



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 03:23 PM UTC

PDB ID : 8D1H / pdb_00008d1h
EMDB ID : EMD-27130
Title : hBest2 Ca²⁺-unbound closed state
Authors : Owji, A.P.; Kittredge, A.; Hendrickson, W.A.; Tingting, Y.
Deposited on : 2022-05-27
Resolution : 1.94 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>.

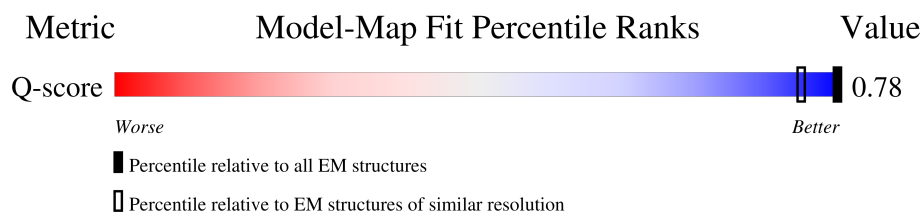
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

i

ELECTRON MICROSCOPY

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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	1283 (1.45 - 2.44)

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

2 Entry composition ⓘ

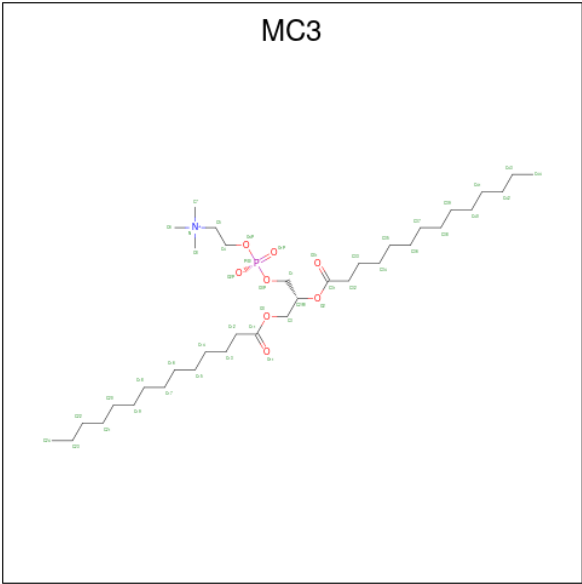
There are 5 unique types of molecules in this entry. The entry contains 17416 atoms, of which 260 are hydrogens and 0 are deuteriums.

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 Bestrophin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	376	Total	C	N	O	S	2	0
			3096	2026	511	542	17		
1	B	376	Total	C	N	O	S	2	0
			3096	2026	511	542	17		
1	A	376	Total	C	N	O	S	2	0
			3096	2026	511	542	17		
1	C	376	Total	C	N	O	S	2	0
			3096	2026	511	542	17		
1	D	376	Total	C	N	O	S	2	0
			3096	2026	511	542	17		

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: MC3) (formula: C₃₆H₇₂NO₈P).



Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	O	P	0
			38	29	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	O	P	0
			37	28	8	1	
2	E	1	Total	C			0
			14	14			
2	E	1	Total	C			0
			14	14			
2	E	1	Total	C			0
			11	11			
2	E	1	Total	C			0
			9	9			
2	E	1	Total	C			0
			7	7			
2	E	1	Total	C	O	P	0
			33	24	8	1	
2	E	1	Total	C			0
			14	14			
2	B	1	Total	C	O	P	0
			38	29	8	1	
2	B	1	Total	C	O	P	0
			37	28	8	1	
2	B	1	Total	C			0
			14	14			
2	B	1	Total	C			0
			14	14			
2	B	1	Total	C			0
			11	11			
2	B	1	Total	C			0
			9	9			
2	B	1	Total	C			0
			7	7			
2	B	1	Total	C	O	P	0
			33	24	8	1	
2	B	1	Total	C			0
			14	14			
2	A	1	Total	C	O	P	0
			33	24	8	1	
2	A	1	Total	C			0
			14	14			
2	A	1	Total	C	O	P	0
			38	29	8	1	
2	A	1	Total	C	O	P	0
			37	28	8	1	

Continued on next page...

Continued from previous page...

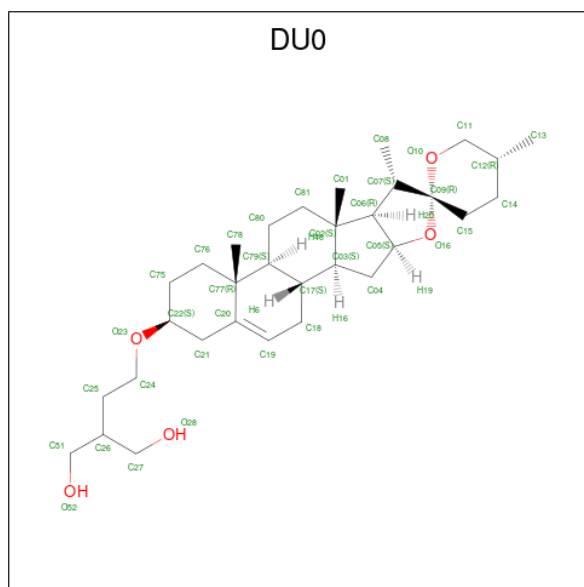
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C			0
			14	14			
2	A	1	Total	C			0
			14	14			
2	A	1	Total	C			0
			11	11			
2	A	1	Total	C			0
			9	9			
2	A	1	Total	C			0
			7	7			
2	C	1	Total	C	O	P	0
			38	29	8	1	
2	C	1	Total	C	O	P	0
			37	28	8	1	
2	C	1	Total	C			0
			14	14			
2	C	1	Total	C			0
			14	14			
2	C	1	Total	C			0
			11	11			
2	C	1	Total	C			0
			9	9			
2	C	1	Total	C			0
			7	7			
2	C	1	Total	C	O	P	0
			33	24	8	1	
2	C	1	Total	C			0
			14	14			
2	D	1	Total	C	O	P	0
			33	24	8	1	
2	D	1	Total	C			0
			14	14			
2	D	1	Total	C	O	P	0
			38	29	8	1	
2	D	1	Total	C	O	P	0
			37	28	8	1	
2	D	1	Total	C			0
			14	14			
2	D	1	Total	C			0
			14	14			
2	D	1	Total	C			0
			11	11			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
2	D	1	Total	C	0
			9	9	
2	D	1	Total	C	0
			7	7	

- Molecule 3 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (CCD ID: DU0) (formula: C₃₂H₅₂O₅).



Mol	Chain	Residues	Atoms				AltConf
3	E	1	Total	C	H	O	0
			89	32	52	5	
3	B	1	Total	C	H	O	0
			89	32	52	5	
3	A	1	Total	C	H	O	0
			89	32	52	5	
3	C	1	Total	C	H	O	0
			89	32	52	5	
3	D	1	Total	C	H	O	0
			89	32	52	5	

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Cl	0
			1	1	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	E	122	Total 122	O 122	0
5	B	120	Total 120	O 120	0
5	A	121	Total 121	O 121	0
5	C	121	Total 121	O 121	0
5	D	121	Total 121	O 121	0

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

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	656860	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	9.774	Depositor
Minimum map value	-5.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.588	Depositor
Recommended contour level	0.6	Depositor
Map size ($\text{\AA}$)	112.87872, 112.87872, 112.87872	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.39194, 0.39194, 0.39194	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

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](#)

Of 51 ligands modelled in this entry, 1 is monoatomic - leaving 50 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	$\# Z > 2$
2	MC3	D	507	-	10,10,45	0.16	0	9,9,53	0.09	0
2	MC3	A	502	-	13,13,45	0.13	0	12,12,53	0.11	0
2	MC3	D	504	-	36,36,45	0.44	0	39,41,53	0.61	1 (2%)
2	MC3	C	609	-	32,32,45	0.46	0	35,37,53	0.59	1 (2%)
2	MC3	B	610	-	13,13,45	0.13	0	12,12,53	0.11	0
2	MC3	B	607	-	6,6,45	0.12	0	5,5,53	0.11	0
2	MC3	B	604	-	13,13,45	0.27	0	12,12,53	0.87	0
2	MC3	A	505	-	13,13,45	0.26	0	12,12,53	0.87	0
2	MC3	B	606	-	8,8,45	0.13	0	7,7,53	0.13	0
2	MC3	D	502	-	13,13,45	0.13	0	12,12,53	0.11	0
2	MC3	D	506	-	13,13,45	0.27	0	12,12,53	0.87	0
2	MC3	C	606	-	8,8,45	0.13	0	7,7,53	0.13	0
2	MC3	A	507	-	10,10,45	0.17	0	9,9,53	0.09	0
2	MC3	C	607	-	6,6,45	0.12	0	5,5,53	0.12	0
2	MC3	C	603	-	13,13,45	0.26	0	12,12,53	0.87	0
2	MC3	D	505	-	13,13,45	0.26	0	12,12,53	0.86	0
2	MC3	D	503	-	37,37,45	0.43	0	40,42,53	0.60	1 (2%)
2	MC3	D	508	-	8,8,45	0.13	0	7,7,53	0.13	0
2	MC3	B	603	-	13,13,45	0.26	0	12,12,53	0.86	0
2	MC3	D	509	-	6,6,45	0.12	0	5,5,53	0.12	0
2	MC3	C	605	-	10,10,45	0.17	0	9,9,53	0.09	0
2	MC3	E	606	-	8,8,45	0.13	0	7,7,53	0.13	0
2	MC3	E	601	-	37,37,45	0.42	0	40,42,53	0.59	1 (2%)
2	MC3	C	604	-	13,13,45	0.27	0	12,12,53	0.87	0
2	MC3	A	501	-	32,32,45	0.45	0	35,37,53	0.59	1 (2%)
2	MC3	B	605	-	10,10,45	0.17	0	9,9,53	0.08	0
2	MC3	E	609	-	32,32,45	0.46	0	35,37,53	0.59	1 (2%)
2	MC3	A	506	-	13,13,45	0.27	0	12,12,53	0.87	0
2	MC3	C	610	-	13,13,45	0.13	0	12,12,53	0.11	0
2	MC3	A	503	-	37,37,45	0.43	0	40,42,53	0.59	1 (2%)
2	MC3	B	601	-	37,37,45	0.43	0	40,42,53	0.59	1 (2%)
3	DU0	C	608	-	42,42,42	0.70	0	64,66,66	0.94	4 (6%)
2	MC3	A	508	-	8,8,45	0.13	0	7,7,53	0.13	0
2	MC3	E	605	-	10,10,45	0.17	0	9,9,53	0.09	0
2	MC3	E	604	-	13,13,45	0.27	0	12,12,53	0.87	0
2	MC3	E	610	-	13,13,45	0.13	0	12,12,53	0.11	0
2	MC3	B	602	-	36,36,45	0.44	0	39,41,53	0.61	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	D	501	-	32,32,45	0.46	0	35,37,53	0.59	1 (2%)
3	DU0	A	510	-	42,42,42	0.69	0	64,66,66	0.94	4 (6%)
3	DU0	D	510	-	42,42,42	0.70	0	64,66,66	0.95	4 (6%)
2	MC3	A	509	-	6,6,45	0.12	0	5,5,53	0.12	0
2	MC3	A	504	-	36,36,45	0.44	0	39,41,53	0.61	1 (2%)
3	DU0	B	608	-	42,42,42	0.70	0	64,66,66	0.94	4 (6%)
2	MC3	C	602	-	36,36,45	0.44	0	39,41,53	0.61	1 (2%)
2	MC3	E	607	-	6,6,45	0.12	0	5,5,53	0.12	0
2	MC3	E	603	-	13,13,45	0.26	0	12,12,53	0.87	0
2	MC3	B	609	-	32,32,45	0.46	0	35,37,53	0.59	1 (2%)
2	MC3	E	602	-	36,36,45	0.44	0	39,41,53	0.61	1 (2%)
2	MC3	C	601	-	37,37,45	0.43	0	40,42,53	0.59	1 (2%)
3	DU0	E	608	-	42,42,42	0.69	0	64,66,66	0.95	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	D	507	-	-	6/8/8/49	-
2	MC3	A	502	-	-	8/11/11/49	-
2	MC3	D	504	-	-	17/38/38/49	-
2	MC3	C	609	-	-	24/34/34/49	-
2	MC3	B	610	-	-	8/11/11/49	-
2	MC3	B	607	-	-	3/4/4/49	-
2	MC3	B	604	-	-	8/11/11/49	-
2	MC3	A	505	-	-	7/11/11/49	-
2	MC3	B	606	-	-	5/6/6/49	-
2	MC3	D	502	-	-	8/11/11/49	-
2	MC3	D	506	-	-	8/11/11/49	-
2	MC3	C	606	-	-	5/6/6/49	-
2	MC3	A	507	-	-	6/8/8/49	-
2	MC3	C	607	-	-	3/4/4/49	-
2	MC3	C	603	-	-	7/11/11/49	-
2	MC3	D	505	-	-	7/11/11/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	D	503	-	-	19/39/39/49	-
2	MC3	D	508	-	-	5/6/6/49	-
2	MC3	B	603	-	-	7/11/11/49	-
2	MC3	D	509	-	-	3/4/4/49	-
2	MC3	C	605	-	-	6/8/8/49	-
2	MC3	E	606	-	-	5/6/6/49	-
2	MC3	E	601	-	-	19/39/39/49	-
2	MC3	C	604	-	-	8/11/11/49	-
2	MC3	A	501	-	-	24/34/34/49	-
2	MC3	B	605	-	-	6/8/8/49	-
2	MC3	E	609	-	-	24/34/34/49	-
2	MC3	A	506	-	-	8/11/11/49	-
2	MC3	C	610	-	-	8/11/11/49	-
2	MC3	A	503	-	-	19/39/39/49	-
2	MC3	B	601	-	-	19/39/39/49	-
3	DU0	C	608	-	-	3/10/98/98	0/6/6/6
2	MC3	A	508	-	-	5/6/6/49	-
2	MC3	E	605	-	-	6/8/8/49	-
2	MC3	E	604	-	-	8/11/11/49	-
2	MC3	E	610	-	-	8/11/11/49	-
2	MC3	B	602	-	-	17/38/38/49	-
2	MC3	D	501	-	-	24/34/34/49	-
3	DU0	A	510	-	-	3/10/98/98	0/6/6/6
3	DU0	D	510	-	-	3/10/98/98	0/6/6/6
2	MC3	A	509	-	-	3/4/4/49	-
2	MC3	A	504	-	-	17/38/38/49	-
3	DU0	B	608	-	-	3/10/98/98	0/6/6/6
2	MC3	C	602	-	-	17/38/38/49	-
2	MC3	E	607	-	-	3/4/4/49	-
2	MC3	E	603	-	-	7/11/11/49	-
2	MC3	B	609	-	-	24/34/34/49	-
2	MC3	E	602	-	-	17/38/38/49	-
2	MC3	C	601	-	-	19/39/39/49	-
3	DU0	E	608	-	-	3/10/98/98	0/6/6/6

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	608	DU0	O10-C09-C15	2.69	113.11	110.76
3	B	608	DU0	O10-C09-C15	2.65	113.07	110.76
3	E	608	DU0	O10-C09-C15	2.65	113.07	110.76
3	A	510	DU0	O10-C09-C15	2.64	113.06	110.76
3	D	510	DU0	O10-C09-C15	2.63	113.05	110.76
3	D	510	DU0	C14-C12-C11	2.59	111.74	108.59
3	E	608	DU0	C14-C12-C11	2.59	111.73	108.59
3	A	510	DU0	C14-C12-C11	2.58	111.72	108.59
3	B	608	DU0	C14-C12-C11	2.58	111.72	108.59
3	C	608	DU0	C14-C12-C11	2.55	111.68	108.59
3	A	510	DU0	O16-C09-C07	2.54	107.93	104.56
3	B	608	DU0	O16-C09-C07	2.52	107.90	104.56
3	D	510	DU0	O16-C09-C07	2.52	107.90	104.56
3	E	608	DU0	O16-C09-C07	2.51	107.90	104.56
3	C	608	DU0	O16-C09-C07	2.51	107.89	104.56
2	D	504	MC3	O2P-P-O1P	2.39	120.15	110.83
2	A	504	MC3	O2P-P-O1P	2.39	120.14	110.83
2	E	602	MC3	O2P-P-O1P	2.38	120.12	110.83
2	C	602	MC3	O2P-P-O1P	2.37	120.08	110.83
2	B	602	MC3	O2P-P-O1P	2.37	120.08	110.83
2	D	503	MC3	O2P-P-O1P	2.32	119.88	110.83
2	C	601	MC3	O2P-P-O1P	2.32	119.88	110.83
2	B	601	MC3	O2P-P-O1P	2.32	119.86	110.83
2	E	601	MC3	O2P-P-O1P	2.31	119.85	110.83
2	A	503	MC3	O2P-P-O1P	2.31	119.85	110.83
2	E	609	MC3	O2P-P-O1P	2.24	119.58	110.83
2	A	501	MC3	O2P-P-O1P	2.24	119.57	110.83
2	D	501	MC3	O2P-P-O1P	2.24	119.57	110.83
2	B	609	MC3	O2P-P-O1P	2.24	119.56	110.83
2	C	609	MC3	O2P-P-O1P	2.24	119.55	110.83
3	C	608	DU0	O10-C09-O16	-2.19	104.67	109.88
3	A	510	DU0	O10-C09-O16	-2.18	104.70	109.88
3	E	608	DU0	O10-C09-O16	-2.17	104.72	109.88
3	B	608	DU0	O10-C09-O16	-2.16	104.74	109.88
3	D	510	DU0	O10-C09-O16	-2.15	104.75	109.88

There are no chirality outliers.

All (500) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	601	MC3	O2-C2-C3-O3
2	E	601	MC3	C1-O3P-P-O2P
2	E	601	MC3	C1-O3P-P-O4P
2	E	609	MC3	O3P-C1-C2-O2
2	E	609	MC3	C32-C31-O2-C2
2	E	609	MC3	C1-O3P-P-O1P
2	E	609	MC3	C1-O3P-P-O2P
2	E	609	MC3	C1-O3P-P-O4P
2	B	601	MC3	O2-C2-C3-O3
2	B	601	MC3	C1-O3P-P-O2P
2	B	601	MC3	C1-O3P-P-O4P
2	B	609	MC3	O3P-C1-C2-O2
2	B	609	MC3	C32-C31-O2-C2
2	B	609	MC3	C1-O3P-P-O1P
2	B	609	MC3	C1-O3P-P-O2P
2	B	609	MC3	C1-O3P-P-O4P
2	A	501	MC3	O3P-C1-C2-O2
2	A	501	MC3	C32-C31-O2-C2
2	A	501	MC3	C1-O3P-P-O1P
2	A	501	MC3	C1-O3P-P-O2P
2	A	501	MC3	C1-O3P-P-O4P
2	A	503	MC3	O2-C2-C3-O3
2	A	503	MC3	C1-O3P-P-O2P
2	A	503	MC3	C1-O3P-P-O4P
2	C	601	MC3	O2-C2-C3-O3
2	C	601	MC3	C1-O3P-P-O2P
2	C	601	MC3	C1-O3P-P-O4P
2	C	609	MC3	O3P-C1-C2-O2
2	C	609	MC3	C32-C31-O2-C2
2	C	609	MC3	C1-O3P-P-O1P
2	C	609	MC3	C1-O3P-P-O2P
2	C	609	MC3	C1-O3P-P-O4P
2	D	501	MC3	O3P-C1-C2-O2
2	D	501	MC3	C32-C31-O2-C2
2	D	501	MC3	C1-O3P-P-O1P
2	D	501	MC3	C1-O3P-P-O2P
2	D	501	MC3	C1-O3P-P-O4P
2	D	503	MC3	O2-C2-C3-O3
2	D	503	MC3	C1-O3P-P-O2P
2	D	503	MC3	C1-O3P-P-O4P
2	E	609	MC3	O31-C31-O2-C2
2	B	609	MC3	O31-C31-O2-C2
2	A	501	MC3	O31-C31-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	609	MC3	O31-C31-O2-C2
2	D	501	MC3	O31-C31-O2-C2
2	E	609	MC3	C14-C15-C16-C17
2	B	609	MC3	C14-C15-C16-C17
2	A	501	MC3	C14-C15-C16-C17
2	C	609	MC3	C14-C15-C16-C17
2	D	501	MC3	C14-C15-C16-C17
2	E	602	MC3	C12-C11-O3-C3
2	B	602	MC3	C12-C11-O3-C3
2	A	504	MC3	C12-C11-O3-C3
2	C	602	MC3	C12-C11-O3-C3
2	D	504	MC3	C12-C11-O3-C3
3	E	608	DU0	O23-C24-C25-C26
3	B	608	DU0	O23-C24-C25-C26
3	A	510	DU0	O23-C24-C25-C26
3	C	608	DU0	O23-C24-C25-C26
3	D	510	DU0	O23-C24-C25-C26
2	E	601	MC3	C33-C34-C35-C36
2	B	601	MC3	C33-C34-C35-C36
2	A	503	MC3	C33-C34-C35-C36
2	C	601	MC3	C33-C34-C35-C36
2	D	503	MC3	C33-C34-C35-C36
2	E	601	MC3	C20-C21-C22-C23
2	B	601	MC3	C20-C21-C22-C23
2	A	503	MC3	C20-C21-C22-C23
2	C	601	MC3	C20-C21-C22-C23
2	D	503	MC3	C20-C21-C22-C23
2	E	605	MC3	C37-C38-C39-C40
2	B	605	MC3	C37-C38-C39-C40
2	A	507	MC3	C37-C38-C39-C40
2	C	605	MC3	C37-C38-C39-C40
2	D	507	MC3	C37-C38-C39-C40
2	B	603	MC3	C32-C33-C34-C35
2	A	505	MC3	C32-C33-C34-C35
2	C	603	MC3	C32-C33-C34-C35
2	E	603	MC3	C32-C33-C34-C35
2	D	505	MC3	C32-C33-C34-C35
2	E	604	MC3	C37-C38-C39-C40
2	B	604	MC3	C37-C38-C39-C40
2	A	506	MC3	C37-C38-C39-C40
2	C	604	MC3	C37-C38-C39-C40
2	D	506	MC3	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	602	MC3	O11-C11-O3-C3
2	B	602	MC3	O11-C11-O3-C3
2	A	504	MC3	O11-C11-O3-C3
2	C	602	MC3	O11-C11-O3-C3
2	D	504	MC3	O11-C11-O3-C3
2	E	602	MC3	C11-C12-C13-C14
2	B	602	MC3	C11-C12-C13-C14
2	A	504	MC3	C11-C12-C13-C14
2	C	602	MC3	C11-C12-C13-C14
2	D	504	MC3	C11-C12-C13-C14
2	E	601	MC3	C12-C13-C14-C15
2	B	601	MC3	C12-C13-C14-C15
2	A	503	MC3	C12-C13-C14-C15
2	C	601	MC3	C12-C13-C14-C15
2	D	503	MC3	C12-C13-C14-C15
2	E	602	MC3	C34-C35-C36-C37
2	E	603	MC3	C37-C38-C39-C40
2	E	606	MC3	C32-C33-C34-C35
2	B	602	MC3	C17-C18-C19-C20
2	B	602	MC3	C34-C35-C36-C37
2	B	603	MC3	C37-C38-C39-C40
2	B	606	MC3	C32-C33-C34-C35
2	A	504	MC3	C34-C35-C36-C37
2	A	505	MC3	C37-C38-C39-C40
2	A	508	MC3	C32-C33-C34-C35
2	C	602	MC3	C34-C35-C36-C37
2	C	603	MC3	C37-C38-C39-C40
2	C	606	MC3	C32-C33-C34-C35
2	D	504	MC3	C34-C35-C36-C37
2	D	505	MC3	C37-C38-C39-C40
2	D	508	MC3	C32-C33-C34-C35
2	E	602	MC3	C17-C18-C19-C20
2	A	504	MC3	C17-C18-C19-C20
2	C	602	MC3	C17-C18-C19-C20
2	D	504	MC3	C17-C18-C19-C20
2	E	603	MC3	C36-C37-C38-C39
2	B	603	MC3	C36-C37-C38-C39
2	C	603	MC3	C36-C37-C38-C39
2	D	505	MC3	C36-C37-C38-C39
2	E	602	MC3	C32-C33-C34-C35
2	E	610	MC3	C33-C34-C35-C36
2	B	602	MC3	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	603	MC3	C34-C35-C36-C37
2	B	610	MC3	C33-C34-C35-C36
2	A	502	MC3	C33-C34-C35-C36
2	A	504	MC3	C32-C33-C34-C35
2	A	505	MC3	C34-C35-C36-C37
2	A	505	MC3	C36-C37-C38-C39
2	C	602	MC3	C32-C33-C34-C35
2	C	610	MC3	C33-C34-C35-C36
2	D	502	MC3	C33-C34-C35-C36
2	D	504	MC3	C32-C33-C34-C35
2	E	603	MC3	C34-C35-C36-C37
2	C	603	MC3	C34-C35-C36-C37
2	D	505	MC3	C34-C35-C36-C37
2	E	609	MC3	C16-C17-C18-C19
2	B	609	MC3	C16-C17-C18-C19
2	A	501	MC3	C16-C17-C18-C19
2	C	609	MC3	C16-C17-C18-C19
2	D	501	MC3	C16-C17-C18-C19
2	E	604	MC3	C36-C37-C38-C39
2	B	604	MC3	C36-C37-C38-C39
2	A	506	MC3	C36-C37-C38-C39
2	D	501	MC3	C13-C14-C15-C16
2	E	606	MC3	C35-C36-C37-C38
2	E	609	MC3	C12-C13-C14-C15
2	E	609	MC3	C13-C14-C15-C16
2	B	606	MC3	C35-C36-C37-C38
2	B	609	MC3	C12-C13-C14-C15
2	B	609	MC3	C13-C14-C15-C16
2	A	501	MC3	C12-C13-C14-C15
2	A	501	MC3	C13-C14-C15-C16
2	A	508	MC3	C35-C36-C37-C38
2	C	604	MC3	C36-C37-C38-C39
2	C	606	MC3	C35-C36-C37-C38
2	C	609	MC3	C12-C13-C14-C15
2	C	609	MC3	C13-C14-C15-C16
2	D	501	MC3	C12-C13-C14-C15
2	D	506	MC3	C36-C37-C38-C39
2	D	508	MC3	C35-C36-C37-C38
2	E	609	MC3	C35-C36-C37-C38
2	B	609	MC3	C35-C36-C37-C38
2	A	501	MC3	C35-C36-C37-C38
2	C	609	MC3	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	501	MC3	C35-C36-C37-C38
2	D	504	MC3	C15-C16-C17-C18
2	E	602	MC3	C15-C16-C17-C18
2	B	602	MC3	C15-C16-C17-C18
2	A	504	MC3	C15-C16-C17-C18
2	C	602	MC3	C15-C16-C17-C18
2	E	604	MC3	C34-C35-C36-C37
2	A	506	MC3	C34-C35-C36-C37
2	D	506	MC3	C34-C35-C36-C37
2	B	604	MC3	C34-C35-C36-C37
2	C	604	MC3	C34-C35-C36-C37
2	E	601	MC3	C14-C15-C16-C17
2	B	601	MC3	C14-C15-C16-C17
2	A	503	MC3	C32-C33-C34-C35
2	C	601	MC3	C14-C15-C16-C17
2	C	601	MC3	C32-C33-C34-C35
2	D	503	MC3	C14-C15-C16-C17
2	E	601	MC3	C16-C17-C18-C19
2	E	601	MC3	C32-C33-C34-C35
2	B	601	MC3	C16-C17-C18-C19
2	B	601	MC3	C32-C33-C34-C35
2	A	503	MC3	C14-C15-C16-C17
2	A	503	MC3	C16-C17-C18-C19
2	C	601	MC3	C16-C17-C18-C19
2	D	503	MC3	C16-C17-C18-C19
2	D	503	MC3	C32-C33-C34-C35
2	E	610	MC3	C37-C38-C39-C40
2	B	610	MC3	C37-C38-C39-C40
2	A	502	MC3	C37-C38-C39-C40
2	C	610	MC3	C37-C38-C39-C40
2	D	502	MC3	C37-C38-C39-C40
2	A	502	MC3	C38-C39-C40-C41
2	D	502	MC3	C38-C39-C40-C41
2	E	610	MC3	C38-C39-C40-C41
2	B	610	MC3	C38-C39-C40-C41
2	A	501	MC3	C34-C35-C36-C37
2	C	610	MC3	C38-C39-C40-C41
2	E	609	MC3	C34-C35-C36-C37
2	B	609	MC3	C34-C35-C36-C37
2	C	609	MC3	C34-C35-C36-C37
2	D	501	MC3	C34-C35-C36-C37
2	A	503	MC3	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	601	MC3	C15-C16-C17-C18
2	E	601	MC3	C15-C16-C17-C18
2	B	601	MC3	C15-C16-C17-C18
2	D	503	MC3	C15-C16-C17-C18
2	A	501	MC3	C33-C34-C35-C36
2	E	609	MC3	C33-C34-C35-C36
2	B	609	MC3	C33-C34-C35-C36
2	C	609	MC3	C33-C34-C35-C36
2	D	501	MC3	C33-C34-C35-C36
2	C	605	MC3	C40-C41-C42-C43
2	D	507	MC3	C40-C41-C42-C43
2	E	602	MC3	C33-C34-C35-C36
2	E	605	MC3	C40-C41-C42-C43
2	B	602	MC3	C33-C34-C35-C36
2	B	605	MC3	C40-C41-C42-C43
2	A	504	MC3	C33-C34-C35-C36
2	A	507	MC3	C40-C41-C42-C43
2	C	602	MC3	C33-C34-C35-C36
2	D	504	MC3	C33-C34-C35-C36
2	D	501	MC3	C32-C33-C34-C35
2	E	609	MC3	C32-C33-C34-C35
2	B	609	MC3	C32-C33-C34-C35
2	A	501	MC3	C32-C33-C34-C35
2	C	609	MC3	C32-C33-C34-C35
2	C	609	MC3	C18-C19-C20-C21
2	E	609	MC3	C18-C19-C20-C21
2	B	609	MC3	C18-C19-C20-C21
2	A	501	MC3	C18-C19-C20-C21
2	D	501	MC3	C18-C19-C20-C21
2	E	610	MC3	C32-C33-C34-C35
2	A	502	MC3	C32-C33-C34-C35
2	B	610	MC3	C32-C33-C34-C35
2	C	610	MC3	C32-C33-C34-C35
2	D	502	MC3	C32-C33-C34-C35
2	E	609	MC3	C17-C18-C19-C20
2	C	609	MC3	C17-C18-C19-C20
2	D	501	MC3	C17-C18-C19-C20
2	D	506	MC3	C38-C39-C40-C41
2	E	604	MC3	C38-C39-C40-C41
2	B	604	MC3	C38-C39-C40-C41
2	B	609	MC3	C17-C18-C19-C20
2	A	501	MC3	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	506	MC3	C38-C39-C40-C41
2	C	604	MC3	C38-C39-C40-C41
2	E	609	MC3	C37-C38-C39-C40
2	E	610	MC3	C31-C32-C33-C34
2	A	501	MC3	C37-C38-C39-C40
2	A	502	MC3	C31-C32-C33-C34
2	C	609	MC3	C37-C38-C39-C40
2	D	502	MC3	C31-C32-C33-C34
2	B	609	MC3	C37-C38-C39-C40
2	B	610	MC3	C31-C32-C33-C34
2	C	610	MC3	C31-C32-C33-C34
2	D	501	MC3	C37-C38-C39-C40
2	E	605	MC3	C41-C42-C43-C44
2	B	605	MC3	C41-C42-C43-C44
2	C	605	MC3	C41-C42-C43-C44
2	D	507	MC3	C41-C42-C43-C44
2	A	507	MC3	C41-C42-C43-C44
2	E	602	MC3	C31-C32-C33-C34
2	B	602	MC3	C31-C32-C33-C34
2	A	504	MC3	C31-C32-C33-C34
2	C	602	MC3	C31-C32-C33-C34
2	D	504	MC3	C31-C32-C33-C34
2	E	609	MC3	C12-C11-O3-C3
2	B	609	MC3	C12-C11-O3-C3
2	A	501	MC3	C12-C11-O3-C3
2	C	609	MC3	C12-C11-O3-C3
2	D	501	MC3	C12-C11-O3-C3
2	E	606	MC3	C31-C32-C33-C34
2	B	606	MC3	C31-C32-C33-C34
2	A	508	MC3	C31-C32-C33-C34
2	C	606	MC3	C31-C32-C33-C34
2	D	508	MC3	C31-C32-C33-C34
2	C	605	MC3	C39-C40-C41-C42
2	E	605	MC3	C39-C40-C41-C42
2	B	605	MC3	C39-C40-C41-C42
2	D	507	MC3	C39-C40-C41-C42
2	E	609	MC3	O3P-C1-C2-C3
2	B	609	MC3	O3P-C1-C2-C3
2	A	501	MC3	O3P-C1-C2-C3
2	C	609	MC3	O3P-C1-C2-C3
2	D	501	MC3	O3P-C1-C2-C3
2	A	507	MC3	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	605	MC3	C35-C36-C37-C38
2	C	605	MC3	C35-C36-C37-C38
2	E	605	MC3	C35-C36-C37-C38
2	A	507	MC3	C35-C36-C37-C38
2	E	603	MC3	C35-C36-C37-C38
2	B	603	MC3	C35-C36-C37-C38
2	C	603	MC3	C35-C36-C37-C38
2	D	505	MC3	C35-C36-C37-C38
2	A	505	MC3	C35-C36-C37-C38
2	D	507	MC3	C35-C36-C37-C38
2	E	601	MC3	C1-C2-C3-O3
2	B	601	MC3	C1-C2-C3-O3
2	C	601	MC3	C1-C2-C3-O3
2	D	503	MC3	C1-C2-C3-O3
2	D	505	MC3	C38-C39-C40-C41
2	E	603	MC3	C38-C39-C40-C41
2	B	603	MC3	C38-C39-C40-C41
2	A	505	MC3	C38-C39-C40-C41
2	C	603	MC3	C38-C39-C40-C41
2	E	609	MC3	O11-C11-O3-C3
2	A	501	MC3	O11-C11-O3-C3
2	C	609	MC3	O11-C11-O3-C3
2	D	501	MC3	O11-C11-O3-C3
2	B	609	MC3	O11-C11-O3-C3
3	E	608	DU0	C75-C22-O23-C24
3	B	608	DU0	C75-C22-O23-C24
3	A	510	DU0	C75-C22-O23-C24
3	C	608	DU0	C75-C22-O23-C24
3	D	510	DU0	C75-C22-O23-C24
2	E	609	MC3	C1-C2-C3-O3
2	B	609	MC3	C1-C2-C3-O3
2	A	501	MC3	C1-C2-C3-O3
2	A	503	MC3	C1-C2-C3-O3
2	C	609	MC3	C1-C2-C3-O3
2	D	501	MC3	C1-C2-C3-O3
2	D	503	MC3	C36-C37-C38-C39
2	E	601	MC3	C36-C37-C38-C39
2	B	601	MC3	C36-C37-C38-C39
2	A	503	MC3	C36-C37-C38-C39
2	C	601	MC3	C36-C37-C38-C39
2	C	602	MC3	C13-C14-C15-C16
2	D	504	MC3	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	602	MC3	C13-C14-C15-C16
2	A	504	MC3	C13-C14-C15-C16
2	B	602	MC3	C13-C14-C15-C16
2	E	610	MC3	C35-C36-C37-C38
2	B	610	MC3	C35-C36-C37-C38
2	A	502	MC3	C35-C36-C37-C38
2	C	606	MC3	C34-C35-C36-C37
2	C	610	MC3	C35-C36-C37-C38
2	D	502	MC3	C35-C36-C37-C38
2	A	508	MC3	C34-C35-C36-C37
2	E	606	MC3	C34-C35-C36-C37
2	D	508	MC3	C34-C35-C36-C37
2	B	606	MC3	C34-C35-C36-C37
2	E	602	MC3	C38-C39-C40-C41
2	B	602	MC3	C38-C39-C40-C41
2	A	504	MC3	C38-C39-C40-C41
2	D	504	MC3	C38-C39-C40-C41
2	C	602	MC3	C38-C39-C40-C41
2	B	601	MC3	C31-C32-C33-C34
2	E	601	MC3	C31-C32-C33-C34
2	A	503	MC3	C31-C32-C33-C34
2	C	601	MC3	C31-C32-C33-C34
2	D	503	MC3	C31-C32-C33-C34
2	E	604	MC3	C40-C41-C42-C43
2	B	604	MC3	C40-C41-C42-C43
2	A	506	MC3	C40-C41-C42-C43
2	C	604	MC3	C40-C41-C42-C43
2	D	506	MC3	C40-C41-C42-C43
2	E	610	MC3	C36-C37-C38-C39
2	B	610	MC3	C36-C37-C38-C39
2	C	610	MC3	C36-C37-C38-C39
2	D	502	MC3	C36-C37-C38-C39
2	A	502	MC3	C36-C37-C38-C39
2	E	609	MC3	O2-C2-C3-O3
2	B	609	MC3	O2-C2-C3-O3
2	A	501	MC3	O2-C2-C3-O3
2	C	609	MC3	O2-C2-C3-O3
2	D	501	MC3	O2-C2-C3-O3
2	A	509	MC3	C40-C41-C42-C43
2	C	607	MC3	C40-C41-C42-C43
2	D	509	MC3	C40-C41-C42-C43
2	E	607	MC3	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	607	MC3	C40-C41-C42-C43
2	E	601	MC3	C32-C31-O2-C2
2	B	601	MC3	C32-C31-O2-C2
2	A	503	MC3	C32-C31-O2-C2
2	C	601	MC3	C32-C31-O2-C2
2	D	503	MC3	C32-C31-O2-C2
2	B	607	MC3	C37-C38-C39-C40
2	A	509	MC3	C37-C38-C39-C40
2	C	607	MC3	C37-C38-C39-C40
2	D	509	MC3	C37-C38-C39-C40
2	E	607	MC3	C37-C38-C39-C40
2	E	607	MC3	C38-C39-C40-C41
2	B	607	MC3	C38-C39-C40-C41
2	D	509	MC3	C38-C39-C40-C41
2	A	509	MC3	C38-C39-C40-C41
2	C	607	MC3	C38-C39-C40-C41
2	A	504	MC3	C16-C17-C18-C19
2	C	602	MC3	C16-C17-C18-C19
2	B	602	MC3	C16-C17-C18-C19
2	D	504	MC3	C16-C17-C18-C19
2	E	602	MC3	C16-C17-C18-C19
2	E	601	MC3	O31-C31-O2-C2
2	C	601	MC3	O31-C31-O2-C2
2	D	503	MC3	O31-C31-O2-C2
2	B	601	MC3	O31-C31-O2-C2
2	A	503	MC3	O31-C31-O2-C2
2	A	503	MC3	C21-C22-C23-C24
2	E	601	MC3	C21-C22-C23-C24
2	B	601	MC3	C21-C22-C23-C24
2	C	601	MC3	C21-C22-C23-C24
2	D	503	MC3	C21-C22-C23-C24
2	D	504	MC3	C37-C38-C39-C40
2	A	504	MC3	C37-C38-C39-C40
2	E	602	MC3	C37-C38-C39-C40
2	B	602	MC3	C37-C38-C39-C40
2	C	602	MC3	C37-C38-C39-C40
2	E	602	MC3	C2-C1-O3P-P
2	B	602	MC3	C2-C1-O3P-P
2	A	504	MC3	C2-C1-O3P-P
2	C	602	MC3	C2-C1-O3P-P
2	D	504	MC3	C2-C1-O3P-P
2	E	605	MC3	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	507	MC3	C36-C37-C38-C39
2	C	605	MC3	C36-C37-C38-C39
2	D	507	MC3	C36-C37-C38-C39
2	B	605	MC3	C36-C37-C38-C39
2	E	601	MC3	C2-C1-O3P-P
2	B	601	MC3	C2-C1-O3P-P
2	A	503	MC3	C2-C1-O3P-P
2	C	601	MC3	C2-C1-O3P-P
2	D	503	MC3	C2-C1-O3P-P
2	E	610	MC3	C40-C41-C42-C43
2	B	610	MC3	C40-C41-C42-C43
2	D	502	MC3	C40-C41-C42-C43
2	A	502	MC3	C40-C41-C42-C43
2	C	610	MC3	C40-C41-C42-C43
2	E	603	MC3	C40-C41-C42-C43
2	B	603	MC3	C40-C41-C42-C43
2	C	603	MC3	C40-C41-C42-C43
2	D	505	MC3	C40-C41-C42-C43
2	A	505	MC3	C40-C41-C42-C43
3	E	608	DU0	C21-C22-O23-C24
3	B	608	DU0	C21-C22-O23-C24
3	A	510	DU0	C21-C22-O23-C24
3	C	608	DU0	C21-C22-O23-C24
3	D	510	DU0	C21-C22-O23-C24
2	E	602	MC3	O2-C31-C32-C33
2	A	504	MC3	O2-C31-C32-C33
2	D	504	MC3	O2-C31-C32-C33
2	B	602	MC3	O2-C31-C32-C33
2	C	602	MC3	O2-C31-C32-C33
2	B	604	MC3	C32-C33-C34-C35
2	C	604	MC3	C32-C33-C34-C35
2	D	506	MC3	C32-C33-C34-C35
2	E	604	MC3	C32-C33-C34-C35
2	A	506	MC3	C32-C33-C34-C35
2	E	609	MC3	C15-C16-C17-C18
2	A	501	MC3	C15-C16-C17-C18
2	C	609	MC3	C15-C16-C17-C18
2	D	501	MC3	C15-C16-C17-C18
2	B	609	MC3	C15-C16-C17-C18
2	C	609	MC3	C31-C32-C33-C34
2	A	506	MC3	C39-C40-C41-C42
2	E	604	MC3	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

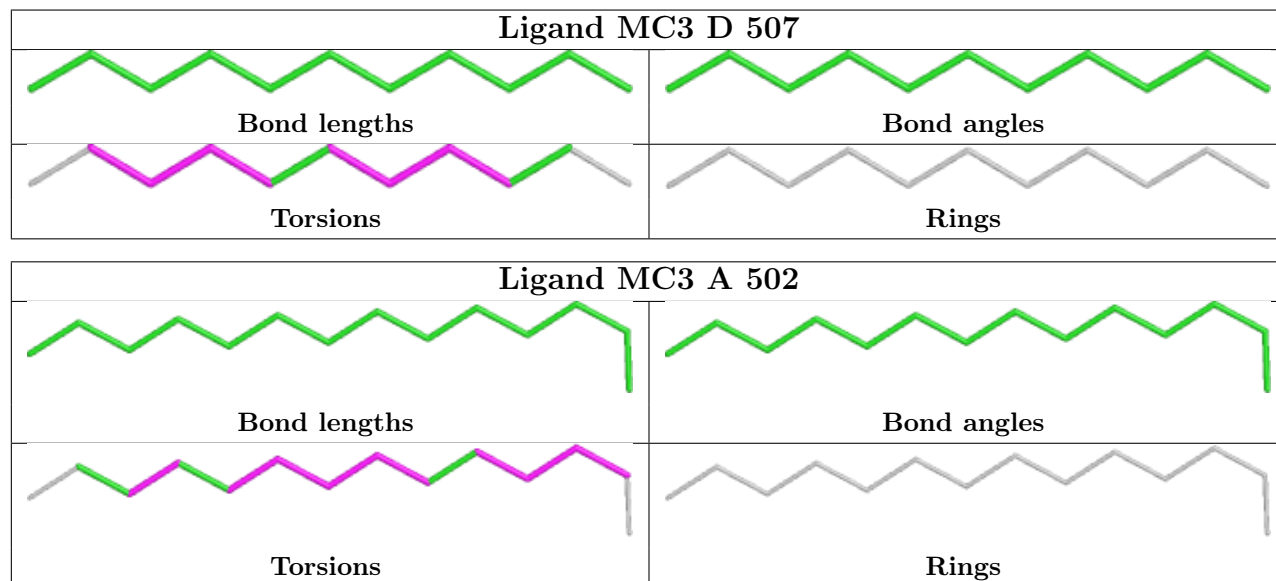
Mol	Chain	Res	Type	Atoms
2	B	604	MC3	C39-C40-C41-C42
2	C	604	MC3	C39-C40-C41-C42
2	E	609	MC3	C31-C32-C33-C34
2	B	609	MC3	C31-C32-C33-C34
2	A	501	MC3	C31-C32-C33-C34
2	D	501	MC3	C31-C32-C33-C34
2	D	506	MC3	C39-C40-C41-C42
2	E	601	MC3	O3-C11-C12-C13
2	A	503	MC3	O3-C11-C12-C13
2	D	503	MC3	O3-C11-C12-C13
2	B	601	MC3	O3-C11-C12-C13
2	C	601	MC3	O3-C11-C12-C13
2	B	602	MC3	C12-C13-C14-C15
2	B	604	MC3	C35-C36-C37-C38
2	D	504	MC3	C12-C13-C14-C15
2	E	602	MC3	C12-C13-C14-C15
2	E	604	MC3	C35-C36-C37-C38
2	A	504	MC3	C12-C13-C14-C15
2	C	604	MC3	C35-C36-C37-C38
2	D	506	MC3	C35-C36-C37-C38
2	A	506	MC3	C35-C36-C37-C38
2	C	602	MC3	C12-C13-C14-C15
2	E	602	MC3	O31-C31-C32-C33
2	B	602	MC3	O31-C31-C32-C33
2	D	504	MC3	O31-C31-C32-C33
2	A	504	MC3	O31-C31-C32-C33
2	C	602	MC3	O31-C31-C32-C33
2	E	606	MC3	C36-C37-C38-C39
2	A	508	MC3	C36-C37-C38-C39
2	B	606	MC3	C36-C37-C38-C39
2	C	606	MC3	C36-C37-C38-C39
2	D	508	MC3	C36-C37-C38-C39
2	D	503	MC3	O2-C31-C32-C33
2	E	601	MC3	O2-C31-C32-C33
2	B	601	MC3	O2-C31-C32-C33
2	A	503	MC3	O2-C31-C32-C33
2	C	601	MC3	O2-C31-C32-C33

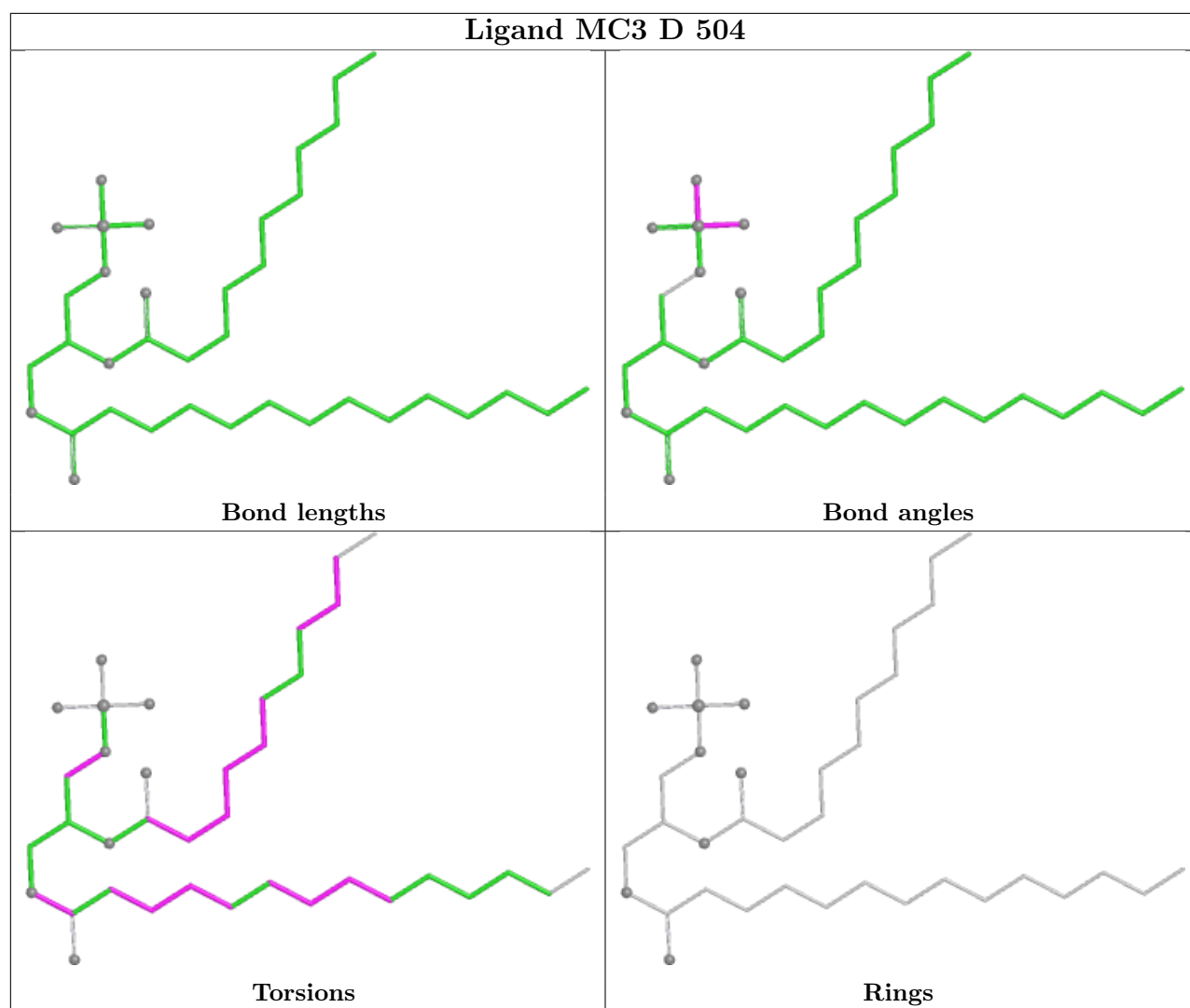
There are no ring outliers.

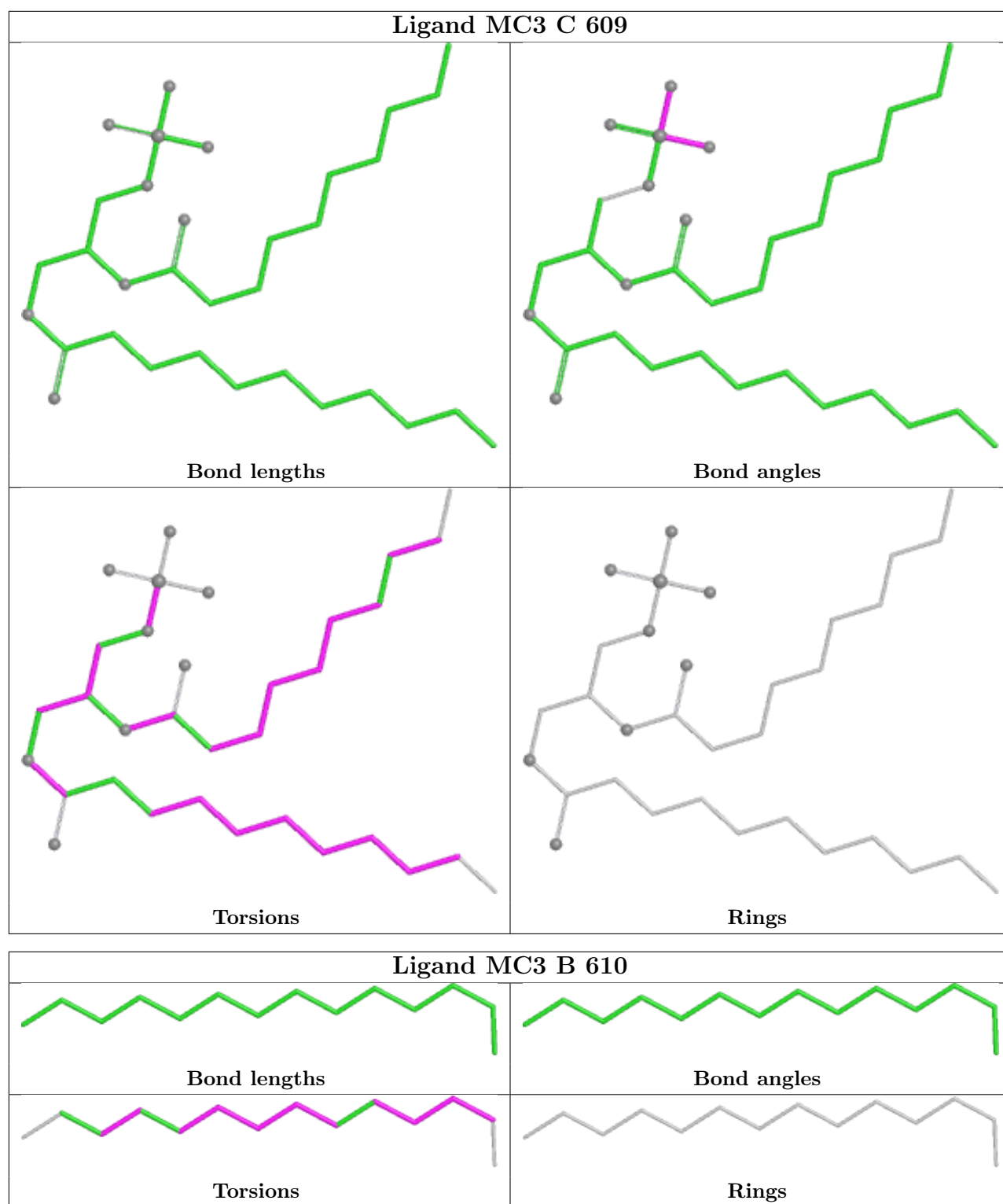
No monomer is involved in short contacts.

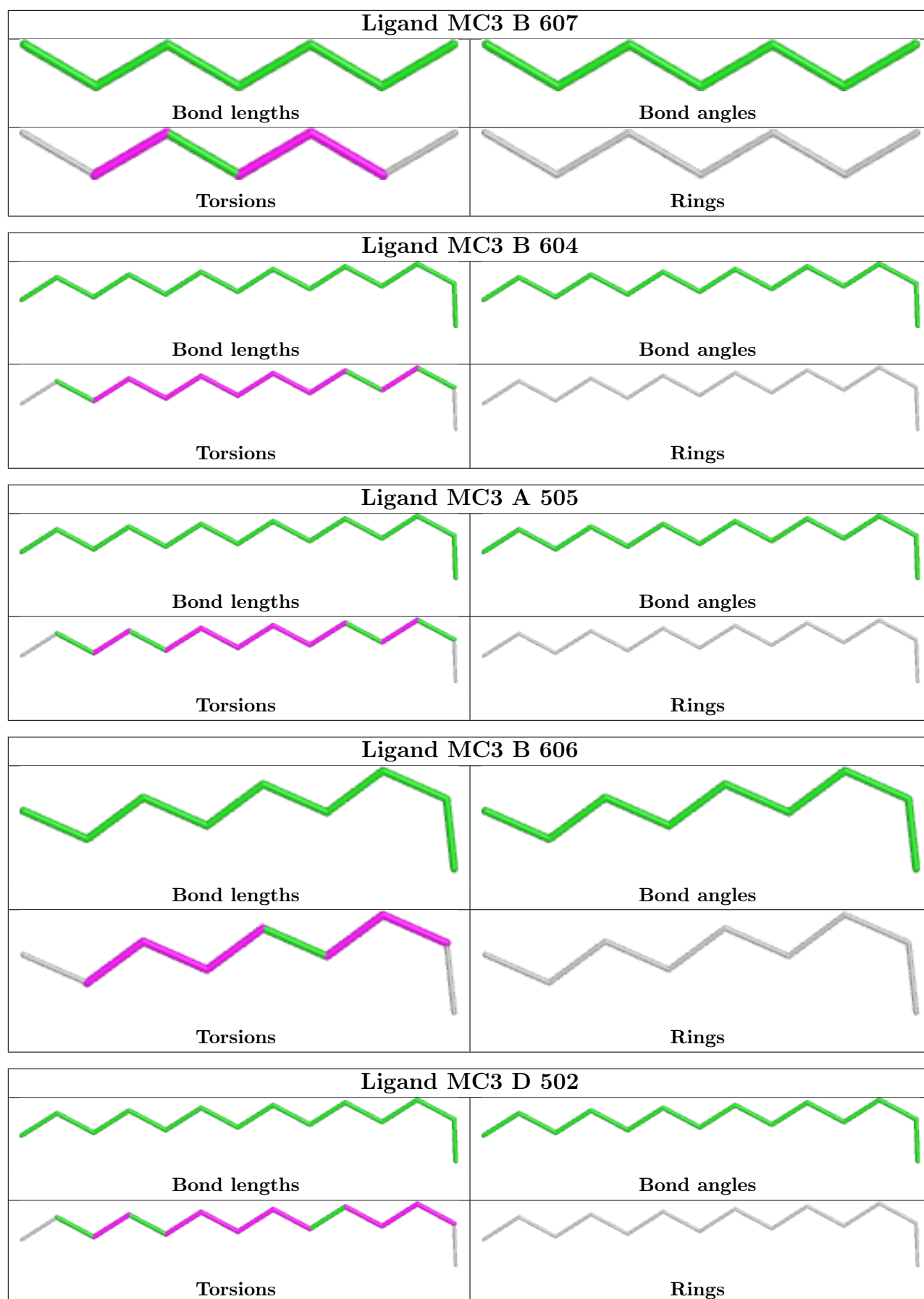
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

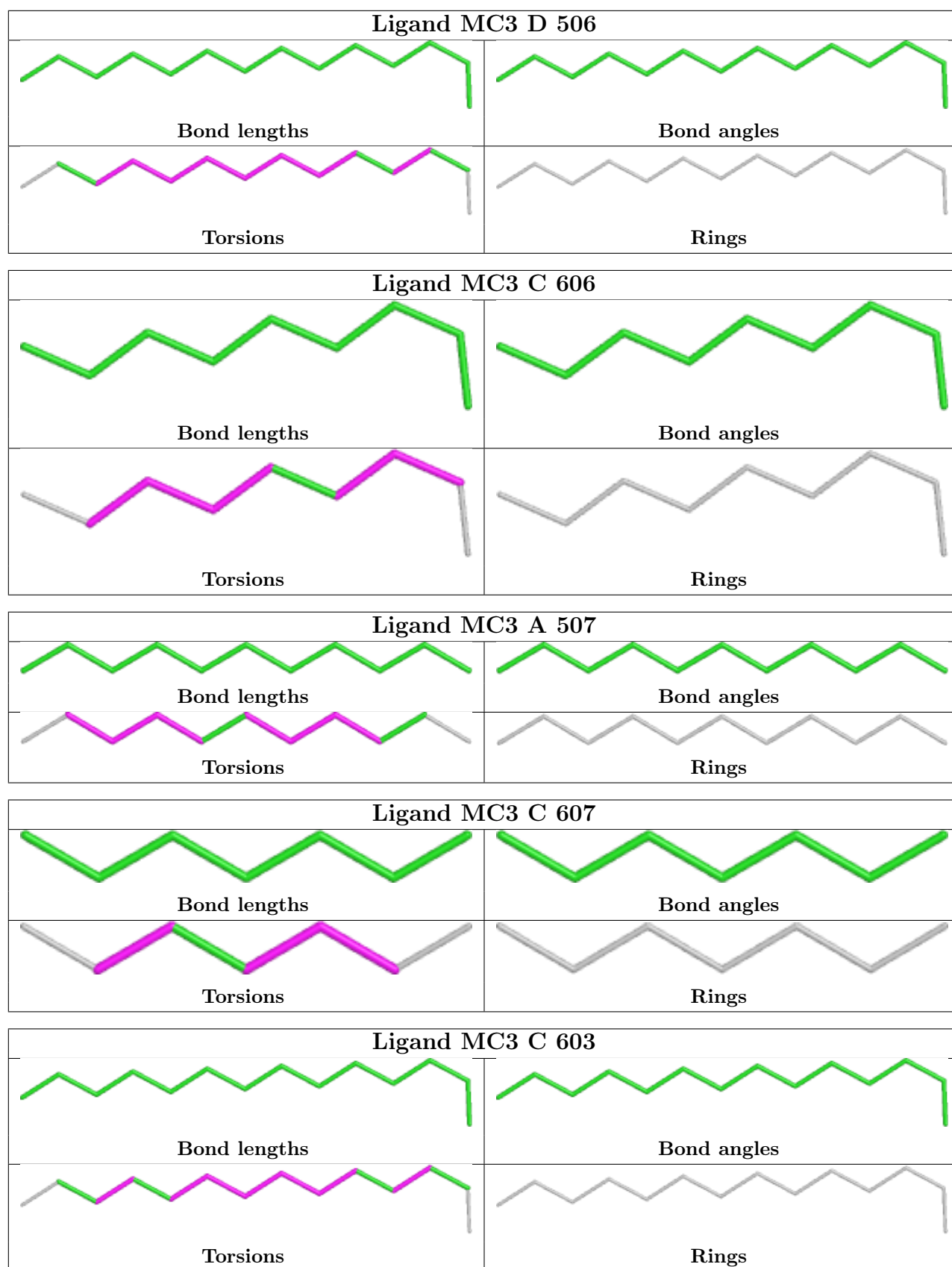
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

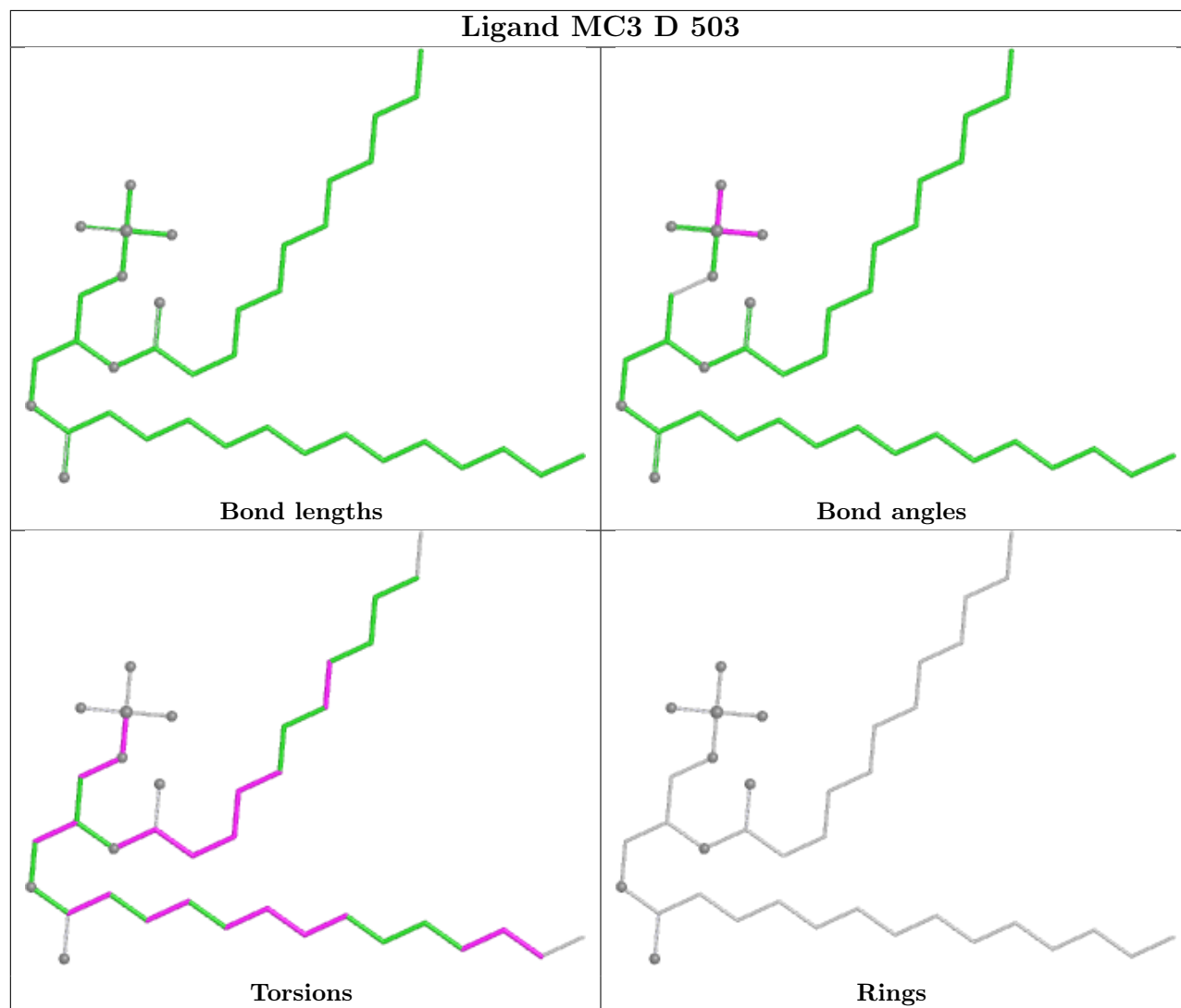
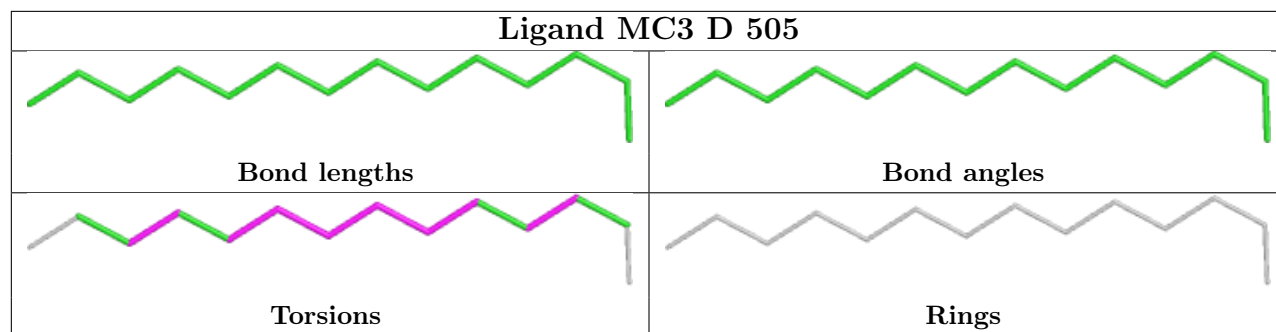


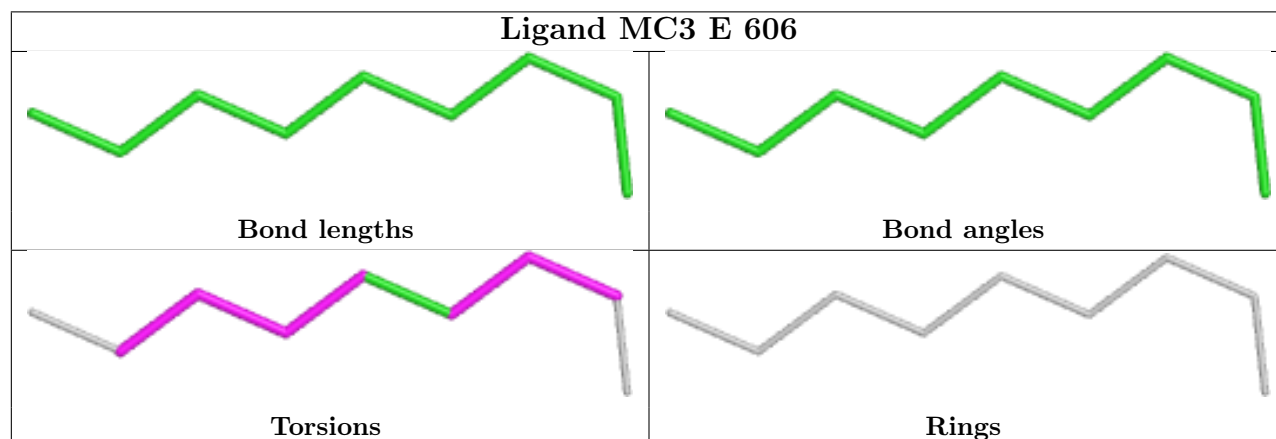
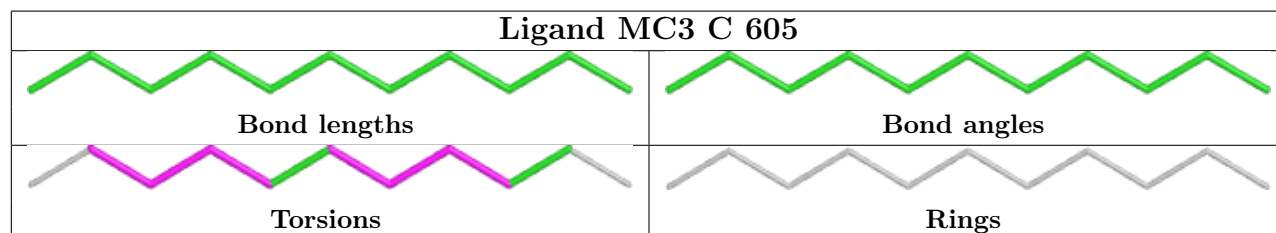
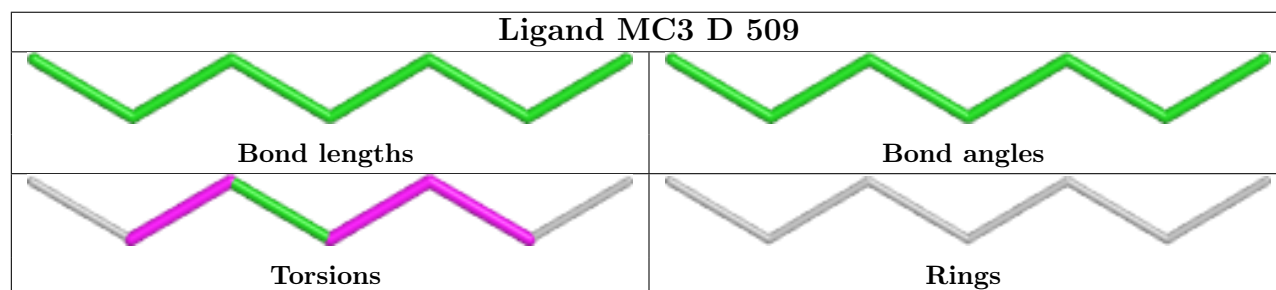
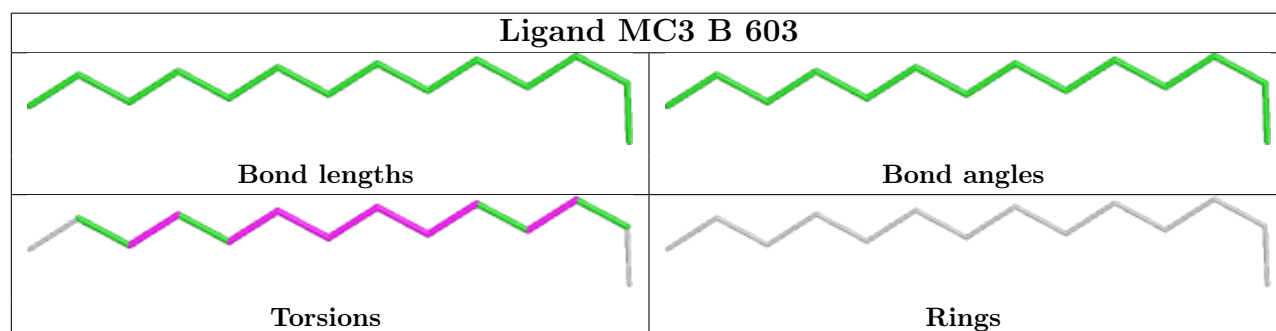
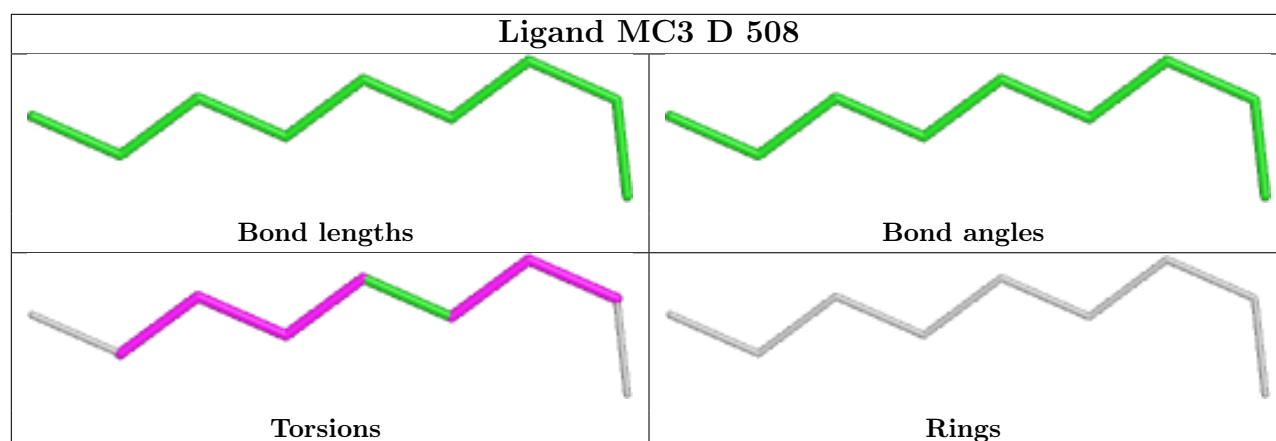


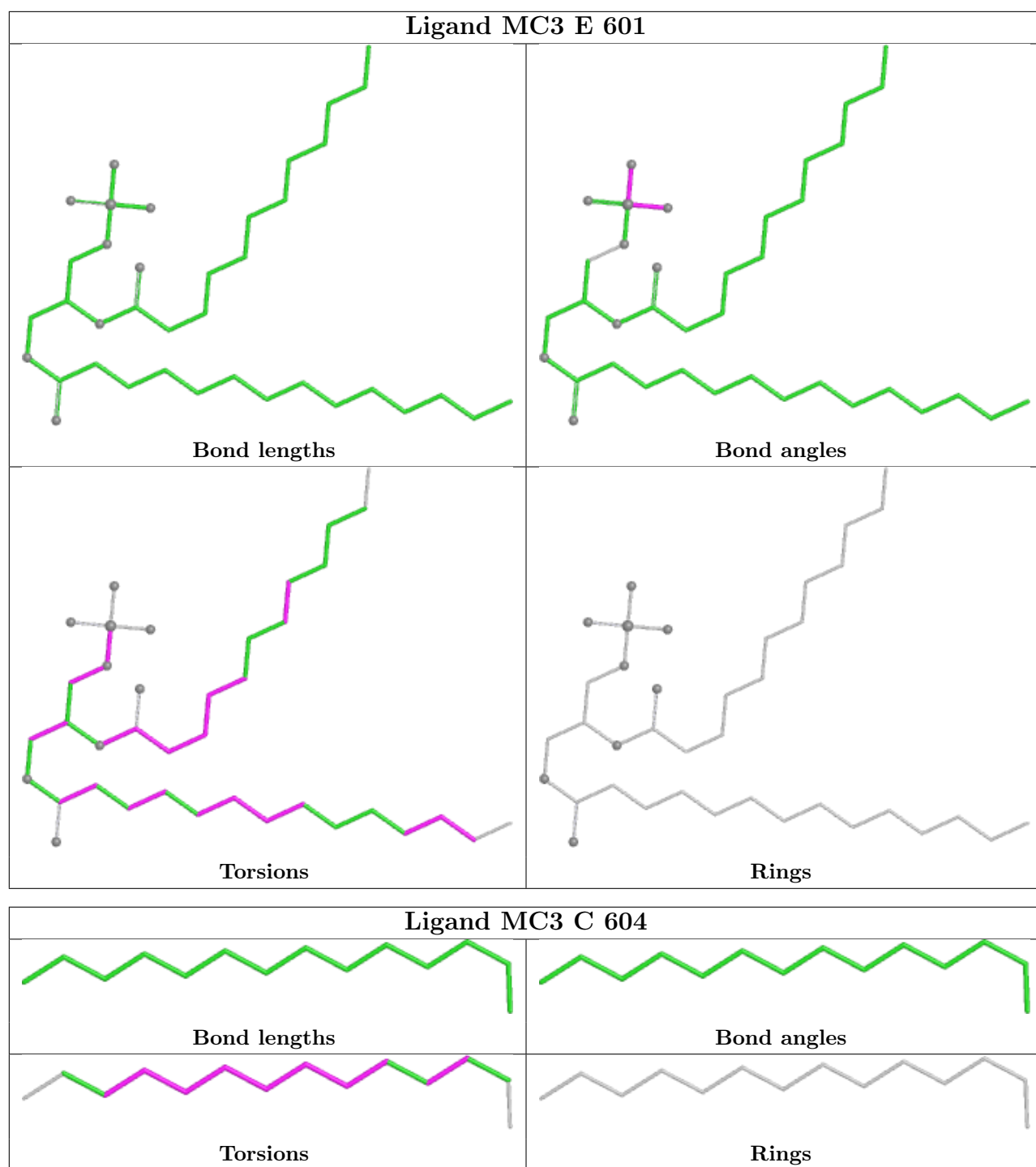


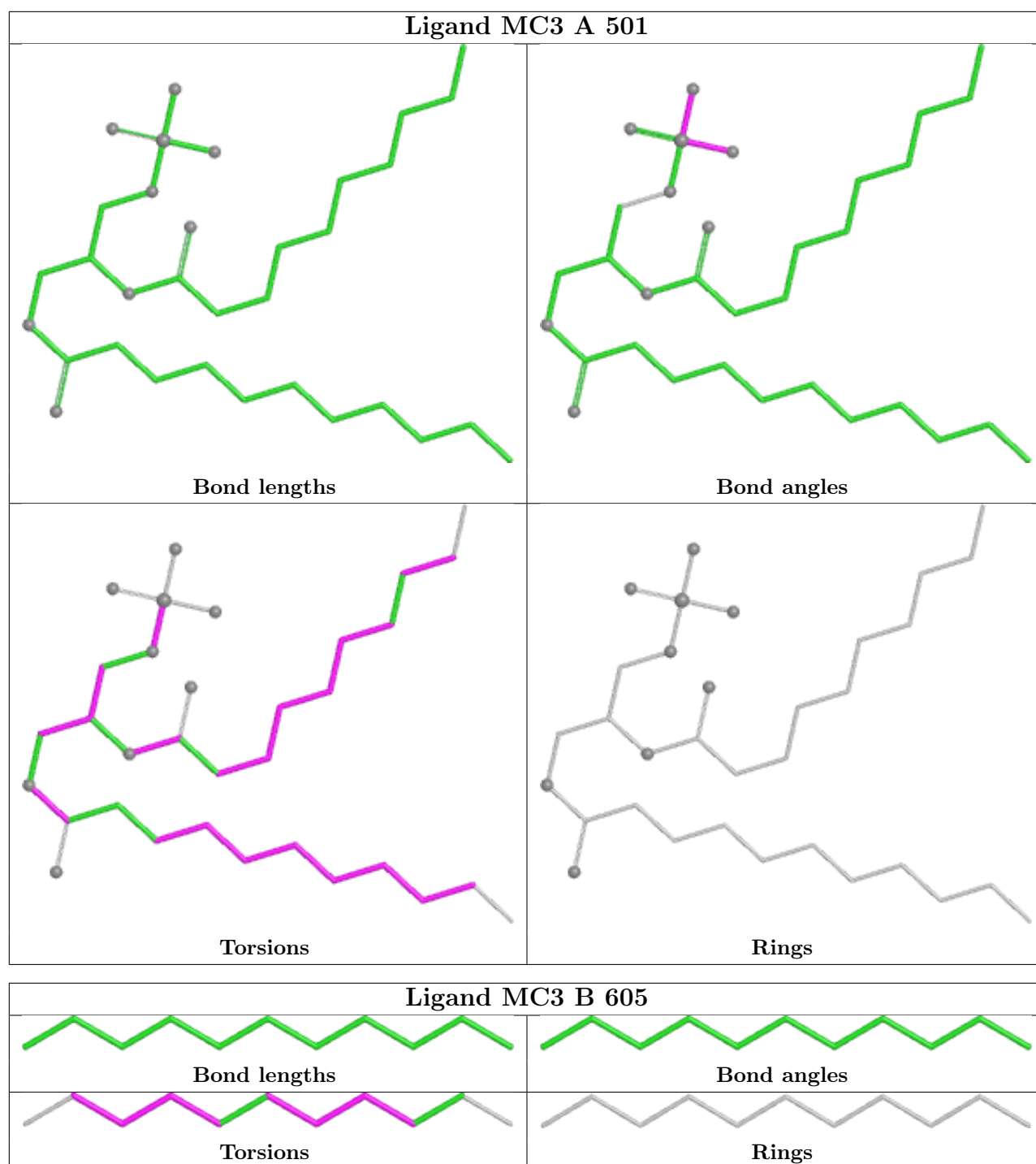


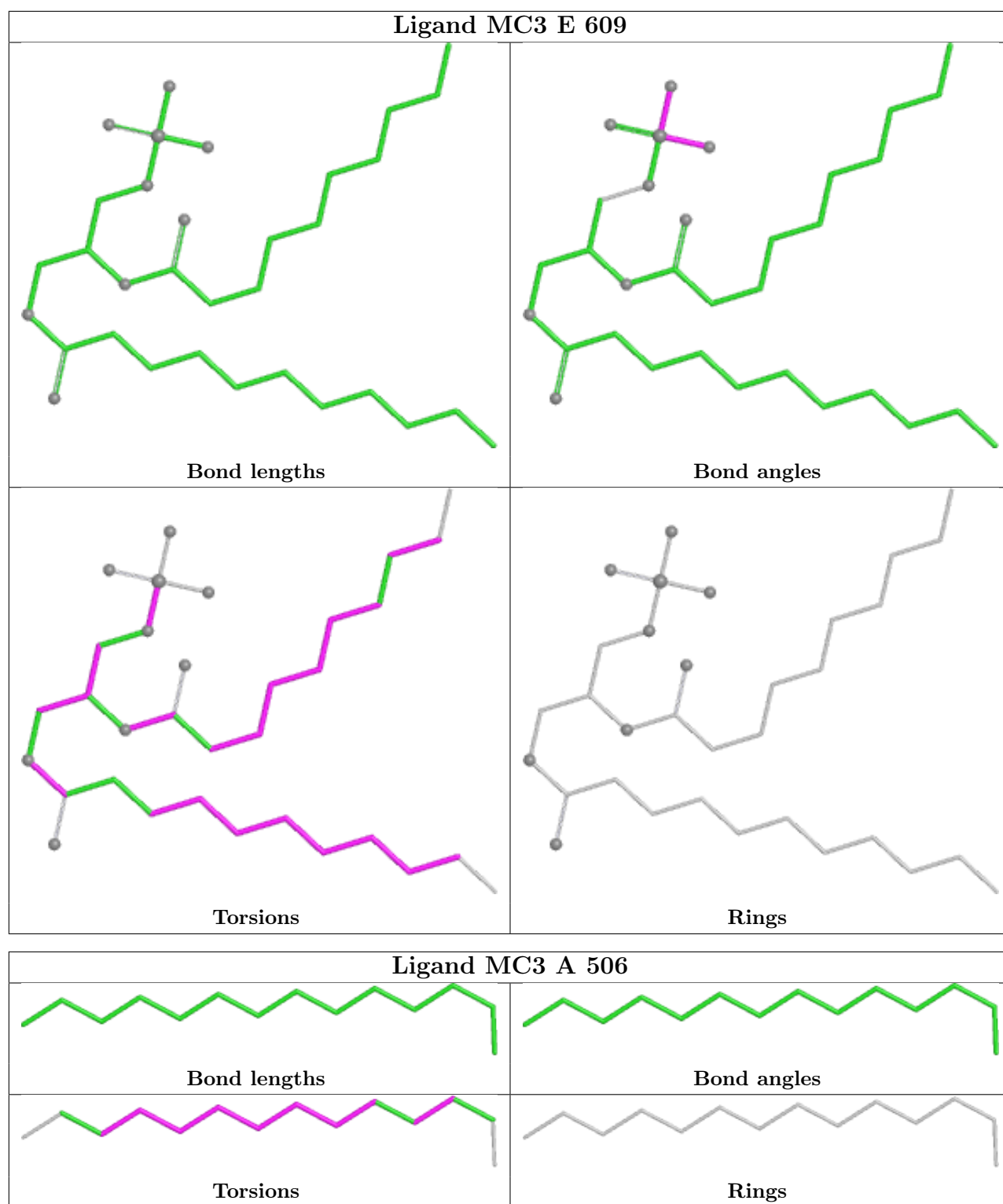


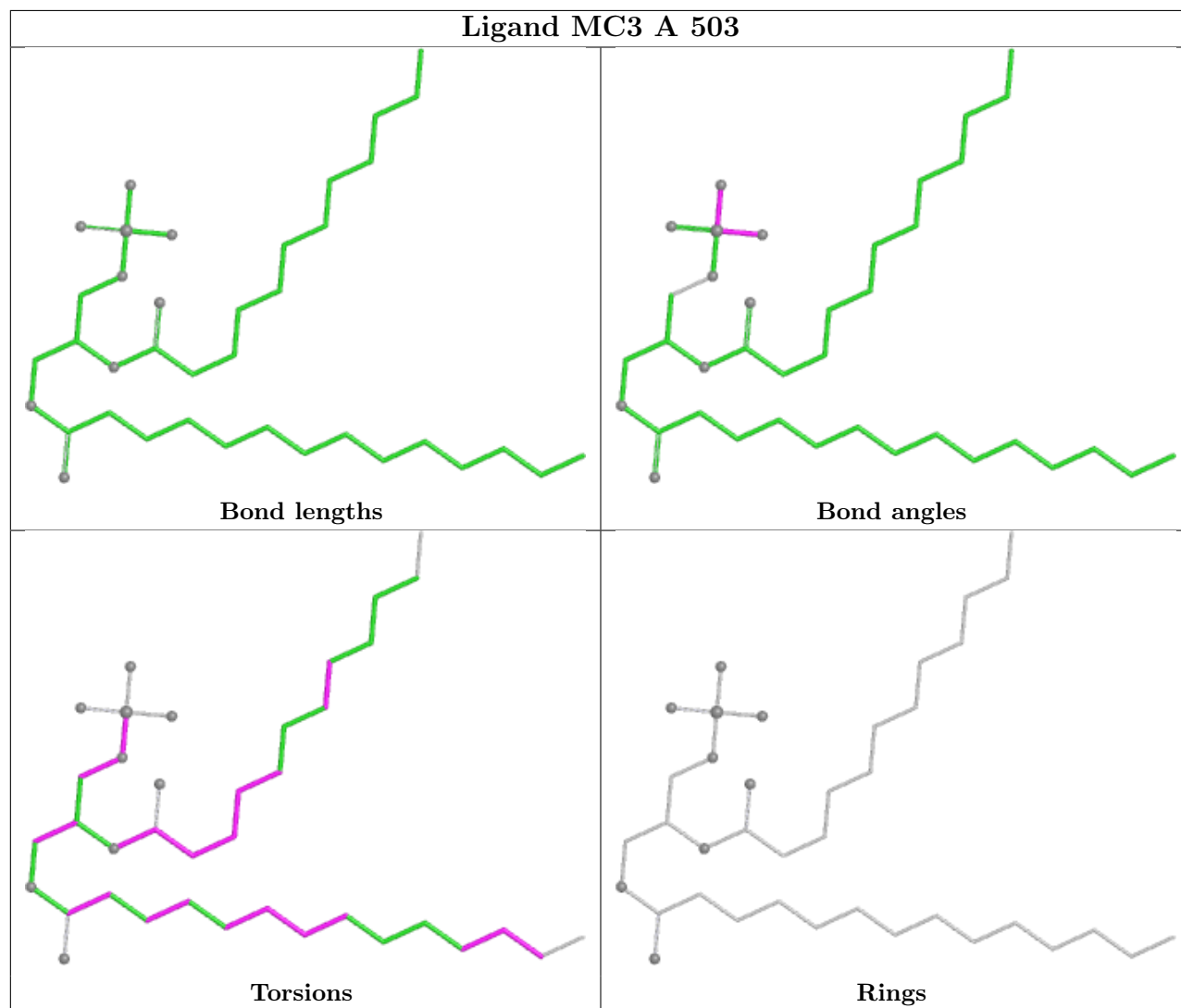
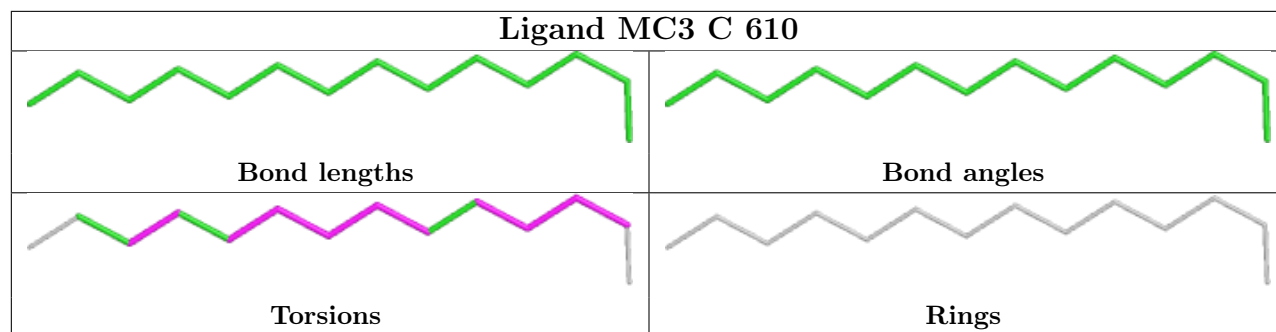




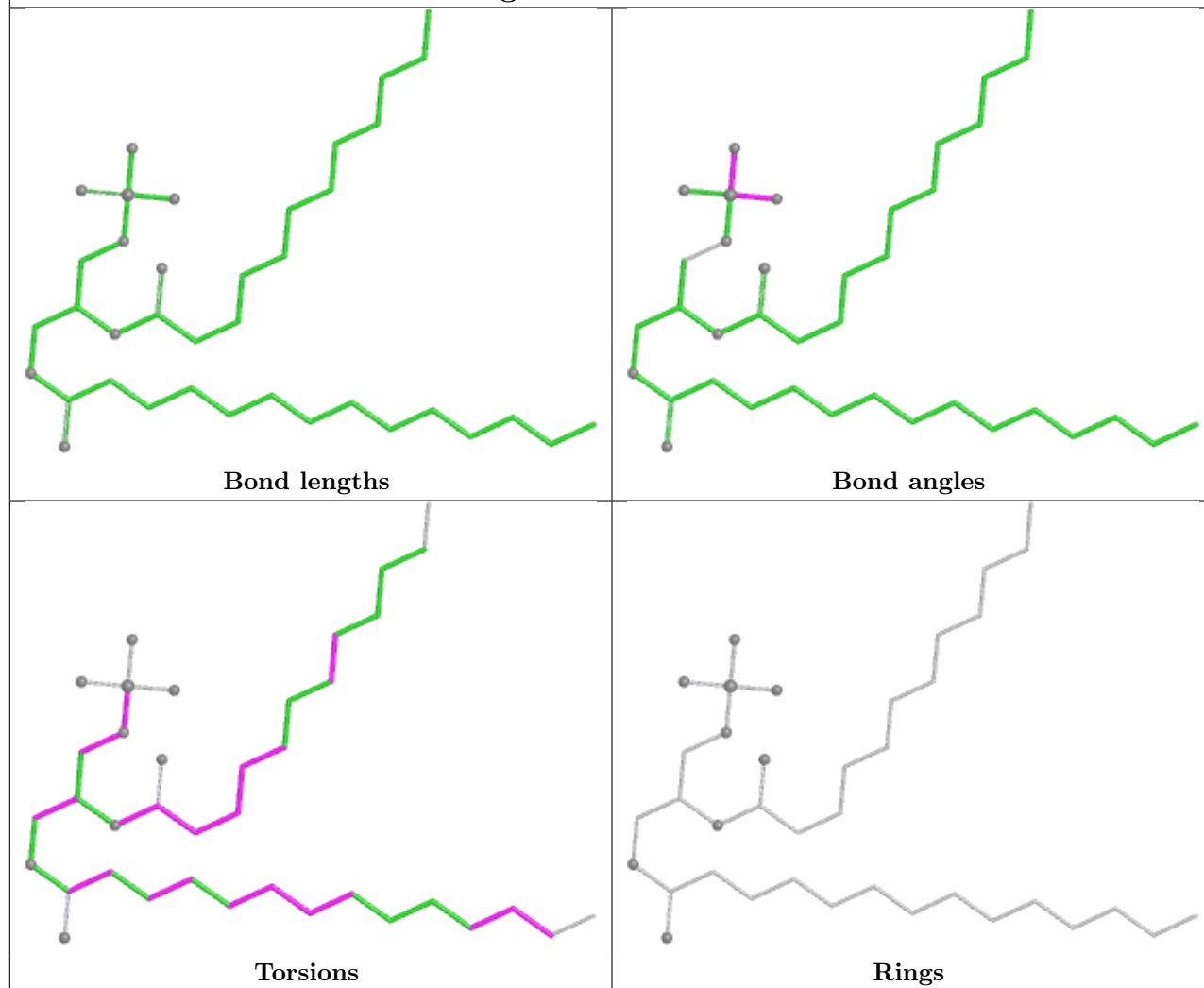




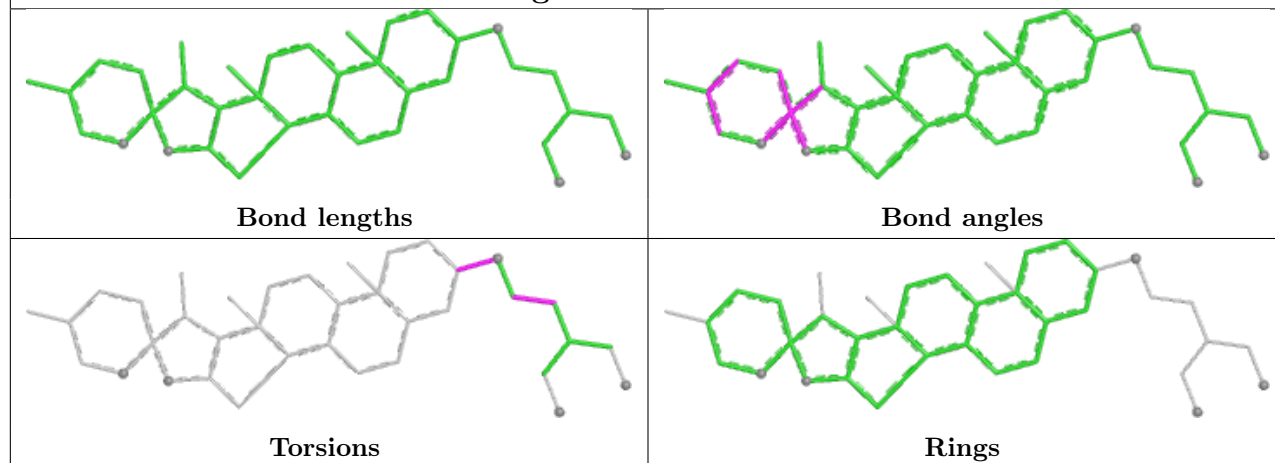


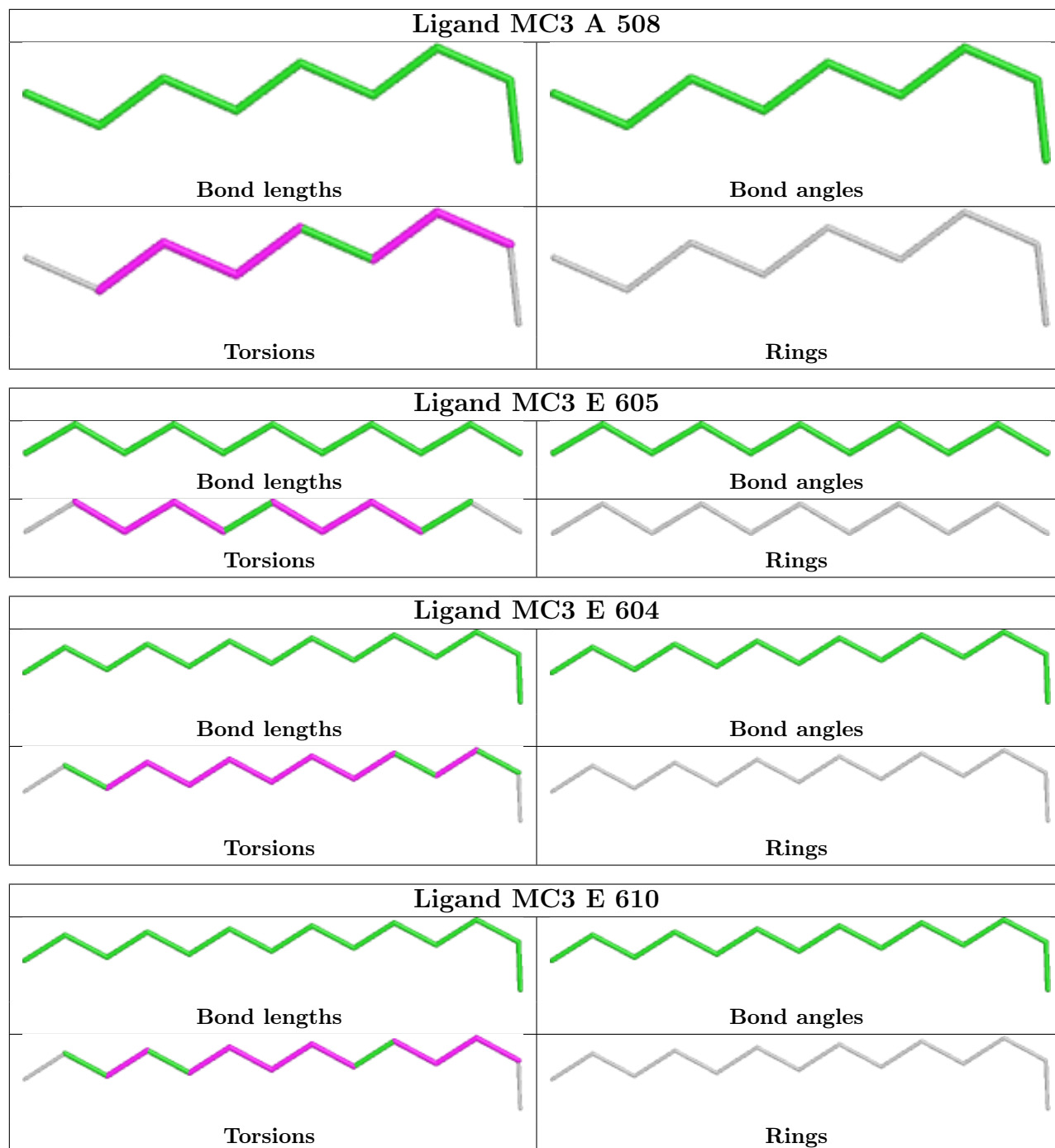


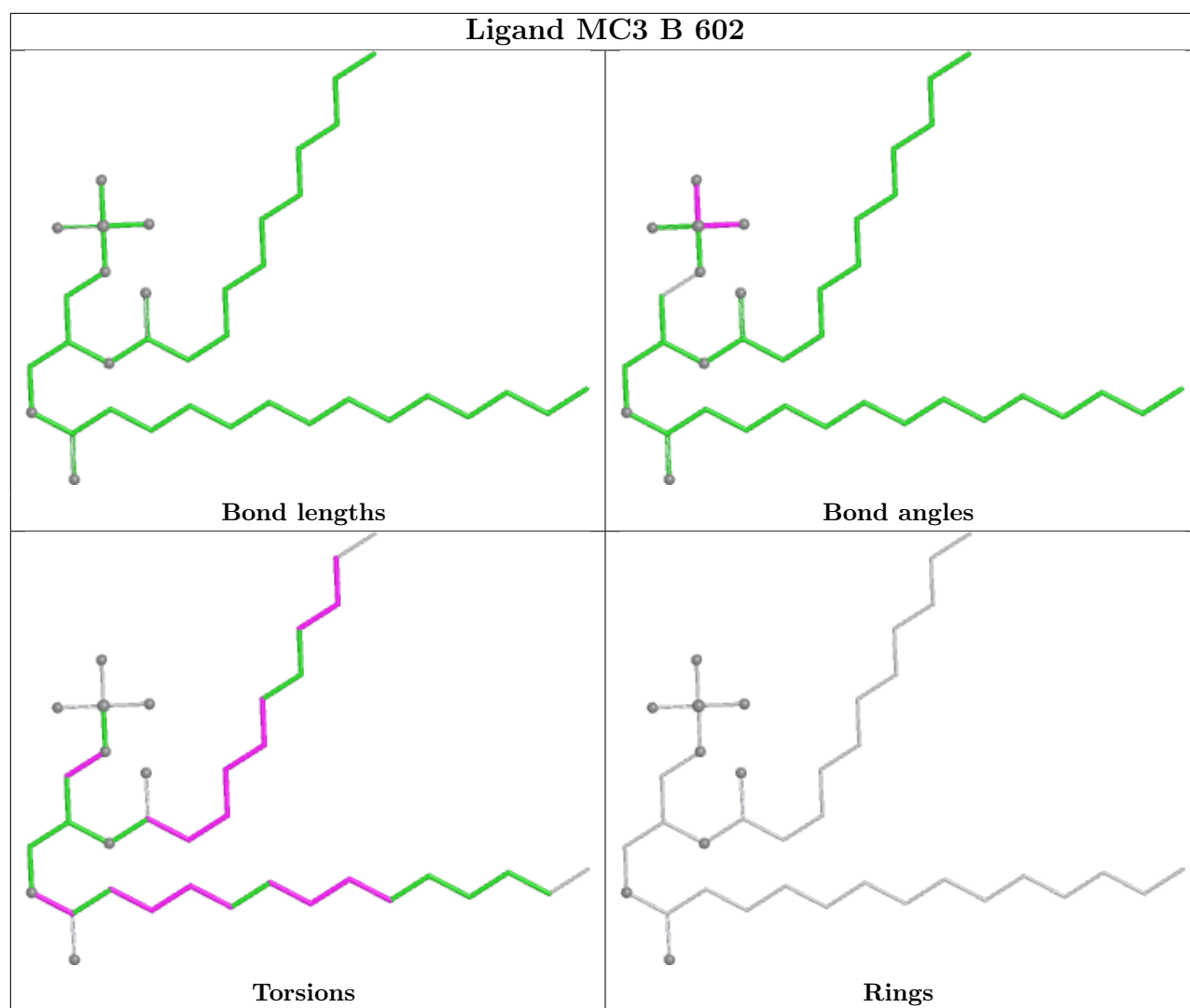
Ligand MC3 B 601

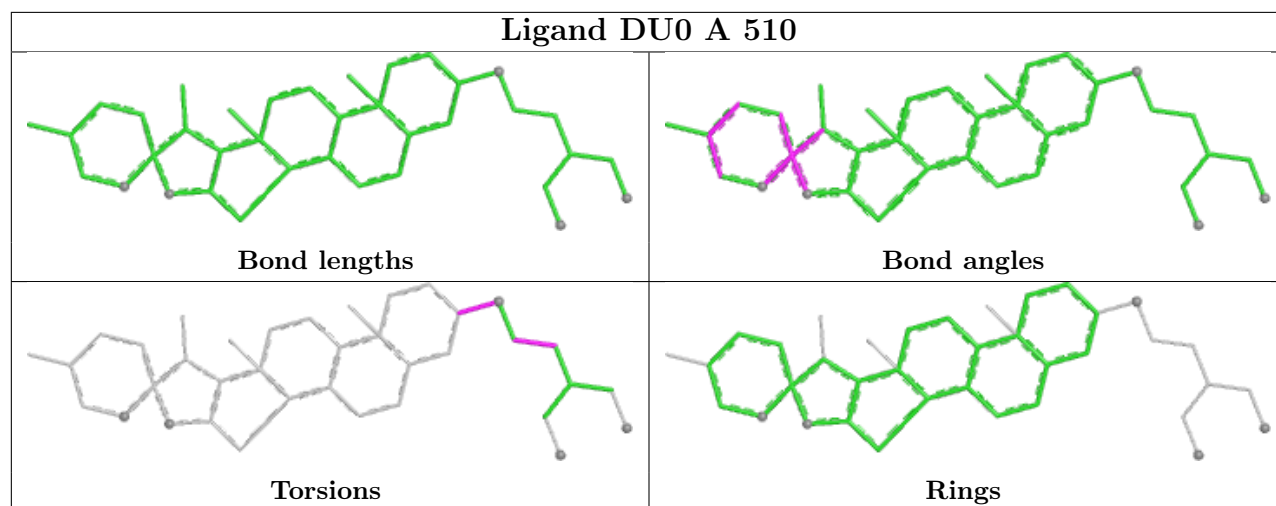
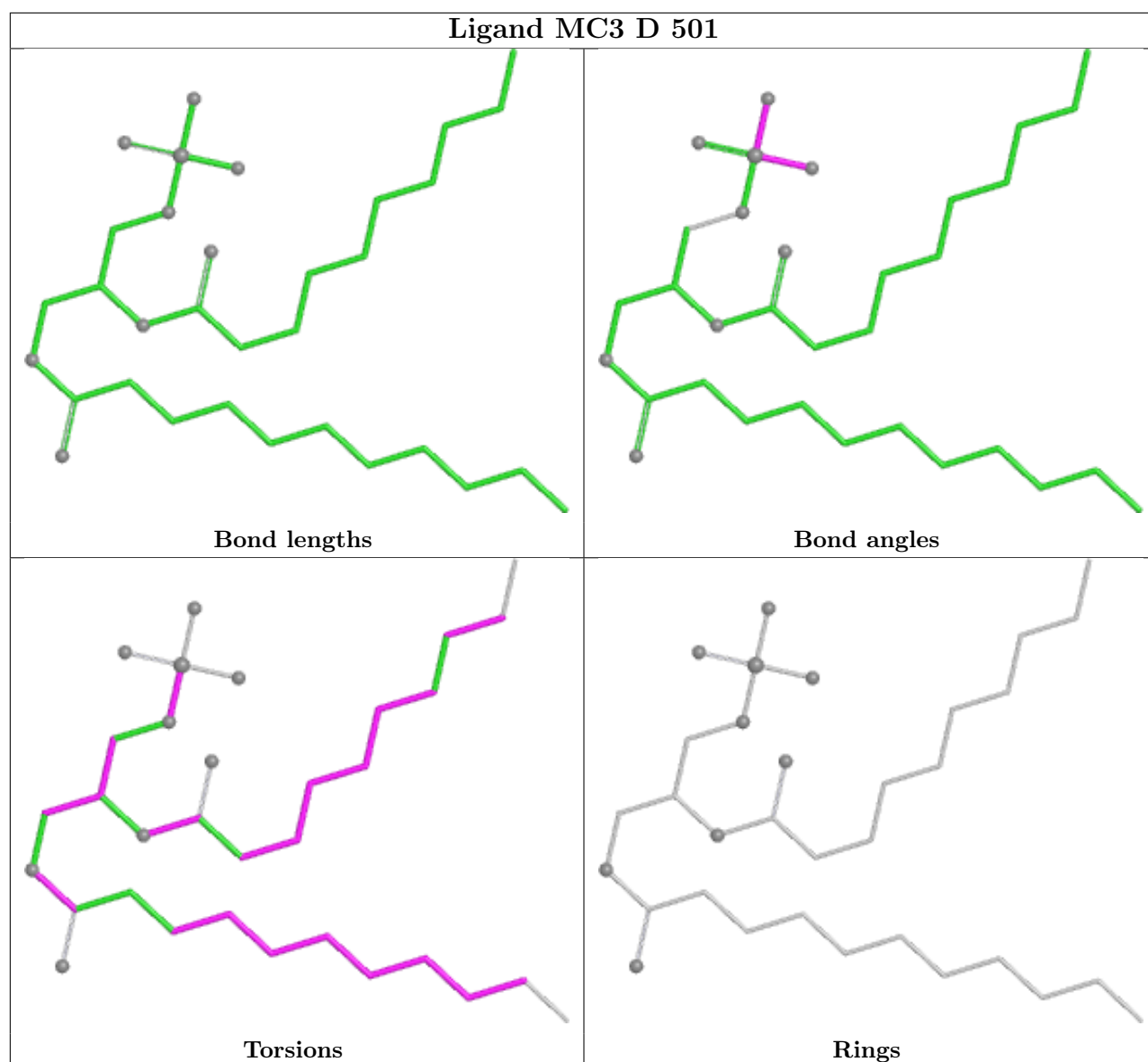


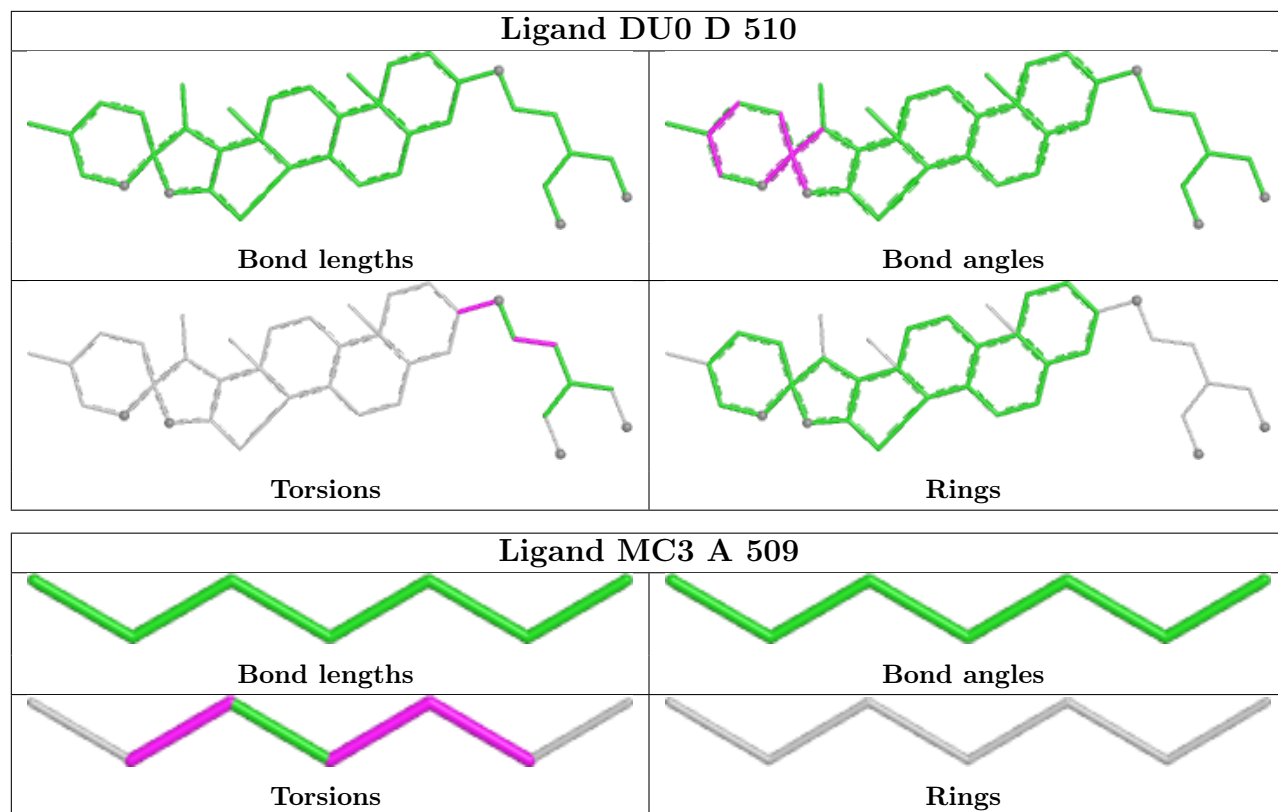
Ligand DU0 C 608

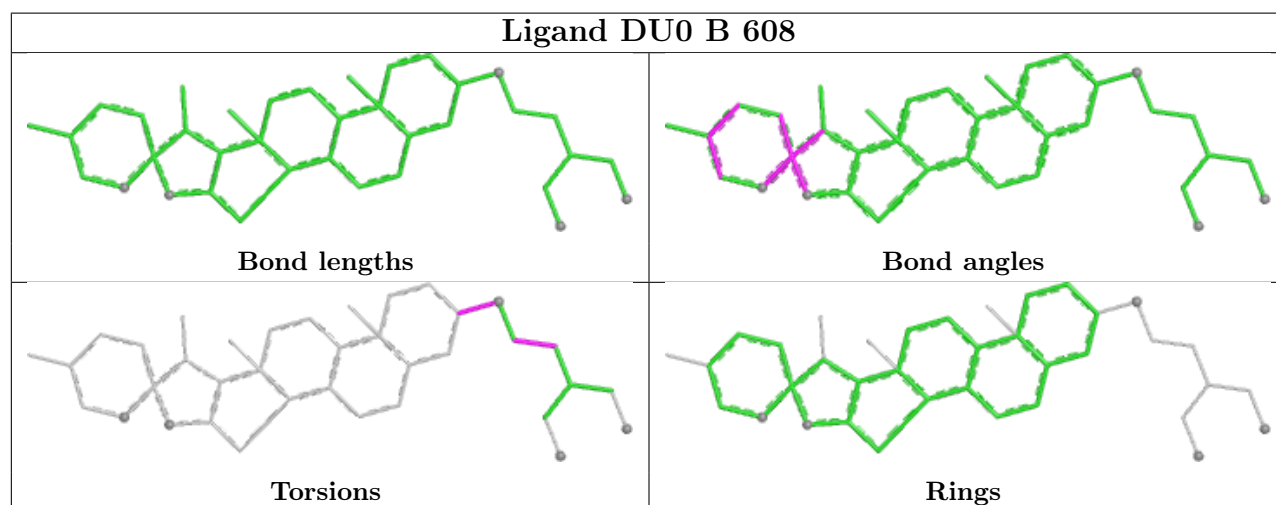
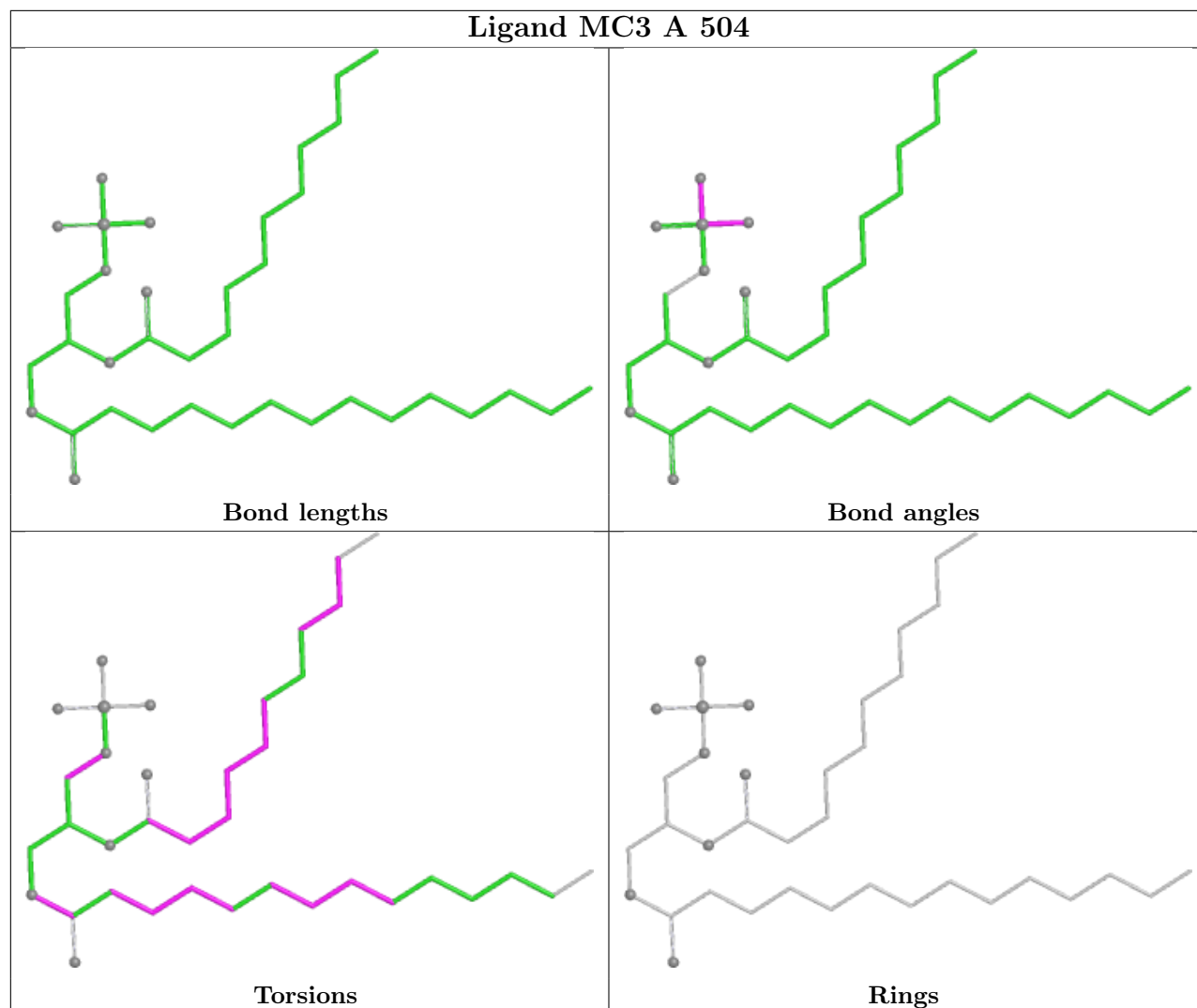


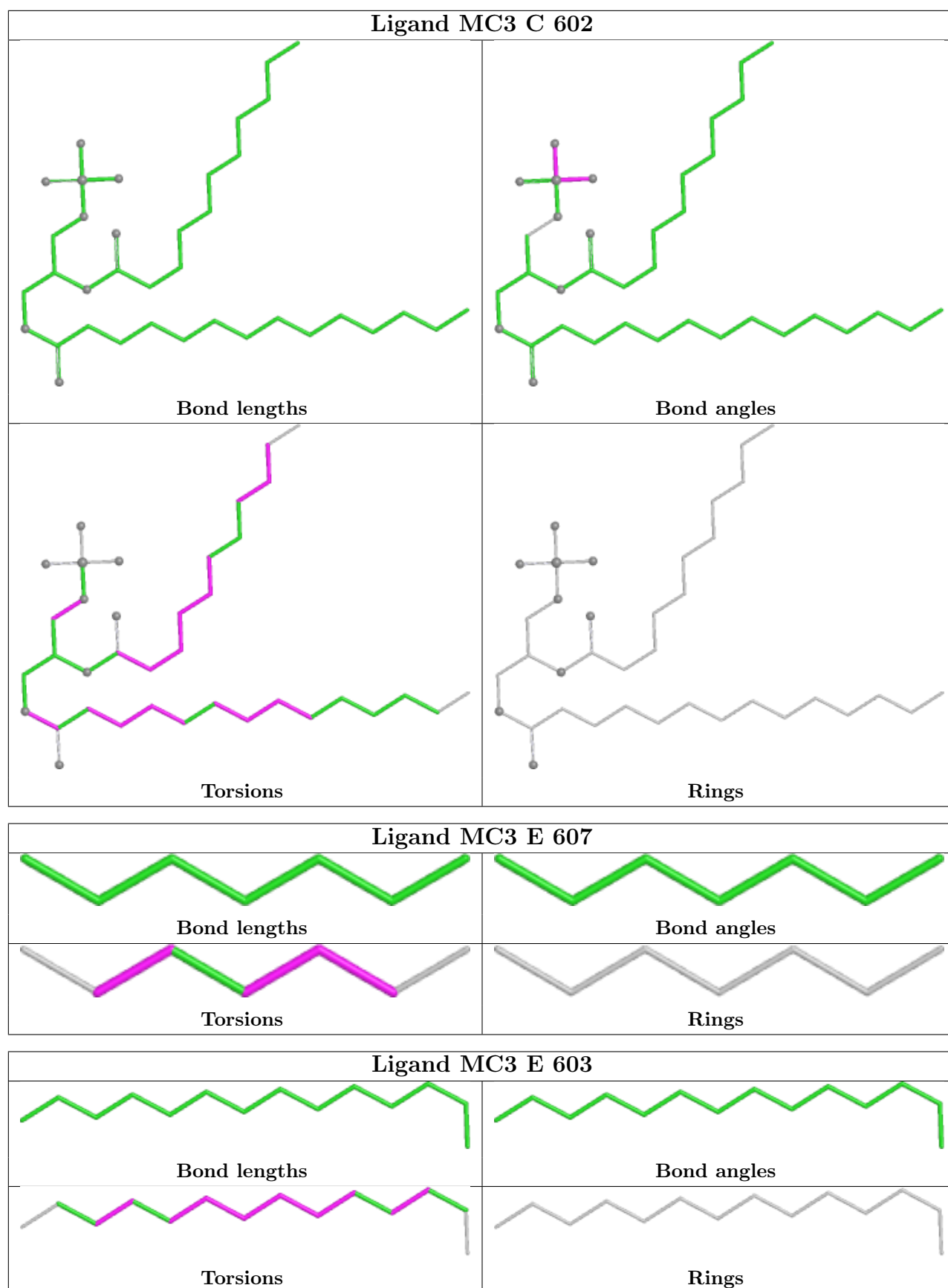


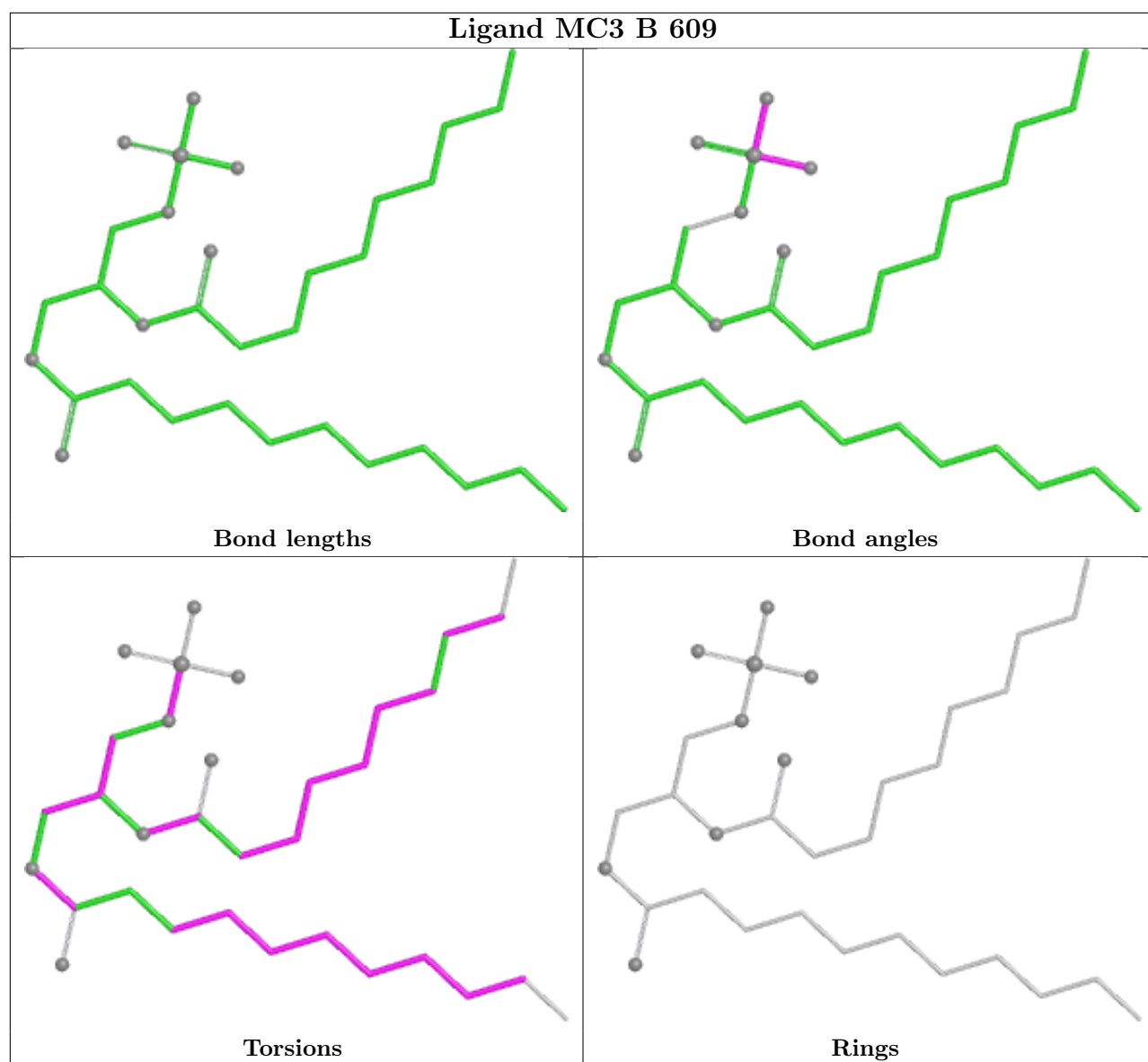


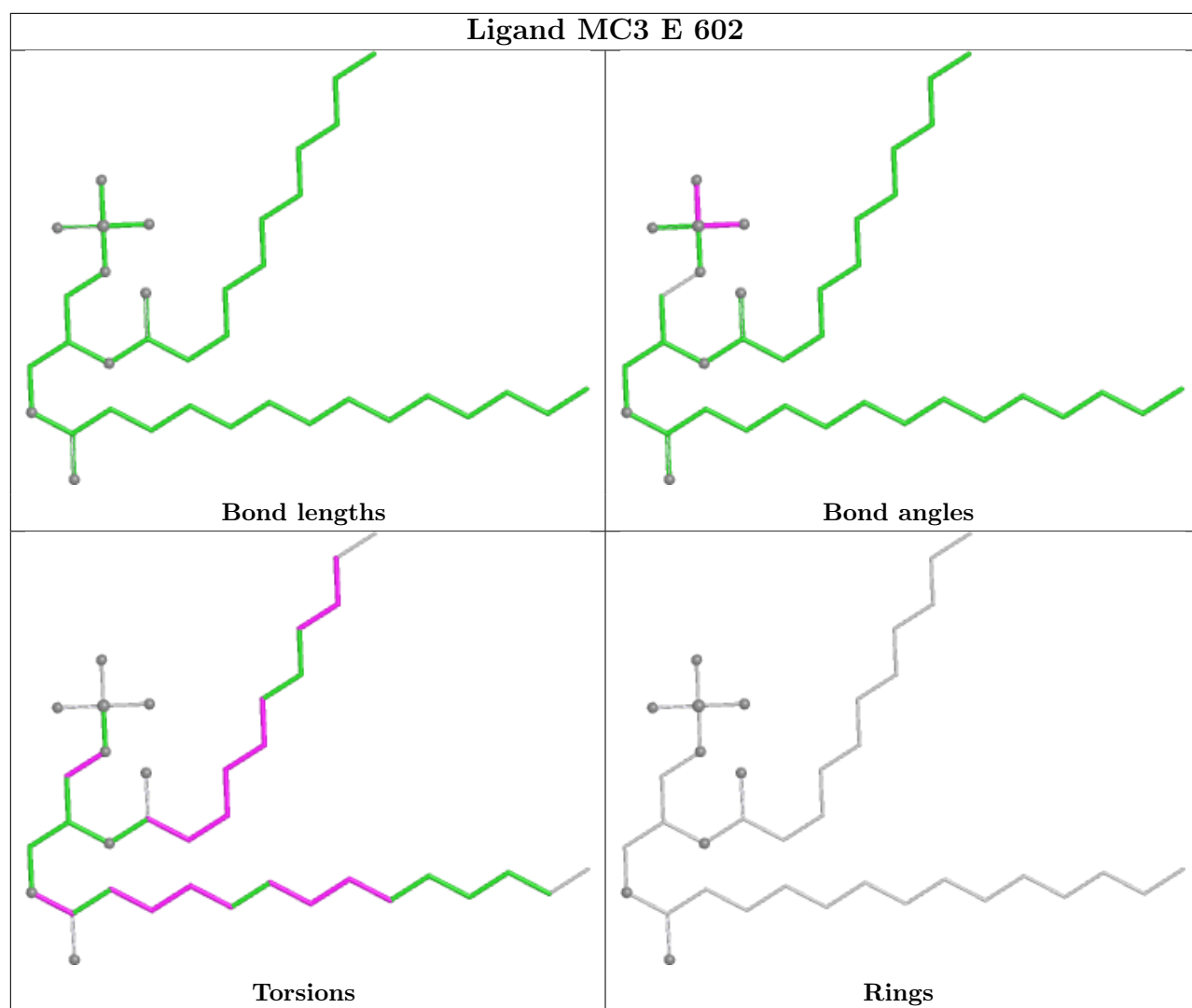


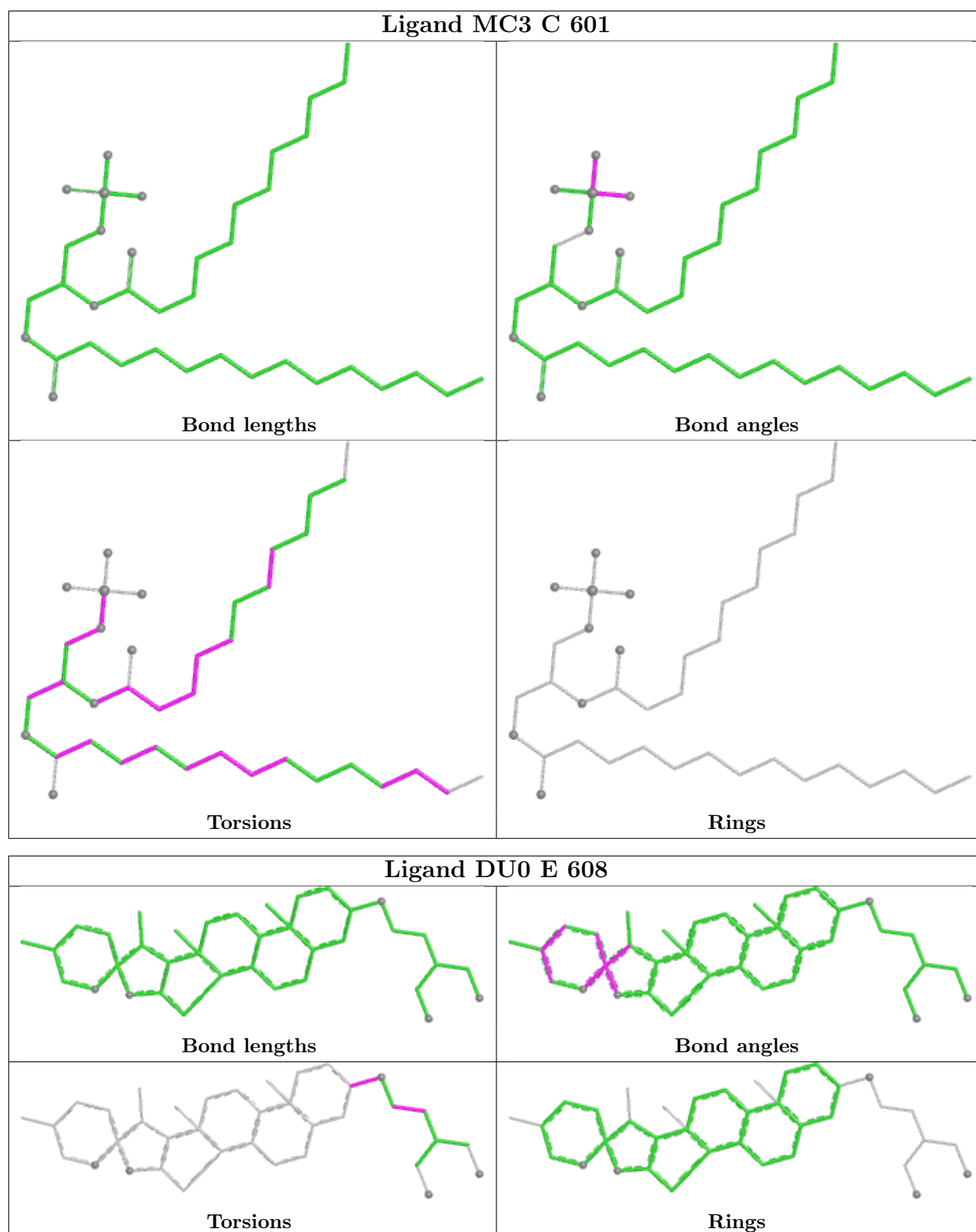












4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

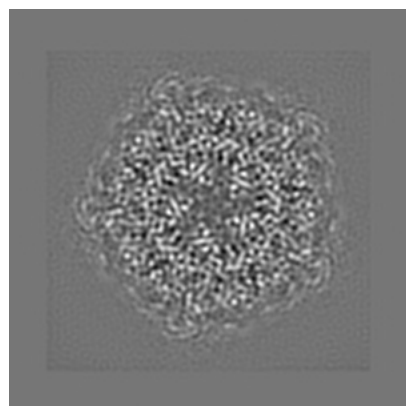
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27130. These allow visual inspection of the internal detail of the map and identification of artifacts.

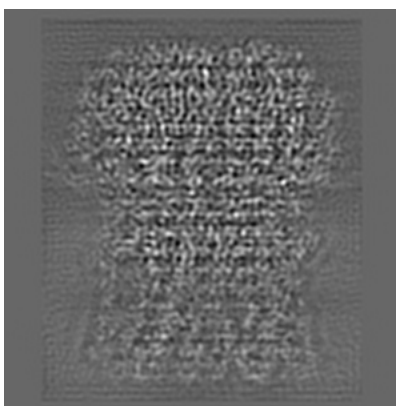
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

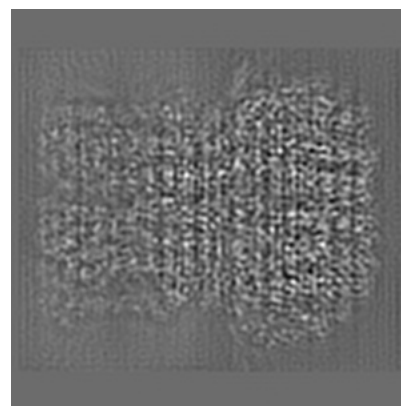
5.1.1 Primary map



X

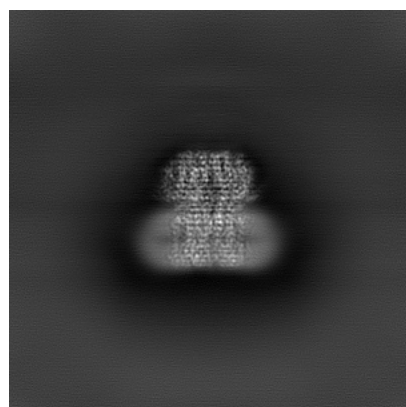


Y

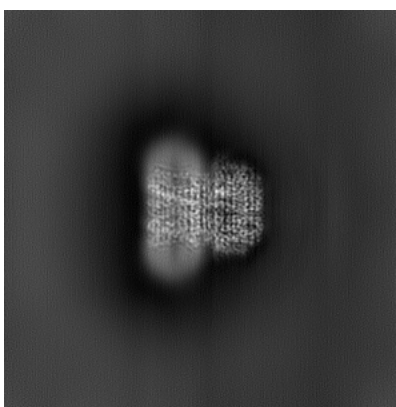


Z

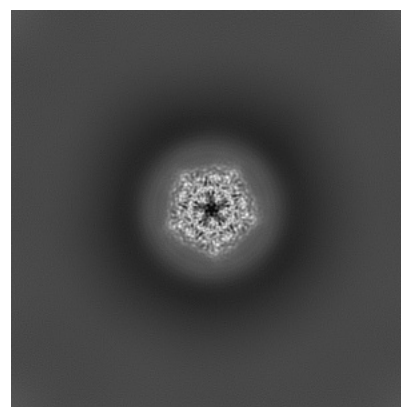
5.1.2 Raw map



X



Y

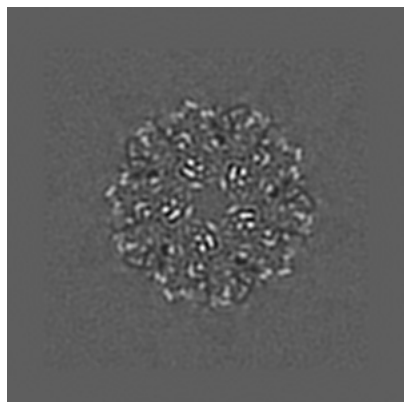


Z

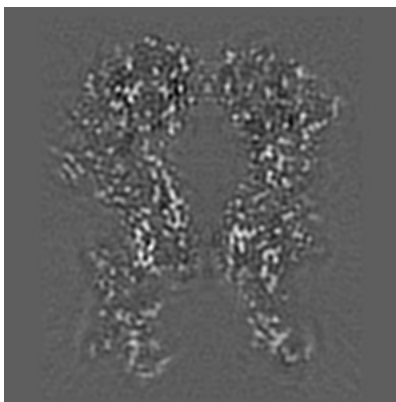
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

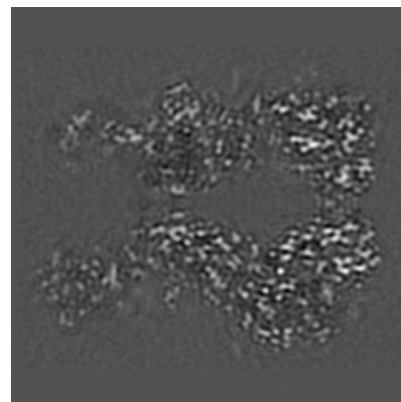
5.2.1 Primary map



X Index: 144

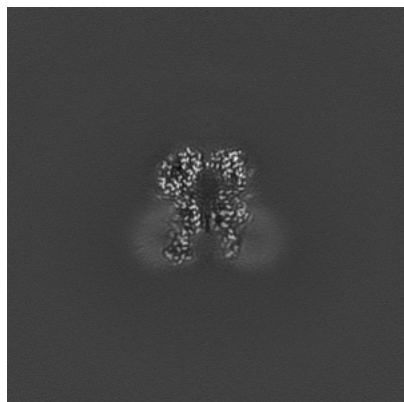


Y Index: 144

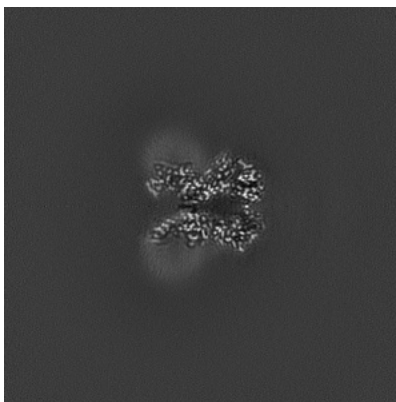


Z Index: 144

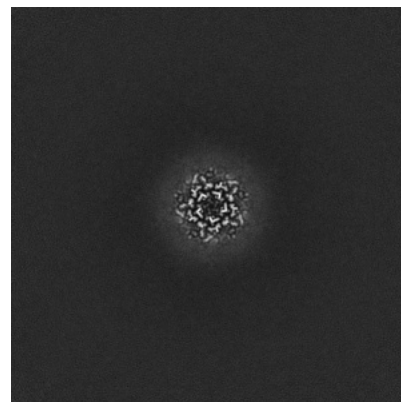
5.2.2 Raw map



X Index: 200



Y Index: 200

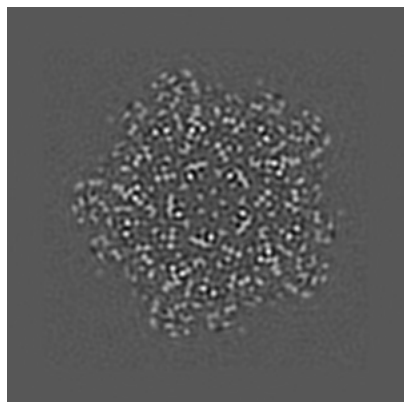


Z Index: 200

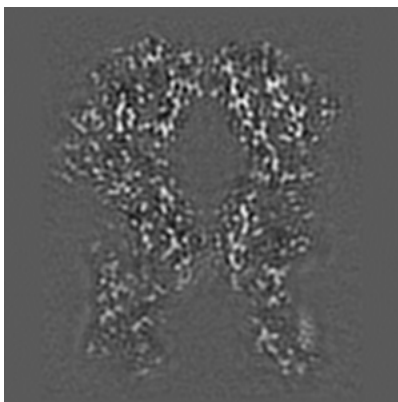
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

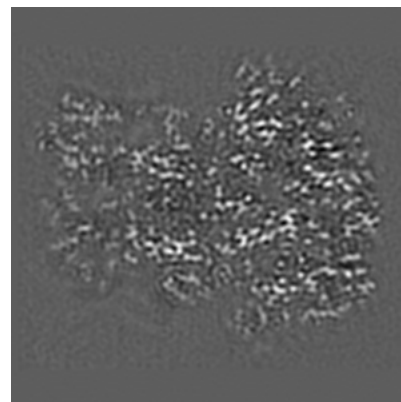
5.3.1 Primary map



X Index: 224

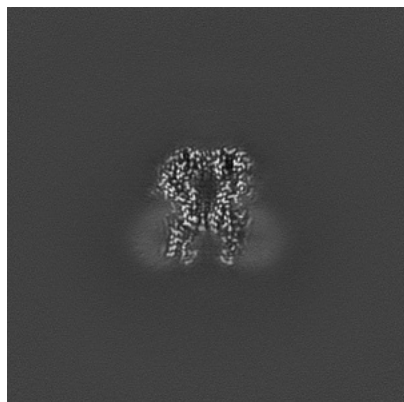


Y Index: 139

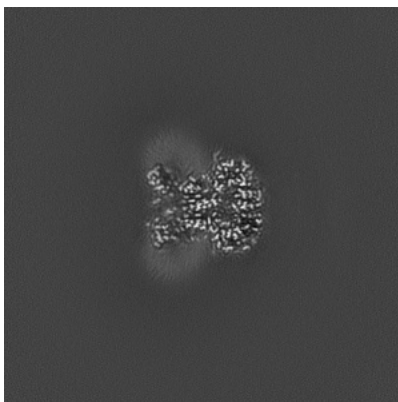


Z Index: 109

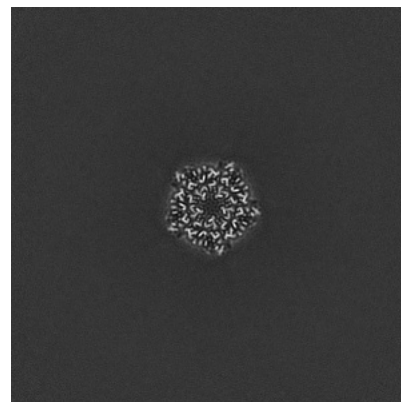
5.3.2 Raw map



X Index: 206



Y Index: 187

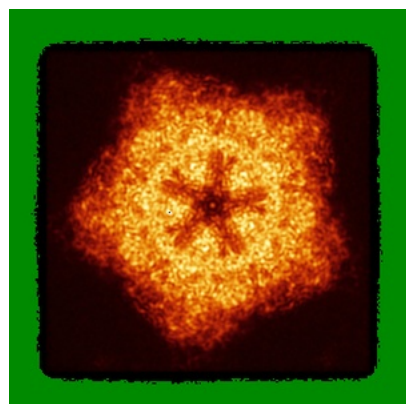


Z Index: 230

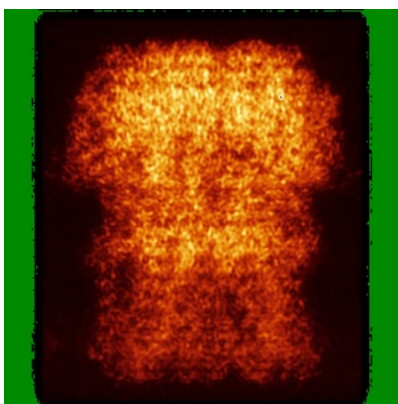
The images above show the largest variance slices of the map in three orthogonal directions.

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

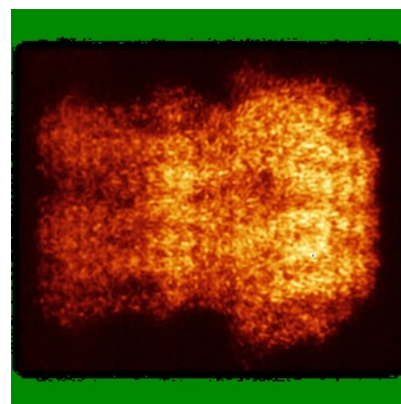
5.4.1 Primary map



X

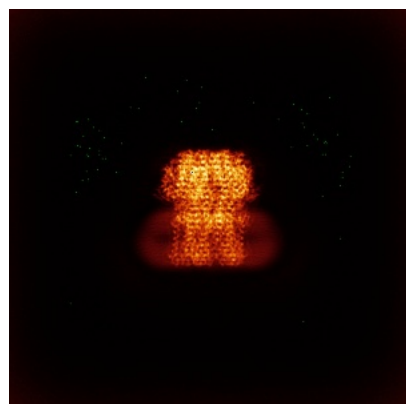


Y

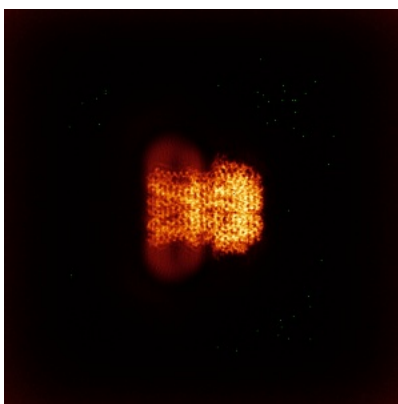


Z

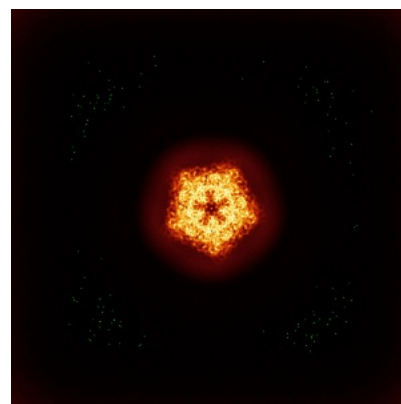
5.4.2 Raw map



X



Y

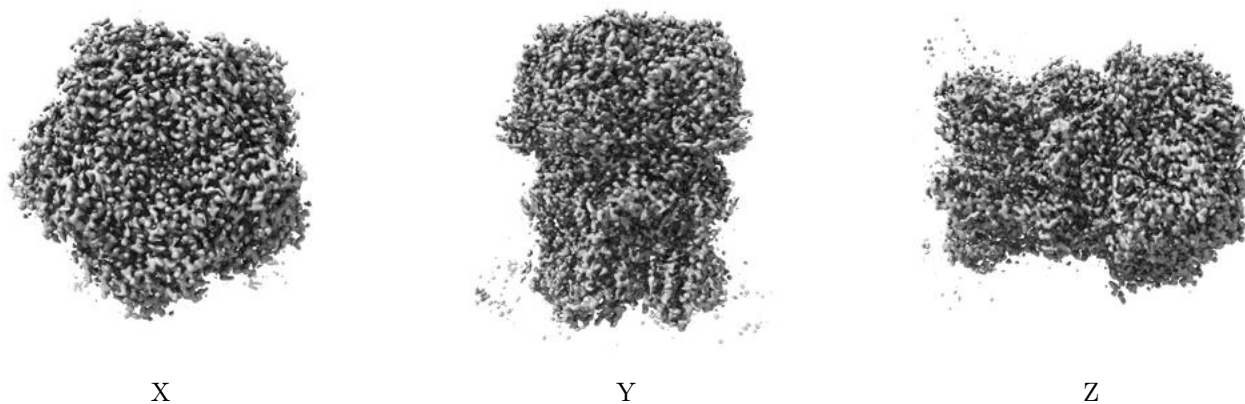


Z

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.

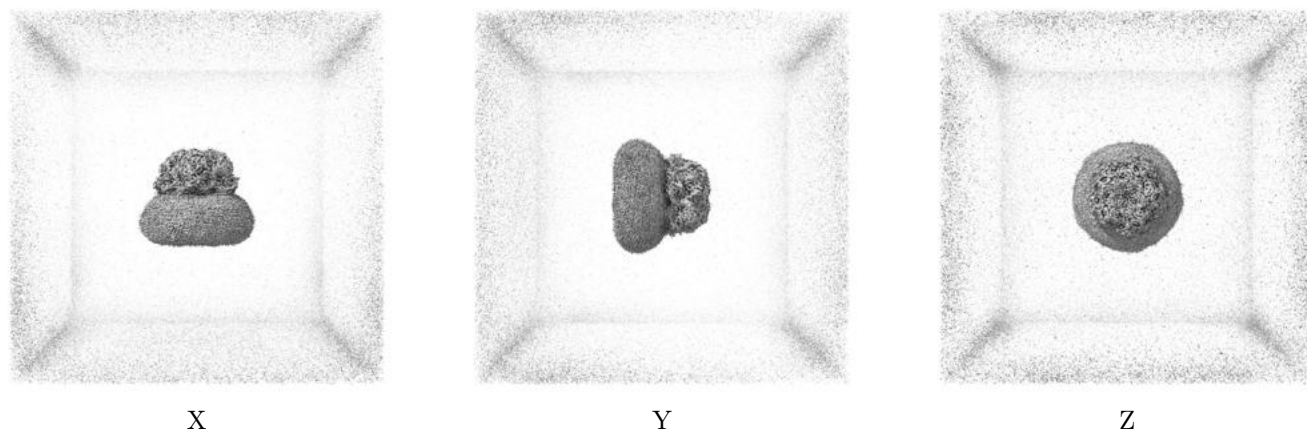
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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.

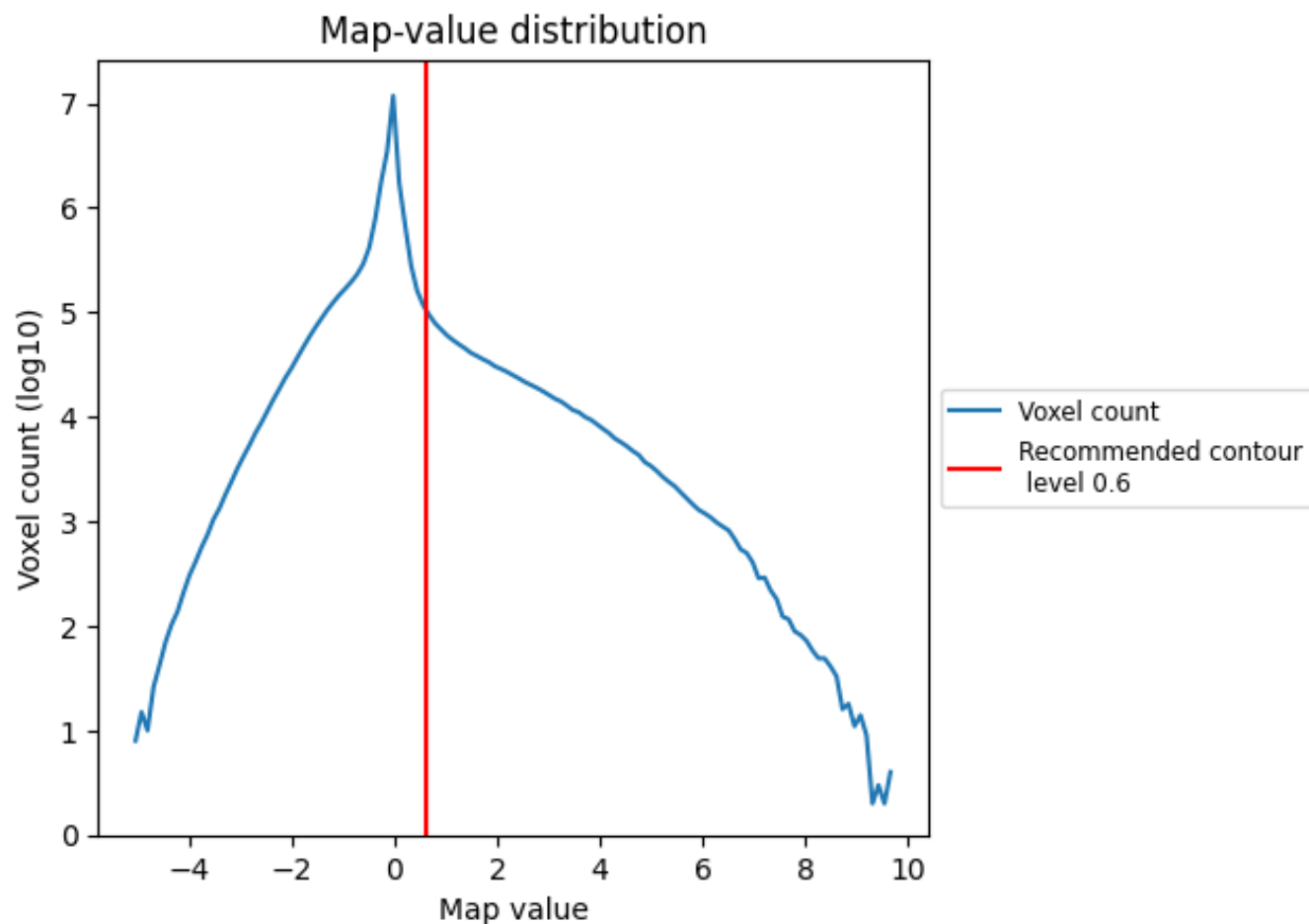
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

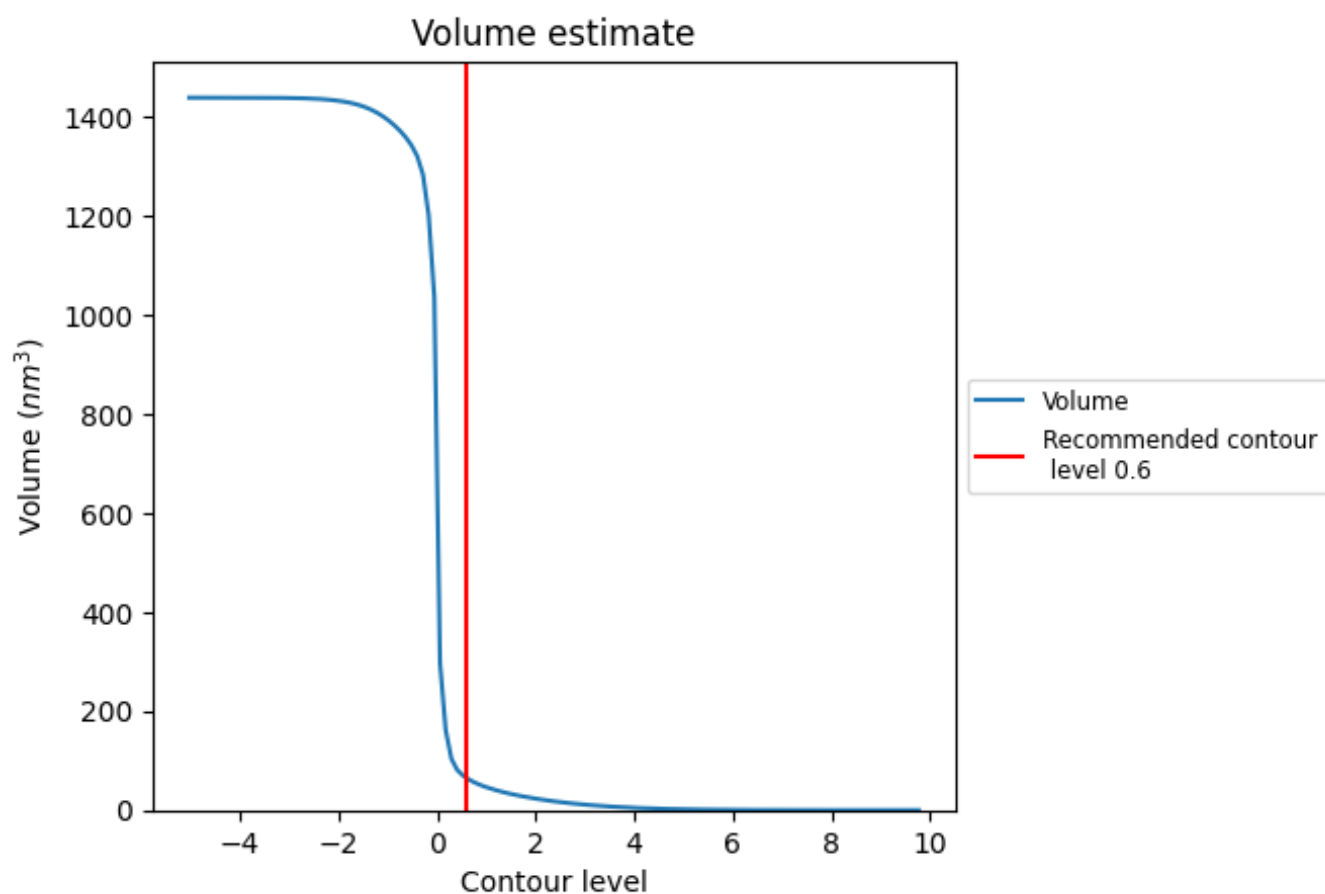
This section contains the results of statistical analysis of the map.

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.

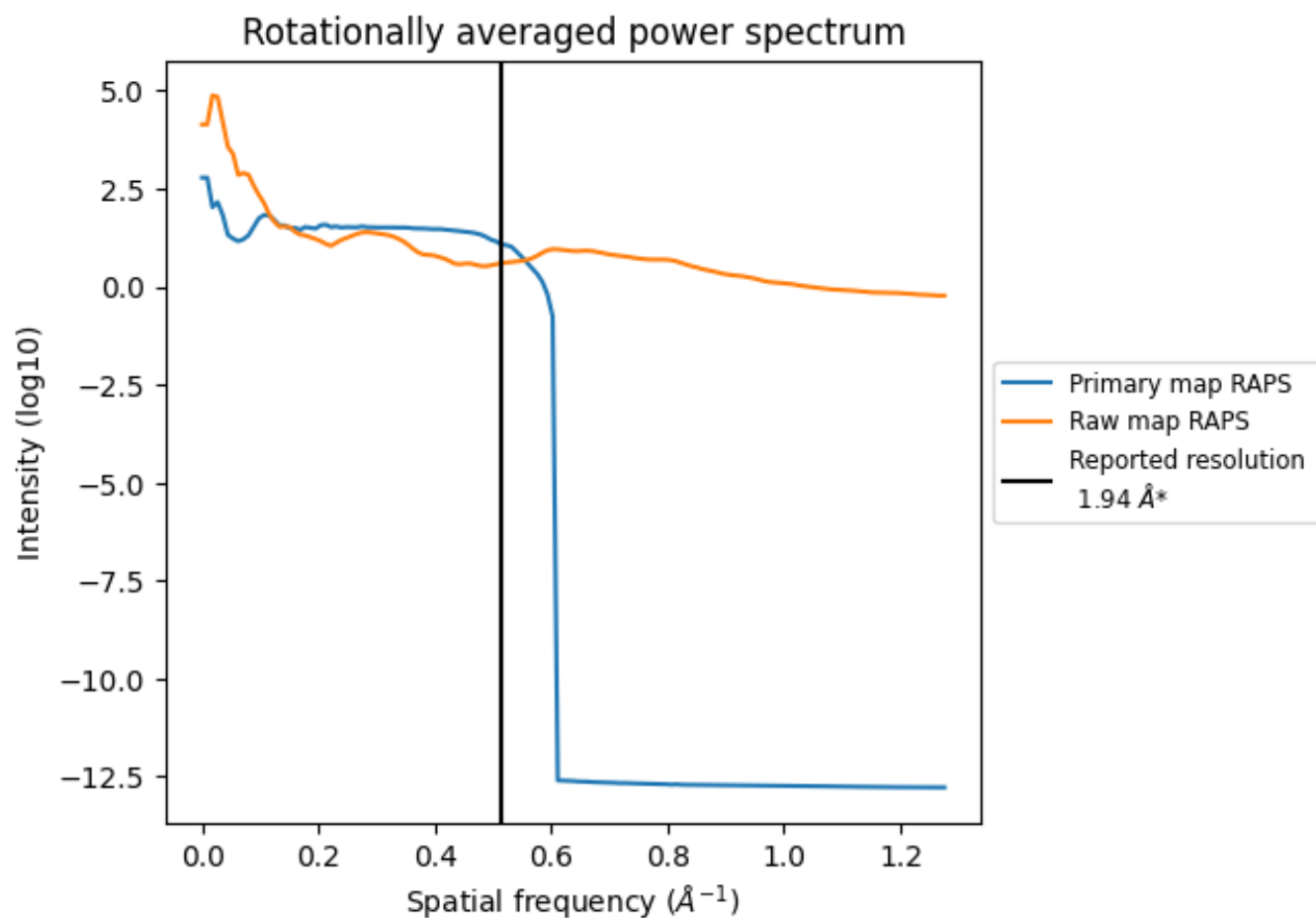
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 nm³; this corresponds to an approximate mass of 58 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 ⓘ

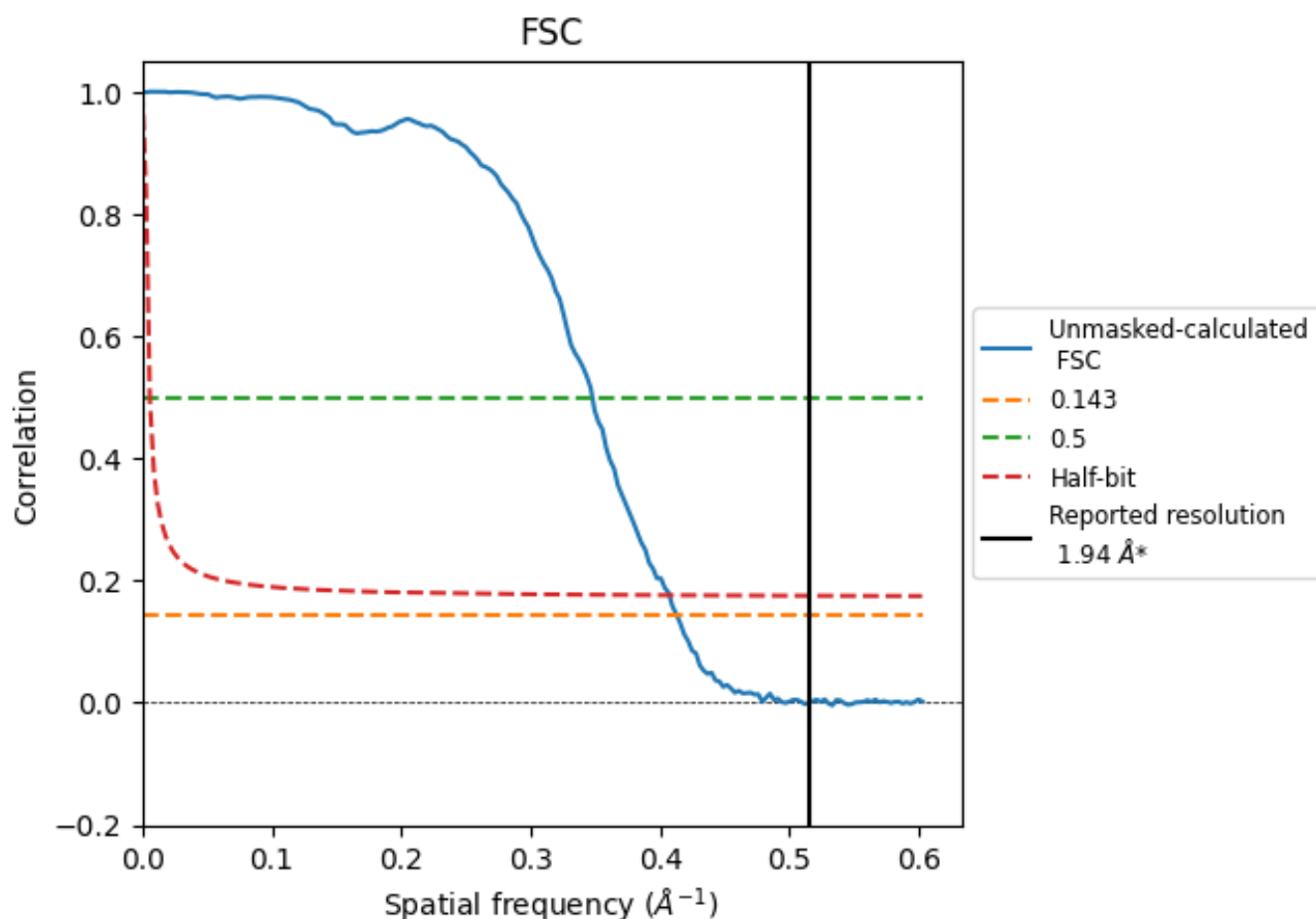


*Reported resolution corresponds to spatial frequency of 0.515 Å⁻¹

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 $0.515 \text{ \AA}^{-1}$

7.2 Resolution estimates [i](#)

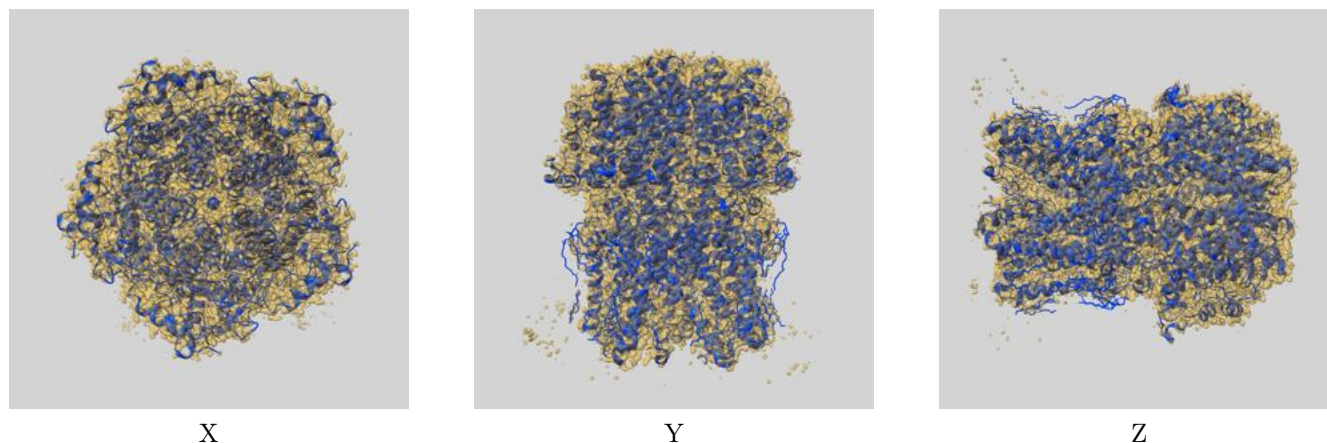
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.94	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.42	2.88	2.46

*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 2.42 differs from the reported value 1.94 by more than 10 %

8 Map-model fit [i](#)

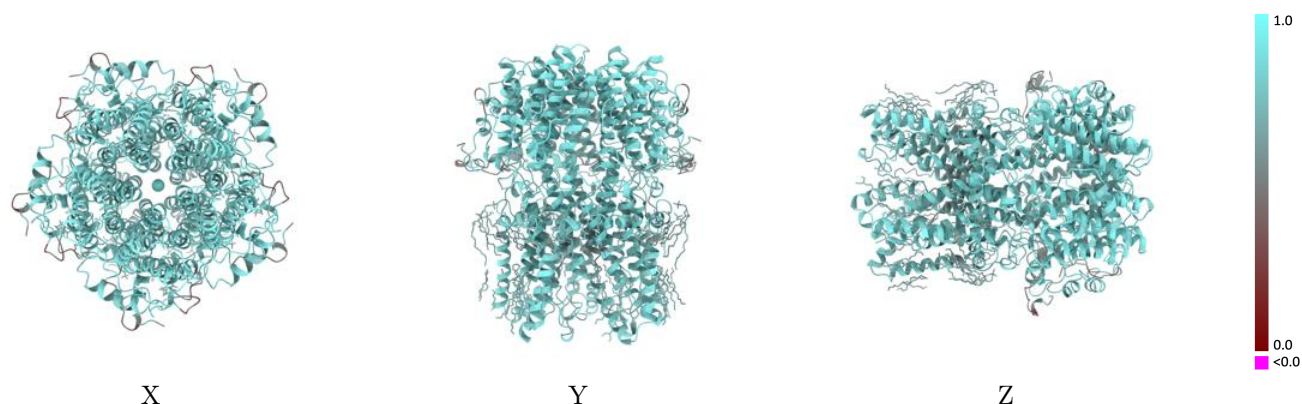
This section contains information regarding the fit between EMDB map EMD-27130 and PDB model 8D1H. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



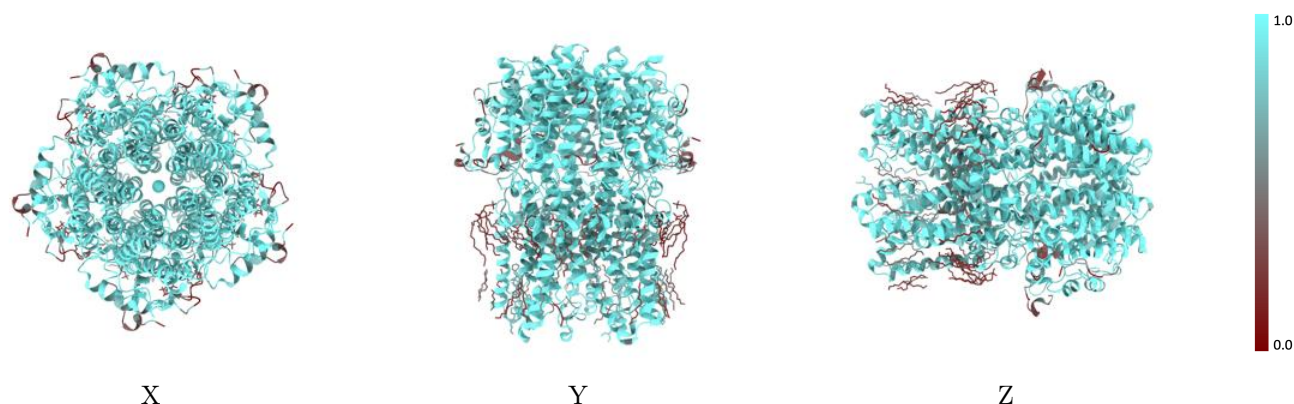
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



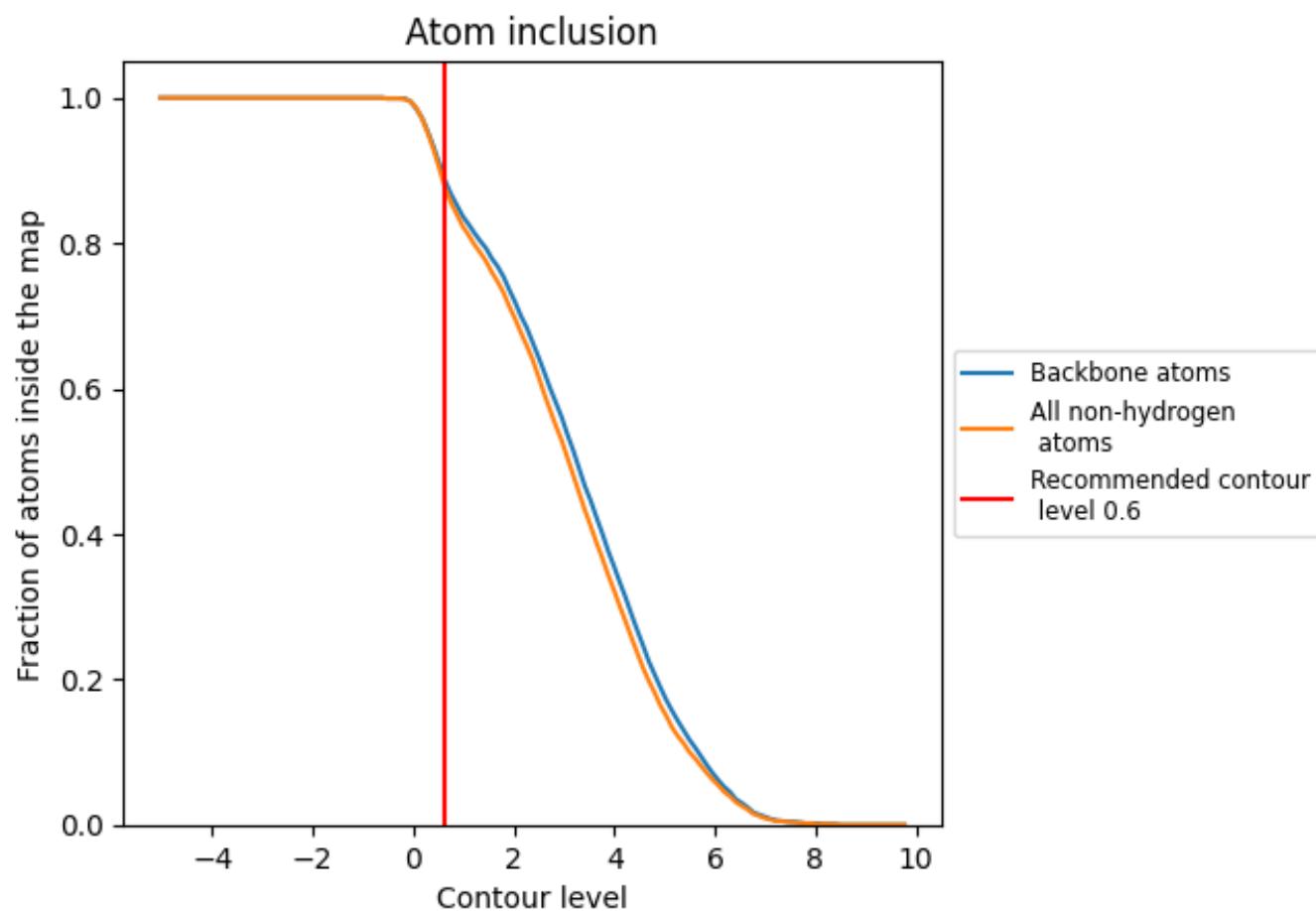
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

8.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8830	0.7800
A	0.8850	0.7810
B	0.8820	0.7780
C	0.8850	0.7790
D	0.8840	0.7810
E	0.8830	0.7800

