



Full wwPDB EM Validation Report ⓘ

Dec 30, 2024 – 02:09 PM EST

PDB ID : 8D1E
EMDB ID : EMD-27127
Title : hBest2 1uM Ca²⁺ (Ca²⁺-bound) closed state
Authors : Owji, A.P.; Kittredge, A.; Hendrickson, W.A.; Tingting, Y.
Deposited on : 2022-05-27
Resolution : 1.78 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
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) : 2.40

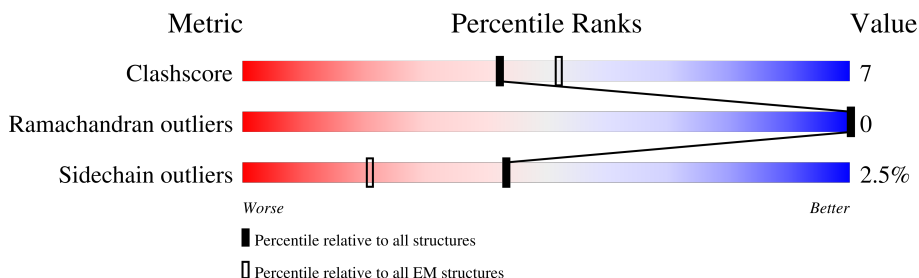
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	406	
1	B	406	
1	C	406	
1	D	406	
1	E	406	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17600 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.

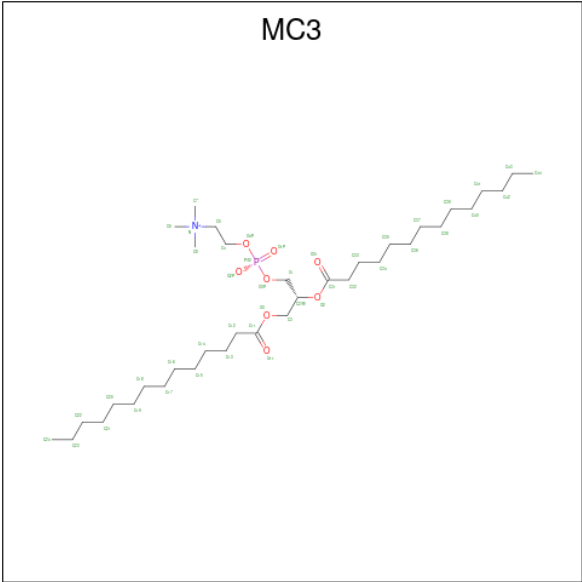
- Molecule 1 is a protein called Bestrophin-2.

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

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	D	1	Total	Ca	0
			1	1	
2	E	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	
2	A	1	Total	Ca	0
			1	1	
2	B	1	Total	Ca	0
			1	1	

- Molecule 3 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: MC3) (formula: C₃₆H₇₂NO₈P).



Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	O	P	0
			40	31	8	1	
3	D	1	Total	C	O	P	0
			40	31	8	1	
3	D	1	Total	C	O	P	0
			40	31	8	1	
3	D	1	Total	C			0
			14	14			
3	D	1	Total	C			0
			14	14			
3	D	1	Total	C			0
			12	12			
3	D	1	Total	C			0
			14	14			
3	D	1	Total	C			0
			12	12			
3	D	1	Total	C			0
			8	8			
3	D	1	Total	C			0
			14	14			
3	E	1	Total	C	O	P	0
			40	31	8	1	
3	E	1	Total	C	O	P	0
			40	31	8	1	
3	E	1	Total	C	O	P	0
			40	31	8	1	
3	E	1	Total	C			0
			14	14			

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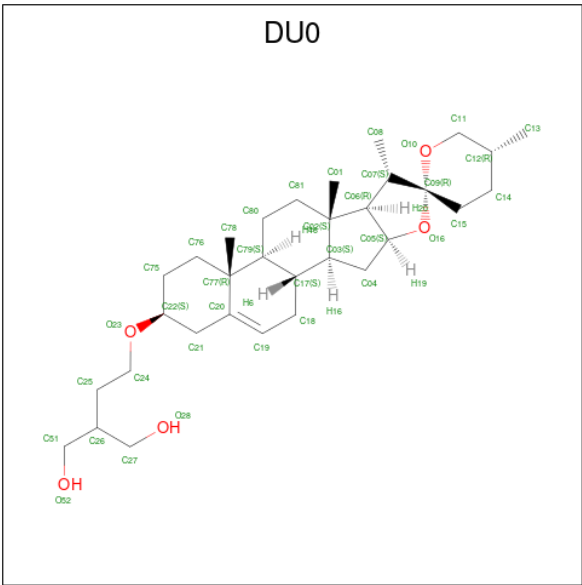
Mol	Chain	Residues	Atoms				AltConf
3	E	1	Total	C			0
			14	14			
3	E	1	Total	C			0
			12	12			
3	E	1	Total	C			0
			14	14			
3	E	1	Total	C			0
			12	12			
3	E	1	Total	C			0
			8	8			
3	E	1	Total	C			0
			14	14			
3	C	1	Total	C			0
			14	14			
3	C	1	Total	C	O	P	0
			40	31	8	1	
3	C	1	Total	C	O	P	0
			40	31	8	1	
3	C	1	Total	C	O	P	0
			40	31	8	1	
3	C	1	Total	C			0
			14	14			
3	C	1	Total	C			0
			14	14			
3	C	1	Total	C			0
			12	12			
3	C	1	Total	C			0
			14	14			
3	C	1	Total	C			0
			12	12			
3	C	1	Total	C			0
			8	8			
3	A	1	Total	C	O	P	0
			40	31	8	1	
3	A	1	Total	C	O	P	0
			40	31	8	1	
3	A	1	Total	C	O	P	0
			40	31	8	1	
3	A	1	Total	C			0
			14	14			
3	A	1	Total	C			0
			14	14			

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C			0
			12	12			
3	A	1	Total	C			0
			14	14			
3	A	1	Total	C			0
			12	12			
3	A	1	Total	C			0
			8	8			
3	A	1	Total	C			0
			14	14			
3	B	1	Total	C			0
			14	14			
3	B	1	Total	C	O	P	0
			40	31	8	1	
3	B	1	Total	C	O	P	0
			40	31	8	1	
3	B	1	Total	C	O	P	0
			40	31	8	1	
3	B	1	Total	C			0
			14	14			
3	B	1	Total	C			0
			14	14			
3	B	1	Total	C			0
			12	12			
3	B	1	Total	C			0
			14	14			
3	B	1	Total	C			0
			12	12			
3	B	1	Total	C			0
			8	8			

- Molecule 4 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 (three-letter code: DU0) (formula: C₃₂H₅₂O₅).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	D	125	Total	O	0
			125	125	
6	E	126	Total	O	0
			126	126	
6	C	126	Total	O	0
			126	126	

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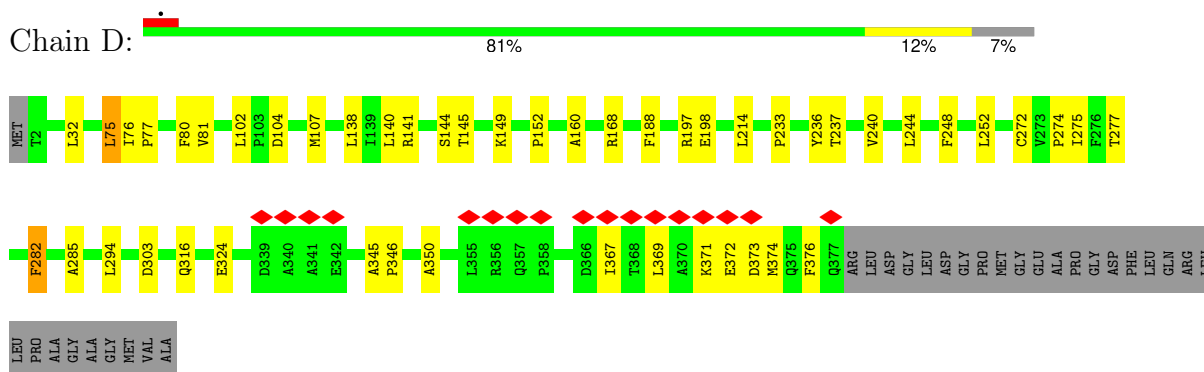
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Mol	Chain	Residues	Atoms		AltConf
6	A	126	Total 126	O 126	0
6	B	126	Total 126	O 126	0

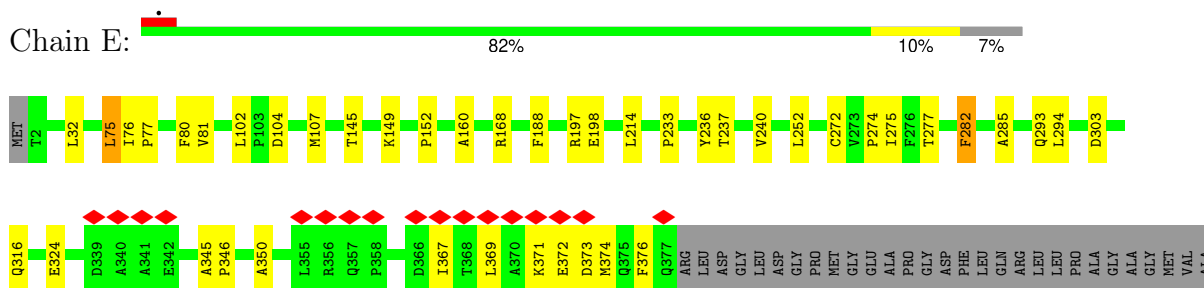
3 Residue-property plots [i](#)

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

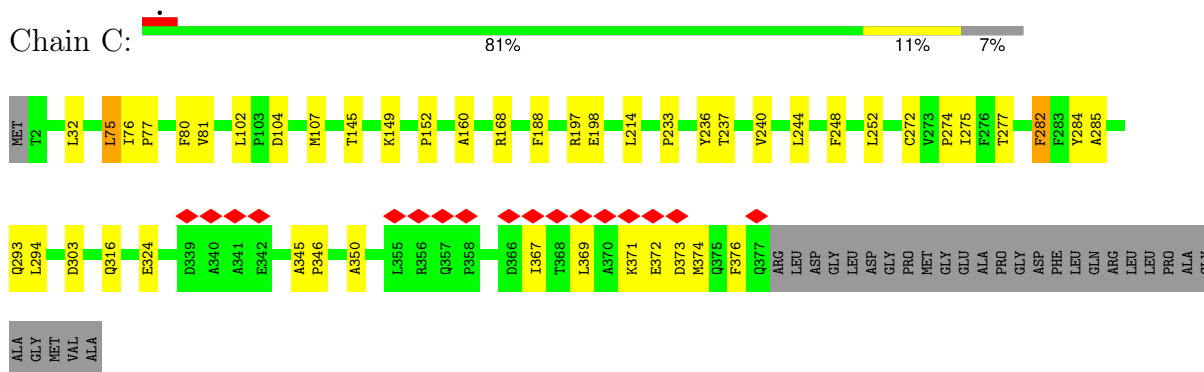
• Molecule 1: Bestrophin-2



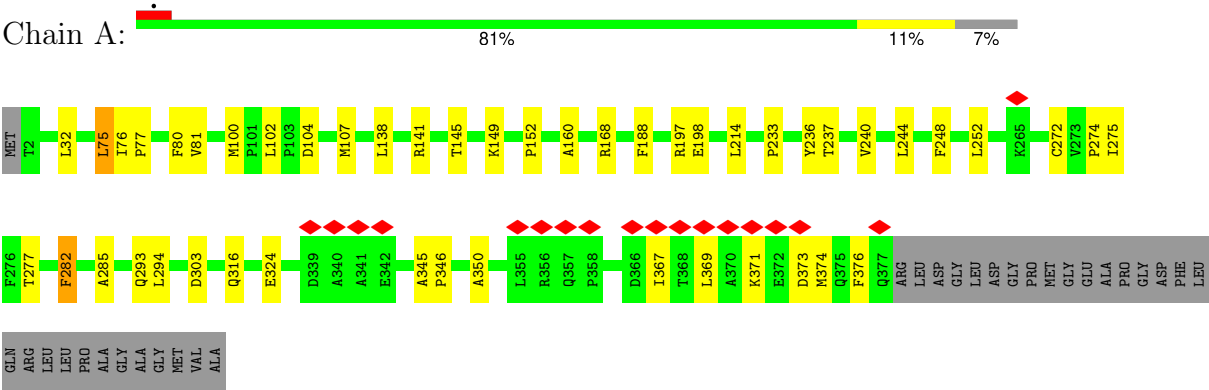
• Molecule 1: Bestrophin-2



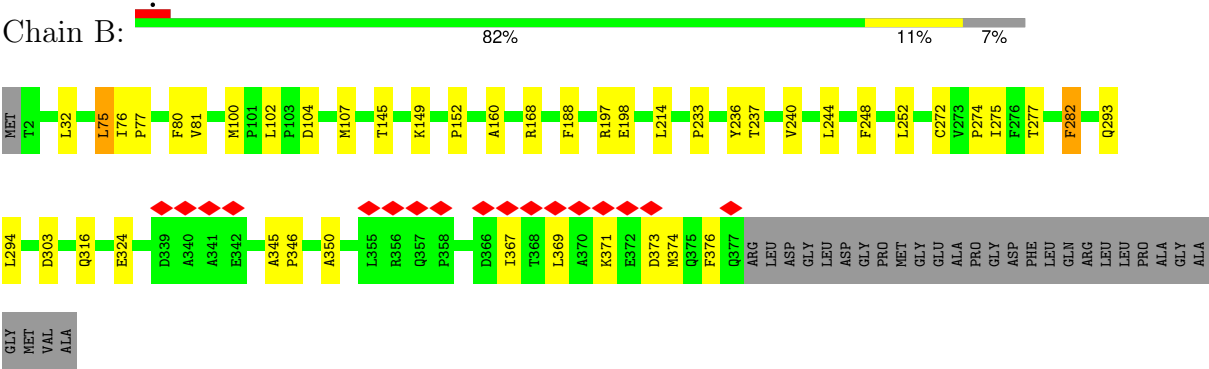
• Molecule 1: Bestrophin-2



• Molecule 1: Bestrophin-2



• Molecule 1: Bestrophin-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	399281	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	16.422	Depositor
Minimum map value	-5.979	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.668	Depositor
Recommended contour level	0.858	Depositor
Map size (\AA)	109.56, 109.56, 109.56	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.40577778, 0.40577778, 0.40577778	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MC3, DU0, CL, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/3185	0.62	0/4323
1	B	0.62	0/3185	0.62	0/4323
1	C	0.62	0/3185	0.62	0/4323
1	D	0.62	0/3185	0.62	0/4323
1	E	0.62	0/3185	0.62	0/4323
All	All	0.62	0/15925	0.62	0/21615

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3096	0	3063	59	0
1	B	3096	0	3063	56	0
1	C	3096	0	3063	58	0
1	D	3096	0	3063	54	0
1	E	3096	0	3063	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	208	0	346	8	0
3	B	208	0	346	8	0
3	C	208	0	346	8	0
3	D	208	0	346	8	0
3	E	208	0	346	8	0
4	A	37	52	0	3	0
4	B	37	52	0	3	0
4	C	37	52	0	3	0
4	D	37	52	0	3	0
4	E	37	52	0	3	0
5	A	1	0	0	0	0
6	A	126	0	0	9	0
6	B	126	0	0	9	0
6	C	126	0	0	7	0
6	D	125	0	0	3	0
6	E	126	0	0	8	0
All	All	17340	260	17045	220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (220) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:504:MC3:H441	3:E:502:MC3:H212	1.18	1.17
3:D:502:MC3:H212	3:C:505:MC3:H441	1.18	1.17
3:C:503:MC3:H212	3:B:505:MC3:H441	1.18	1.17
3:E:504:MC3:H441	3:A:502:MC3:H212	1.18	1.12
3:A:504:MC3:H441	3:B:503:MC3:H212	1.18	1.10
1:D:252:LEU:HD23	4:D:511:DU0:C13	1.97	0.95
1:C:252:LEU:HD23	4:C:512:DU0:C13	1.97	0.95
1:E:252:LEU:HD23	4:E:511:DU0:C13	1.97	0.95
1:B:252:LEU:HD23	4:B:512:DU0:C13	1.97	0.95
1:A:252:LEU:HD23	4:A:511:DU0:C13	1.97	0.93
3:A:504:MC3:H441	3:B:503:MC3:C21	2.05	0.87
3:D:504:MC3:H441	3:E:502:MC3:C21	2.05	0.86
1:C:77:PRO:HG3	1:B:75:LEU:HD13	1.57	0.86
3:C:503:MC3:C21	3:B:505:MC3:H441	2.05	0.86
1:D:77:PRO:HG3	1:C:75:LEU:HD13	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:LEU:CD2	6:E:709:HOH:O	2.22	0.86
3:E:504:MC3:H441	3:A:502:MC3:C21	2.05	0.85
1:A:75:LEU:HD13	1:B:77:PRO:HG3	1.57	0.85
1:D:75:LEU:HD13	1:E:77:PRO:HG3	1.57	0.85
1:E:75:LEU:HD13	1:A:77:PRO:HG3	1.57	0.84
1:A:102:LEU:CD2	6:A:702:HOH:O	2.27	0.82
1:A:252:LEU:CD2	4:A:511:DU0:C13	2.57	0.82
1:E:252:LEU:CD2	4:E:511:DU0:C13	2.57	0.82
1:B:252:LEU:CD2	4:B:512:DU0:C13	2.57	0.82
1:D:252:LEU:CD2	4:D:511:DU0:C13	2.57	0.81
1:C:252:LEU:CD2	4:C:512:DU0:C13	2.57	0.81
3:D:502:MC3:C21	3:C:505:MC3:H441	2.05	0.81
1:C:102:LEU:CD2	6:C:706:HOH:O	2.29	0.80
1:E:102:LEU:HD23	6:E:709:HOH:O	1.82	0.79
1:C:102:LEU:HD23	6:C:706:HOH:O	1.86	0.76
1:A:102:LEU:HD23	6:A:702:HOH:O	1.83	0.76
1:B:102:LEU:CD2	6:B:702:HOH:O	2.36	0.74
1:D:75:LEU:HD12	1:D:76:ILE:N	2.03	0.73
1:A:75:LEU:HD12	1:A:76:ILE:N	2.03	0.73
1:B:75:LEU:HD12	1:B:76:ILE:N	2.03	0.73
1:E:75:LEU:HD12	1:E:76:ILE:N	2.03	0.72
1:C:75:LEU:HD12	1:C:76:ILE:N	2.03	0.72
1:B:102:LEU:HD23	6:B:702:HOH:O	1.89	0.72
1:D:102:LEU:CD2	6:D:703:HOH:O	2.38	0.71
1:D:374:MET:HE3	1:A:152:PRO:HB2	1.74	0.69
1:E:374:MET:HE3	1:B:152:PRO:HB2	1.74	0.69
3:D:504:MC3:C44	3:E:502:MC3:H212	2.11	0.68
1:C:152:PRO:HB2	1:A:374:MET:HE3	1.76	0.67
1:D:152:PRO:HB2	1:B:374:MET:HE3	1.76	0.67
1:D:102:LEU:HD23	6:D:703:HOH:O	1.93	0.66
3:A:504:MC3:C44	3:B:503:MC3:H212	2.12	0.66
3:D:502:MC3:H212	3:C:505:MC3:C44	2.11	0.64
1:A:80:PHE:CZ	1:B:80:PHE:HZ	2.16	0.64
1:D:80:PHE:HZ	1:C:80:PHE:CZ	2.16	0.64
1:C:80:PHE:HZ	1:B:80:PHE:CZ	2.16	0.63
1:E:80:PHE:CZ	1:A:80:PHE:HZ	2.16	0.63
1:D:80:PHE:CZ	1:E:80:PHE:HZ	2.16	0.63
1:D:294:LEU:HD11	1:E:233:PRO:HG2	1.82	0.62
1:A:81:VAL:HG22	1:A:240[A]:VAL:HG12	1.82	0.62
1:D:81:VAL:HG22	1:D:240[A]:VAL:HG12	1.82	0.62
1:C:233:PRO:HG2	1:B:294:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:LEU:HD11	1:A:233:PRO:HG2	1.82	0.61
1:B:81:VAL:HG22	1:B:240[A]:VAL:HG12	1.82	0.61
1:D:233:PRO:HG2	1:C:294:LEU:HD11	1.82	0.61
1:C:81:VAL:HG22	1:C:240[A]:VAL:HG12	1.82	0.60
1:E:81:VAL:HG22	1:E:240[A]:VAL:HG12	1.82	0.60
1:A:294:LEU:HD11	1:B:233:PRO:HG2	1.82	0.60
3:E:504:MC3:C44	3:A:502:MC3:H212	2.12	0.59
1:A:80:PHE:CZ	1:B:80:PHE:CZ	2.92	0.58
1:D:80:PHE:CZ	1:E:80:PHE:CZ	2.92	0.58
1:E:80:PHE:CZ	1:A:80:PHE:CZ	2.92	0.57
1:E:102:LEU:HD21	6:E:709:HOH:O	1.98	0.57
1:E:152:PRO:HB2	1:C:374:MET:HE3	1.87	0.57
1:C:80:PHE:CZ	1:B:80:PHE:CZ	2.92	0.57
1:D:80:PHE:CZ	1:C:80:PHE:CZ	2.92	0.57
1:E:152:PRO:CG	1:C:374:MET:HE2	2.36	0.56
1:A:293:GLN:CB	6:A:683:HOH:O	2.55	0.55
1:B:252:LEU:HD21	4:B:512:DU0:C13	2.37	0.55
1:C:252:LEU:HD21	4:C:512:DU0:C13	2.37	0.55
1:A:293:GLN:HB2	6:A:683:HOH:O	2.06	0.54
1:B:293:GLN:HB2	6:B:683:HOH:O	2.07	0.54
1:E:252:LEU:HD21	4:E:511:DU0:C13	2.37	0.54
1:C:293:GLN:CB	6:C:677:HOH:O	2.56	0.54
1:C:293:GLN:HB2	6:C:677:HOH:O	2.08	0.53
3:C:503:MC3:H212	3:B:505:MC3:C44	2.12	0.52
1:A:102:LEU:HD21	6:A:702:HOH:O	2.02	0.52
1:E:80:PHE:CE2	1:A:80:PHE:CE2	2.97	0.52
1:D:252:LEU:HD21	4:D:511:DU0:C13	2.37	0.52
1:E:81:VAL:HG22	1:E:240[B]:VAL:HG22	1.92	0.52
1:A:80:PHE:CE2	1:B:80:PHE:CE2	2.97	0.52
1:B:293:GLN:CB	6:B:683:HOH:O	2.56	0.52
1:C:80:PHE:CE2	1:B:80:PHE:CE2	2.97	0.52
1:C:293:GLN:CG	6:C:677:HOH:O	2.58	0.52
1:A:81:VAL:HG22	1:A:240[B]:VAL:HG22	1.92	0.52
1:A:252:LEU:HD21	4:A:511:DU0:C13	2.37	0.52
1:D:80:PHE:CE2	1:E:80:PHE:CE2	2.97	0.51
1:D:81:VAL:HG22	1:D:240[B]:VAL:HG22	1.92	0.51
1:E:293:GLN:CB	6:E:678:HOH:O	2.57	0.51
1:D:80:PHE:CE2	1:C:80:PHE:CE2	2.97	0.51
1:B:81:VAL:HG22	1:B:240[B]:VAL:HG22	1.92	0.51
1:E:293:GLN:HB2	6:E:678:HOH:O	2.09	0.51
1:A:293:GLN:CG	6:A:683:HOH:O	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLN:CG	6:B:683:HOH:O	2.59	0.50
1:E:374:MET:CE	1:B:152:PRO:HB2	2.42	0.50
1:E:152:PRO:HB2	1:C:374:MET:CE	2.41	0.50
1:D:374:MET:CE	1:A:152:PRO:HB2	2.41	0.50
1:D:152:PRO:HB2	1:B:374:MET:CE	2.41	0.49
1:C:81:VAL:HG22	1:C:240[B]:VAL:HG22	1.92	0.49
1:E:293:GLN:CG	6:E:678:HOH:O	2.60	0.49
1:C:152:PRO:HB2	1:A:374:MET:CE	2.41	0.49
1:D:75:LEU:HD22	1:E:77:PRO:HG2	1.95	0.49
1:E:152:PRO:HG2	1:C:374:MET:HE2	1.94	0.49
1:A:75:LEU:HD22	1:B:77:PRO:HG2	1.95	0.49
1:E:75:LEU:HD22	1:A:77:PRO:HG2	1.95	0.49
1:D:77:PRO:HG2	1:C:75:LEU:HD22	1.95	0.48
1:C:152:PRO:CG	1:A:374:MET:HE2	2.43	0.48
1:D:272:CYS:O	1:D:272:CYS:SG	2.72	0.48
1:A:272:CYS:O	1:A:272:CYS:SG	2.72	0.48
1:C:77:PRO:HG2	1:B:75:LEU:HD22	1.95	0.47
1:E:272:CYS:O	1:E:272:CYS:SG	2.72	0.47
1:D:152:PRO:CG	1:B:374:MET:HE2	2.43	0.47
1:B:272:CYS:O	1:B:272:CYS:SG	2.72	0.47
1:C:272:CYS:O	1:C:272:CYS:SG	2.72	0.46
1:E:374:MET:HE2	1:B:152:PRO:CG	2.45	0.46
1:B:324:GLU:N	1:B:324:GLU:OE1	2.49	0.46
1:A:324:GLU:OE1	1:A:324:GLU:N	2.49	0.46
1:D:275:ILE:HD11	3:D:509:MC3:H442	1.98	0.46
1:C:275:ILE:HD11	3:C:510:MC3:H442	1.98	0.46
1:D:374:MET:HE2	1:A:152:PRO:CG	2.45	0.45
1:B:188:PHE:CD1	1:B:214:LEU:HD22	2.52	0.45
1:E:188:PHE:CD1	1:E:214:LEU:HD22	2.52	0.45
1:C:152:PRO:HG2	1:A:374:MET:HE2	1.97	0.45
1:D:374:MET:HE2	1:A:152:PRO:HG2	1.99	0.45
1:D:152:PRO:HG2	1:B:374:MET:HE2	1.98	0.45
1:D:188:PHE:CD1	1:D:214:LEU:HD22	2.52	0.45
1:E:324:GLU:N	1:E:324:GLU:OE1	2.49	0.45
1:C:324:GLU:N	1:C:324:GLU:OE1	2.49	0.45
1:B:102:LEU:HD21	6:B:702:HOH:O	2.13	0.45
1:D:324:GLU:OE1	1:D:324:GLU:N	2.49	0.45
1:C:188:PHE:CD1	1:C:214:LEU:HD22	2.52	0.45
1:A:188:PHE:CD1	1:A:214:LEU:HD22	2.52	0.45
1:E:374:MET:HE2	1:B:152:PRO:HG2	1.99	0.45
1:E:275:ILE:HD11	3:E:509:MC3:H442	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ILE:CD1	3:D:509:MC3:H442	2.47	0.44
1:E:275:ILE:CD1	3:E:509:MC3:H442	2.47	0.44
1:B:275:ILE:HD11	3:B:510:MC3:H442	1.98	0.44
1:E:104:ASP:O	1:E:107:MET:HG2	2.17	0.44
1:A:275:ILE:HD11	3:A:509:MC3:H442	1.98	0.44
1:B:104:ASP:O	1:B:107:MET:HG2	2.17	0.44
1:B:275:ILE:CD1	3:B:510:MC3:H442	2.47	0.44
1:C:104:ASP:O	1:C:107:MET:HG2	2.17	0.44
1:C:346:PRO:HB2	1:B:376:PHE:CD1	2.54	0.43
1:C:350:ALA:HB2	1:B:373:ASP:HB3	2.00	0.43
1:C:275:ILE:CD1	3:C:510:MC3:H442	2.47	0.43
1:A:275:ILE:CD1	3:A:509:MC3:H442	2.47	0.43
1:D:104:ASP:O	1:D:107:MET:HG2	2.17	0.43
1:D:350:ALA:HB2	1:C:373:ASP:HB3	2.00	0.43
1:E:373:ASP:HB3	1:A:350:ALA:HB2	2.00	0.43
1:C:293:GLN:HG3	6:C:677:HOH:O	2.16	0.43
1:A:373:ASP:HB3	1:B:350:ALA:HB2	2.00	0.43
1:D:373:ASP:HB3	1:E:350:ALA:HB2	2.00	0.43
1:D:376:PHE:CD1	1:E:346:PRO:HB2	2.53	0.43
1:E:237:THR:O	1:E:240[A]:VAL:HG22	2.19	0.43
1:B:293:GLN:HG3	6:B:683:HOH:O	2.18	0.43
1:D:367:ILE:HD11	1:A:145:THR:HG22	2.01	0.42
1:E:376:PHE:CD1	1:A:346:PRO:HB2	2.53	0.42
1:A:293:GLN:HG3	6:A:683:HOH:O	2.18	0.42
1:D:369:LEU:HD11	1:A:149:LYS:HA	2.01	0.42
1:E:149:LYS:HA	1:C:369:LEU:HD11	2.01	0.42
1:A:376:PHE:CD1	1:B:346:PRO:HB2	2.54	0.42
1:C:149:LYS:HA	1:A:369:LEU:HD11	2.02	0.42
1:A:104:ASP:O	1:A:107:MET:HG2	2.17	0.42
1:D:237:THR:O	1:D:240[A]:VAL:HG22	2.20	0.42
1:D:346:PRO:HB2	1:C:376:PHE:CD1	2.53	0.42
1:D:32:LEU:HD23	1:D:282:PHE:CD1	2.55	0.42
1:E:369:LEU:HD11	1:B:149:LYS:HA	2.01	0.42
1:A:237:THR:O	1:A:240[A]:VAL:HG22	2.20	0.42
1:C:237:THR:O	1:C:240[A]:VAL:HG22	2.19	0.42
1:A:32:LEU:HD23	1:A:282:PHE:CD1	2.55	0.42
1:E:145:THR:HG22	1:C:367:ILE:HD11	2.01	0.41
1:B:32:LEU:HD23	1:B:282:PHE:CD1	2.55	0.41
1:C:198:GLU:HG3	6:C:637:HOH:O	2.21	0.41
1:C:372:GLU:OE1	1:C:372:GLU:N	2.51	0.41
1:D:198:GLU:HG3	6:D:637:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:GLN:HG3	6:E:678:HOH:O	2.18	0.41
1:E:345:ALA:HB1	1:A:160:ALA:HB1	2.03	0.41
1:D:345:ALA:HB1	1:E:160:ALA:HB1	2.03	0.41
1:E:274:PRO:HB2	1:E:277:THR:HB	2.02	0.41
1:C:32:LEU:HD23	1:C:282:PHE:CD1	2.55	0.41
1:B:237:THR:O	1:B:240[A]:VAL:HG22	2.19	0.41
1:E:198:GLU:HG3	6:E:636:HOH:O	2.21	0.41
1:C:160:ALA:HB1	1:B:345:ALA:HB1	2.02	0.41
1:A:198:GLU:HG3	6:A:637:HOH:O	2.21	0.41
1:D:145:THR:HG22	1:B:367:ILE:HD11	2.01	0.41
1:D:149:LYS:HA	1:B:369:LEU:HD11	2.02	0.41
1:A:274:PRO:HB2	1:A:277:THR:HB	2.02	0.41
1:D:274:PRO:HB2	1:D:277:THR:HB	2.02	0.41
1:C:145:THR:HG22	1:A:367:ILE:HD11	2.01	0.41
1:A:32:LEU:HD11	1:A:285:ALA:HB1	2.03	0.41
1:D:369:LEU:HD11	1:A:149:LYS:HG2	2.03	0.41
1:D:160:ALA:HB1	1:C:345:ALA:HB1	2.03	0.41
1:E:149:LYS:HG2	1:C:369:LEU:HD11	2.03	0.41
1:C:32:LEU:HD11	1:C:285:ALA:HB1	2.02	0.41
1:C:149:LYS:HG2	1:A:369:LEU:HD11	2.03	0.41
1:C:244:LEU:HD11	1:C:248:PHE:CZ	2.56	0.41
1:C:274:PRO:HB2	1:C:277:THR:HB	2.02	0.41
1:A:244:LEU:HD11	1:A:248:PHE:CZ	2.56	0.41
1:B:244:LEU:HD11	1:B:248:PHE:CZ	2.56	0.41
1:B:274:PRO:HB2	1:B:277:THR:HB	2.02	0.41
1:E:32:LEU:HD23	1:E:282:PHE:CD1	2.55	0.41
1:E:369:LEU:HD11	1:B:149:LYS:HG2	2.03	0.41
1:A:138:LEU:O	1:A:141:ARG:HG2	2.21	0.41
1:A:345:ALA:HB1	1:B:160:ALA:HB1	2.03	0.41
1:B:100:MET:HG2	6:B:702:HOH:O	2.21	0.41
1:C:75:LEU:HB2	1:C:284:TYR:OH	2.21	0.40
1:D:138:LEU:O	1:D:141:ARG:HG2	2.21	0.40
1:D:32:LEU:HD11	1:D:285:ALA:HB1	2.03	0.40
1:D:140:LEU:O	1:D:144:SER:N	2.52	0.40
1:D:244:LEU:HD11	1:D:248:PHE:CZ	2.56	0.40
1:E:372:GLU:OE1	1:E:372:GLU:N	2.51	0.40
1:B:198:GLU:HG3	6:B:636:HOH:O	2.21	0.40
1:E:32:LEU:HD11	1:E:285:ALA:HB1	2.03	0.40
1:A:100:MET:HG2	6:A:702:HOH:O	2.21	0.40
1:D:372:GLU:OE1	1:D:372:GLU:N	2.51	0.40
1:E:367:ILE:HD11	1:B:145:THR:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/406 (93%)	370 (98%)	6 (2%)	0	100	100
1	B	376/406 (93%)	370 (98%)	6 (2%)	0	100	100
1	C	376/406 (93%)	370 (98%)	6 (2%)	0	100	100
1	D	376/406 (93%)	370 (98%)	6 (2%)	0	100	100
1	E	376/406 (93%)	370 (98%)	6 (2%)	0	100	100
All	All	1880/2030 (93%)	1850 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/346 (95%)	320 (98%)	8 (2%)	44	24
1	B	328/346 (95%)	320 (98%)	8 (2%)	44	24
1	C	328/346 (95%)	320 (98%)	8 (2%)	44	24
1	D	328/346 (95%)	320 (98%)	8 (2%)	44	24
1	E	328/346 (95%)	320 (98%)	8 (2%)	44	24
All	All	1640/1730 (95%)	1600 (98%)	40 (2%)	43	24

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	75	LEU
1	D	168	ARG
1	D	197	ARG
1	D	236	TYR
1	D	282	PHE
1	D	303	ASP
1	D	316	GLN
1	D	371	LYS
1	E	75	LEU
1	E	168	ARG
1	E	197	ARG
1	E	236	TYR
1	E	282	PHE
1	E	303	ASP
1	E	316	GLN
1	E	371	LYS
1	C	75	LEU
1	C	168	ARG
1	C	197	ARG
1	C	236	TYR
1	C	282	PHE
1	C	303	ASP
1	C	316	GLN
1	C	371	LYS
1	A	75	LEU
1	A	168	ARG
1	A	197	ARG
1	A	236	TYR
1	A	282	PHE
1	A	303	ASP
1	A	316	GLN
1	A	371	LYS
1	B	75	LEU
1	B	168	ARG
1	B	197	ARG
1	B	236	TYR
1	B	282	PHE
1	B	303	ASP
1	B	316	GLN
1	B	371	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 61 ligands modelled in this entry, 6 are monoatomic - leaving 55 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	$\# Z > 2$
3	MC3	E	503	-	39,39,45	1.03	5 (12%)	42,44,53	0.97	2 (4%)
3	MC3	E	506	-	13,13,45	0.33	0	12,12,53	0.67	0
3	MC3	E	502	-	39,39,45	1.09	5 (12%)	42,44,53	1.10	2 (4%)
3	MC3	B	506	-	13,13,45	0.37	0	12,12,53	0.59	0
3	MC3	B	510	-	11,11,45	0.32	0	10,10,53	0.67	0
3	MC3	C	504	-	39,39,45	1.03	5 (12%)	42,44,53	0.97	2 (4%)
3	MC3	A	503	-	39,39,45	1.04	5 (12%)	42,44,53	0.97	2 (4%)
3	MC3	C	510	-	11,11,45	0.32	0	10,10,53	0.67	0
3	MC3	D	509	-	11,11,45	0.32	0	10,10,53	0.67	0
3	MC3	E	507	-	11,11,45	0.32	0	10,10,53	0.73	0
3	MC3	D	508	-	13,13,45	0.34	0	12,12,53	0.63	0
3	MC3	A	505	-	13,13,45	0.37	0	12,12,53	0.59	0
3	MC3	B	511	-	7,7,45	0.32	0	6,6,53	0.67	0
3	MC3	E	504	-	39,39,45	1.04	5 (12%)	42,44,53	1.27	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MC3	C	501	-	13,13,45	0.30	0	12,12,53	0.79	0
3	MC3	C	511	-	7,7,45	0.32	0	6,6,53	0.67	0
3	MC3	B	509	-	13,13,45	0.34	0	12,12,53	0.63	0
3	MC3	A	502	-	39,39,45	1.10	5 (12%)	42,44,53	1.10	2 (4%)
3	MC3	D	507	-	11,11,45	0.32	0	10,10,53	0.73	0
3	MC3	C	505	-	39,39,45	1.04	5 (12%)	42,44,53	1.28	3 (7%)
3	MC3	B	508	-	11,11,45	0.32	0	10,10,53	0.73	0
4	DU0	A	511	-	42,42,42	0.33	0	64,66,66	0.47	0
3	MC3	E	509	-	11,11,45	0.32	0	10,10,53	0.67	0
3	MC3	E	512	-	13,13,45	0.30	0	12,12,53	0.79	0
3	MC3	D	504	-	39,39,45	1.04	5 (12%)	42,44,53	1.27	3 (7%)
3	MC3	A	510	-	7,7,45	0.32	0	6,6,53	0.67	0
3	MC3	E	508	-	13,13,45	0.34	0	12,12,53	0.63	0
3	MC3	A	504	-	39,39,45	1.03	5 (12%)	42,44,53	1.28	3 (7%)
3	MC3	B	507	-	13,13,45	0.33	0	12,12,53	0.67	0
4	DU0	E	511	-	42,42,42	0.32	0	64,66,66	0.46	0
3	MC3	D	505	-	13,13,45	0.37	0	12,12,53	0.59	0
4	DU0	C	512	-	42,42,42	0.33	0	64,66,66	0.47	0
3	MC3	C	507	-	13,13,45	0.33	0	12,12,53	0.67	0
3	MC3	C	506	-	13,13,45	0.37	0	12,12,53	0.59	0
3	MC3	D	502	-	39,39,45	1.10	5 (12%)	42,44,53	1.10	2 (4%)
3	MC3	A	512	-	13,13,45	0.30	0	12,12,53	0.80	0
3	MC3	D	506	-	13,13,45	0.33	0	12,12,53	0.67	0
3	MC3	E	510	-	7,7,45	0.32	0	6,6,53	0.67	0
3	MC3	B	504	-	39,39,45	1.03	5 (12%)	42,44,53	0.97	2 (4%)
4	DU0	D	511	-	42,42,42	0.33	0	64,66,66	0.46	0
3	MC3	B	501	-	13,13,45	0.30	0	12,12,53	0.80	0
3	MC3	B	503	-	39,39,45	1.10	5 (12%)	42,44,53	1.10	2 (4%)
3	MC3	A	509	-	11,11,45	0.33	0	10,10,53	0.67	0
3	MC3	A	508	-	13,13,45	0.33	0	12,12,53	0.63	0
3	MC3	C	503	-	39,39,45	1.10	5 (12%)	42,44,53	1.10	2 (4%)
3	MC3	D	503	-	39,39,45	1.03	5 (12%)	42,44,53	0.97	2 (4%)
3	MC3	C	509	-	13,13,45	0.34	0	12,12,53	0.63	0
3	MC3	B	505	-	39,39,45	1.04	5 (12%)	42,44,53	1.28	3 (7%)
3	MC3	E	505	-	13,13,45	0.37	0	12,12,53	0.59	0
3	MC3	A	506	-	13,13,45	0.34	0	12,12,53	0.67	0
3	MC3	C	508	-	11,11,45	0.32	0	10,10,53	0.73	0
3	MC3	A	507	-	11,11,45	0.32	0	10,10,53	0.73	0
4	DU0	B	512	-	42,42,42	0.32	0	64,66,66	0.46	0
3	MC3	D	510	-	7,7,45	0.32	0	6,6,53	0.67	0
3	MC3	D	512	-	13,13,45	0.30	0	12,12,53	0.79	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
3	MC3	E	503	-	-	21/41/41/49	-
3	MC3	E	506	-	-	8/11/11/49	-
3	MC3	E	502	-	-	21/41/41/49	-
3	MC3	B	506	-	-	6/11/11/49	-
3	MC3	B	510	-	-	4/9/9/49	-
3	MC3	C	504	-	-	21/41/41/49	-
3	MC3	A	503	-	-	21/41/41/49	-
3	MC3	C	510	-	-	4/9/9/49	-
3	MC3	D	509	-	-	4/9/9/49	-
3	MC3	E	507	-	-	4/9/9/49	-
3	MC3	D	508	-	-	7/11/11/49	-
3	MC3	A	505	-	-	6/11/11/49	-
3	MC3	B	511	-	-	3/5/5/49	-
3	MC3	E	504	-	-	19/41/41/49	-
3	MC3	C	501	-	-	4/11/11/49	-
3	MC3	C	511	-	-	3/5/5/49	-
3	MC3	B	509	-	-	7/11/11/49	-
3	MC3	A	502	-	-	21/41/41/49	-
3	MC3	D	507	-	-	4/9/9/49	-
3	MC3	C	505	-	-	19/41/41/49	-
3	MC3	B	508	-	-	4/9/9/49	-
4	DU0	A	511	-	-	3/10/98/98	0/6/6/6
3	MC3	E	509	-	-	4/9/9/49	-
3	MC3	E	512	-	-	4/11/11/49	-
3	MC3	D	504	-	-	19/41/41/49	-
3	MC3	A	510	-	-	3/5/5/49	-
3	MC3	E	508	-	-	7/11/11/49	-
3	MC3	A	504	-	-	19/41/41/49	-
3	MC3	B	507	-	-	8/11/11/49	-
4	DU0	E	511	-	-	3/10/98/98	0/6/6/6
3	MC3	D	505	-	-	6/11/11/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DU0	C	512	-	-	3/10/98/98	0/6/6/6
3	MC3	C	507	-	-	8/11/11/49	-
3	MC3	C	506	-	-	6/11/11/49	-
3	MC3	D	502	-	-	21/41/41/49	-
3	MC3	A	512	-	-	4/11/11/49	-
3	MC3	D	506	-	-	8/11/11/49	-
3	MC3	E	510	-	-	3/5/5/49	-
3	MC3	B	504	-	-	21/41/41/49	-
4	DU0	D	511	-	-	3/10/98/98	0/6/6/6
3	MC3	B	501	-	-	4/11/11/49	-
3	MC3	B	503	-	-	21/41/41/49	-
3	MC3	A	509	-	-	4/9/9/49	-
3	MC3	A	508	-	-	7/11/11/49	-
3	MC3	C	503	-	-	21/41/41/49	-
3	MC3	D	503	-	-	21/41/41/49	-
3	MC3	C	509	-	-	7/11/11/49	-
3	MC3	B	505	-	-	19/41/41/49	-
3	MC3	E	505	-	-	6/11/11/49	-
3	MC3	A	506	-	-	8/11/11/49	-
3	MC3	C	508	-	-	4/9/9/49	-
3	MC3	A	507	-	-	4/9/9/49	-
4	DU0	B	512	-	-	3/10/98/98	0/6/6/6
3	MC3	D	510	-	-	3/5/5/49	-
3	MC3	D	512	-	-	4/11/11/49	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	MC3	O3-C3	-2.85	1.38	1.45
3	B	504	MC3	P-O4P	2.84	1.65	1.54
3	B	503	MC3	O3-C3	-2.84	1.38	1.45
3	E	503	MC3	P-O4P	2.84	1.65	1.54
3	A	503	MC3	P-O4P	2.84	1.65	1.54
3	C	504	MC3	P-O4P	2.83	1.65	1.54
3	D	503	MC3	P-O4P	2.83	1.65	1.54
3	D	502	MC3	O3-C3	-2.83	1.38	1.45
3	C	503	MC3	O3-C3	-2.83	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	MC3	O3-C3	-2.80	1.38	1.45
3	A	502	MC3	P-O4P	2.78	1.65	1.54
3	C	503	MC3	P-O4P	2.78	1.65	1.54
3	E	502	MC3	P-O4P	2.78	1.65	1.54
3	B	503	MC3	P-O4P	2.78	1.65	1.54
3	D	502	MC3	P-O4P	2.78	1.65	1.54
3	C	505	MC3	P-O4P	2.74	1.65	1.54
3	B	505	MC3	P-O4P	2.74	1.65	1.54
3	D	504	MC3	P-O4P	2.73	1.65	1.54
3	E	504	MC3	P-O4P	2.73	1.64	1.54
3	A	504	MC3	P-O4P	2.72	1.64	1.54
3	B	503	MC3	O2-C2	-2.67	1.40	1.46
3	D	502	MC3	O2-C2	-2.64	1.40	1.46
3	A	502	MC3	O2-C2	-2.64	1.40	1.46
3	E	502	MC3	O2-C2	-2.62	1.40	1.46
3	C	503	MC3	O2-C2	-2.62	1.40	1.46
3	A	503	MC3	O2-C2	-2.47	1.40	1.46
3	B	505	MC3	O3-C3	-2.46	1.39	1.45
3	A	504	MC3	O3-C3	-2.46	1.39	1.45
3	E	504	MC3	O3-C3	-2.46	1.39	1.45
3	D	504	MC3	O3-C3	-2.45	1.39	1.45
3	E	504	MC3	O3-C11	2.45	1.40	1.33
3	E	503	MC3	O2-C2	-2.45	1.40	1.46
3	C	505	MC3	O3-C3	-2.45	1.39	1.45
3	D	503	MC3	O2-C2	-2.44	1.40	1.46
3	B	505	MC3	O3-C11	2.44	1.40	1.33
3	D	504	MC3	O3-C11	2.44	1.40	1.33
3	B	504	MC3	O2-C2	-2.43	1.40	1.46
3	C	505	MC3	O3-C11	2.42	1.40	1.33
3	C	504	MC3	O2-C2	-2.41	1.40	1.46
3	A	503	MC3	O3-C3	-2.41	1.39	1.45
3	A	504	MC3	O3-C11	2.41	1.40	1.33
3	C	504	MC3	O3-C3	-2.41	1.39	1.45
3	D	503	MC3	O3-C3	-2.40	1.39	1.45
3	E	503	MC3	O3-C3	-2.40	1.39	1.45
3	B	504	MC3	O3-C3	-2.40	1.39	1.45
3	C	504	MC3	O3-C11	2.39	1.40	1.33
3	C	505	MC3	O2-C2	-2.37	1.41	1.46
3	B	504	MC3	O3-C11	2.37	1.40	1.33
3	D	503	MC3	O3-C11	2.37	1.40	1.33
3	A	503	MC3	O3-C11	2.36	1.40	1.33
3	E	503	MC3	O3-C11	2.34	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	504	MC3	O2-C2	-2.33	1.41	1.46
3	E	504	MC3	O2-C2	-2.33	1.41	1.46
3	A	504	MC3	O2-C2	-2.33	1.41	1.46
3	A	502	MC3	O3-C11	2.32	1.40	1.33
3	B	505	MC3	O2-C2	-2.32	1.41	1.46
3	B	503	MC3	O3-C11	2.32	1.40	1.33
3	C	503	MC3	O3-C11	2.31	1.40	1.33
3	D	502	MC3	O3-C11	2.31	1.40	1.33
3	E	502	MC3	O3-C11	2.29	1.40	1.33
3	E	504	MC3	O2-C31	2.26	1.40	1.34
3	C	505	MC3	O2-C31	2.26	1.40	1.34
3	D	504	MC3	O2-C31	2.25	1.40	1.34
3	A	504	MC3	O2-C31	2.24	1.40	1.34
3	B	505	MC3	O2-C31	2.24	1.40	1.34
3	B	503	MC3	O2-C31	2.21	1.40	1.34
3	D	502	MC3	O2-C31	2.20	1.40	1.34
3	A	502	MC3	O2-C31	2.20	1.40	1.34
3	C	503	MC3	O2-C31	2.19	1.40	1.34
3	E	502	MC3	O2-C31	2.19	1.40	1.34
3	E	503	MC3	O2-C31	2.07	1.40	1.34
3	C	504	MC3	O2-C31	2.06	1.40	1.34
3	B	504	MC3	O2-C31	2.06	1.40	1.34
3	A	503	MC3	O2-C31	2.06	1.40	1.34
3	D	503	MC3	O2-C31	2.06	1.40	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	MC3	O2-C31-C32	4.04	120.22	111.48
3	E	502	MC3	O2-C31-C32	4.04	120.21	111.48
3	B	503	MC3	O2-C31-C32	4.03	120.20	111.48
3	C	505	MC3	O2-C31-C32	4.03	120.20	111.48
3	D	502	MC3	O2-C31-C32	4.03	120.19	111.48
3	C	503	MC3	O2-C31-C32	4.02	120.19	111.48
3	E	504	MC3	O2-C31-C32	4.02	120.18	111.48
3	A	502	MC3	O2-C31-C32	4.02	120.17	111.48
3	B	505	MC3	O2-C31-C32	4.01	120.16	111.48
3	D	504	MC3	O2-C31-C32	4.01	120.15	111.48
3	B	505	MC3	O3-C11-C12	3.28	121.84	111.83
3	A	504	MC3	O3-C11-C12	3.27	121.81	111.83
3	C	505	MC3	O3-C11-C12	3.27	121.81	111.83
3	D	504	MC3	O3-C11-C12	3.27	121.79	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	504	MC3	O3-C11-C12	3.26	121.77	111.83
3	A	503	MC3	O2-C31-C32	3.20	118.40	111.48
3	E	503	MC3	O2-C31-C32	3.20	118.40	111.48
3	D	503	MC3	O2-C31-C32	3.19	118.39	111.48
3	C	504	MC3	O2-C31-C32	3.19	118.37	111.48
3	B	504	MC3	O2-C31-C32	3.18	118.36	111.48
3	B	503	MC3	O3-C11-C12	2.89	120.66	111.83
3	E	502	MC3	O3-C11-C12	2.89	120.64	111.83
3	A	502	MC3	O3-C11-C12	2.89	120.64	111.83
3	D	502	MC3	O3-C11-C12	2.89	120.64	111.83
3	C	503	MC3	O3-C11-C12	2.88	120.63	111.83
3	E	503	MC3	O3-C11-C12	2.57	119.67	111.83
3	A	503	MC3	O3-C11-C12	2.57	119.67	111.83
3	D	503	MC3	O3-C11-C12	2.57	119.66	111.83
3	C	504	MC3	O3-C11-C12	2.56	119.64	111.83
3	B	504	MC3	O3-C11-C12	2.55	119.62	111.83
3	C	505	MC3	C3-C2-C1	-2.02	107.07	111.78
3	B	505	MC3	C3-C2-C1	-2.02	107.08	111.78
3	A	504	MC3	C3-C2-C1	-2.01	107.09	111.78
3	D	504	MC3	C3-C2-C1	-2.01	107.10	111.78

There are no chirality outliers.

All (500) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	MC3	C1-O3P-P-O1P
3	D	503	MC3	C32-C31-O2-C2
3	E	502	MC3	C1-O3P-P-O1P
3	E	503	MC3	C32-C31-O2-C2
3	C	503	MC3	C1-O3P-P-O1P
3	C	504	MC3	C32-C31-O2-C2
3	A	502	MC3	C1-O3P-P-O1P
3	A	503	MC3	C32-C31-O2-C2
3	B	503	MC3	C1-O3P-P-O1P
3	B	504	MC3	C32-C31-O2-C2
3	D	503	MC3	O31-C31-O2-C2
3	D	504	MC3	O31-C31-O2-C2
3	E	503	MC3	O31-C31-O2-C2
3	E	504	MC3	O31-C31-O2-C2
3	C	504	MC3	O31-C31-O2-C2
3	C	505	MC3	O31-C31-O2-C2
3	A	503	MC3	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
3	A	504	MC3	O31-C31-O2-C2
3	B	504	MC3	O31-C31-O2-C2
3	B	505	MC3	O31-C31-O2-C2
3	D	502	MC3	O11-C11-O3-C3
3	E	502	MC3	O11-C11-O3-C3
3	C	503	MC3	O11-C11-O3-C3
3	A	502	MC3	O11-C11-O3-C3
3	B	503	MC3	O11-C11-O3-C3
3	D	502	MC3	C12-C11-O3-C3
3	E	502	MC3	C12-C11-O3-C3
3	C	503	MC3	C12-C11-O3-C3
3	A	502	MC3	C12-C11-O3-C3
3	B	503	MC3	C12-C11-O3-C3
3	D	504	MC3	C32-C31-O2-C2
3	E	504	MC3	C32-C31-O2-C2
3	C	505	MC3	C32-C31-O2-C2
3	A	504	MC3	C32-C31-O2-C2
3	B	505	MC3	C32-C31-O2-C2
3	D	502	MC3	C15-C16-C17-C18
3	E	502	MC3	C15-C16-C17-C18
3	C	503	MC3	C15-C16-C17-C18
3	A	502	MC3	C15-C16-C17-C18
3	B	503	MC3	C15-C16-C17-C18
4	D	511	DU0	C21-C22-O23-C24
4	D	511	DU0	C75-C22-O23-C24
4	E	511	DU0	C21-C22-O23-C24
4	E	511	DU0	C75-C22-O23-C24
4	C	512	DU0	C21-C22-O23-C24
4	C	512	DU0	C75-C22-O23-C24
4	A	511	DU0	C21-C22-O23-C24
4	A	511	DU0	C75-C22-O23-C24
4	B	512	DU0	C21-C22-O23-C24
4	B	512	DU0	C75-C22-O23-C24
3	D	504	MC3	C1-C2-O2-C31
3	E	504	MC3	C1-C2-O2-C31
3	C	505	MC3	C1-C2-O2-C31
3	A	504	MC3	C1-C2-O2-C31
3	B	505	MC3	C1-C2-O2-C31
3	E	503	MC3	C19-C20-C21-C22
3	D	503	MC3	C19-C20-C21-C22
3	D	503	MC3	C37-C38-C39-C40
3	E	503	MC3	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
3	C	504	MC3	C19-C20-C21-C22
3	C	504	MC3	C37-C38-C39-C40
3	A	503	MC3	C19-C20-C21-C22
3	A	503	MC3	C37-C38-C39-C40
3	B	504	MC3	C19-C20-C21-C22
3	B	504	MC3	C37-C38-C39-C40
3	D	502	MC3	C12-C13-C14-C15
3	E	502	MC3	C12-C13-C14-C15
3	C	503	MC3	C12-C13-C14-C15
3	A	502	MC3	C12-C13-C14-C15
3	B	503	MC3	C12-C13-C14-C15
3	D	505	MC3	C36-C37-C38-C39
3	E	505	MC3	C36-C37-C38-C39
3	C	506	MC3	C36-C37-C38-C39
3	A	505	MC3	C36-C37-C38-C39
3	B	506	MC3	C36-C37-C38-C39
3	D	505	MC3	C34-C35-C36-C37
3	D	506	MC3	C34-C35-C36-C37
3	E	505	MC3	C34-C35-C36-C37
3	C	506	MC3	C34-C35-C36-C37
3	C	507	MC3	C34-C35-C36-C37
3	A	505	MC3	C34-C35-C36-C37
3	A	506	MC3	C34-C35-C36-C37
3	B	507	MC3	C34-C35-C36-C37
3	E	506	MC3	C34-C35-C36-C37
3	B	506	MC3	C34-C35-C36-C37
3	A	508	MC3	C39-C40-C41-C42
3	D	505	MC3	C38-C39-C40-C41
3	D	507	MC3	C34-C35-C36-C37
3	D	508	MC3	C39-C40-C41-C42
3	E	505	MC3	C32-C33-C34-C35
3	E	505	MC3	C38-C39-C40-C41
3	E	507	MC3	C34-C35-C36-C37
3	E	508	MC3	C39-C40-C41-C42
3	C	506	MC3	C38-C39-C40-C41
3	C	508	MC3	C34-C35-C36-C37
3	C	509	MC3	C39-C40-C41-C42
3	A	505	MC3	C38-C39-C40-C41
3	A	507	MC3	C34-C35-C36-C37
3	B	506	MC3	C32-C33-C34-C35
3	B	506	MC3	C38-C39-C40-C41
3	B	508	MC3	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
3	B	509	MC3	C39-C40-C41-C42
3	D	505	MC3	C32-C33-C34-C35
3	A	505	MC3	C32-C33-C34-C35
3	C	506	MC3	C32-C33-C34-C35
3	D	512	MC3	C33-C34-C35-C36
3	D	504	MC3	C37-C38-C39-C40
3	E	504	MC3	C37-C38-C39-C40
3	E	512	MC3	C33-C34-C35-C36
3	C	501	MC3	C33-C34-C35-C36
3	C	505	MC3	C37-C38-C39-C40
3	A	504	MC3	C37-C38-C39-C40
3	A	512	MC3	C33-C34-C35-C36
3	B	501	MC3	C33-C34-C35-C36
3	B	505	MC3	C37-C38-C39-C40
3	D	502	MC3	C17-C18-C19-C20
3	E	502	MC3	C17-C18-C19-C20
3	C	503	MC3	C17-C18-C19-C20
3	B	503	MC3	C17-C18-C19-C20
3	A	502	MC3	C17-C18-C19-C20
3	D	505	MC3	C37-C38-C39-C40
3	D	503	MC3	C32-C33-C34-C35
3	E	503	MC3	C32-C33-C34-C35
3	E	505	MC3	C37-C38-C39-C40
3	C	504	MC3	C32-C33-C34-C35
3	C	506	MC3	C37-C38-C39-C40
3	A	503	MC3	C32-C33-C34-C35
3	A	505	MC3	C37-C38-C39-C40
3	B	504	MC3	C32-C33-C34-C35
3	B	506	MC3	C37-C38-C39-C40
3	C	504	MC3	C40-C41-C42-C43
3	B	504	MC3	C40-C41-C42-C43
3	D	503	MC3	C40-C41-C42-C43
3	D	504	MC3	C16-C17-C18-C19
3	D	509	MC3	C40-C41-C42-C43
3	E	503	MC3	C40-C41-C42-C43
3	E	509	MC3	C40-C41-C42-C43
3	C	505	MC3	C16-C17-C18-C19
3	C	510	MC3	C40-C41-C42-C43
3	A	503	MC3	C40-C41-C42-C43
3	A	504	MC3	C16-C17-C18-C19
3	A	509	MC3	C40-C41-C42-C43
3	B	505	MC3	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
3	B	510	MC3	C40-C41-C42-C43
3	E	504	MC3	C16-C17-C18-C19
3	D	505	MC3	C35-C36-C37-C38
3	E	505	MC3	C35-C36-C37-C38
3	C	506	MC3	C35-C36-C37-C38
3	A	505	MC3	C35-C36-C37-C38
3	B	506	MC3	C35-C36-C37-C38
3	D	503	MC3	C15-C16-C17-C18
3	C	504	MC3	C15-C16-C17-C18
3	D	504	MC3	C12-C11-O3-C3
3	E	504	MC3	C12-C11-O3-C3
3	C	505	MC3	C12-C11-O3-C3
3	A	504	MC3	C12-C11-O3-C3
3	B	505	MC3	C12-C11-O3-C3
3	E	503	MC3	C15-C16-C17-C18
3	B	504	MC3	C15-C16-C17-C18
3	D	512	MC3	C38-C39-C40-C41
3	E	512	MC3	C38-C39-C40-C41
3	C	501	MC3	C38-C39-C40-C41
3	A	503	MC3	C15-C16-C17-C18
3	B	501	MC3	C38-C39-C40-C41
3	A	512	MC3	C38-C39-C40-C41
3	D	506	MC3	C32-C33-C34-C35
3	D	510	MC3	C40-C41-C42-C43
3	E	506	MC3	C32-C33-C34-C35
3	E	510	MC3	C40-C41-C42-C43
3	C	507	MC3	C32-C33-C34-C35
3	A	506	MC3	C32-C33-C34-C35
3	A	510	MC3	C40-C41-C42-C43
3	B	507	MC3	C32-C33-C34-C35
3	B	511	MC3	C40-C41-C42-C43
3	C	511	MC3	C40-C41-C42-C43
3	D	502	MC3	C32-C31-O2-C2
3	E	502	MC3	C32-C31-O2-C2
3	C	503	MC3	C32-C31-O2-C2
3	A	502	MC3	C32-C31-O2-C2
3	B	503	MC3	C32-C31-O2-C2
4	D	511	DU0	O23-C24-C25-C26
4	E	511	DU0	O23-C24-C25-C26
4	C	512	DU0	O23-C24-C25-C26
4	A	511	DU0	O23-C24-C25-C26
4	B	512	DU0	O23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	D	506	MC3	C39-C40-C41-C42
3	C	507	MC3	C39-C40-C41-C42
3	B	507	MC3	C39-C40-C41-C42
3	E	506	MC3	C39-C40-C41-C42
3	A	506	MC3	C39-C40-C41-C42
3	E	504	MC3	C19-C20-C21-C22
3	D	504	MC3	C19-C20-C21-C22
3	C	505	MC3	C19-C20-C21-C22
3	A	504	MC3	C19-C20-C21-C22
3	B	505	MC3	C19-C20-C21-C22
3	D	504	MC3	O11-C11-O3-C3
3	E	504	MC3	O11-C11-O3-C3
3	C	505	MC3	O11-C11-O3-C3
3	A	504	MC3	O11-C11-O3-C3
3	B	505	MC3	O11-C11-O3-C3
3	D	502	MC3	C38-C39-C40-C41
3	A	502	MC3	C38-C39-C40-C41
3	E	502	MC3	C38-C39-C40-C41
3	C	503	MC3	C38-C39-C40-C41
3	B	503	MC3	C32-C33-C34-C35
3	B	503	MC3	C38-C39-C40-C41
3	D	502	MC3	C32-C33-C34-C35
3	D	508	MC3	C40-C41-C42-C43
3	E	502	MC3	C32-C33-C34-C35
3	E	508	MC3	C40-C41-C42-C43
3	C	503	MC3	C32-C33-C34-C35
3	A	502	MC3	C32-C33-C34-C35
3	C	509	MC3	C40-C41-C42-C43
3	A	508	MC3	C40-C41-C42-C43
3	B	509	MC3	C40-C41-C42-C43
3	D	502	MC3	O31-C31-O2-C2
3	E	502	MC3	O31-C31-O2-C2
3	C	503	MC3	O31-C31-O2-C2
3	A	502	MC3	O31-C31-O2-C2
3	B	503	MC3	O31-C31-O2-C2
3	D	504	MC3	C35-C36-C37-C38
3	C	505	MC3	C35-C36-C37-C38
3	B	505	MC3	C35-C36-C37-C38
3	E	504	MC3	C35-C36-C37-C38
3	A	504	MC3	C35-C36-C37-C38
3	E	507	MC3	C38-C39-C40-C41
3	B	508	MC3	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
3	D	507	MC3	C38-C39-C40-C41
3	C	508	MC3	C38-C39-C40-C41
3	A	507	MC3	C38-C39-C40-C41
3	D	510	MC3	C38-C39-C40-C41
3	E	510	MC3	C38-C39-C40-C41
3	C	511	MC3	C38-C39-C40-C41
3	A	510	MC3	C38-C39-C40-C41
3	B	511	MC3	C38-C39-C40-C41
3	B	503	MC3	C33-C34-C35-C36
3	D	502	MC3	C33-C34-C35-C36
3	E	502	MC3	C33-C34-C35-C36
3	C	503	MC3	C33-C34-C35-C36
3	A	502	MC3	C33-C34-C35-C36
3	D	503	MC3	C14-C15-C16-C17
3	E	503	MC3	C14-C15-C16-C17
3	C	504	MC3	C14-C15-C16-C17
3	A	503	MC3	C14-C15-C16-C17
3	B	504	MC3	C14-C15-C16-C17
3	E	504	MC3	C38-C39-C40-C41
3	D	504	MC3	C38-C39-C40-C41
3	C	505	MC3	C33-C34-C35-C36
3	C	505	MC3	C38-C39-C40-C41
3	A	504	MC3	C33-C34-C35-C36
3	A	504	MC3	C38-C39-C40-C41
3	B	505	MC3	C33-C34-C35-C36
3	B	505	MC3	C38-C39-C40-C41
3	D	504	MC3	C33-C34-C35-C36
3	E	504	MC3	C33-C34-C35-C36
3	D	512	MC3	C40-C41-C42-C43
3	E	512	MC3	C40-C41-C42-C43
3	C	501	MC3	C40-C41-C42-C43
3	A	512	MC3	C40-C41-C42-C43
3	B	501	MC3	C40-C41-C42-C43
3	D	503	MC3	C41-C42-C43-C44
3	E	503	MC3	C41-C42-C43-C44
3	C	504	MC3	C41-C42-C43-C44
3	A	503	MC3	C41-C42-C43-C44
3	B	504	MC3	C41-C42-C43-C44
3	D	504	MC3	C32-C33-C34-C35
3	E	504	MC3	C32-C33-C34-C35
3	C	505	MC3	C32-C33-C34-C35
3	A	504	MC3	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	B	505	MC3	C32-C33-C34-C35
3	D	504	MC3	C41-C42-C43-C44
3	E	504	MC3	C41-C42-C43-C44
3	A	504	MC3	C41-C42-C43-C44
3	C	505	MC3	C41-C42-C43-C44
3	B	505	MC3	C41-C42-C43-C44
3	D	502	MC3	C13-C14-C15-C16
3	E	502	MC3	C13-C14-C15-C16
3	C	503	MC3	C13-C14-C15-C16
3	A	502	MC3	C13-C14-C15-C16
3	B	503	MC3	C13-C14-C15-C16
3	E	503	MC3	C38-C39-C40-C41
3	A	503	MC3	C38-C39-C40-C41
3	D	503	MC3	C38-C39-C40-C41
3	C	504	MC3	C38-C39-C40-C41
3	B	504	MC3	C38-C39-C40-C41
3	B	509	MC3	C38-C39-C40-C41
3	D	508	MC3	C38-C39-C40-C41
3	E	508	MC3	C38-C39-C40-C41
3	C	509	MC3	C38-C39-C40-C41
3	A	508	MC3	C38-C39-C40-C41
3	D	502	MC3	C19-C20-C21-C22
3	E	502	MC3	C19-C20-C21-C22
3	C	503	MC3	C19-C20-C21-C22
3	A	502	MC3	C19-C20-C21-C22
3	B	503	MC3	C19-C20-C21-C22
3	D	502	MC3	C11-C12-C13-C14
3	E	502	MC3	C11-C12-C13-C14
3	C	503	MC3	C11-C12-C13-C14
3	A	502	MC3	C11-C12-C13-C14
3	B	503	MC3	C11-C12-C13-C14
3	D	509	MC3	C34-C35-C36-C37
3	A	509	MC3	C34-C35-C36-C37
3	E	509	MC3	C34-C35-C36-C37
3	C	510	MC3	C34-C35-C36-C37
3	B	510	MC3	C34-C35-C36-C37
3	A	503	MC3	C34-C35-C36-C37
3	D	503	MC3	C34-C35-C36-C37
3	E	503	MC3	C34-C35-C36-C37
3	C	504	MC3	C34-C35-C36-C37
3	B	504	MC3	C34-C35-C36-C37
3	D	502	MC3	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
3	E	502	MC3	C1-O3P-P-O4P
3	C	503	MC3	C1-O3P-P-O4P
3	A	502	MC3	C1-O3P-P-O4P
3	B	503	MC3	C1-O3P-P-O4P
3	E	508	MC3	C34-C35-C36-C37
3	B	509	MC3	C34-C35-C36-C37
3	D	508	MC3	C34-C35-C36-C37
3	C	509	MC3	C34-C35-C36-C37
3	A	508	MC3	C34-C35-C36-C37
3	D	509	MC3	C37-C38-C39-C40
3	E	509	MC3	C37-C38-C39-C40
3	C	510	MC3	C37-C38-C39-C40
3	A	509	MC3	C37-C38-C39-C40
3	B	510	MC3	C37-C38-C39-C40
3	A	506	MC3	C36-C37-C38-C39
3	B	507	MC3	C36-C37-C38-C39
3	E	506	MC3	C36-C37-C38-C39
3	C	507	MC3	C36-C37-C38-C39
3	D	506	MC3	C36-C37-C38-C39
3	E	503	MC3	C20-C21-C22-C23
3	C	504	MC3	C20-C21-C22-C23
3	D	503	MC3	C20-C21-C22-C23
3	D	502	MC3	O3P-C1-C2-C3
3	E	502	MC3	O3P-C1-C2-C3
3	C	503	MC3	O3P-C1-C2-C3
3	A	502	MC3	O3P-C1-C2-C3
3	B	503	MC3	O3P-C1-C2-C3
3	A	503	MC3	C20-C21-C22-C23
3	B	504	MC3	C20-C21-C22-C23
3	D	502	MC3	O3P-C1-C2-O2
3	E	502	MC3	O3P-C1-C2-O2
3	C	503	MC3	O3P-C1-C2-O2
3	A	502	MC3	O3P-C1-C2-O2
3	B	503	MC3	O3P-C1-C2-O2
3	C	508	MC3	C37-C38-C39-C40
3	A	507	MC3	C37-C38-C39-C40
3	B	508	MC3	C37-C38-C39-C40
3	D	507	MC3	C37-C38-C39-C40
3	E	507	MC3	C37-C38-C39-C40
3	C	507	MC3	C37-C38-C39-C40
3	B	507	MC3	C37-C38-C39-C40
3	D	506	MC3	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
3	E	506	MC3	C37-C38-C39-C40
3	A	506	MC3	C37-C38-C39-C40
3	C	504	MC3	C35-C36-C37-C38
3	B	504	MC3	C35-C36-C37-C38
3	D	503	MC3	C35-C36-C37-C38
3	E	503	MC3	C35-C36-C37-C38
3	A	503	MC3	C35-C36-C37-C38
3	C	511	MC3	C41-C42-C43-C44
3	A	510	MC3	C41-C42-C43-C44
3	B	511	MC3	C41-C42-C43-C44
3	D	510	MC3	C41-C42-C43-C44
3	E	510	MC3	C41-C42-C43-C44
3	C	507	MC3	C38-C39-C40-C41
3	A	506	MC3	C38-C39-C40-C41
3	D	506	MC3	C38-C39-C40-C41
3	E	506	MC3	C38-C39-C40-C41
3	B	507	MC3	C38-C39-C40-C41
3	C	507	MC3	C35-C36-C37-C38
3	D	506	MC3	C35-C36-C37-C38
3	E	506	MC3	C35-C36-C37-C38
3	B	507	MC3	C35-C36-C37-C38
3	A	506	MC3	C35-C36-C37-C38
3	D	512	MC3	C31-C32-C33-C34
3	B	501	MC3	C31-C32-C33-C34
3	E	512	MC3	C31-C32-C33-C34
3	C	501	MC3	C31-C32-C33-C34
3	A	512	MC3	C31-C32-C33-C34
3	D	503	MC3	C12-C11-O3-C3
3	E	503	MC3	C12-C11-O3-C3
3	C	504	MC3	C12-C11-O3-C3
3	A	503	MC3	C12-C11-O3-C3
3	B	504	MC3	C12-C11-O3-C3
3	D	504	MC3	O2-C31-C32-C33
3	D	503	MC3	C21-C22-C23-C24
3	C	504	MC3	C21-C22-C23-C24
3	E	503	MC3	C21-C22-C23-C24
3	A	503	MC3	C21-C22-C23-C24
3	B	504	MC3	C21-C22-C23-C24
3	E	504	MC3	O2-C31-C32-C33
3	C	505	MC3	O2-C31-C32-C33
3	A	504	MC3	O2-C31-C32-C33
3	B	505	MC3	O2-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
3	D	503	MC3	O11-C11-O3-C3
3	E	503	MC3	O11-C11-O3-C3
3	C	504	MC3	O11-C11-O3-C3
3	A	503	MC3	O11-C11-O3-C3
3	B	504	MC3	O11-C11-O3-C3
3	A	508	MC3	C32-C33-C34-C35
3	D	508	MC3	C32-C33-C34-C35
3	E	508	MC3	C32-C33-C34-C35
3	B	509	MC3	C32-C33-C34-C35
3	C	509	MC3	C32-C33-C34-C35
3	E	504	MC3	C12-C13-C14-C15
3	C	505	MC3	C12-C13-C14-C15
3	A	504	MC3	C12-C13-C14-C15
3	B	505	MC3	C12-C13-C14-C15
3	D	504	MC3	C12-C13-C14-C15
3	D	503	MC3	C1-C2-O2-C31
3	D	503	MC3	C3-C2-O2-C31
3	E	503	MC3	C1-C2-O2-C31
3	E	503	MC3	C3-C2-O2-C31
3	C	504	MC3	C1-C2-O2-C31
3	C	504	MC3	C3-C2-O2-C31
3	A	503	MC3	C1-C2-O2-C31
3	A	503	MC3	C3-C2-O2-C31
3	B	504	MC3	C1-C2-O2-C31
3	B	504	MC3	C3-C2-O2-C31
3	D	506	MC3	C40-C41-C42-C43
3	A	506	MC3	C40-C41-C42-C43
3	E	506	MC3	C40-C41-C42-C43
3	C	507	MC3	C40-C41-C42-C43
3	B	507	MC3	C40-C41-C42-C43
3	E	503	MC3	C33-C34-C35-C36
3	D	503	MC3	C33-C34-C35-C36
3	D	502	MC3	C1-C2-C3-O3
3	E	502	MC3	C1-C2-C3-O3
3	C	503	MC3	C1-C2-C3-O3
3	A	502	MC3	C1-C2-C3-O3
3	B	503	MC3	C1-C2-C3-O3
3	A	503	MC3	C33-C34-C35-C36
3	B	504	MC3	C33-C34-C35-C36
3	C	504	MC3	C33-C34-C35-C36
3	E	507	MC3	C40-C41-C42-C43
3	D	507	MC3	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
3	C	508	MC3	C40-C41-C42-C43
3	A	507	MC3	C40-C41-C42-C43
3	B	508	MC3	C40-C41-C42-C43
3	A	502	MC3	C35-C36-C37-C38
3	D	502	MC3	C35-C36-C37-C38
3	E	502	MC3	C35-C36-C37-C38
3	B	503	MC3	C35-C36-C37-C38
3	C	503	MC3	C35-C36-C37-C38
3	C	504	MC3	C12-C13-C14-C15
3	D	503	MC3	C12-C13-C14-C15
3	A	503	MC3	C12-C13-C14-C15
3	B	504	MC3	C12-C13-C14-C15
3	E	503	MC3	C12-C13-C14-C15
3	E	504	MC3	C13-C14-C15-C16
3	C	505	MC3	C13-C14-C15-C16
3	A	504	MC3	C13-C14-C15-C16
3	D	504	MC3	C13-C14-C15-C16
3	B	505	MC3	C13-C14-C15-C16
3	D	508	MC3	C35-C36-C37-C38
3	E	508	MC3	C35-C36-C37-C38
3	C	509	MC3	C35-C36-C37-C38
3	A	508	MC3	C35-C36-C37-C38
3	B	509	MC3	C35-C36-C37-C38
3	E	504	MC3	C36-C37-C38-C39
3	A	504	MC3	C36-C37-C38-C39
3	D	504	MC3	C36-C37-C38-C39
3	C	505	MC3	C36-C37-C38-C39
3	B	505	MC3	C36-C37-C38-C39
3	D	502	MC3	O3-C11-C12-C13
3	E	502	MC3	O3-C11-C12-C13
3	C	503	MC3	O3-C11-C12-C13
3	A	502	MC3	O3-C11-C12-C13
3	B	503	MC3	O3-C11-C12-C13
3	A	509	MC3	C35-C36-C37-C38
3	D	509	MC3	C35-C36-C37-C38
3	B	510	MC3	C35-C36-C37-C38
3	E	509	MC3	C35-C36-C37-C38
3	C	510	MC3	C35-C36-C37-C38
3	D	508	MC3	C36-C37-C38-C39
3	C	509	MC3	C36-C37-C38-C39
3	A	508	MC3	C36-C37-C38-C39
3	E	508	MC3	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
3	B	509	MC3	C36-C37-C38-C39
3	A	502	MC3	O11-C11-C12-C13
3	B	503	MC3	O11-C11-C12-C13
3	D	502	MC3	O11-C11-C12-C13
3	E	502	MC3	O11-C11-C12-C13
3	C	503	MC3	O11-C11-C12-C13
3	A	504	MC3	C31-C32-C33-C34
3	D	503	MC3	O3-C11-C12-C13
3	E	503	MC3	O3-C11-C12-C13
3	C	504	MC3	O3-C11-C12-C13
3	A	503	MC3	O3-C11-C12-C13
3	B	504	MC3	O3-C11-C12-C13
3	E	504	MC3	O3-C11-C12-C13
3	C	505	MC3	O3-C11-C12-C13
3	A	504	MC3	O3-C11-C12-C13
3	B	505	MC3	O3-C11-C12-C13
3	D	504	MC3	C31-C32-C33-C34
3	E	504	MC3	C31-C32-C33-C34
3	C	505	MC3	C31-C32-C33-C34
3	B	505	MC3	C31-C32-C33-C34
3	D	504	MC3	O3-C11-C12-C13

There are no ring outliers.

20 monomers are involved in 40 short contacts:

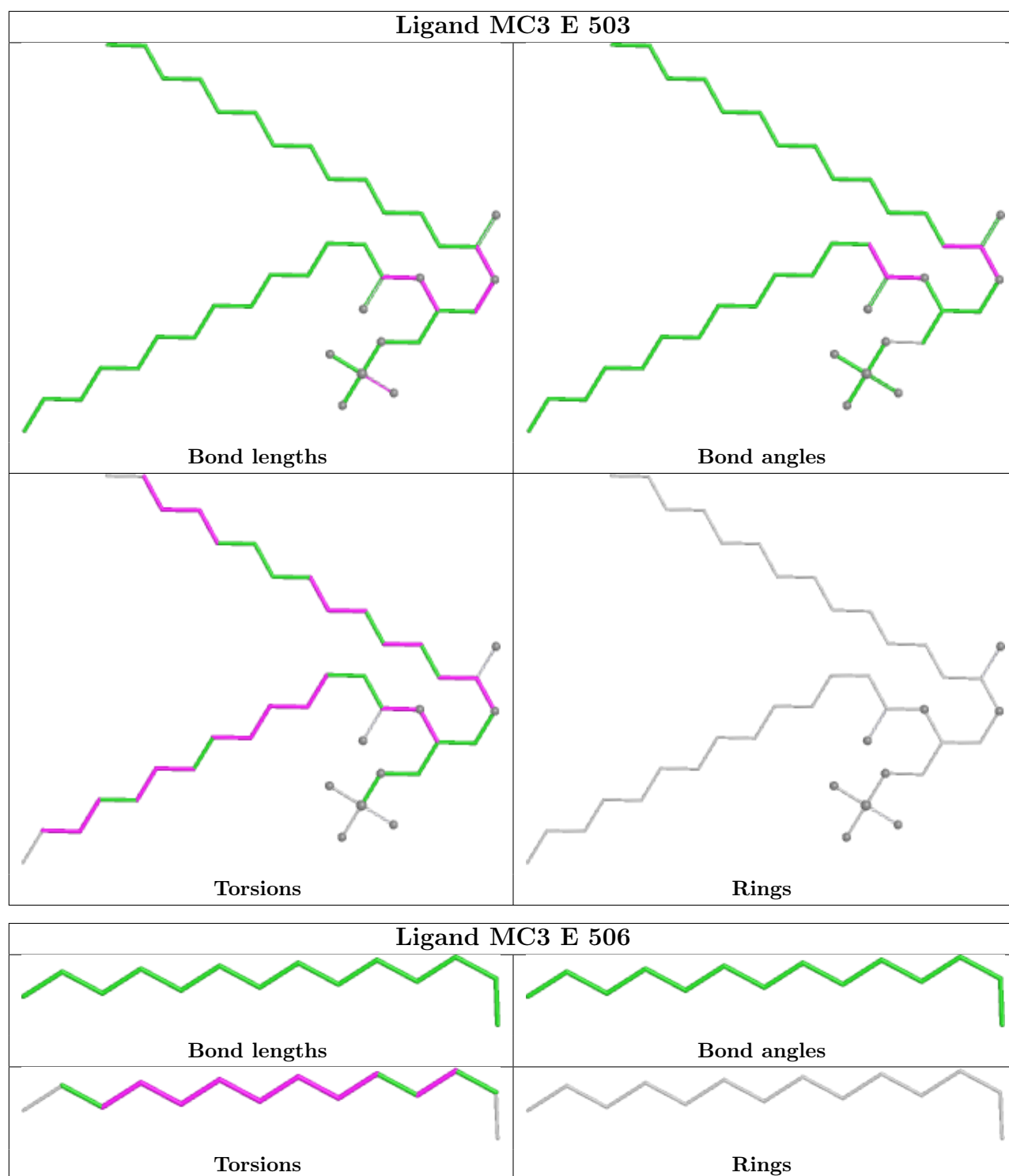
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	502	MC3	3	0
3	B	510	MC3	2	0
3	C	510	MC3	2	0
3	D	509	MC3	2	0
3	E	504	MC3	3	0
3	A	502	MC3	3	0
3	C	505	MC3	3	0
4	A	511	DU0	3	0
3	E	509	MC3	2	0
3	D	504	MC3	3	0
3	A	504	MC3	3	0
4	E	511	DU0	3	0
4	C	512	DU0	3	0
3	D	502	MC3	3	0
4	D	511	DU0	3	0
3	B	503	MC3	3	0

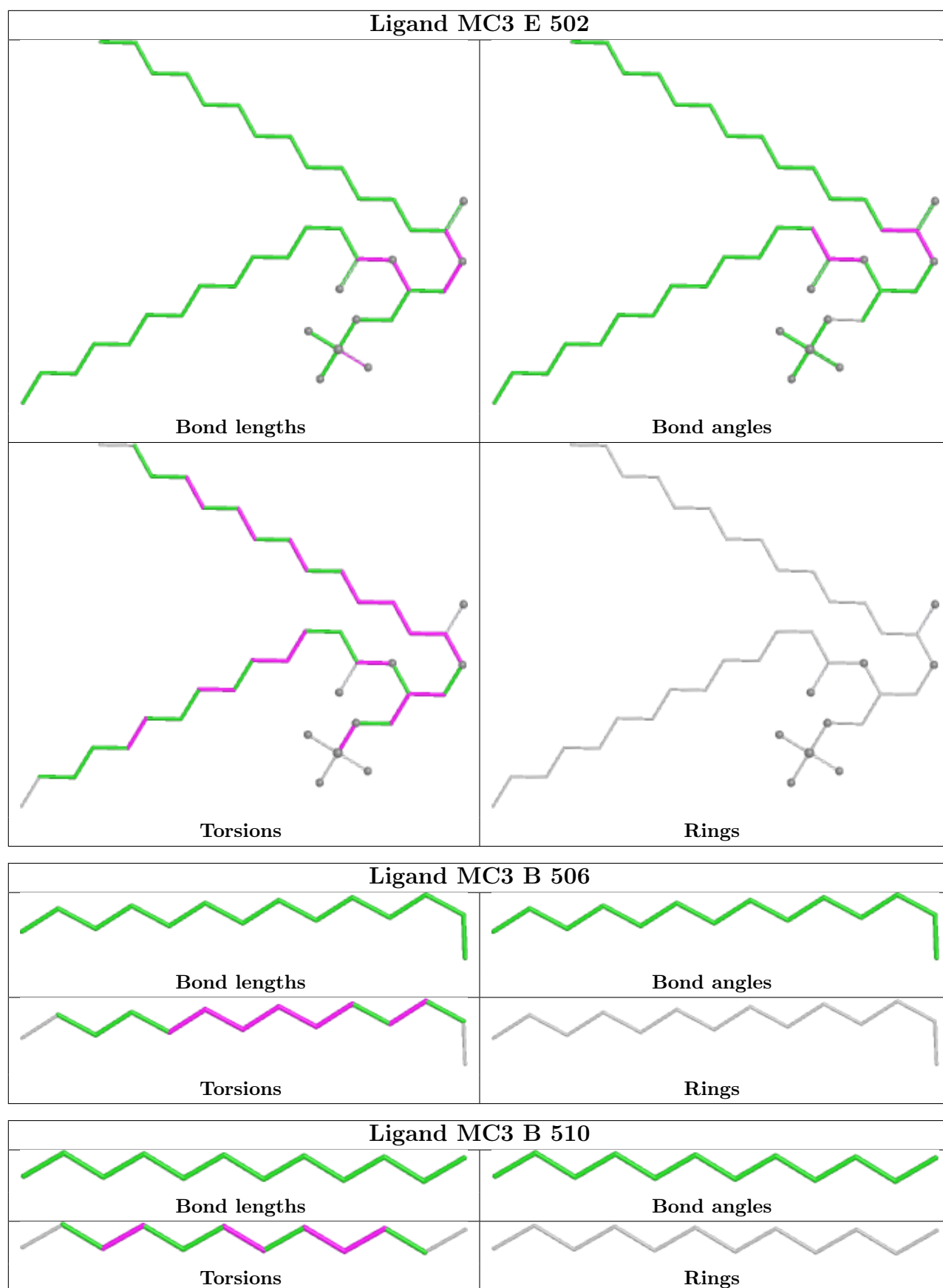
Continued on next page...

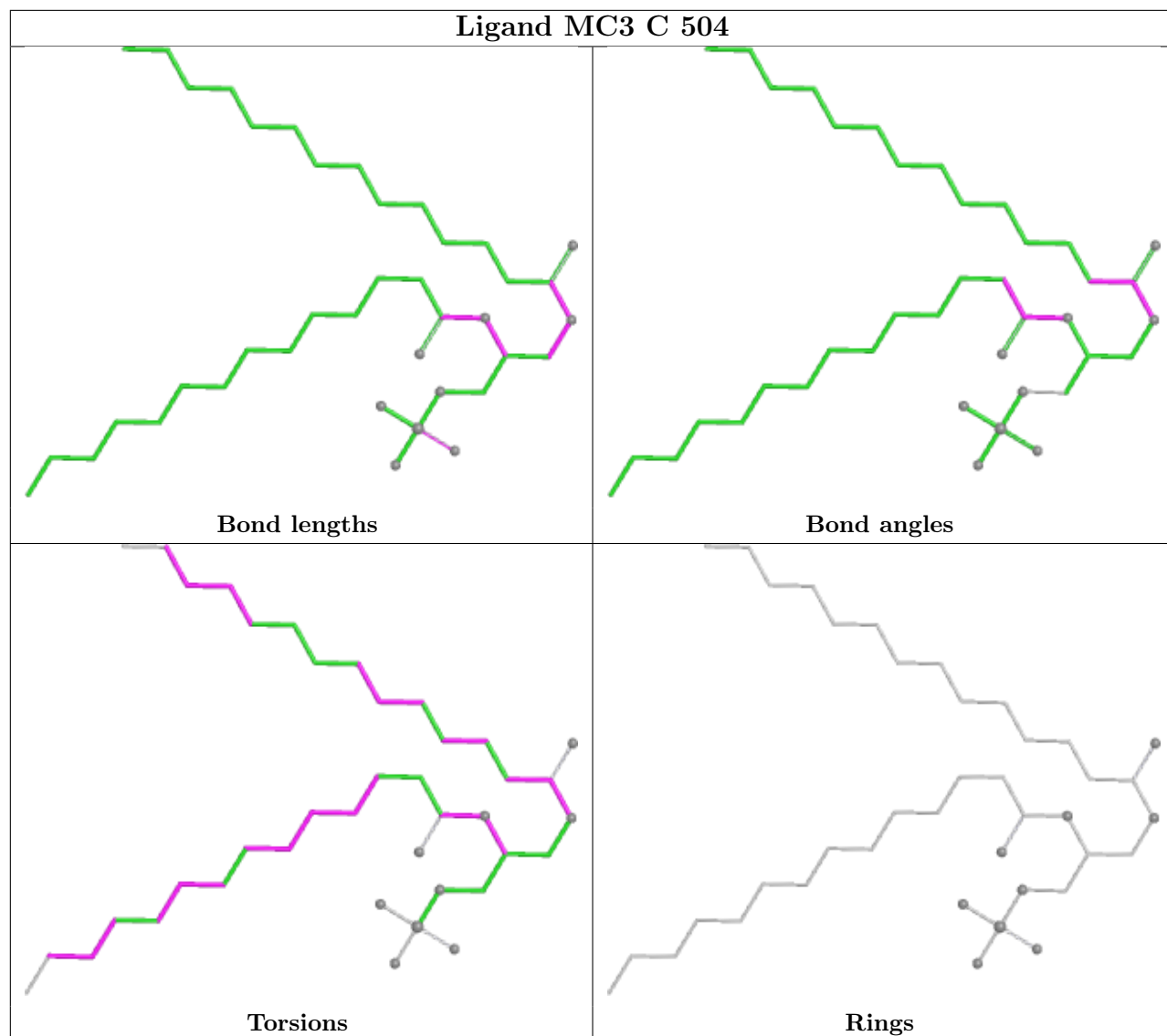
Continued from previous page...

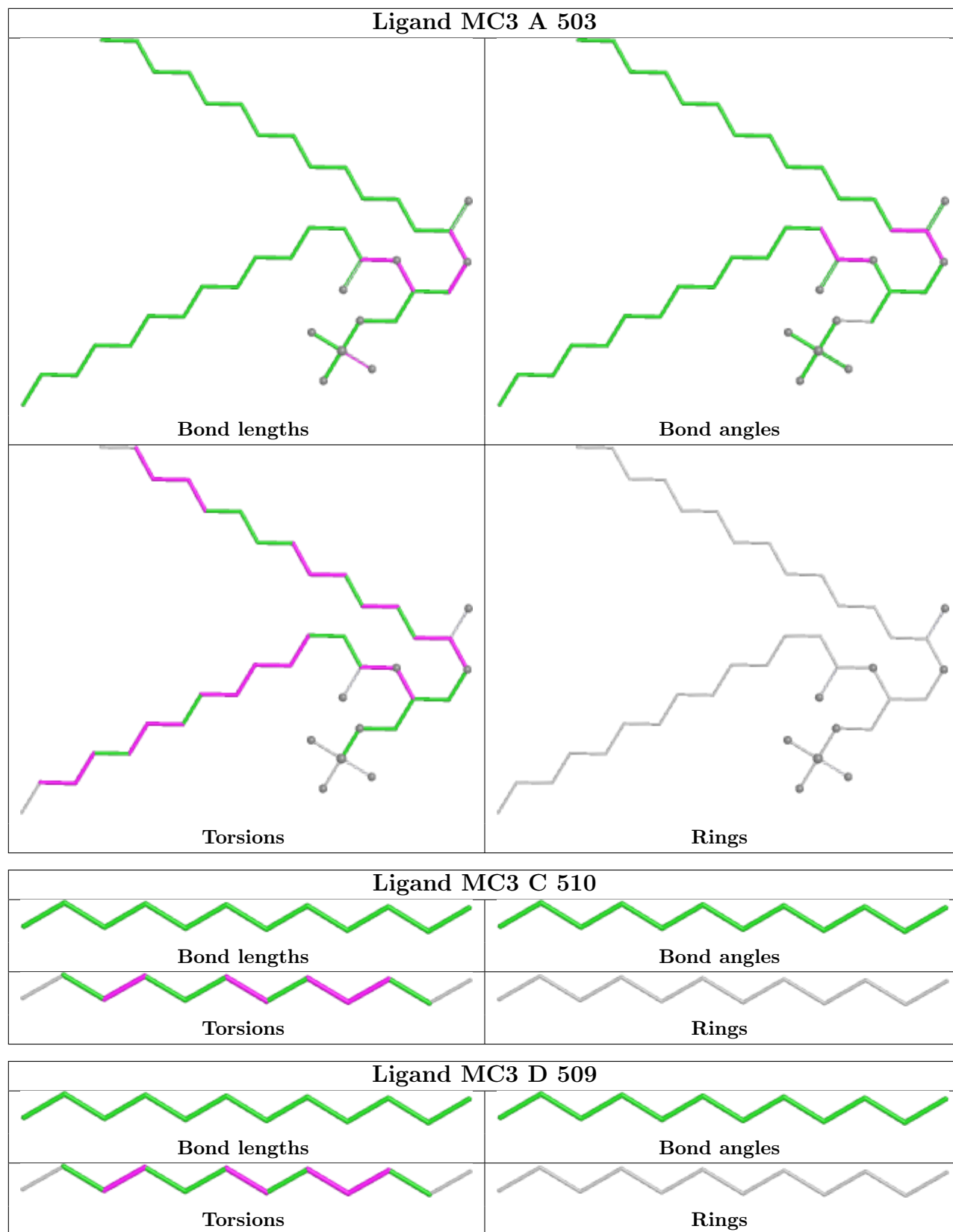
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	509	MC3	2	0
3	C	503	MC3	3	0
3	B	505	MC3	3	0
4	B	512	DU0	3	0

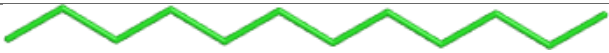
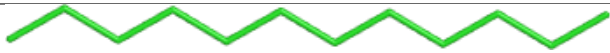


The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



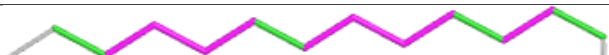















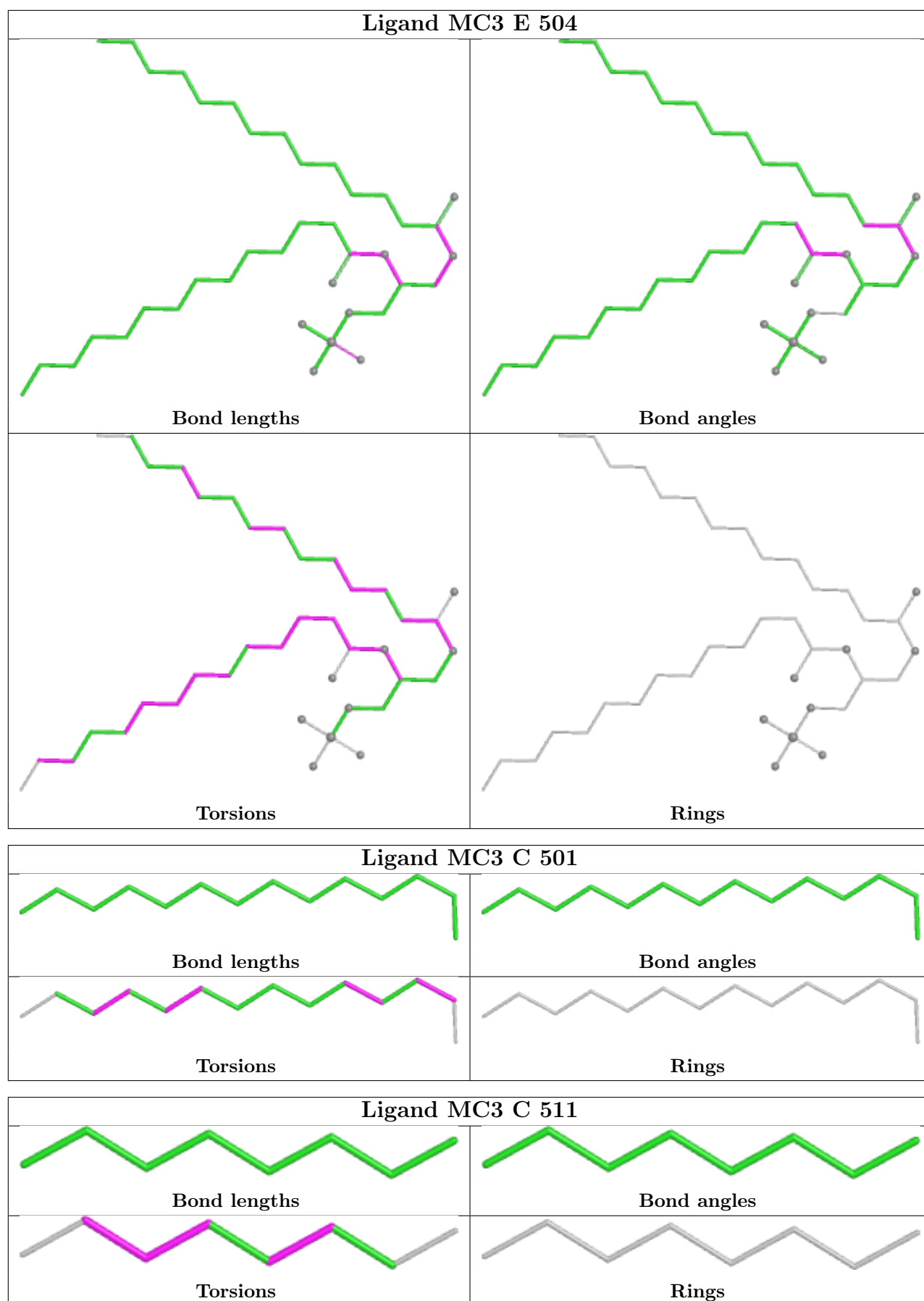


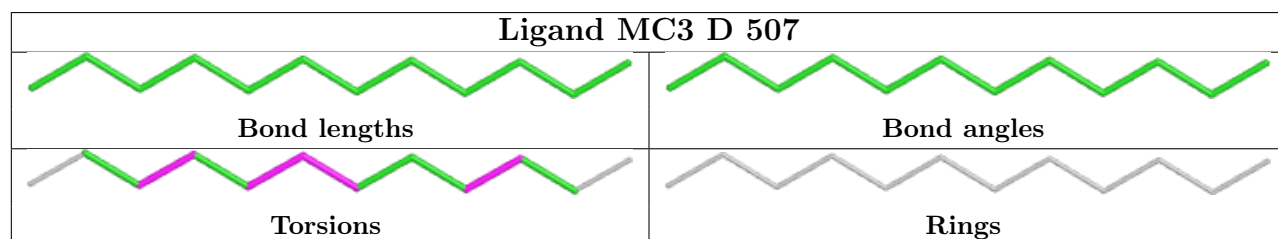
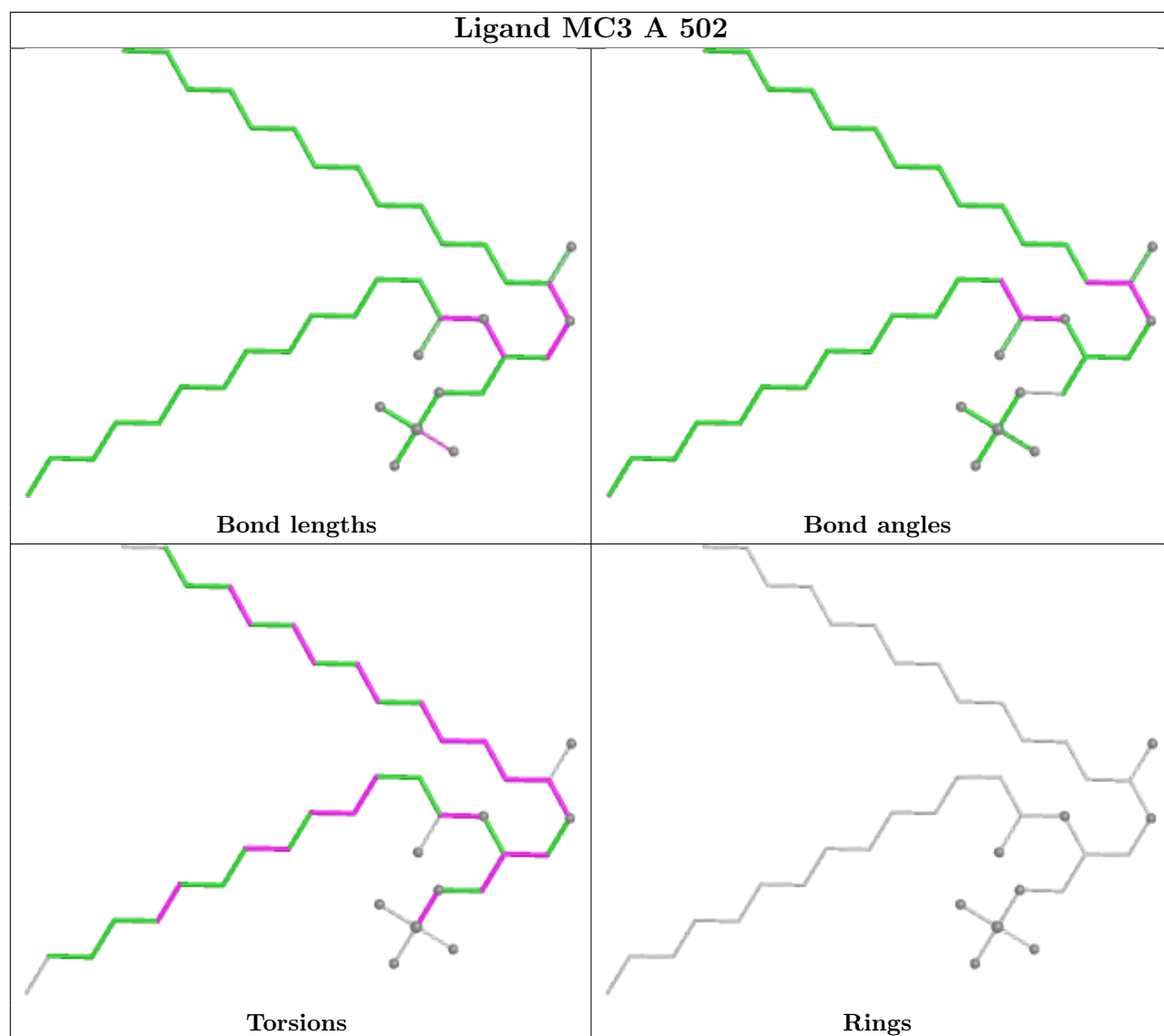
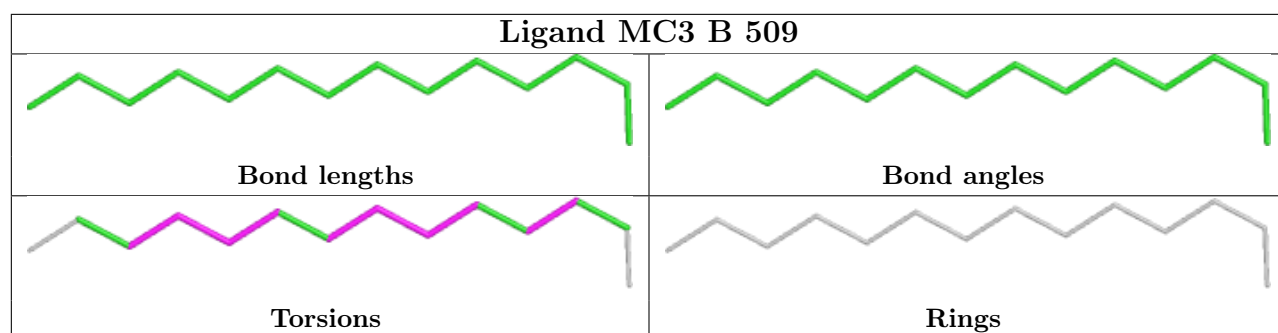
Ligand MC3 E 507			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

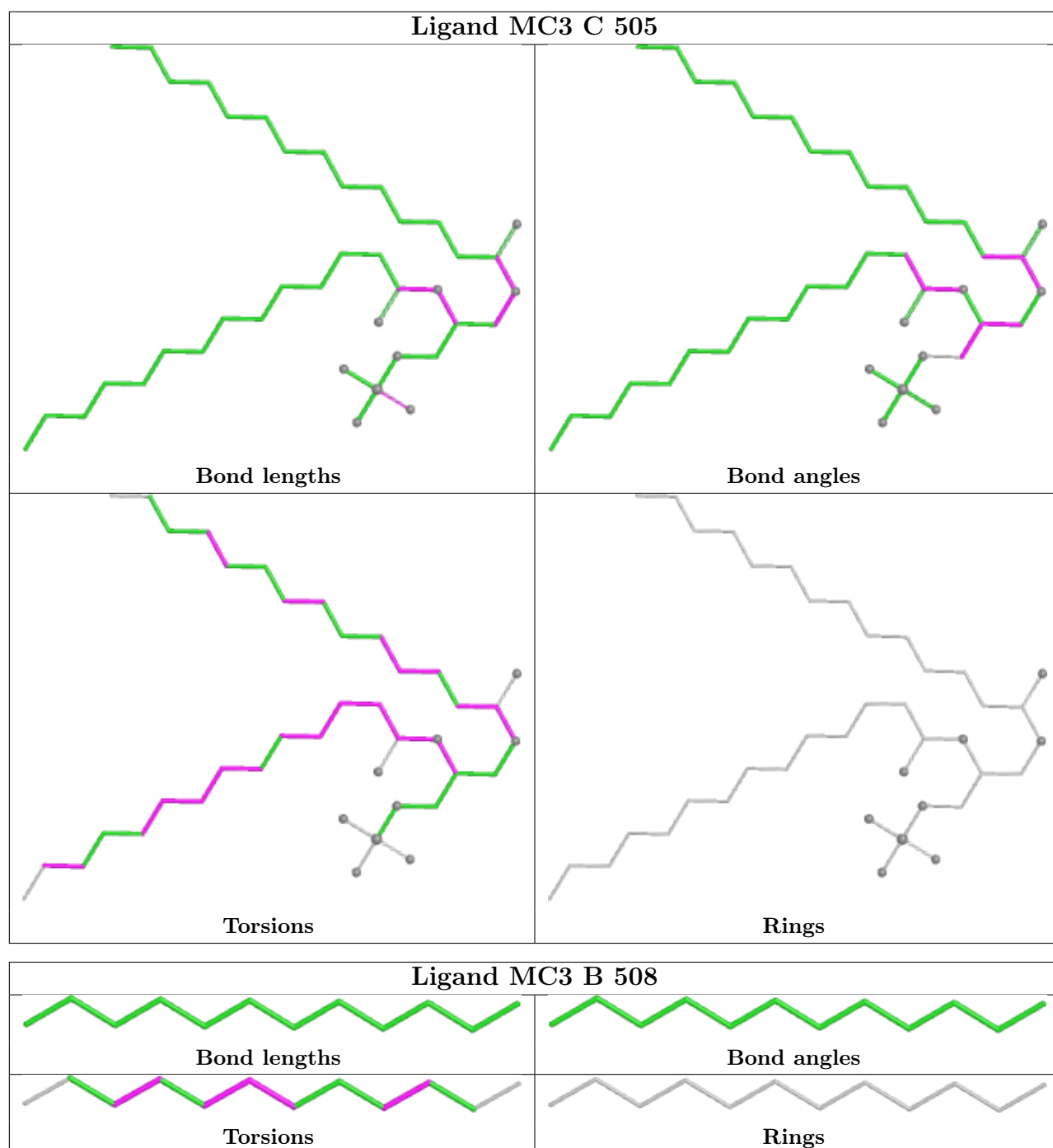
Ligand MC3 D 508			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

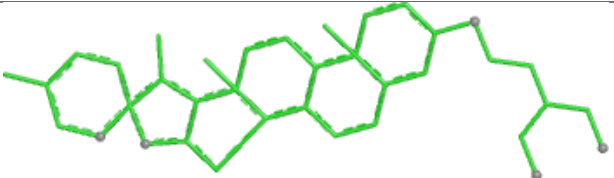
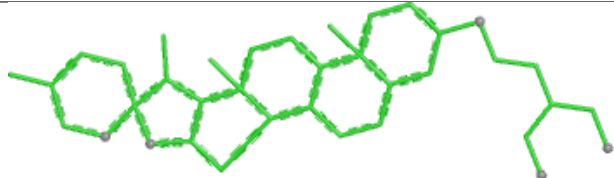
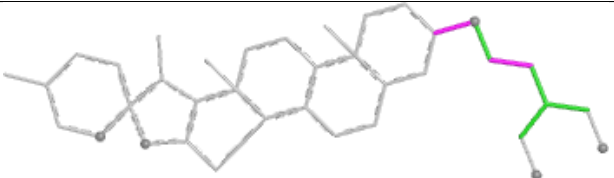
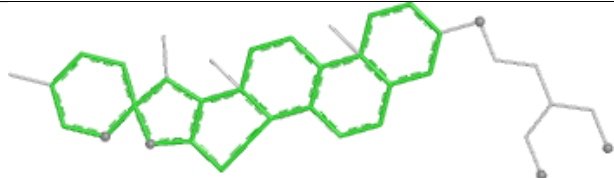
Ligand MC3 A 505			
 Bond lengths		 Bond angles	
 Torsions		 Rings	





Ligand MC3 B 511			
 Bond lengths		 Bond angles	
 Torsions		 Rings	







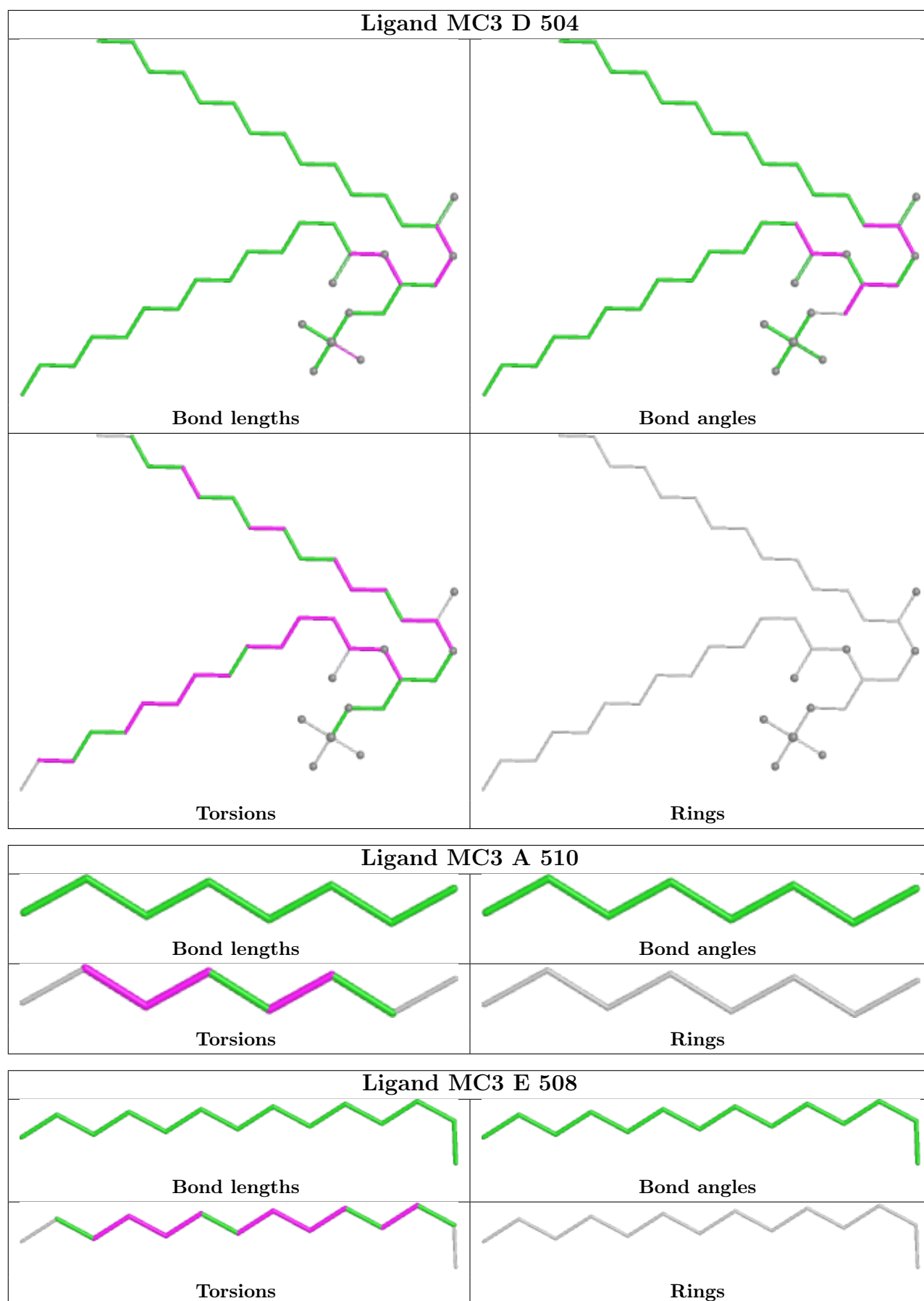


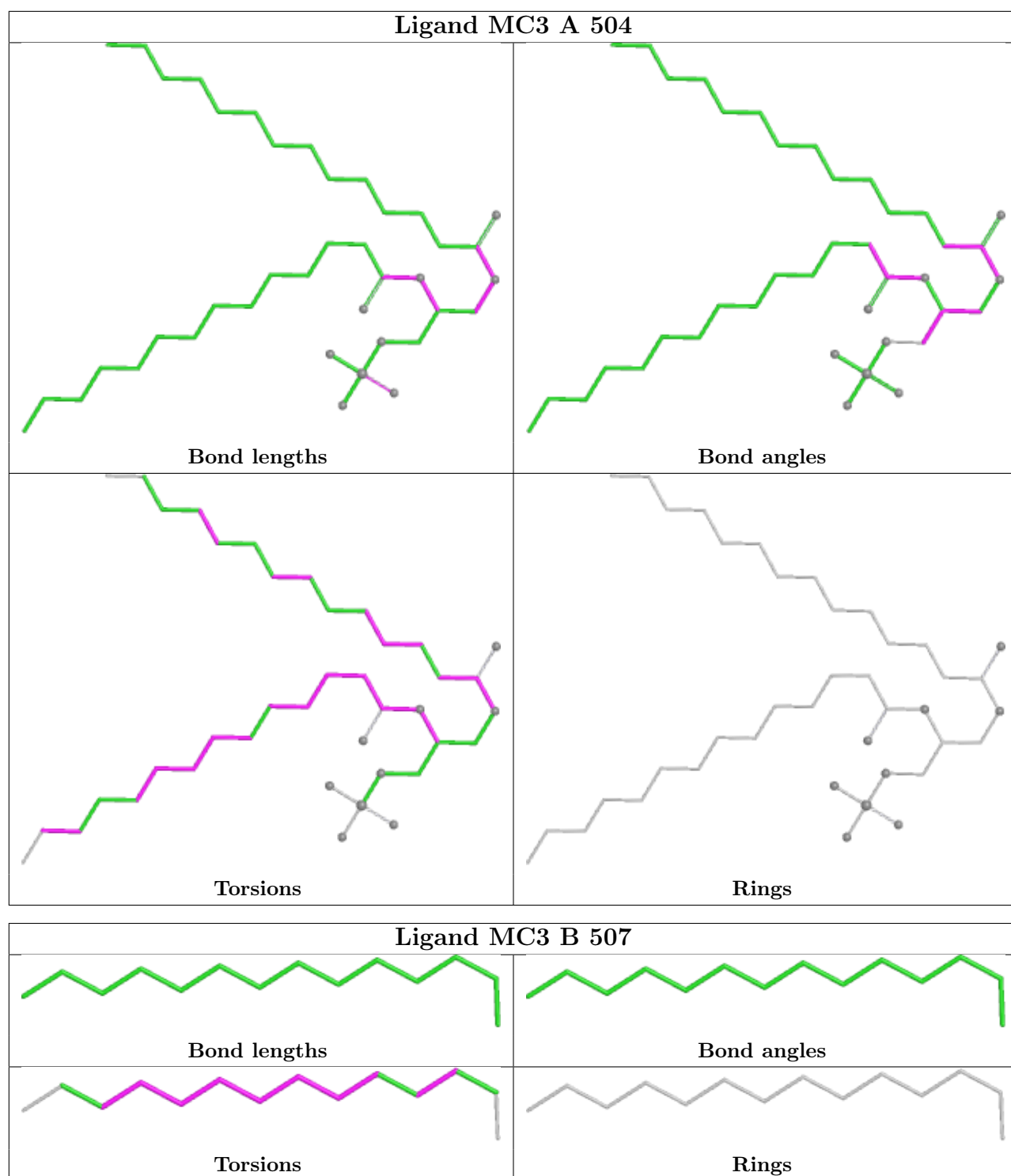


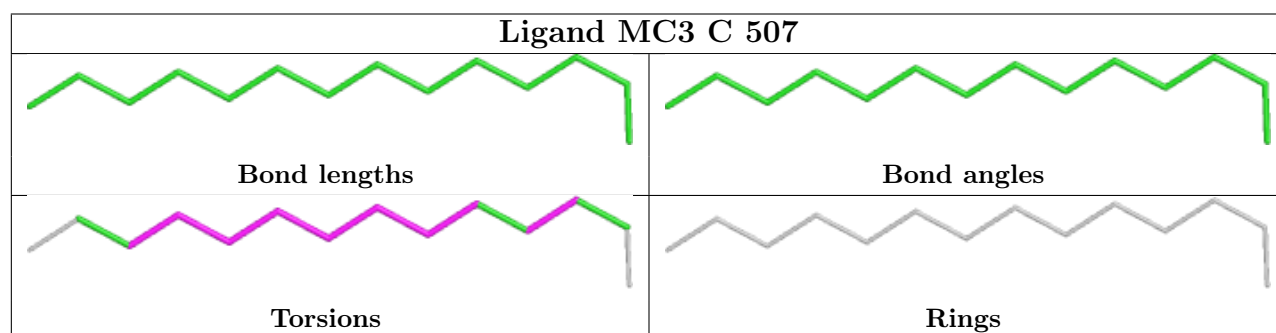
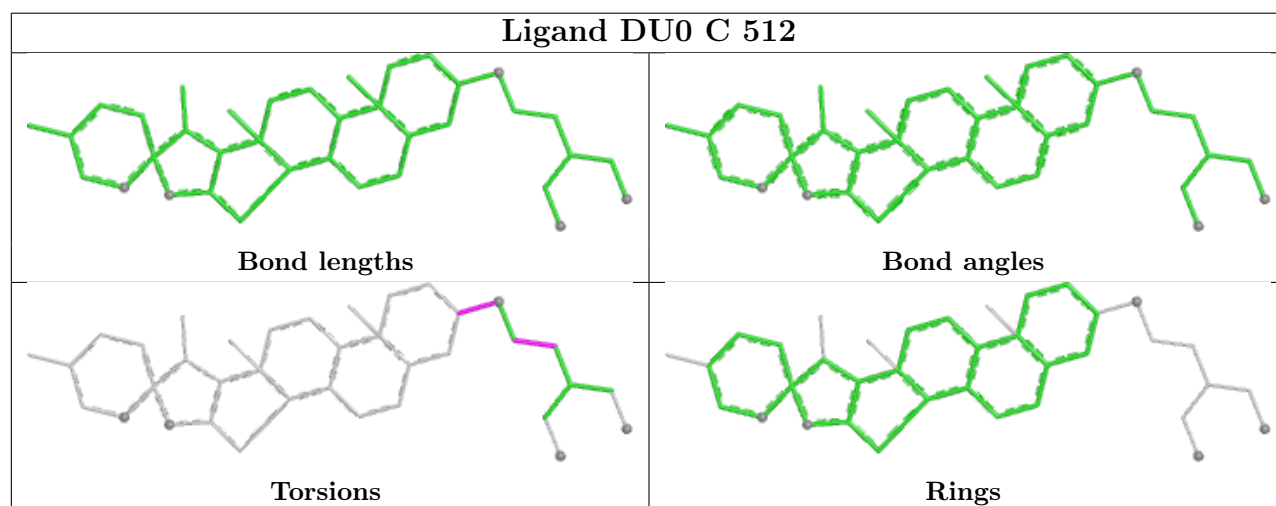
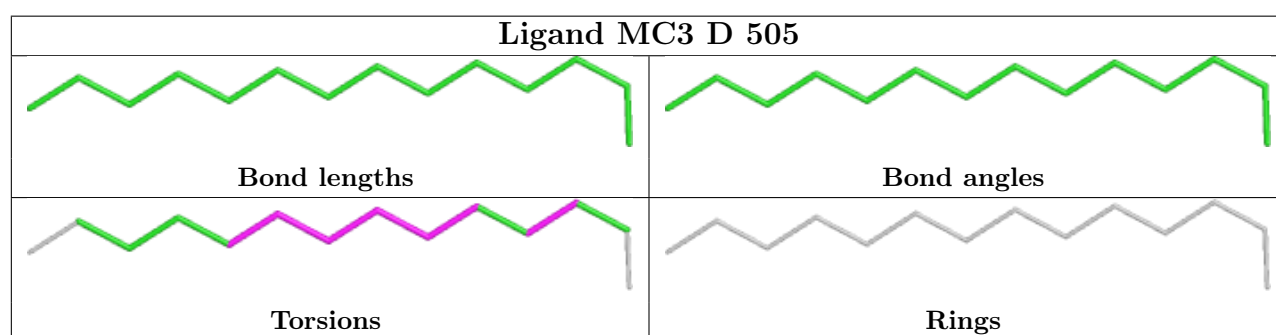
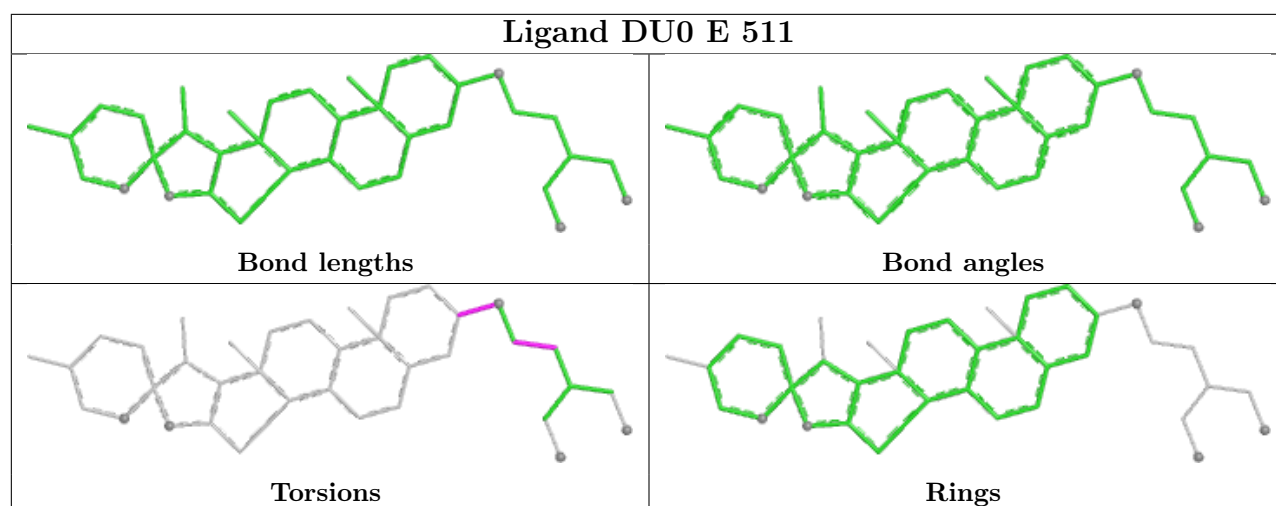
Ligand DU0 A 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

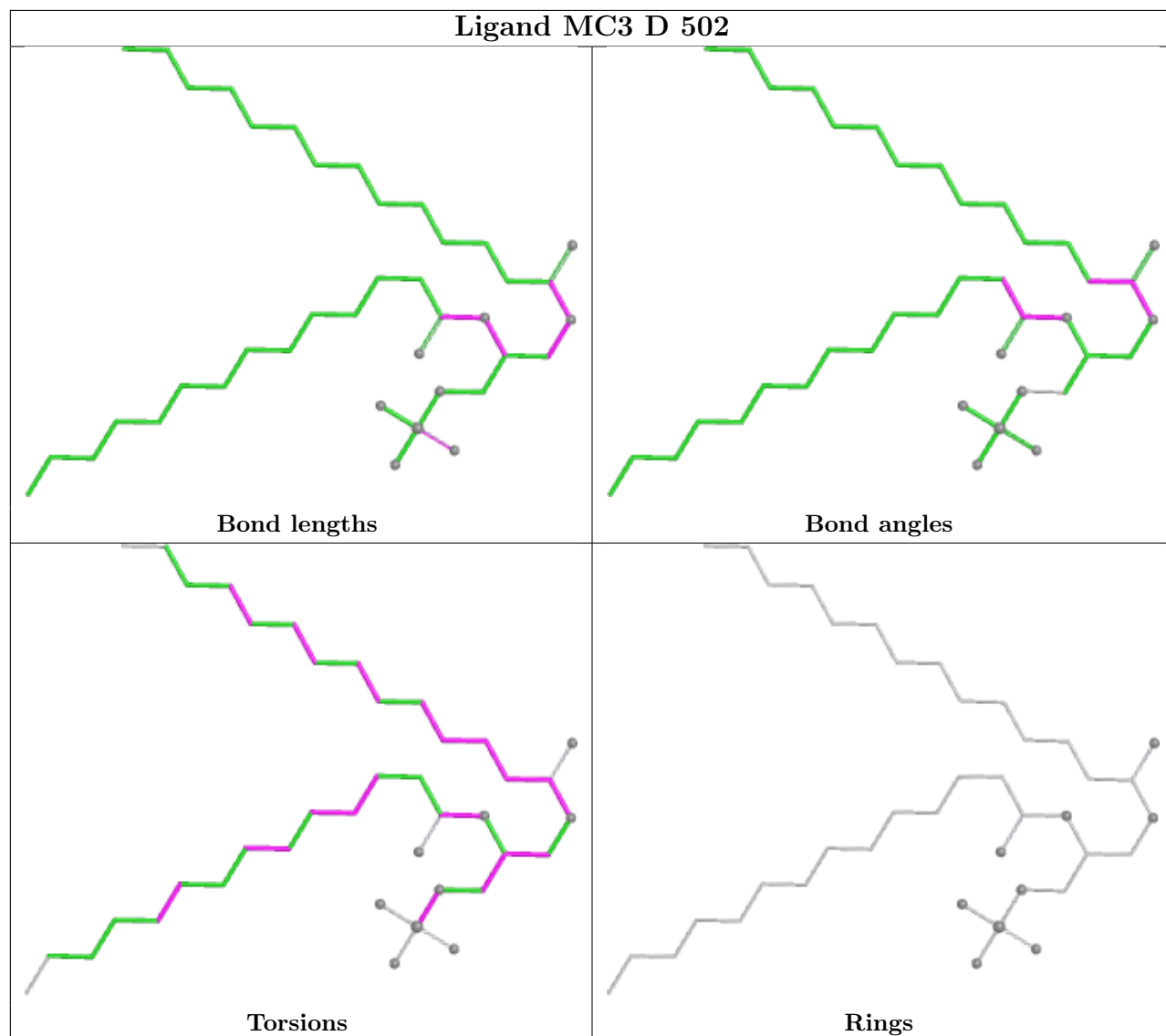
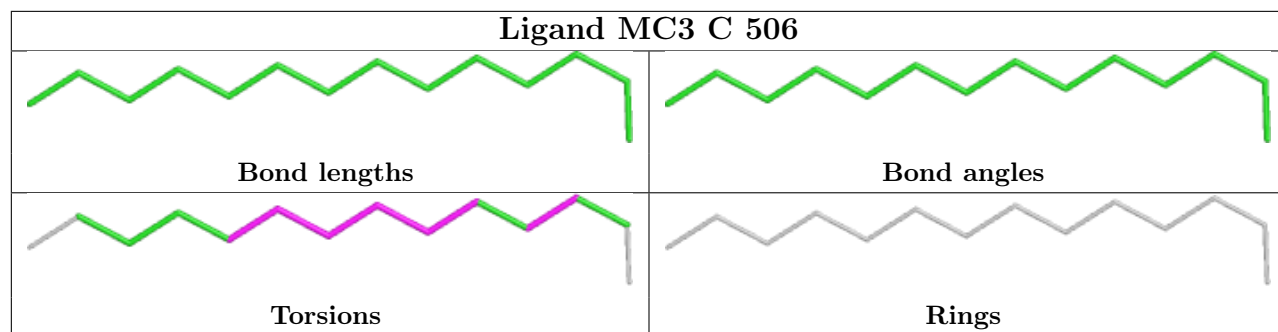
Ligand MC3 E 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

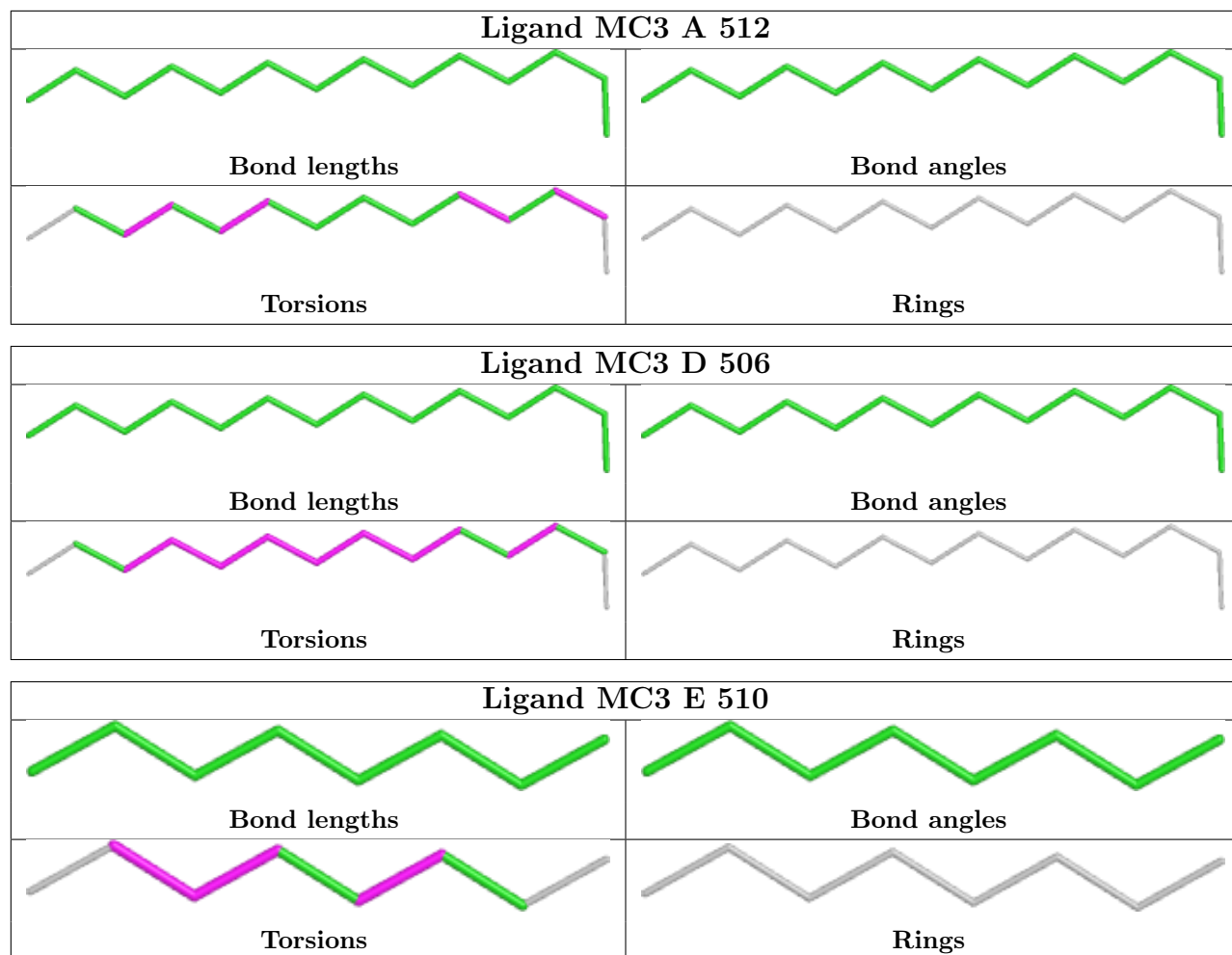
Ligand MC3 E 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

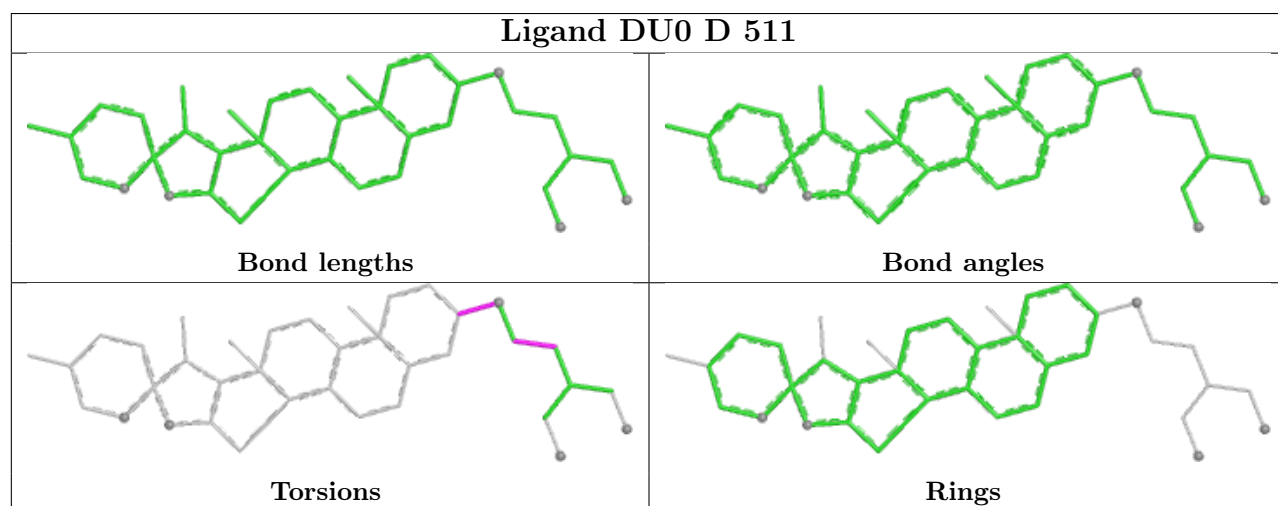
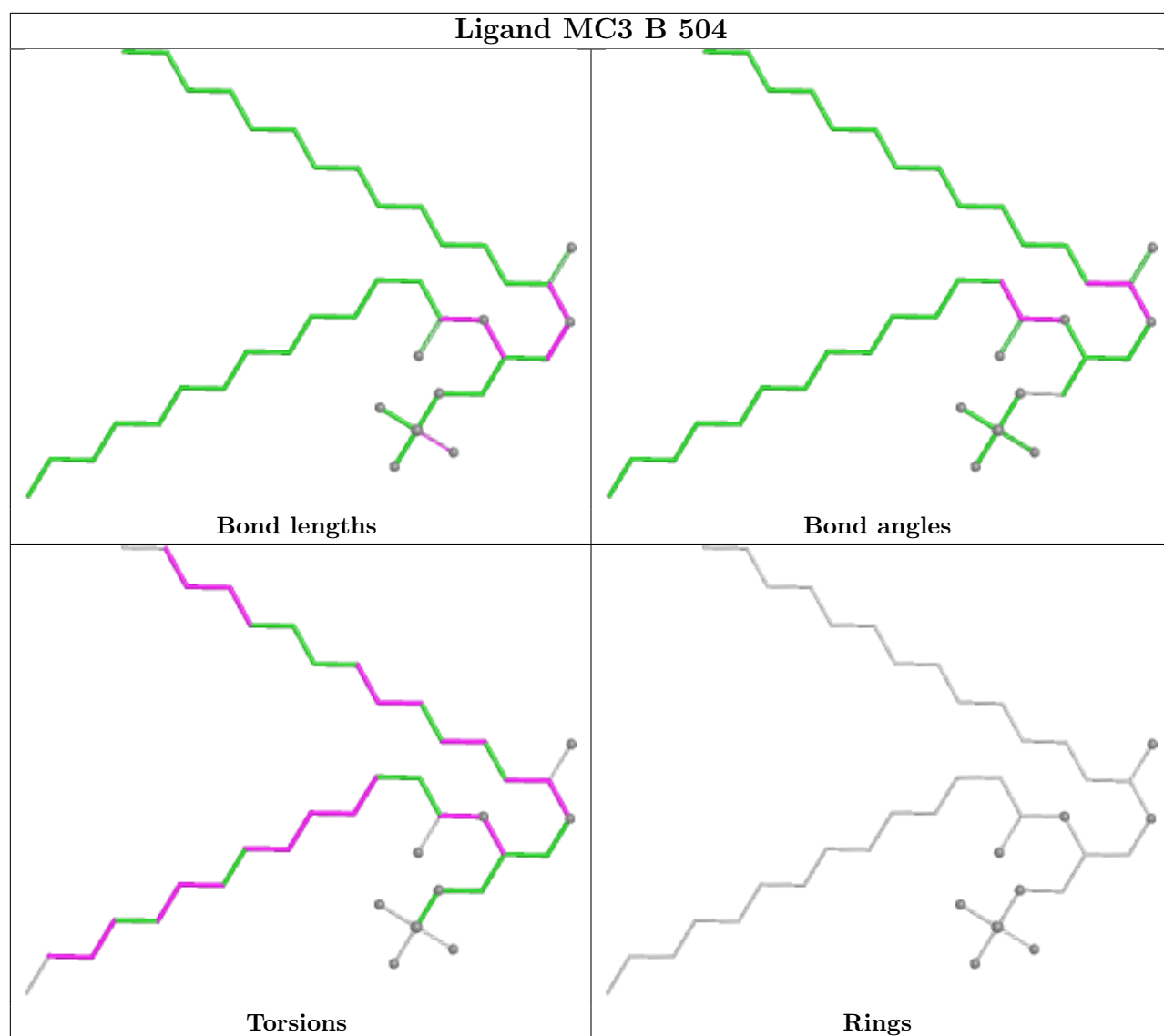


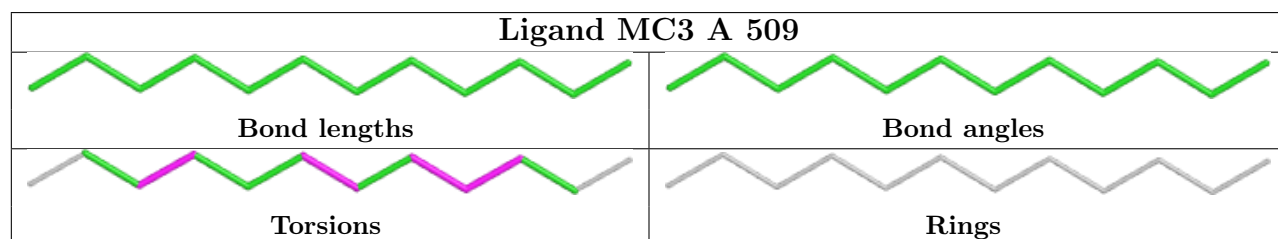
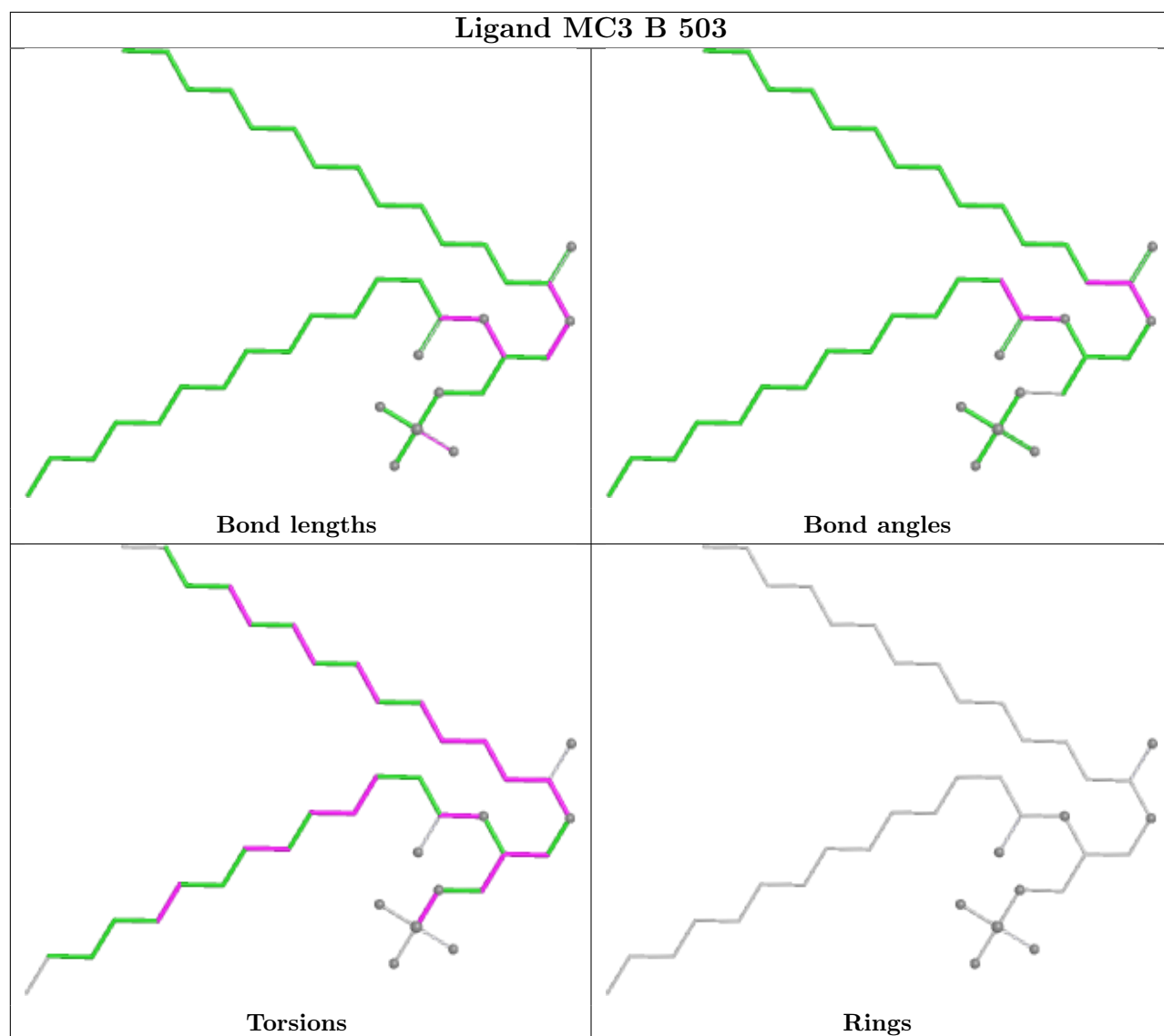
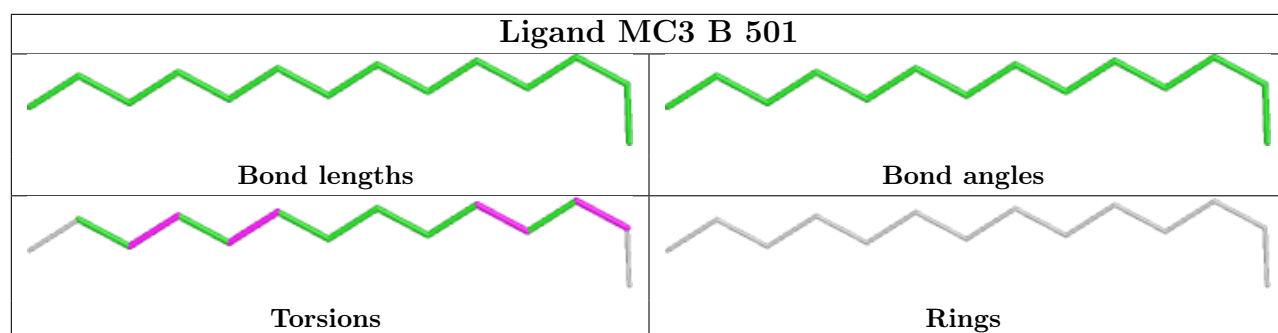


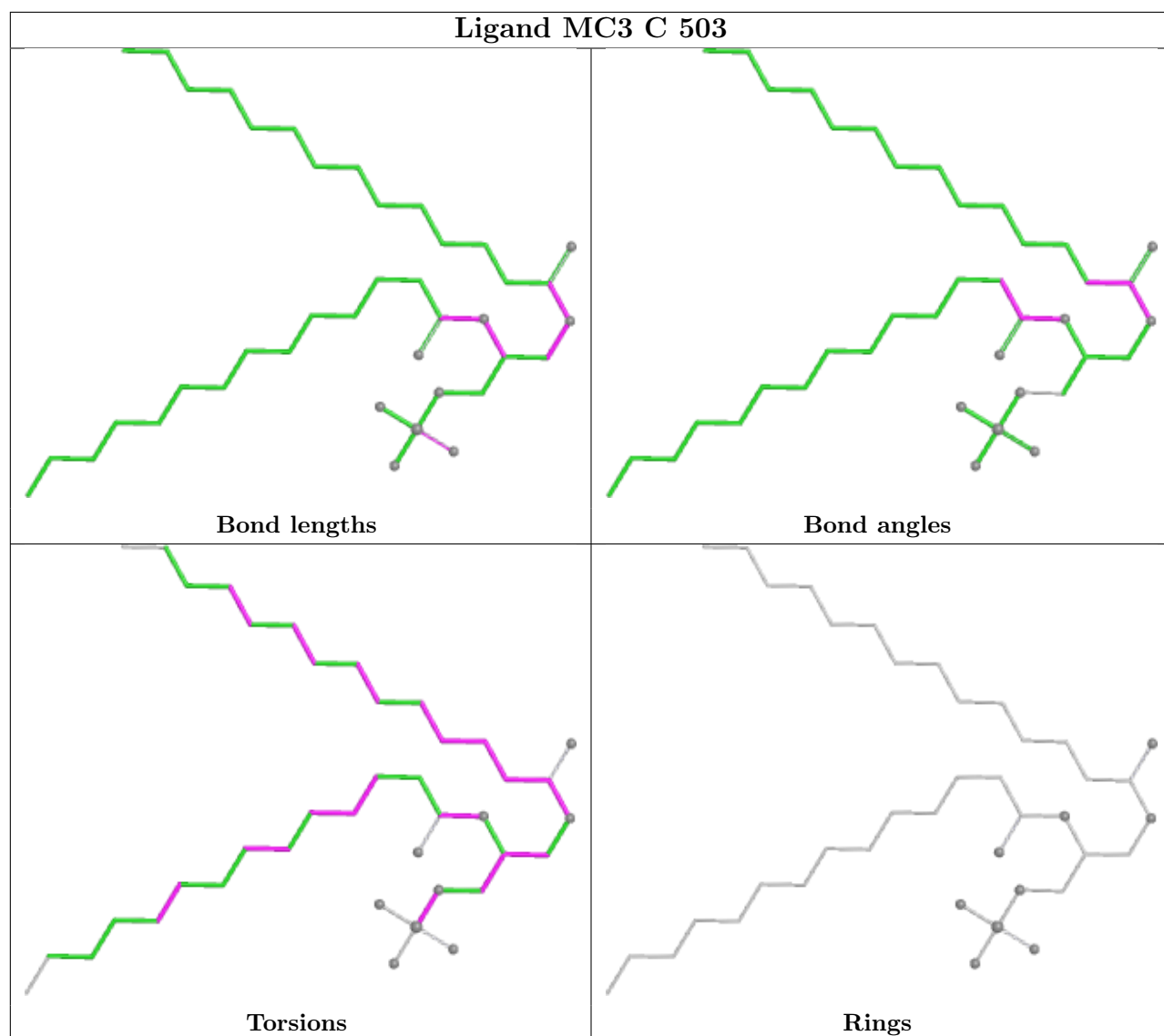
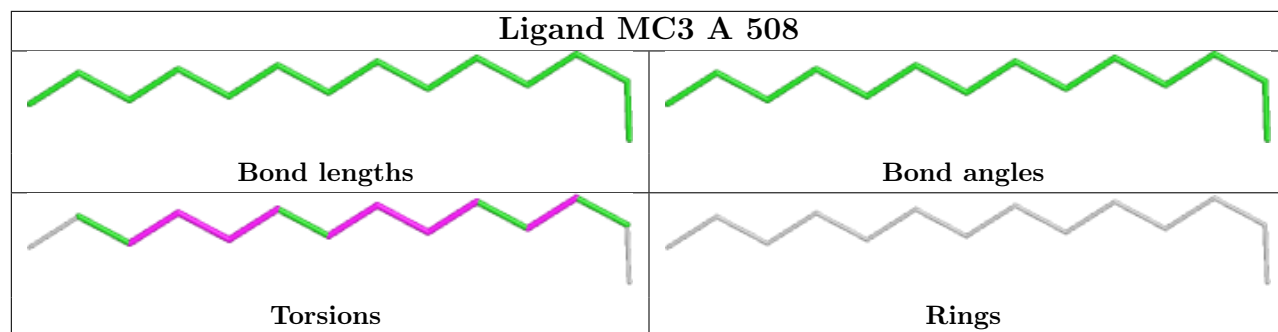


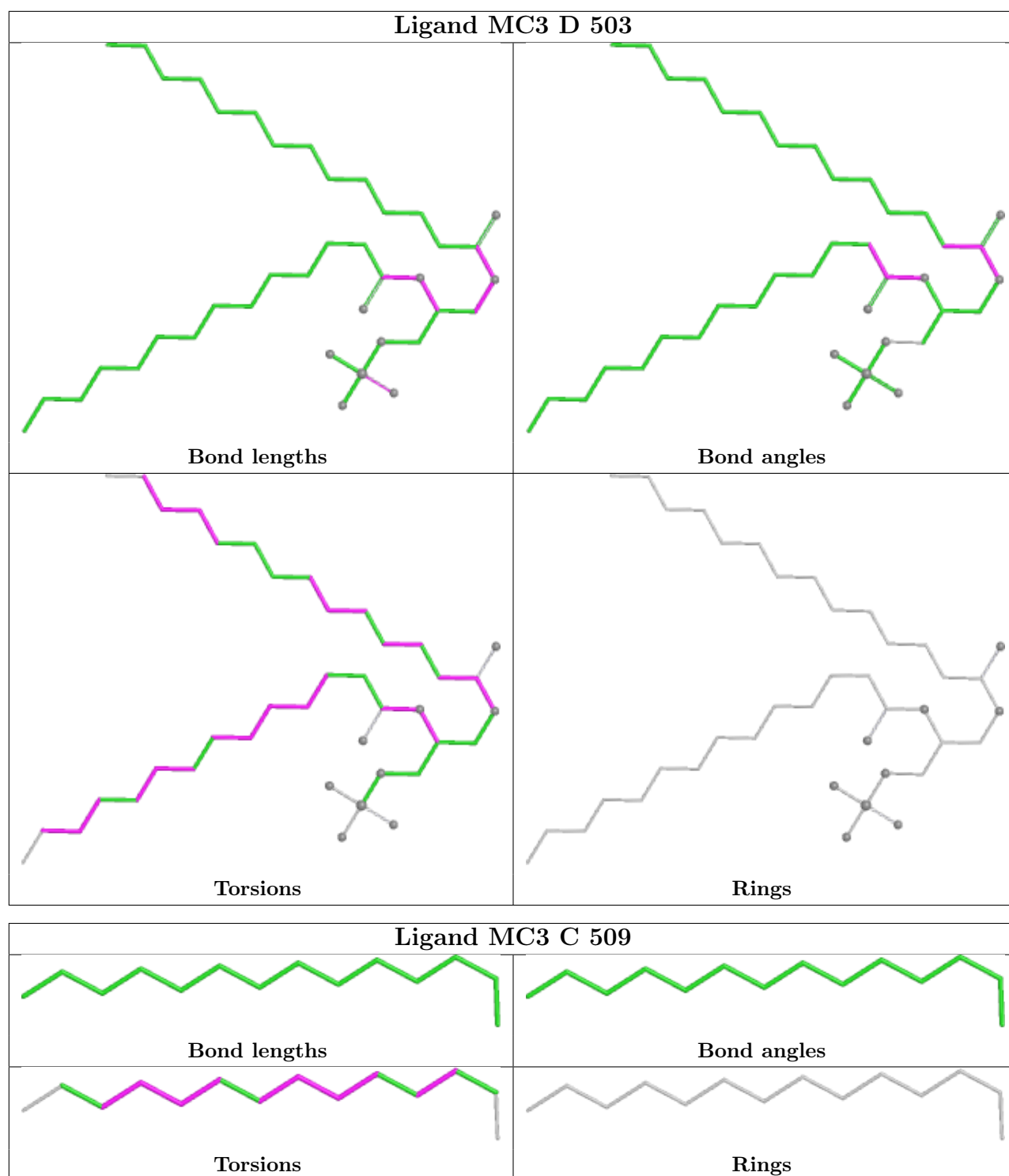


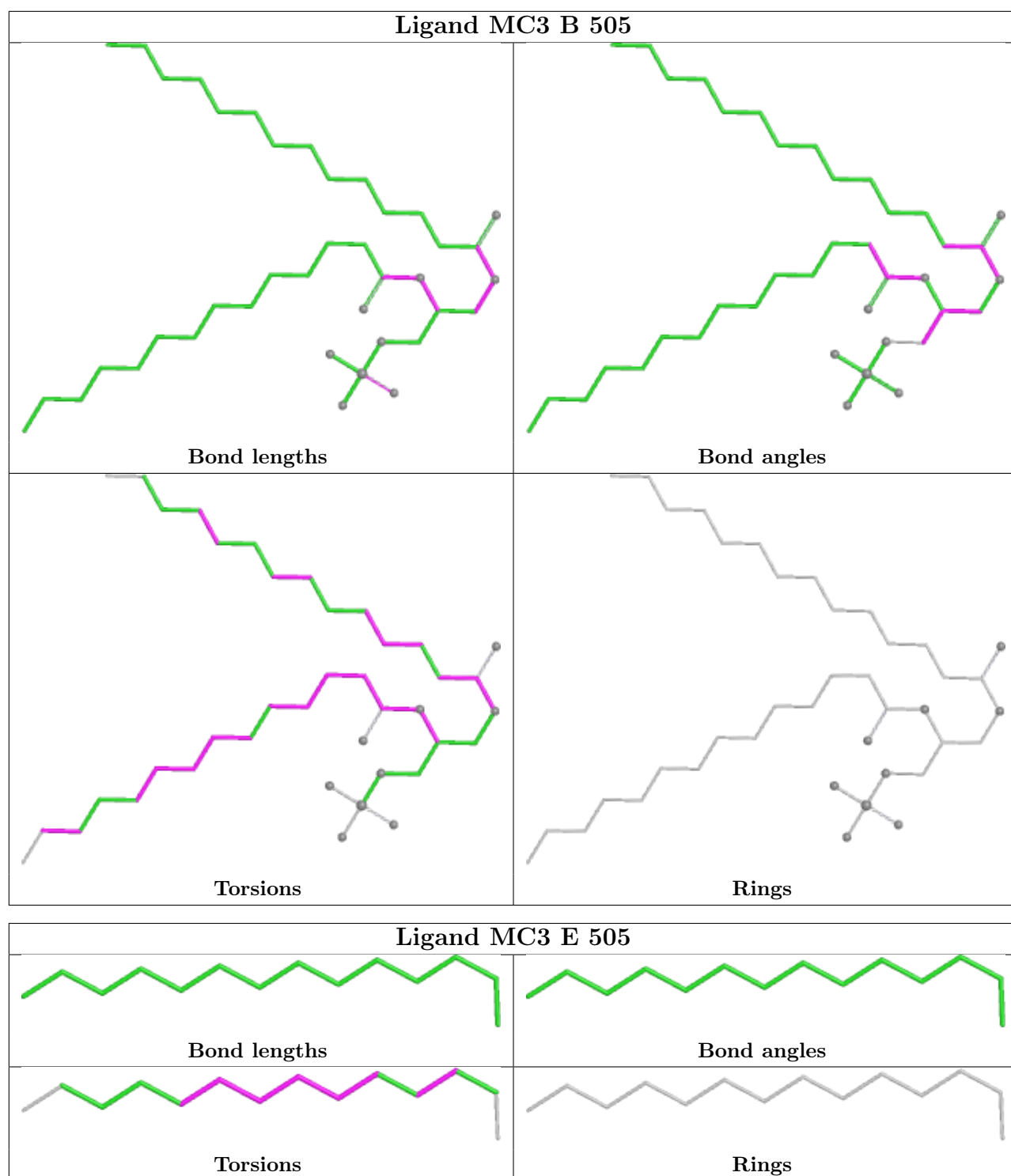


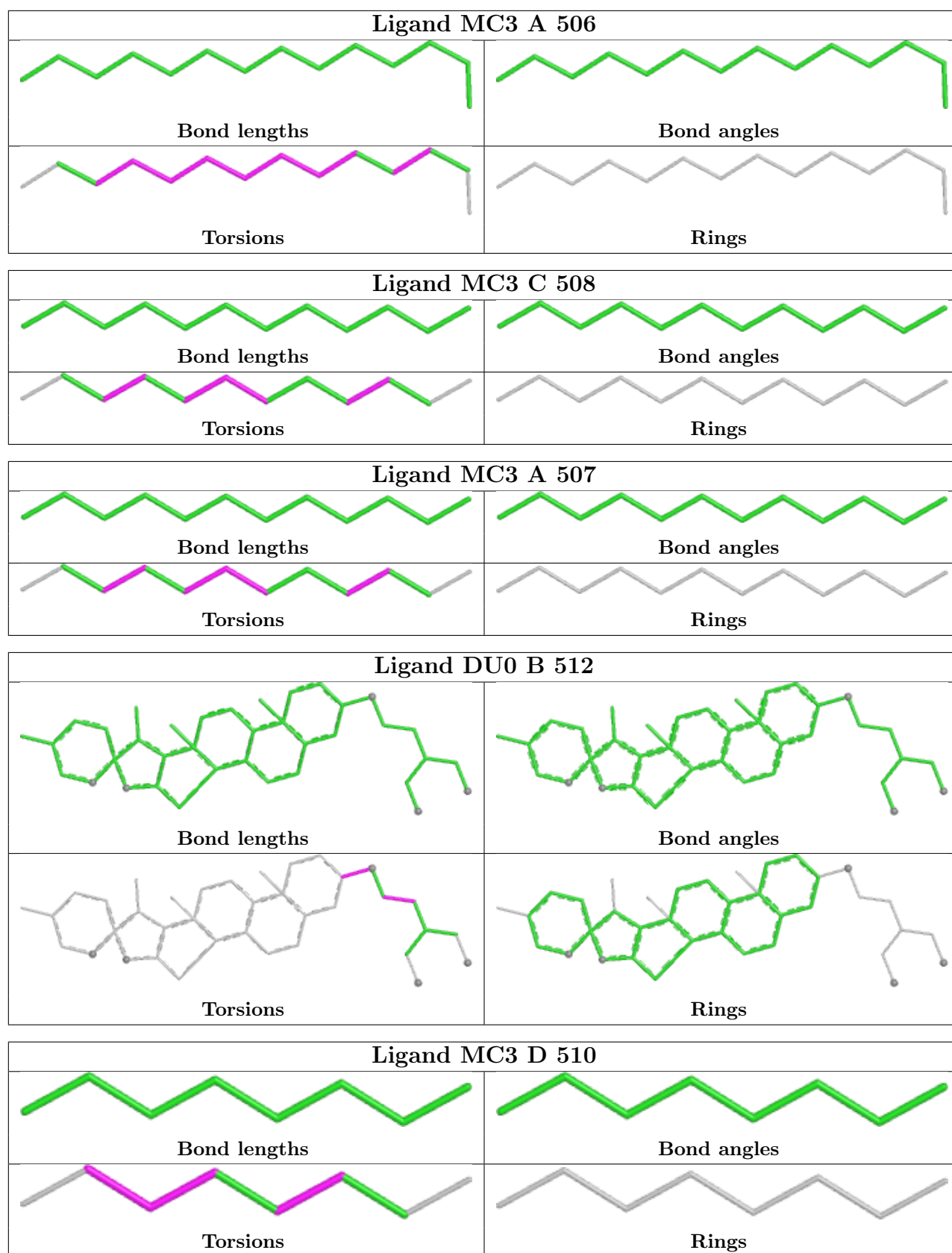


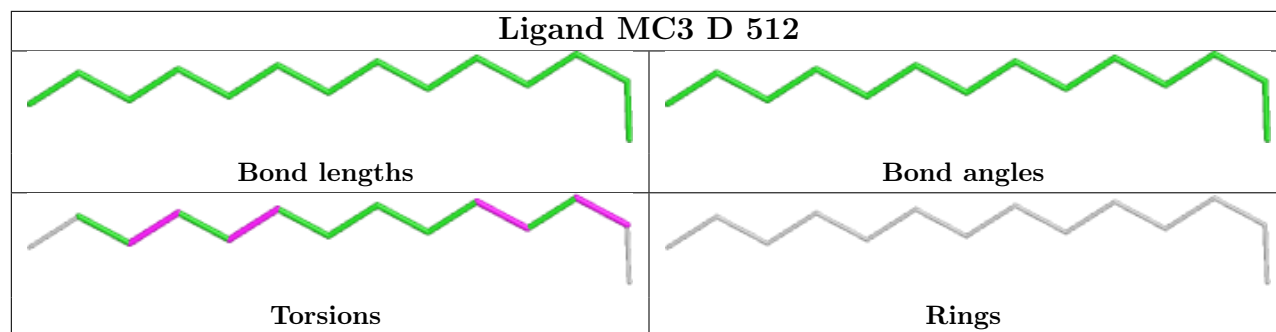












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

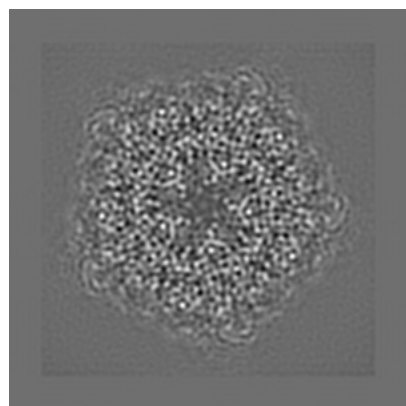
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27127. These allow visual inspection of the internal detail of the map and identification of artifacts.

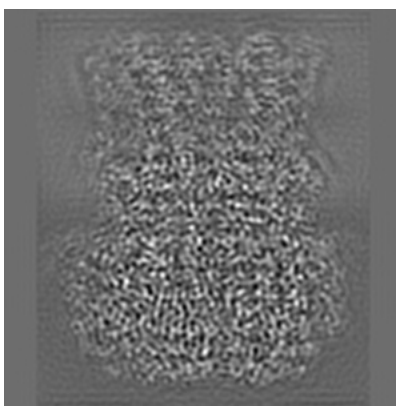
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

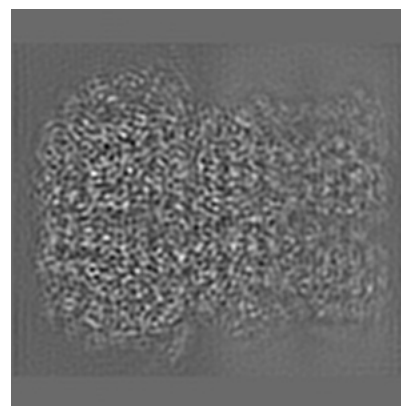
6.1.1 Primary map



X

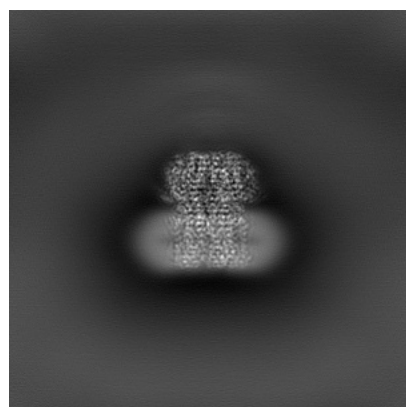


Y

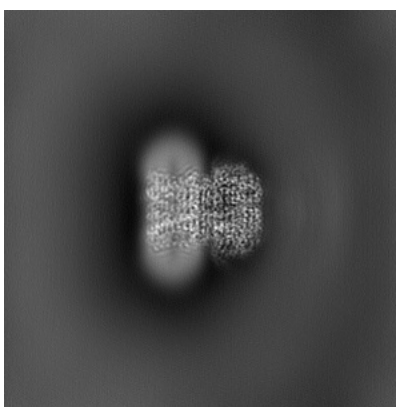


Z

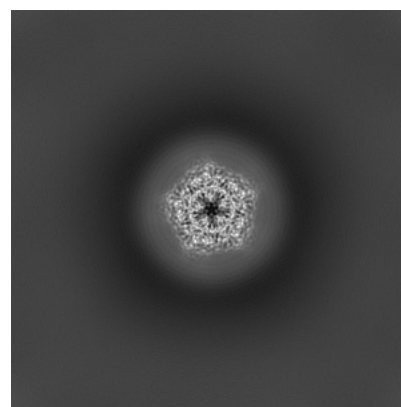
6.1.2 Raw map



X



Y

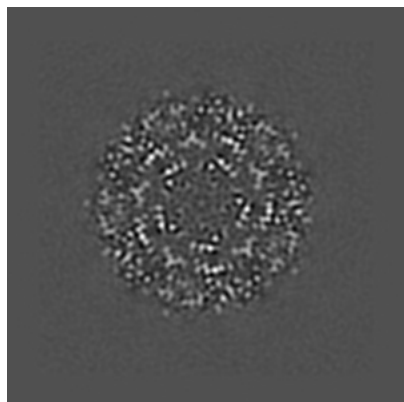


Z

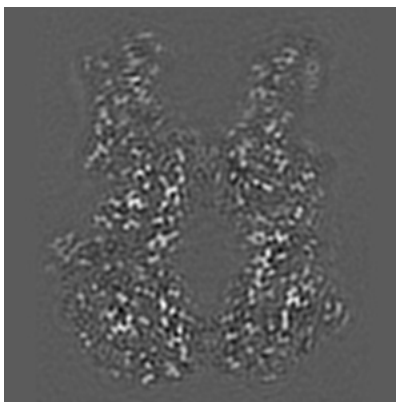
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

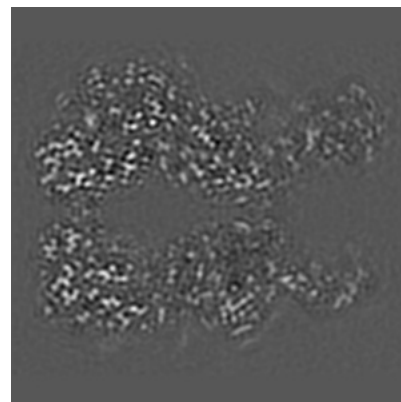
6.2.1 Primary map



X Index: 135

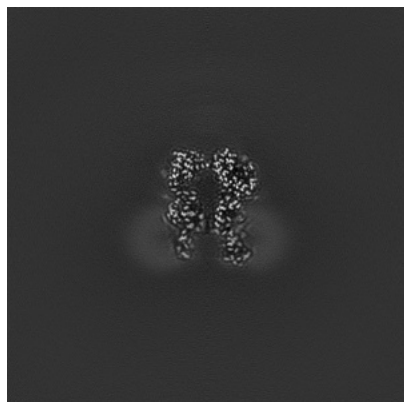


Y Index: 135

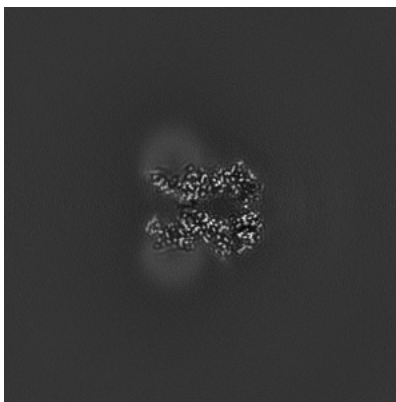


Z Index: 135

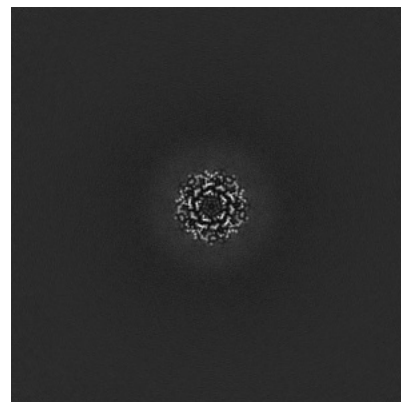
6.2.2 Raw map



X Index: 200



Y Index: 200

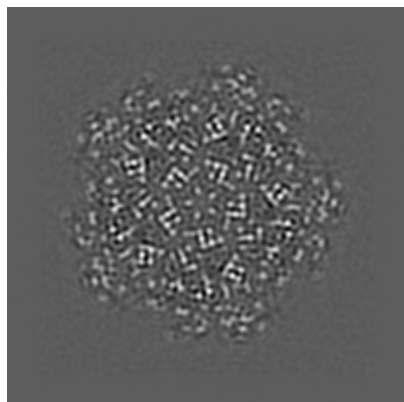


Z Index: 200

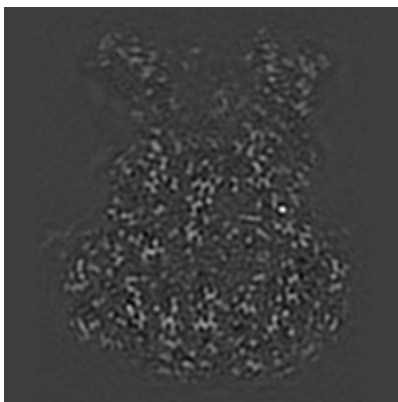
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

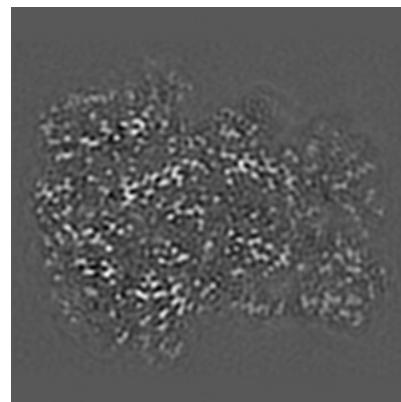
6.3.1 Primary map



X Index: 54

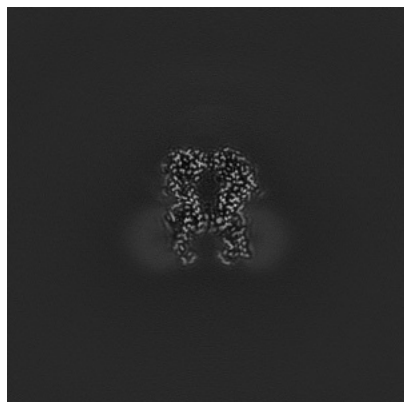


Y Index: 159

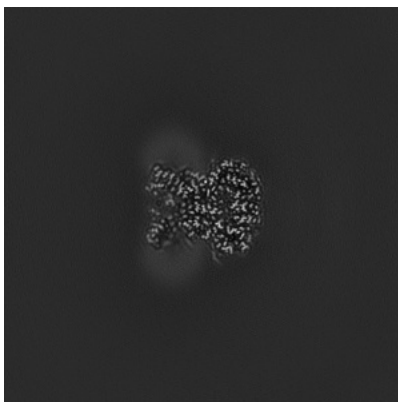


Z Index: 101

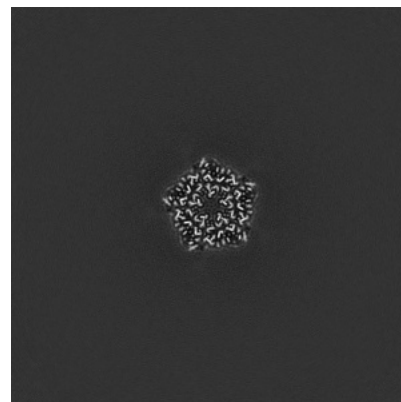
6.3.2 Raw map



X Index: 195



Y Index: 214

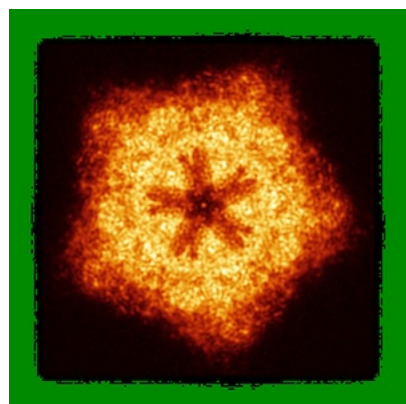


Z Index: 229

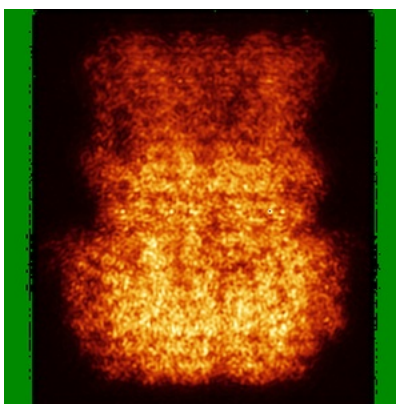
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

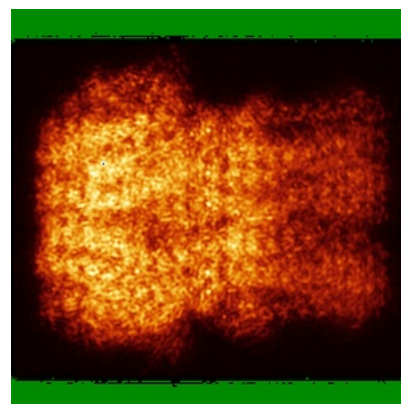
6.4.1 Primary map



X

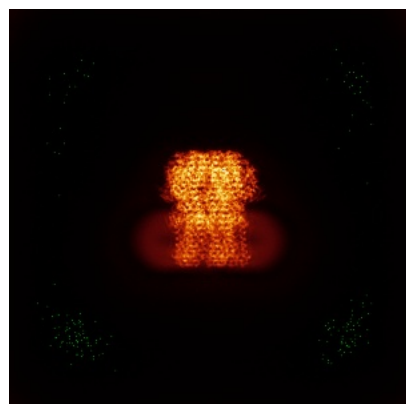


Y

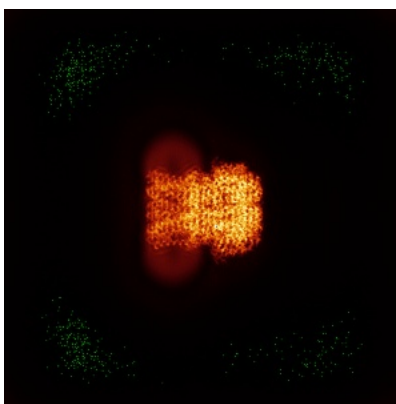


Z

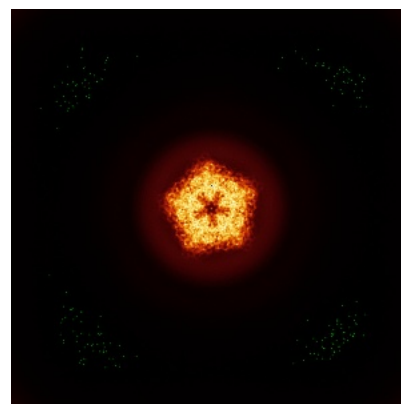
6.4.2 Raw map



X



Y

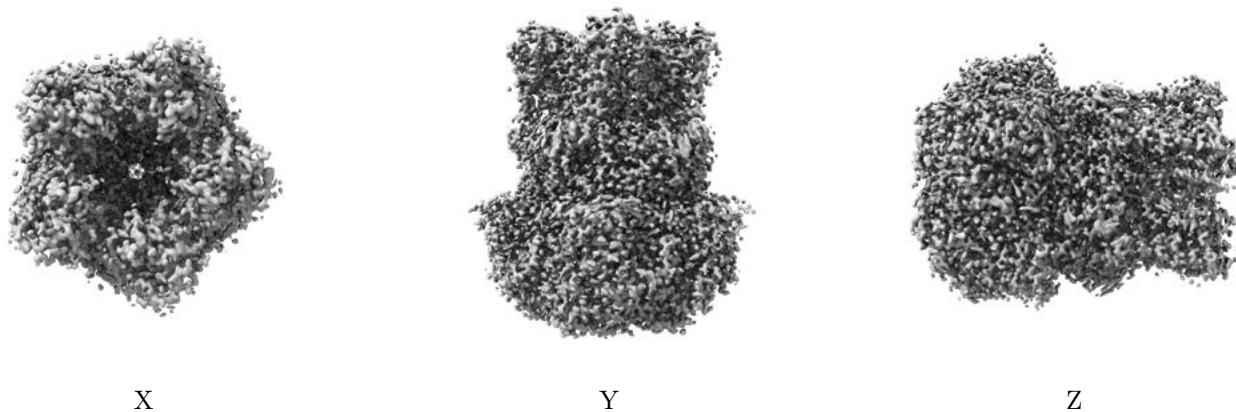


Z

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

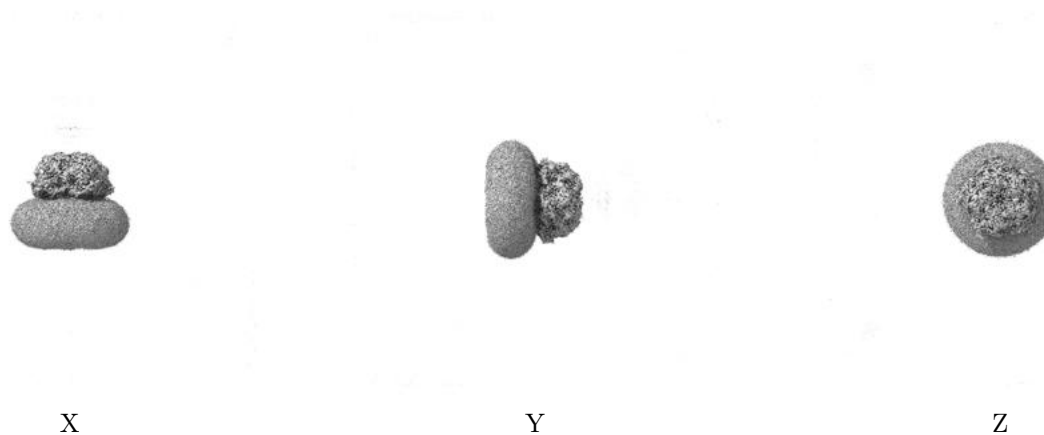
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.858. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

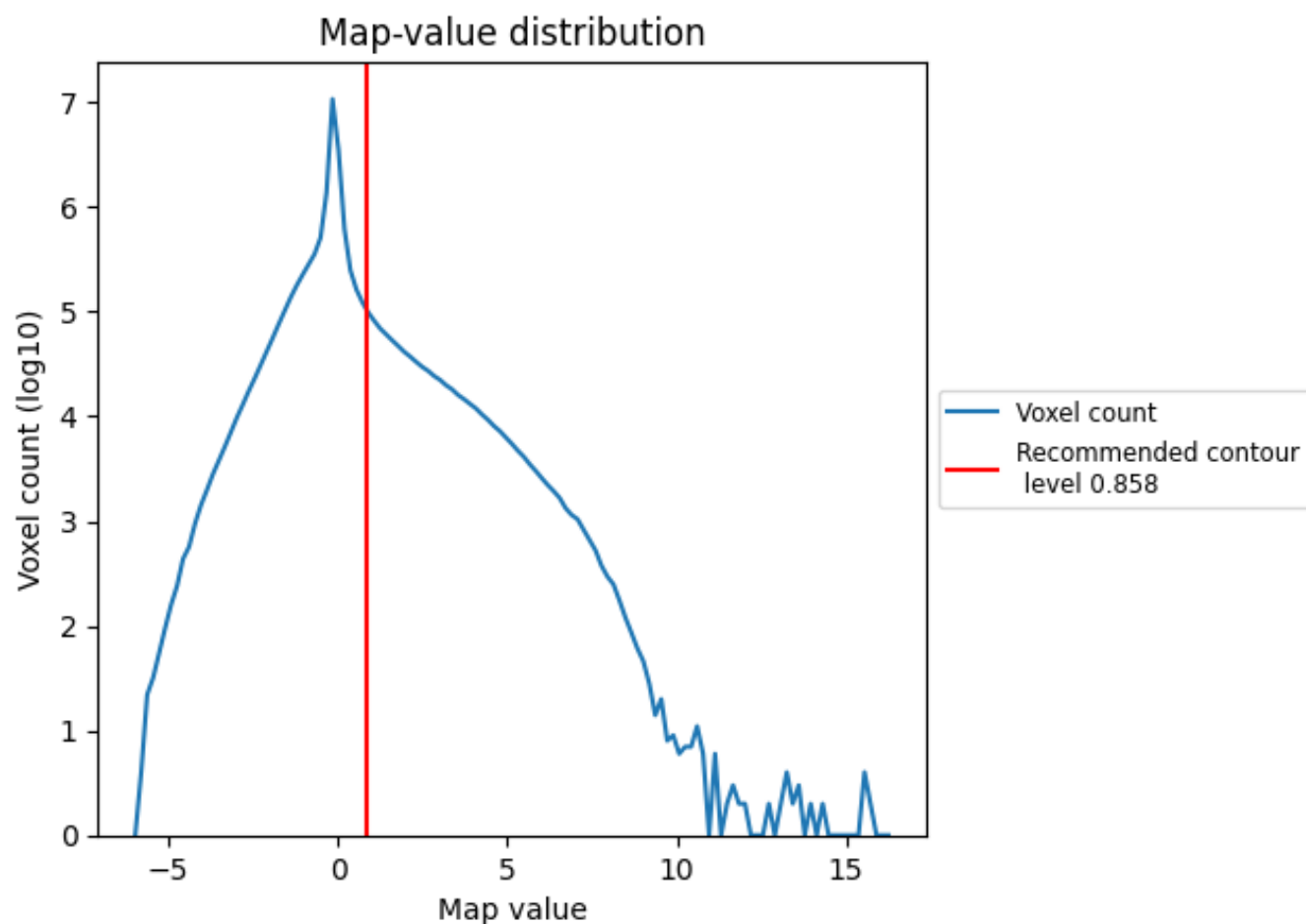
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

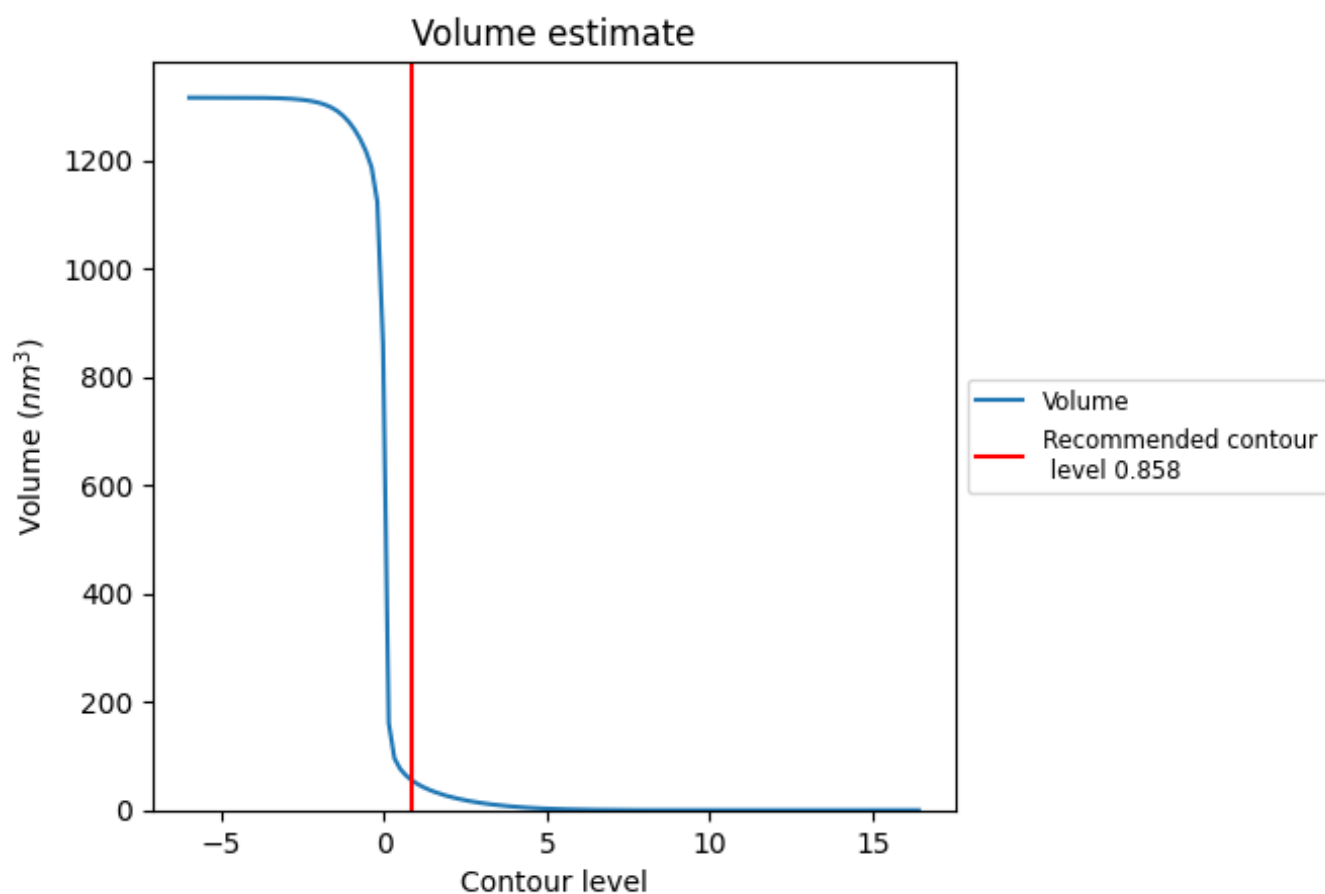
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

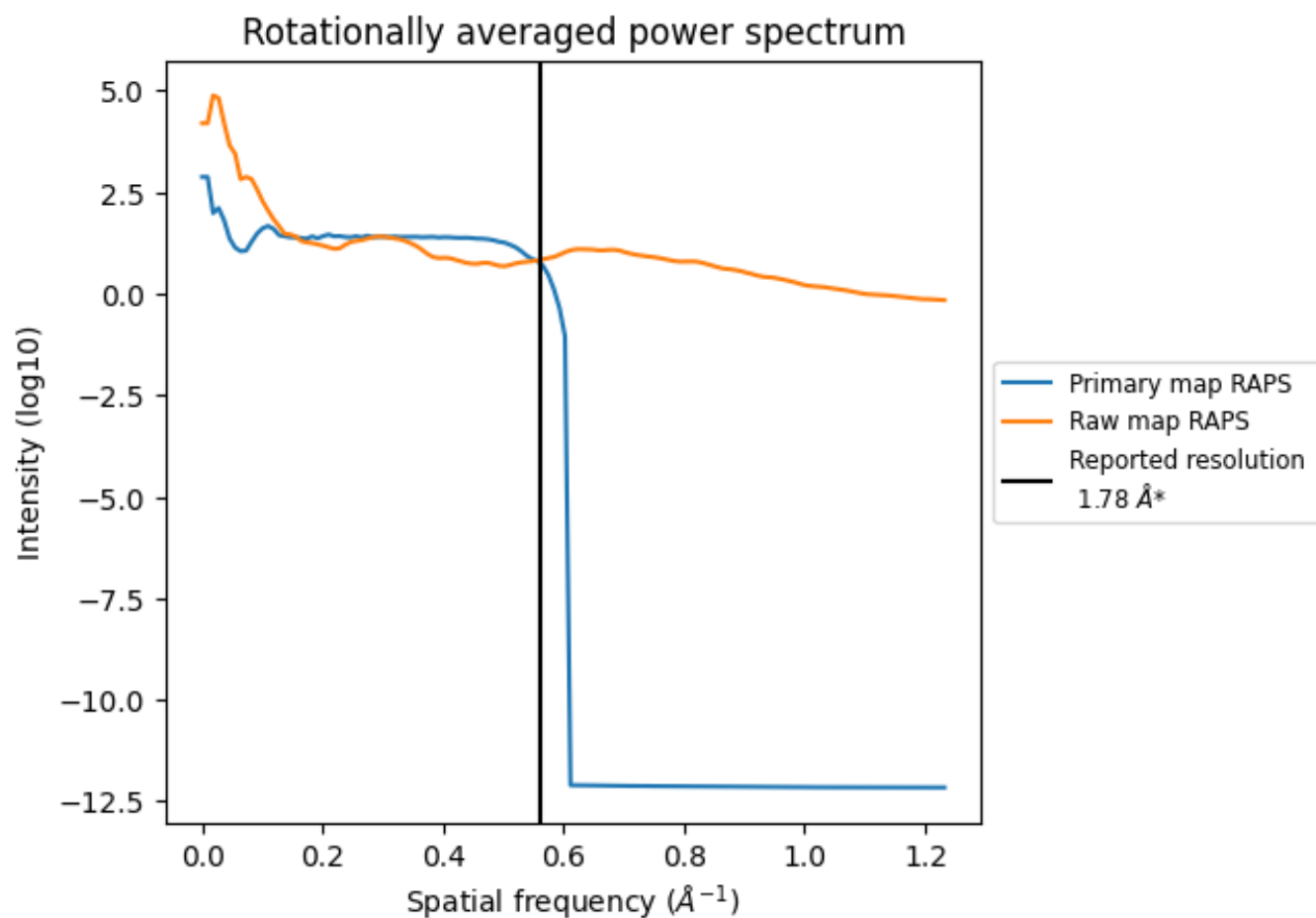
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 55 nm³; this corresponds to an approximate mass of 50 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

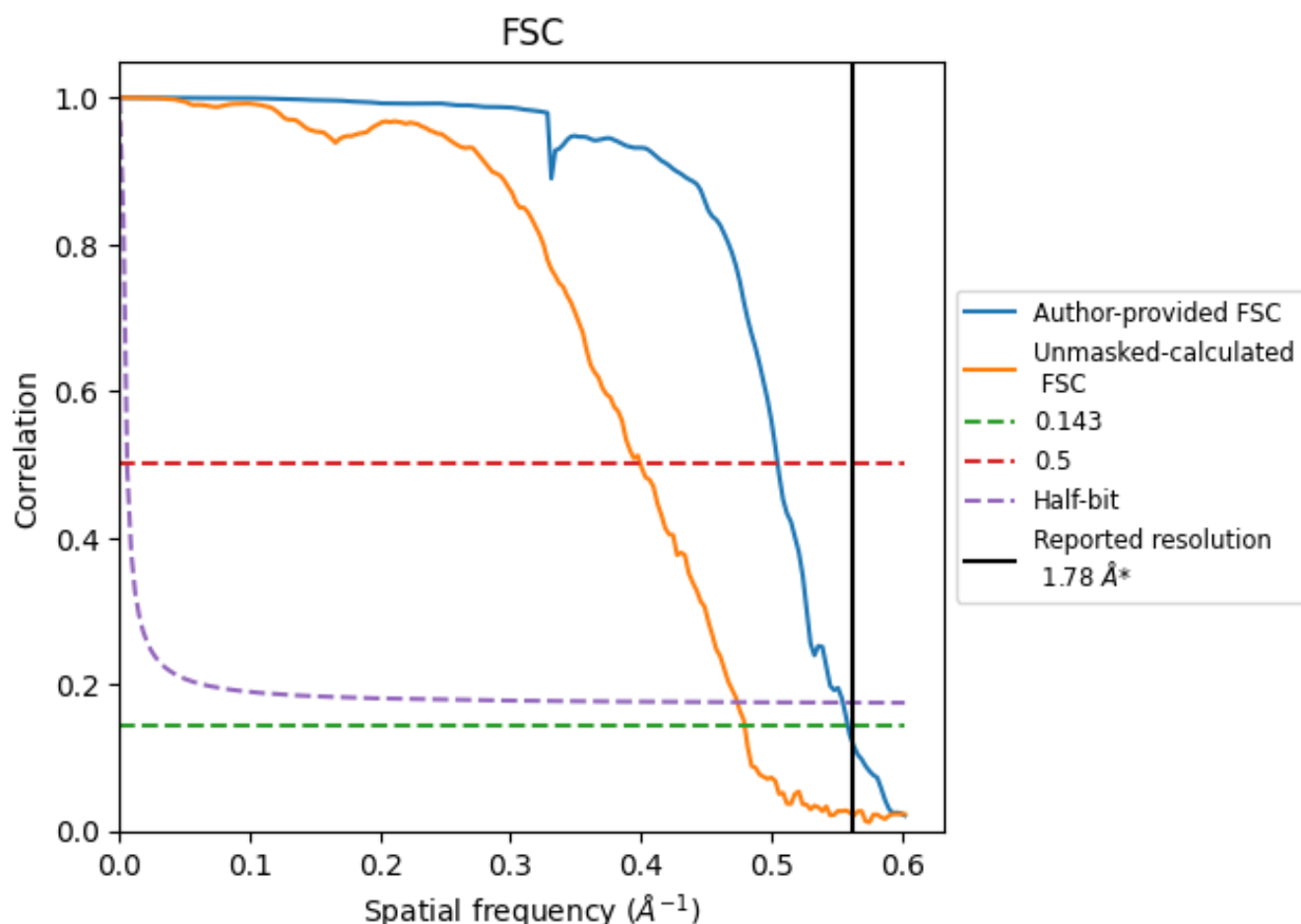


*Reported resolution corresponds to spatial frequency of 0.562 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.562 Å⁻¹

8.2 Resolution estimates [i](#)

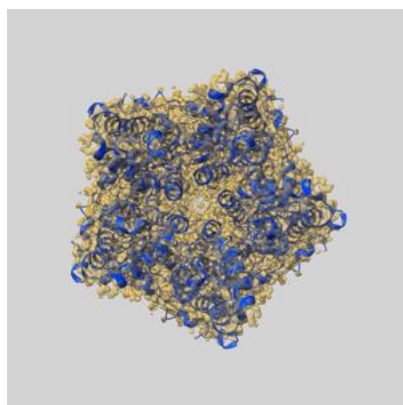
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.78	-	-
Author-provided FSC curve	1.79	1.98	1.80
Unmasked-calculated*	2.09	2.50	2.11

*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 2.09 differs from the reported value 1.78 by more than 10 %

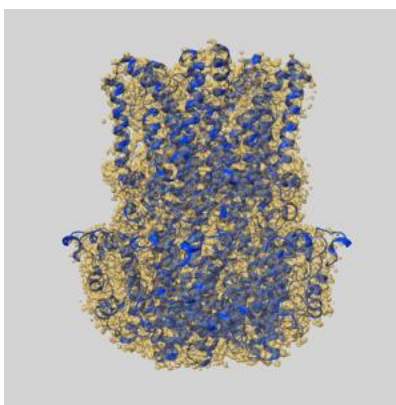
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27127 and PDB model 8D1E. Per-residue inclusion information can be found in section [3](#) on page [9](#).

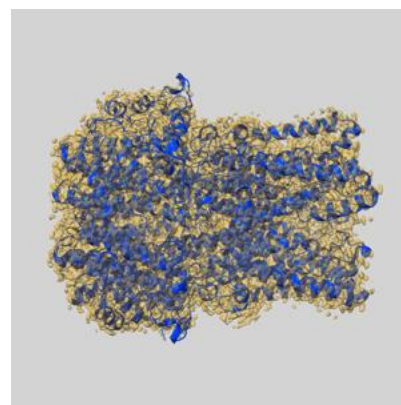
9.1 Map-model overlay [i](#)



X



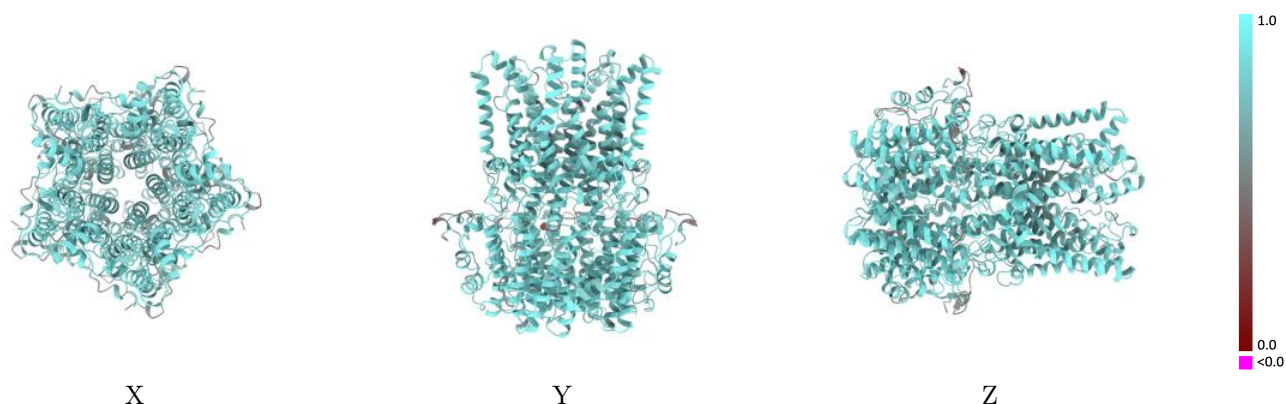
Y



Z

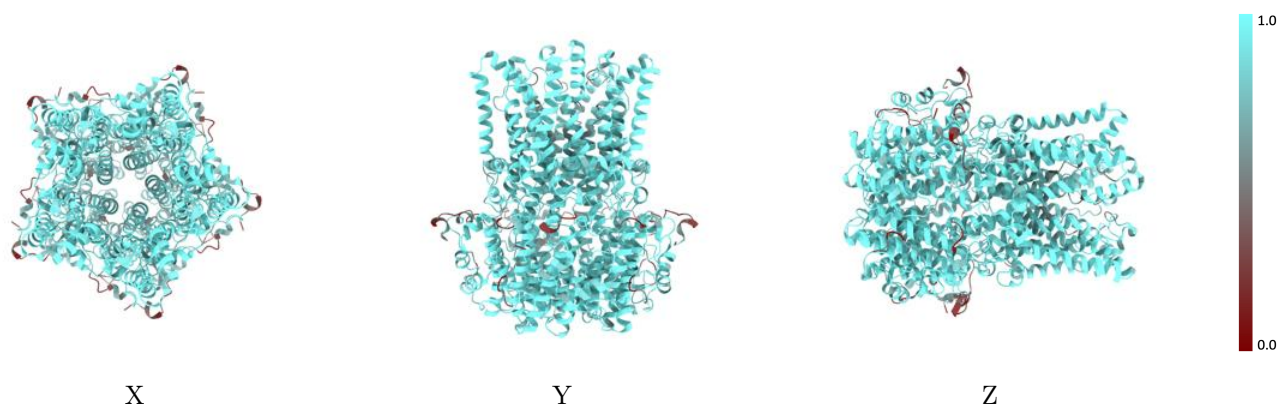
The images above show the 3D surface view of the map at the recommended contour level 0.858 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



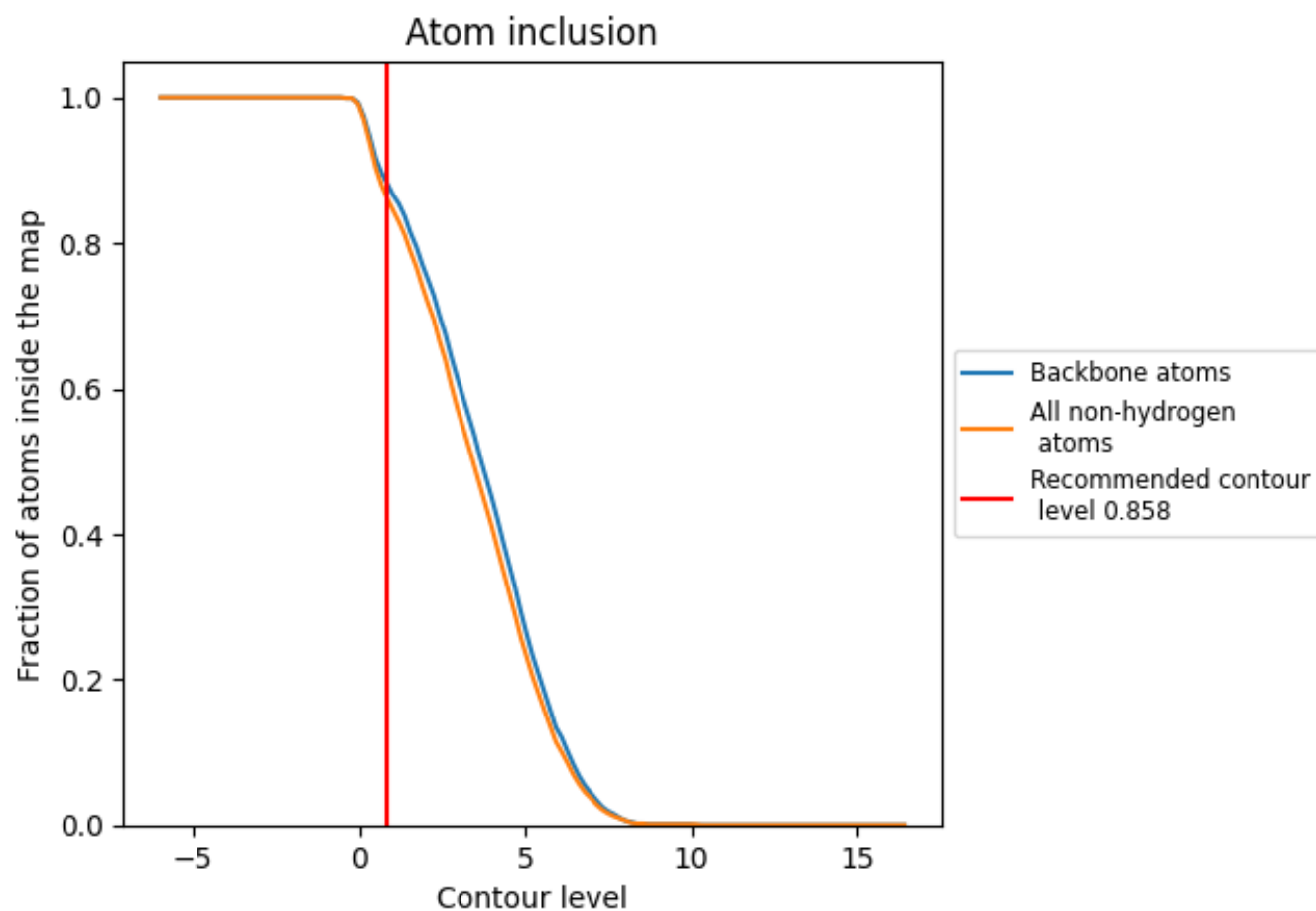
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.858).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.858) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8600	<div><div></div></div> 0.7890
A	<div><div></div></div> 0.8630	<div><div></div></div> 0.7880
B	<div><div></div></div> 0.8610	<div><div></div></div> 0.7890
C	<div><div></div></div> 0.8640	<div><div></div></div> 0.7880
D	<div><div></div></div> 0.8630	<div><div></div></div> 0.7900
E	<div><div></div></div> 0.8630	<div><div></div></div> 0.7880

