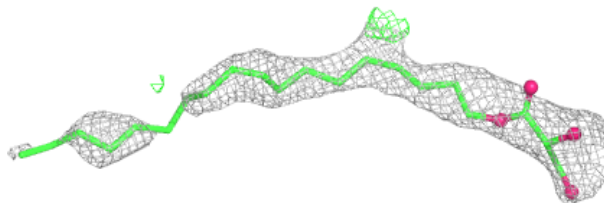


Electron density around LDA A 306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

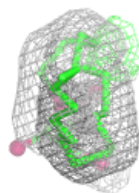
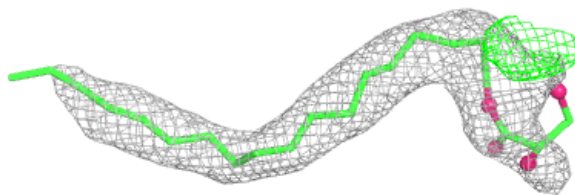
**Electron density around MPG A 321:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

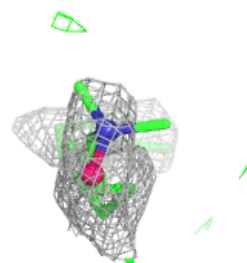
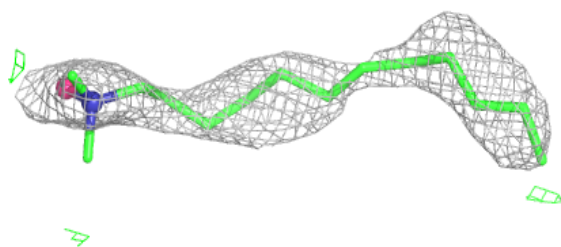
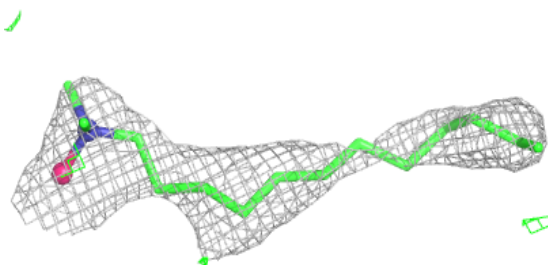


Electron density around MPG A 318:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

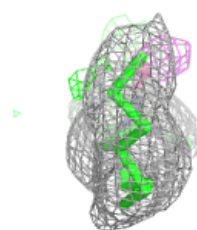
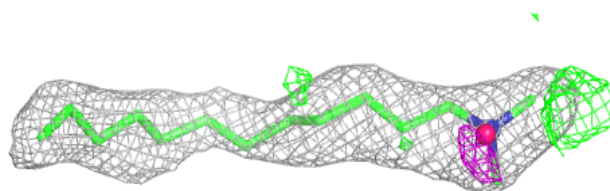
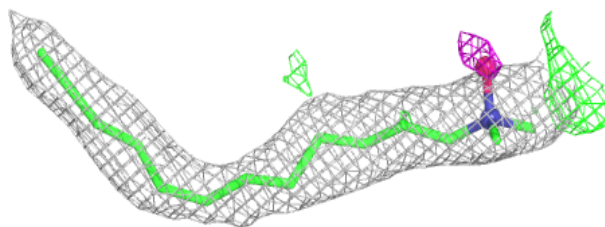
**Electron density around LDA A 310:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

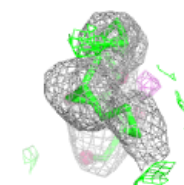
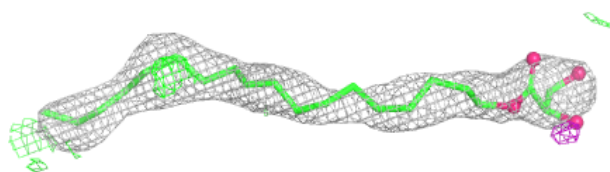
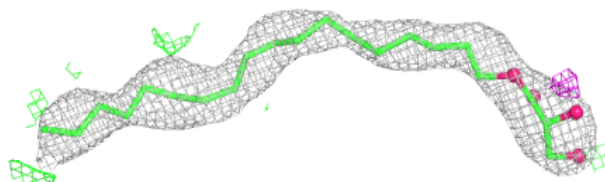


Electron density around LDA A 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

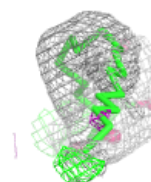
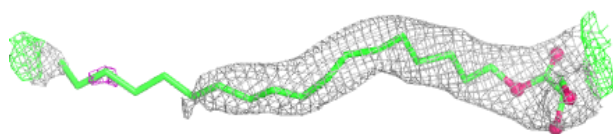
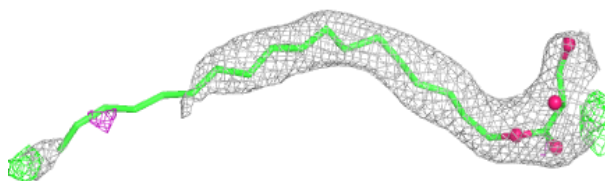
**Electron density around MPG A 320:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

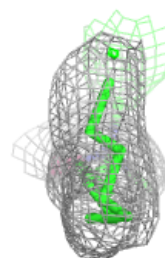
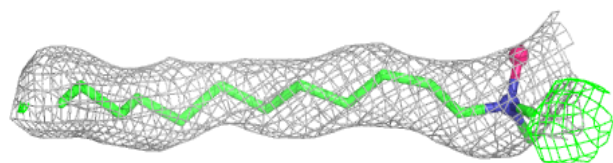
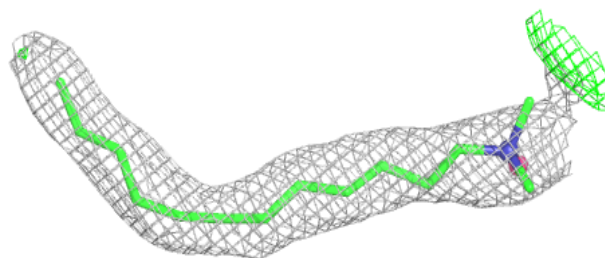


Electron density around MPG A 317:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

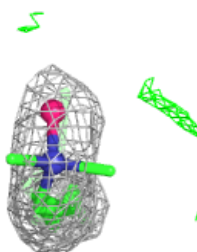
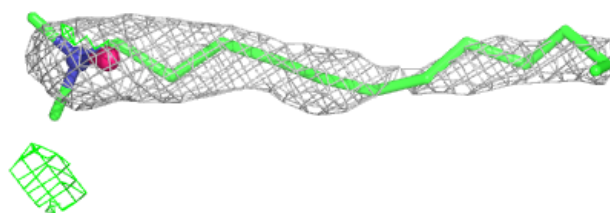
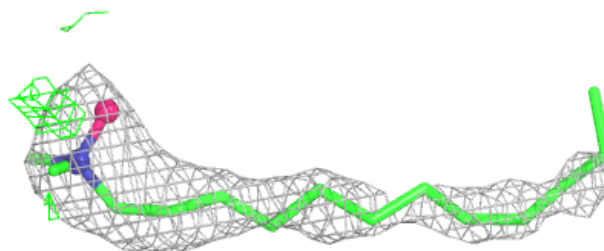
**Electron density around LDA A 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

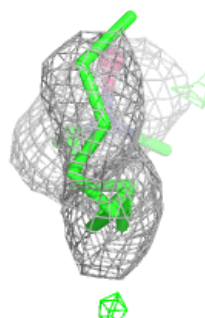
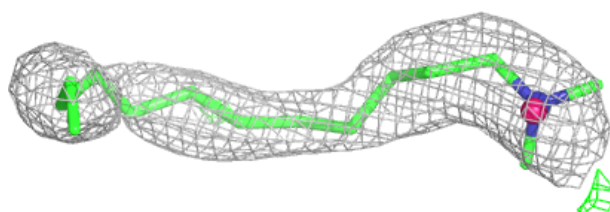
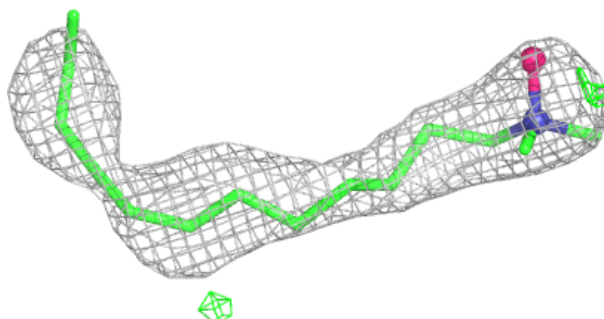


Electron density around LDA A 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

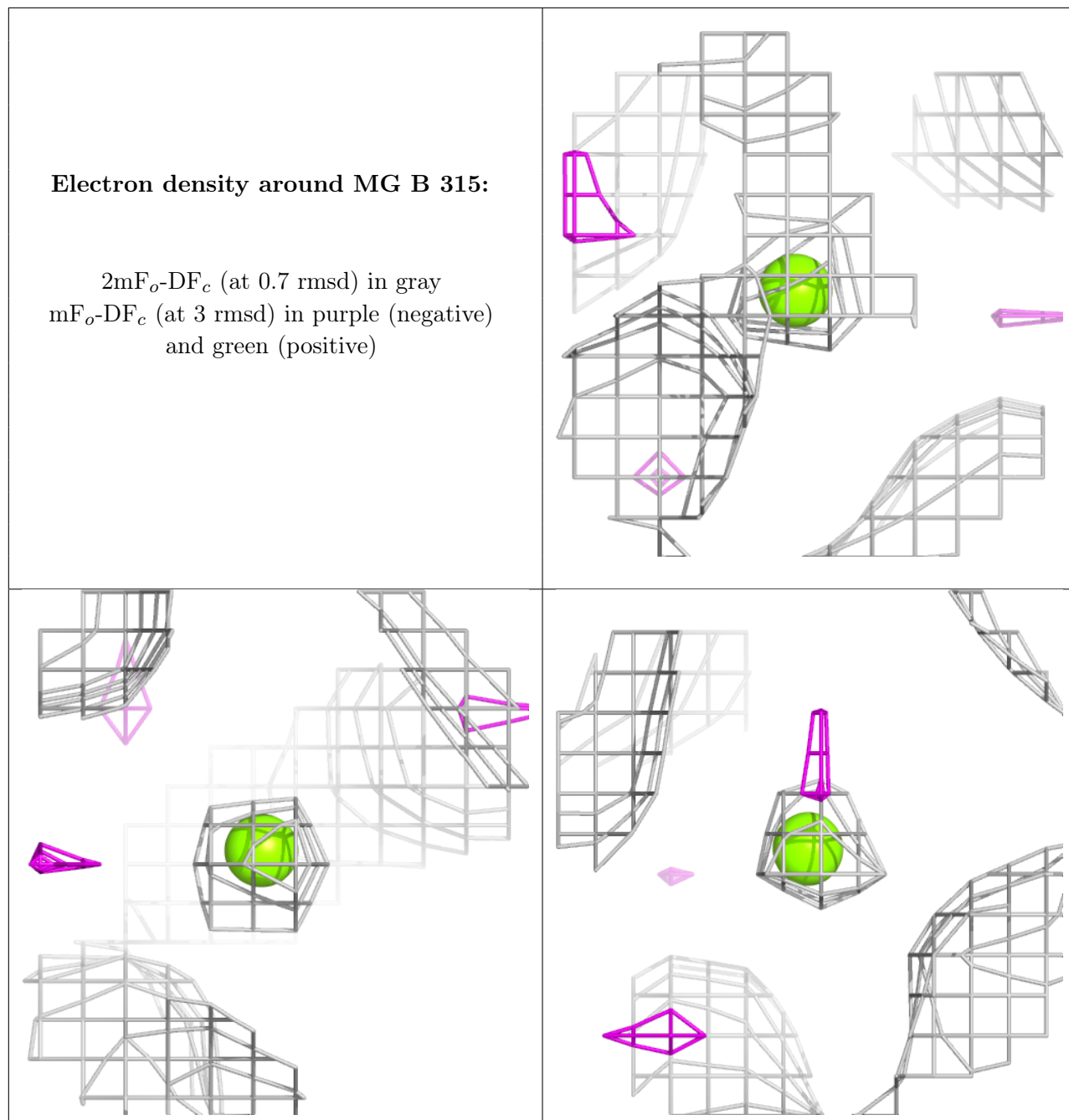
**Electron density around LDA A 307:**

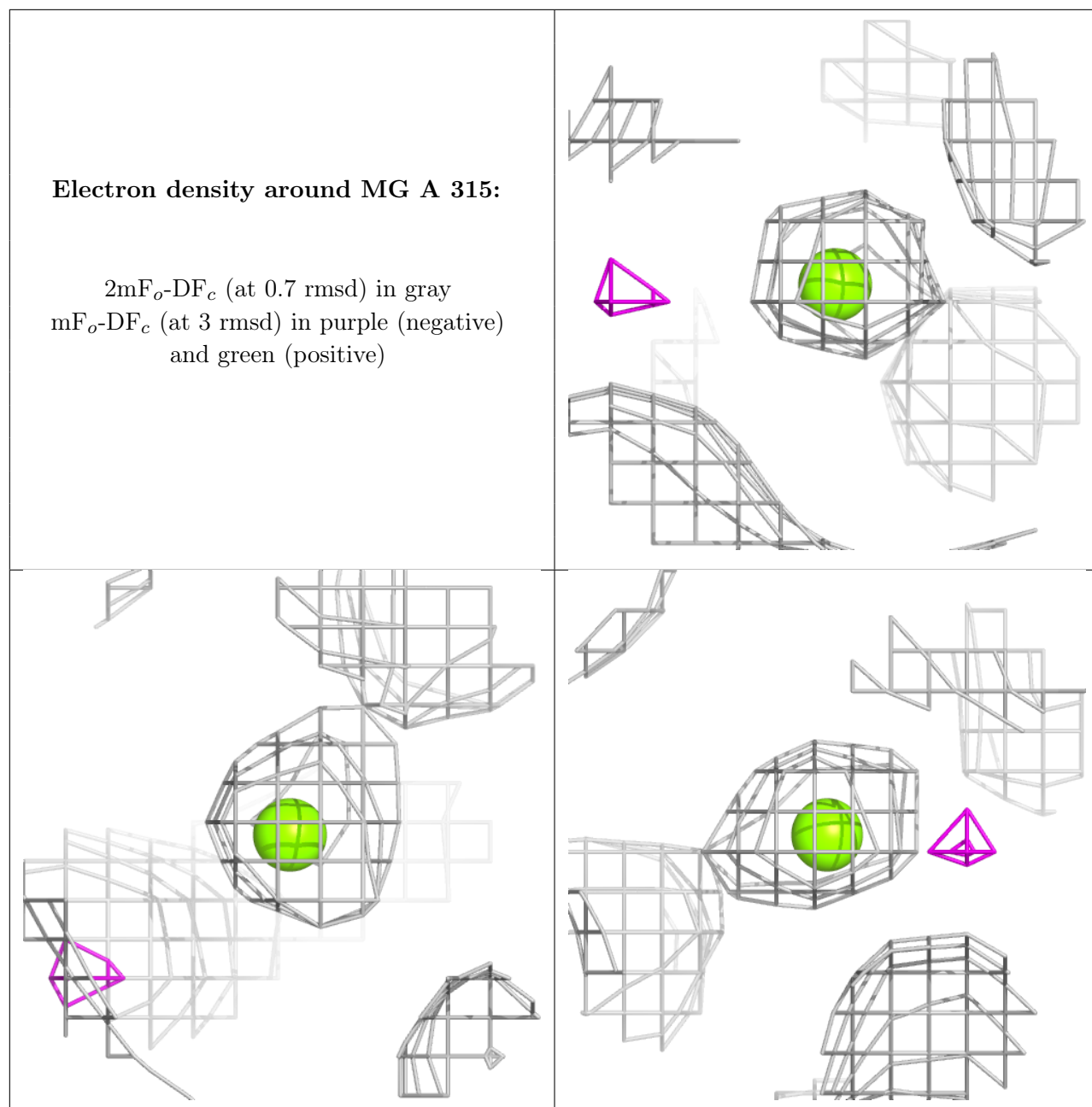
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG B 315:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.