



Full wwPDB EM Validation Report ⓘ

Sep 7, 2025 – 07:21 am BST

PDB ID : 9R21 / pdb_00009r21
EMDB ID : EMD-53519
Title : Cryo-EM structure of the flotillin-associated rhodopsin PsFAR in detergent micelle
Authors : Kovalev, K.; Stetsenko, A.; Marin, E.; Guskov, A.
Deposited on : 2025-04-29
Resolution : 2.56 Å(reported)

This is a Full wwPDB EM Validation 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.dev126
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

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 2.56 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

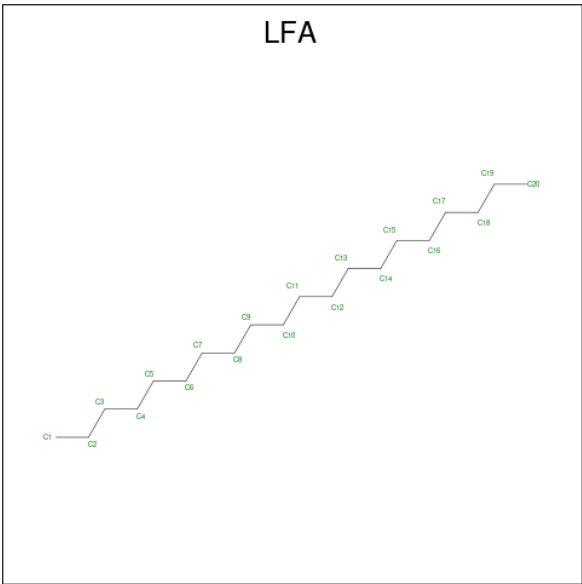
There are 3 unique types of molecules in this entry. The entry contains 10231 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called flotillin-associated rhodopsin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	236	Total	C	N	O	S	0	0
			1846	1221	295	318	12		
1	B	236	Total	C	N	O	S	0	0
			1846	1221	295	318	12		
1	C	236	Total	C	N	O	S	0	0
			1846	1221	295	318	12		
1	D	236	Total	C	N	O	S	0	0
			1846	1221	295	318	12		
1	E	236	Total	C	N	O	S	0	0
			1846	1221	295	318	12		

- Molecule 2 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	C	0
			13	13	
2	A	1	Total	C	0
			20	20	

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Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C 11 11	0
2	A	1	Total C 8 8	0
2	A	1	Total C 10 10	0
2	A	1	Total C 13 13	0
2	A	1	Total C 12 12	0
2	A	1	Total C 12 12	0
2	A	1	Total C 9 9	0
2	A	1	Total C 12 12	0
2	A	1	Total C 9 9	0
2	A	1	Total C 10 10	0
2	A	1	Total C 10 10	0
2	A	1	Total C 7 7	0
2	A	1	Total C 6 6	0
2	A	1	Total C 17 17	0
2	A	1	Total C 9 9	0
2	A	1	Total C 10 10	0
2	B	1	Total C 14 14	0
2	B	1	Total C 17 17	0
2	B	1	Total C 20 20	0
2	B	1	Total C 10 10	0
2	B	1	Total C 9 9	0

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Mol	Chain	Residues	Atoms	AltConf
2	B	1	Total C 11 11	0
2	B	1	Total C 8 8	0
2	B	1	Total C 11 11	0
2	B	1	Total C 12 12	0
2	B	1	Total C 12 12	0
2	B	1	Total C 9 9	0
2	B	1	Total C 8 8	0
2	B	1	Total C 7 7	0
2	B	1	Total C 10 10	0
2	B	1	Total C 11 11	0
2	B	1	Total C 6 6	0
2	B	1	Total C 14 14	0
2	C	1	Total C 20 20	0
2	C	1	Total C 17 17	0
2	C	1	Total C 9 9	0
2	C	1	Total C 11 11	0
2	C	1	Total C 13 13	0
2	C	1	Total C 13 13	0
2	C	1	Total C 12 12	0
2	C	1	Total C 10 10	0
2	C	1	Total C 9 9	0

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Mol	Chain	Residues	Atoms	AltConf
2	C	1	Total C 11 11	0
2	C	1	Total C 9 9	0
2	C	1	Total C 10 10	0
2	C	1	Total C 10 10	0
2	C	1	Total C 7 7	0
2	C	1	Total C 10 10	0
2	C	1	Total C 14 14	0
2	C	1	Total C 6 6	0
2	D	1	Total C 20 20	0
2	D	1	Total C 13 13	0
2	D	1	Total C 13 13	0
2	D	1	Total C 10 10	0
2	D	1	Total C 9 9	0
2	D	1	Total C 9 9	0
2	D	1	Total C 6 6	0
2	D	1	Total C 11 11	0
2	D	1	Total C 9 9	0
2	D	1	Total C 10 10	0
2	D	1	Total C 11 11	0
2	D	1	Total C 7 7	0
2	D	1	Total C 10 10	0

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Mol	Chain	Residues	Atoms	AltConf
2	D	1	Total C 15 15	0
2	D	1	Total C 17 17	0
2	E	1	Total C 16 16	0
2	E	1	Total C 17 17	0
2	E	1	Total C 12 12	0
2	E	1	Total C 14 14	0
2	E	1	Total C 13 13	0
2	E	1	Total C 8 8	0
2	E	1	Total C 10 10	0
2	E	1	Total C 10 10	0
2	E	1	Total C 9 9	0
2	E	1	Total C 12 12	0
2	E	1	Total C 7 7	0
2	E	1	Total C 10 10	0
2	E	1	Total C 11 11	0
2	E	1	Total C 7 7	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	AltConf
3	A	19	Total O 19 19	0
3	B	19	Total O 19 19	0
3	C	20	Total O 20 20	0

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Mol	Chain	Residues	Atoms		AltConf
3	D	19	Total	O	0
			19	19	
3	E	20	Total	O	0
			20	20	

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3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212403	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.554	Depositor
Minimum map value	-1.083	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	321.02402, 321.02402, 321.02402	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.836, 0.836, 0.836	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

81 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	LFA	C	308	-	9,9,19	0.55	0	8,8,18	0.47	0
2	LFA	D	301	-	19,19,19	0.48	0	18,18,18	0.67	0
2	LFA	E	303	-	11,11,19	0.47	0	10,10,18	0.52	0
2	LFA	E	305	-	12,12,19	0.41	0	11,11,18	0.55	0
2	LFA	E	307	-	9,9,19	0.54	0	8,8,18	0.39	0
2	LFA	C	312	-	9,9,19	0.35	0	8,8,18	0.70	0
2	LFA	C	316	-	13,13,19	0.65	0	12,12,18	0.55	0
2	LFA	A	311	-	8,8,19	0.35	0	7,7,18	0.56	0
2	LFA	D	306	-	8,8,19	0.48	0	7,7,18	0.44	0
2	LFA	A	307	-	11,11,19	0.46	0	10,10,18	0.64	0
2	LFA	D	309	-	8,8,19	0.30	0	7,7,18	0.62	0
2	LFA	E	314	-	6,6,19	0.36	0	5,5,18	0.77	0
2	LFA	C	303	-	8,8,19	0.37	0	7,7,18	0.85	0
2	LFA	B	308	-	10,10,19	0.45	0	9,9,18	0.69	0
2	LFA	A	314	-	6,6,19	0.33	0	5,5,18	0.58	0
2	LFA	C	310	-	10,10,19	0.50	0	9,9,18	0.46	0
2	LFA	D	303	-	12,12,19	0.42	0	11,11,18	0.71	0
2	LFA	D	311	-	10,10,19	0.41	0	9,9,18	0.57	0
2	LFA	B	311	-	8,8,19	0.52	0	7,7,18	0.31	0
2	LFA	A	316	-	16,16,19	0.41	0	15,15,18	0.79	0
2	LFA	C	315	-	9,9,19	0.51	0	8,8,18	0.48	0
2	LFA	B	316	-	5,5,19	0.44	0	4,4,18	0.53	0
2	LFA	C	311	-	8,8,19	0.37	0	7,7,18	0.54	0
2	LFA	C	313	-	9,9,19	0.36	0	8,8,18	0.69	0
2	LFA	C	302	-	16,16,19	0.43	0	15,15,18	0.77	0
2	LFA	A	305	-	9,9,19	0.54	0	8,8,18	0.54	0
2	LFA	C	314	-	6,6,19	0.34	0	5,5,18	0.68	0
2	LFA	A	309	-	8,8,19	0.49	0	7,7,18	0.46	0
2	LFA	D	304	-	9,9,19	0.52	0	8,8,18	0.47	0
2	LFA	D	310	-	9,9,19	0.33	0	8,8,18	0.76	0
2	LFA	B	310	-	11,11,19	0.42	0	10,10,18	0.69	0
2	LFA	D	312	-	6,6,19	0.33	0	5,5,18	0.63	0
2	LFA	B	309	-	11,11,19	0.51	0	10,10,18	0.48	0
2	LFA	A	315	-	5,5,19	0.42	0	4,4,18	0.60	0
2	LFA	B	312	-	7,7,19	0.37	0	6,6,18	0.58	0
2	LFA	D	315	-	16,16,19	0.38	0	15,15,18	0.82	0
2	LFA	B	315	-	10,10,19	0.31	0	9,9,18	0.76	0
2	LFA	A	301	-	12,12,19	0.65	0	11,11,18	0.64	0
2	LFA	E	306	-	7,7,19	0.54	0	6,6,18	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LFA	E	310	-	11,11,19	0.44	0	10,10,18	0.49	0
2	LFA	E	312	-	9,9,19	0.34	0	8,8,18	0.58	0
2	LFA	A	302	-	19,19,19	0.52	0	18,18,18	0.68	0
2	LFA	B	305	-	8,8,19	0.35	0	7,7,18	0.66	0
2	LFA	A	306	-	12,12,19	0.42	0	11,11,18	0.57	0
2	LFA	A	304	-	7,7,19	0.42	0	6,6,18	0.61	0
2	LFA	D	313	-	9,9,19	0.44	0	8,8,18	0.50	0
2	LFA	A	308	-	11,11,19	0.41	0	10,10,18	0.66	0
2	LFA	B	301	-	13,13,19	0.49	0	12,12,18	1.02	1 (8%)
2	LFA	B	302	-	16,16,19	0.39	0	15,15,18	0.74	0
2	LFA	D	314	-	14,14,19	0.51	0	13,13,18	0.86	0
2	LFA	B	306	-	10,10,19	0.51	0	9,9,18	0.45	0
2	LFA	C	305	-	12,12,19	0.40	0	11,11,18	0.63	0
2	LFA	C	309	-	8,8,19	0.47	0	7,7,18	0.35	0
2	LFA	E	301	-	15,15,19	0.51	0	14,14,18	0.42	0
2	LFA	E	313	-	10,10,19	0.36	0	9,9,18	0.73	0
2	LFA	E	302	-	16,16,19	0.40	0	15,15,18	0.75	0
2	LFA	A	318	-	9,9,19	0.41	0	8,8,18	0.66	0
2	LFA	D	302	-	12,12,19	0.47	0	11,11,18	0.70	0
2	LFA	C	317	-	5,5,19	0.46	0	4,4,18	0.77	0
2	LFA	B	304	-	9,9,19	0.43	0	8,8,18	0.64	0
2	LFA	E	304	-	13,13,19	0.46	0	12,12,18	0.70	0
2	LFA	E	308	-	9,9,19	0.42	0	8,8,18	0.52	0
2	LFA	E	309	-	8,8,19	0.31	0	7,7,18	0.70	0
2	LFA	C	304	-	10,10,19	0.46	0	9,9,18	0.54	0
2	LFA	A	312	-	9,9,19	0.37	0	8,8,18	0.58	0
2	LFA	D	307	-	5,5,19	0.40	0	4,4,18	0.44	0
2	LFA	B	307	-	7,7,19	0.50	0	6,6,18	0.43	0
2	LFA	A	310	-	11,11,19	0.44	0	10,10,18	0.44	0
2	LFA	C	306	-	12,12,19	0.47	0	11,11,18	0.49	0
2	LFA	A	313	-	9,9,19	0.37	0	8,8,18	0.70	0
2	LFA	C	301	-	19,19,19	0.45	0	18,18,18	0.80	0
2	LFA	E	311	-	6,6,19	0.34	0	5,5,18	0.65	0
2	LFA	D	308	-	10,10,19	0.52	0	9,9,18	0.43	0
2	LFA	B	313	-	6,6,19	0.34	0	5,5,18	0.56	0
2	LFA	A	303	-	10,10,19	0.48	0	9,9,18	0.56	0
2	LFA	A	317	-	8,8,19	0.30	0	7,7,18	0.70	0
2	LFA	B	314	-	9,9,19	0.40	0	8,8,18	0.64	0
2	LFA	B	303	-	19,19,19	0.52	0	18,18,18	0.77	0
2	LFA	B	317	-	13,13,19	0.52	0	12,12,18	0.88	0
2	LFA	D	305	-	8,8,19	0.37	0	7,7,18	0.69	0
2	LFA	C	307	-	11,11,19	0.42	0	10,10,18	0.56	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
2	LFA	C	308	-	-	4/7/7/17	-
2	LFA	D	301	-	-	8/17/17/17	-
2	LFA	E	303	-	-	3/9/9/17	-
2	LFA	E	305	-	-	4/10/10/17	-
2	LFA	E	307	-	-	3/7/7/17	-
2	LFA	C	312	-	-	1/7/7/17	-
2	LFA	C	316	-	-	5/11/11/17	-
2	LFA	A	311	-	-	4/6/6/17	-
2	LFA	D	306	-	-	1/6/6/17	-
2	LFA	A	307	-	-	1/9/9/17	-
2	LFA	D	309	-	-	3/6/6/17	-
2	LFA	E	314	-	-	1/4/4/17	-
2	LFA	C	303	-	-	0/6/6/17	-
2	LFA	B	308	-	-	2/8/8/17	-
2	LFA	A	314	-	-	0/4/4/17	-
2	LFA	C	310	-	-	4/8/8/17	-
2	LFA	D	303	-	-	1/10/10/17	-
2	LFA	D	311	-	-	5/8/8/17	-
2	LFA	B	311	-	-	1/6/6/17	-
2	LFA	A	316	-	-	5/14/14/17	-
2	LFA	C	315	-	-	3/7/7/17	-
2	LFA	B	316	-	-	1/3/3/17	-
2	LFA	C	311	-	-	4/6/6/17	-
2	LFA	C	313	-	-	1/7/7/17	-
2	LFA	C	302	-	-	5/14/14/17	-
2	LFA	A	305	-	-	2/7/7/17	-
2	LFA	C	314	-	-	0/4/4/17	-
2	LFA	A	309	-	-	0/6/6/17	-
2	LFA	D	304	-	-	3/7/7/17	-
2	LFA	D	310	-	-	1/7/7/17	-
2	LFA	B	310	-	-	0/9/9/17	-
2	LFA	D	312	-	-	1/4/4/17	-
2	LFA	B	309	-	-	1/9/9/17	-
2	LFA	A	315	-	-	0/3/3/17	-
2	LFA	B	312	-	-	1/5/5/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	D	315	-	-	6/14/14/17	-
2	LFA	B	315	-	-	3/8/8/17	-
2	LFA	A	301	-	-	3/10/10/17	-
2	LFA	E	306	-	-	1/5/5/17	-
2	LFA	E	310	-	-	0/9/9/17	-
2	LFA	E	312	-	-	5/7/7/17	-
2	LFA	A	302	-	-	5/17/17/17	-
2	LFA	B	305	-	-	2/6/6/17	-
2	LFA	A	306	-	-	3/10/10/17	-
2	LFA	A	304	-	-	1/5/5/17	-
2	LFA	D	313	-	-	3/7/7/17	-
2	LFA	A	308	-	-	3/9/9/17	-
2	LFA	B	301	-	-	4/11/11/17	-
2	LFA	B	302	-	-	5/14/14/17	-
2	LFA	D	314	-	-	3/12/12/17	-
2	LFA	B	306	-	-	3/8/8/17	-
2	LFA	C	305	-	-	3/10/10/17	-
2	LFA	C	309	-	-	3/6/6/17	-
2	LFA	E	301	-	-	5/13/13/17	-
2	LFA	E	313	-	-	4/8/8/17	-
2	LFA	E	302	-	-	4/14/14/17	-
2	LFA	A	318	-	-	2/7/7/17	-
2	LFA	D	302	-	-	2/10/10/17	-
2	LFA	C	317	-	-	0/3/3/17	-
2	LFA	B	304	-	-	2/7/7/17	-
2	LFA	E	304	-	-	2/11/11/17	-
2	LFA	E	308	-	-	2/7/7/17	-
2	LFA	E	309	-	-	3/6/6/17	-
2	LFA	C	304	-	-	2/8/8/17	-
2	LFA	A	312	-	-	3/7/7/17	-
2	LFA	D	307	-	-	1/3/3/17	-
2	LFA	B	307	-	-	0/5/5/17	-
2	LFA	A	310	-	-	3/9/9/17	-
2	LFA	C	306	-	-	4/10/10/17	-
2	LFA	A	313	-	-	0/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	C	301	-	-	6/17/17/17	-
2	LFA	E	311	-	-	1/4/4/17	-
2	LFA	D	308	-	-	2/8/8/17	-
2	LFA	B	313	-	-	0/4/4/17	-
2	LFA	A	303	-	-	6/8/8/17	-
2	LFA	A	317	-	-	0/6/6/17	-
2	LFA	B	314	-	-	1/7/7/17	-
2	LFA	B	303	-	-	5/17/17/17	-
2	LFA	B	317	-	-	2/11/11/17	-
2	LFA	D	305	-	-	1/6/6/17	-
2	LFA	C	307	-	-	4/9/9/17	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	LFA	C12-C11-C10	-2.09	103.80	114.42

There are no chirality outliers.

All (202) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	316	LFA	C10-C11-C12-C13
2	C	301	LFA	C16-C17-C18-C19
2	D	314	LFA	C11-C12-C13-C14
2	B	306	LFA	C6-C7-C8-C9
2	C	310	LFA	C7-C8-C9-C10
2	C	309	LFA	C3-C4-C5-C6
2	C	311	LFA	C3-C4-C5-C6
2	A	307	LFA	C12-C13-C14-C15
2	B	301	LFA	C2-C3-C4-C5
2	C	302	LFA	C6-C7-C8-C9
2	A	311	LFA	C4-C5-C6-C7
2	B	315	LFA	C3-C4-C5-C6
2	C	309	LFA	C4-C5-C6-C7
2	C	304	LFA	C7-C8-C9-C10
2	D	308	LFA	C7-C8-C9-C10
2	E	304	LFA	C9-C10-C11-C12
2	B	315	LFA	C6-C7-C8-C9
2	C	301	LFA	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
2	D	310	LFA	C12-C13-C14-C15
2	D	308	LFA	C11-C10-C9-C8
2	D	311	LFA	C4-C5-C6-C7
2	C	315	LFA	C5-C6-C7-C8
2	E	308	LFA	C3-C4-C5-C6
2	E	313	LFA	C3-C4-C5-C6
2	A	303	LFA	C4-C5-C6-C7
2	C	305	LFA	C5-C6-C7-C8
2	E	301	LFA	C2-C3-C4-C5
2	C	307	LFA	C5-C6-C7-C8
2	D	304	LFA	C5-C6-C7-C8
2	A	316	LFA	C12-C13-C14-C15
2	A	318	LFA	C3-C4-C5-C6
2	B	317	LFA	C1-C2-C3-C4
2	A	305	LFA	C3-C4-C5-C6
2	C	302	LFA	C5-C6-C7-C8
2	A	301	LFA	C7-C8-C9-C10
2	B	301	LFA	C7-C8-C9-C10
2	B	304	LFA	C13-C14-C15-C16
2	D	315	LFA	C7-C8-C9-C10
2	A	306	LFA	C6-C7-C8-C9
2	C	308	LFA	C6-C7-C8-C9
2	D	302	LFA	C3-C4-C5-C6
2	E	309	LFA	C14-C15-C16-C17
2	A	308	LFA	C16-C17-C18-C19
2	B	309	LFA	C7-C8-C9-C10
2	E	302	LFA	C6-C7-C8-C9
2	D	301	LFA	C9-C10-C11-C12
2	B	306	LFA	C2-C3-C4-C5
2	C	311	LFA	C2-C3-C4-C5
2	D	315	LFA	C9-C10-C11-C12
2	D	315	LFA	C6-C7-C8-C9
2	E	309	LFA	C12-C13-C14-C15
2	E	308	LFA	C5-C6-C7-C8
2	C	315	LFA	C3-C4-C5-C6
2	C	316	LFA	C3-C4-C5-C6
2	E	305	LFA	C14-C15-C16-C17
2	B	312	LFA	C1-C2-C3-C4
2	D	307	LFA	C15-C16-C17-C18
2	D	312	LFA	C14-C15-C16-C17
2	D	309	LFA	C1-C2-C3-C4
2	E	301	LFA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	C	316	LFA	C1-C2-C3-C4
2	A	304	LFA	C5-C6-C7-C8
2	B	303	LFA	C6-C7-C8-C9
2	D	301	LFA	C10-C11-C12-C13
2	A	301	LFA	C10-C11-C12-C13
2	D	315	LFA	C3-C4-C5-C6
2	B	305	LFA	C3-C4-C5-C6
2	C	309	LFA	C2-C3-C4-C5
2	E	303	LFA	C7-C8-C9-C10
2	A	312	LFA	C11-C12-C13-C14
2	C	301	LFA	C5-C6-C7-C8
2	D	304	LFA	C2-C3-C4-C5
2	B	308	LFA	C1-C2-C3-C4
2	A	303	LFA	C6-C7-C8-C9
2	D	306	LFA	C2-C3-C4-C5
2	A	301	LFA	C6-C7-C8-C9
2	E	301	LFA	C7-C8-C9-C10
2	D	309	LFA	C4-C5-C6-C7
2	E	306	LFA	C12-C13-C14-C15
2	D	301	LFA	C15-C16-C17-C18
2	D	315	LFA	C14-C15-C16-C17
2	B	317	LFA	C5-C6-C7-C8
2	B	311	LFA	C6-C7-C8-C9
2	B	304	LFA	C11-C12-C13-C14
2	D	301	LFA	C3-C4-C5-C6
2	E	311	LFA	C14-C15-C16-C17
2	A	310	LFA	C1-C2-C3-C4
2	A	308	LFA	C14-C15-C16-C17
2	B	306	LFA	C4-C5-C6-C7
2	C	311	LFA	C6-C7-C8-C9
2	E	313	LFA	C5-C6-C7-C8
2	D	301	LFA	C11-C10-C9-C8
2	C	310	LFA	C6-C7-C8-C9
2	B	302	LFA	C7-C8-C9-C10
2	E	307	LFA	C4-C5-C6-C7
2	C	308	LFA	C2-C3-C4-C5
2	C	306	LFA	C5-C6-C7-C8
2	C	311	LFA	C4-C5-C6-C7
2	A	311	LFA	C5-C6-C7-C8
2	D	314	LFA	C1-C2-C3-C4
2	C	308	LFA	C5-C6-C7-C8
2	E	312	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	A	312	LFA	C17-C18-C19-C20
2	A	318	LFA	C4-C5-C6-C7
2	E	305	LFA	C13-C14-C15-C16
2	A	302	LFA	C7-C8-C9-C10
2	A	302	LFA	C5-C6-C7-C8
2	D	311	LFA	C3-C4-C5-C6
2	B	301	LFA	C10-C11-C12-C13
2	B	303	LFA	C3-C4-C5-C6
2	D	314	LFA	C6-C7-C8-C9
2	A	316	LFA	C11-C10-C9-C8
2	C	302	LFA	C1-C2-C3-C4
2	C	315	LFA	C6-C7-C8-C9
2	C	302	LFA	C9-C10-C11-C12
2	E	301	LFA	C5-C6-C7-C8
2	E	302	LFA	C1-C2-C3-C4
2	C	304	LFA	C5-C6-C7-C8
2	D	301	LFA	C14-C15-C16-C17
2	E	304	LFA	C12-C13-C14-C15
2	E	312	LFA	C3-C4-C5-C6
2	C	312	LFA	C11-C12-C13-C14
2	A	312	LFA	C16-C17-C18-C19
2	A	310	LFA	C2-C3-C4-C5
2	C	316	LFA	C6-C7-C8-C9
2	A	311	LFA	C1-C2-C3-C4
2	B	301	LFA	C4-C5-C6-C7
2	C	316	LFA	C7-C8-C9-C10
2	C	302	LFA	C14-C15-C16-C17
2	D	302	LFA	C2-C3-C4-C5
2	D	301	LFA	C13-C14-C15-C16
2	B	302	LFA	C2-C3-C4-C5
2	E	307	LFA	C7-C8-C9-C10
2	D	311	LFA	C7-C8-C9-C10
2	B	302	LFA	C6-C7-C8-C9
2	C	301	LFA	C7-C8-C9-C10
2	E	313	LFA	C11-C10-C9-C8
2	C	313	LFA	C13-C14-C15-C16
2	D	313	LFA	C4-C5-C6-C7
2	C	310	LFA	C4-C5-C6-C7
2	D	303	LFA	C10-C11-C12-C13
2	A	311	LFA	C3-C4-C5-C6
2	B	302	LFA	C5-C6-C7-C8
2	C	301	LFA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
2	A	308	LFA	C12-C13-C14-C15
2	D	311	LFA	C5-C6-C7-C8
2	A	316	LFA	C9-C10-C11-C12
2	B	316	LFA	C17-C18-C19-C20
2	D	313	LFA	C7-C8-C9-C10
2	D	305	LFA	C3-C4-C5-C6
2	E	302	LFA	C2-C3-C4-C5
2	A	303	LFA	C7-C8-C9-C10
2	D	313	LFA	C2-C3-C4-C5
2	A	303	LFA	C5-C6-C7-C8
2	E	302	LFA	C11-C12-C13-C14
2	C	307	LFA	C6-C7-C8-C9
2	C	308	LFA	C1-C2-C3-C4
2	C	307	LFA	C7-C8-C9-C10
2	A	302	LFA	C10-C11-C12-C13
2	E	301	LFA	C11-C10-C9-C8
2	A	316	LFA	C11-C12-C13-C14
2	D	311	LFA	C11-C10-C9-C8
2	B	308	LFA	C11-C10-C9-C8
2	C	301	LFA	C11-C10-C9-C8
2	A	302	LFA	C13-C14-C15-C16
2	D	309	LFA	C5-C6-C7-C8
2	A	303	LFA	C1-C2-C3-C4
2	D	304	LFA	C1-C2-C3-C4
2	B	305	LFA	C1-C2-C3-C4
2	B	303	LFA	C7-C8-C9-C10
2	A	302	LFA	C9-C10-C11-C12
2	A	306	LFA	C7-C8-C9-C10
2	A	303	LFA	C11-C10-C9-C8
2	E	307	LFA	C6-C7-C8-C9
2	A	316	LFA	C1-C2-C3-C4
2	C	306	LFA	C1-C2-C3-C4
2	E	309	LFA	C15-C16-C17-C18
2	C	306	LFA	C3-C4-C5-C6
2	B	302	LFA	C11-C10-C9-C8
2	D	301	LFA	C16-C17-C18-C19
2	B	315	LFA	C11-C10-C9-C8
2	E	305	LFA	C12-C13-C14-C15
2	E	303	LFA	C11-C10-C9-C8
2	A	310	LFA	C7-C8-C9-C10
2	E	303	LFA	C6-C7-C8-C9
2	E	312	LFA	C2-C3-C4-C5

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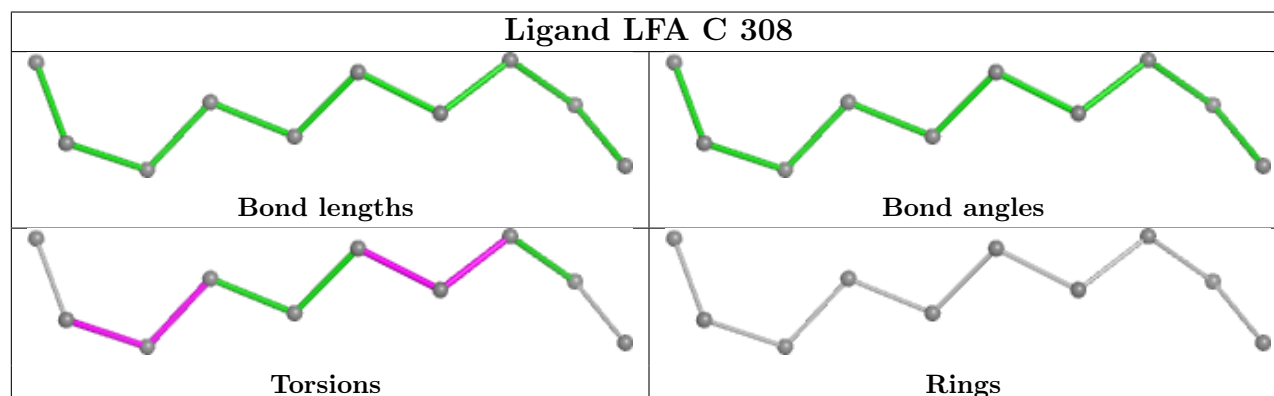
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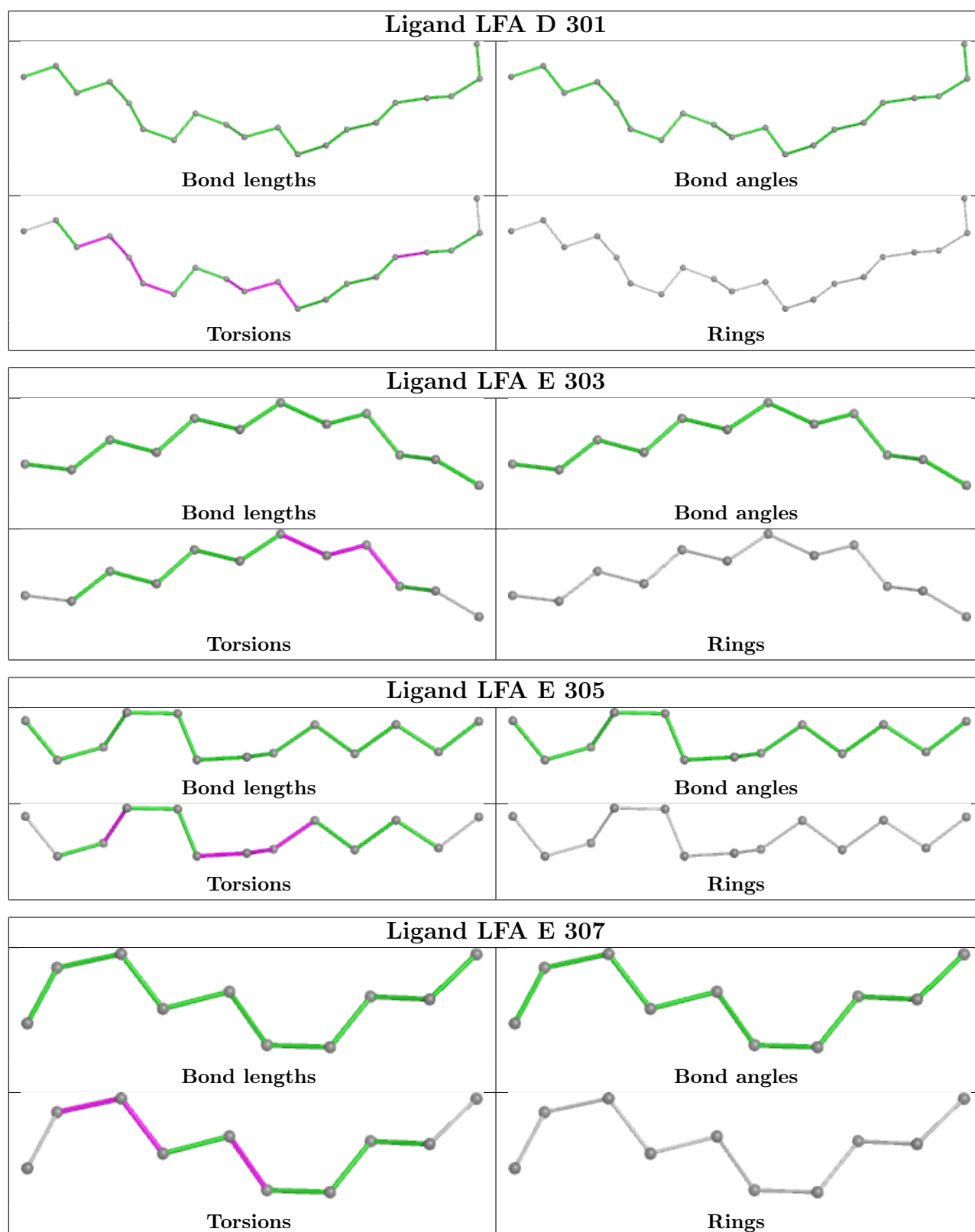
Mol	Chain	Res	Type	Atoms
2	C	306	LFA	C2-C3-C4-C5
2	A	305	LFA	C5-C6-C7-C8
2	C	305	LFA	C6-C7-C8-C9
2	C	310	LFA	C3-C4-C5-C6
2	C	305	LFA	C1-C2-C3-C4
2	A	306	LFA	C2-C3-C4-C5
2	E	305	LFA	C9-C10-C11-C12
2	E	313	LFA	C2-C3-C4-C5
2	E	314	LFA	C16-C17-C18-C19
2	C	307	LFA	C4-C5-C6-C7
2	B	314	LFA	C6-C7-C8-C9
2	E	312	LFA	C1-C2-C3-C4
2	B	303	LFA	C14-C15-C16-C17
2	D	315	LFA	C5-C6-C7-C8
2	B	303	LFA	C13-C14-C15-C16
2	E	312	LFA	C6-C7-C8-C9

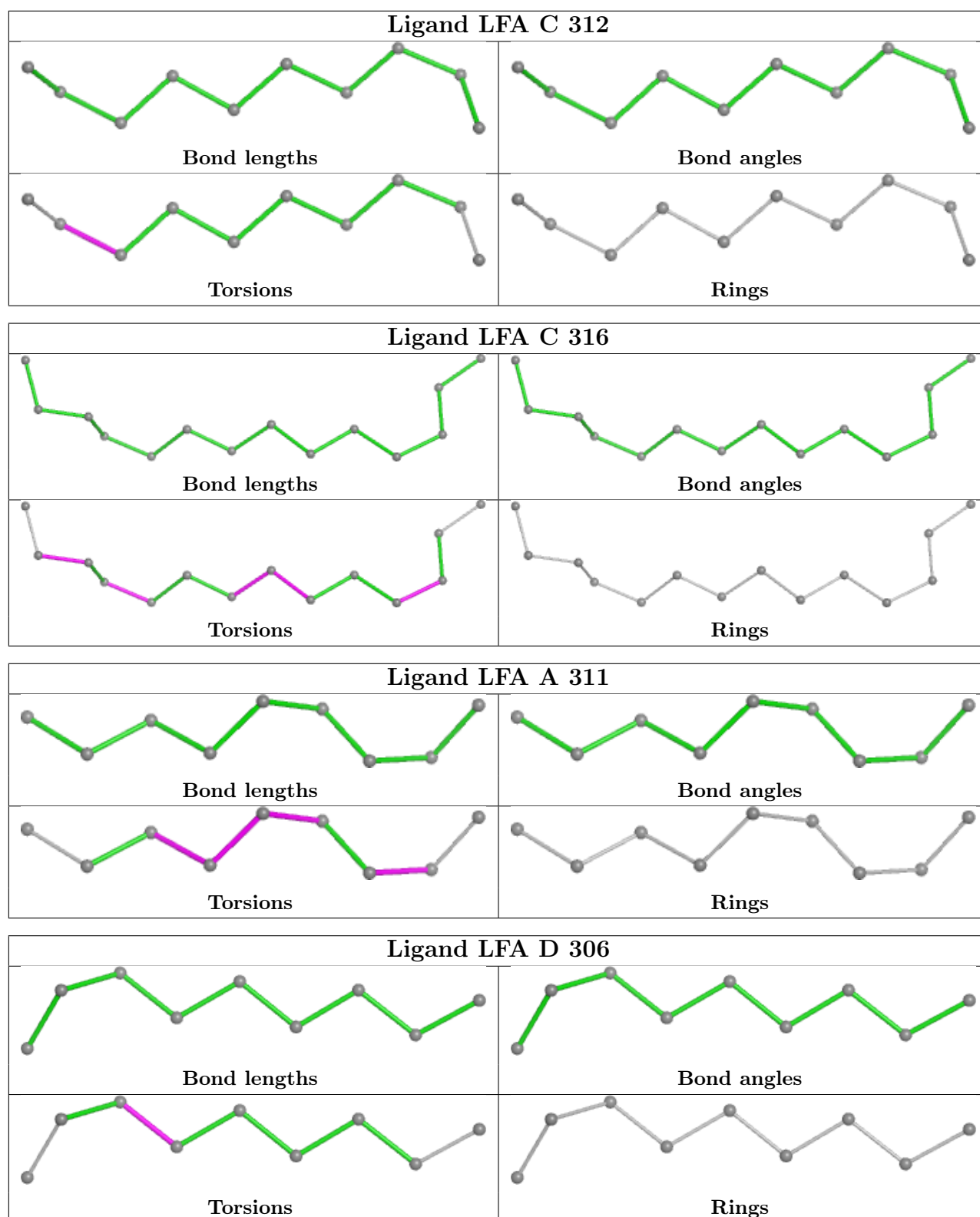
There are no ring outliers.

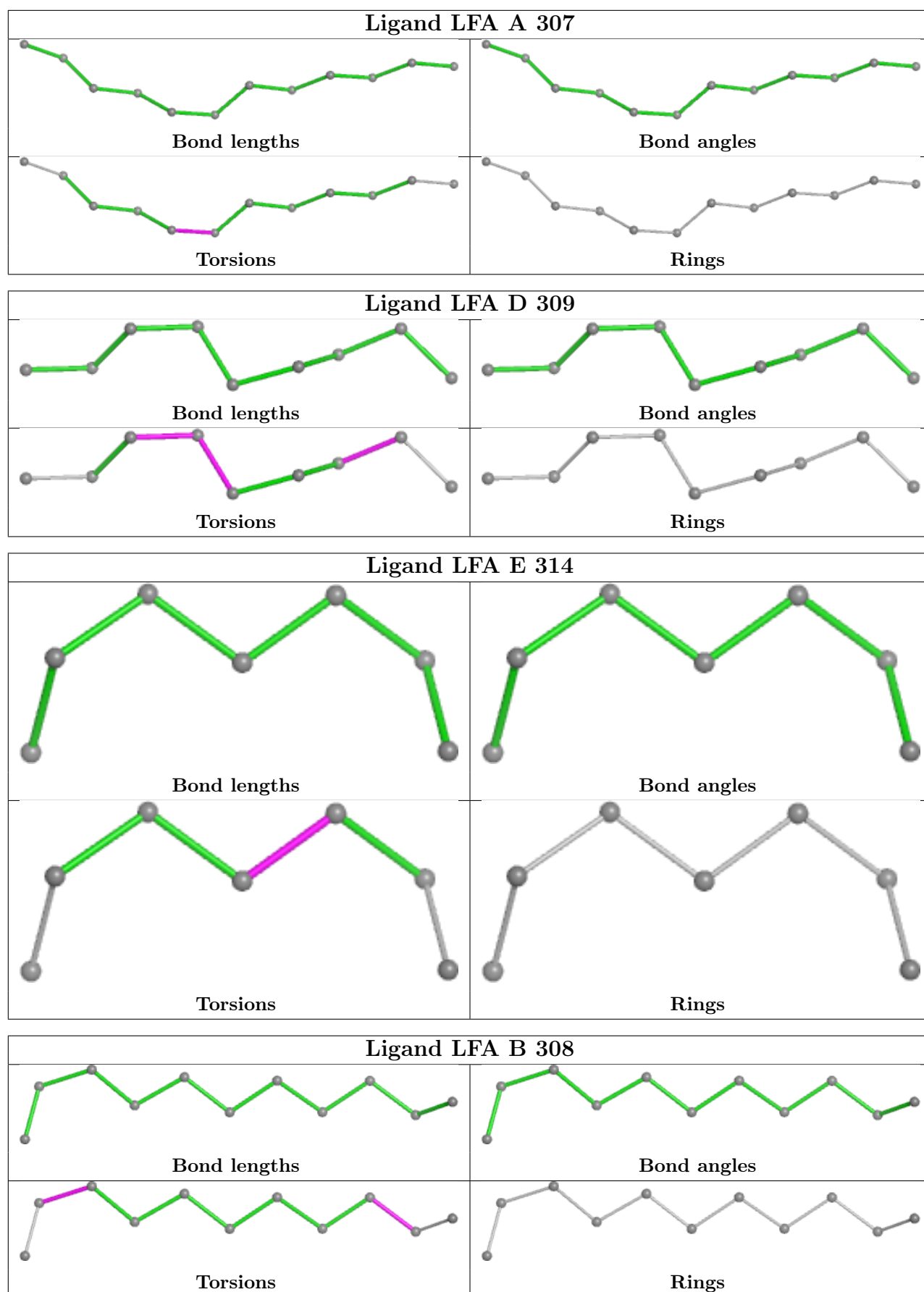
No monomer is involved in short contacts.

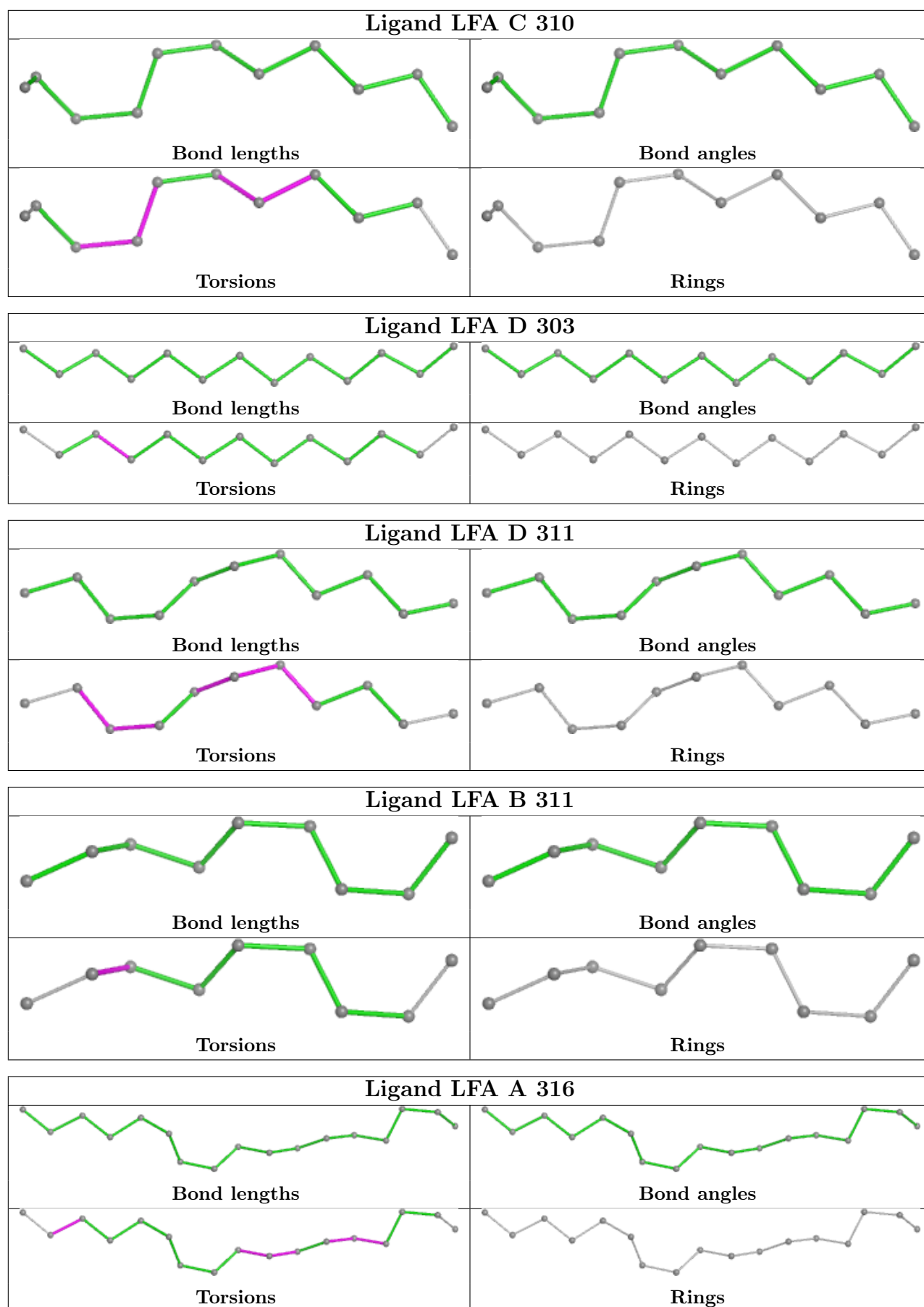
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

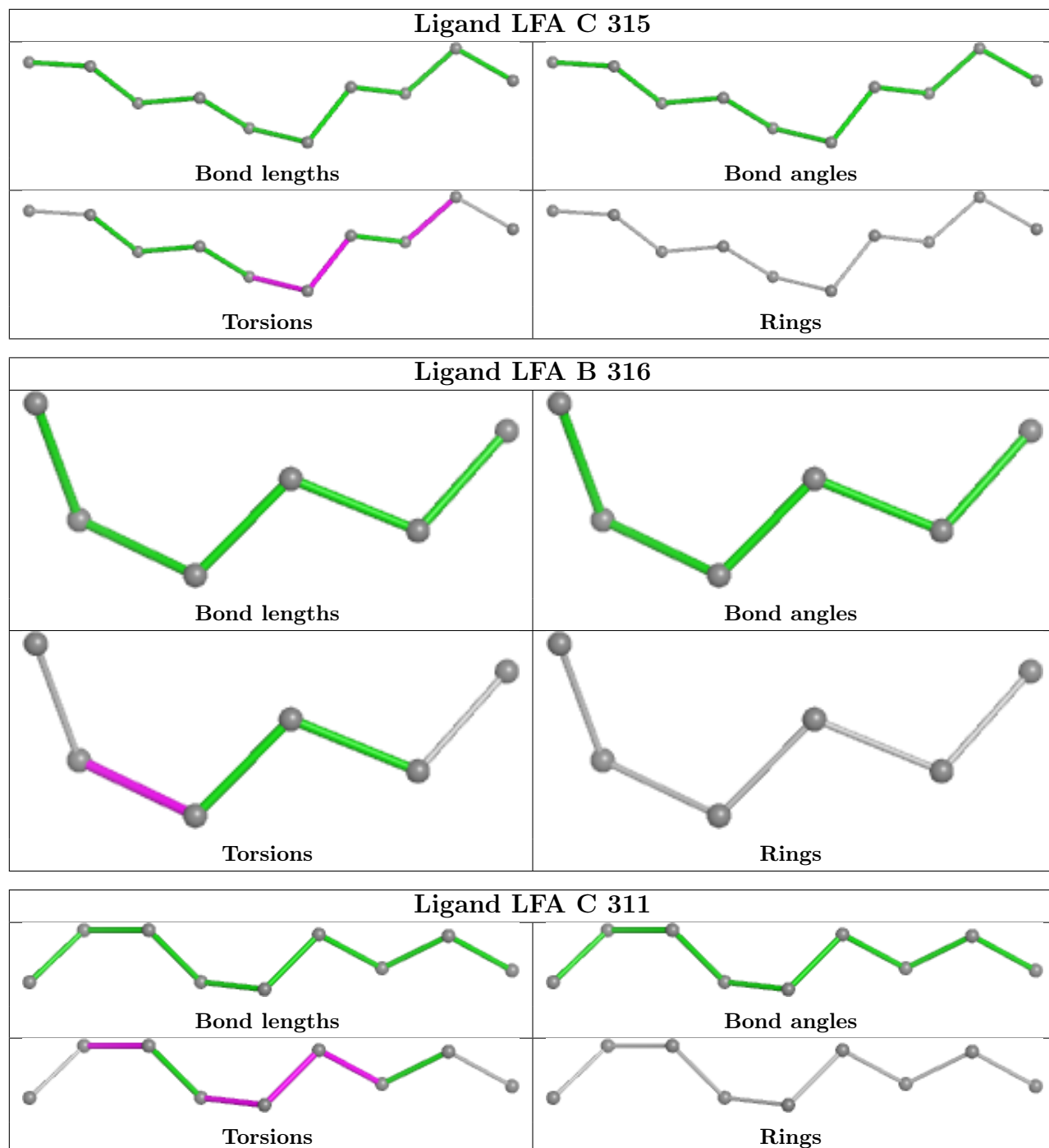


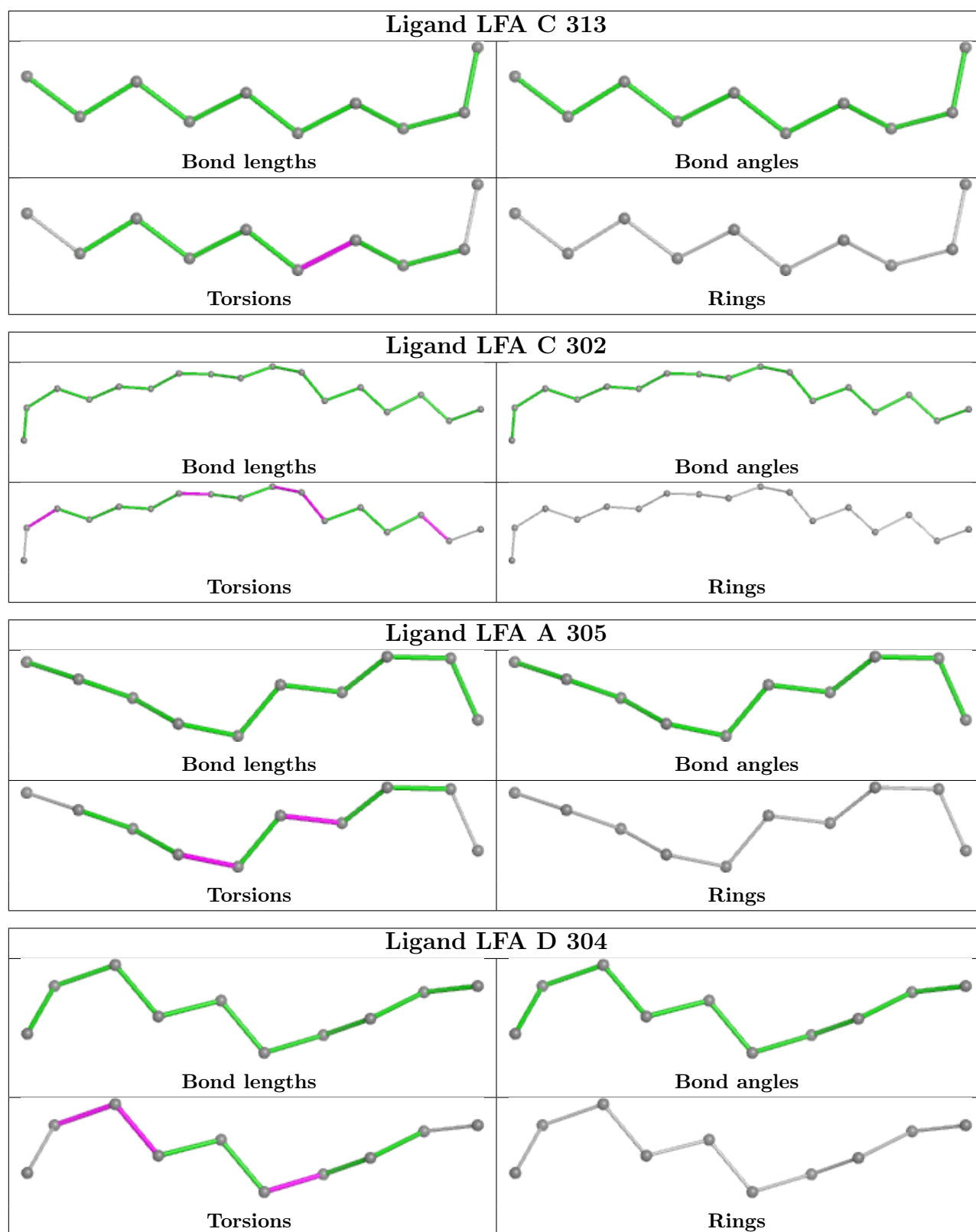


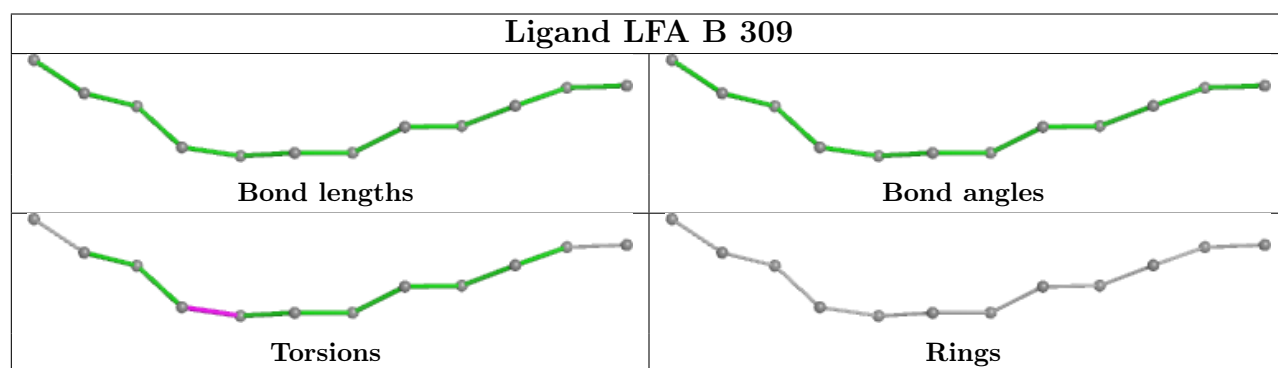
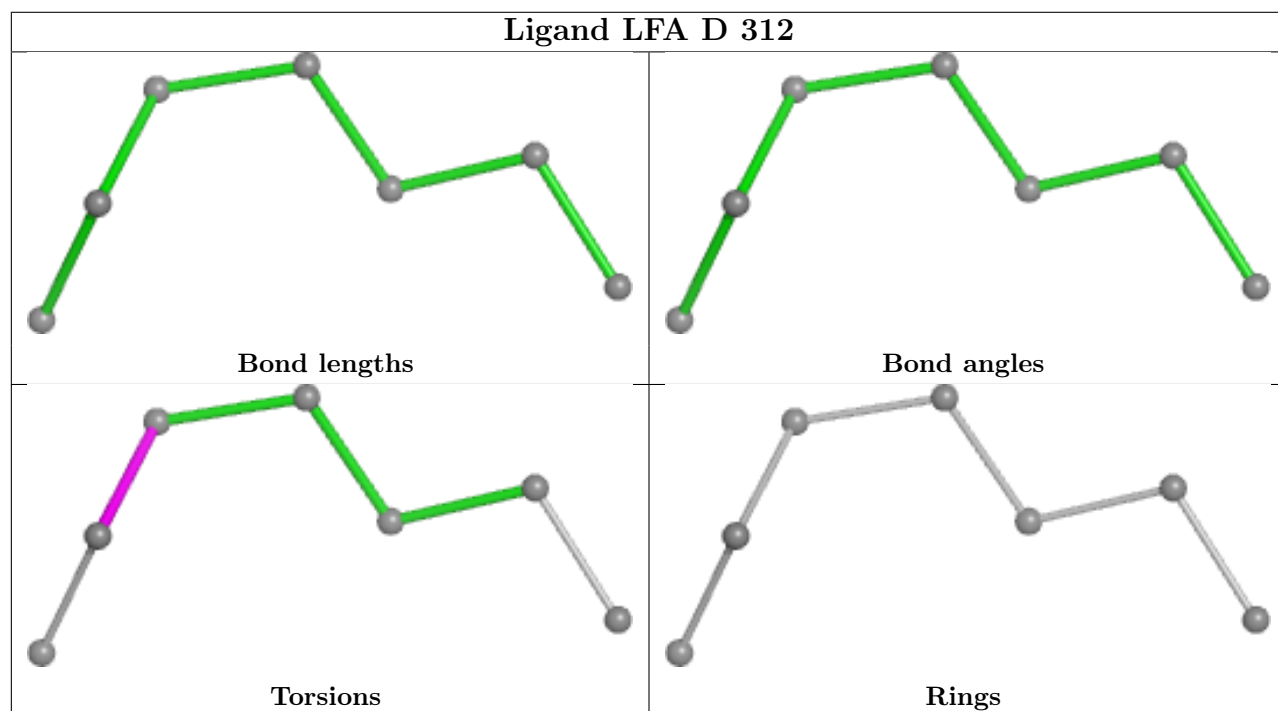
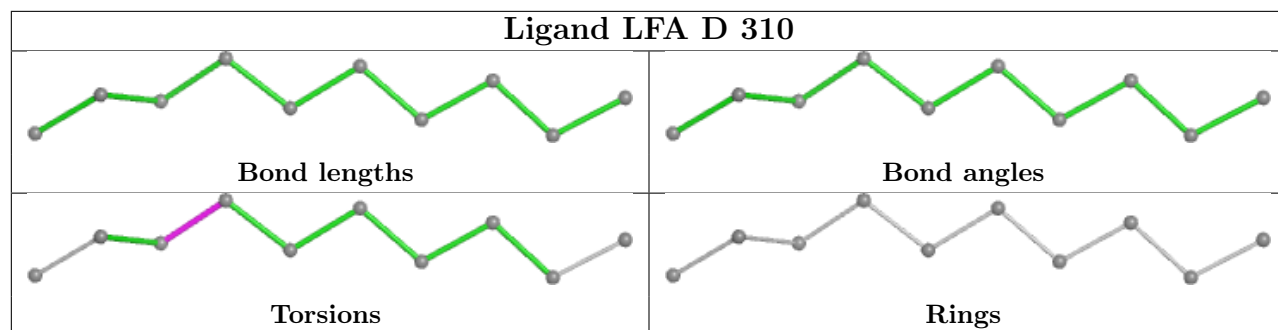


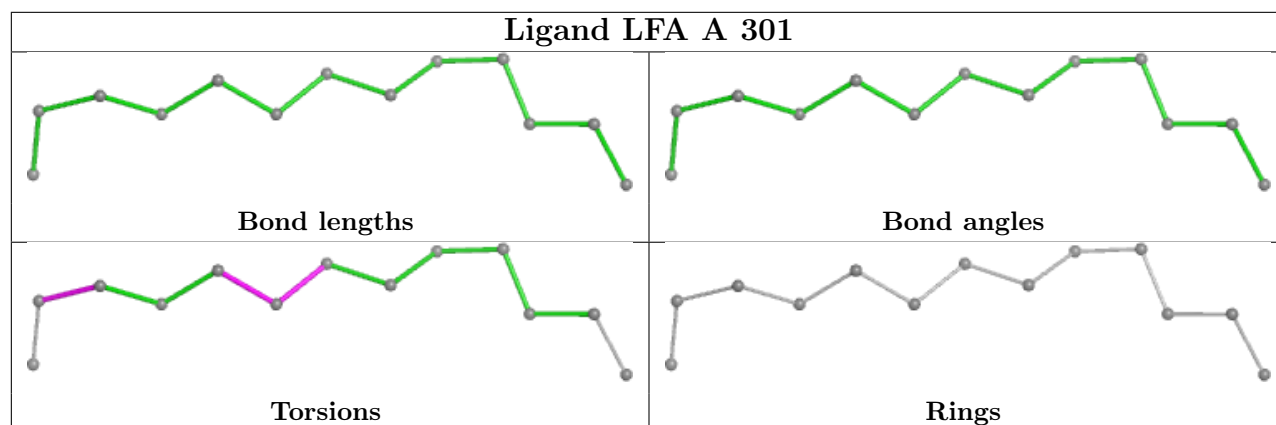
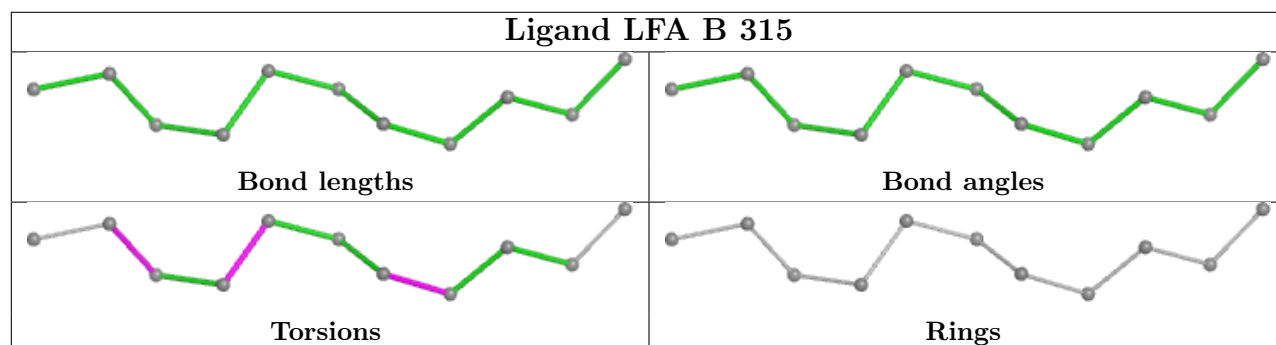
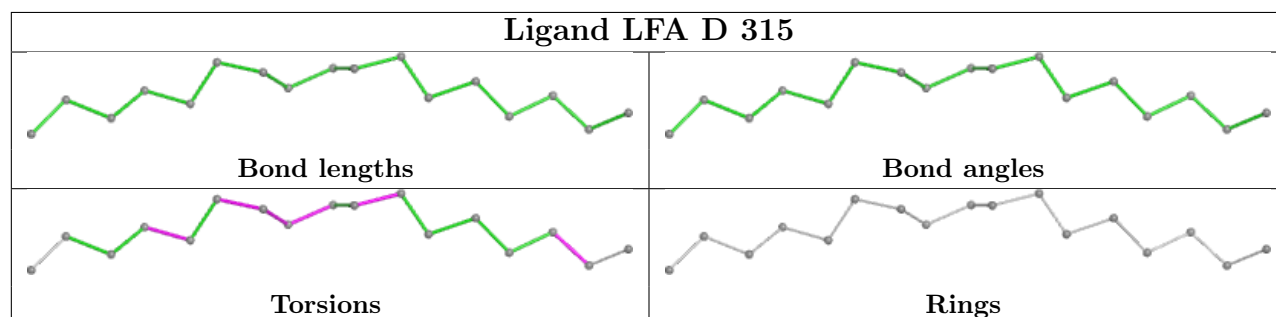
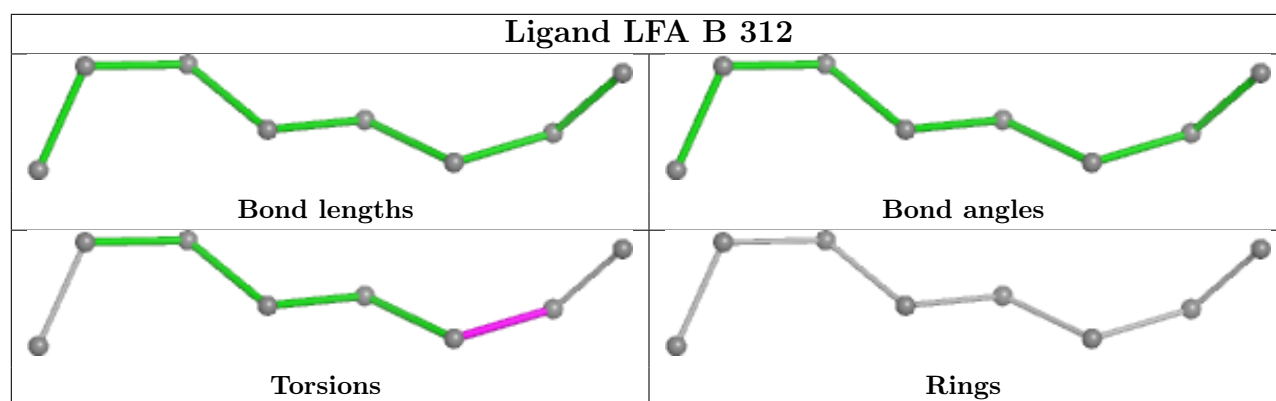


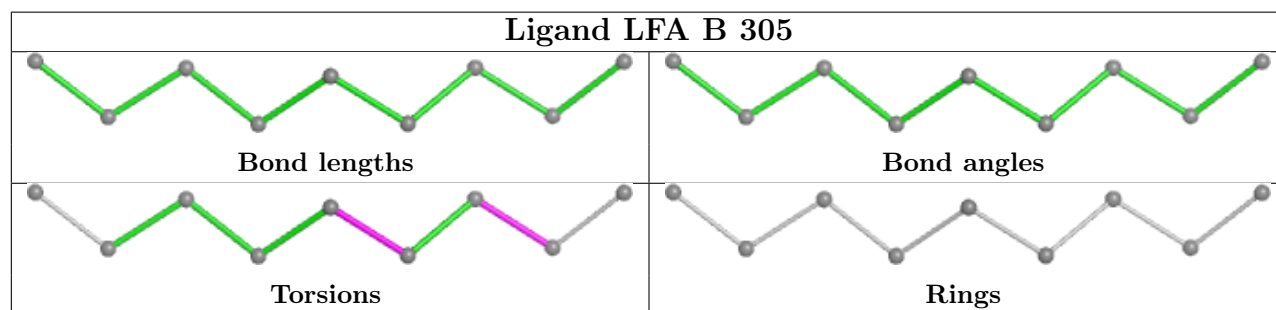
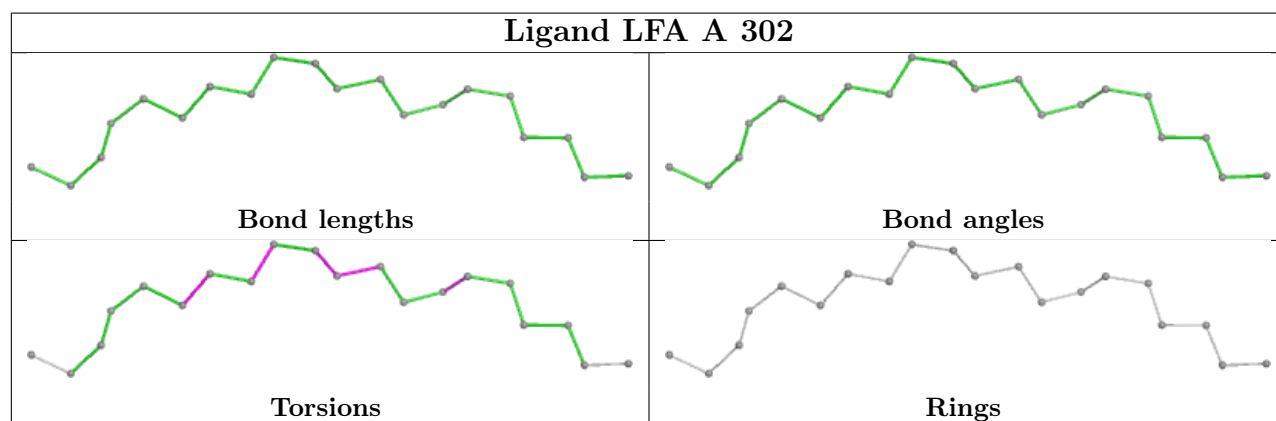
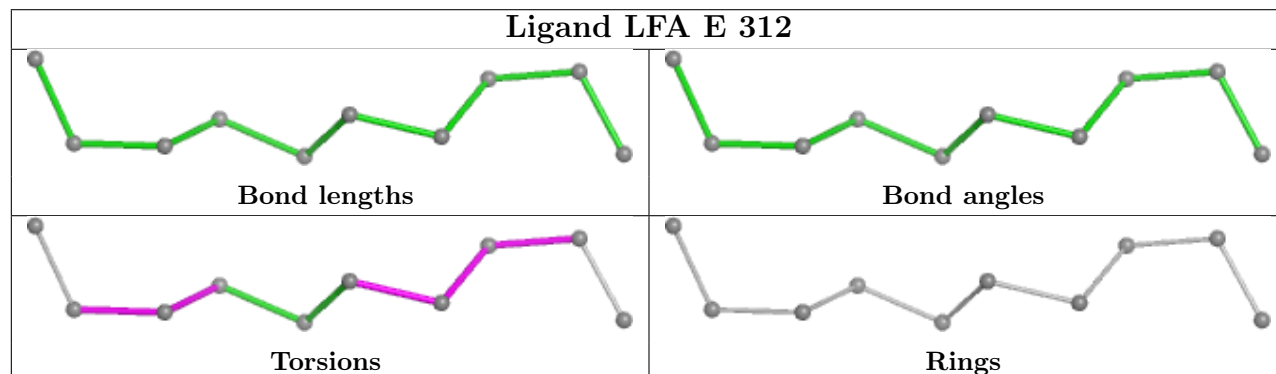
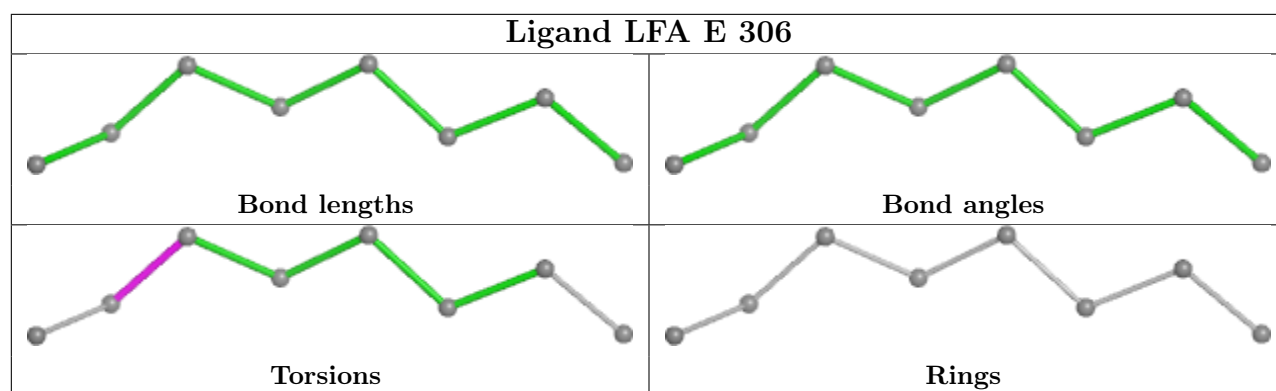


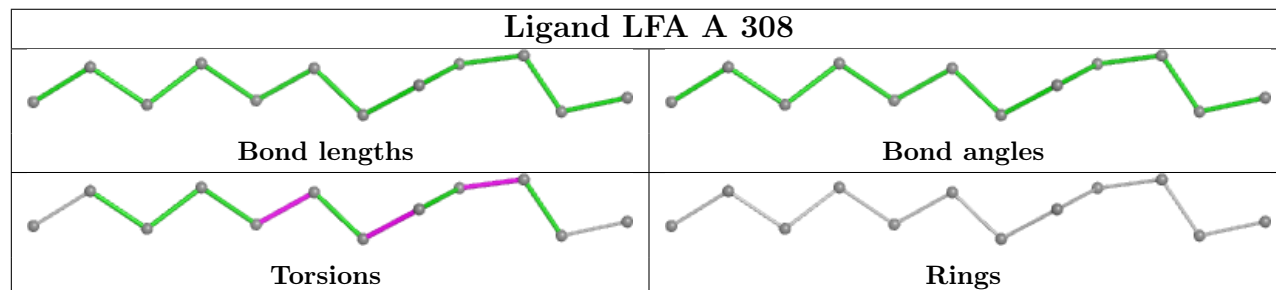
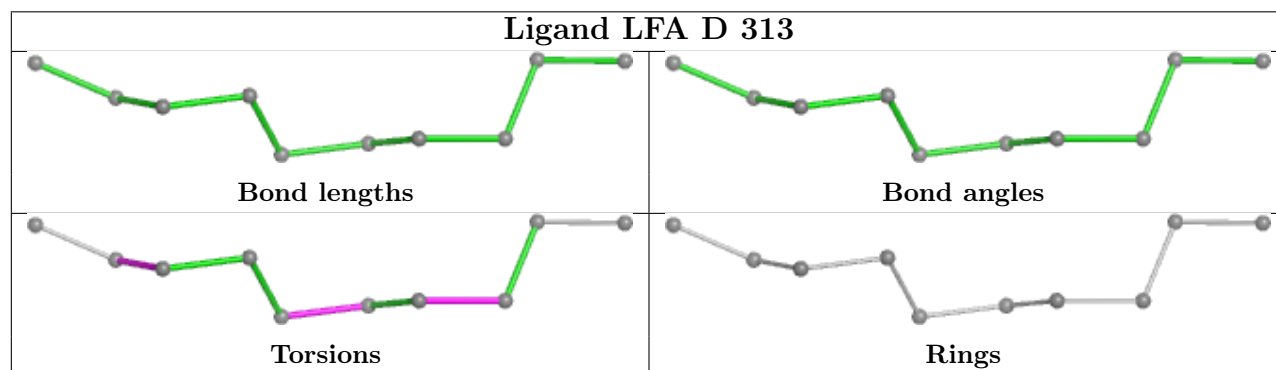
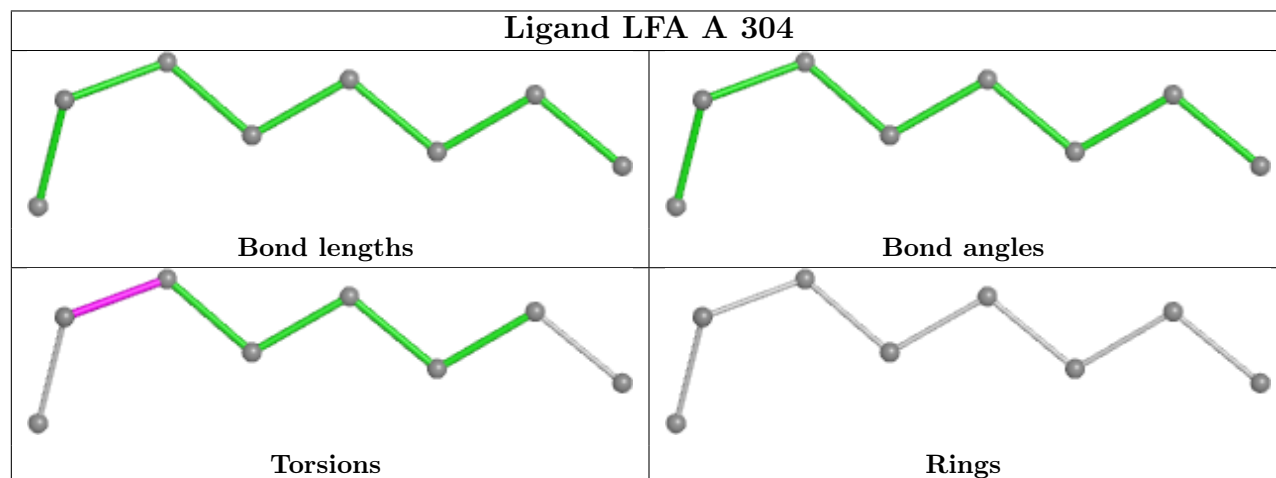
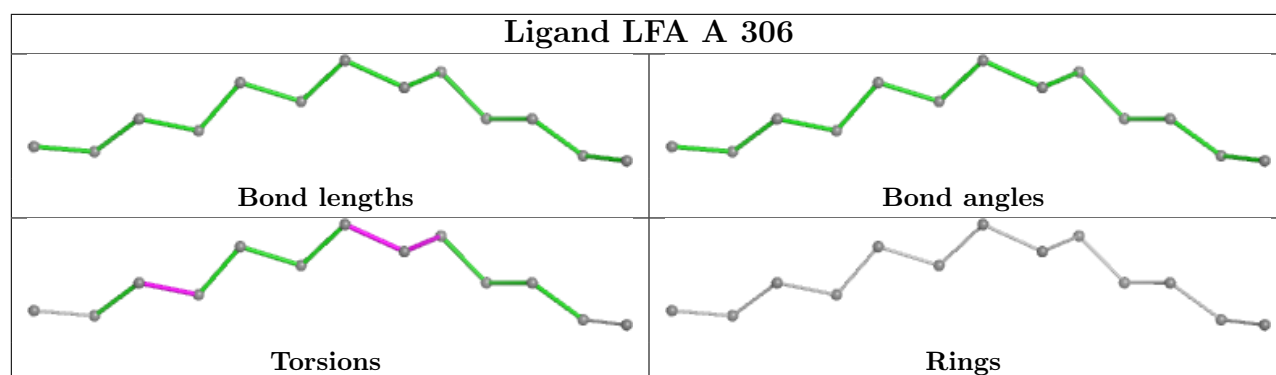


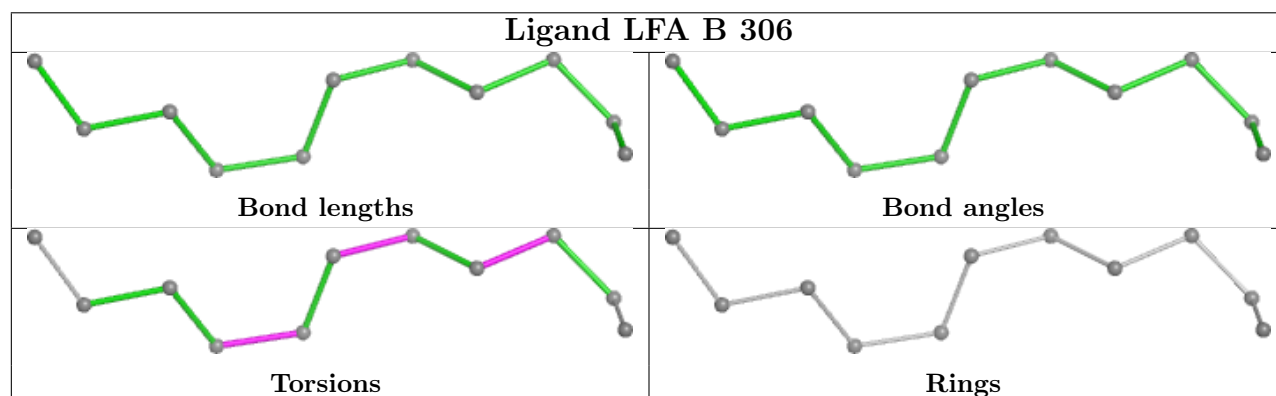
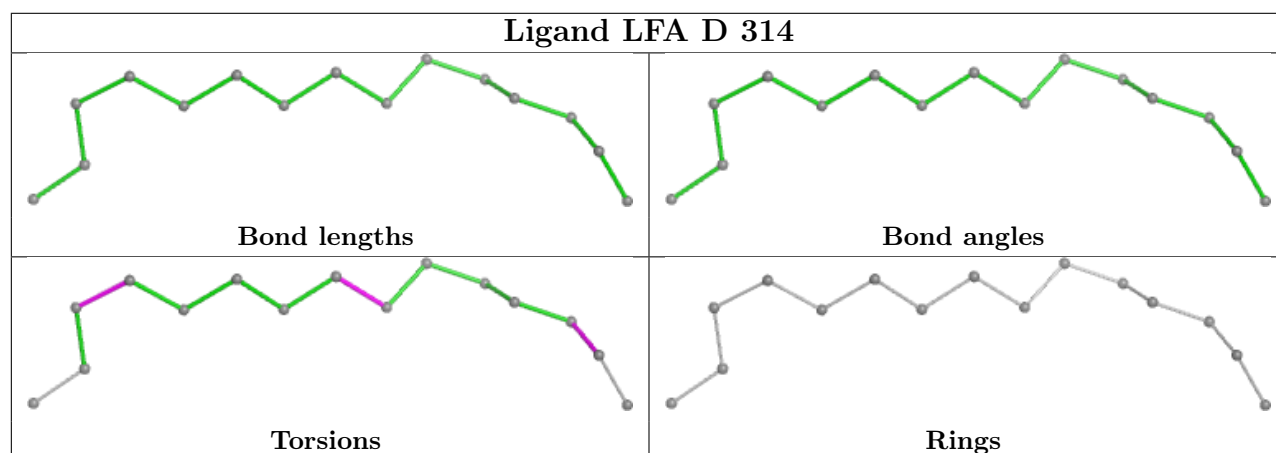
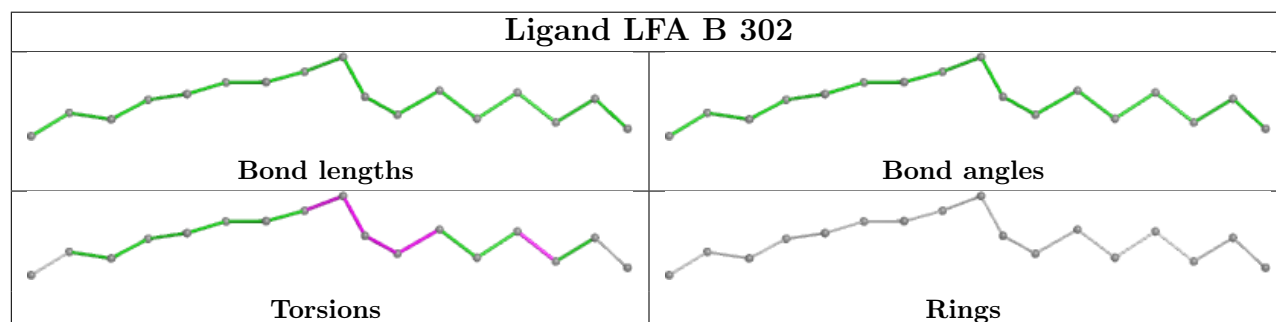
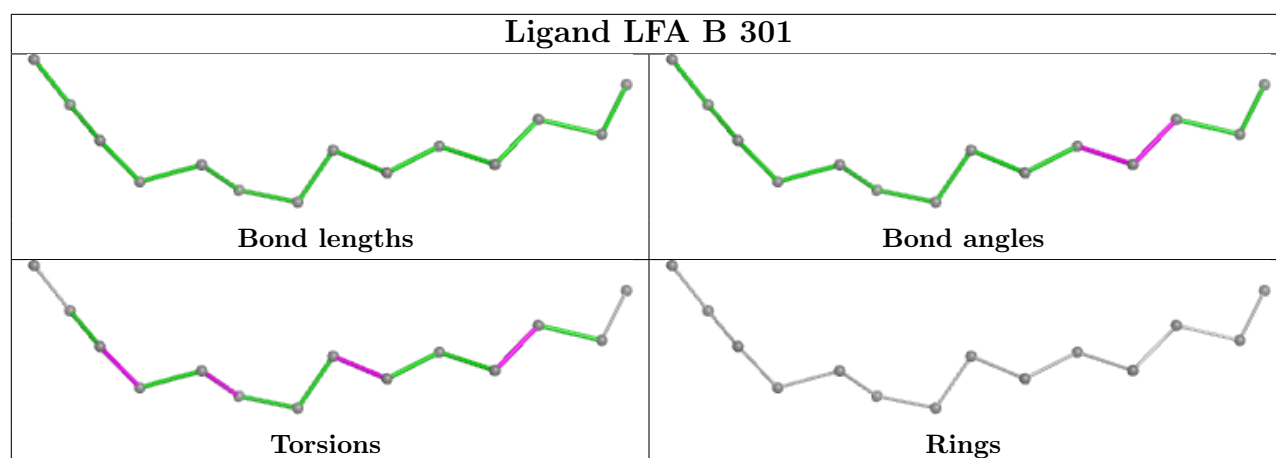


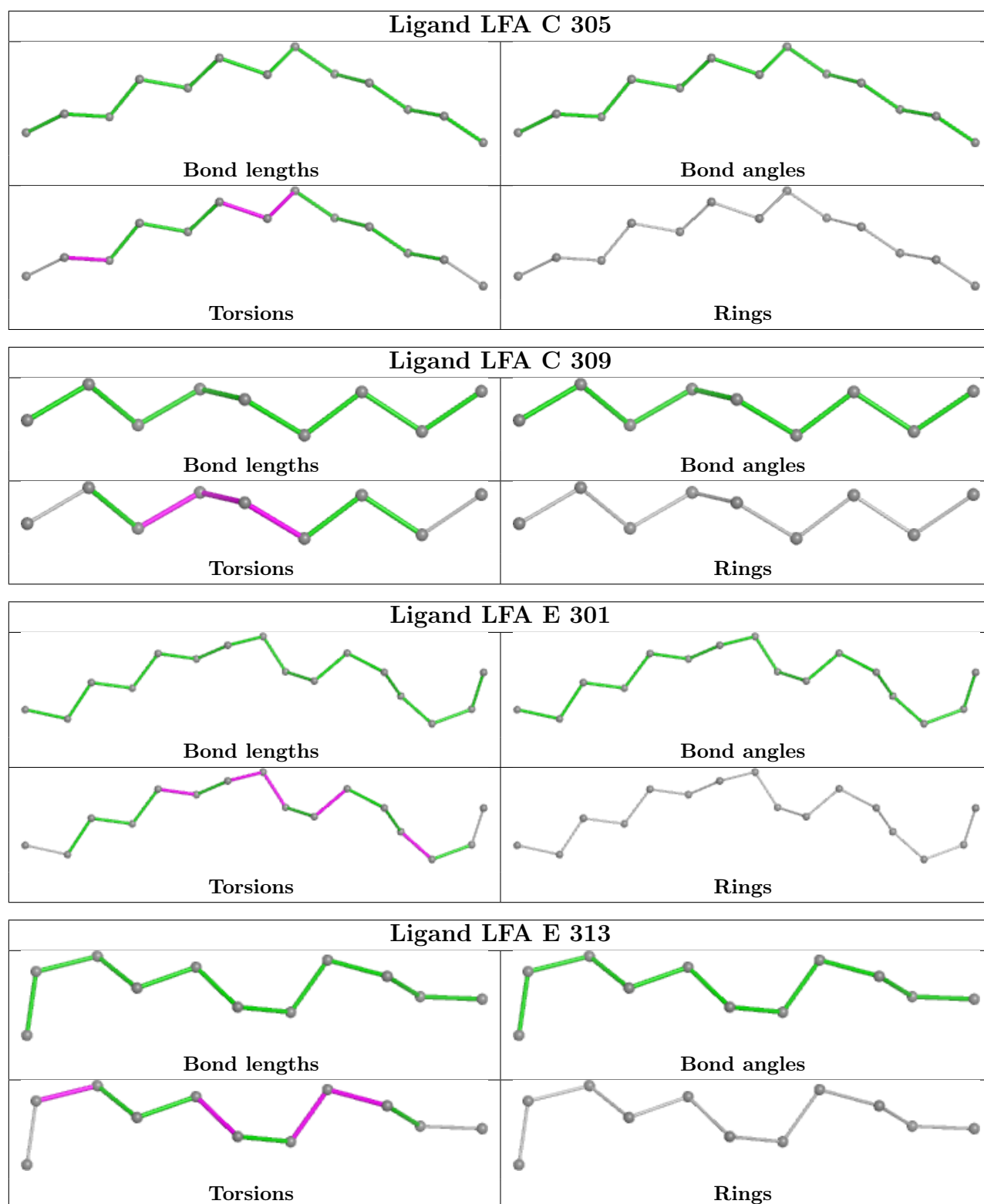


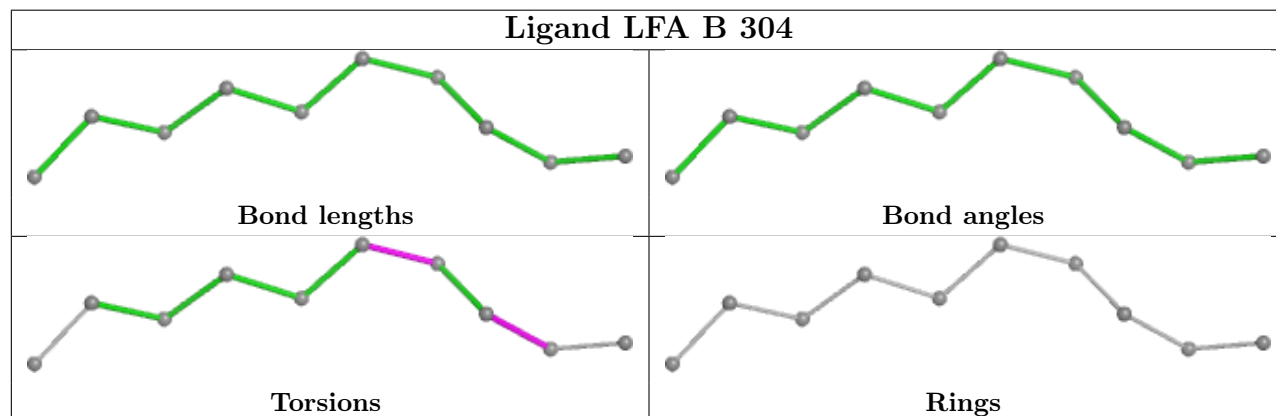
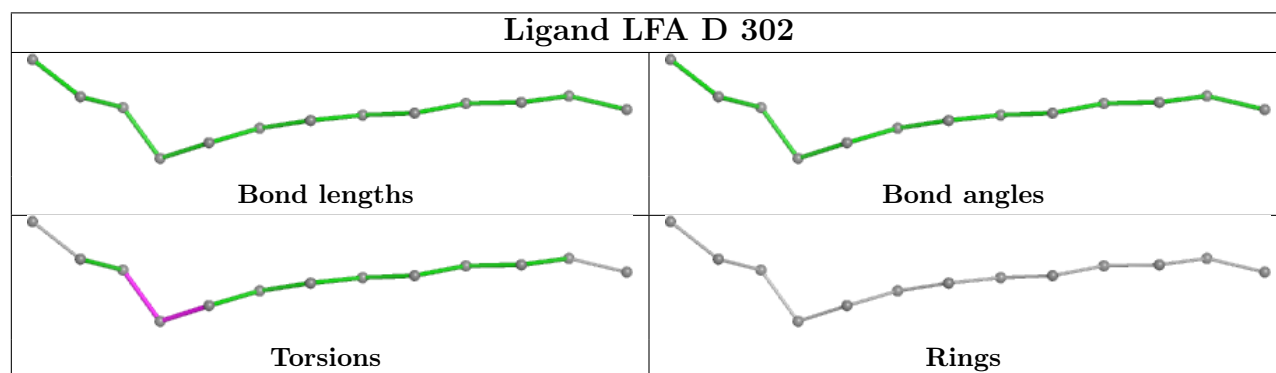
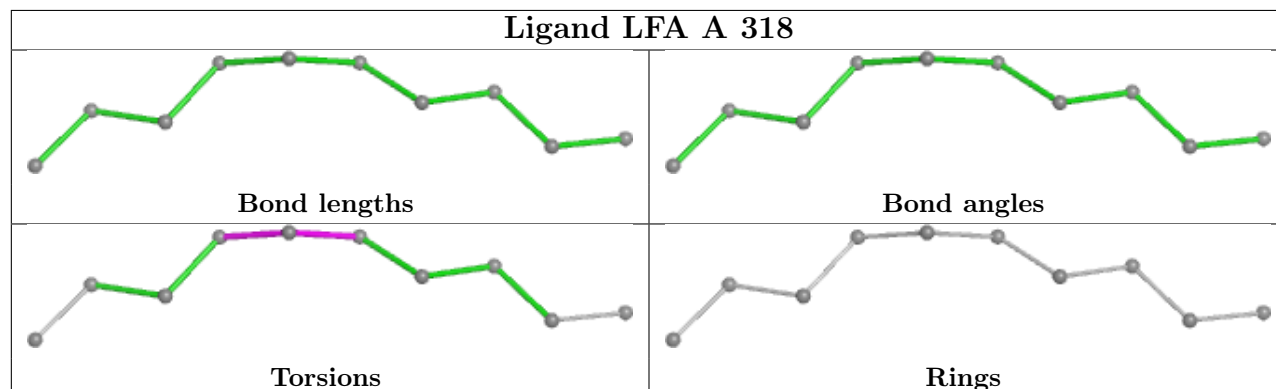
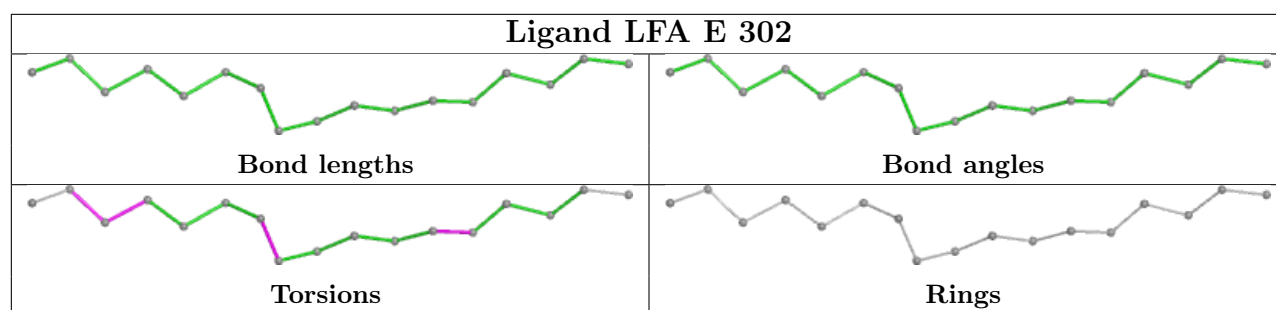


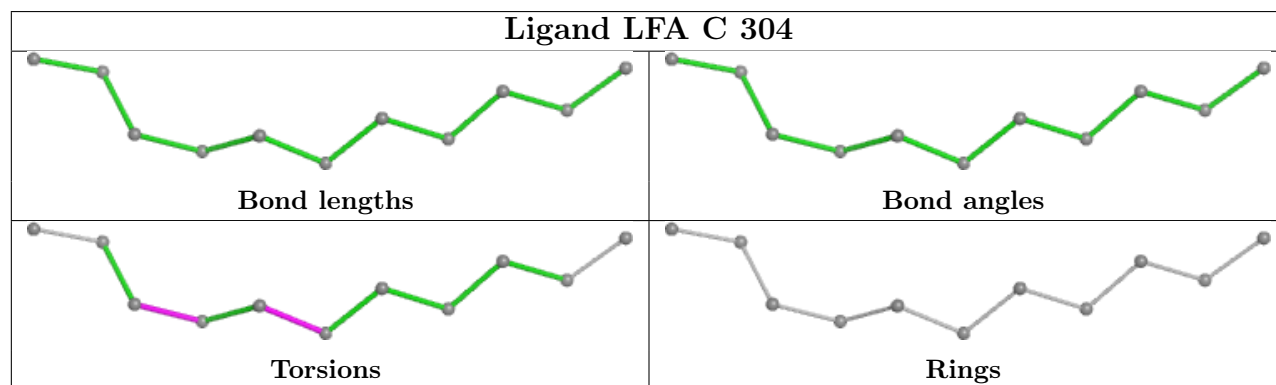
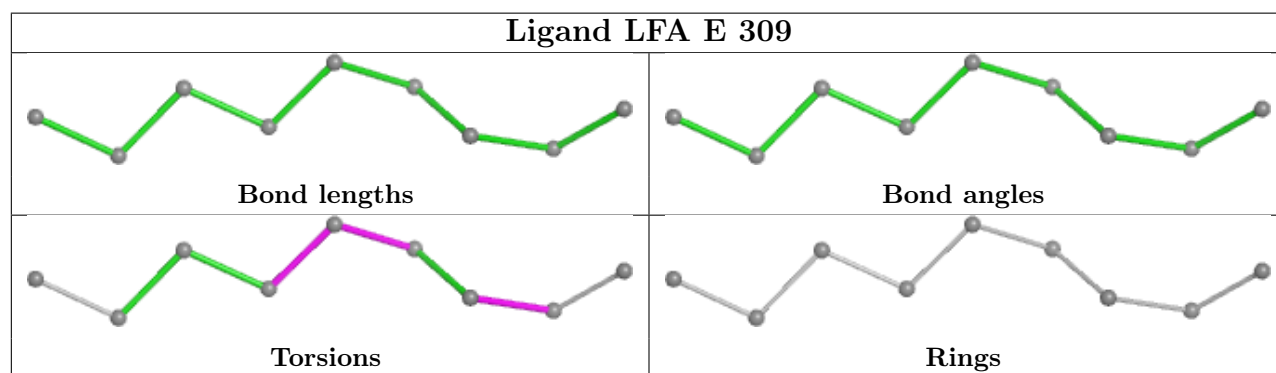
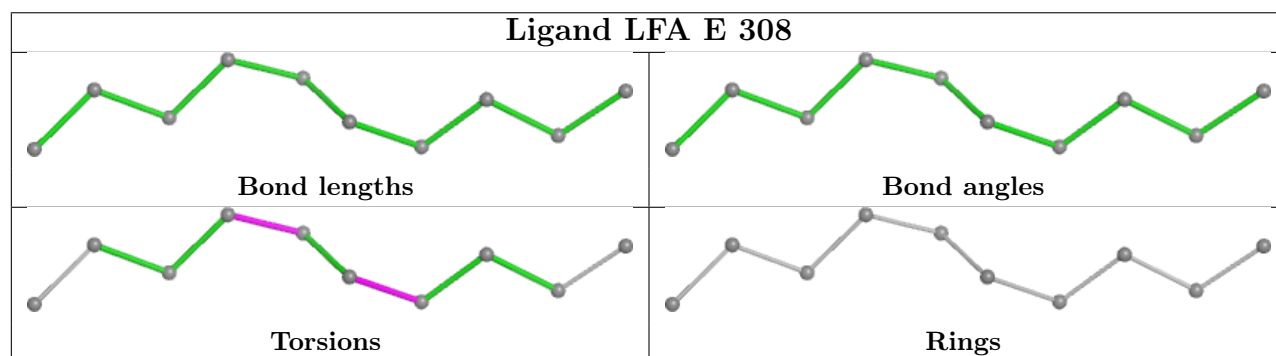
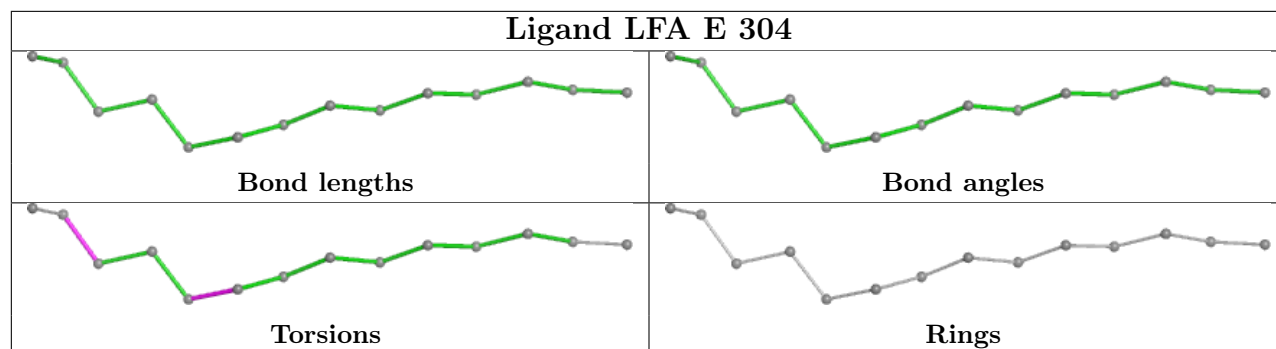


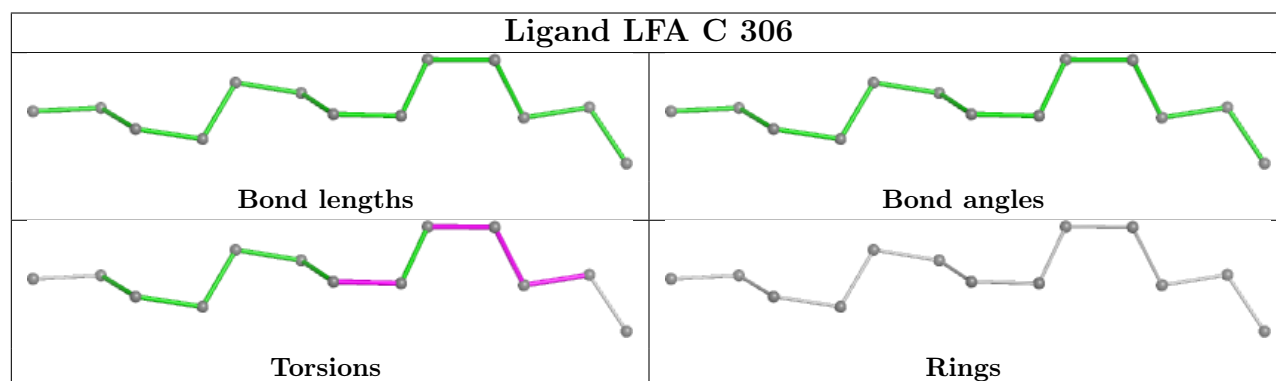
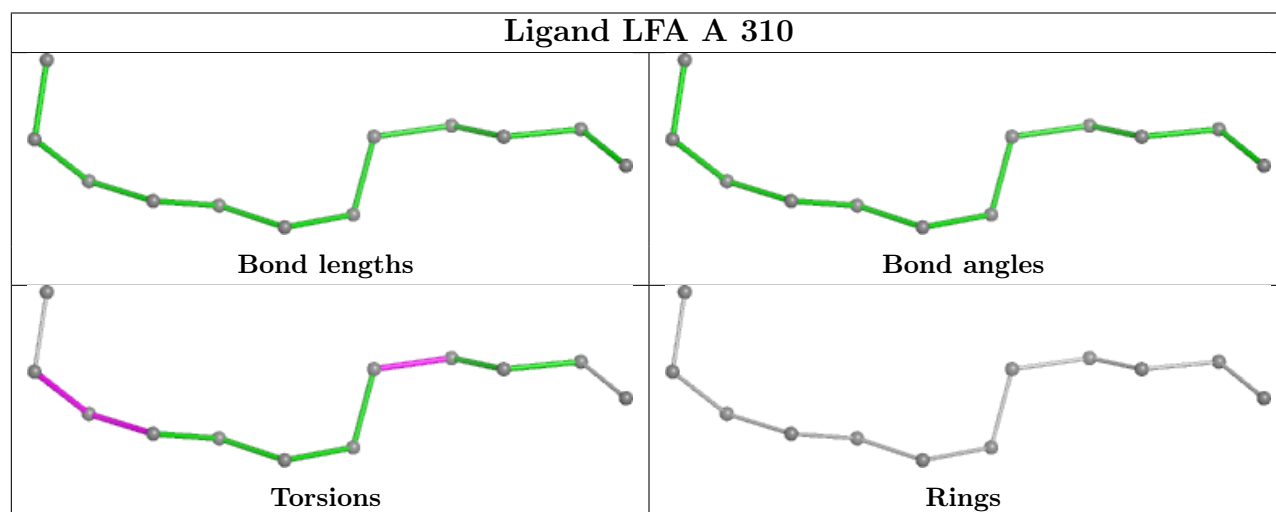
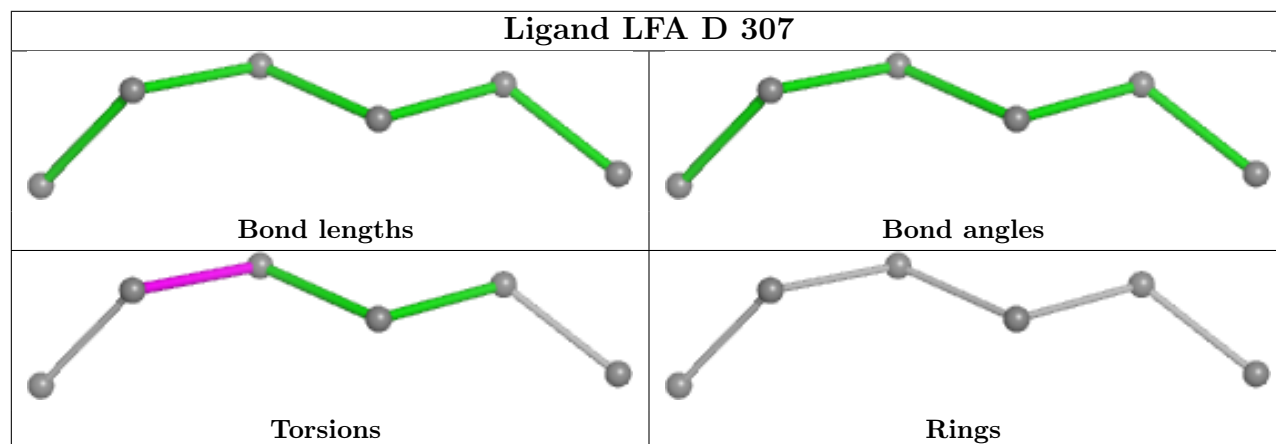
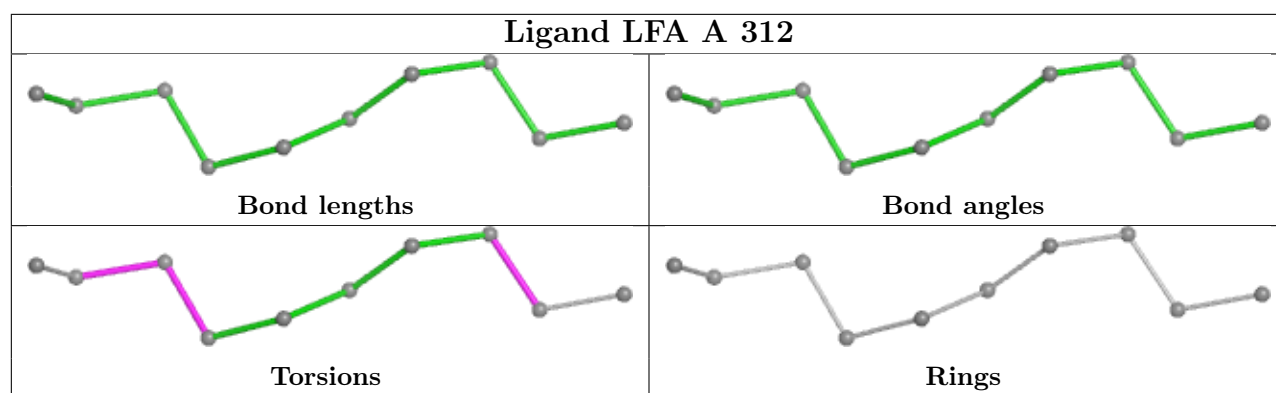


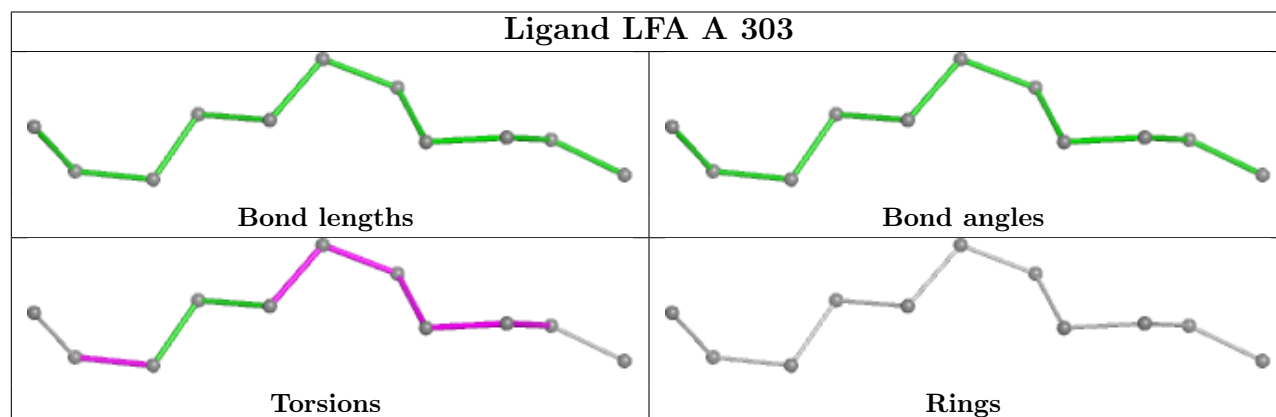
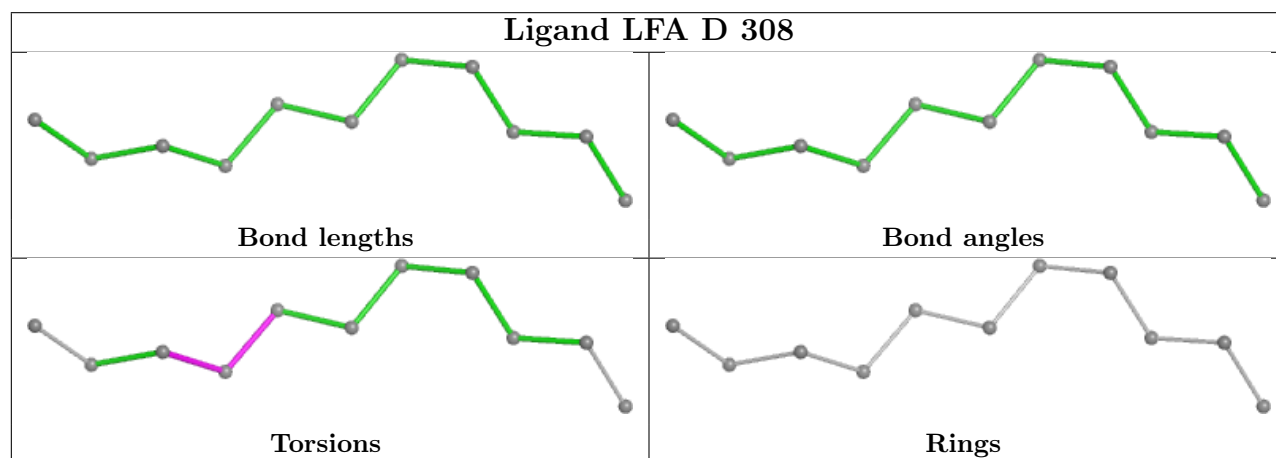
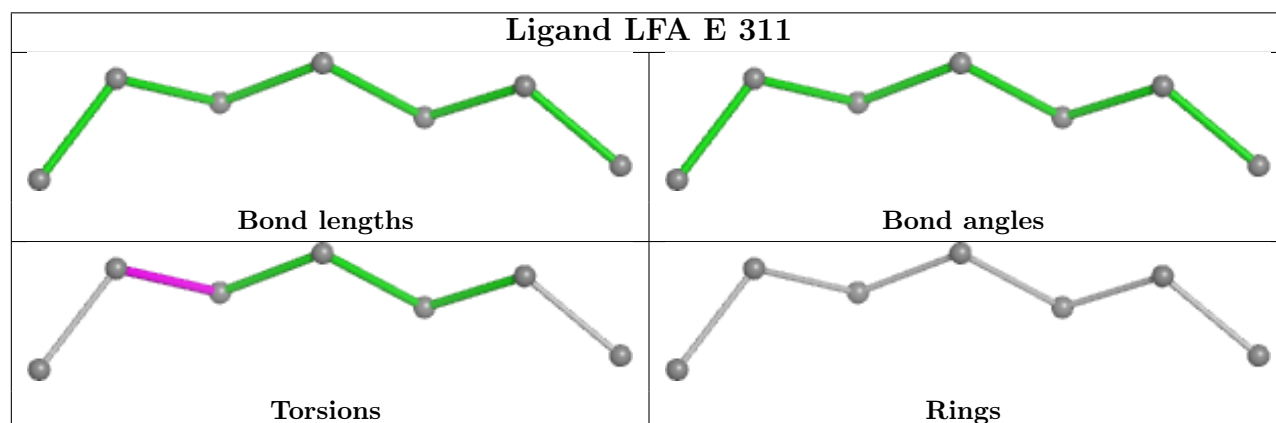
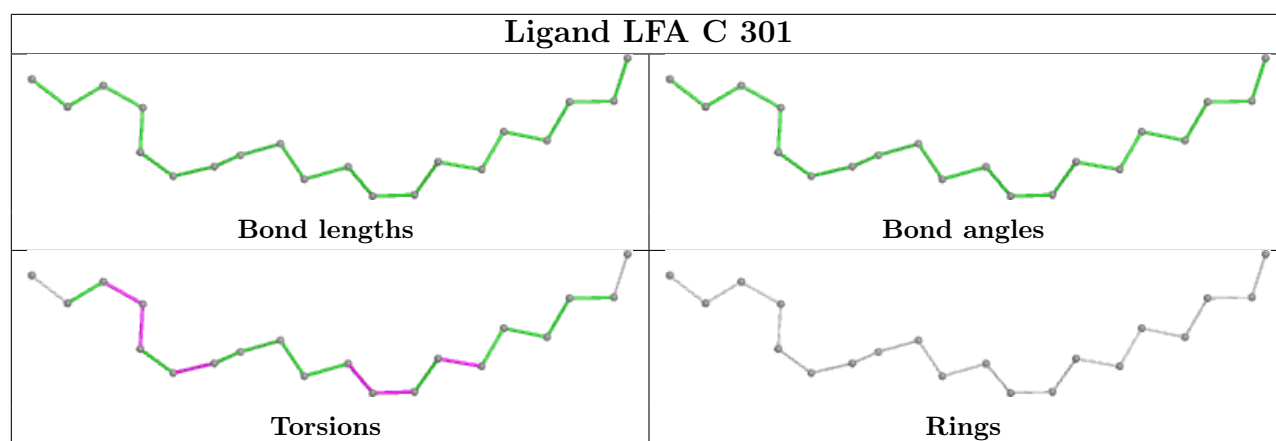


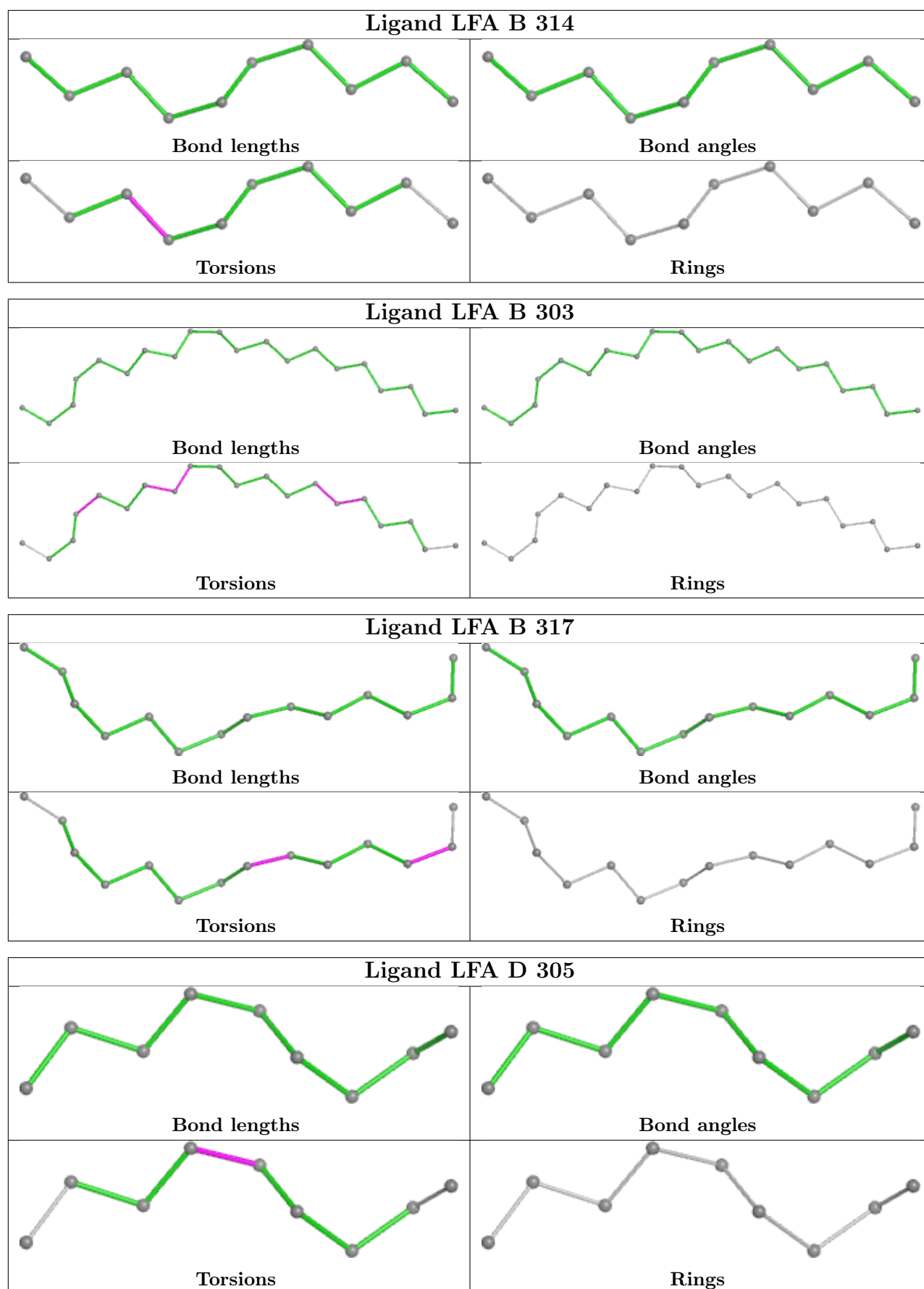


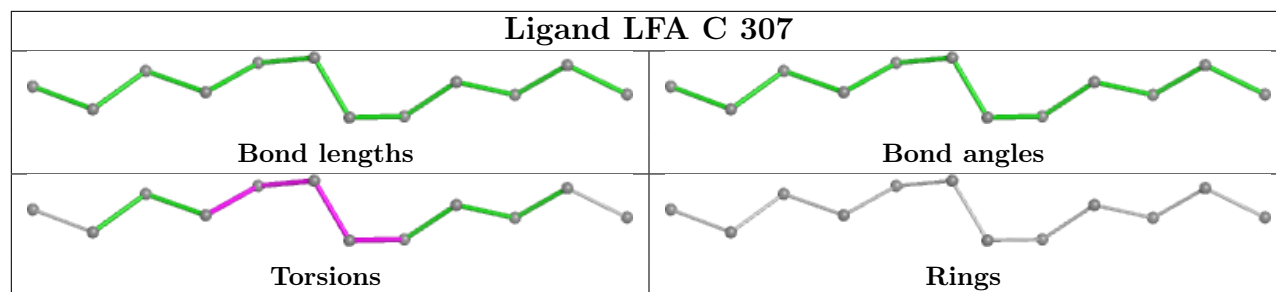












4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

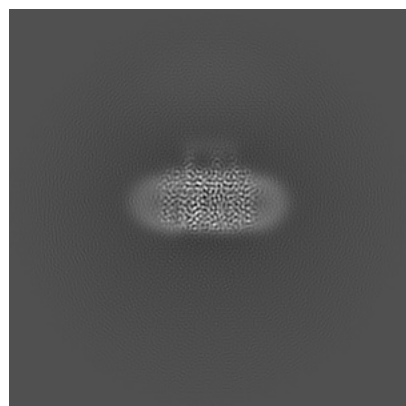
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53519. These allow visual inspection of the internal detail of the map and identification of artifacts.

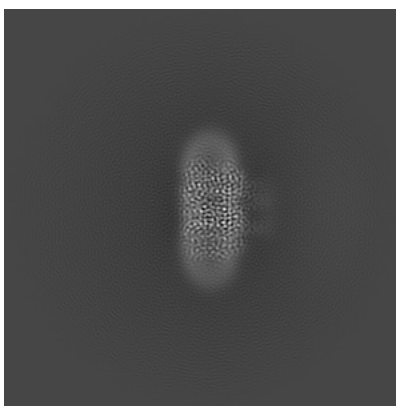
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

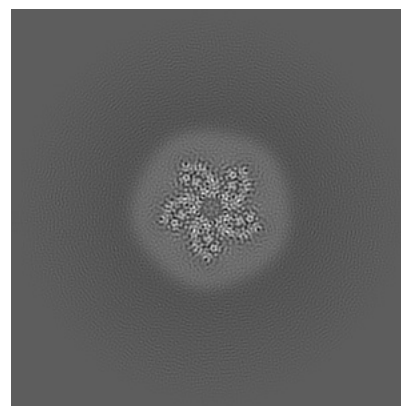
5.1.1 Primary map



X

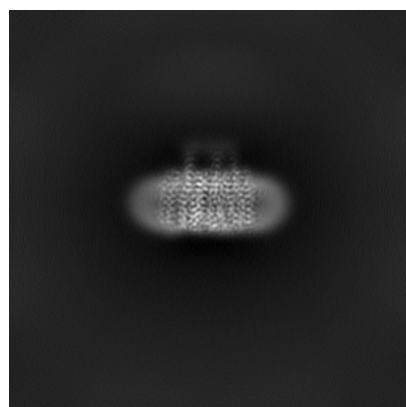


Y

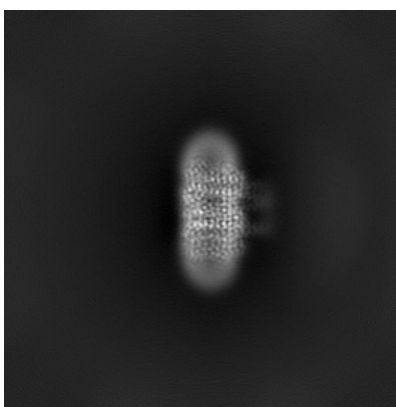


Z

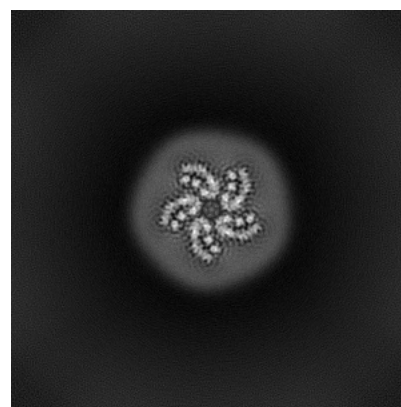
5.1.2 Raw map



X



Y

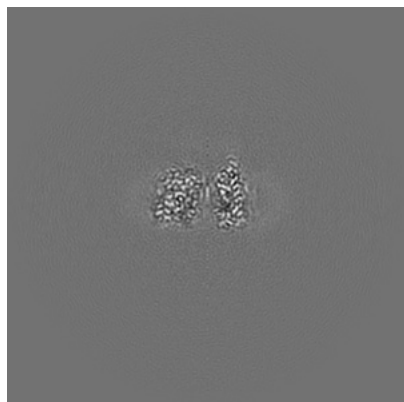


Z

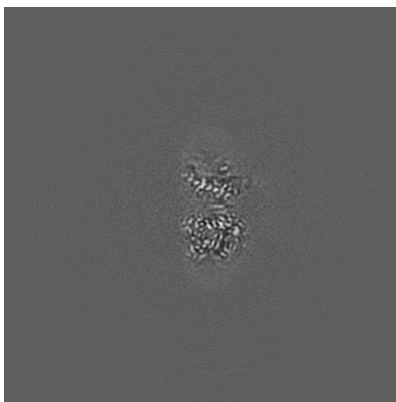
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

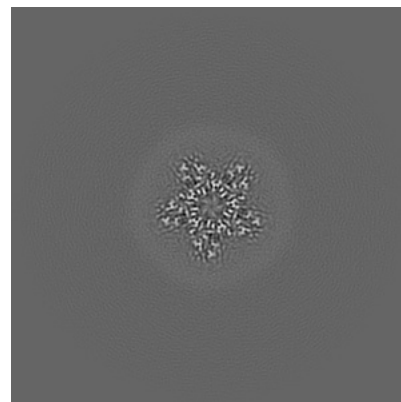
5.2.1 Primary map



X Index: 192

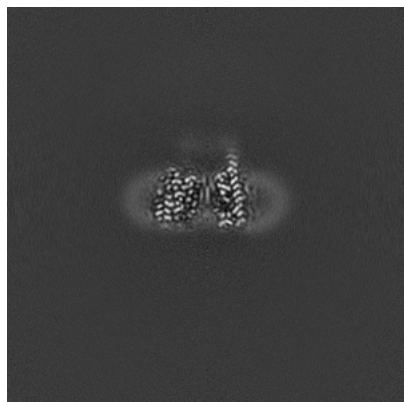


Y Index: 192

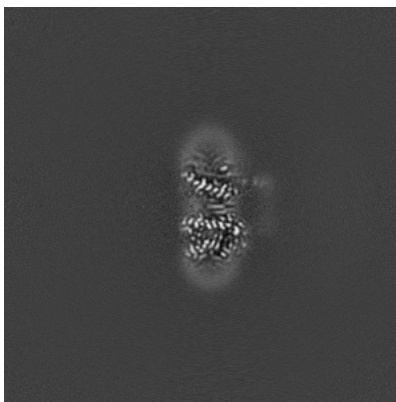


Z Index: 192

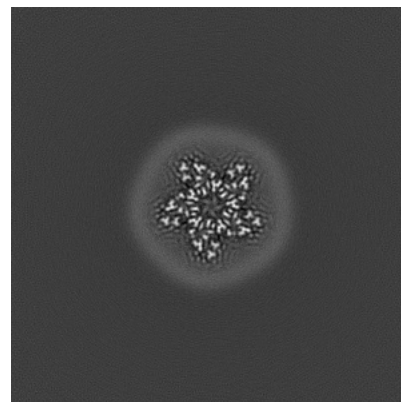
5.2.2 Raw map



X Index: 192



Y Index: 192

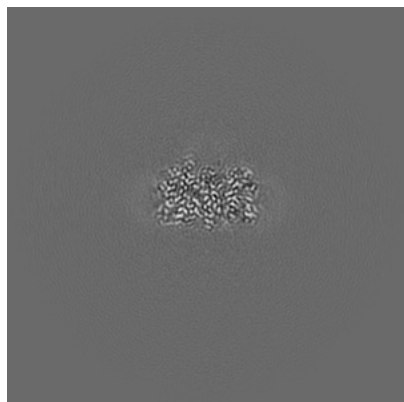


Z Index: 192

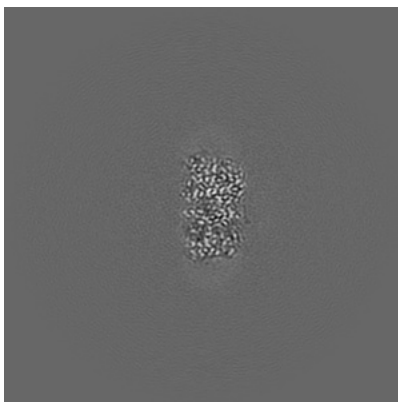
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

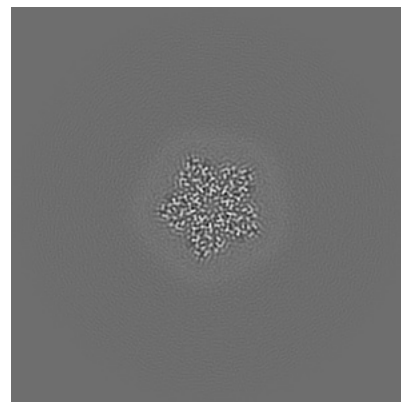
5.3.1 Primary map



X Index: 177

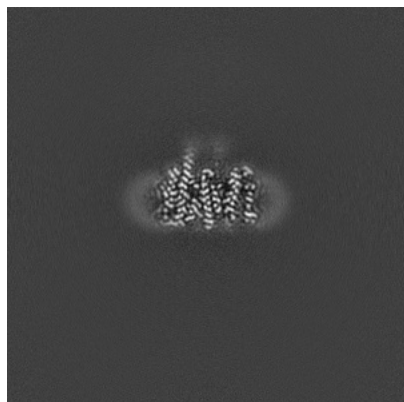


Y Index: 181

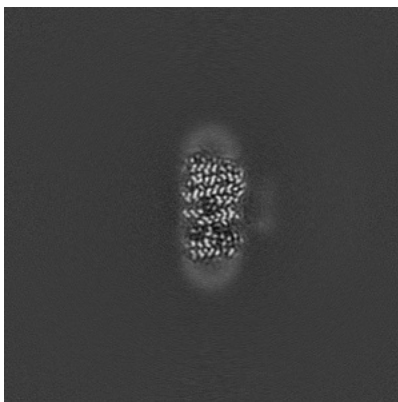


Z Index: 211

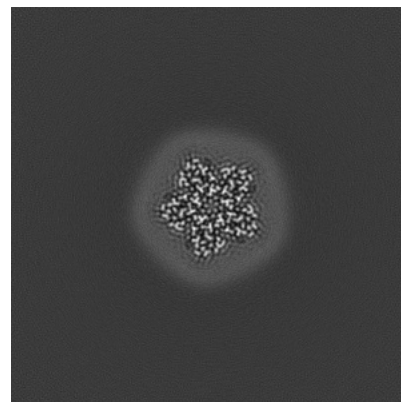
5.3.2 Raw map



X Index: 176



Y Index: 181

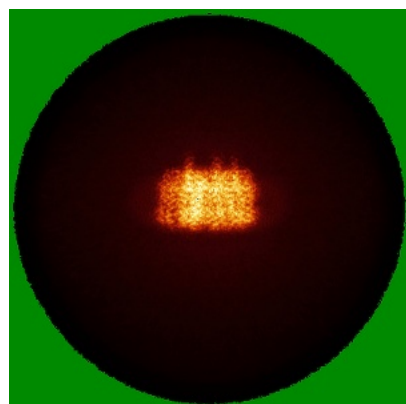


Z Index: 211

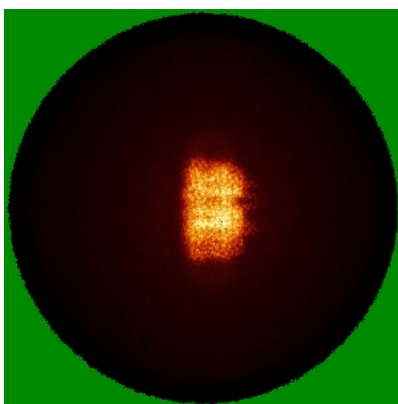
The images above show the largest variance slices of the map in three orthogonal directions.

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

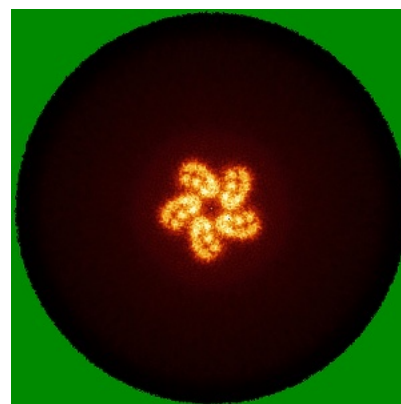
5.4.1 Primary map



X

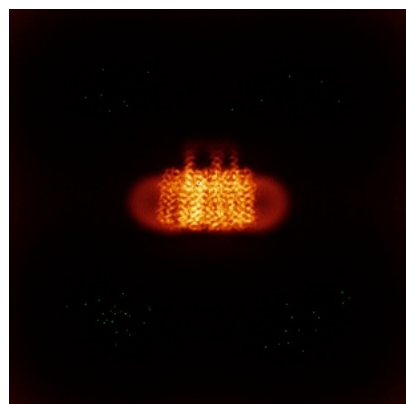


Y

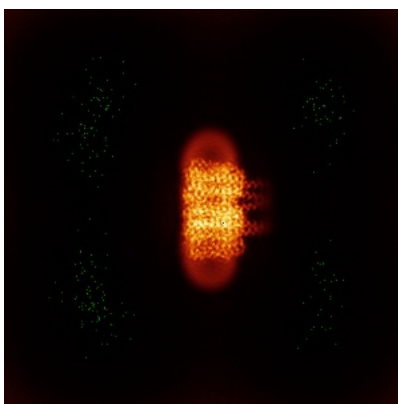


Z

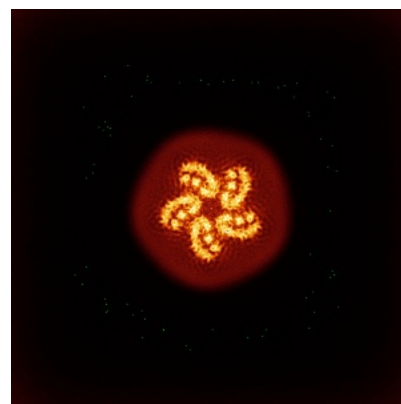
5.4.2 Raw map



X



Y

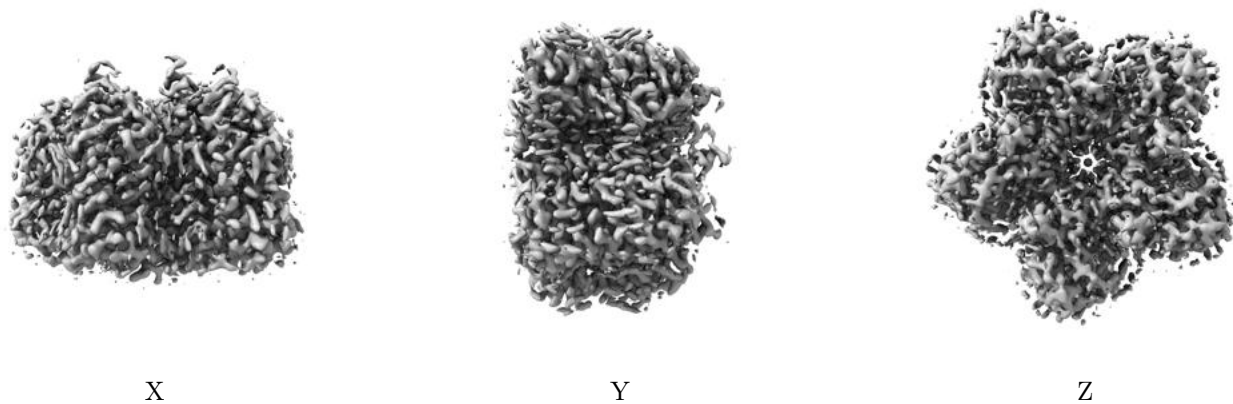


Z

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.

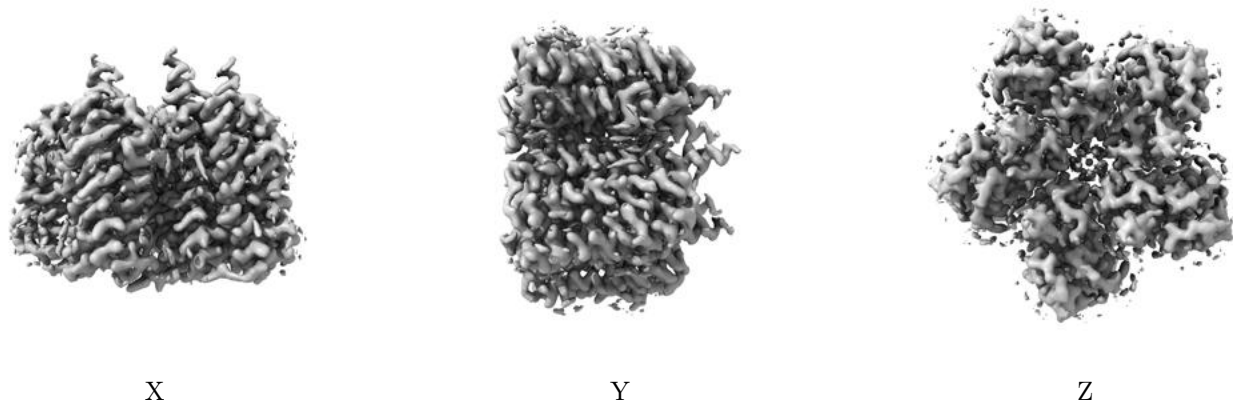
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 Raw map



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

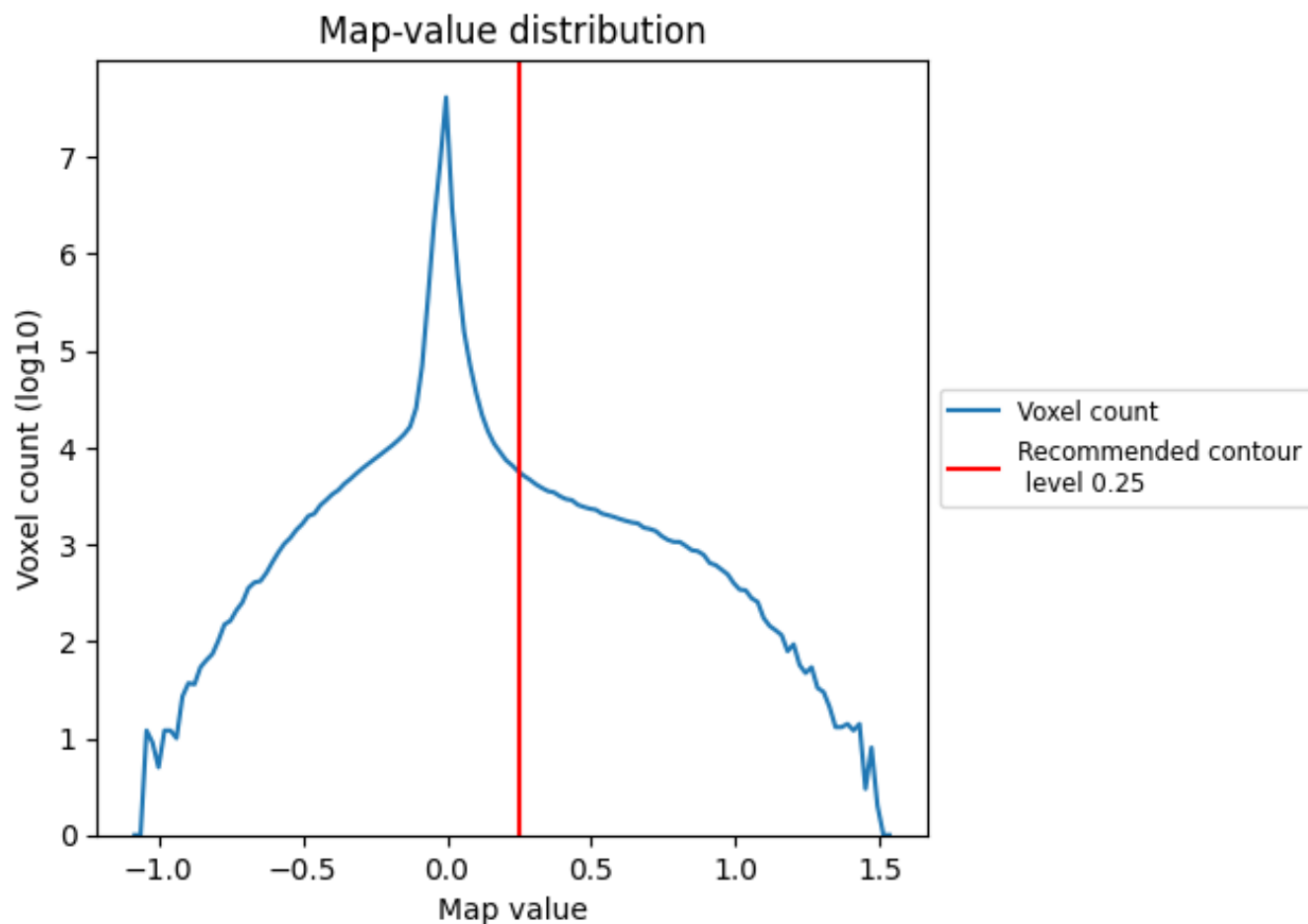
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

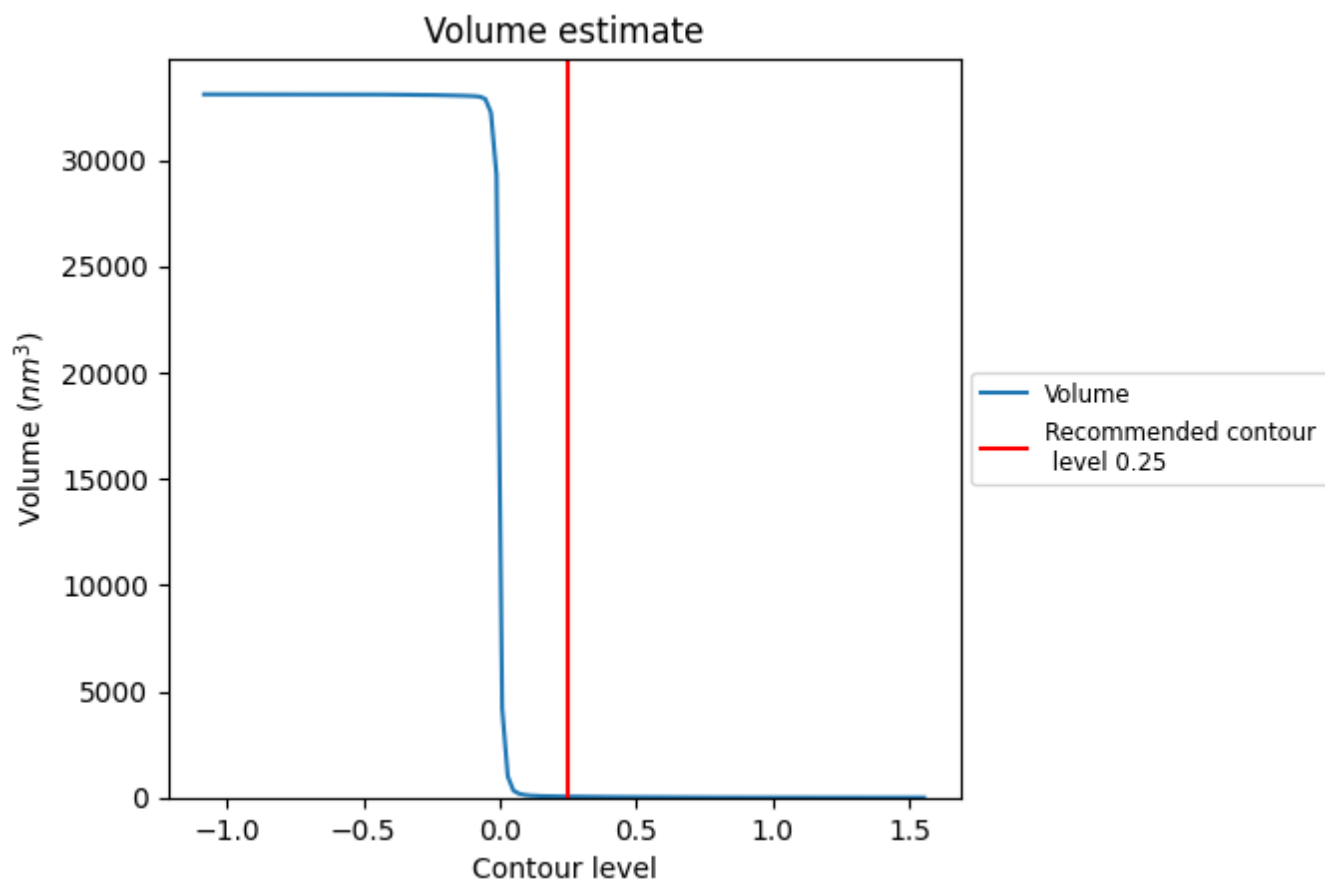
This section contains the results of statistical analysis of the map.

6.1 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.

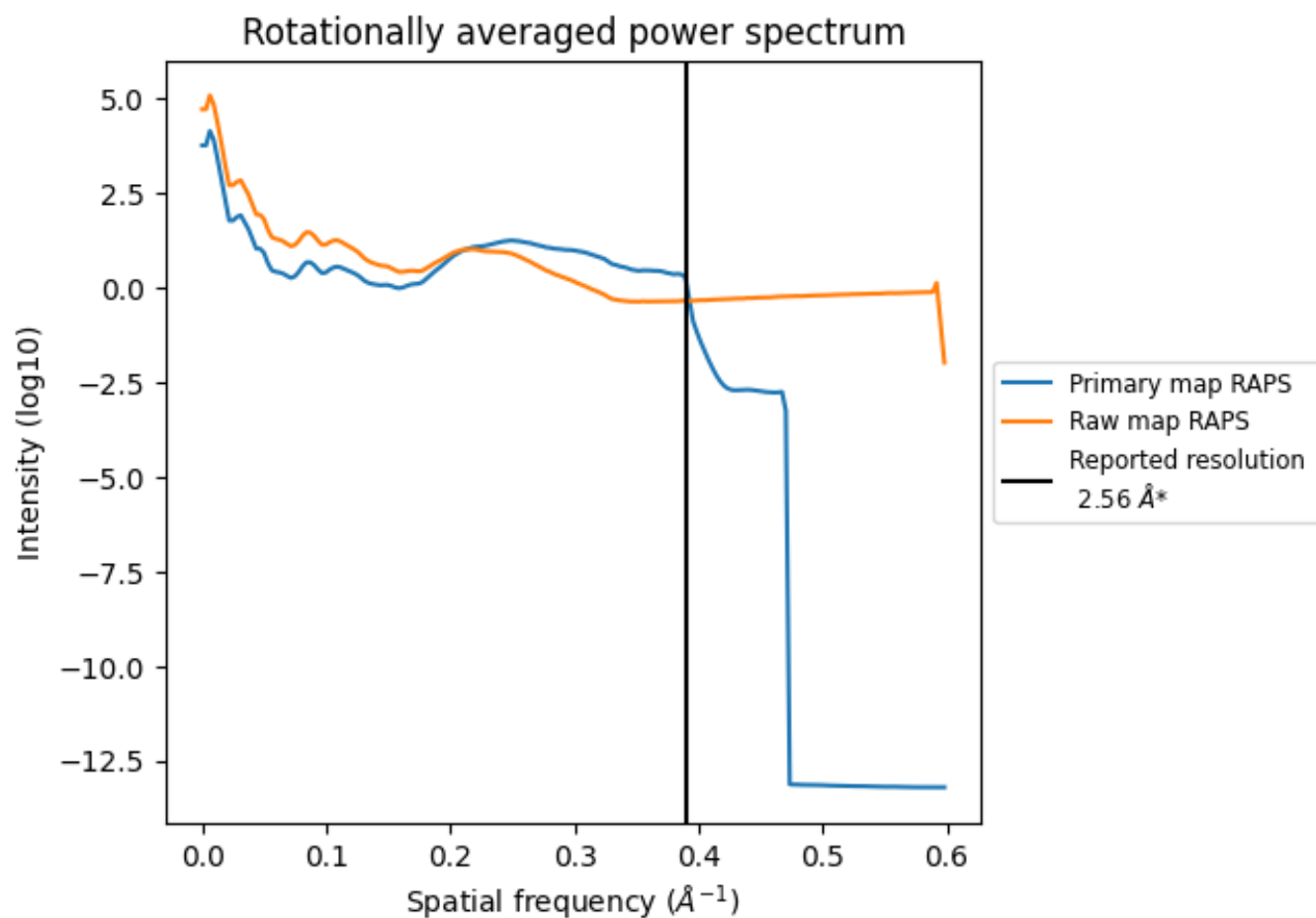
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm³; this corresponds to an approximate mass of 41 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.

6.3 Rotationally averaged power spectrum ⓘ

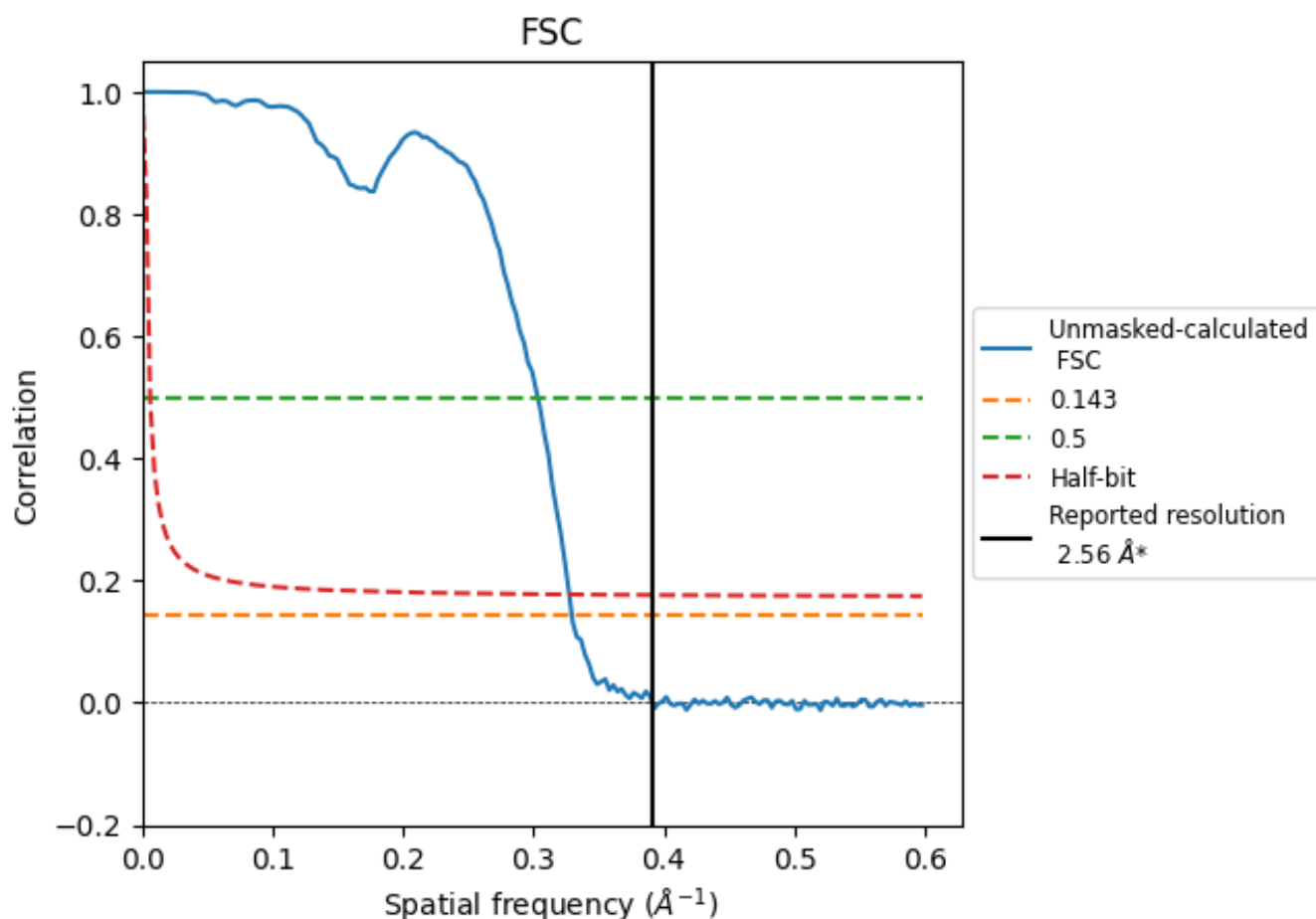


*Reported resolution corresponds to spatial frequency of 0.391 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.391 \AA^{-1}

7.2 Resolution estimates [i](#)

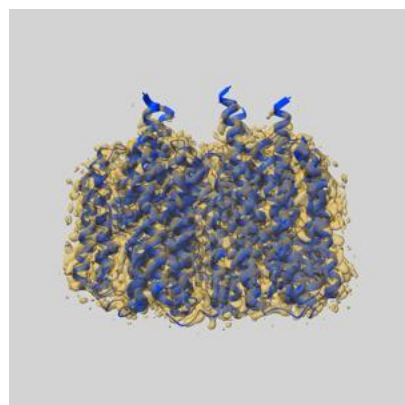
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.03	3.30	3.05

*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 3.03 differs from the reported value 2.56 by more than 10 %

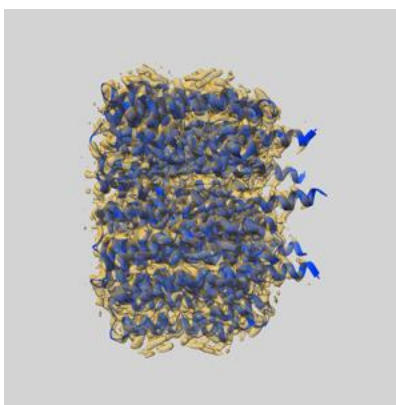
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53519 and PDB model 9R21. Per-residue inclusion information can be found in section ?? on page ??.

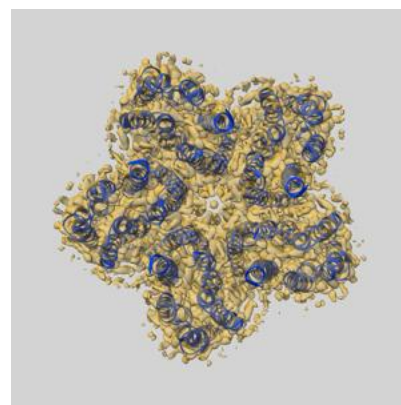
8.1 Map-model overlay [i](#)



X



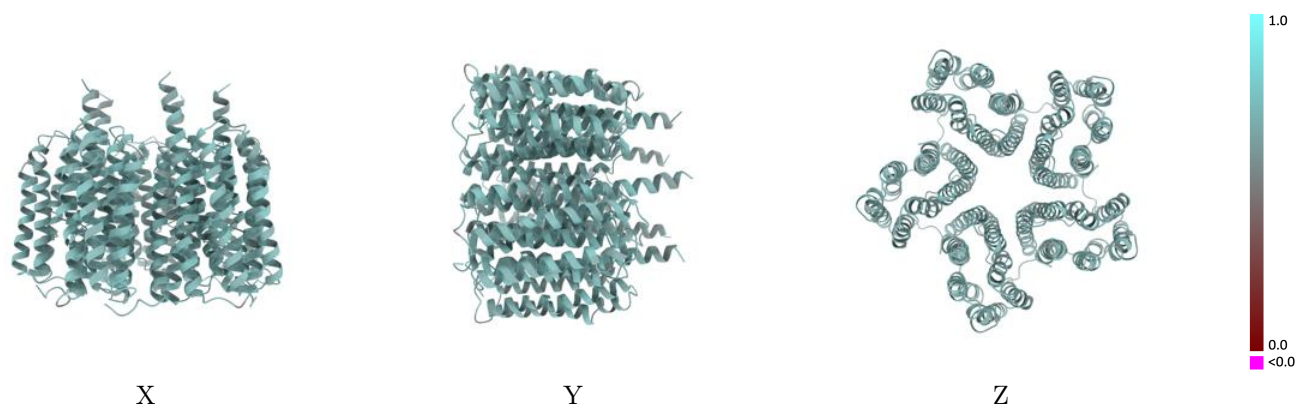
Y



Z

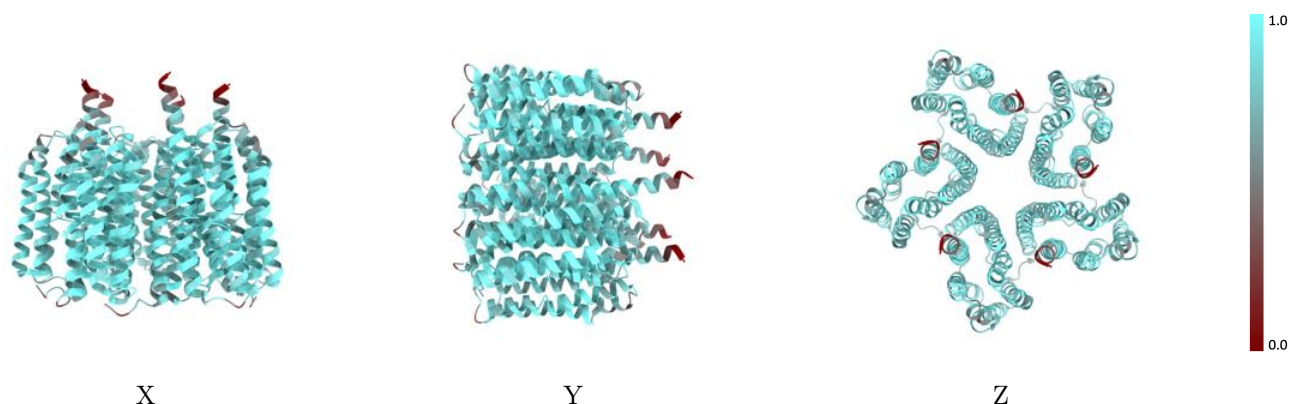
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



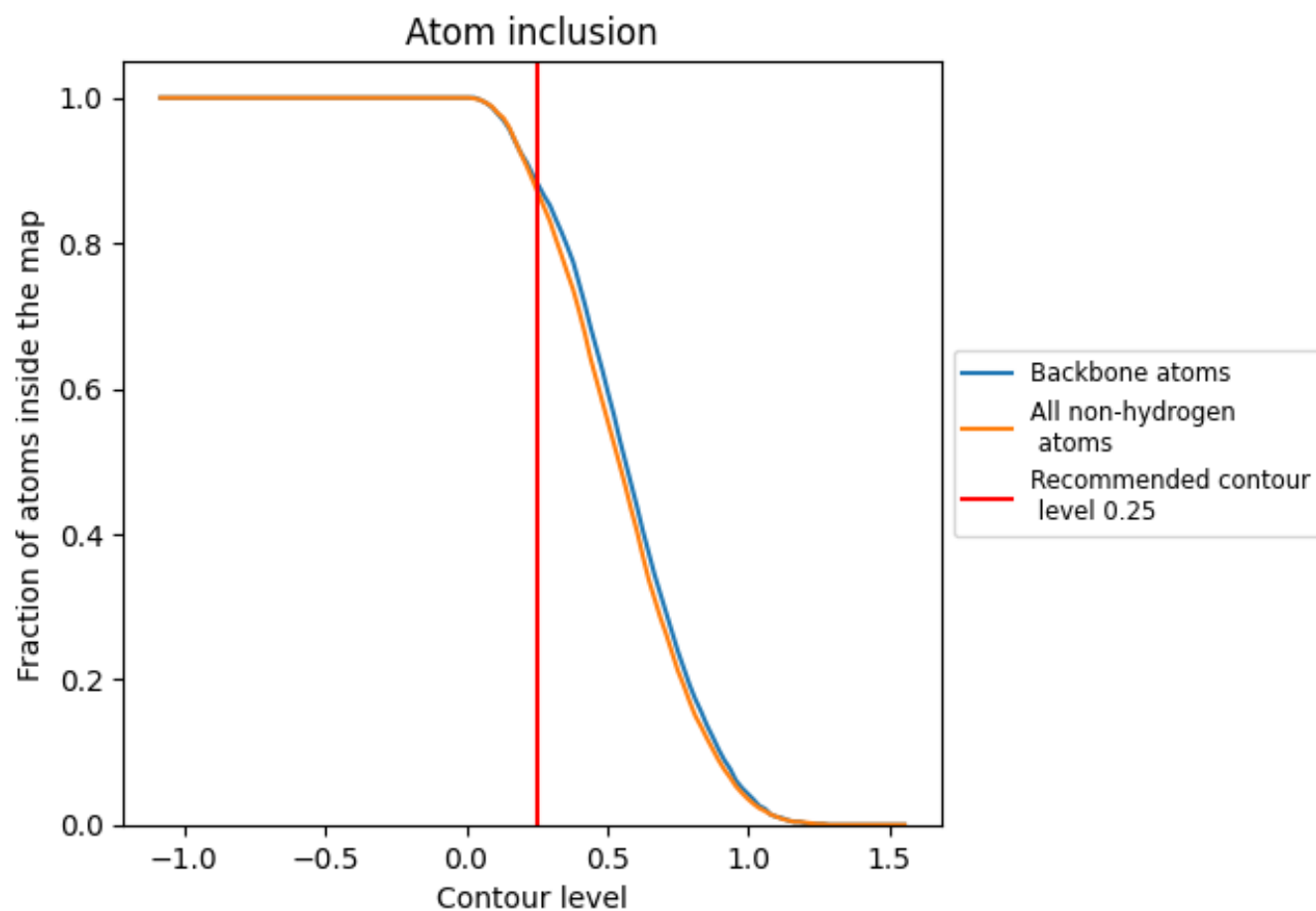
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 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 (0.25).

8.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8730	<div></div> 0.6570
A	<div></div> 0.8770	<div></div> 0.6570
B	<div></div> 0.8770	<div></div> 0.6570
C	<div></div> 0.8700	<div></div> 0.6550
D	<div></div> 0.8770	<div></div> 0.6580
E	<div></div> 0.8690	<div></div> 0.6560

