



Full wwPDB EM Validation Report ⓘ

Jun 29, 2025 – 07:29 am BST

PDB ID : 8AP7 / pdb_00008ap7
EMDB ID : EMD-15560
Title : membrane region of the Trypanosoma brucei mitochondrial ATP synthase dimer
Authors : Muehleip, A.; Gahura, O.; Zikova, A.; Amunts, A.
Deposited on : 2022-08-09
Resolution : 2.70 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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

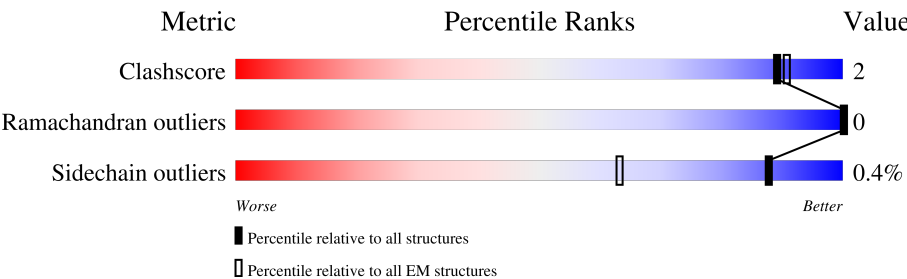
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.





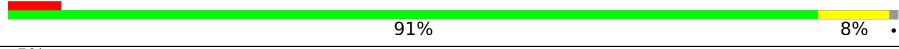
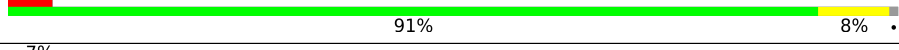
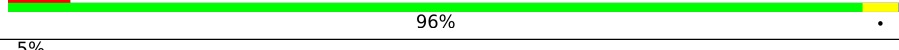
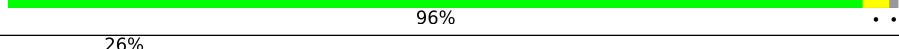
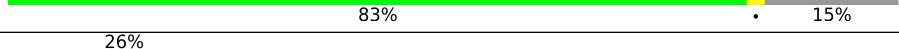
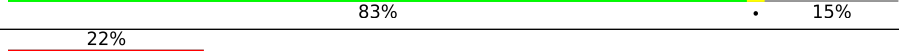
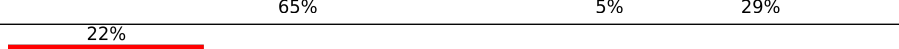
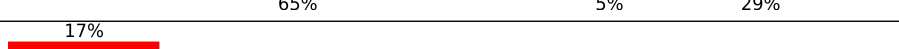
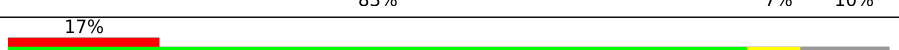

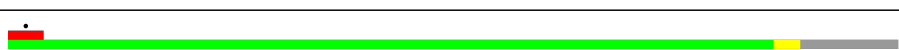
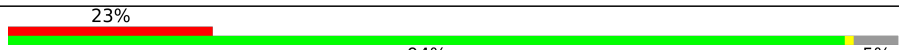
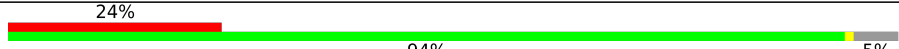




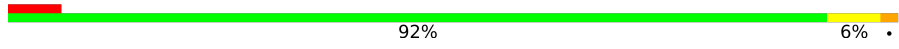
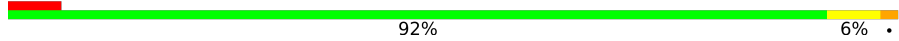
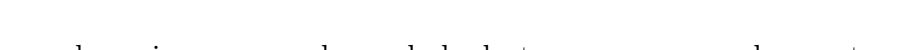
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	231	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>
1	a	231	<div> <div>5%</div> <div>96%</div> <div>.</div> </div>
2	C	114	<div> <div>52%</div> <div>44%</div> </div>
2	c	114	<div> <div>49%</div> <div>7%</div> <div>44%</div> </div>
3	D	370	<div> <div>26%</div> <div>49%</div> <div>48%</div> </div>
3	d	370	<div> <div>26%</div> <div>49%</div> <div>48%</div> </div>
4	E	396	<div> <div>93%</div> <div>.</div> <div>.</div> </div>
4	e	396	<div> <div>93%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	145	
5	f	145	
6	I	104	
6	i	104	
7	J	169	
7	j	169	
8	K	124	
8	k	124	
9	L	92	
9	l	92	
10	M	144	
10	m	144	
11	N	156	
11	n	156	
12	O	101	
12	o	101	
13	P	105	
13	p	105	
14	Q	98	
14	q	98	
15	R	62	
15	r	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	Q7G	E	407	X	-	-	-
18	Q7G	N	201	X	-	-	-
18	Q7G	e	407	X	-	-	-
18	Q7G	n	201	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 76690 atoms, of which 38834 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 ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	231	Total	C	H	N	O	S	0	0
			4076	1459	2044	261	284	28		
1	a	231	Total	C	H	N	O	S	0	0
			4076	1459	2044	261	284	28		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	TRP	-	insertion	UNP P24499
A	180	TRP	-	insertion	UNP P24499
a	23	TRP	-	insertion	UNP P24499
a	180	TRP	-	insertion	UNP P24499

- Molecule 2 is a protein called subunit-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	64	Total	C	H	N	O	S	0	0
			1115	385	549	86	90	5		
2	c	64	Total	C	H	N	O	S	0	0
			1115	385	549	86	90	5		

- Molecule 3 is a protein called subunit-d.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	193	Total	C	H	N	O	S	0	0
			3212	1008	1607	293	297	7		
3	d	193	Total	C	H	N	O	S	0	0
			3212	1008	1607	293	297	7		

- Molecule 4 is a protein called ATPTB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	383	Total	C	H	N	O	S	0	0
			6281	2060	3061	558	585	17		
4	e	383	Total	C	H	N	O	S	0	0
			6281	2060	3061	558	585	17		

- Molecule 5 is a protein called subunit-f.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	135	Total	C	H	N	O	S	0	0
			2256	744	1111	201	195	5		
5	f	135	Total	C	H	N	O	S	0	0
			2256	744	1111	201	195	5		

- Molecule 6 is a protein called subunit-i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	103	Total	C	H	N	O	S	0	0
			1740	574	857	152	151	6		
6	i	103	Total	C	H	N	O	S	0	0
			1740	574	857	152	151	6		

- Molecule 7 is a protein called ATPTB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	168	Total	C	H	N	O	S	0	0
			2835	919	1411	249	249	7		
7	j	168	Total	C	H	N	O	S	0	0
			2835	919	1411	249	249	7		

- Molecule 8 is a protein called subunit-k.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	K	105	Total	C	H	N	O	S	0	0
			1749	577	876	149	141	6		
8	k	105	Total	C	H	N	O	S	0	0
			1749	577	876	149	141	6		

- Molecule 9 is a protein called subunit-e.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	L	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
9	l	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		

- Molecule 10 is a protein called subunit-g.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	M	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		
10	m	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		

- Molecule 11 is a protein called ATPTB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	N	139	Total	C	H	N	O	S	0	0
			2210	730	1082	183	208	7		
11	n	139	Total	C	H	N	O	S	0	0
			2210	730	1082	183	208	7		

- Molecule 12 is a protein called ATPTB12.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	O	96	Total	C	H	N	O	S	0	0
			1556	506	767	140	140	3		
12	o	96	Total	C	H	N	O	S	0	0
			1556	506	767	140	140	3		

- Molecule 13 is a protein called subunit-b.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	P	80	Total	C	H	N	O	S	0	0
			1335	448	651	108	125	3		
13	p	80	Total	C	H	N	O	S	0	0
			1335	448	651	108	125	3		

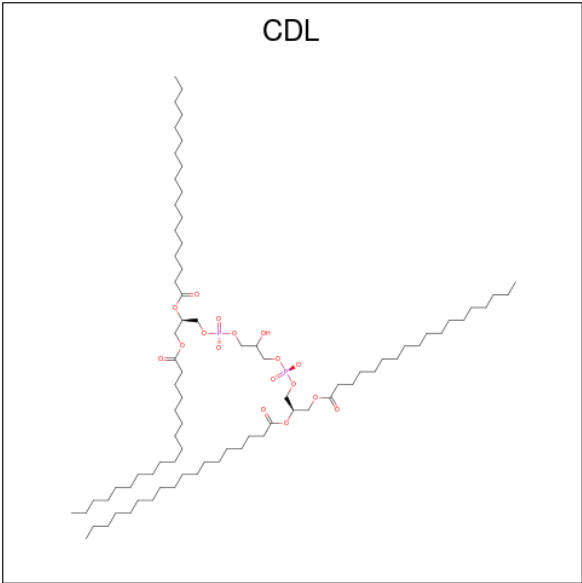
- Molecule 14 is a protein called ATPEG3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	85	Total	C	H	N	O	0	0
			1486	499	720	142	125		
14	q	85	Total	C	H	N	O	0	0
			1486	499	720	142	125		

- Molecule 15 is a protein called ATPEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	R	62	Total	C	H	N	O	S	0	0
			1040	358	498	94	85	5		
15	r	62	Total	C	H	N	O	S	0	0
			1040	358	498	94	85	5		

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



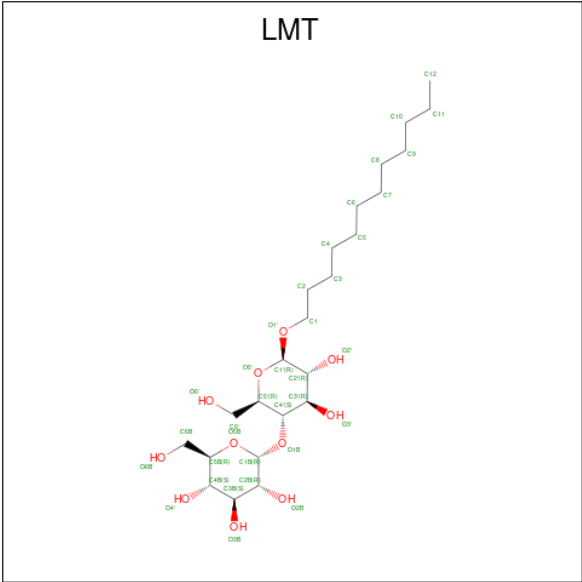
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
16	C	1	Total	C	H	O	P	0
			256	81	156	17	2	
16	E	1	Total	C	H	O	P	0
			256	81	156	17	2	
16	E	1	Total	C	H	O	P	0
			256	81	156	17	2	
16	E	1	Total	C	H	O	P	0
			256	81	156	17	2	
16	E	1	Total	C	H	O	P	0
			256	81	156	17	2	
16	F	1	Total	C	H	O	P	0
			256	81	156	17	2	
16	J	1	Total	C	H	O	P	0
			256	81	156	17	2	

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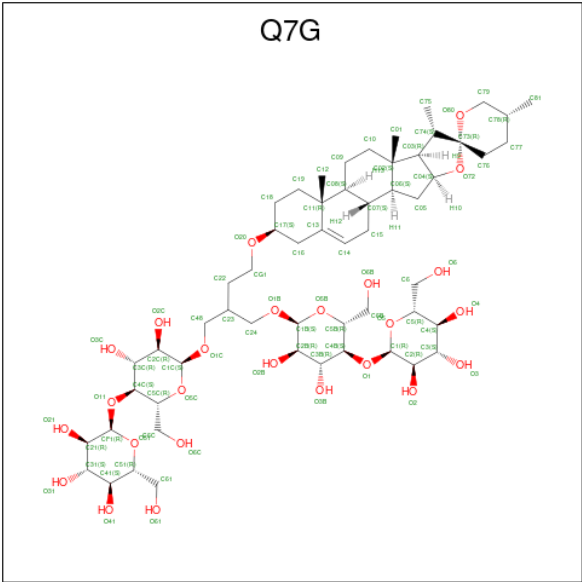
Mol	Chain	Residues	Atoms					AltConf
16	J	1	Total 256	C 81	H 156	O 17	P 2	0
16	L	1	Total 256	C 81	H 156	O 17	P 2	0
16	M	1	Total 256	C 81	H 156	O 17	P 2	0
16	Q	1	Total 256	C 81	H 156	O 17	P 2	0
16	c	1	Total 256	C 81	H 156	O 17	P 2	0
16	e	1	Total 256	C 81	H 156	O 17	P 2	0
16	e	1	Total 256	C 81	H 156	O 17	P 2	0
16	e	1	Total 256	C 81	H 156	O 17	P 2	0
16	e	1	Total 256	C 81	H 156	O 17	P 2	0
16	e	1	Total 256	C 81	H 156	O 17	P 2	0
16	f	1	Total 256	C 81	H 156	O 17	P 2	0
16	j	1	Total 256	C 81	H 156	O 17	P 2	0
16	j	1	Total 256	C 81	H 156	O 17	P 2	0
16	l	1	Total 256	C 81	H 156	O 17	P 2	0
16	m	1	Total 256	C 81	H 156	O 17	P 2	0
16	q	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 17 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



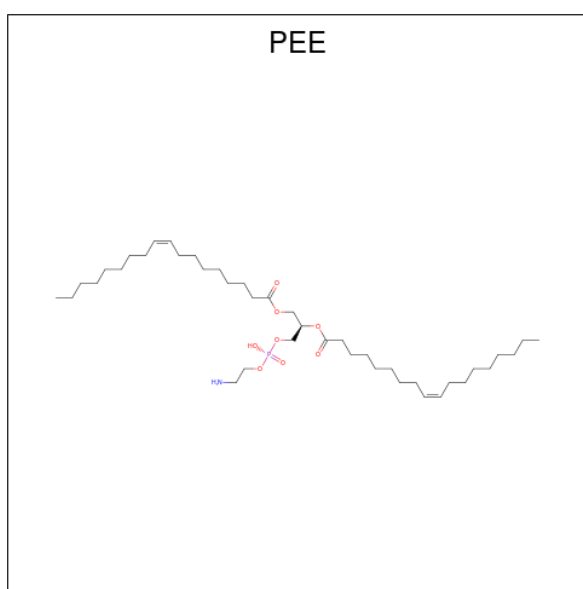
Mol	Chain	Residues	Atoms				AltConf
17	E	1	Total	C	H	O	0
			74	24	39	11	
17	J	1	Total	C	H	O	0
			74	24	39	11	
17	e	1	Total	C	H	O	0
			74	24	39	11	
17	j	1	Total	C	H	O	0
			74	24	39	11	

- Molecule 18 is 2-[[[(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl]-4-[[[(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (CCD ID: Q7G) (formula: C₅₆H₉₂O₂₅).



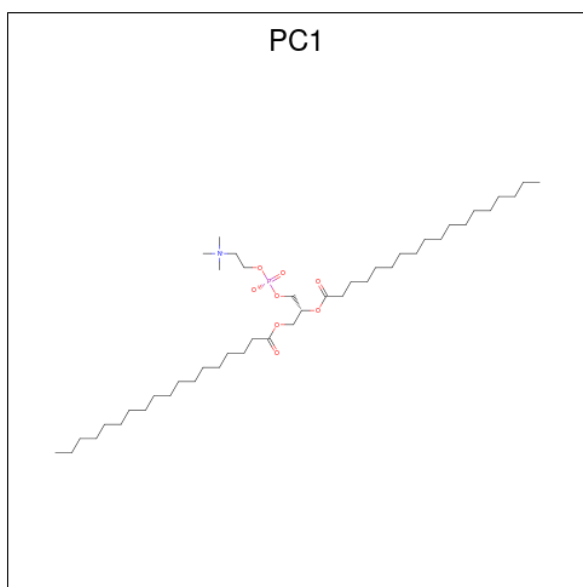
Mol	Chain	Residues	Atoms				AltConf
18	E	1	Total	C	H	O	0
			108	38	60	10	
18	N	1	Total	C	H	O	0
			129	44	70	15	
18	e	1	Total	C	H	O	0
			108	38	60	10	
18	n	1	Total	C	H	O	0
			129	44	70	15	

- Molecule 19 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
19	F	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
19	R	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
19	f	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
19	r	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 20 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
20	F	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
20	F	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
20	I	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
20	J	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
20	f	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
20	f	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
20	i	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
20	j	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	5	Total	O	0
			5	5	
21	F	5	Total	O	0
			5	5	
21	I	1	Total	O	0
			1	1	
21	Q	1	Total	O	0
			1	1	

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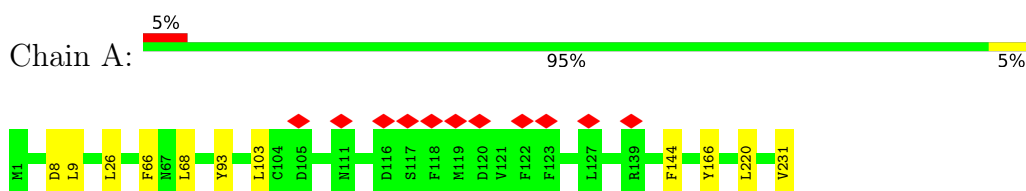
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Mol	Chain	Residues	Atoms		AltConf
21	a	5	Total 5	O 5	0
21	f	5	Total 5	O 5	0
21	i	1	Total 1	O 1	0
21	q	1	Total 1	O 1	0

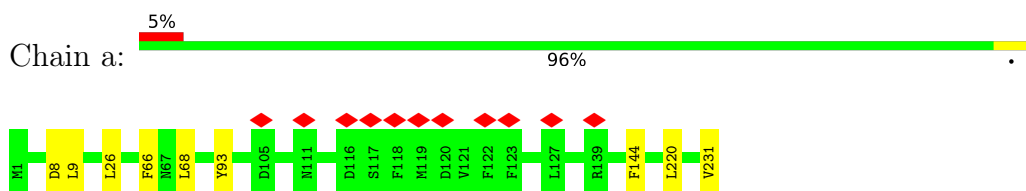
3 Residue-property plots

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

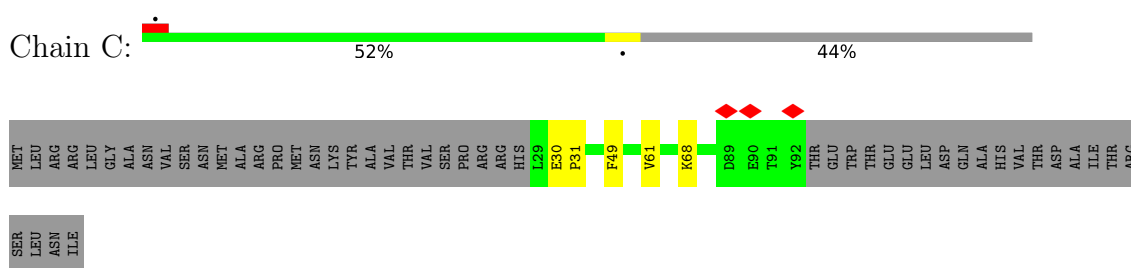
- Molecule 1: ATP synthase subunit a



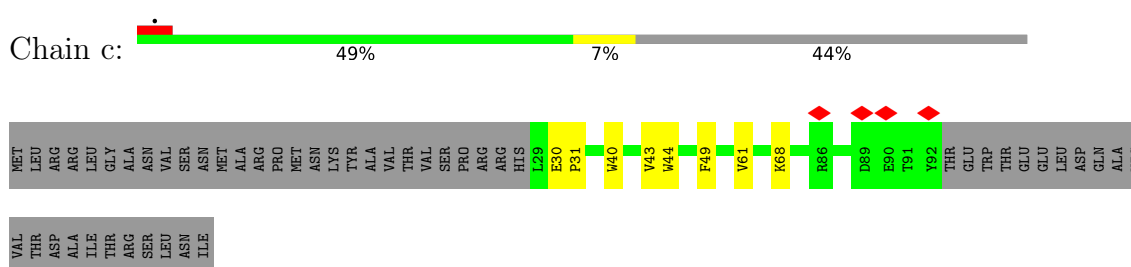
- Molecule 1: ATP synthase subunit a



- Molecule 2: subunit-8

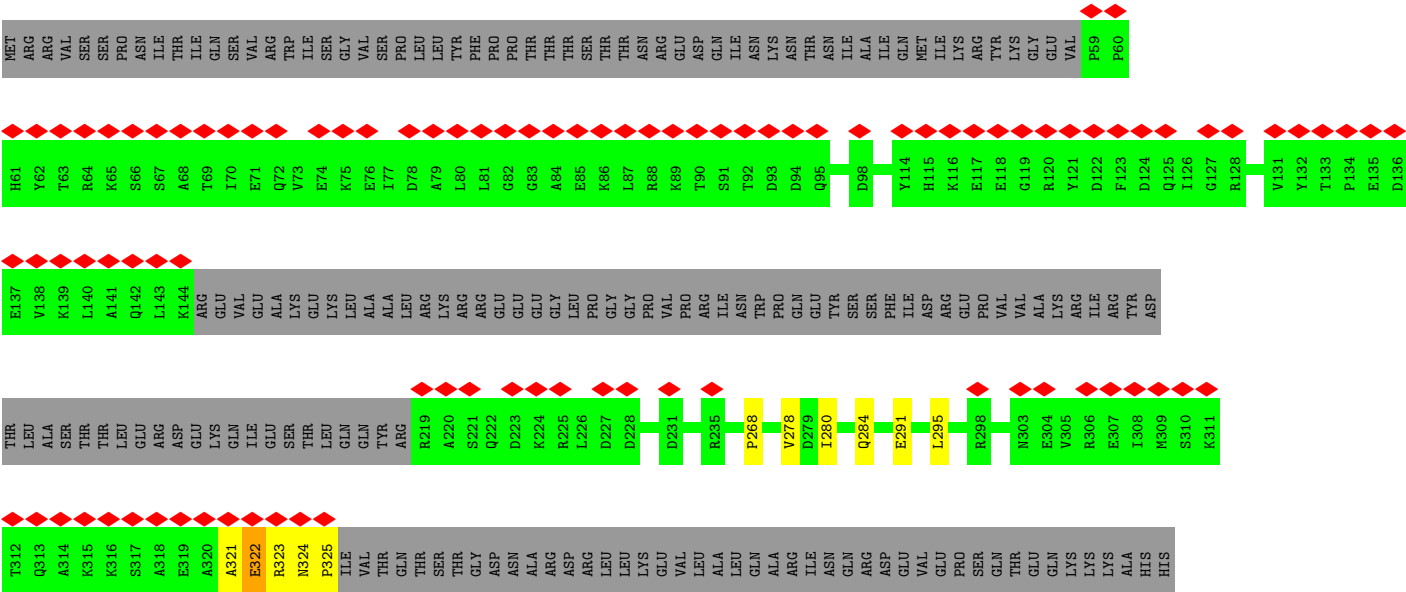


- Molecule 2: subunit-8

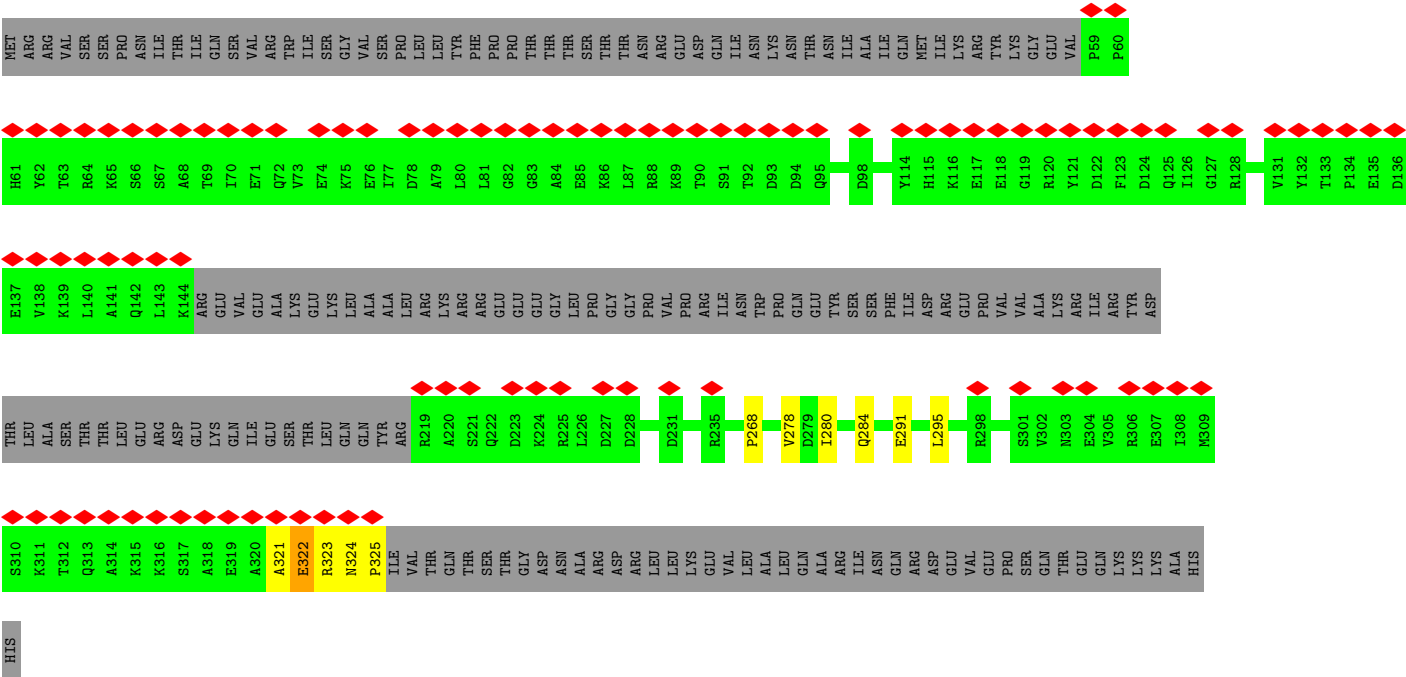


- Molecule 3: subunit-d

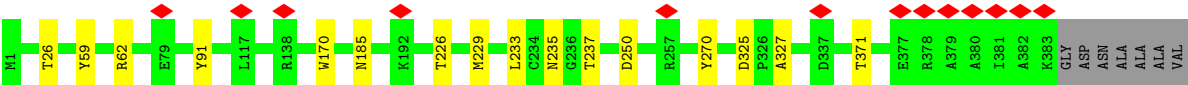
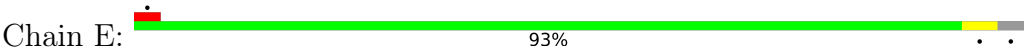




• Molecule 3: subunit-d



• Molecule 4: ATPTB1



GLU
GLY
ARG
HIS
THR
ALA


• Molecule 4: ATPTB1

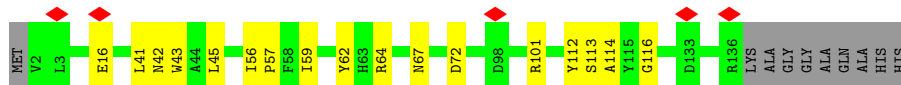
Chain e:  93%




GLY
ARG
HIS
THR
ALA

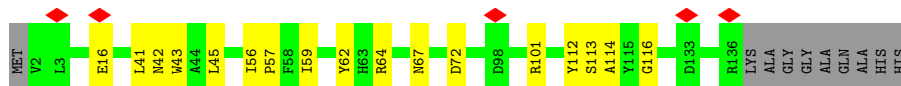
• Molecule 5: subunit-f

Chain F:  81% 12% 7%

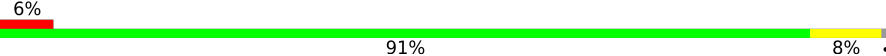


• Molecule 5: subunit-f

Chain f:  81% 12% 7%

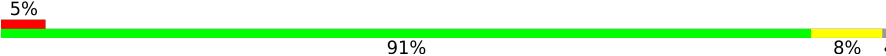


• Molecule 6: subunit-i/j

Chain I:  6% 91% 8%



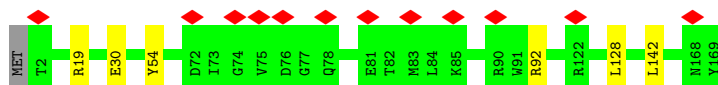
• Molecule 6: subunit-i/j

Chain i:  5% 91% 8%

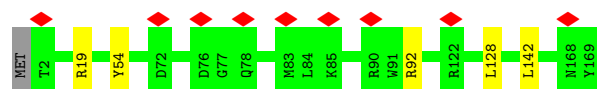
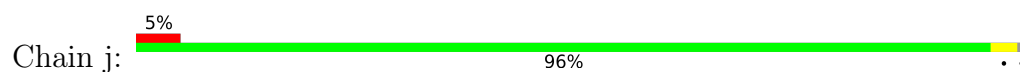


• Molecule 7: ATPTB6

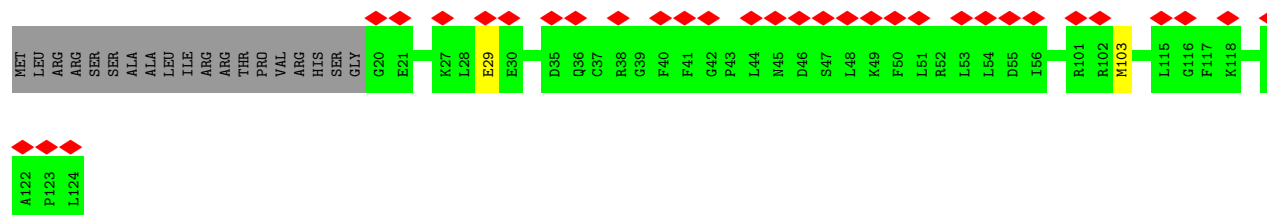
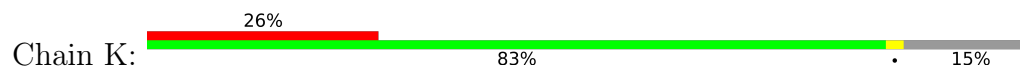
Chain J:  7% 96%



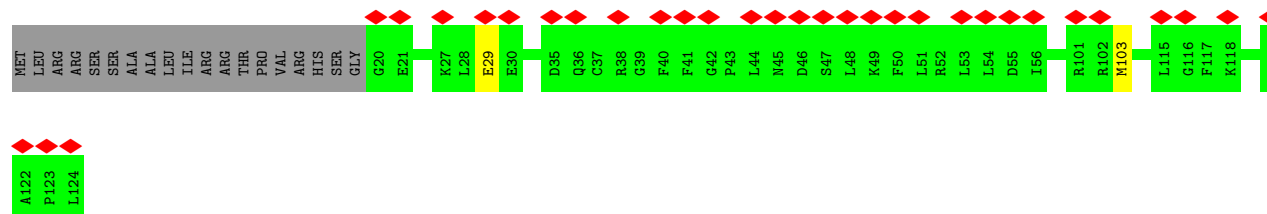
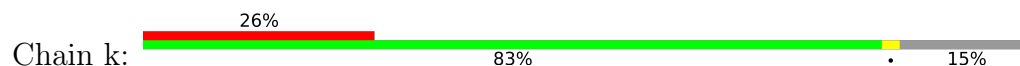
• Molecule 7: ATPTB6



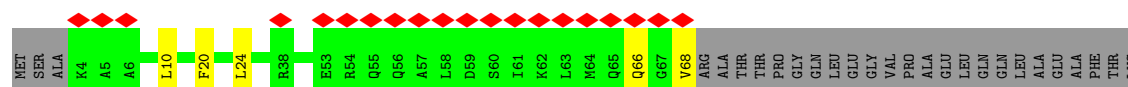
- Molecule 8: subunit-k



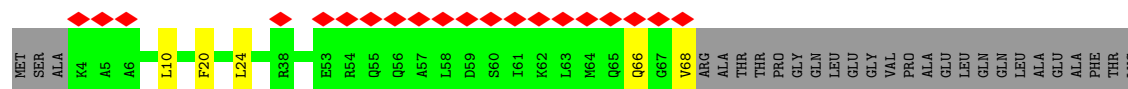
- Molecule 8: subunit-k



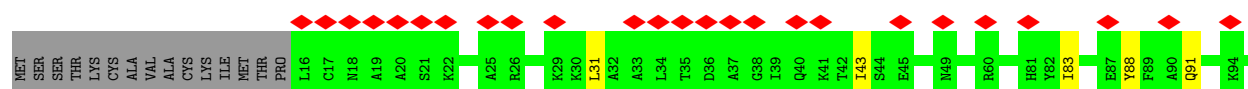
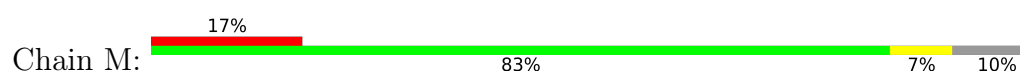
- Molecule 9: subunit-e



- Molecule 9: subunit-e

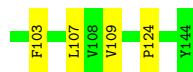
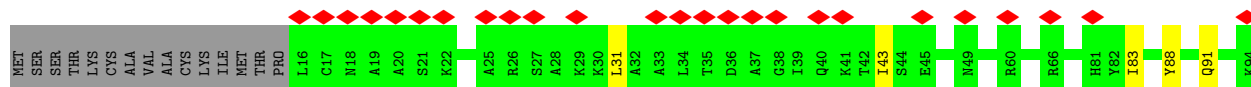
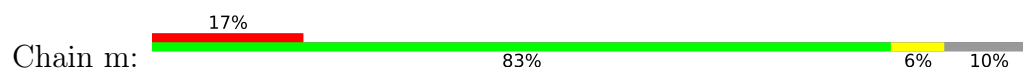


- Molecule 10: subunit-g

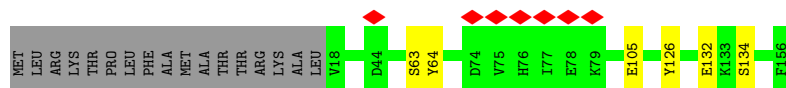
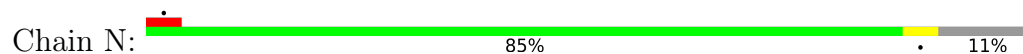




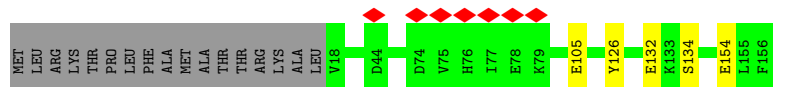
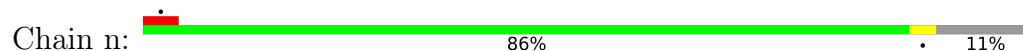
- Molecule 10: subunit-g



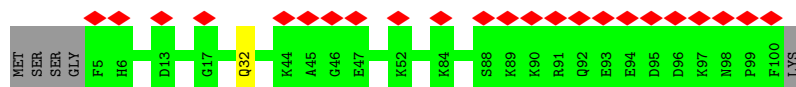
- Molecule 11: ATPTB11



- Molecule 11: ATPTB11



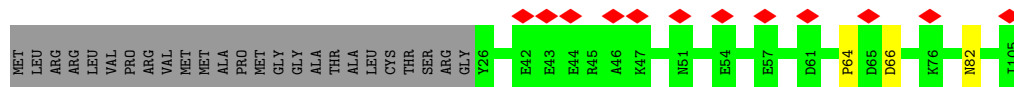
- Molecule 12: ATPTB12



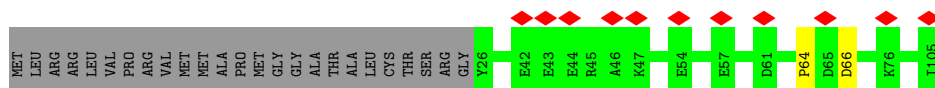
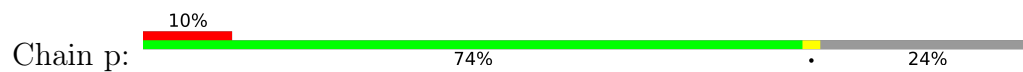
- Molecule 12: ATPTB12



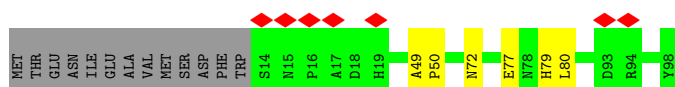
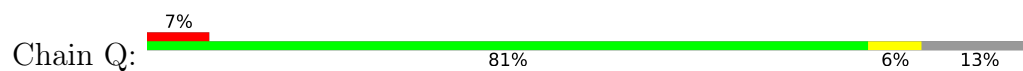
- Molecule 13: subunit-b



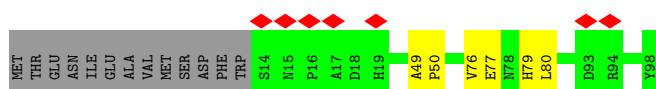
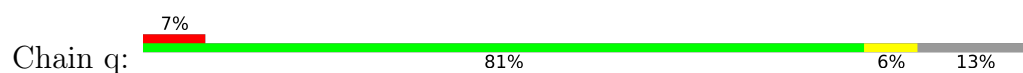
• Molecule 13: subunit-b



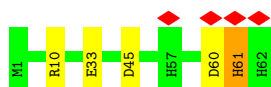
• Molecule 14: ATPEG3



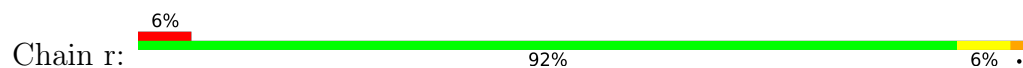
• Molecule 14: ATPEG3



• Molecule 15: ATPEG4



• Molecule 15: ATPEG4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	100605	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.202	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AME, PEE, CDL, PC1, Q7G, LMT

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	0.20	0/2111	0.25	0/2861
1	a	0.20	0/2111	0.25	0/2861
2	C	0.16	0/590	0.25	0/805
2	c	0.17	0/590	0.30	0/805
3	D	0.13	0/1636	0.26	1/2204 (0.0%)
3	d	0.13	0/1636	0.26	1/2204 (0.0%)
4	E	0.14	0/3305	0.21	0/4482
4	e	0.14	0/3305	0.21	0/4482
5	F	0.19	0/1183	0.34	0/1601
5	f	0.19	0/1183	0.34	0/1601
6	I	0.14	0/913	0.23	0/1240
6	i	0.14	0/913	0.22	0/1240
7	J	0.12	0/1462	0.20	0/1973
7	j	0.12	0/1462	0.20	0/1973
8	K	0.12	0/904	0.23	0/1228
8	k	0.12	0/904	0.23	0/1228
9	L	0.11	0/547	0.18	0/735
9	l	0.11	0/547	0.18	0/735
10	M	0.13	0/1049	0.22	0/1423
10	m	0.13	0/1049	0.22	0/1423
11	N	0.14	0/1166	0.23	0/1581
11	n	0.14	0/1166	0.23	0/1581
12	O	0.12	0/814	0.20	0/1100
12	o	0.12	0/814	0.20	0/1100
13	P	0.12	0/707	0.22	0/957
13	p	0.12	0/707	0.22	0/957
14	Q	0.16	0/799	0.26	0/1091
14	q	0.16	0/799	0.27	0/1091
15	R	0.17	0/567	0.27	0/767
15	r	0.18	0/567	0.27	0/767
All	All	0.15	0/35506	0.24	2/48096 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	322	GLU	N-CA-C	5.26	117.01	111.28
3	d	322	GLU	N-CA-C	5.25	117.00	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2032	2044	2044	9	0
1	a	2032	2044	2044	7	0
2	C	566	549	549	4	0
2	c	566	549	549	6	0
3	D	1605	1607	1606	10	0
3	d	1605	1607	1606	10	0
4	E	3220	3061	3061	11	0
4	e	3220	3061	3061	10	0
5	F	1145	1111	1111	12	0
5	f	1145	1111	1111	12	0
6	I	883	857	857	6	0
6	i	883	857	857	6	0
7	J	1424	1411	1411	4	0
7	j	1424	1411	1411	3	0
8	K	873	876	876	2	0
8	k	873	876	876	2	0
9	L	537	545	545	3	0
9	l	537	545	545	3	0
10	M	1027	1042	1042	6	0
10	m	1027	1042	1042	5	0
11	N	1128	1082	1082	3	0
11	n	1128	1082	1082	3	0
12	O	789	767	767	1	0
12	o	789	767	767	1	0
13	P	684	651	651	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	p	684	651	651	3	0
14	Q	766	720	720	5	0
14	q	766	720	720	5	0
15	R	542	498	498	4	0
15	r	542	498	498	4	0
16	C	100	156	156	1	0
16	E	500	780	780	4	0
16	F	100	156	156	0	0
16	J	200	312	312	1	0
16	L	100	156	156	0	0
16	M	100	156	156	0	0
16	Q	100	156	156	0	0
16	c	100	156	156	1	0
16	e	500	780	780	3	0
16	f	100	156	156	0	0
16	j	200	312	312	1	0
16	l	100	156	156	0	0
16	m	100	156	156	0	0
16	q	100	156	156	0	0
17	E	35	39	46	0	0
17	J	35	39	46	0	0
17	e	35	39	46	0	0
17	j	35	39	46	0	0
18	E	48	60	0	0	0
18	N	59	70	0	0	0
18	e	48	60	0	0	0
18	n	59	70	0	0	0
19	F	51	82	82	0	0
19	R	51	82	82	0	0
19	f	51	82	82	0	0
19	r	51	82	82	0	0
20	F	108	176	176	1	0
20	I	54	88	88	0	0
20	J	54	88	88	0	0
20	f	108	176	176	0	0
20	i	54	88	88	0	0
20	j	54	88	88	0	0
21	A	5	0	0	0	0
21	F	5	0	0	0	0
21	I	1	0	0	0	0
21	Q	1	0	0	0	0
21	a	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	f	5	0	0	0	0
21	i	1	0	0	0	0
21	q	1	0	0	0	0
All	All	37856	38834	38600	130	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 2.

All (130) 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)
7:j:19:ARG:NH2	14:q:77:GLU:O	2.21	0.74
7:J:19:ARG:NH2	14:Q:77:GLU:O	2.21	0.73
5:F:112:TYR:HB3	5:F:116:GLY:HA3	1.74	0.69
5:f:112:TYR:HB3	5:f:116:GLY:HA3	1.74	0.68
5:f:113:SER:OG	5:f:114:ALA:N	2.28	0.67
5:F:113:SER:OG	5:F:114:ALA:N	2.28	0.66
5:f:101:ARG:NH2	10:m:124:PRO:O	2.30	0.65
1:A:8:ASP:OD1	11:N:126:TYR:OH	2.15	0.65
5:f:101:ARG:NH1	15:r:45:ASP:O	2.30	0.64
2:C:68:LYS:NZ	3:D:284:GLN:O	2.29	0.64
7:J:128:LEU:HD21	7:J:142:LEU:HD12	1.80	0.63
1:a:8:ASP:OD1	11:n:126:TYR:OH	2.15	0.63
4:e:62:ARG:NH2	16:e:402:CDL:OB4	2.32	0.63
7:j:128:LEU:HD21	7:j:142:LEU:HD12	1.80	0.62
5:F:101:ARG:NH2	10:M:124:PRO:O	2.30	0.62
4:E:62:ARG:NH2	16:E:402:CDL:OB4	2.33	0.62
5:F:101:ARG:NH1	15:R:45:ASP:O	2.32	0.61
2:c:68:LYS:NZ	3:d:284:GLN:O	2.29	0.61
5:F:64:ARG:NH2	15:R:33:GLU:OE2	2.32	0.61
4:E:250:ASP:OD1	4:E:270:TYR:OH	2.14	0.61
1:A:93:TYR:CE1	1:A:220:LEU:HD22	2.36	0.61
5:f:64:ARG:NH2	15:r:33:GLU:OE2	2.31	0.61
2:c:61:VAL:HG13	3:d:278:VAL:HG11	1.83	0.60
4:E:185:ASN:ND2	4:E:325:ASP:OD1	2.35	0.59
1:a:93:TYR:CE1	1:a:220:LEU:HD22	2.36	0.59
2:C:61:VAL:HG13	3:D:278:VAL:HG11	1.85	0.59
4:e:185:ASN:ND2	4:e:325:ASP:OD1	2.35	0.58
3:d:322:GLU:C	3:d:323:ARG:N	2.62	0.57
3:D:322:GLU:C	3:D:323:ARG:N	2.62	0.57
9:l:66:GLN:HG3	9:l:68:VAL:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:66:GLN:HG3	9:L:68:VAL:HG23	1.90	0.54
4:E:229:MET:SD	4:E:235:ASN:ND2	2.81	0.53
1:a:68:LEU:HD13	5:f:45:LEU:HD11	1.91	0.53
1:A:68:LEU:HD13	5:F:45:LEU:HD11	1.90	0.53
13:p:66:ASP:OD2	15:r:10:ARG:NH1	2.43	0.52
4:e:250:ASP:OD1	4:e:270:TYR:OH	2.14	0.52
2:c:40:TRP:O	2:c:43:VAL:HG12	2.09	0.52
13:P:66:ASP:OD2	15:R:10:ARG:NH1	2.41	0.52
14:Q:77:GLU:OE2	14:Q:79:HIS:NE2	2.43	0.51
14:q:77:GLU:OE2	14:q:79:HIS:NE2	2.43	0.51
4:e:229:MET:SD	4:e:235:ASN:ND2	2.81	0.51
6:i:62:ARG:NH2	11:n:134:SER:O	2.43	0.51
1:a:93:TYR:CD1	1:a:220:LEU:HD22	2.46	0.50
7:j:54:TYR:O	7:j:92:ARG:NH1	2.42	0.50
1:A:93:TYR:CD1	1:A:220:LEU:HD22	2.46	0.50
3:D:321:ALA:O	3:D:325:PRO:HD2	2.12	0.50
3:d:321:ALA:O	3:d:325:PRO:CD	2.61	0.49
1:A:231:VAL:O	4:E:170:TRP:NE1	2.45	0.49
3:D:321:ALA:O	3:D:325:PRO:CD	2.61	0.49
3:d:291:GLU:O	3:d:295:LEU:N	2.43	0.49
3:d:321:ALA:O	3:d:325:PRO:HD2	2.12	0.49
6:I:62:ARG:NH2	11:N:134:SER:O	2.43	0.48
16:e:402:CDL:H861	16:e:403:CDL:H673	1.95	0.48
7:J:54:TYR:O	7:J:92:ARG:NH1	2.42	0.48
6:I:16:LEU:O	6:I:20:THR:HG22	2.14	0.48
16:E:402:CDL:H861	16:E:403:CDL:H673	1.95	0.47
15:R:61:HIS:ND1	15:R:61:HIS:C	2.73	0.47
1:a:231:VAL:O	4:e:170:TRP:NE1	2.45	0.47
6:i:16:LEU:O	6:i:20:THR:HG22	2.14	0.47
3:D:291:GLU:O	3:D:295:LEU:N	2.43	0.47
9:l:10:LEU:HD13	10:m:83:ILE:HD11	1.96	0.47
6:I:88:LYS:O	12:O:32:GLN:NE2	2.46	0.47
1:a:26:LEU:HD22	5:f:43:TRP:CZ2	2.50	0.47
6:i:88:LYS:O	12:o:32:GLN:NE2	2.46	0.47
1:A:166:TYR:OH	20:F:204:PC1:O12	2.27	0.46
9:L:10:LEU:HD13	10:M:83:ILE:HD11	1.97	0.46
14:q:49:ALA:N	14:q:50:PRO:CD	2.79	0.46
1:A:26:LEU:HD22	5:F:43:TRP:CZ2	2.51	0.46
6:I:87:PRO:O	6:I:91:GLY:N	2.41	0.46
3:D:280:ILE:HD12	3:D:280:ILE:O	2.16	0.46
3:d:280:ILE:HD12	3:d:280:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:26:THR:HG23	4:E:91:TYR:OH	2.16	0.46
14:Q:49:ALA:N	14:Q:50:PRO:CD	2.79	0.46
8:k:29:GLU:N	8:k:29:GLU:OE1	2.50	0.45
8:K:29:GLU:N	8:K:29:GLU:OE1	2.50	0.45
2:c:30:GLU:N	2:c:31:PRO:CD	2.80	0.45
4:e:26:THR:HG23	4:e:91:TYR:OH	2.16	0.45
2:C:30:GLU:N	2:C:31:PRO:CD	2.80	0.45
4:E:371:THR:HG23	13:P:64:PRO:CG	2.47	0.45
15:r:61:HIS:ND1	15:r:61:HIS:C	2.73	0.45
1:A:9:LEU:HD11	1:A:66:PHE:CE2	2.53	0.44
3:d:268:PRO:HB2	4:e:327:ALA:HB3	2.00	0.44
4:e:371:THR:HG23	13:p:64:PRO:CG	2.47	0.44
4:E:233:LEU:O	4:E:237:THR:OG1	2.30	0.44
3:D:268:PRO:HB2	4:E:327:ALA:HB3	2.00	0.44
10:M:88:TYR:O	10:M:91:GLN:NE2	2.51	0.44
16:e:402:CDL:H151	16:j:202:CDL:H872	2.00	0.43
9:l:20:PHE:CE2	9:l:24:LEU:HD11	2.53	0.43
3:D:324:ASN:CB	3:D:325:PRO:HD3	2.48	0.43
16:E:402:CDL:H151	16:J:202:CDL:H872	2.00	0.43
11:n:154:GLU:OE1	11:n:154:GLU:N	2.46	0.43
1:a:9:LEU:HD11	1:a:66:PHE:CE2	2.53	0.43
5:f:67:ASN:ND2	5:f:72:ASP:OD2	2.52	0.43
3:d:324:ASN:CB	3:d:325:PRO:HD3	2.47	0.43
2:C:49:PHE:O	6:I:15:GLN:NE2	2.51	0.43
5:f:41:LEU:HD23	5:f:45:LEU:HD12	2.00	0.43
16:C:201:CDL:H832	16:C:201:CDL:H872	2.01	0.43
4:E:371:THR:HG23	13:P:64:PRO:HG3	2.00	0.43
9:L:20:PHE:CE2	9:L:24:LEU:HD11	2.52	0.43
8:K:103:MET:HE1	14:Q:80:LEU:HA	2.01	0.43
2:c:43:VAL:HG13	2:c:44:TRP:N	2.34	0.42
3:D:324:ASN:HB2	3:D:325:PRO:HD3	2.00	0.42
5:F:41:LEU:HD23	5:F:45:LEU:HD12	2.00	0.42
3:d:324:ASN:HB2	3:d:325:PRO:HD3	2.00	0.42
4:e:371:THR:HG23	13:p:64:PRO:HG3	2.00	0.42
10:M:31:LEU:HD11	10:M:43:ILE:HD13	2.01	0.42
10:m:88:TYR:O	10:m:91:GLN:NE2	2.51	0.42
5:F:67:ASN:ND2	5:F:72:ASP:OD2	2.52	0.42
16:c:201:CDL:H832	16:c:201:CDL:H872	2.01	0.42
4:e:233:LEU:O	4:e:237:THR:OG1	2.30	0.42
10:m:31:LEU:HD11	10:m:43:ILE:HD13	2.01	0.42
6:i:87:PRO:O	6:i:91:GLY:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:30:GLU:OE1	14:Q:72:ASN:ND2	2.52	0.41
5:f:16:GLU:OE1	5:f:16:GLU:N	2.53	0.41
6:i:17:LYS:HA	6:i:20:THR:HG22	2.02	0.41
2:c:49:PHE:O	6:i:15:GLN:NE2	2.53	0.41
5:F:16:GLU:N	5:F:16:GLU:OE1	2.53	0.41
5:F:56:ILE:HB	5:F:57:PRO:HD3	2.02	0.41
5:f:59:ILE:HA	5:f:62:TYR:CE2	2.55	0.41
6:I:17:LYS:HA	6:I:20:THR:HG22	2.02	0.41
8:k:103:MET:HE1	14:q:80:LEU:HA	2.01	0.41
5:F:59:ILE:HA	5:F:62:TYR:CE2	2.55	0.41
10:M:102:ARG:NH2	13:P:82:ASN:OD1	2.50	0.41
10:M:103:PHE:CZ	10:M:107:LEU:HD11	2.56	0.41
14:q:76:VAL:O	14:q:76:VAL:HG12	2.20	0.41
5:f:56:ILE:HB	5:f:57:PRO:HD3	2.02	0.41
11:N:63:SER:O	11:N:64:TYR:C	2.65	0.40
1:A:103:LEU:HD21	4:E:59:TYR:CG	2.57	0.40
10:m:103:PHE:CZ	10:m:107:LEU:HD11	2.56	0.40
16:E:403:CDL:H651	16:E:403:CDL:H612	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/231 (99%)	227 (99%)	2 (1%)	0	100	100
1	a	229/231 (99%)	227 (99%)	2 (1%)	0	100	100
2	C	62/114 (54%)	62 (100%)	0	0	100	100
2	c	62/114 (54%)	62 (100%)	0	0	100	100
3	D	187/370 (50%)	182 (97%)	5 (3%)	0	100	100
3	d	187/370 (50%)	182 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	381/396 (96%)	376 (99%)	5 (1%)	0	100	100
4	e	381/396 (96%)	376 (99%)	5 (1%)	0	100	100
5	F	133/145 (92%)	131 (98%)	2 (2%)	0	100	100
5	f	133/145 (92%)	131 (98%)	2 (2%)	0	100	100
6	I	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
6	i	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
7	J	166/169 (98%)	164 (99%)	2 (1%)	0	100	100
7	j	166/169 (98%)	163 (98%)	3 (2%)	0	100	100
8	K	103/124 (83%)	100 (97%)	3 (3%)	0	100	100
8	k	103/124 (83%)	100 (97%)	3 (3%)	0	100	100
9	L	63/92 (68%)	63 (100%)	0	0	100	100
9	l	63/92 (68%)	63 (100%)	0	0	100	100
10	M	127/144 (88%)	127 (100%)	0	0	100	100
10	m	127/144 (88%)	127 (100%)	0	0	100	100
11	N	137/156 (88%)	131 (96%)	6 (4%)	0	100	100
11	n	137/156 (88%)	131 (96%)	6 (4%)	0	100	100
12	O	94/101 (93%)	94 (100%)	0	0	100	100
12	o	94/101 (93%)	94 (100%)	0	0	100	100
13	P	78/105 (74%)	77 (99%)	1 (1%)	0	100	100
13	p	78/105 (74%)	77 (99%)	1 (1%)	0	100	100
14	Q	83/98 (85%)	80 (96%)	3 (4%)	0	100	100
14	q	83/98 (85%)	80 (96%)	3 (4%)	0	100	100
15	R	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
15	r	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
All	All	4008/4822 (83%)	3945 (98%)	63 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	225/225 (100%)	224 (100%)	1 (0%)	89	96
1	a	225/225 (100%)	224 (100%)	1 (0%)	89	96
2	C	60/104 (58%)	60 (100%)	0	100	100
2	c	60/104 (58%)	60 (100%)	0	100	100
3	D	173/334 (52%)	173 (100%)	0	100	100
3	d	173/334 (52%)	173 (100%)	0	100	100
4	E	334/341 (98%)	333 (100%)	1 (0%)	91	97
4	e	334/341 (98%)	333 (100%)	1 (0%)	91	97
5	F	119/124 (96%)	118 (99%)	1 (1%)	79	91
5	f	119/124 (96%)	118 (99%)	1 (1%)	79	91
6	I	95/96 (99%)	95 (100%)	0	100	100
6	i	95/96 (99%)	95 (100%)	0	100	100
7	J	149/150 (99%)	149 (100%)	0	100	100
7	j	149/150 (99%)	149 (100%)	0	100	100
8	K	91/107 (85%)	91 (100%)	0	100	100
8	k	91/107 (85%)	91 (100%)	0	100	100
9	L	55/75 (73%)	55 (100%)	0	100	100
9	l	55/75 (73%)	55 (100%)	0	100	100
10	M	111/124 (90%)	110 (99%)	1 (1%)	75	90
10	m	111/124 (90%)	110 (99%)	1 (1%)	75	90
11	N	123/137 (90%)	121 (98%)	2 (2%)	58	82
11	n	123/137 (90%)	121 (98%)	2 (2%)	58	82
12	O	82/86 (95%)	82 (100%)	0	100	100
12	o	82/86 (95%)	82 (100%)	0	100	100
13	P	75/94 (80%)	75 (100%)	0	100	100
13	p	75/94 (80%)	75 (100%)	0	100	100
14	Q	80/92 (87%)	80 (100%)	0	100	100
14	q	80/92 (87%)	80 (100%)	0	100	100
15	R	56/56 (100%)	54 (96%)	2 (4%)	30	59
15	r	56/56 (100%)	54 (96%)	2 (4%)	30	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3656/4290 (85%)	3640 (100%)	16 (0%)	88 96

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	PHE
4	E	226	THR
5	F	42	ASN
10	M	109	VAL
11	N	105	GLU
11	N	132	GLU
15	R	60	ASP
15	R	61	HIS
1	a	144	PHE
4	e	226	THR
5	f	42	ASN
10	m	109	VAL
11	n	105	GLU
11	n	132	GLU
15	r	60	ASP
15	r	61	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
5	F	34	GLN
5	F	75	HIS
9	L	43	HIS
11	N	144	HIS
13	P	39	GLN
13	P	95	GLN
5	f	34	GLN
5	f	75	HIS
9	l	43	HIS
11	n	89	GLN
11	n	91	HIS
11	n	144	HIS
13	p	39	GLN
13	p	95	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	AME	e	1	4	9,10,11	0.23	0	9,11,13	0.50	0
4	AME	E	1	4	9,10,11	0.24	0	9,11,13	0.50	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
4	AME	e	1	4	-	2/9/10/12	-
4	AME	E	1	4	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	AME	N-CA-CB-CG
4	e	1	AME	N-CA-CB-CG
4	E	1	AME	C-CA-CB-CG
4	e	1	AME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

44 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CDL	m	201	-	99,99,99	0.30	0	105,111,111	0.29	0
16	CDL	e	405	-	99,99,99	0.29	0	105,111,111	0.25	0
18	Q7G	e	407	-	54,54,90	0.14	0	82,84,138	0.32	0
18	Q7G	E	407	-	54,54,90	0.14	0	82,84,138	0.32	0
17	LMT	J	204	-	36,36,36	0.20	0	47,47,47	0.42	0
16	CDL	E	403	-	99,99,99	0.29	0	105,111,111	0.26	0
16	CDL	Q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
20	PC1	f	203	-	53,53,53	0.28	0	59,61,61	0.27	0
16	CDL	E	405	-	99,99,99	0.29	0	105,111,111	0.26	0
16	CDL	e	403	-	99,99,99	0.29	0	105,111,111	0.26	0
20	PC1	i	201	-	53,53,53	0.29	0	59,61,61	0.27	0
20	PC1	F	203	-	53,53,53	0.28	0	59,61,61	0.27	0
16	CDL	M	201	-	99,99,99	0.30	0	105,111,111	0.29	0
20	PC1	j	203	-	53,53,53	0.28	0	59,61,61	0.27	0
16	CDL	e	402	-	99,99,99	0.29	0	105,111,111	0.28	0
18	Q7G	N	201	-	66,66,90	0.15	0	100,102,138	0.32	0
20	PC1	f	204	-	53,53,53	0.27	0	59,61,61	0.26	0
19	PEE	F	202	-	50,50,50	0.76	2 (4%)	53,55,55	0.46	0
16	CDL	f	201	-	99,99,99	0.29	0	105,111,111	0.26	0
20	PC1	J	203	-	53,53,53	0.28	0	59,61,61	0.27	0
16	CDL	E	401	-	99,99,99	0.29	0	105,111,111	0.26	0
20	PC1	F	204	-	53,53,53	0.27	0	59,61,61	0.27	0
16	CDL	E	404	-	99,99,99	0.30	0	105,111,111	0.25	0
16	CDL	e	401	-	99,99,99	0.30	0	105,111,111	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CDL	q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
19	PEE	f	202	-	50,50,50	0.76	2 (4%)	53,55,55	0.46	0
17	LMT	E	406	-	36,36,36	0.30	0	47,47,47	0.45	0
18	Q7G	n	201	-	66,66,90	0.15	0	100,102,138	0.32	0
17	LMT	j	204	-	36,36,36	0.20	0	47,47,47	0.42	0
16	CDL	E	402	-	99,99,99	0.29	0	105,111,111	0.28	0
17	LMT	e	406	-	36,36,36	0.30	0	47,47,47	0.45	0
16	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.26	0
16	CDL	L	101	-	99,99,99	0.30	0	105,111,111	0.26	0
16	CDL	l	101	-	99,99,99	0.29	0	105,111,111	0.25	0
16	CDL	J	202	-	99,99,99	0.29	0	105,111,111	0.25	0
16	CDL	j	202	-	99,99,99	0.29	0	105,111,111	0.25	0
16	CDL	c	201	-	99,99,99	0.29	0	105,111,111	0.26	0
16	CDL	J	201	-	99,99,99	0.29	0	105,111,111	0.26	0
16	CDL	F	201	-	99,99,99	0.29	0	105,111,111	0.26	0
19	PEE	R	101	-	50,50,50	0.76	2 (4%)	53,55,55	0.47	0
20	PC1	I	201	-	53,53,53	0.29	0	59,61,61	0.27	0
16	CDL	C	201	-	99,99,99	0.29	0	105,111,111	0.26	0
16	CDL	e	404	-	99,99,99	0.30	0	105,111,111	0.25	0
19	PEE	r	101	-	50,50,50	0.75	2 (4%)	53,55,55	0.47	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
16	CDL	m	201	-	-	43/110/110/110	-
16	CDL	e	404	-	-	20/110/110/110	-
16	CDL	e	405	-	-	35/110/110/110	-
18	Q7G	e	407	-	1/1/19/34	5/15/123/200	0/7/7/10
18	Q7G	E	407	-	1/1/19/34	5/15/123/200	0/7/7/10
17	LMT	J	204	-	-	6/21/61/61	0/2/2/2
16	CDL	E	403	-	-	31/110/110/110	-
16	CDL	Q	101	-	-	27/110/110/110	-
20	PC1	f	203	-	-	10/57/57/57	-
16	CDL	E	405	-	-	35/110/110/110	-
16	CDL	e	403	-	-	31/110/110/110	-
20	PC1	i	201	-	-	10/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PC1	F	203	-	-	10/57/57/57	-
20	PC1	j	203	-	-	14/57/57/57	-
16	CDL	e	402	-	-	29/110/110/110	-
18	Q7G	N	201	-	2/2/24/34	6/20/148/200	0/8/8/10
20	PC1	f	204	-	-	11/57/57/57	-
19	PEE	F	202	-	-	17/54/54/54	-
16	CDL	f	201	-	-	21/110/110/110	-
20	PC1	J	203	-	-	14/57/57/57	-
16	CDL	E	401	-	-	23/110/110/110	-
20	PC1	F	204	-	-	11/57/57/57	-
16	CDL	E	404	-	-	20/110/110/110	-
16	CDL	e	401	-	-	23/110/110/110	-
16	CDL	q	101	-	-	27/110/110/110	-
19	PEE	f	202	-	-	17/54/54/54	-
17	LMT	E	406	-	-	1/21/61/61	0/2/2/2
18	Q7G	n	201	-	2/2/24/34	6/20/148/200	0/8/8/10
17	LMT	j	204	-	-	6/21/61/61	0/2/2/2
16	CDL	E	402	-	-	29/110/110/110	-
17	LMT	e	406	-	-	1/21/61/61	0/2/2/2
16	CDL	j	201	-	-	25/110/110/110	-
16	CDL	L	101	-	-	24/110/110/110	-
16	CDL	l	101	-	-	24/110/110/110	-
16	CDL	J	202	-	-	29/110/110/110	-
16	CDL	j	202	-	-	29/110/110/110	-
16	CDL	c	201	-	-	25/110/110/110	-
16	CDL	J	201	-	-	25/110/110/110	-
16	CDL	F	201	-	-	21/110/110/110	-
19	PEE	R	101	-	-	24/54/54/54	-
20	PC1	I	201	-	-	10/57/57/57	-
16	CDL	C	201	-	-	25/110/110/110	-
16	CDL	M	201	-	-	43/110/110/110	-
19	PEE	r	101	-	-	24/54/54/54	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	f	202	PEE	C39-C38	3.57	1.52	1.31
19	F	202	PEE	C39-C38	3.57	1.52	1.31
19	R	101	PEE	C18-C19	3.53	1.52	1.31
19	r	101	PEE	C18-C19	3.51	1.52	1.31
19	R	101	PEE	C39-C38	3.51	1.52	1.31
19	r	101	PEE	C39-C38	3.50	1.52	1.31
19	F	202	PEE	C18-C19	3.50	1.52	1.31
19	f	202	PEE	C18-C19	3.50	1.52	1.31

There are no bond angle outliers.

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	E	407	Q7G	C1B
18	N	201	Q7G	C1C
18	N	201	Q7G	C1B
18	e	407	Q7G	C1B
18	n	201	Q7G	C1C
18	n	201	Q7G	C1B

All (872) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	C	201	CDL	CB3-OB5-PB2-OB4
16	E	401	CDL	CB2-OB2-PB2-OB3
16	E	401	CDL	CB2-OB2-PB2-OB4
16	E	401	CDL	CB2-OB2-PB2-OB5
16	E	401	CDL	CB3-OB5-PB2-OB3
16	E	402	CDL	CA3-OA5-PA1-OA2
16	E	402	CDL	CA3-OA5-PA1-OA3
16	E	402	CDL	CA3-OA5-PA1-OA4
16	E	404	CDL	CA3-OA5-PA1-OA4
16	E	404	CDL	CB3-OB5-PB2-OB3
16	E	404	CDL	CB3-OB5-PB2-OB4
16	E	405	CDL	CA3-OA5-PA1-OA2
16	E	405	CDL	CA3-OA5-PA1-OA3
16	E	405	CDL	CA3-OA5-PA1-OA4
16	E	405	CDL	CB3-OB5-PB2-OB3
16	E	405	CDL	CB3-OB5-PB2-OB4
16	E	405	CDL	OB5-CB3-CB4-OB6
16	J	201	CDL	CB2-C1-CA2-OA2
16	J	201	CDL	CA2-OA2-PA1-OA3
16	J	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
16	J	201	CDL	CA3-OA5-PA1-OA3
16	J	201	CDL	CA3-OA5-PA1-OA4
16	J	202	CDL	CA2-OA2-PA1-OA4
16	J	202	CDL	CB3-OB5-PB2-OB4
16	L	101	CDL	CA2-OA2-PA1-OA3
16	L	101	CDL	CA2-OA2-PA1-OA4
16	L	101	CDL	CB2-OB2-PB2-OB5
16	M	201	CDL	CA3-OA5-PA1-OA3
16	M	201	CDL	CA3-OA5-PA1-OA4
16	M	201	CDL	OA6-CA4-CA6-OA8
16	M	201	CDL	CB2-OB2-PB2-OB3
16	M	201	CDL	CB2-OB2-PB2-OB4
16	M	201	CDL	CB2-OB2-PB2-OB5
16	M	201	CDL	CB3-OB5-PB2-OB3
16	Q	101	CDL	OA5-CA3-CA4-OA6
16	Q	101	CDL	CB2-OB2-PB2-OB3
16	Q	101	CDL	CB2-OB2-PB2-OB4
16	Q	101	CDL	CB3-OB5-PB2-OB3
16	c	201	CDL	CB3-OB5-PB2-OB4
16	e	401	CDL	CB2-OB2-PB2-OB3
16	e	401	CDL	CB2-OB2-PB2-OB4
16	e	401	CDL	CB2-OB2-PB2-OB5
16	e	401	CDL	CB3-OB5-PB2-OB3
16	e	402	CDL	CA3-OA5-PA1-OA2
16	e	402	CDL	CA3-OA5-PA1-OA3
16	e	402	CDL	CA3-OA5-PA1-OA4
16	e	404	CDL	CA3-OA5-PA1-OA4
16	e	404	CDL	CB3-OB5-PB2-OB3
16	e	404	CDL	CB3-OB5-PB2-OB4
16	e	405	CDL	CA3-OA5-PA1-OA2
16	e	405	CDL	CA3-OA5-PA1-OA3
16	e	405	CDL	CA3-OA5-PA1-OA4
16	e	405	CDL	CB3-OB5-PB2-OB3
16	e	405	CDL	CB3-OB5-PB2-OB4
16	e	405	CDL	OB5-CB3-CB4-OB6
16	j	201	CDL	CB2-C1-CA2-OA2
16	j	201	CDL	CA2-OA2-PA1-OA3
16	j	201	CDL	CA3-OA5-PA1-OA2
16	j	201	CDL	CA3-OA5-PA1-OA3
16	j	201	CDL	CA3-OA5-PA1-OA4
16	j	202	CDL	CA2-OA2-PA1-OA4
16	j	202	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
16	l	101	CDL	CA2-OA2-PA1-OA3
16	l	101	CDL	CA2-OA2-PA1-OA4
16	l	101	CDL	CB2-OB2-PB2-OB5
16	m	201	CDL	CA3-OA5-PA1-OA3
16	m	201	CDL	CA3-OA5-PA1-OA4
16	m	201	CDL	OA6-CA4-CA6-OA8
16	m	201	CDL	CB2-OB2-PB2-OB3
16	m	201	CDL	CB2-OB2-PB2-OB4
16	m	201	CDL	CB2-OB2-PB2-OB5
16	m	201	CDL	CB3-OB5-PB2-OB3
16	q	101	CDL	OA5-CA3-CA4-OA6
16	q	101	CDL	CB2-OB2-PB2-OB3
16	q	101	CDL	CB2-OB2-PB2-OB4
16	q	101	CDL	CB3-OB5-PB2-OB3
17	E	406	LMT	C2-C1-O1'-C1'
17	J	204	LMT	C2'-C1'-O1'-C1
17	J	204	LMT	O5'-C1'-O1'-C1
17	J	204	LMT	C2-C1-O1'-C1'
17	e	406	LMT	C2-C1-O1'-C1'
17	j	204	LMT	C2'-C1'-O1'-C1
17	j	204	LMT	O5'-C1'-O1'-C1
17	j	204	LMT	C2-C1-O1'-C1'
18	E	407	Q7G	C2B-C1B-O1B-C24
18	E	407	Q7G	O5B-C1B-O1B-C24
18	E	407	Q7G	CG1-C22-C23-C48
18	N	201	Q7G	C2B-C1B-O1B-C24
18	N	201	Q7G	O5B-C1B-O1B-C24
18	e	407	Q7G	C2B-C1B-O1B-C24
18	e	407	Q7G	O5B-C1B-O1B-C24
18	e	407	Q7G	CG1-C22-C23-C48
18	n	201	Q7G	C2B-C1B-O1B-C24
18	n	201	Q7G	O5B-C1B-O1B-C24
19	F	202	PEE	C1-O3P-P-O2P
19	F	202	PEE	C1-O3P-P-O1P
19	R	101	PEE	C1-O3P-P-O2P
19	R	101	PEE	C4-O4P-P-O2P
19	R	101	PEE	O4P-C4-C5-N
19	f	202	PEE	C1-O3P-P-O2P
19	f	202	PEE	C1-O3P-P-O1P
19	r	101	PEE	C1-O3P-P-O2P
19	r	101	PEE	C4-O4P-P-O2P
19	r	101	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
20	F	203	PC1	C11-O13-P-O12
20	F	203	PC1	C1-O11-P-O14
20	F	204	PC1	O13-C11-C12-N
20	I	201	PC1	C11-O13-P-O12
20	I	201	PC1	C11-O13-P-O14
20	I	201	PC1	C11-O13-P-O11
20	I	201	PC1	O13-C11-C12-N
20	J	203	PC1	C11-O13-P-O14
20	J	203	PC1	C1-O11-P-O12
20	J	203	PC1	C1-O11-P-O14
20	J	203	PC1	C1-O11-P-O13
20	f	203	PC1	C11-O13-P-O12
20	f	203	PC1	C1-O11-P-O14
20	f	204	PC1	O13-C11-C12-N
20	i	201	PC1	C11-O13-P-O12
20	i	201	PC1	C11-O13-P-O14
20	i	201	PC1	C11-O13-P-O11
20	i	201	PC1	O13-C11-C12-N
20	j	203	PC1	C11-O13-P-O14
20	j	203	PC1	C1-O11-P-O12
20	j	203	PC1	C1-O11-P-O14
20	j	203	PC1	C1-O11-P-O13
16	C	201	CDL	O1-C1-CA2-OA2
16	J	201	CDL	O1-C1-CA2-OA2
16	M	201	CDL	O1-C1-CB2-OB2
16	c	201	CDL	O1-C1-CA2-OA2
16	j	201	CDL	O1-C1-CA2-OA2
16	m	201	CDL	O1-C1-CB2-OB2
16	E	403	CDL	C11-CA5-OA6-CA4
16	e	403	CDL	C11-CA5-OA6-CA4
16	E	401	CDL	C77-C78-C79-C80
16	e	401	CDL	C77-C78-C79-C80
16	E	403	CDL	OA7-CA5-OA6-CA4
16	e	403	CDL	OA7-CA5-OA6-CA4
16	M	201	CDL	CA2-C1-CB2-OB2
16	Q	101	CDL	CA2-C1-CB2-OB2
16	m	201	CDL	CA2-C1-CB2-OB2
16	q	101	CDL	CA2-C1-CB2-OB2
16	M	201	CDL	OA5-CA3-CA4-OA6
16	m	201	CDL	OA5-CA3-CA4-OA6
16	E	404	CDL	O1-C1-CA2-OA2
16	L	101	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
16	e	404	CDL	O1-C1-CA2-OA2
16	l	101	CDL	O1-C1-CA2-OA2
19	R	101	PEE	C31-C32-C33-C34
19	r	101	PEE	C31-C32-C33-C34
16	M	201	CDL	C34-C35-C36-C37
16	m	201	CDL	C34-C35-C36-C37
16	E	402	CDL	C31-CA7-OA8-CA6
16	e	402	CDL	C31-CA7-OA8-CA6
16	E	405	CDL	CA7-C31-C32-C33
16	e	405	CDL	CA7-C31-C32-C33
16	M	201	CDL	CA5-C11-C12-C13
16	m	201	CDL	CA5-C11-C12-C13
16	M	201	CDL	CB5-C51-C52-C53
16	m	201	CDL	CB5-C51-C52-C53
16	Q	101	CDL	O1-C1-CB2-OB2
16	q	101	CDL	O1-C1-CB2-OB2
16	E	402	CDL	OA9-CA7-OA8-CA6
16	e	402	CDL	OA9-CA7-OA8-CA6
16	E	405	CDL	C11-CA5-OA6-CA4
16	M	201	CDL	C51-CB5-OB6-CB4
16	e	405	CDL	C11-CA5-OA6-CA4
16	m	201	CDL	C51-CB5-OB6-CB4
16	C	201	CDL	CB3-OB5-PB2-OB2
16	E	401	CDL	CB3-OB5-PB2-OB2
16	E	404	CDL	CA3-OA5-PA1-OA2
16	E	404	CDL	CB3-OB5-PB2-OB2
16	E	405	CDL	CB3-OB5-PB2-OB2
16	F	201	CDL	CA2-OA2-PA1-OA5
16	F	201	CDL	CB3-OB5-PB2-OB2
16	J	202	CDL	CB3-OB5-PB2-OB2
16	L	101	CDL	CA2-OA2-PA1-OA5
16	L	101	CDL	CA3-OA5-PA1-OA2
16	M	201	CDL	CA3-OA5-PA1-OA2
16	M	201	CDL	CB3-OB5-PB2-OB2
16	Q	101	CDL	CA2-OA2-PA1-OA5
16	Q	101	CDL	CB2-OB2-PB2-OB5
16	c	201	CDL	CB3-OB5-PB2-OB2
16	e	401	CDL	CB3-OB5-PB2-OB2
16	e	404	CDL	CA3-OA5-PA1-OA2
16	e	404	CDL	CB3-OB5-PB2-OB2
16	e	405	CDL	CB3-OB5-PB2-OB2
16	f	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
16	f	201	CDL	CB3-OB5-PB2-OB2
16	j	202	CDL	CB3-OB5-PB2-OB2
16	l	101	CDL	CA2-OA2-PA1-OA5
16	l	101	CDL	CA3-OA5-PA1-OA2
16	m	201	CDL	CA3-OA5-PA1-OA2
16	m	201	CDL	CB3-OB5-PB2-OB2
16	q	101	CDL	CA2-OA2-PA1-OA5
16	q	101	CDL	CB2-OB2-PB2-OB5
19	F	202	PEE	C1-O3P-P-O4P
19	F	202	PEE	C4-O4P-P-O3P
19	f	202	PEE	C1-O3P-P-O4P
19	f	202	PEE	C4-O4P-P-O3P
20	F	203	PC1	C11-O13-P-O11
20	F	203	PC1	C1-O11-P-O13
20	F	204	PC1	C11-O13-P-O11
20	J	203	PC1	C11-O13-P-O11
20	f	203	PC1	C11-O13-P-O11
20	f	203	PC1	C1-O11-P-O13
20	f	204	PC1	C11-O13-P-O11
20	j	203	PC1	C11-O13-P-O11
19	R	101	PEE	C31-C30-O3-C3
19	r	101	PEE	C31-C30-O3-C3
16	E	405	CDL	OA7-CA5-OA6-CA4
16	M	201	CDL	OB7-CB5-OB6-CB4
16	e	405	CDL	OA7-CA5-OA6-CA4
16	m	201	CDL	OB7-CB5-OB6-CB4
16	Q	101	CDL	C11-CA5-OA6-CA4
16	q	101	CDL	C11-CA5-OA6-CA4
16	E	402	CDL	C74-C75-C76-C77
16	e	402	CDL	C74-C75-C76-C77
16	j	201	CDL	CA7-C31-C32-C33
16	E	404	CDL	O1-C1-CB2-OB2
16	J	202	CDL	O1-C1-CB2-OB2
16	e	404	CDL	O1-C1-CB2-OB2
16	j	202	CDL	O1-C1-CB2-OB2
16	J	201	CDL	CA7-C31-C32-C33
19	R	101	PEE	O5-C30-O3-C3
19	r	101	PEE	O5-C30-O3-C3
16	J	202	CDL	C74-C75-C76-C77
16	j	202	CDL	C74-C75-C76-C77
16	J	201	CDL	C13-C14-C15-C16
16	j	201	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
16	Q	101	CDL	OA7-CA5-OA6-CA4
16	q	101	CDL	OA7-CA5-OA6-CA4
16	E	403	CDL	C71-C72-C73-C74
16	J	202	CDL	C78-C79-C80-C81
16	j	202	CDL	C78-C79-C80-C81
16	e	403	CDL	C71-C72-C73-C74
16	C	201	CDL	C55-C56-C57-C58
16	c	201	CDL	C55-C56-C57-C58
16	J	202	CDL	C11-CA5-OA6-CA4
16	j	202	CDL	C11-CA5-OA6-CA4
18	E	407	Q7G	CG1-C22-C23-C24
18	e	407	Q7G	CG1-C22-C23-C24
19	R	101	PEE	C43-C44-C45-C46
19	r	101	PEE	C43-C44-C45-C46
16	C	201	CDL	CB2-C1-CA2-OA2
16	E	404	CDL	CA2-C1-CB2-OB2
16	J	202	CDL	CA2-C1-CB2-OB2
16	c	201	CDL	CB2-C1-CA2-OA2
16	e	404	CDL	CA2-C1-CB2-OB2
16	j	202	CDL	CA2-C1-CB2-OB2
16	E	403	CDL	C14-C15-C16-C17
16	e	403	CDL	C14-C15-C16-C17
16	J	202	CDL	OA7-CA5-OA6-CA4
16	j	202	CDL	OA7-CA5-OA6-CA4
16	E	404	CDL	C17-C18-C19-C20
16	e	404	CDL	C17-C18-C19-C20
16	M	201	CDL	CA7-C31-C32-C33
16	m	201	CDL	CA7-C31-C32-C33
19	f	202	PEE	C11-C10-O2-C2
16	J	202	CDL	C15-C16-C17-C18
16	j	202	CDL	C15-C16-C17-C18
16	Q	101	CDL	CB7-C71-C72-C73
16	q	101	CDL	CB7-C71-C72-C73
16	E	403	CDL	C78-C79-C80-C81
16	e	403	CDL	C78-C79-C80-C81
16	E	405	CDL	C40-C41-C42-C43
16	J	201	CDL	C81-C82-C83-C84
16	e	405	CDL	C40-C41-C42-C43
16	j	201	CDL	C81-C82-C83-C84
16	Q	101	CDL	CA5-C11-C12-C13
16	q	101	CDL	CA5-C11-C12-C13
16	M	201	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
16	m	201	CDL	C36-C37-C38-C39
16	E	404	CDL	C11-CA5-OA6-CA4
16	J	202	CDL	C51-CB5-OB6-CB4
16	e	404	CDL	C11-CA5-OA6-CA4
16	j	202	CDL	C51-CB5-OB6-CB4
19	F	202	PEE	C11-C10-O2-C2
16	E	405	CDL	C57-C58-C59-C60
16	C	201	CDL	C34-C35-C36-C37
16	c	201	CDL	C34-C35-C36-C37
16	e	405	CDL	C57-C58-C59-C60
16	E	403	CDL	O1-C1-CA2-OA2
16	e	403	CDL	O1-C1-CA2-OA2
16	e	404	CDL	OA7-CA5-OA6-CA4
17	J	204	LMT	O5B-C5B-C6B-O6B
17	j	204	LMT	O5B-C5B-C6B-O6B
16	J	201	CDL	C34-C35-C36-C37
16	j	201	CDL	C34-C35-C36-C37
19	f	202	PEE	C42-C43-C44-C45
16	e	405	CDL	C56-C57-C58-C59
19	F	202	PEE	C42-C43-C44-C45
19	R	101	PEE	C22-C23-C24-C25
19	r	101	PEE	C22-C23-C24-C25
19	R	101	PEE	C17-C18-C19-C20
19	r	101	PEE	C17-C18-C19-C20
16	E	405	CDL	C56-C57-C58-C59
18	N	201	Q7G	O5C-C5C-C6C-O6C
18	n	201	Q7G	O5C-C5C-C6C-O6C
16	M	201	CDL	C12-C13-C14-C15
16	m	201	CDL	C12-C13-C14-C15
16	E	404	CDL	OA7-CA5-OA6-CA4
16	J	202	CDL	OB7-CB5-OB6-CB4
16	j	202	CDL	OB7-CB5-OB6-CB4
16	E	403	CDL	C51-CB5-OB6-CB4
16	e	403	CDL	C51-CB5-OB6-CB4
16	E	405	CDL	C71-C72-C73-C74
16	J	202	CDL	CA2-OA2-PA1-OA5
16	j	202	CDL	CA2-OA2-PA1-OA5
19	R	101	PEE	C4-O4P-P-O3P
19	r	101	PEE	C4-O4P-P-O3P
16	e	405	CDL	C71-C72-C73-C74
16	J	202	CDL	OA5-CA3-CA4-CA6
16	M	201	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
16	Q	101	CDL	OA5-CA3-CA4-CA6
16	j	202	CDL	OA5-CA3-CA4-CA6
16	m	201	CDL	OA5-CA3-CA4-CA6
16	q	101	CDL	OA5-CA3-CA4-CA6
16	m	201	CDL	C73-C74-C75-C76
16	M	201	CDL	C73-C74-C75-C76
16	J	201	CDL	C62-C63-C64-C65
16	j	201	CDL	C62-C63-C64-C65
19	R	101	PEE	C39-C40-C41-C42
19	r	101	PEE	C39-C40-C41-C42
16	f	201	CDL	C77-C78-C79-C80
16	F	201	CDL	C77-C78-C79-C80
16	E	403	CDL	C17-C18-C19-C20
16	e	403	CDL	C17-C18-C19-C20
16	C	201	CDL	C51-C52-C53-C54
16	c	201	CDL	C51-C52-C53-C54
16	E	401	CDL	C18-C19-C20-C21
16	e	401	CDL	C18-C19-C20-C21
16	E	402	CDL	C11-C12-C13-C14
16	C	201	CDL	CA4-CA6-OA8-CA7
16	c	201	CDL	CA4-CA6-OA8-CA7
16	e	402	CDL	C11-C12-C13-C14
16	e	405	CDL	C76-C77-C78-C79
16	E	405	CDL	C76-C77-C78-C79
16	L	101	CDL	C14-C15-C16-C17
16	l	101	CDL	C14-C15-C16-C17
16	E	405	CDL	C53-C54-C55-C56
16	e	405	CDL	C53-C54-C55-C56
16	Q	101	CDL	CB3-CB4-OB6-CB5
16	q	101	CDL	CB3-CB4-OB6-CB5
16	E	401	CDL	C81-C82-C83-C84
16	M	201	CDL	C33-C34-C35-C36
16	e	401	CDL	C81-C82-C83-C84
16	m	201	CDL	C33-C34-C35-C36
16	E	405	CDL	OA5-CA3-CA4-OA6
16	e	405	CDL	OA5-CA3-CA4-OA6
16	f	201	CDL	C11-CA5-OA6-CA4
16	e	405	CDL	C11-C12-C13-C14
20	F	204	PC1	C37-C38-C39-C3A
20	f	204	PC1	C37-C38-C39-C3A
16	E	404	CDL	OB6-CB4-CB6-OB8
16	F	201	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
16	L	101	CDL	OA6-CA4-CA6-OA8
16	e	404	CDL	OB6-CB4-CB6-OB8
16	f	201	CDL	OB6-CB4-CB6-OB8
16	l	101	CDL	OA6-CA4-CA6-OA8
16	C	201	CDL	C39-C40-C41-C42
16	E	405	CDL	C11-C12-C13-C14
16	c	201	CDL	C39-C40-C41-C42
19	F	202	PEE	O4-C10-O2-C2
19	f	202	PEE	O4-C10-O2-C2
16	J	202	CDL	C76-C77-C78-C79
16	j	202	CDL	C76-C77-C78-C79
20	i	201	PC1	C32-C31-O31-C3
16	E	402	CDL	C78-C79-C80-C81
16	e	402	CDL	C78-C79-C80-C81
16	F	201	CDL	C11-CA5-OA6-CA4
16	l	101	CDL	C31-C32-C33-C34
20	I	201	PC1	C32-C31-O31-C3
16	L	101	CDL	C31-C32-C33-C34
16	C	201	CDL	OA5-CA3-CA4-CA6
16	E	401	CDL	OB5-CB3-CB4-CB6
16	c	201	CDL	OA5-CA3-CA4-CA6
16	e	401	CDL	OB5-CB3-CB4-CB6
16	J	202	CDL	C79-C80-C81-C82
16	j	202	CDL	C79-C80-C81-C82
16	m	201	CDL	C83-C84-C85-C86
16	M	201	CDL	C83-C84-C85-C86
16	C	201	CDL	CA4-CA3-OA5-PA1
16	J	201	CDL	CA4-CA3-OA5-PA1
16	c	201	CDL	CA4-CA3-OA5-PA1
16	j	201	CDL	CA4-CA3-OA5-PA1
16	L	101	CDL	C64-C65-C66-C67
16	l	101	CDL	C64-C65-C66-C67
16	E	405	CDL	CB3-CB4-CB6-OB8
16	e	405	CDL	CB3-CB4-CB6-OB8
19	F	202	PEE	C1-C2-C3-O3
19	f	202	PEE	C1-C2-C3-O3
20	F	203	PC1	C1-C2-C3-O31
20	f	203	PC1	C1-C2-C3-O31
16	E	403	CDL	OB7-CB5-OB6-CB4
16	e	403	CDL	OB7-CB5-OB6-CB4
16	E	403	CDL	CB5-C51-C52-C53
16	e	403	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
16	E	403	CDL	C83-C84-C85-C86
16	e	403	CDL	C83-C84-C85-C86
16	F	201	CDL	C12-C13-C14-C15
16	e	403	CDL	C12-C13-C14-C15
16	f	201	CDL	C12-C13-C14-C15
16	J	201	CDL	CA2-OA2-PA1-OA5
16	j	201	CDL	CA2-OA2-PA1-OA5
16	E	405	CDL	CB7-C71-C72-C73
16	e	405	CDL	CB7-C71-C72-C73
16	E	403	CDL	C12-C13-C14-C15
16	C	201	CDL	OA5-CA3-CA4-OA6
16	E	401	CDL	OB5-CB3-CB4-OB6
16	c	201	CDL	OA5-CA3-CA4-OA6
16	e	401	CDL	OB5-CB3-CB4-OB6
20	i	201	PC1	C2C-C2D-C2E-C2F
16	f	201	CDL	C13-C14-C15-C16
20	I	201	PC1	C2C-C2D-C2E-C2F
20	f	203	PC1	O21-C2-C3-O31
16	F	201	CDL	C13-C14-C15-C16
16	J	202	CDL	C72-C73-C74-C75
16	j	202	CDL	C72-C73-C74-C75
16	E	404	CDL	CB2-C1-CA2-OA2
16	Q	101	CDL	CB2-C1-CA2-OA2
16	e	404	CDL	CB2-C1-CA2-OA2
16	q	101	CDL	CB2-C1-CA2-OA2
18	N	201	Q7G	C24-C23-C48-O1C
18	n	201	Q7G	C24-C23-C48-O1C
16	F	201	CDL	OA7-CA5-OA6-CA4
16	f	201	CDL	OA7-CA5-OA6-CA4
16	E	401	CDL	C43-C44-C45-C46
16	e	401	CDL	C43-C44-C45-C46
16	E	405	CDL	C78-C79-C80-C81
16	J	201	CDL	C55-C56-C57-C58
16	e	405	CDL	C78-C79-C80-C81
16	j	201	CDL	C55-C56-C57-C58
16	E	401	CDL	CB4-CB3-OB5-PB2
16	J	201	CDL	C1-CB2-OB2-PB2
16	L	101	CDL	CA4-CA3-OA5-PA1
16	e	401	CDL	CB4-CB3-OB5-PB2
16	j	201	CDL	C1-CB2-OB2-PB2
16	j	202	CDL	CB4-CB3-OB5-PB2
16	l	101	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
20	J	203	PC1	C2-C1-O11-P
20	j	203	PC1	C2-C1-O11-P
20	I	201	PC1	O32-C31-O31-C3
17	J	204	LMT	C2-C3-C4-C5
17	j	204	LMT	C2-C3-C4-C5
16	m	201	CDL	C78-C79-C80-C81
16	M	201	CDL	C78-C79-C80-C81
16	E	401	CDL	C56-C57-C58-C59
16	e	401	CDL	C56-C57-C58-C59
16	E	405	CDL	C59-C60-C61-C62
16	e	405	CDL	C59-C60-C61-C62
20	i	201	PC1	O32-C31-O31-C3
16	E	405	CDL	OB5-CB3-CB4-CB6
16	e	405	CDL	OB5-CB3-CB4-CB6
16	E	405	CDL	C52-C53-C54-C55
16	e	405	CDL	C52-C53-C54-C55
19	R	101	PEE	C23-C24-C25-C26
19	r	101	PEE	C23-C24-C25-C26
16	L	101	CDL	C31-CA7-OA8-CA6
16	l	101	CDL	C31-CA7-OA8-CA6
16	E	402	CDL	CA6-CA4-OA6-CA5
16	e	402	CDL	CA6-CA4-OA6-CA5
16	j	201	CDL	C77-C78-C79-C80
16	C	201	CDL	CA3-CA4-CA6-OA8
16	E	402	CDL	CA4-CA3-OA5-PA1
16	E	404	CDL	CB3-CB4-CB6-OB8
16	F	201	CDL	CB4-CB3-OB5-PB2
16	J	202	CDL	CB4-CB3-OB5-PB2
16	M	201	CDL	CA3-CA4-CA6-OA8
16	c	201	CDL	CA3-CA4-CA6-OA8
16	e	402	CDL	CA4-CA3-OA5-PA1
16	e	402	CDL	C1-CB2-OB2-PB2
16	e	404	CDL	CB3-CB4-CB6-OB8
16	f	201	CDL	CB4-CB3-OB5-PB2
16	m	201	CDL	CA3-CA4-CA6-OA8
16	E	402	CDL	C81-C82-C83-C84
16	j	202	CDL	C61-C62-C63-C64
16	E	402	CDL	OB5-CB3-CB4-OB6
16	E	404	CDL	OA5-CA3-CA4-OA6
16	F	201	CDL	OA5-CA3-CA4-OA6
16	J	202	CDL	OA5-CA3-CA4-OA6
16	e	402	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
16	e	404	CDL	OA5-CA3-CA4-OA6
16	f	201	CDL	OA5-CA3-CA4-OA6
16	j	202	CDL	OA5-CA3-CA4-OA6
16	C	201	CDL	C83-C84-C85-C86
16	J	201	CDL	C77-C78-C79-C80
16	J	202	CDL	C61-C62-C63-C64
16	e	402	CDL	C81-C82-C83-C84
16	E	401	CDL	C13-C14-C15-C16
16	c	201	CDL	C83-C84-C85-C86
16	e	401	CDL	C13-C14-C15-C16
16	m	201	CDL	C42-C43-C44-C45
16	M	201	CDL	C42-C43-C44-C45
16	E	402	CDL	C75-C76-C77-C78
16	e	402	CDL	C75-C76-C77-C78
16	E	403	CDL	OA6-CA4-CA6-OA8
16	e	403	CDL	OA6-CA4-CA6-OA8
20	F	203	PC1	O21-C2-C3-O31
16	E	402	CDL	C34-C35-C36-C37
16	e	402	CDL	C34-C35-C36-C37
19	R	101	PEE	C34-C35-C36-C37
19	r	101	PEE	C34-C35-C36-C37
18	N	201	Q7G	C16-C17-O20-CG1
18	N	201	Q7G	C18-C17-O20-CG1
18	n	201	Q7G	C16-C17-O20-CG1
18	n	201	Q7G	C18-C17-O20-CG1
20	J	203	PC1	C3C-C3D-C3E-C3F
20	j	203	PC1	C3C-C3D-C3E-C3F
19	R	101	PEE	C1-O3P-P-O4P
19	r	101	PEE	C1-O3P-P-O4P
16	E	402	CDL	C1-CB2-OB2-PB2
16	E	405	CDL	CA4-CA3-OA5-PA1
16	e	405	CDL	CA4-CA3-OA5-PA1
16	L	101	CDL	OA9-CA7-OA8-CA6
16	l	101	CDL	OA9-CA7-OA8-CA6
16	E	401	CDL	CB3-OB5-PB2-OB4
16	E	404	CDL	CA3-OA5-PA1-OA3
16	F	201	CDL	CA2-OA2-PA1-OA4
16	F	201	CDL	CB3-OB5-PB2-OB3
16	J	201	CDL	CA2-OA2-PA1-OA4
16	J	202	CDL	CA2-OA2-PA1-OA3
16	L	101	CDL	CA3-OA5-PA1-OA3
16	L	101	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
16	M	201	CDL	CB3-OB5-PB2-OB4
16	Q	101	CDL	CA2-OA2-PA1-OA3
16	e	401	CDL	CB3-OB5-PB2-OB4
16	e	404	CDL	CA3-OA5-PA1-OA3
16	f	201	CDL	CA2-OA2-PA1-OA4
16	f	201	CDL	CB3-OB5-PB2-OB3
16	j	201	CDL	CA2-OA2-PA1-OA4
16	j	202	CDL	CA2-OA2-PA1-OA3
16	l	101	CDL	CA3-OA5-PA1-OA3
16	l	101	CDL	CB2-OB2-PB2-OB4
16	m	201	CDL	CB3-OB5-PB2-OB4
16	q	101	CDL	CA2-OA2-PA1-OA3
19	F	202	PEE	C4-O4P-P-O2P
19	F	202	PEE	C4-O4P-P-O1P
19	R	101	PEE	C1-O3P-P-O1P
19	R	101	PEE	C4-O4P-P-O1P
19	f	202	PEE	C4-O4P-P-O2P
19	f	202	PEE	C4-O4P-P-O1P
19	r	101	PEE	C1-O3P-P-O1P
19	r	101	PEE	C4-O4P-P-O1P
20	F	203	PC1	C1-O11-P-O12
20	F	204	PC1	C11-O13-P-O12
20	f	203	PC1	C1-O11-P-O12
20	f	204	PC1	C11-O13-P-O12
16	E	402	CDL	OB5-CB3-CB4-CB6
16	E	404	CDL	OA5-CA3-CA4-CA6
16	J	201	CDL	OB5-CB3-CB4-CB6
16	e	402	CDL	OB5-CB3-CB4-CB6
16	e	404	CDL	OA5-CA3-CA4-CA6
16	j	201	CDL	OB5-CB3-CB4-CB6
16	Q	101	CDL	C77-C78-C79-C80
16	q	101	CDL	C77-C78-C79-C80
16	C	201	CDL	C62-C63-C64-C65
16	c	201	CDL	C62-C63-C64-C65
20	F	204	PC1	C21-C22-C23-C24
20	f	204	PC1	C21-C22-C23-C24
16	j	201	CDL	C72-C73-C74-C75
16	J	201	CDL	OB5-CB3-CB4-OB6
16	j	201	CDL	OB5-CB3-CB4-OB6
18	E	407	Q7G	C23-C24-O1B-C1B
18	e	407	Q7G	C23-C24-O1B-C1B
16	J	201	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
16	M	201	CDL	C20-C21-C22-C23
16	m	201	CDL	C20-C21-C22-C23
20	F	203	PC1	O13-C11-C12-N
20	J	203	PC1	O13-C11-C12-N
20	f	203	PC1	O13-C11-C12-N
20	j	203	PC1	O13-C11-C12-N
16	E	405	CDL	OB6-CB4-CB6-OB8
16	e	405	CDL	OB6-CB4-CB6-OB8
19	F	202	PEE	O2-C2-C3-O3
19	f	202	PEE	O2-C2-C3-O3
16	E	403	CDL	C62-C63-C64-C65
16	e	403	CDL	C62-C63-C64-C65
19	R	101	PEE	C13-C14-C15-C16
19	r	101	PEE	C13-C14-C15-C16
16	e	402	CDL	C17-C18-C19-C20
16	e	402	CDL	C79-C80-C81-C82
16	E	402	CDL	C17-C18-C19-C20
16	E	402	CDL	C53-C54-C55-C56
16	e	402	CDL	C53-C54-C55-C56
16	E	402	CDL	C79-C80-C81-C82
16	E	404	CDL	CA6-CA4-OA6-CA5
16	J	202	CDL	CB3-CB4-OB6-CB5
16	e	404	CDL	CA6-CA4-OA6-CA5
16	j	202	CDL	CB3-CB4-OB6-CB5
16	E	405	CDL	OA5-CA3-CA4-CA6
16	e	405	CDL	OA5-CA3-CA4-CA6
16	E	402	CDL	C55-C56-C57-C58
16	e	402	CDL	C55-C56-C57-C58
19	r	101	PEE	C41-C42-C43-C44
19	R	101	PEE	C41-C42-C43-C44
16	E	403	CDL	C1-CA2-OA2-PA1
16	e	403	CDL	C1-CA2-OA2-PA1
16	e	401	CDL	C53-C54-C55-C56
16	E	401	CDL	C53-C54-C55-C56
16	E	403	CDL	C51-C52-C53-C54
20	I	201	PC1	C2A-C2B-C2C-C2D
20	i	201	PC1	C2A-C2B-C2C-C2D
16	e	403	CDL	C51-C52-C53-C54
16	C	201	CDL	OA6-CA4-CA6-OA8
16	E	403	CDL	OB6-CB4-CB6-OB8
16	c	201	CDL	OA6-CA4-CA6-OA8
16	e	403	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
16	C	201	CDL	CA3-OA5-PA1-OA2
16	E	403	CDL	CB2-OB2-PB2-OB5
16	Q	101	CDL	CA3-OA5-PA1-OA2
16	Q	101	CDL	CB3-OB5-PB2-OB2
16	c	201	CDL	CA3-OA5-PA1-OA2
16	e	403	CDL	CB2-OB2-PB2-OB5
16	q	101	CDL	CA3-OA5-PA1-OA2
16	q	101	CDL	CB3-OB5-PB2-OB2
16	C	201	CDL	C35-C36-C37-C38
16	c	201	CDL	C35-C36-C37-C38
16	E	403	CDL	CA3-CA4-CA6-OA8
16	E	403	CDL	CB3-CB4-CB6-OB8
16	F	201	CDL	CB3-CB4-CB6-OB8
16	J	202	CDL	CB3-CB4-CB6-OB8
16	e	403	CDL	CA3-CA4-CA6-OA8
16	e	403	CDL	CB3-CB4-CB6-OB8
16	f	201	CDL	CB3-CB4-CB6-OB8
16	j	202	CDL	CB3-CB4-CB6-OB8
20	F	204	PC1	C22-C21-O21-C2
20	f	204	PC1	C22-C21-O21-C2
16	Q	101	CDL	C1-CB2-OB2-PB2
16	q	101	CDL	C1-CB2-OB2-PB2
19	F	202	PEE	C16-C17-C18-C19
19	R	101	PEE	C36-C37-C38-C39
19	f	202	PEE	C16-C17-C18-C19
19	r	101	PEE	C36-C37-C38-C39
20	f	204	PC1	O31-C31-C32-C33
20	F	204	PC1	O31-C31-C32-C33
16	E	401	CDL	C80-C81-C82-C83
16	e	401	CDL	C80-C81-C82-C83
20	J	203	PC1	O11-C1-C2-O21
20	j	203	PC1	O11-C1-C2-O21
16	F	201	CDL	C78-C79-C80-C81
16	f	201	CDL	C78-C79-C80-C81
16	f	201	CDL	O1-C1-CB2-OB2
16	c	201	CDL	C40-C41-C42-C43
16	l	101	CDL	C36-C37-C38-C39
16	L	101	CDL	C36-C37-C38-C39
16	C	201	CDL	C40-C41-C42-C43
19	r	101	PEE	C33-C34-C35-C36
16	C	201	CDL	C1-CB2-OB2-PB2
16	c	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
19	R	101	PEE	C33-C34-C35-C36
16	M	201	CDL	C72-C73-C74-C75
16	E	402	CDL	OA7-CA5-OA6-CA4
16	e	402	CDL	OA7-CA5-OA6-CA4
16	m	201	CDL	C72-C73-C74-C75
16	C	201	CDL	C42-C43-C44-C45
16	E	402	CDL	C54-C55-C56-C57
16	e	402	CDL	C54-C55-C56-C57
16	c	201	CDL	C42-C43-C44-C45
16	m	201	CDL	C21-C22-C23-C24
16	L	101	CDL	CA3-CA4-CA6-OA8
16	l	101	CDL	CA3-CA4-CA6-OA8
19	R	101	PEE	C1-C2-C3-O3
19	r	101	PEE	C1-C2-C3-O3
20	F	204	PC1	O22-C21-O21-C2
20	f	204	PC1	O22-C21-O21-C2
16	M	201	CDL	C21-C22-C23-C24
16	E	401	CDL	C16-C17-C18-C19
16	e	401	CDL	C16-C17-C18-C19
16	F	201	CDL	O1-C1-CB2-OB2
16	E	404	CDL	C78-C79-C80-C81
16	e	404	CDL	C78-C79-C80-C81
16	J	201	CDL	CA3-CA4-OA6-CA5
16	j	201	CDL	CA3-CA4-OA6-CA5
20	F	203	PC1	O22-C21-O21-C2
20	f	203	PC1	O22-C21-O21-C2
16	l	101	CDL	C39-C40-C41-C42
16	L	101	CDL	C39-C40-C41-C42
16	M	201	CDL	C75-C76-C77-C78
16	m	201	CDL	C75-C76-C77-C78
16	Q	101	CDL	C75-C76-C77-C78
16	q	101	CDL	C75-C76-C77-C78
16	C	201	CDL	C38-C39-C40-C41
16	c	201	CDL	C38-C39-C40-C41
16	e	401	CDL	C11-C12-C13-C14
16	E	401	CDL	C11-C12-C13-C14
16	l	101	CDL	CB2-C1-CA2-OA2
16	C	201	CDL	C56-C57-C58-C59
16	c	201	CDL	C56-C57-C58-C59
16	e	402	CDL	C77-C78-C79-C80
16	E	402	CDL	C77-C78-C79-C80
16	J	201	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
16	j	201	CDL	C71-C72-C73-C74
16	j	202	CDL	C37-C38-C39-C40
19	R	101	PEE	C38-C39-C40-C41
19	r	101	PEE	C38-C39-C40-C41
16	J	202	CDL	C37-C38-C39-C40
20	F	203	PC1	C22-C21-O21-C2
20	f	203	PC1	C22-C21-O21-C2
16	E	401	CDL	C37-C38-C39-C40
20	F	204	PC1	C24-C25-C26-C27
20	f	204	PC1	C24-C25-C26-C27
16	e	403	CDL	C23-C24-C25-C26
16	E	403	CDL	C23-C24-C25-C26
16	e	401	CDL	C37-C38-C39-C40
20	J	203	PC1	O11-C1-C2-C3
20	j	203	PC1	O11-C1-C2-C3
16	E	403	CDL	C18-C19-C20-C21
16	M	201	CDL	C12-C11-CA5-OA6
16	L	101	CDL	CB2-C1-CA2-OA2
16	e	403	CDL	C18-C19-C20-C21
16	f	201	CDL	C12-C11-CA5-OA6
16	m	201	CDL	C12-C11-CA5-OA6
16	E	405	CDL	C79-C80-C81-C82
16	e	405	CDL	C79-C80-C81-C82
16	F	201	CDL	C12-C11-CA5-OA6
19	F	202	PEE	O2-C10-C11-C12
16	e	401	CDL	C17-C18-C19-C20
16	f	201	CDL	C37-C38-C39-C40
16	F	201	CDL	C37-C38-C39-C40
16	E	401	CDL	C32-C31-CA7-OA8
16	e	401	CDL	C32-C31-CA7-OA8
16	E	401	CDL	C17-C18-C19-C20
16	M	201	CDL	C19-C20-C21-C22
16	m	201	CDL	C19-C20-C21-C22
19	f	202	PEE	O2-C10-C11-C12
16	L	101	CDL	OA7-CA5-OA6-CA4
16	l	101	CDL	OA7-CA5-OA6-CA4
16	E	402	CDL	C52-C51-CB5-OB6
16	M	201	CDL	C72-C71-CB7-OB8
16	m	201	CDL	C72-C71-CB7-OB8
16	L	101	CDL	C60-C61-C62-C63
16	l	101	CDL	C60-C61-C62-C63
16	e	403	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
19	F	202	PEE	C36-C37-C38-C39
19	f	202	PEE	C36-C37-C38-C39
16	Q	101	CDL	OB5-CB3-CB4-OB6
16	q	101	CDL	OB5-CB3-CB4-OB6
16	J	202	CDL	C12-C11-CA5-OA6
16	e	402	CDL	C52-C51-CB5-OB6
16	j	202	CDL	C12-C11-CA5-OA6
16	E	403	CDL	OB9-CB7-OB8-CB6
19	R	101	PEE	C18-C19-C20-C21
19	r	101	PEE	C18-C19-C20-C21
16	E	404	CDL	C18-C19-C20-C21
16	e	404	CDL	C18-C19-C20-C21
20	I	201	PC1	C3B-C3C-C3D-C3E
16	E	403	CDL	C71-CB7-OB8-CB6
16	e	403	CDL	C71-CB7-OB8-CB6
16	E	403	CDL	OA5-CA3-CA4-CA6
16	Q	101	CDL	OB5-CB3-CB4-CB6
16	e	403	CDL	OA5-CA3-CA4-CA6
16	q	101	CDL	OB5-CB3-CB4-CB6
20	i	201	PC1	C3B-C3C-C3D-C3E
16	F	201	CDL	C72-C71-CB7-OB8
16	f	201	CDL	C72-C71-CB7-OB8
16	j	201	CDL	C52-C51-CB5-OB6
20	J	203	PC1	O31-C31-C32-C33
20	j	203	PC1	O31-C31-C32-C33
16	J	201	CDL	C52-C51-CB5-OB6
19	f	202	PEE	O4-C10-C11-C12
19	F	202	PEE	C18-C19-C20-C21
19	R	101	PEE	C16-C17-C18-C19
19	f	202	PEE	C18-C19-C20-C21
19	r	101	PEE	C16-C17-C18-C19
16	E	405	CDL	C12-C11-CA5-OA6
16	e	405	CDL	C12-C11-CA5-OA6
19	F	202	PEE	O4-C10-C11-C12
16	M	201	CDL	C71-CB7-OB8-CB6
16	m	201	CDL	C71-CB7-OB8-CB6
16	Q	101	CDL	C72-C71-CB7-OB8
16	E	402	CDL	C11-CA5-OA6-CA4
16	e	402	CDL	C11-CA5-OA6-CA4
16	q	101	CDL	C72-C71-CB7-OB8
16	j	202	CDL	C38-C39-C40-C41
16	J	202	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
16	J	202	CDL	C12-C11-CA5-OA7
16	j	202	CDL	C12-C11-CA5-OA7
16	m	201	CDL	C31-CA7-OA8-CA6
16	M	201	CDL	C31-CA7-OA8-CA6
16	F	201	CDL	C12-C11-CA5-OA7
16	M	201	CDL	C72-C71-CB7-OB9
16	m	201	CDL	C72-C71-CB7-OB9
16	E	405	CDL	O1-C1-CA2-OA2
16	Q	101	CDL	O1-C1-CA2-OA2
16	e	405	CDL	O1-C1-CA2-OA2
16	q	101	CDL	O1-C1-CA2-OA2
16	E	401	CDL	C32-C31-CA7-OA9
16	M	201	CDL	C12-C11-CA5-OA7
16	e	401	CDL	C32-C31-CA7-OA9
16	f	201	CDL	C12-C11-CA5-OA7
16	f	201	CDL	C72-C71-CB7-OB9
16	m	201	CDL	C12-C11-CA5-OA7
16	E	405	CDL	C81-C82-C83-C84
16	e	405	CDL	C81-C82-C83-C84
16	E	403	CDL	C52-C51-CB5-OB6
16	e	403	CDL	C52-C51-CB5-OB6
16	E	402	CDL	CB4-CB3-OB5-PB2
16	e	402	CDL	CB4-CB3-OB5-PB2
16	F	201	CDL	C72-C71-CB7-OB9
16	C	201	CDL	CA3-OA5-PA1-OA3
16	C	201	CDL	CB2-OB2-PB2-OB3
16	E	403	CDL	CB2-OB2-PB2-OB3
16	c	201	CDL	CA3-OA5-PA1-OA3
16	c	201	CDL	CB2-OB2-PB2-OB3
16	e	403	CDL	CB2-OB2-PB2-OB3
20	J	203	PC1	C11-O13-P-O12
20	j	203	PC1	C11-O13-P-O12
16	l	101	CDL	C80-C81-C82-C83
16	E	405	CDL	C12-C11-CA5-OA7
16	e	405	CDL	C12-C11-CA5-OA7
16	L	101	CDL	C80-C81-C82-C83
16	E	403	CDL	C32-C31-CA7-OA8
16	E	405	CDL	C32-C31-CA7-OA8
16	e	403	CDL	C32-C31-CA7-OA8
16	e	405	CDL	C32-C31-CA7-OA8
16	L	101	CDL	C58-C59-C60-C61
16	m	201	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
16	l	101	CDL	C58-C59-C60-C61
20	F	204	PC1	C2B-C2C-C2D-C2E
16	M	201	CDL	C53-C54-C55-C56
16	E	402	CDL	C32-C31-CA7-OA8
16	e	402	CDL	C32-C31-CA7-OA8
16	M	201	CDL	C51-C52-C53-C54
16	Q	101	CDL	C73-C74-C75-C76
16	m	201	CDL	C51-C52-C53-C54
16	l	101	CDL	C11-CA5-OA6-CA4
16	m	201	CDL	C53-C54-C55-C56
16	q	101	CDL	C73-C74-C75-C76
20	f	204	PC1	C2B-C2C-C2D-C2E
16	E	405	CDL	CA3-CA4-OA6-CA5
16	J	201	CDL	CA6-CA4-OA6-CA5
16	e	405	CDL	CA3-CA4-OA6-CA5
16	j	201	CDL	CA6-CA4-OA6-CA5
20	J	203	PC1	C12-C11-O13-P
20	j	203	PC1	C12-C11-O13-P
16	M	201	CDL	OB9-CB7-OB8-CB6
20	F	204	PC1	O32-C31-O31-C3
20	f	204	PC1	O32-C31-O31-C3
16	Q	101	CDL	C72-C71-CB7-OB9
20	J	203	PC1	O32-C31-C32-C33
20	j	203	PC1	O32-C31-C32-C33
17	J	204	LMT	C5-C6-C7-C8
16	q	101	CDL	C72-C71-CB7-OB9
16	E	403	CDL	C32-C33-C34-C35
17	j	204	LMT	C5-C6-C7-C8
16	e	403	CDL	C32-C33-C34-C35
16	m	201	CDL	OA9-CA7-OA8-CA6
16	M	201	CDL	OA9-CA7-OA8-CA6
16	E	402	CDL	C32-C31-CA7-OA9
16	e	402	CDL	C32-C31-CA7-OA9
20	I	201	PC1	O21-C21-C22-C23
20	i	201	PC1	O21-C21-C22-C23
16	J	202	CDL	C59-C60-C61-C62
16	j	202	CDL	C71-C72-C73-C74
16	J	202	CDL	C71-C72-C73-C74
16	L	101	CDL	C11-CA5-OA6-CA4
16	j	202	CDL	C59-C60-C61-C62
16	E	402	CDL	O1-C1-CA2-OA2
16	e	402	CDL	O1-C1-CA2-OA2

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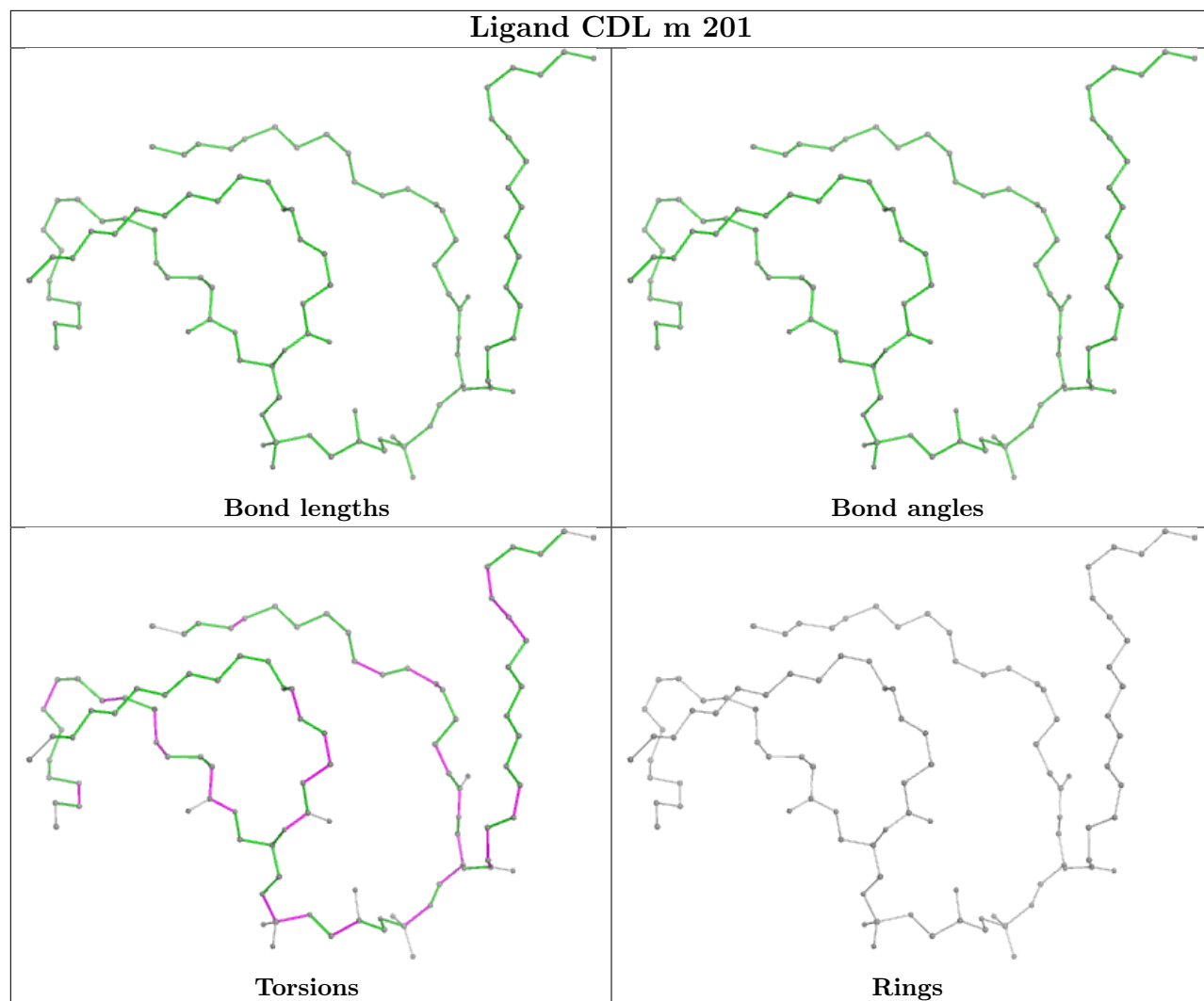
Mol	Chain	Res	Type	Atoms
16	F	201	CDL	C52-C51-CB5-OB6
16	f	201	CDL	C52-C51-CB5-OB6
16	E	403	CDL	C32-C31-CA7-OA9
16	E	403	CDL	C52-C51-CB5-OB7
16	E	405	CDL	C32-C31-CA7-OA9
16	J	201	CDL	C52-C51-CB5-OB7
16	e	403	CDL	C32-C31-CA7-OA9
16	e	403	CDL	C52-C51-CB5-OB7
16	e	405	CDL	C32-C31-CA7-OA9
16	j	201	CDL	C52-C51-CB5-OB7
19	F	202	PEE	O3-C30-C31-C32
19	f	202	PEE	O3-C30-C31-C32

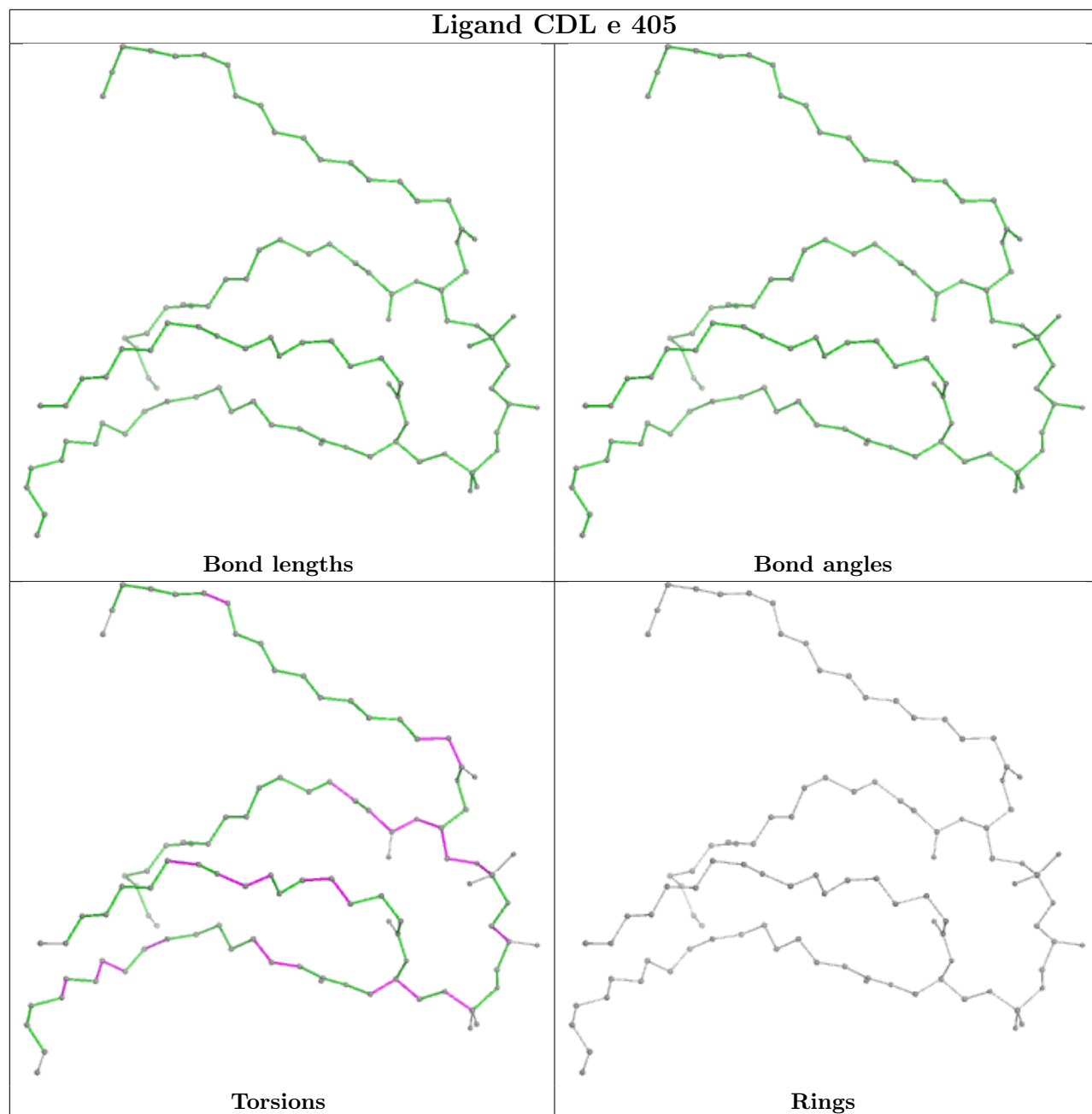
There are no ring outliers.

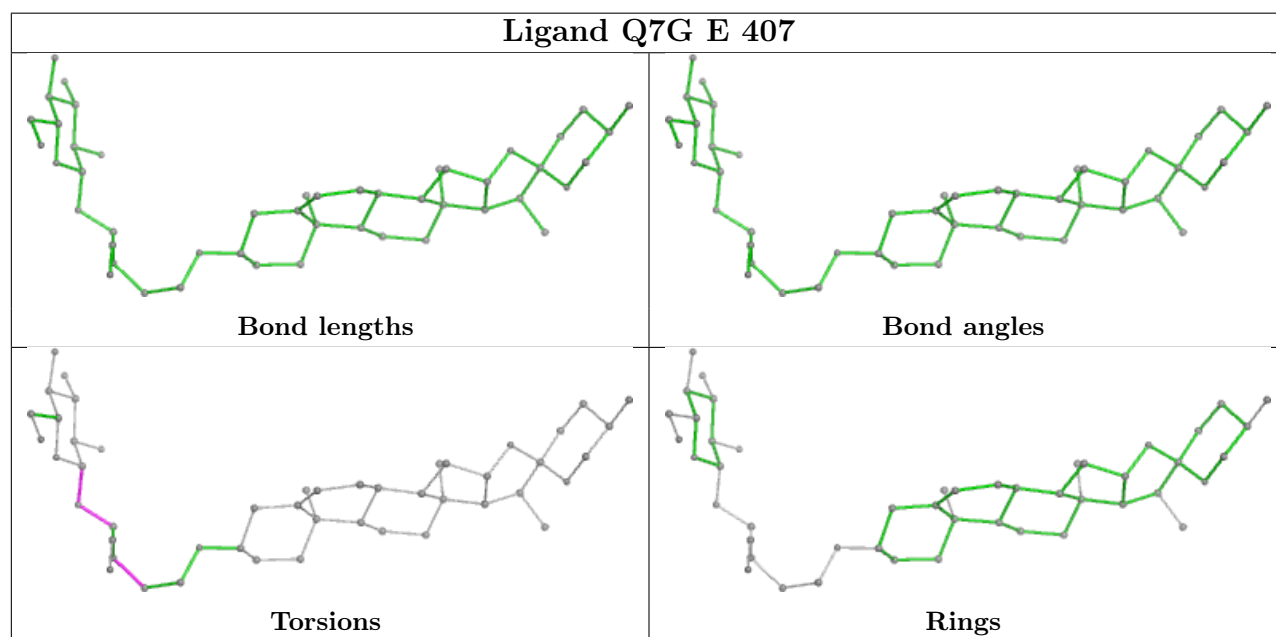
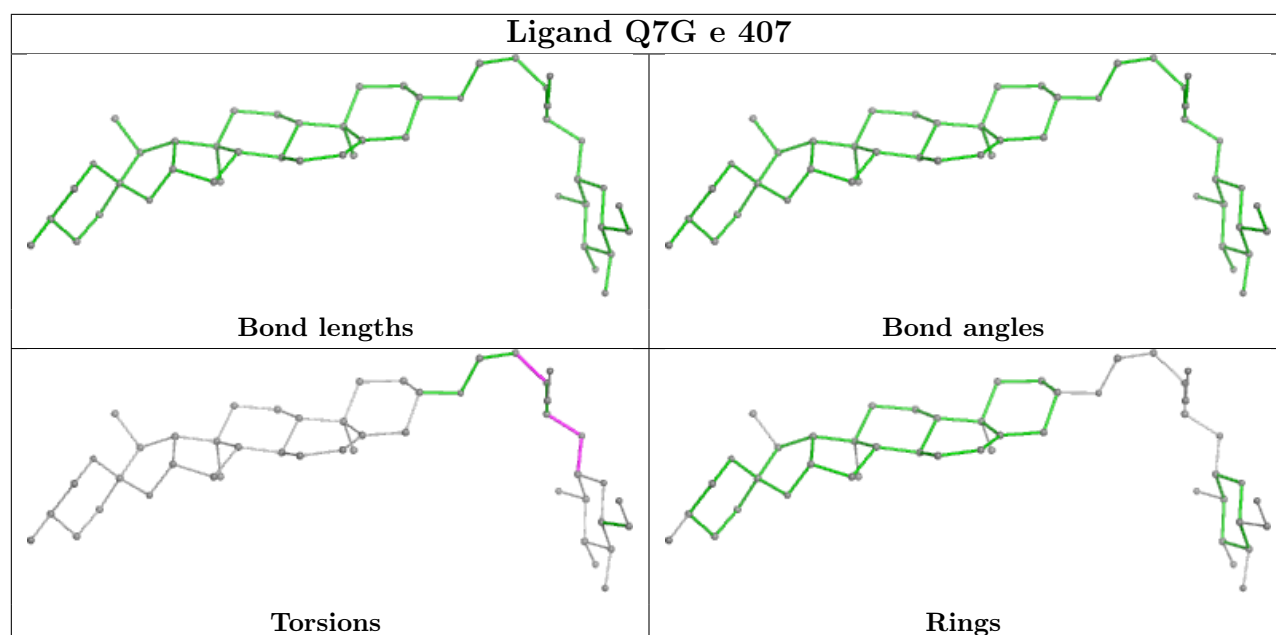
9 monomers are involved in 10 short contacts:

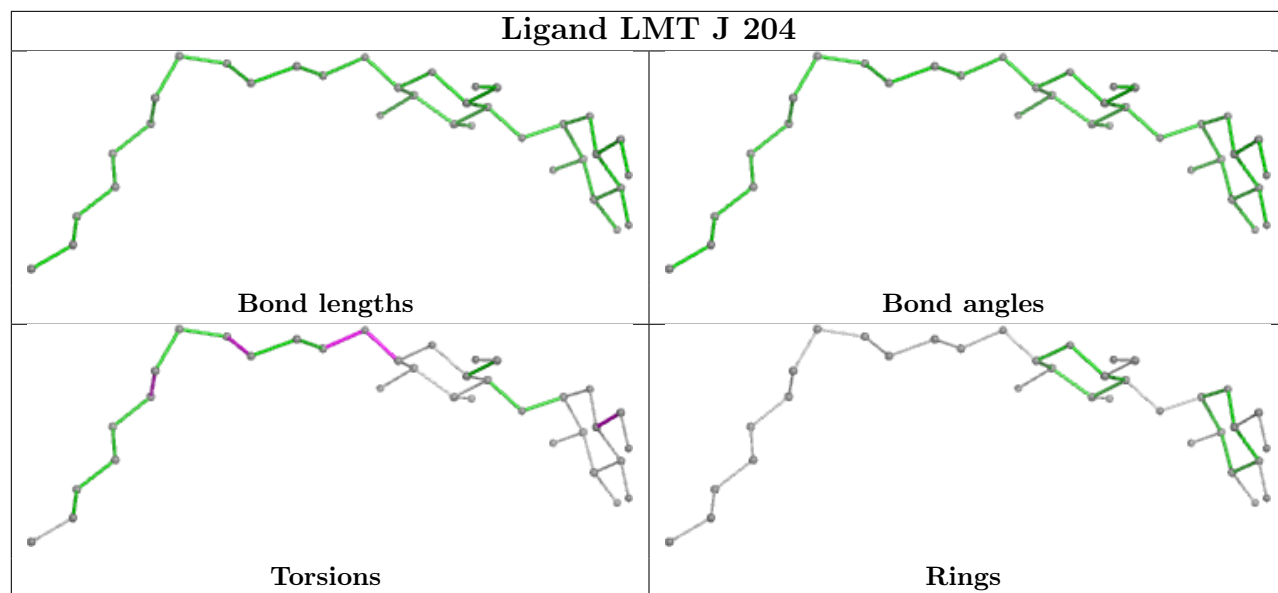
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	E	403	CDL	2	0
16	e	403	CDL	1	0
16	e	402	CDL	3	0
20	F	204	PC1	1	0
16	E	402	CDL	3	0
16	J	202	CDL	1	0
16	j	202	CDL	1	0
16	c	201	CDL	1	0
16	C	201	CDL	1	0

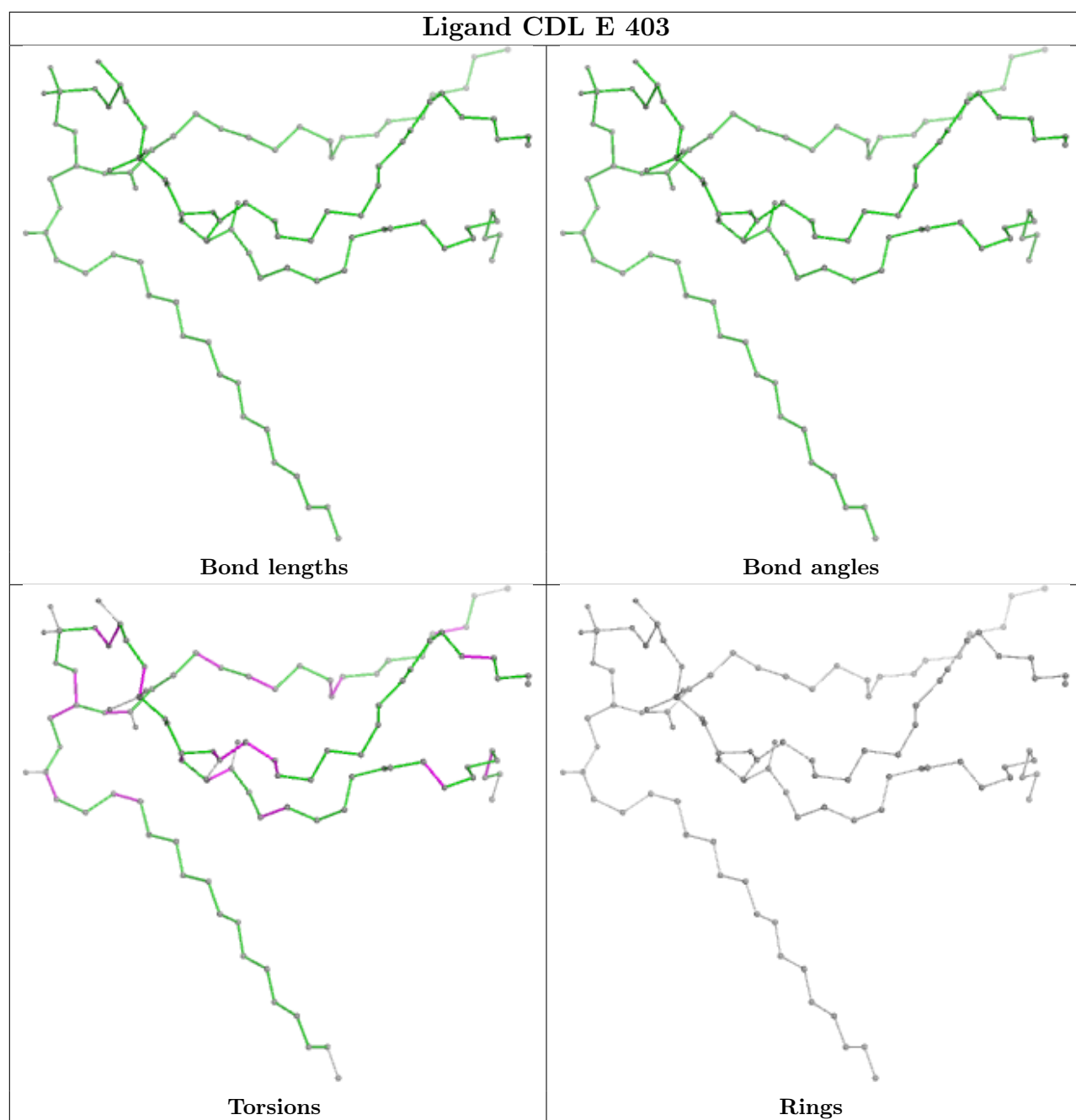
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

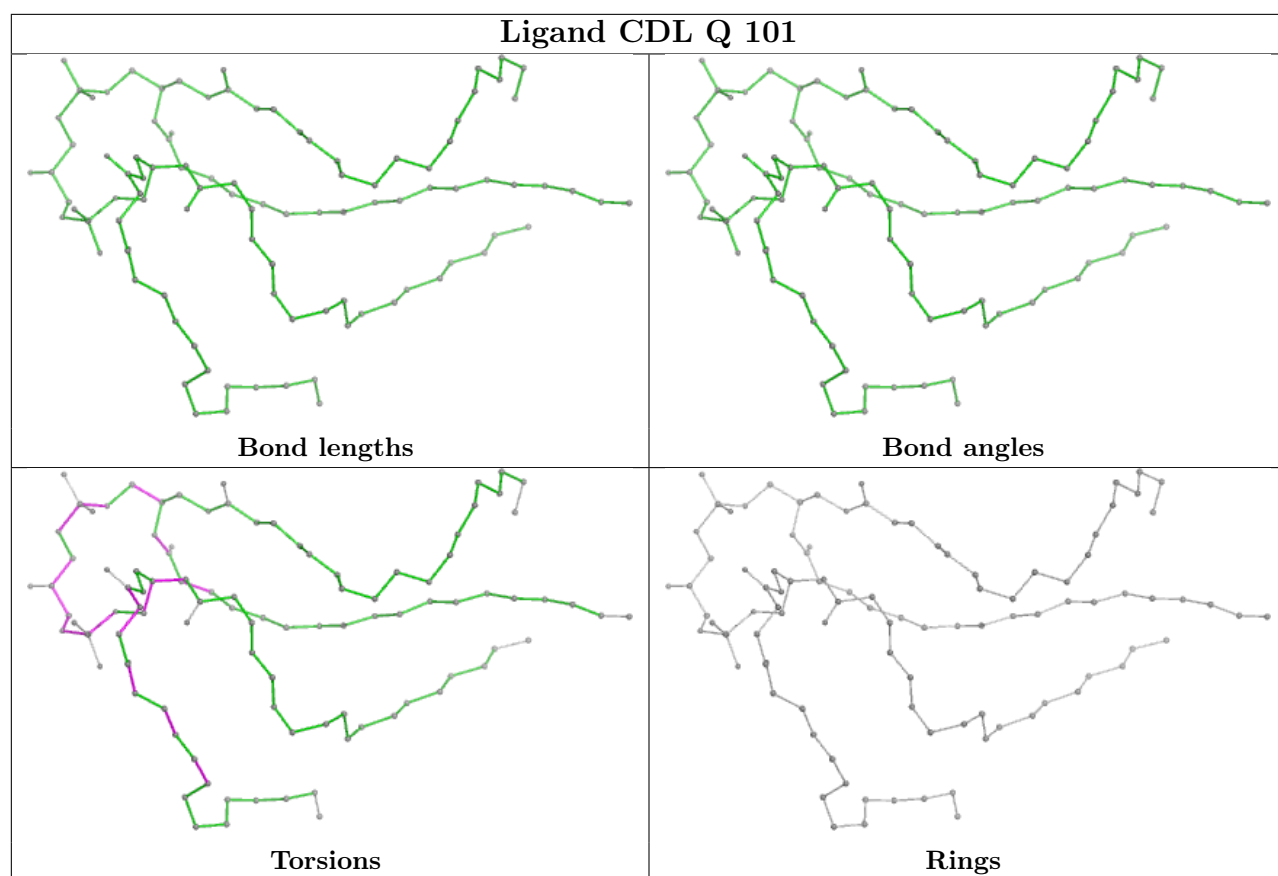


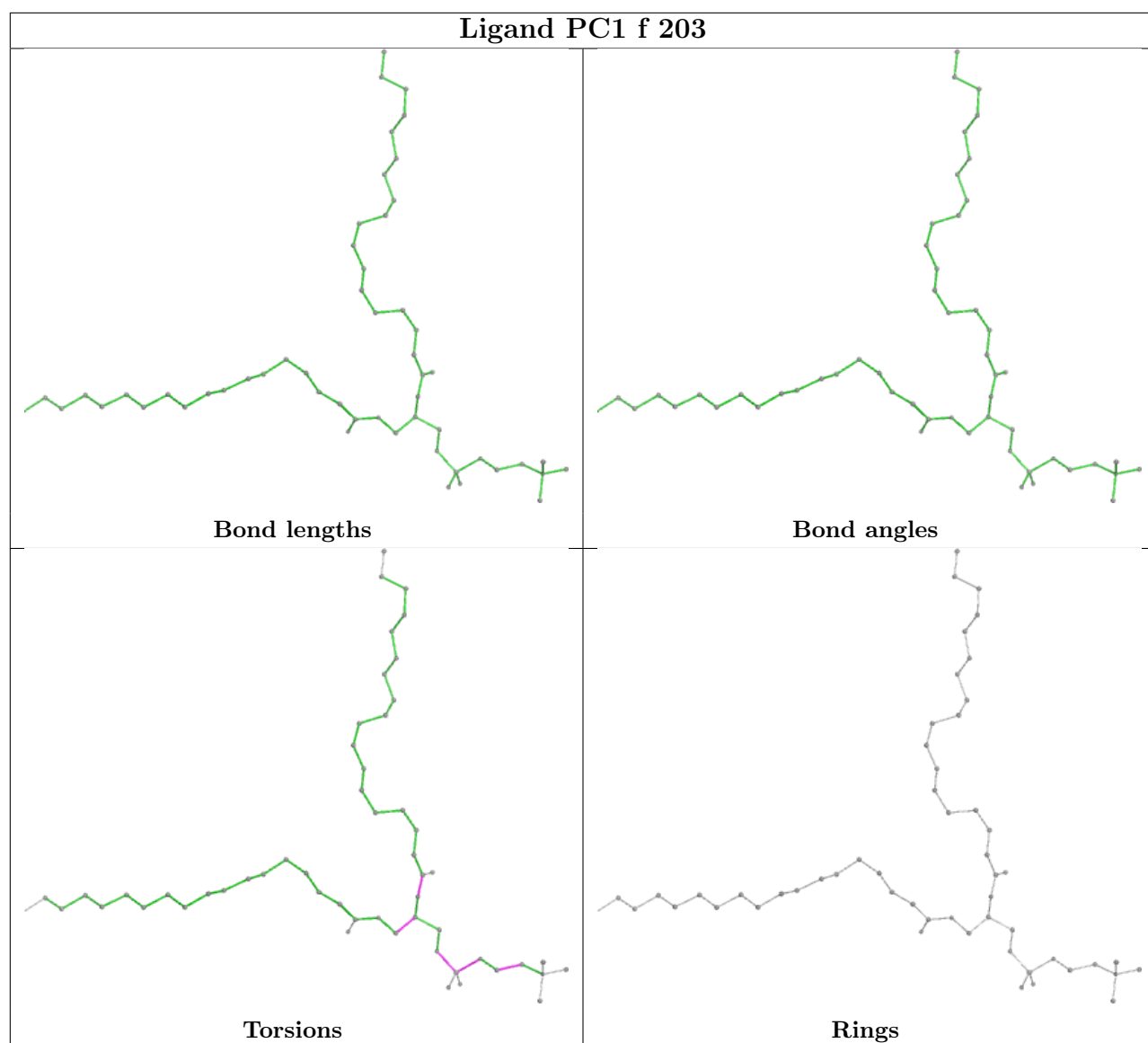


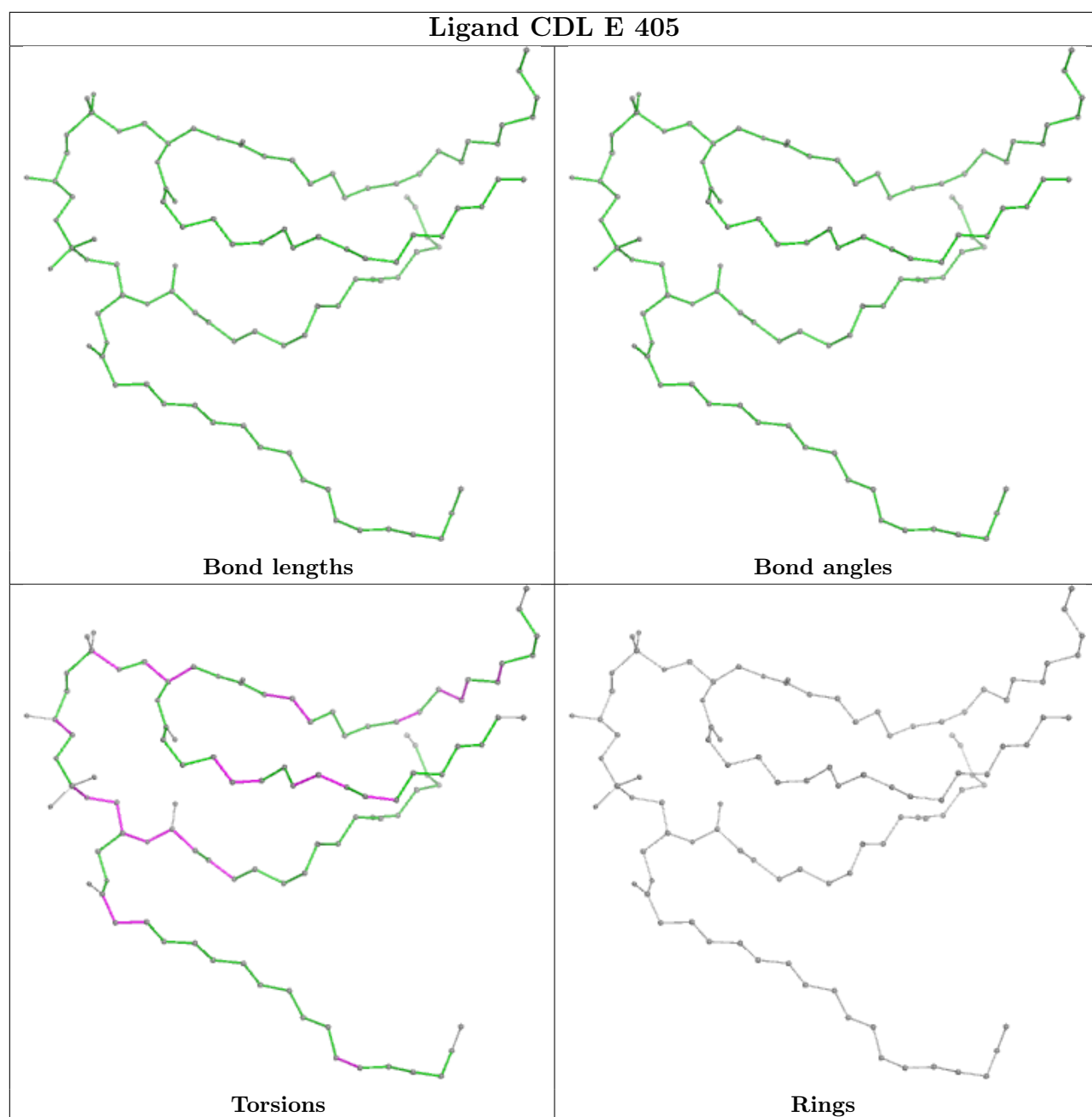


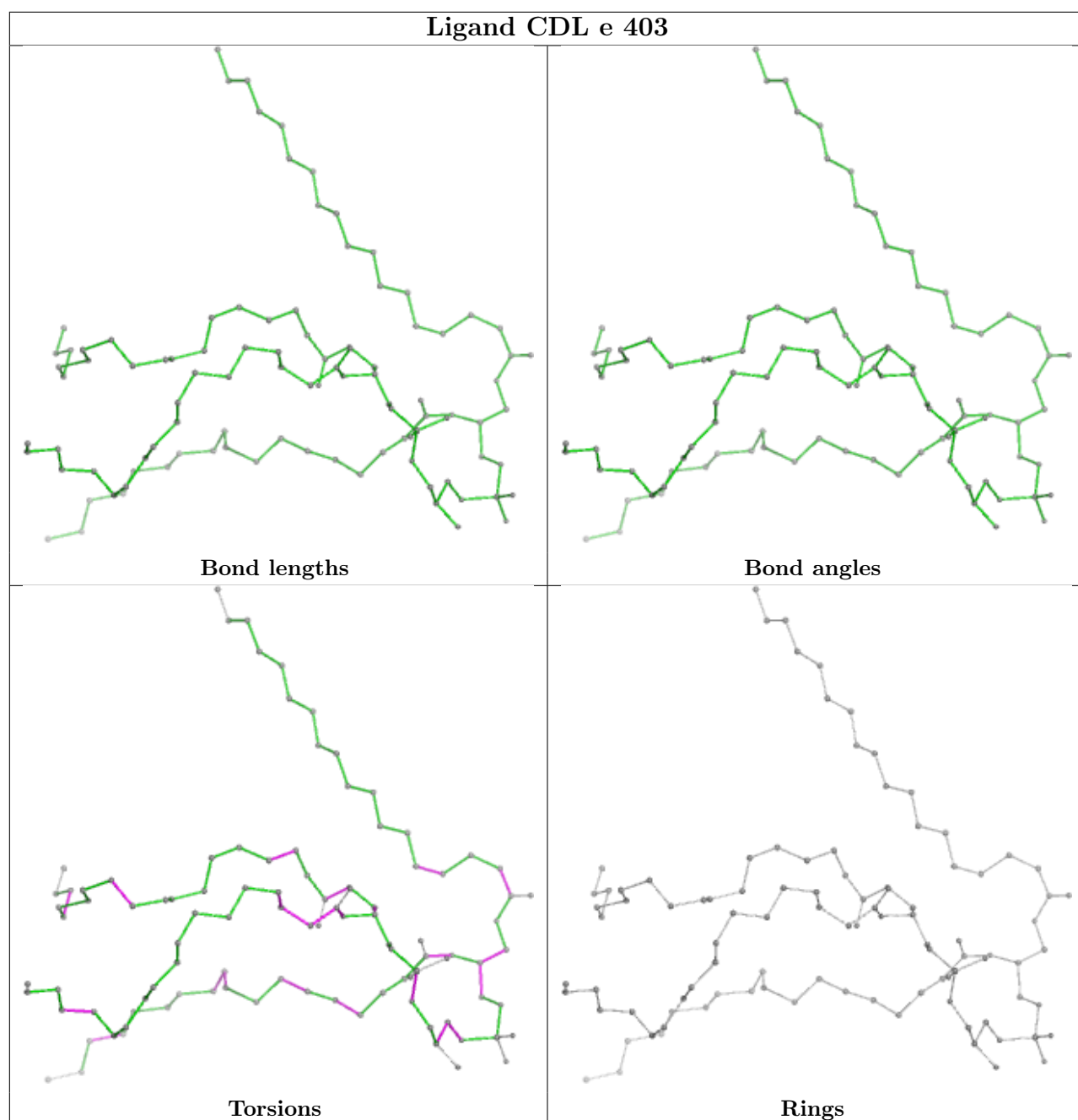


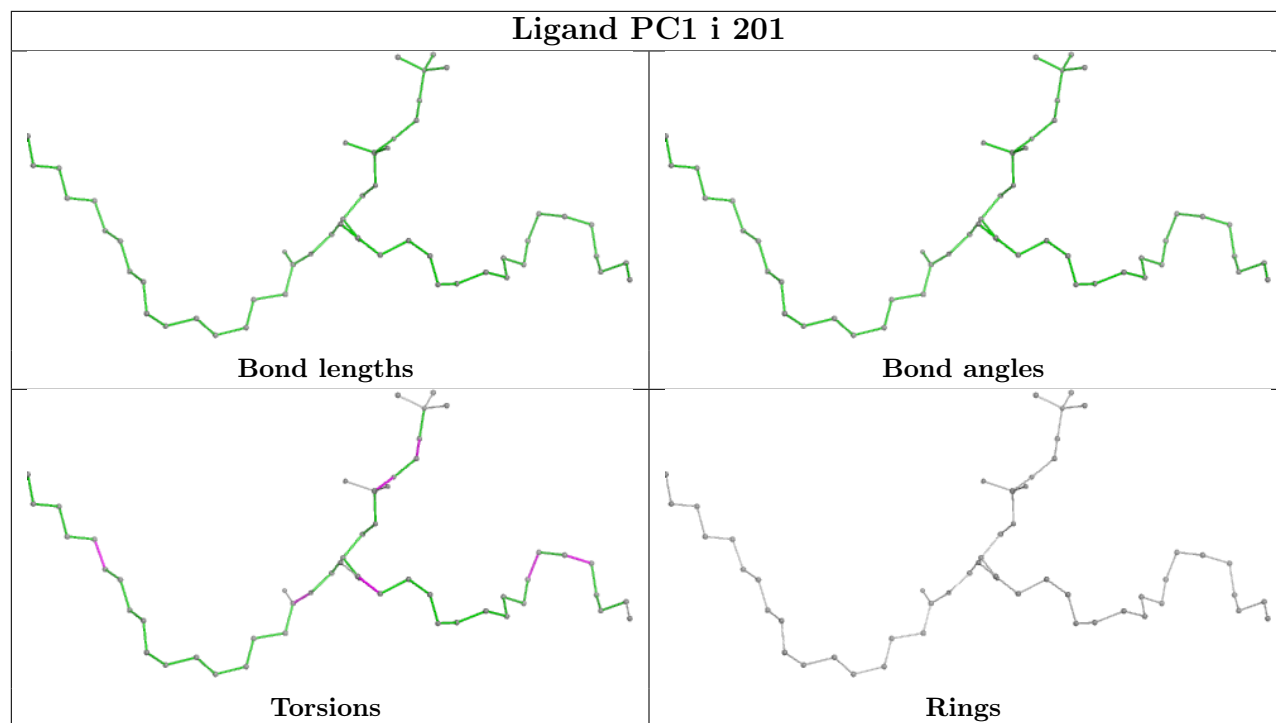


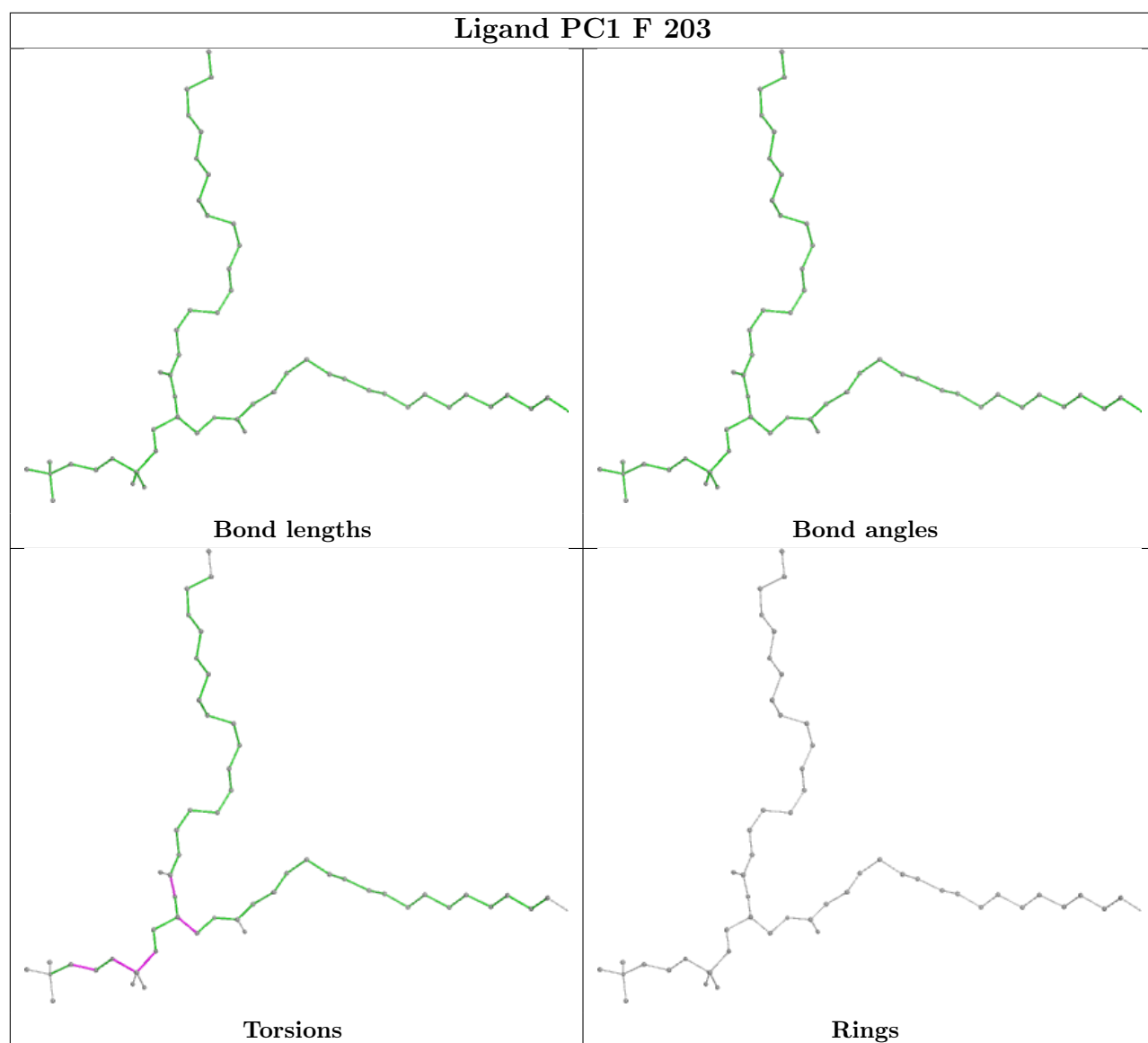


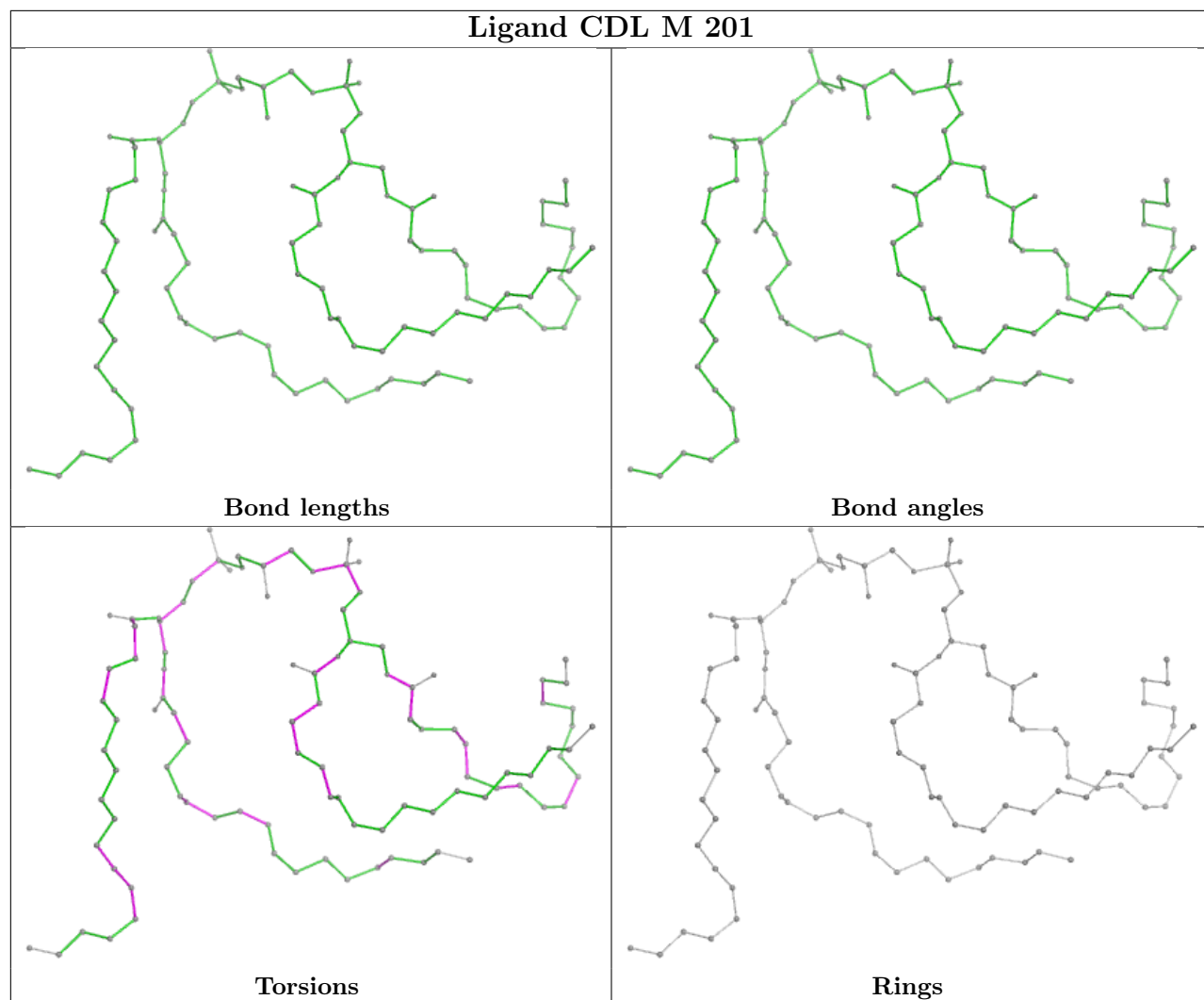


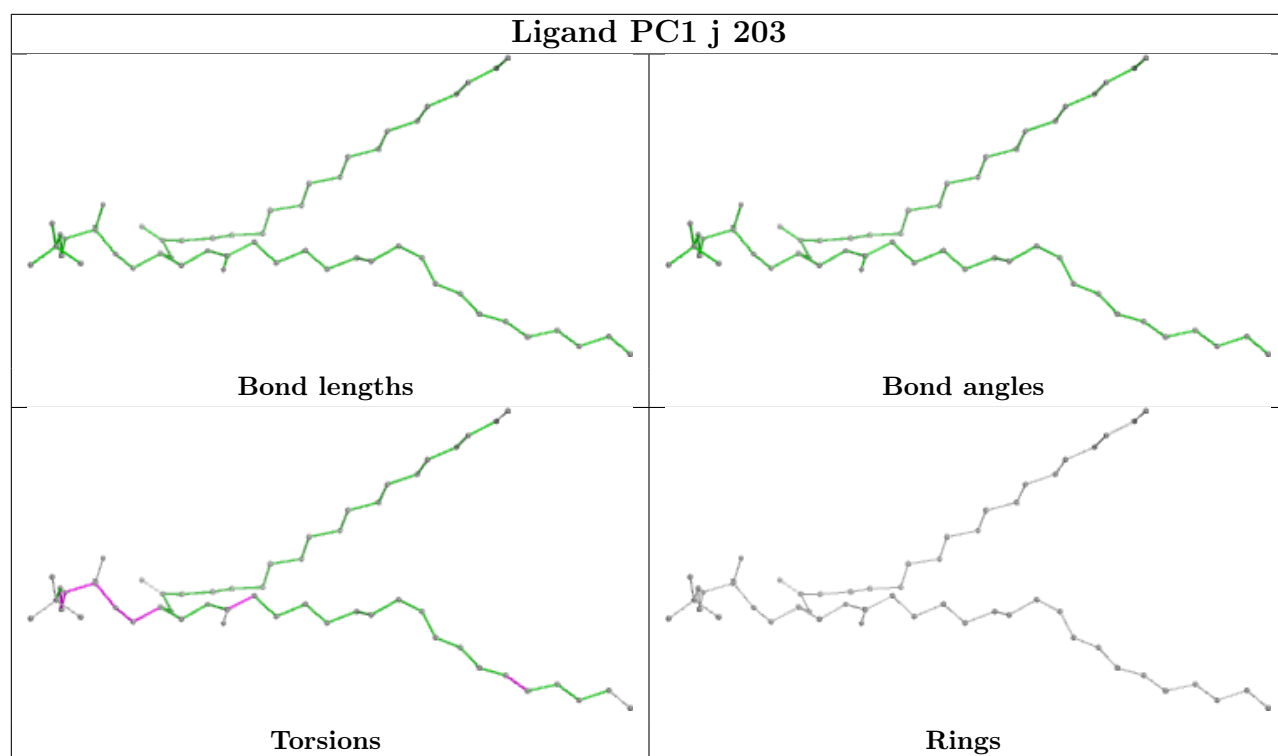


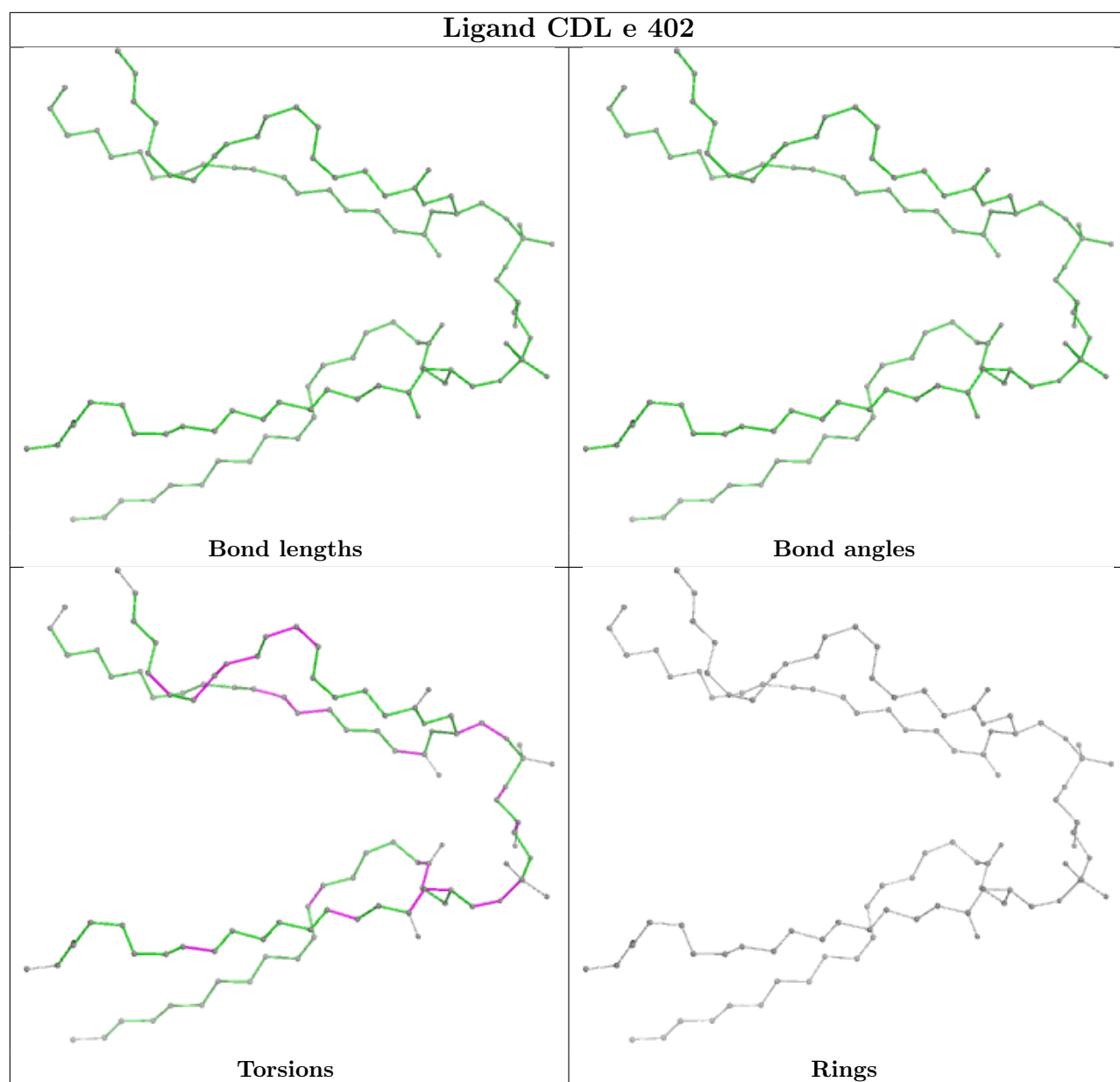


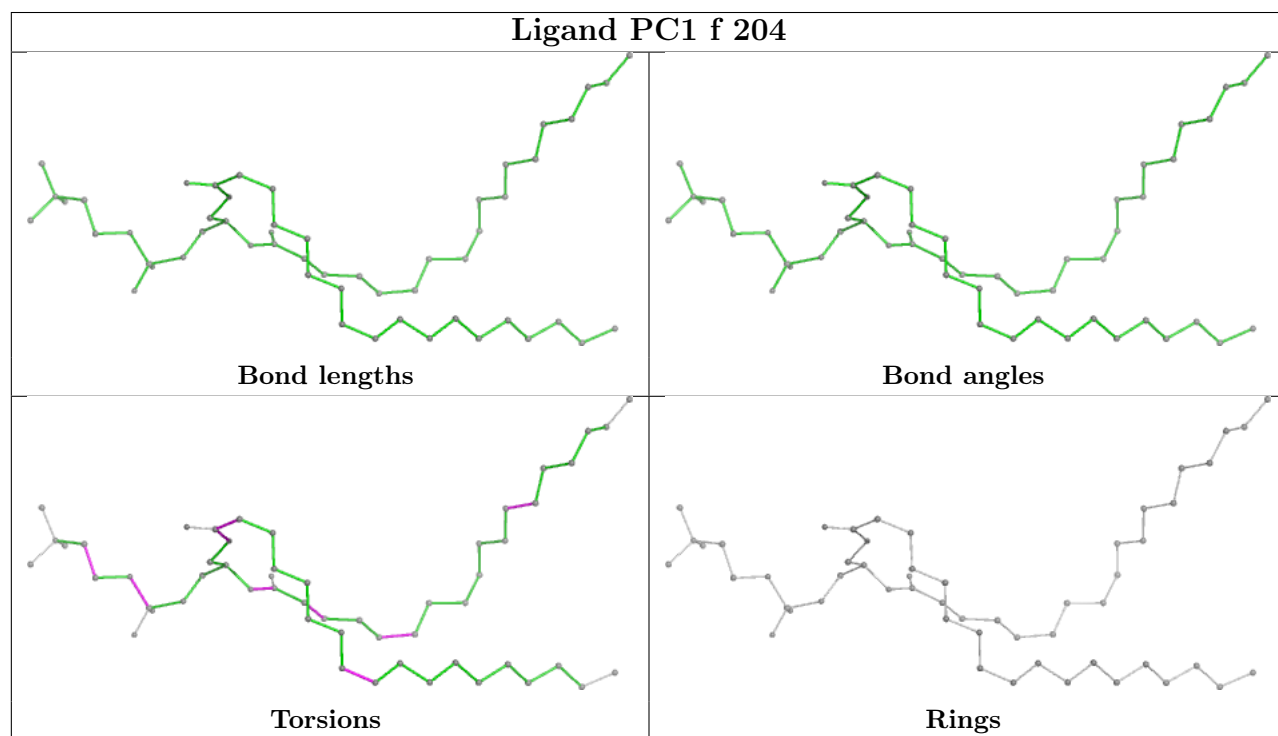
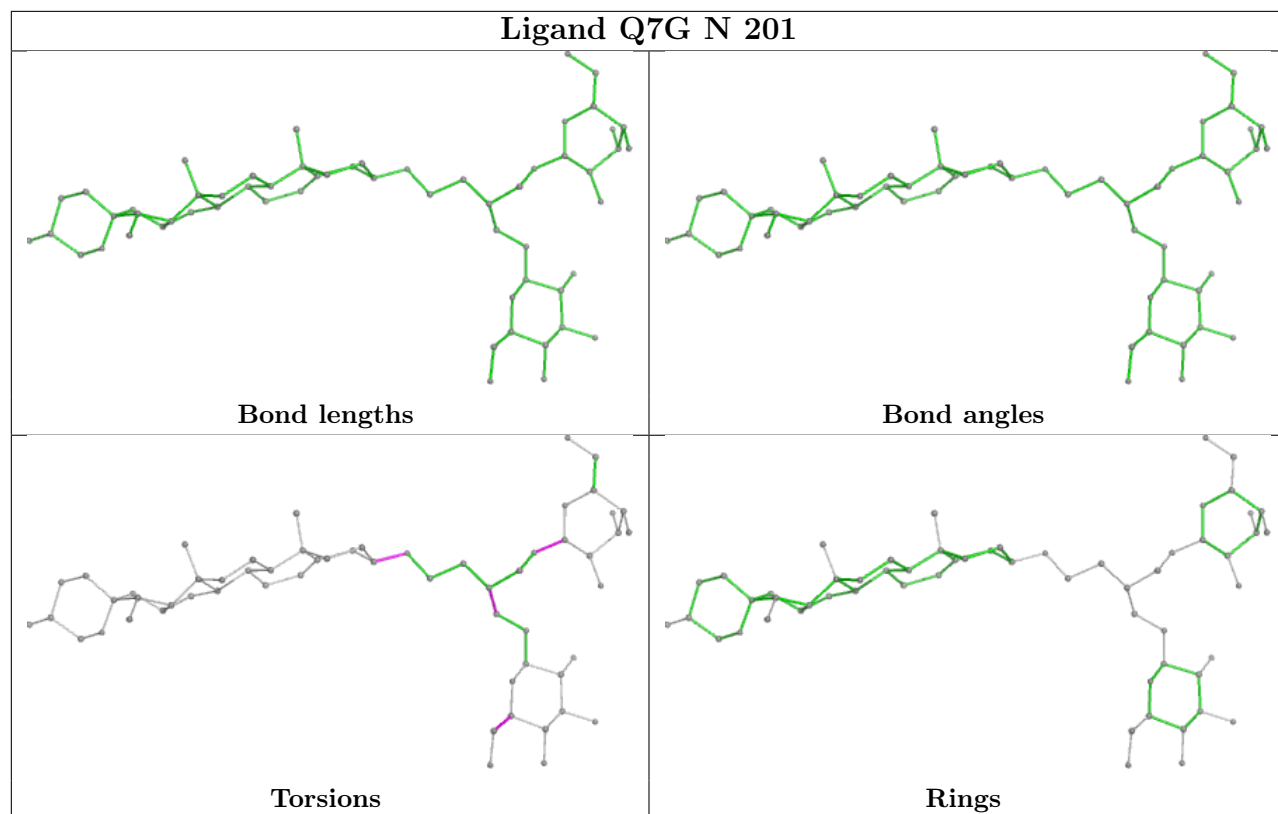


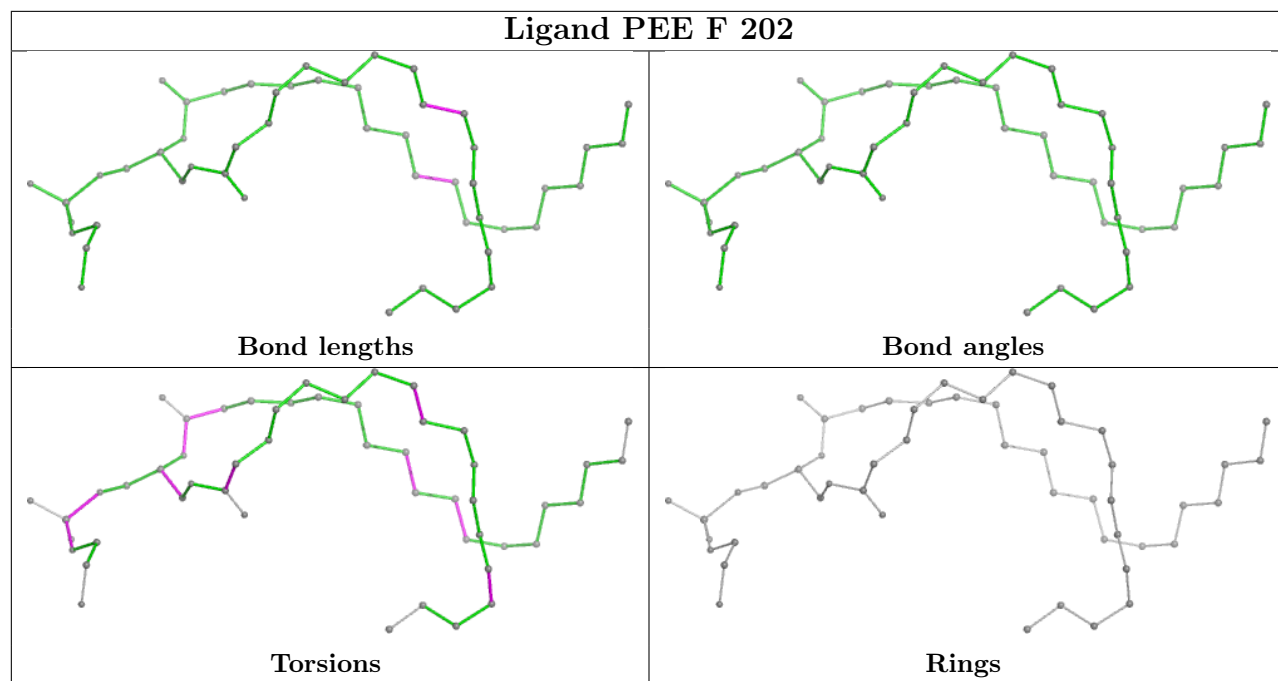


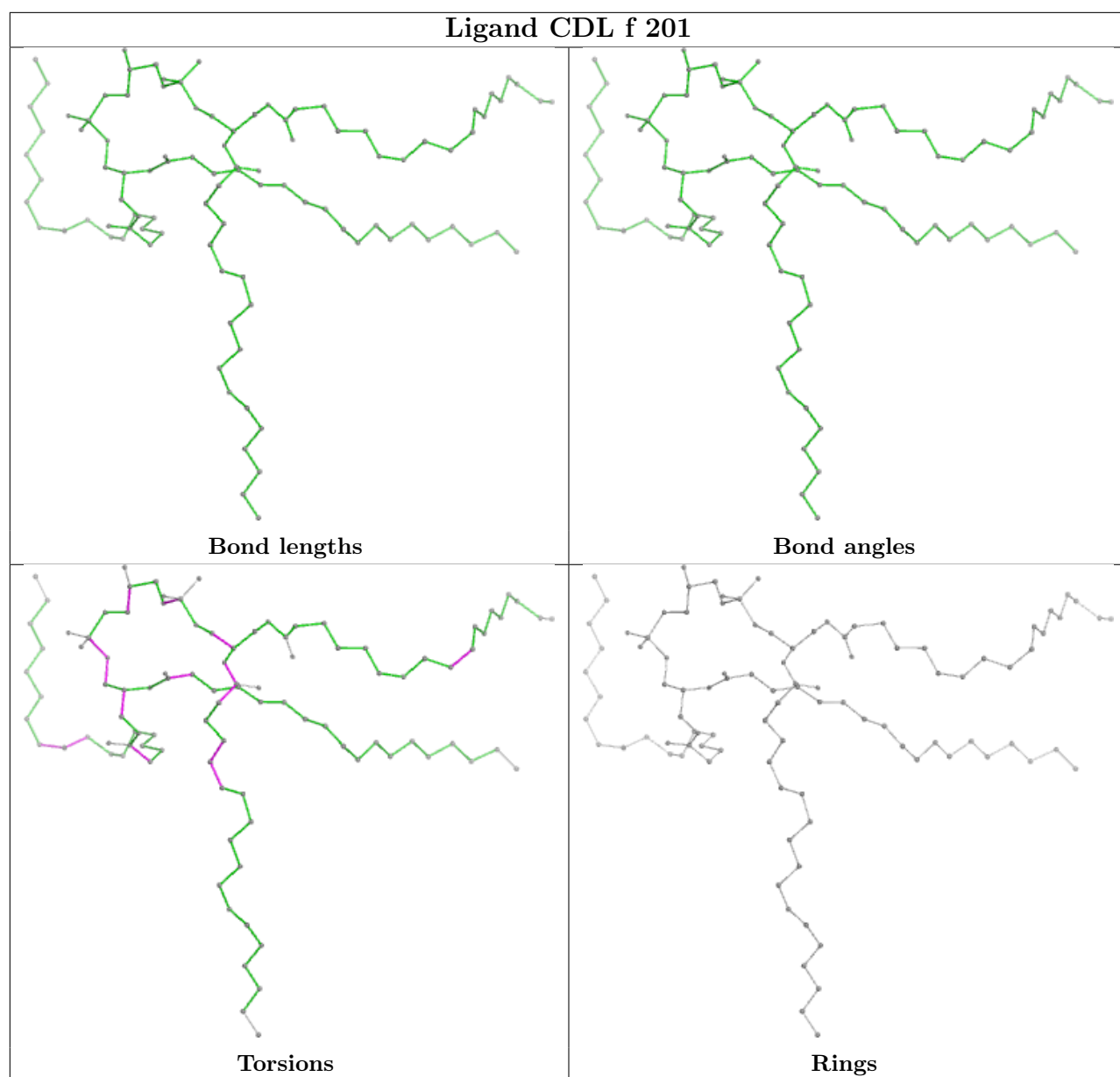


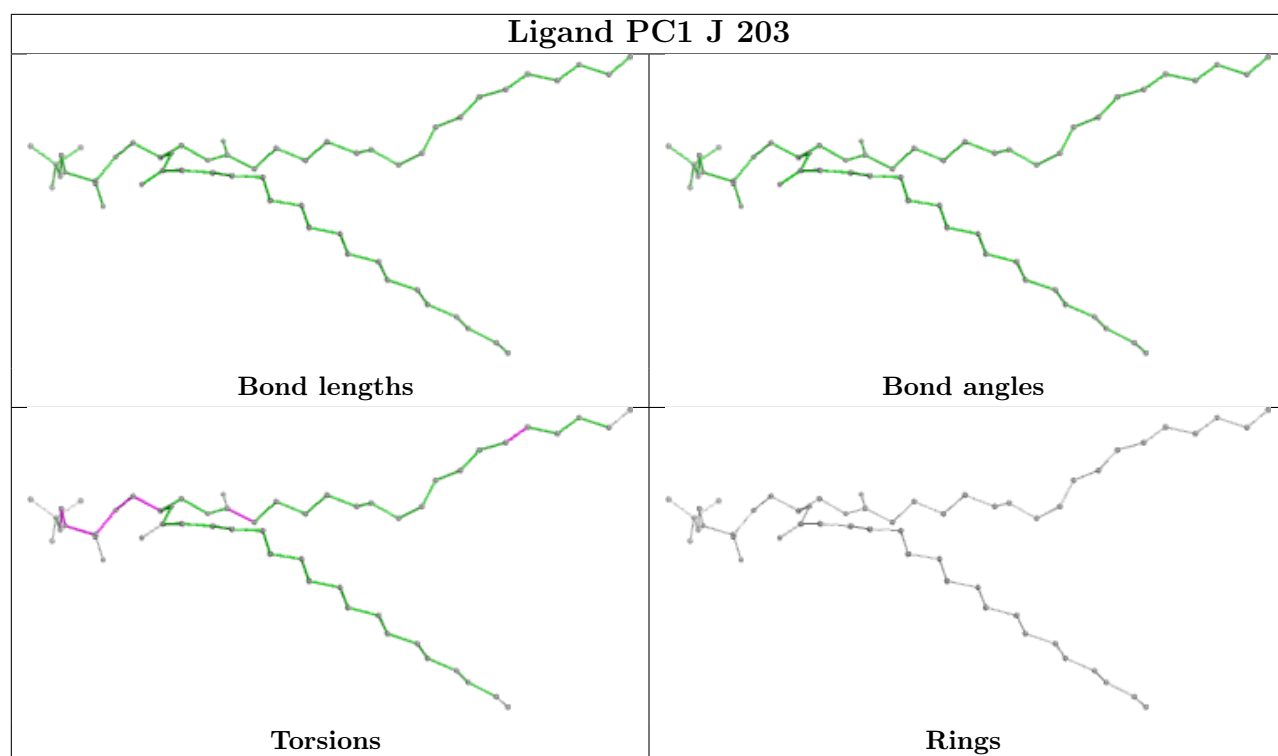


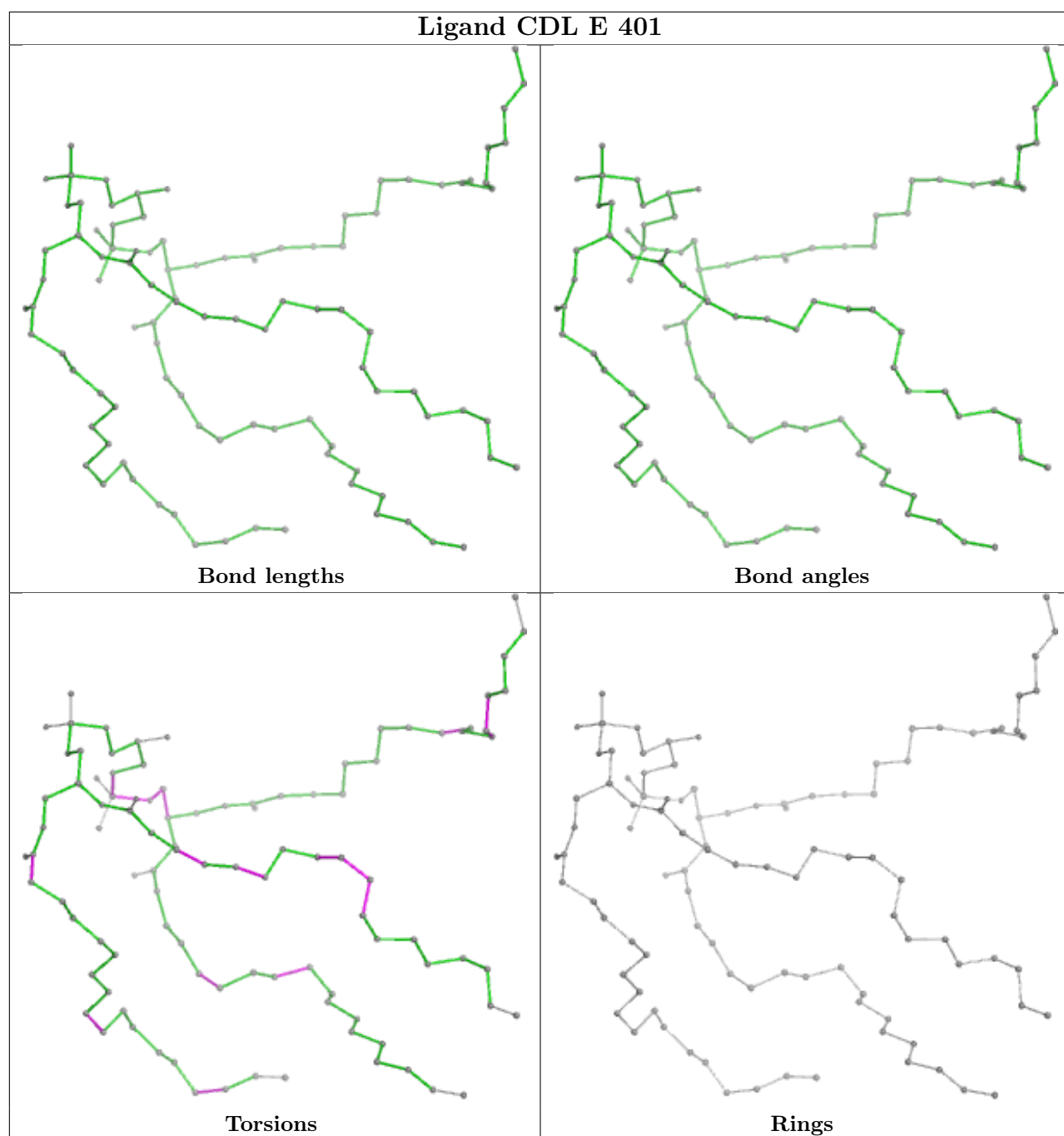


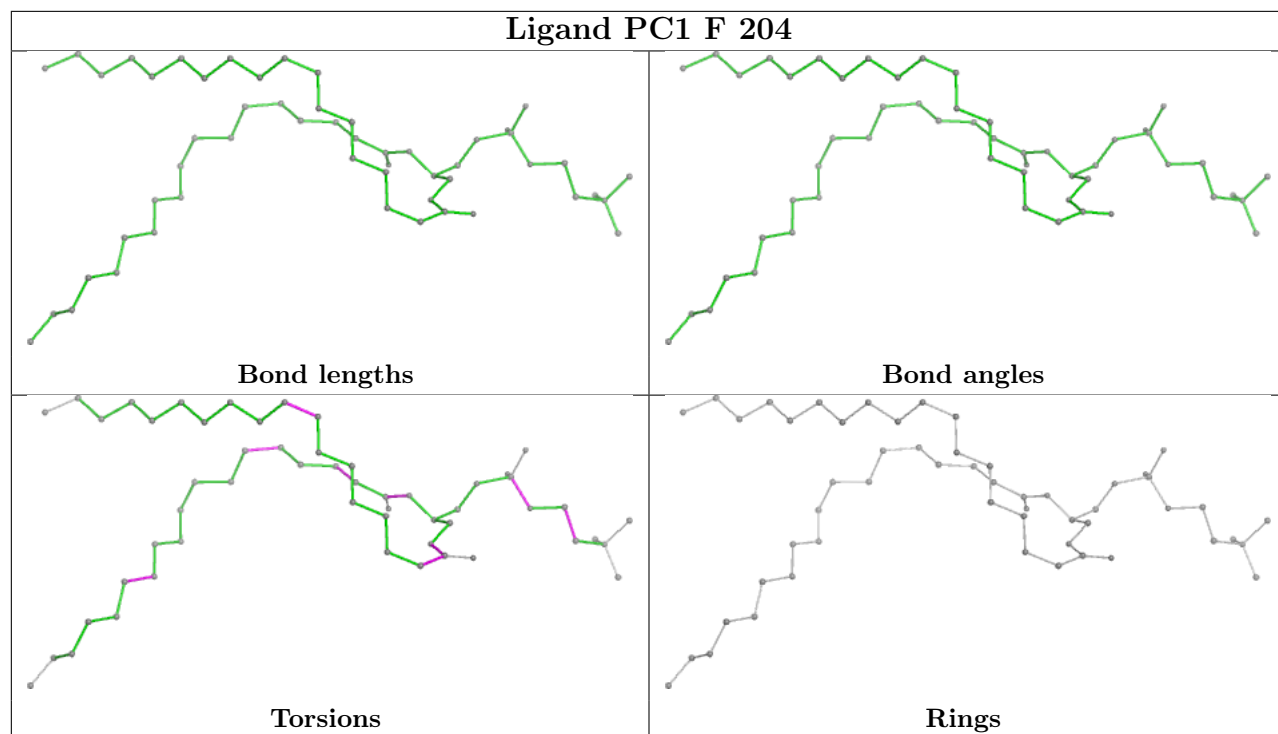


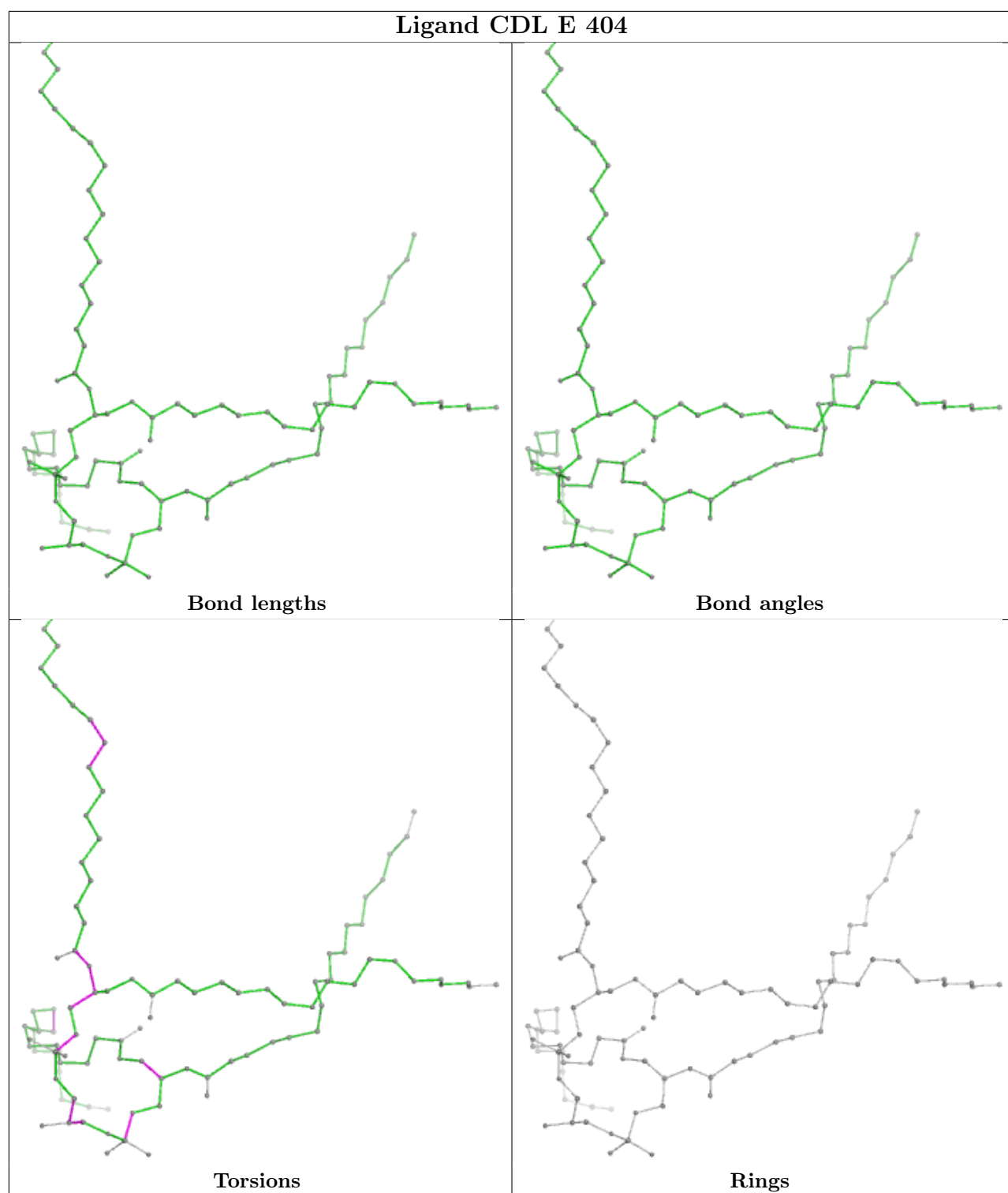


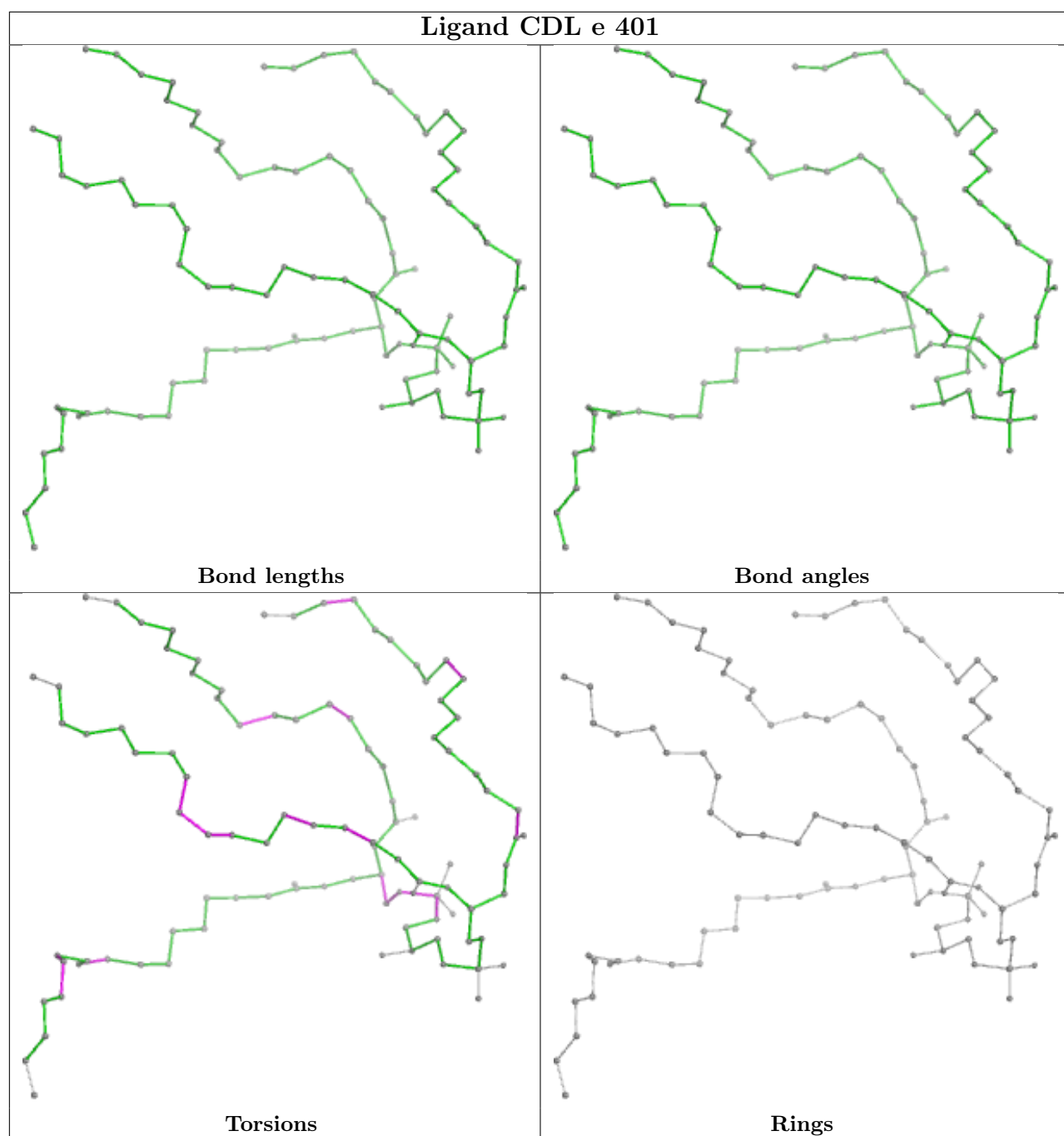


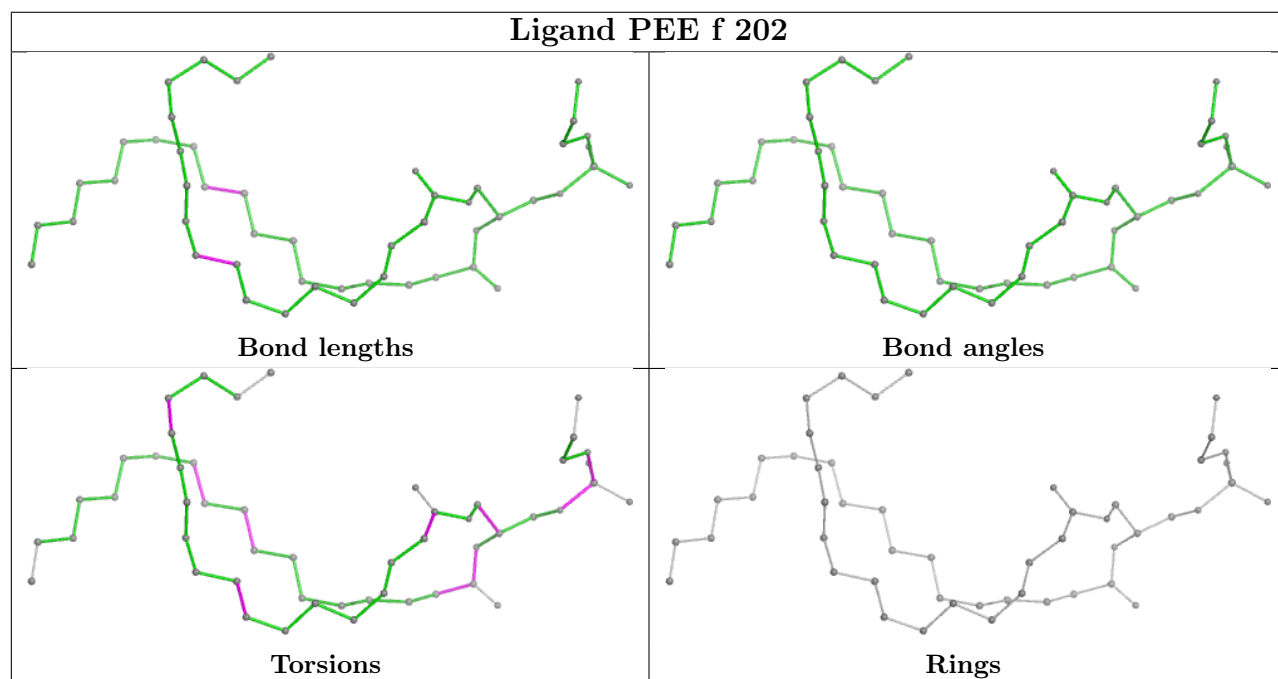
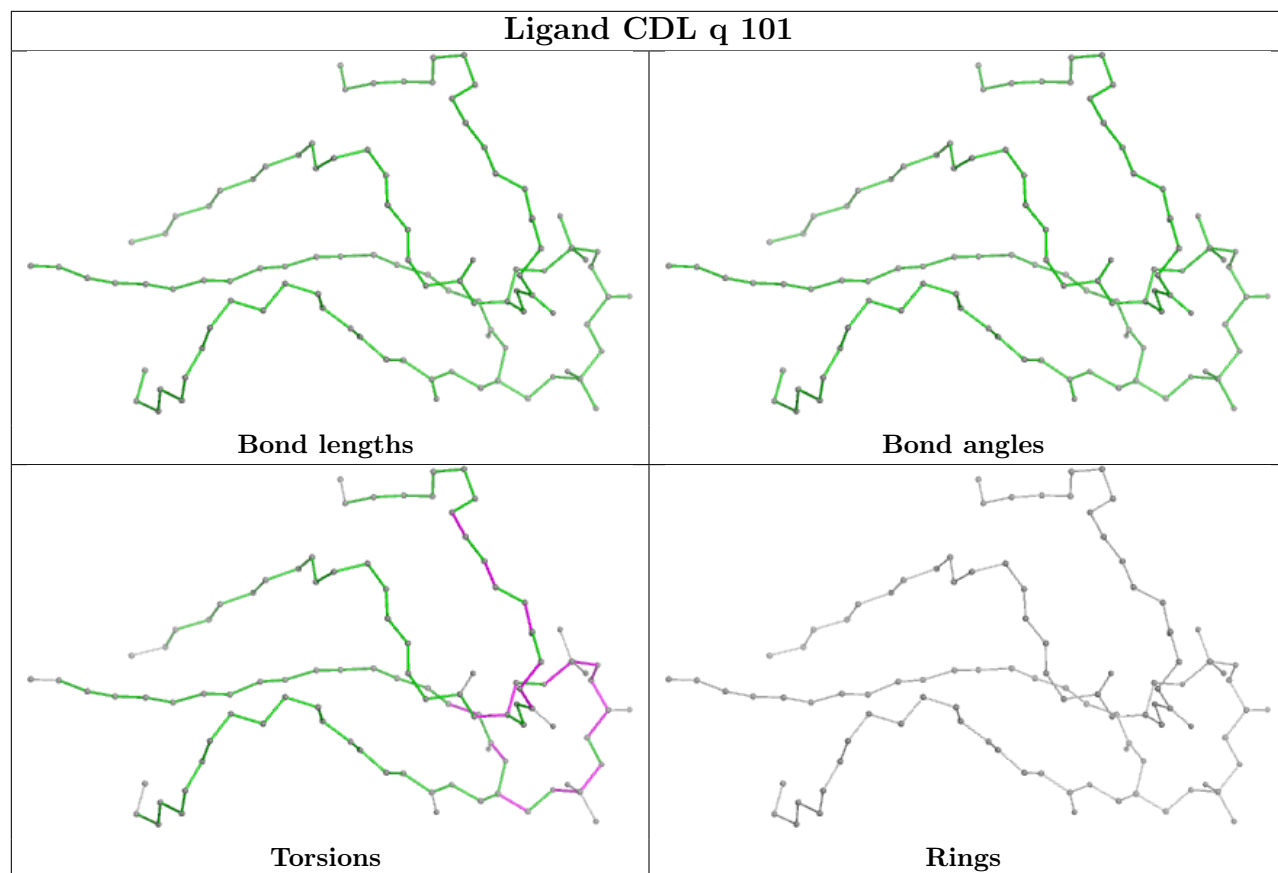


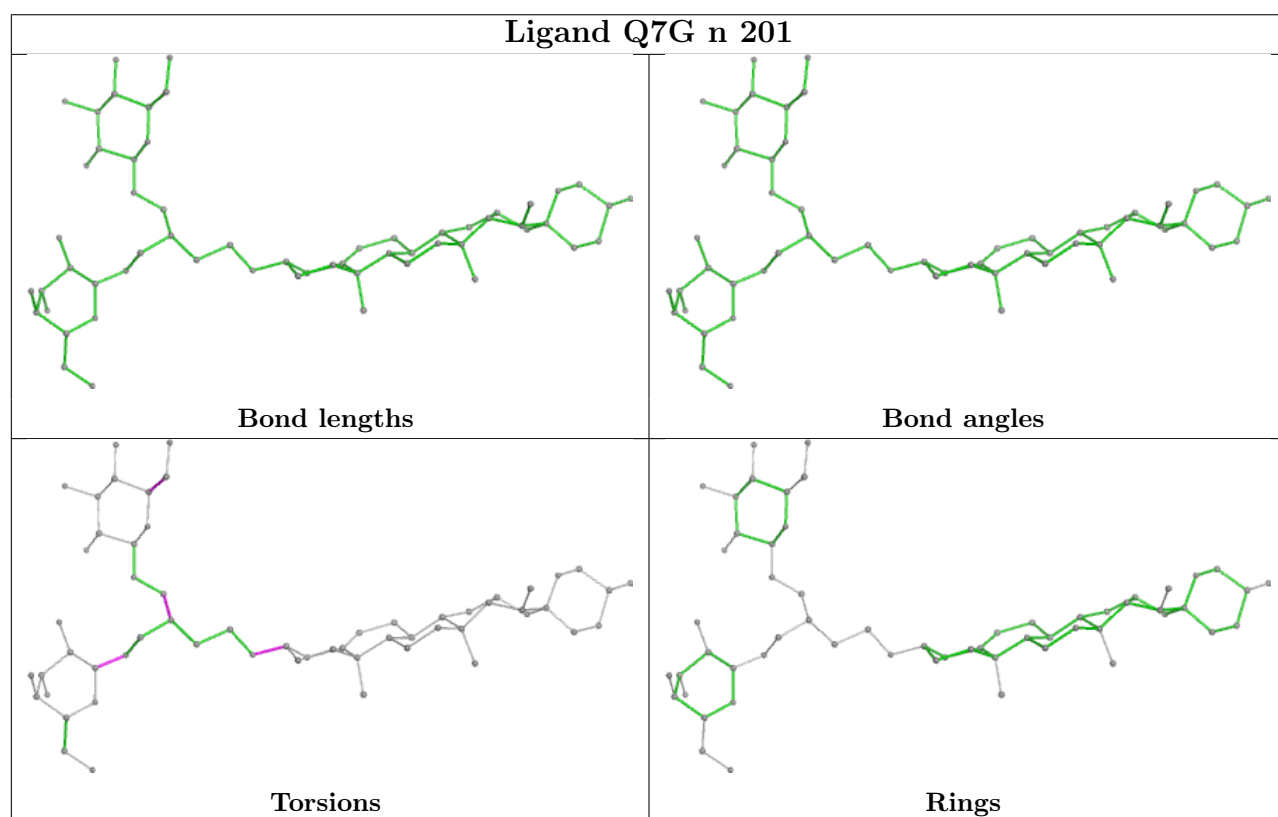
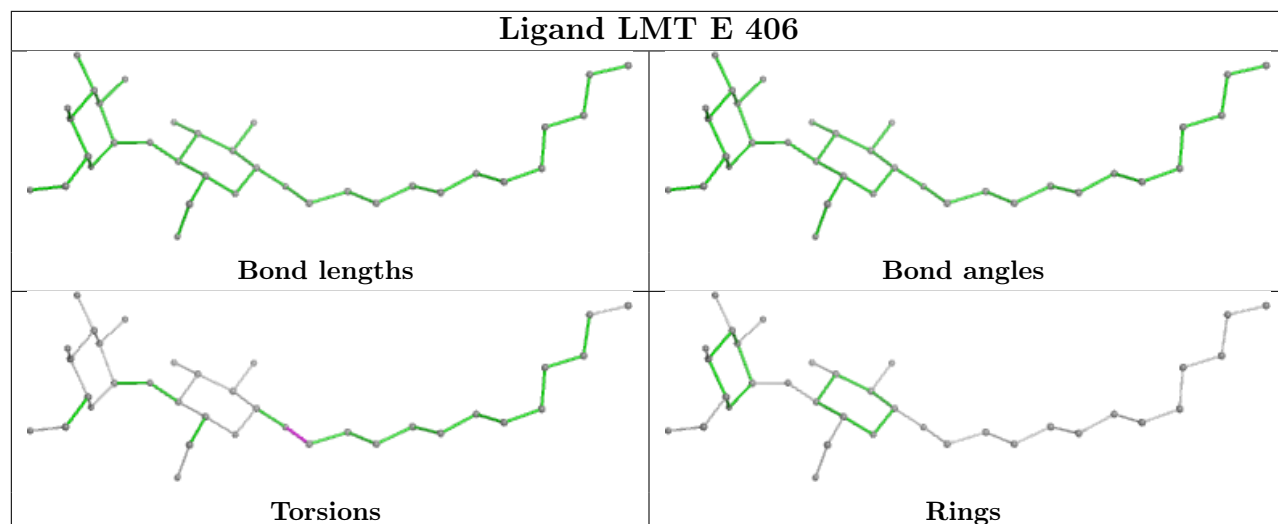


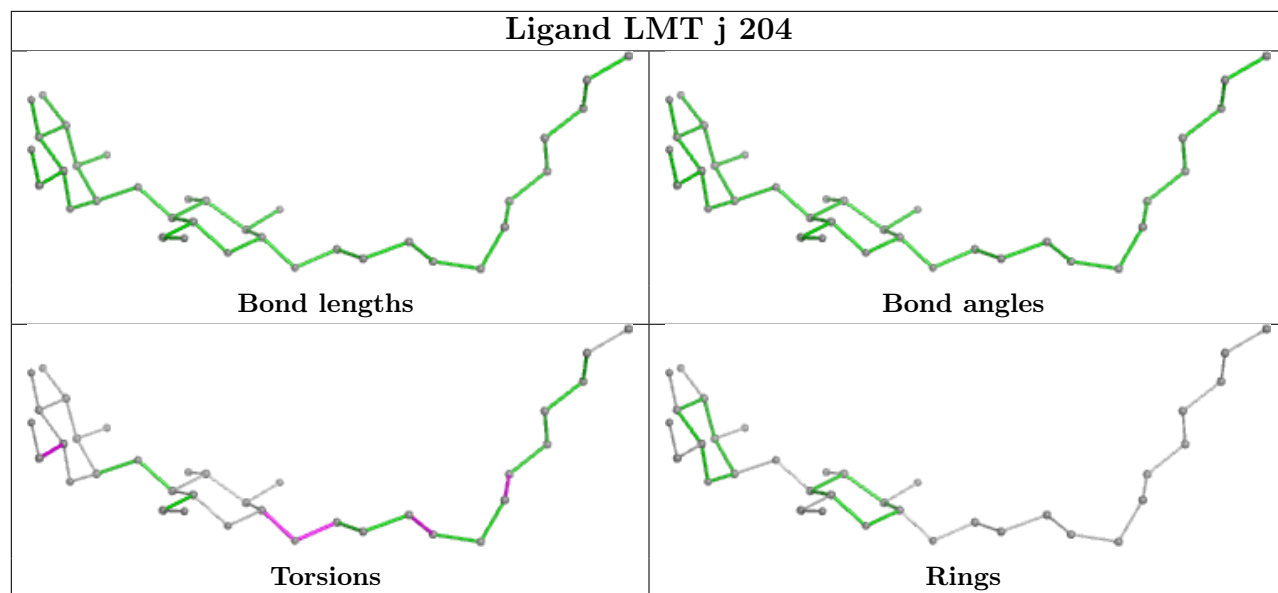


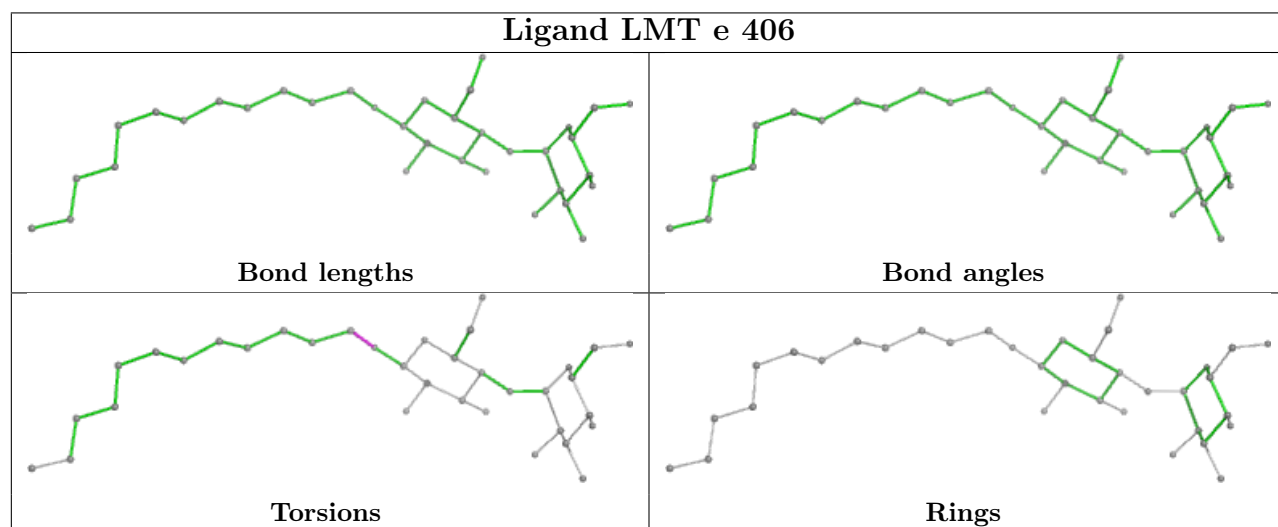
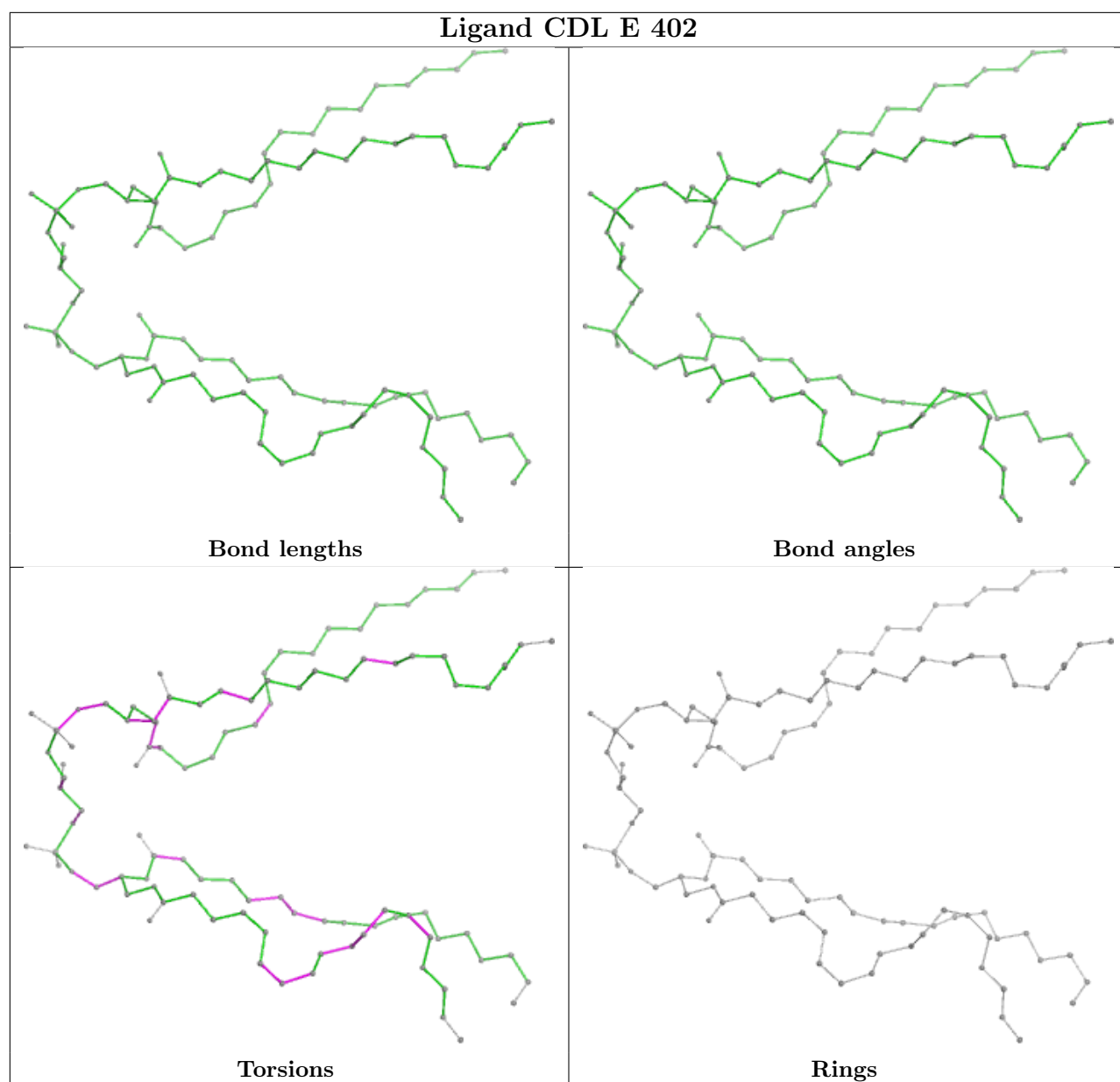


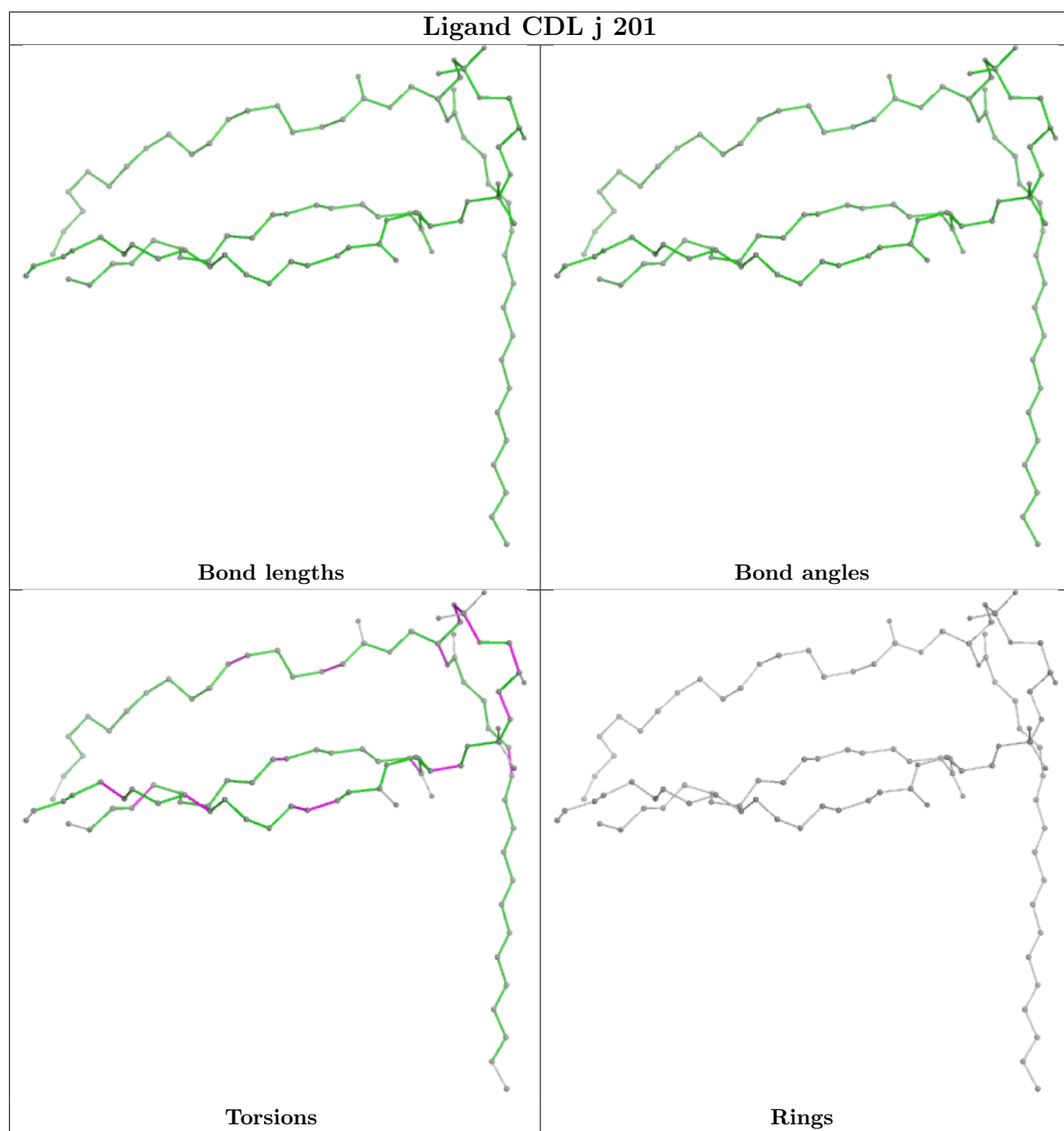


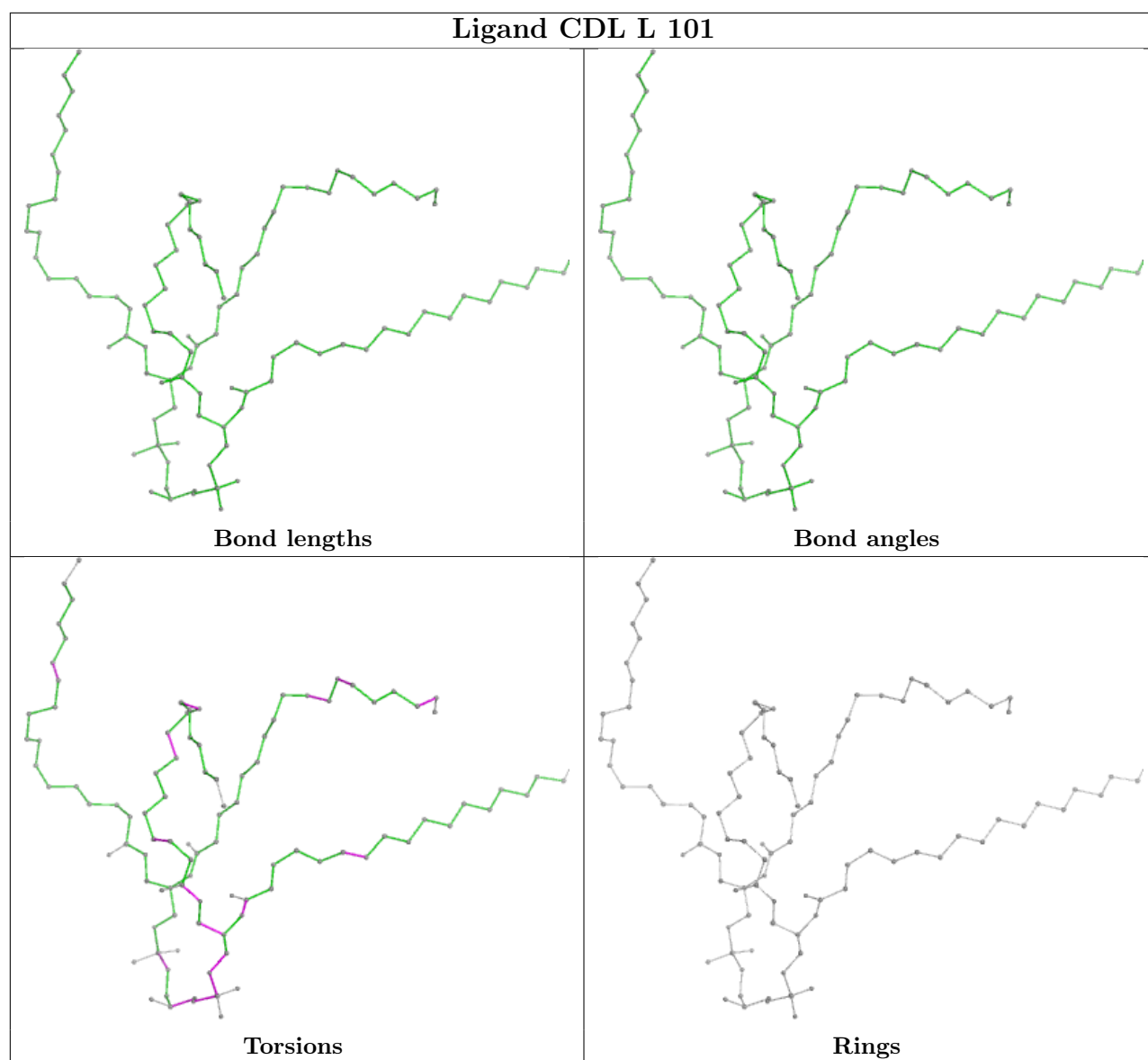


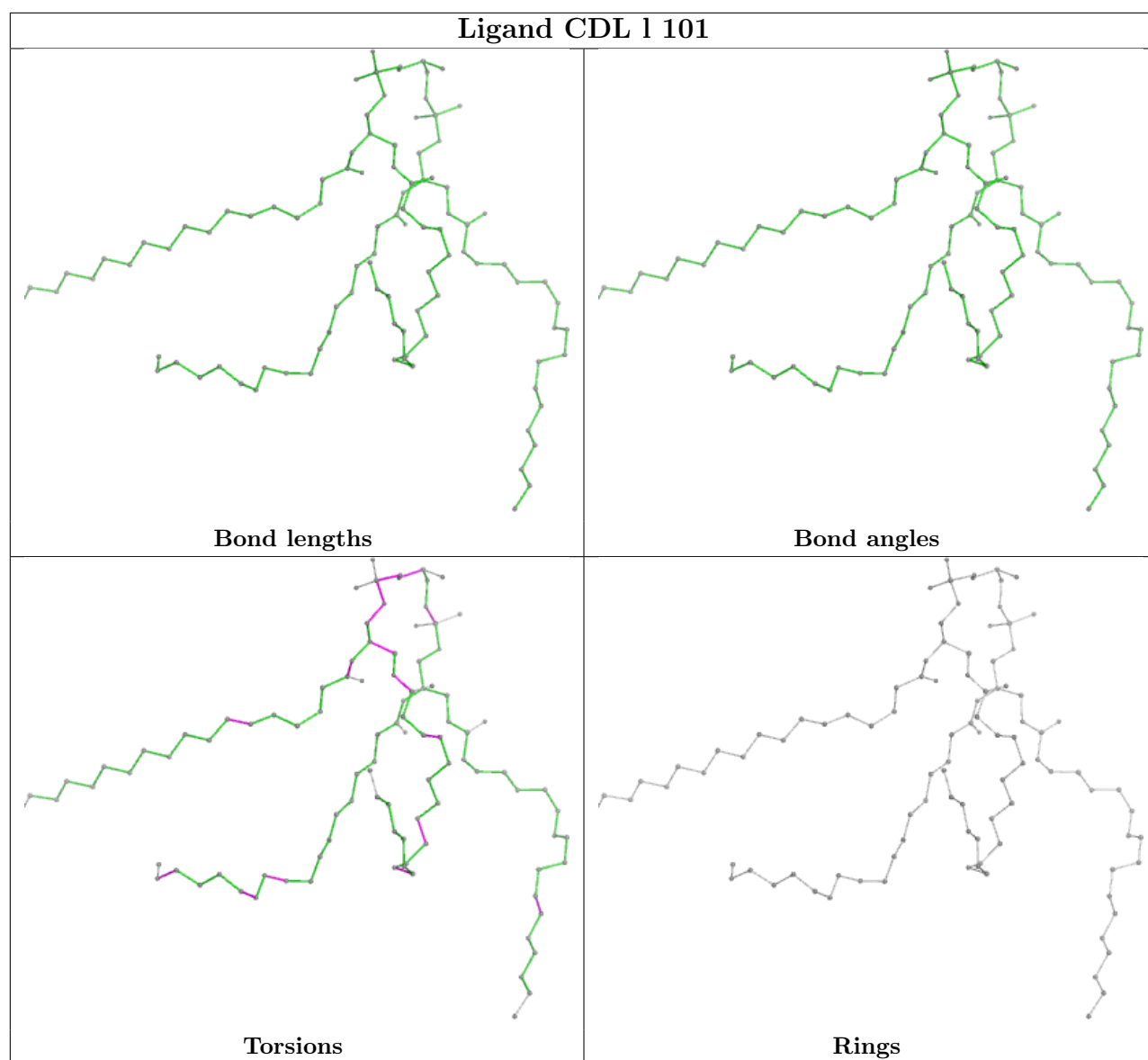


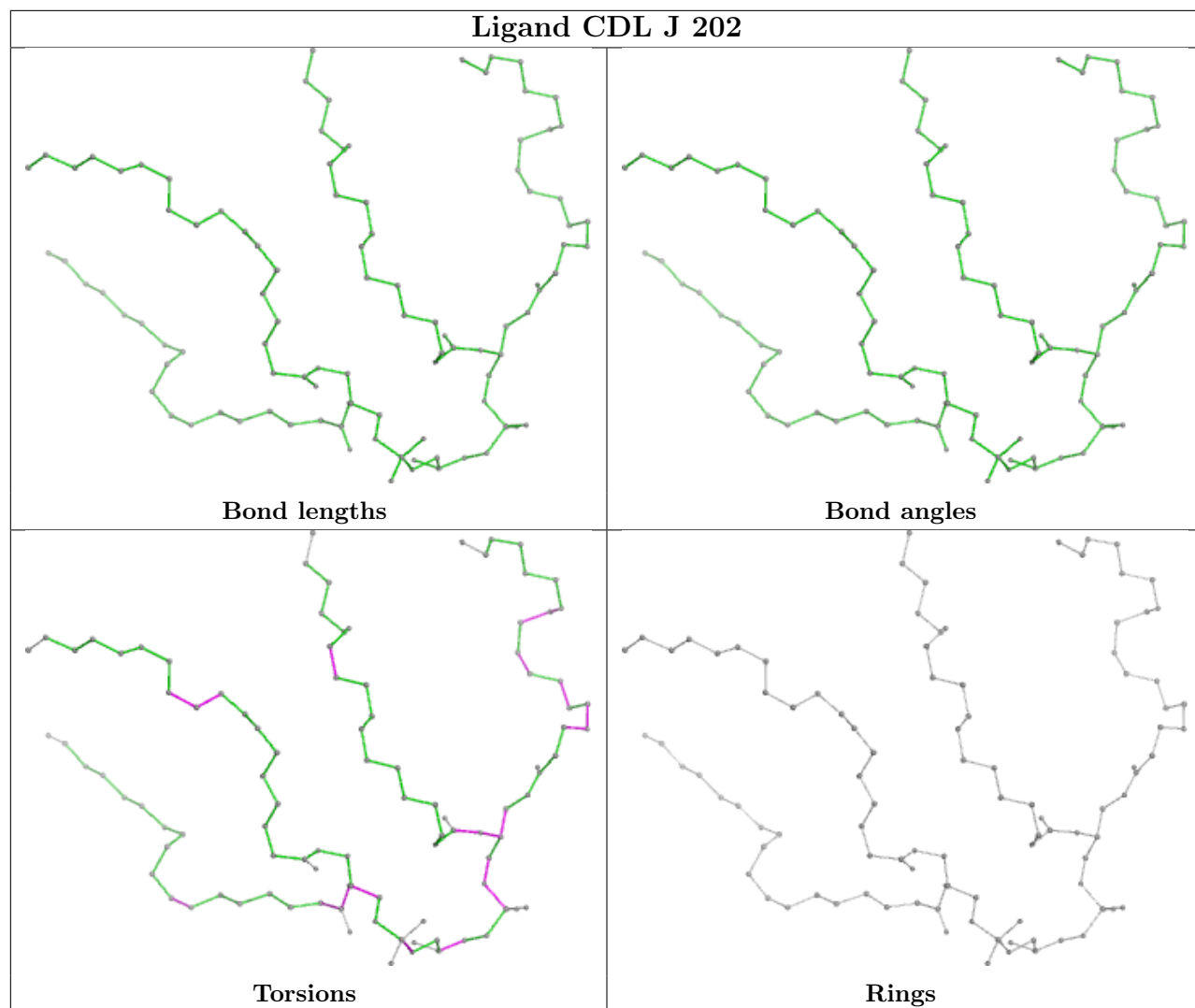


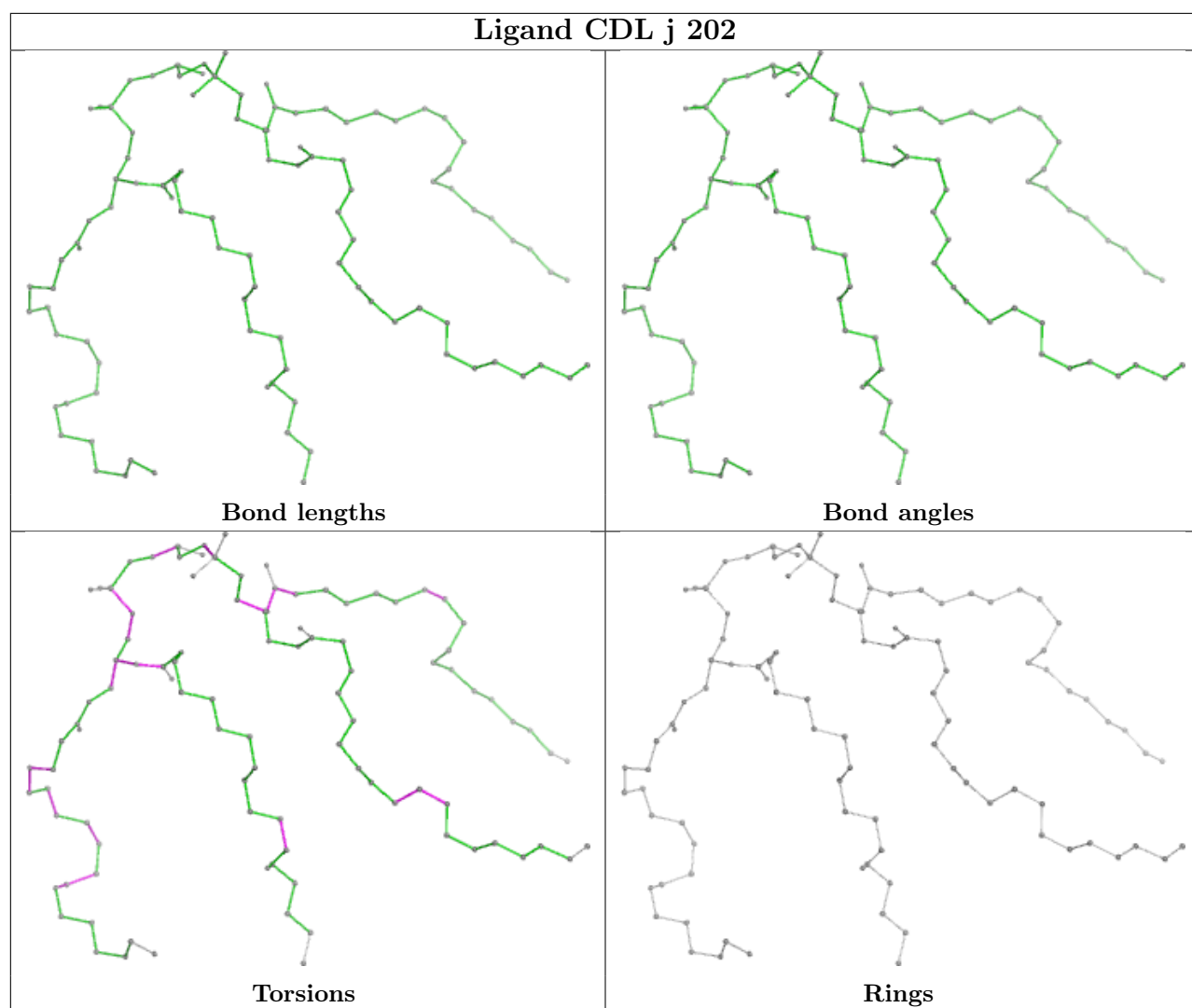


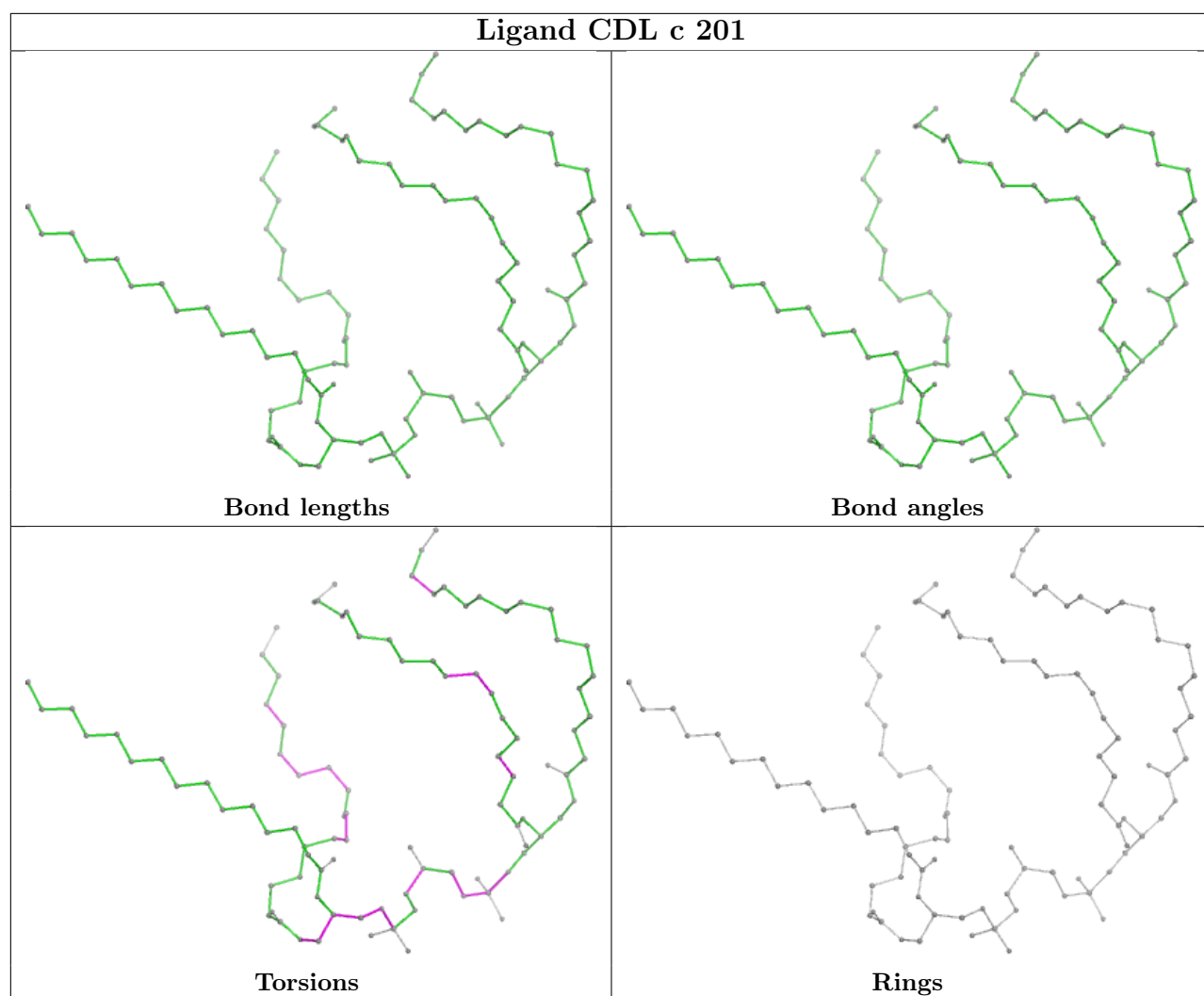


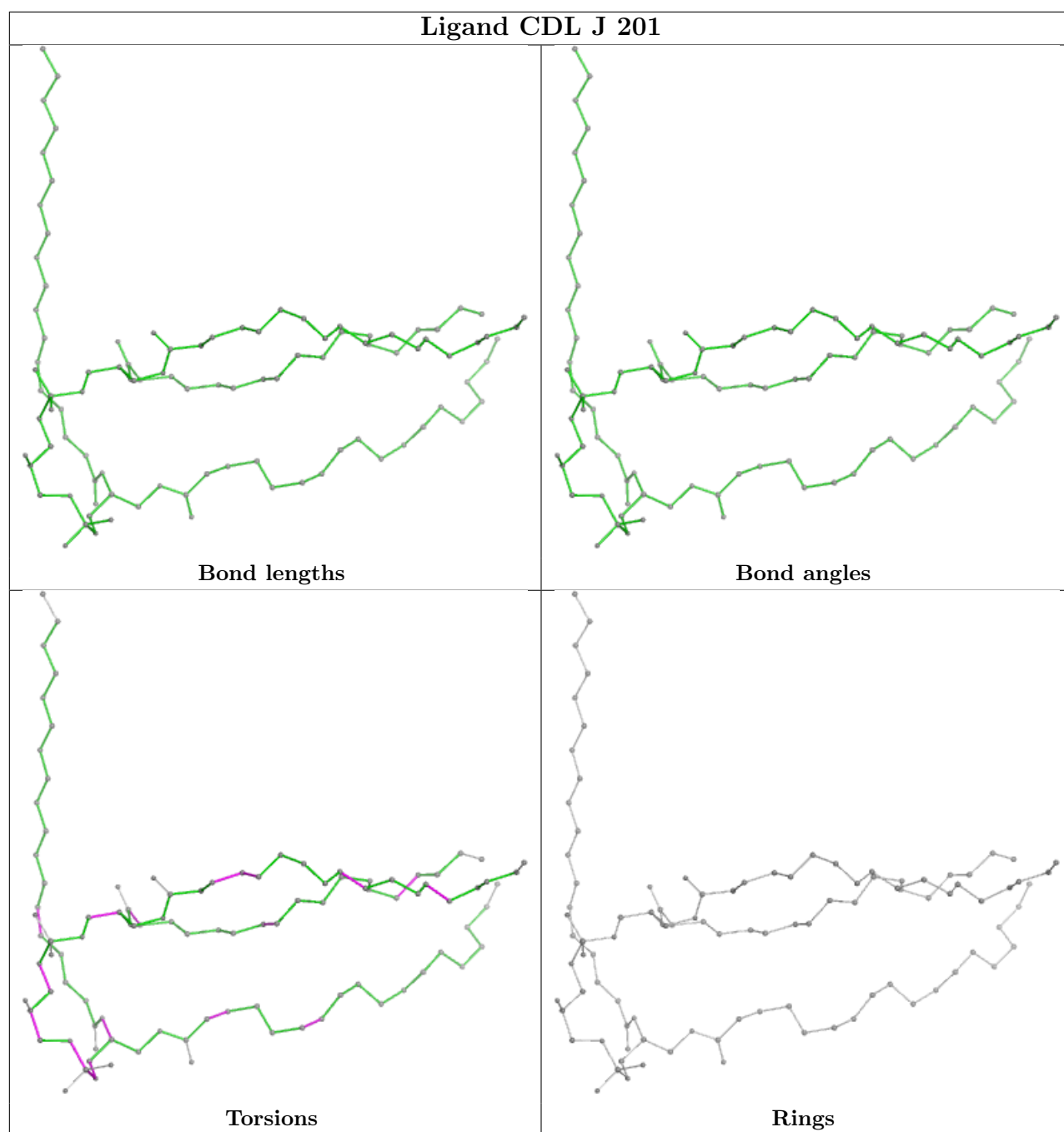


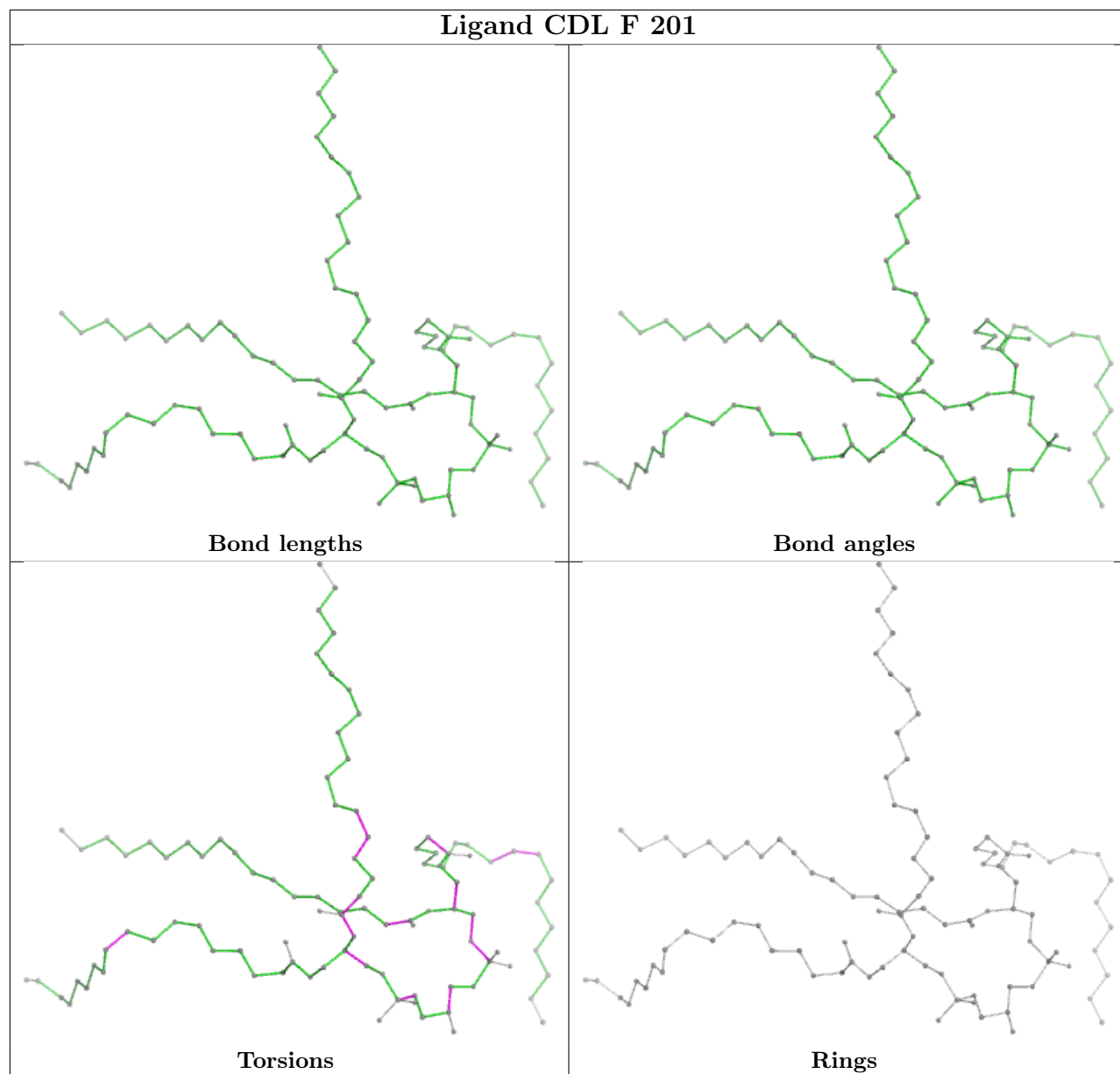


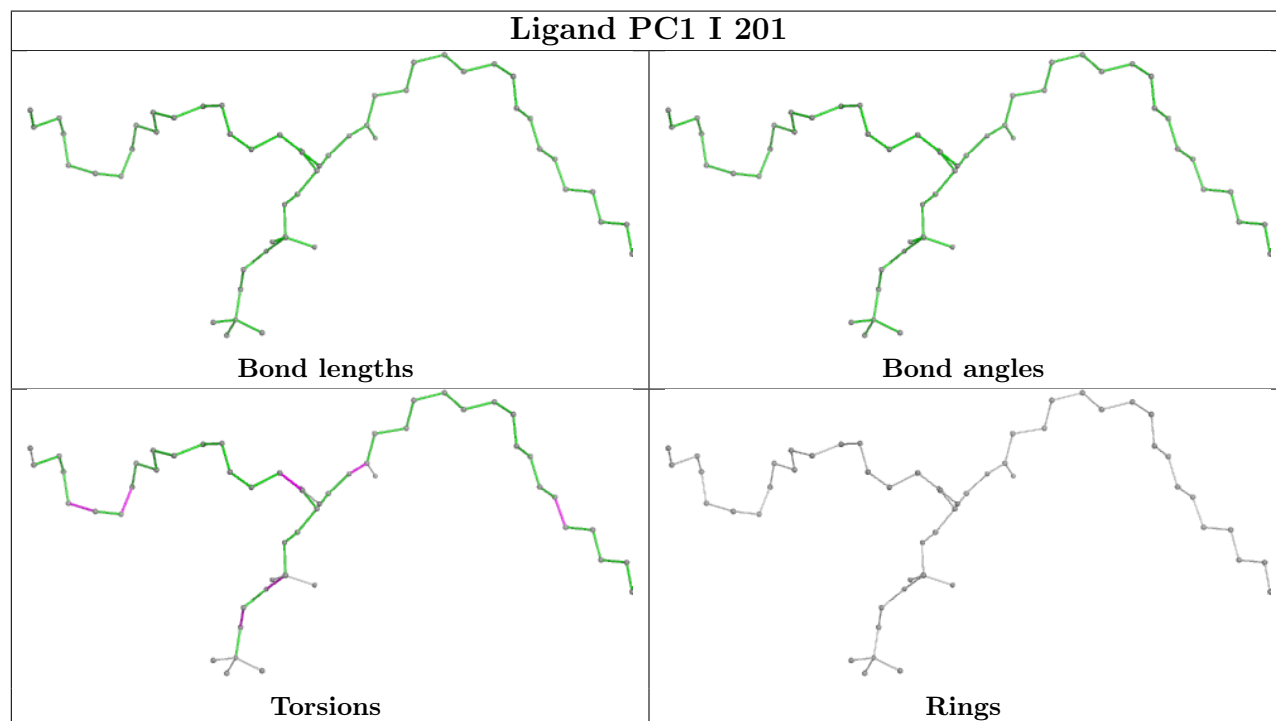
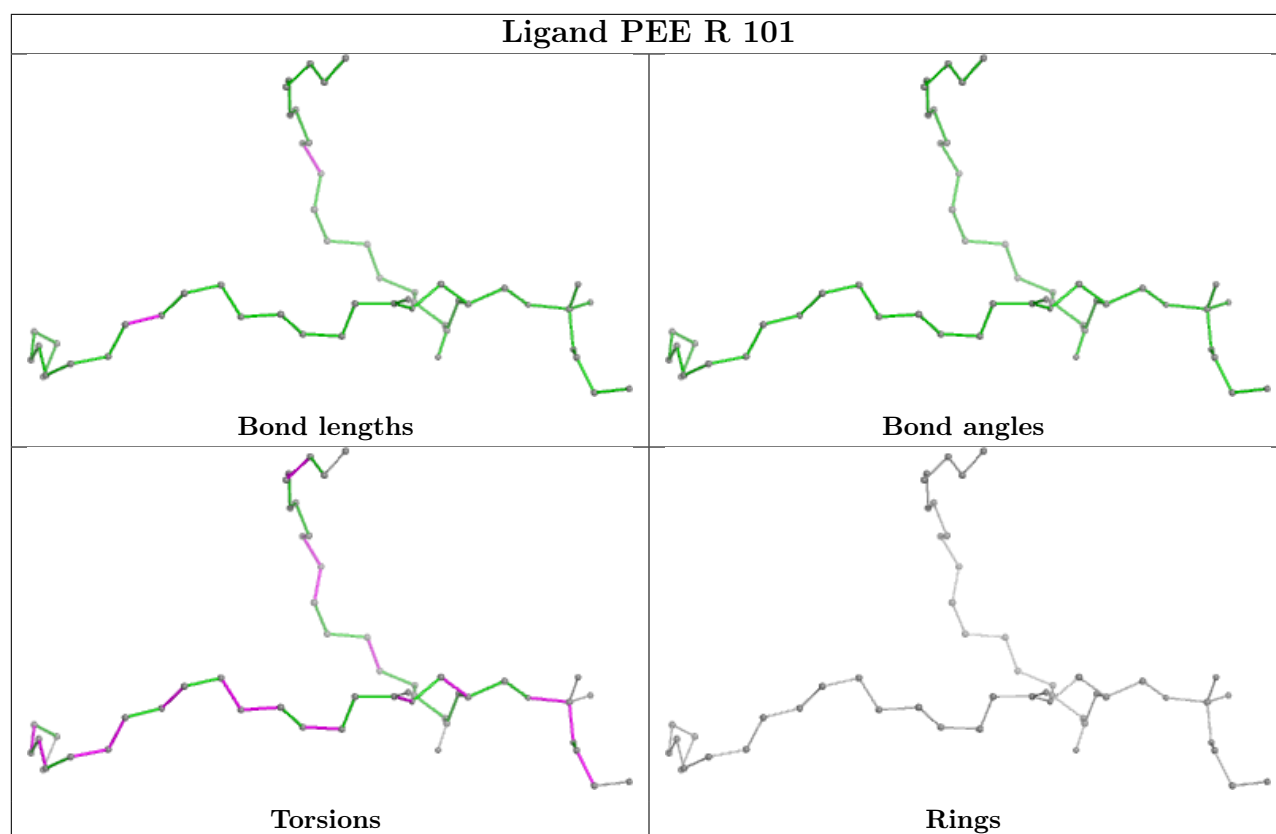


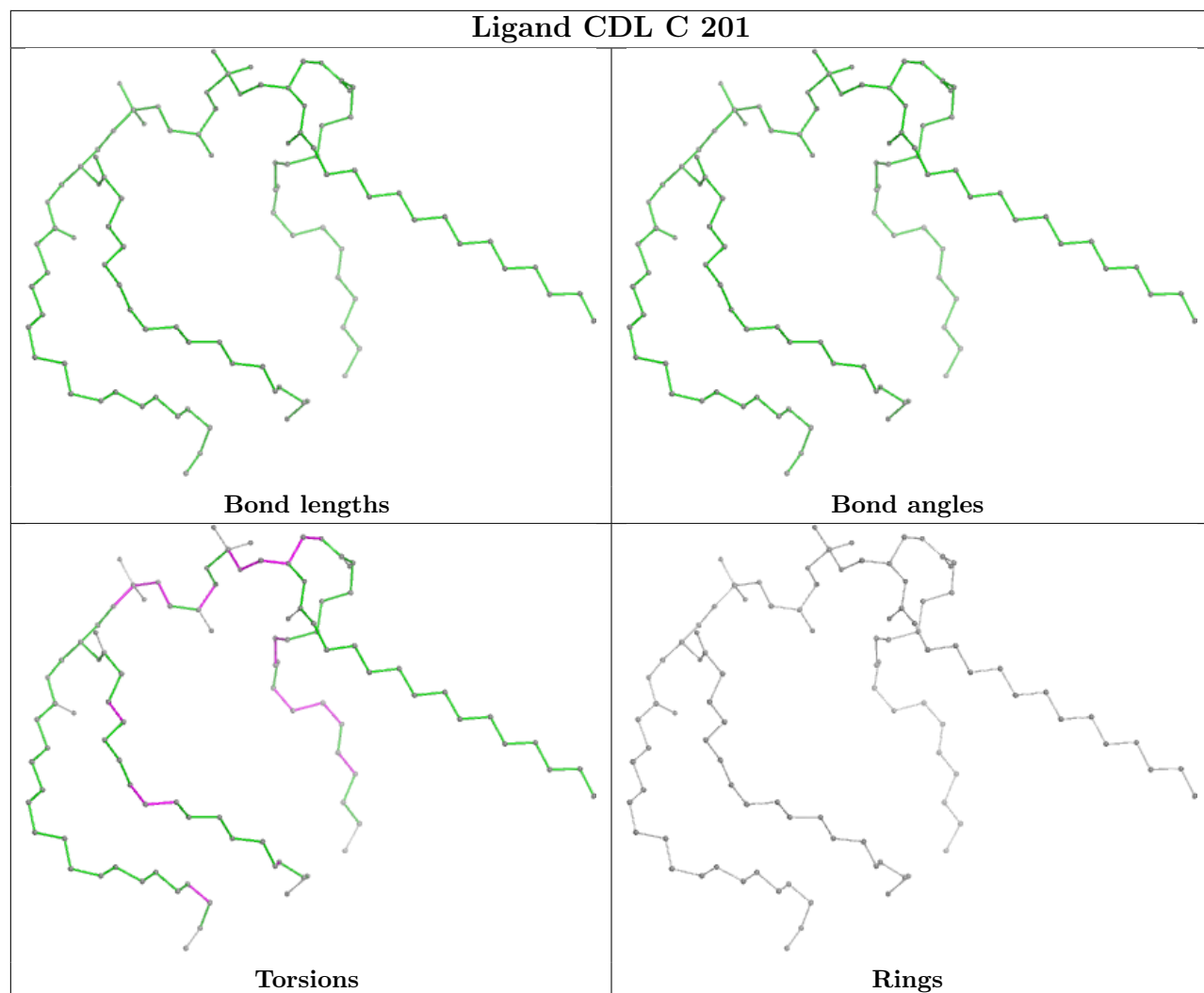


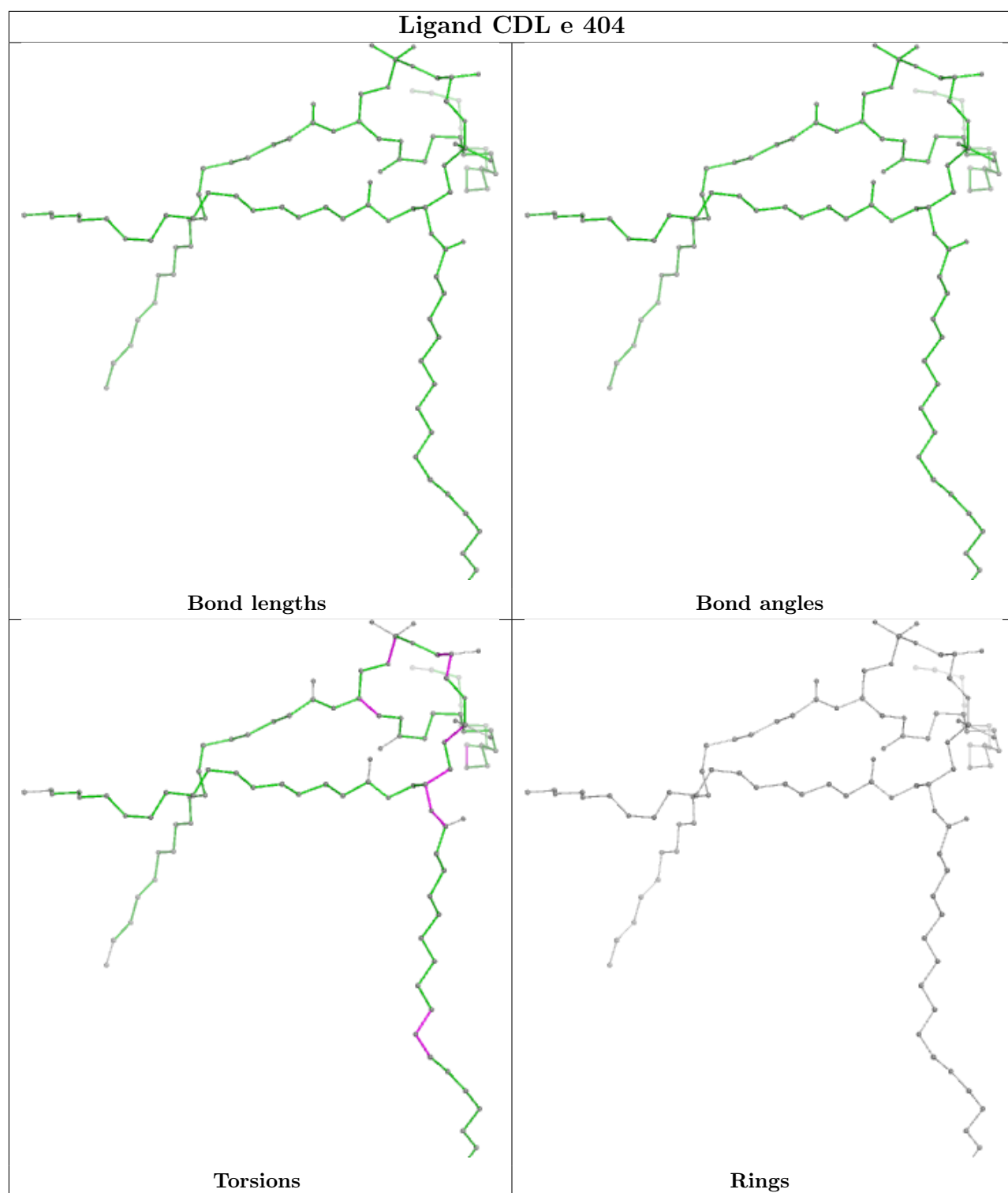


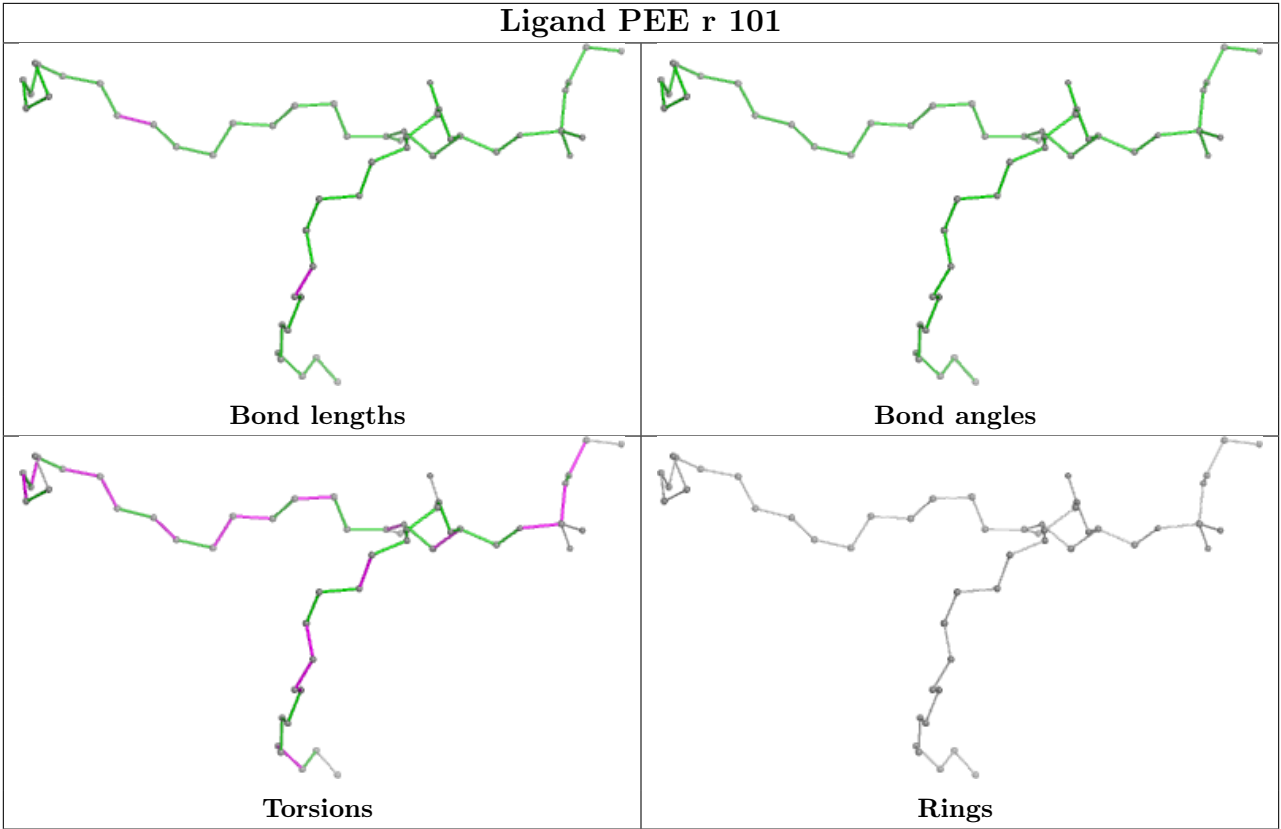












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	1
3	d	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	322:GLU	C	323:ARG	N	2.62
1	d	322:GLU	C	323:ARG	N	2.62

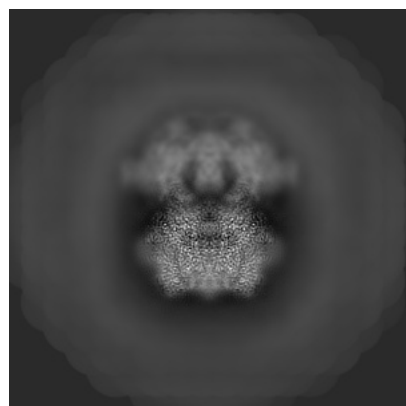
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15560. These allow visual inspection of the internal detail of the map and identification of artifacts.

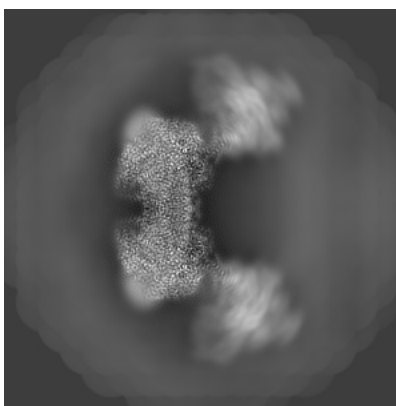
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

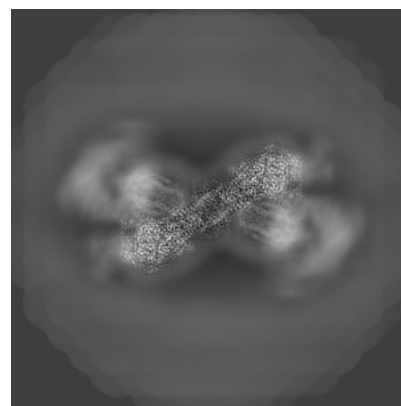
6.1.1 Primary map



X

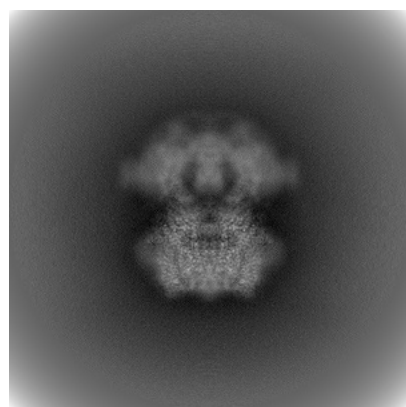


Y

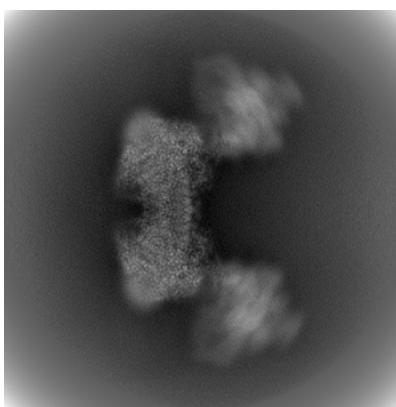


Z

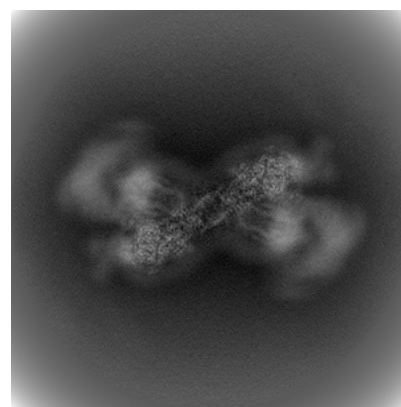
6.1.2 Raw map



X



Y

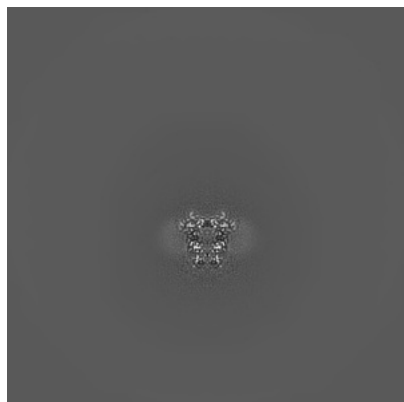


Z

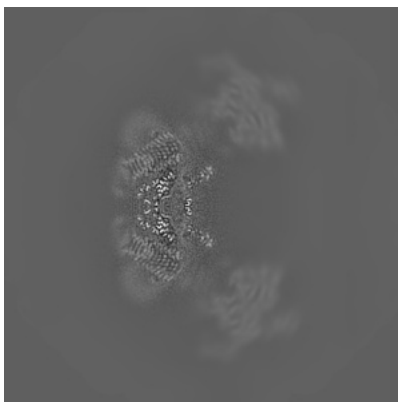
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

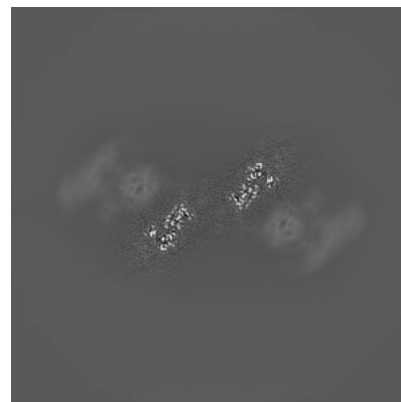
6.2.1 Primary map



X Index: 280

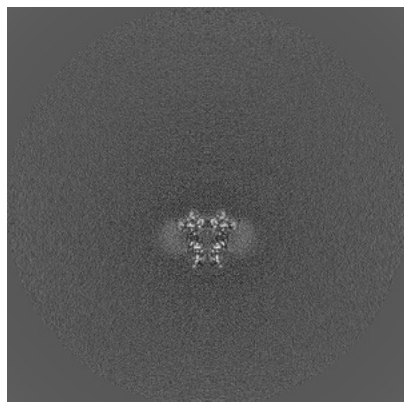


Y Index: 280

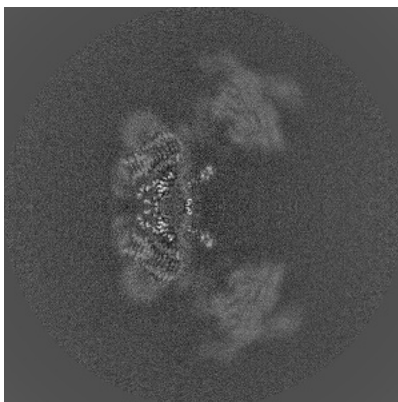


Z Index: 280

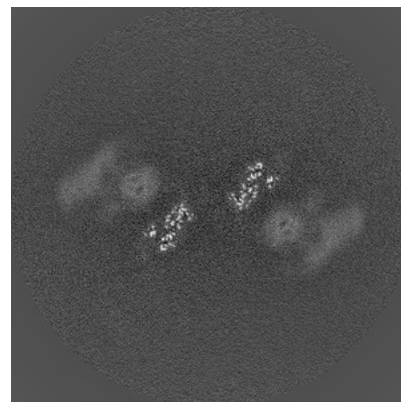
6.2.2 Raw map



X Index: 280



Y Index: 280

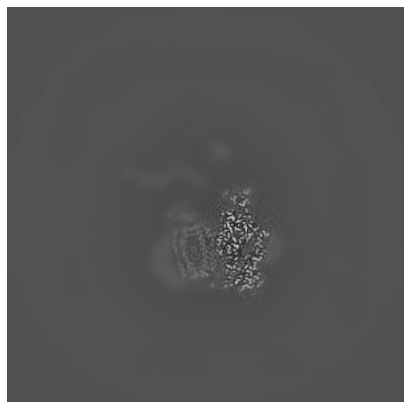


Z Index: 280

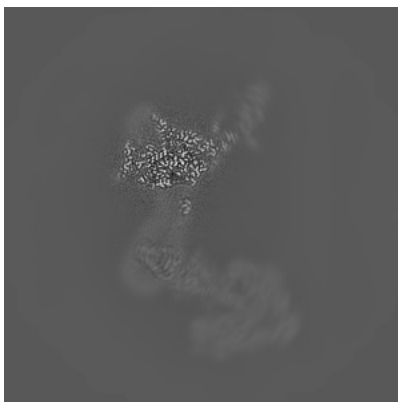
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

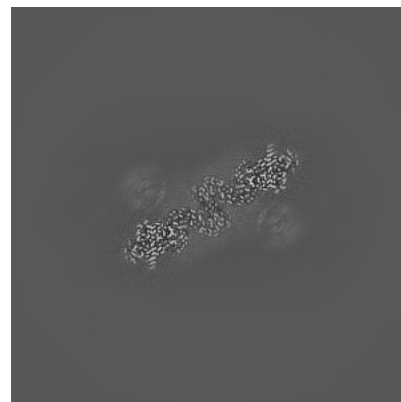
6.3.1 Primary map



X Index: 353

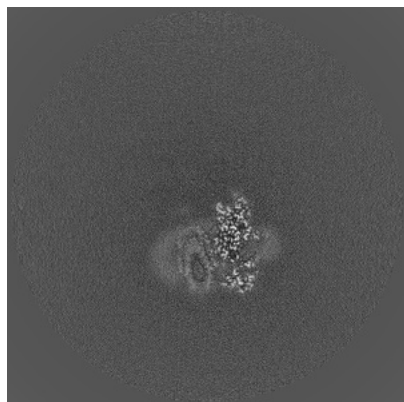


Y Index: 319

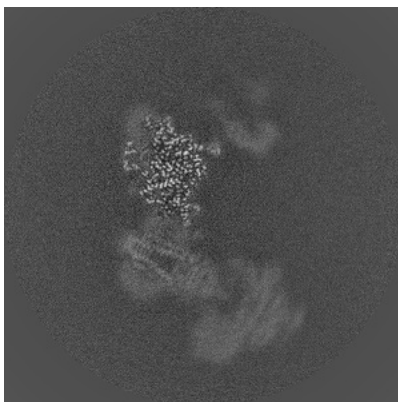


Z Index: 254

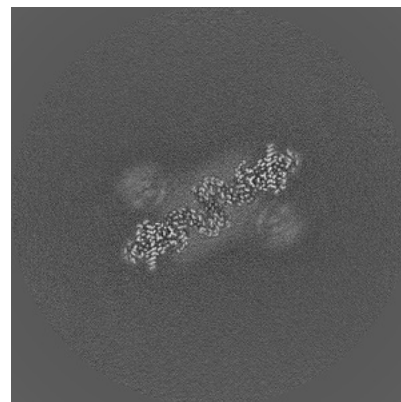
6.3.2 Raw map



X Index: 341



Y Index: 304

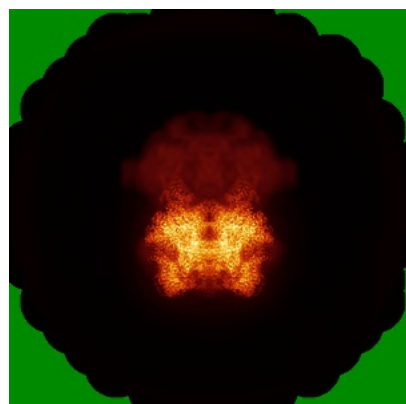


Z Index: 254

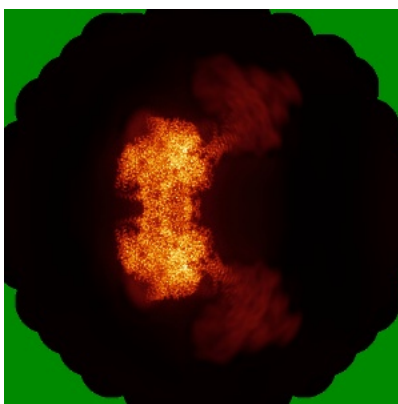
The images above show the largest variance slices of the map in three orthogonal directions.

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

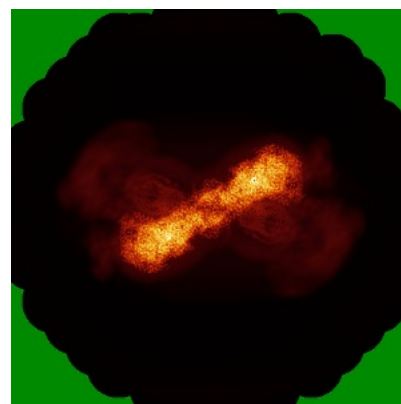
6.4.1 Primary map



X

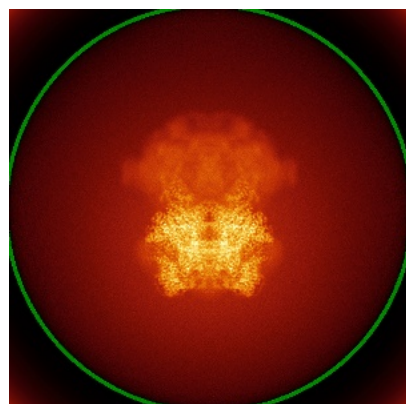


Y

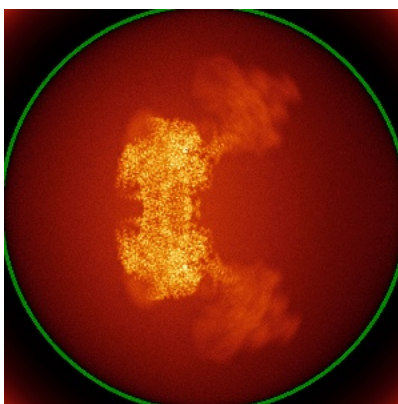


Z

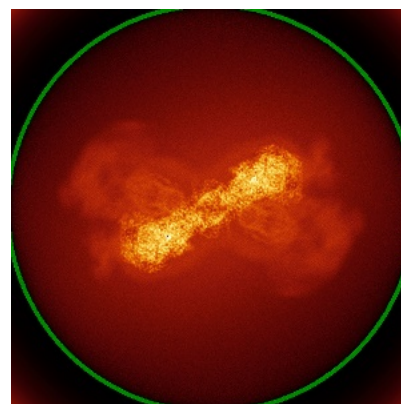
6.4.2 Raw map



X



Y

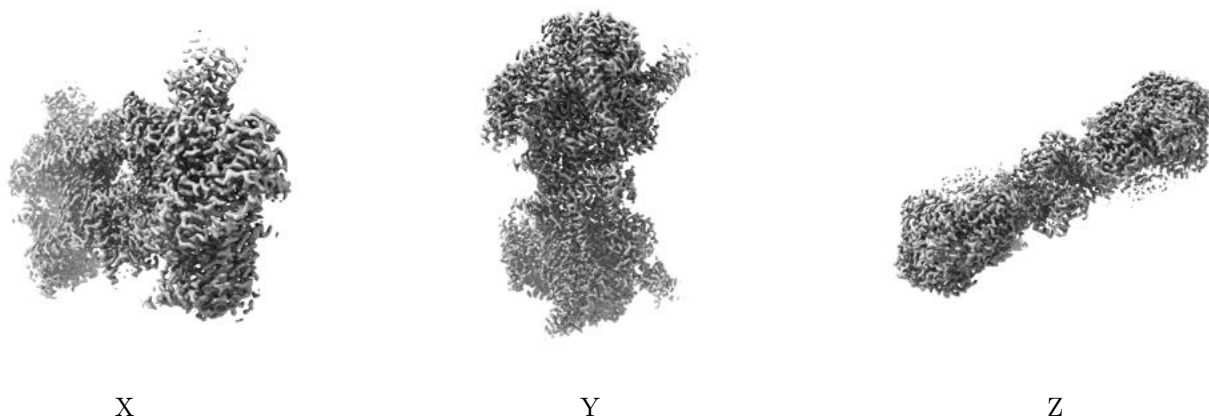


Z

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

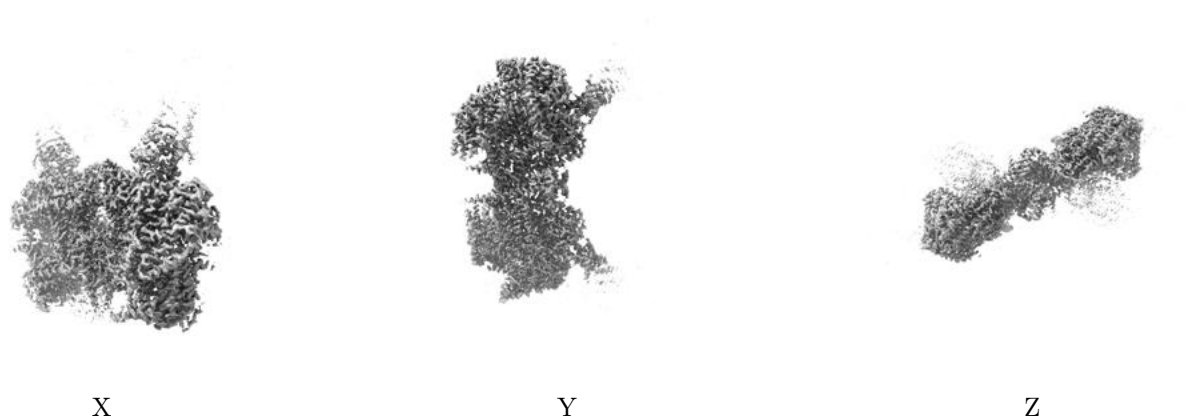
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

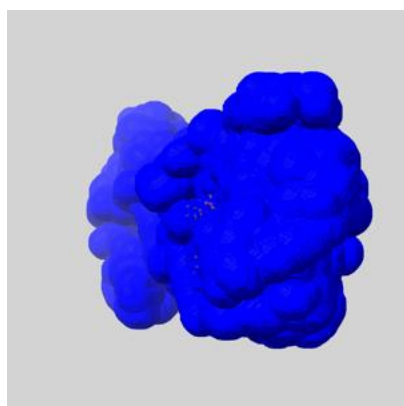
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

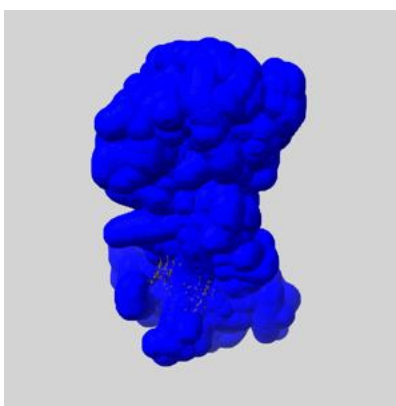
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

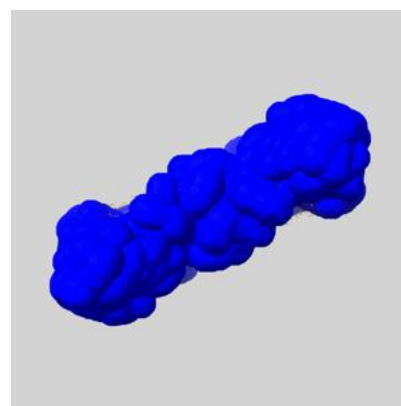
6.6.1 emd_15560_msk_1.map [i](#)



X



Y

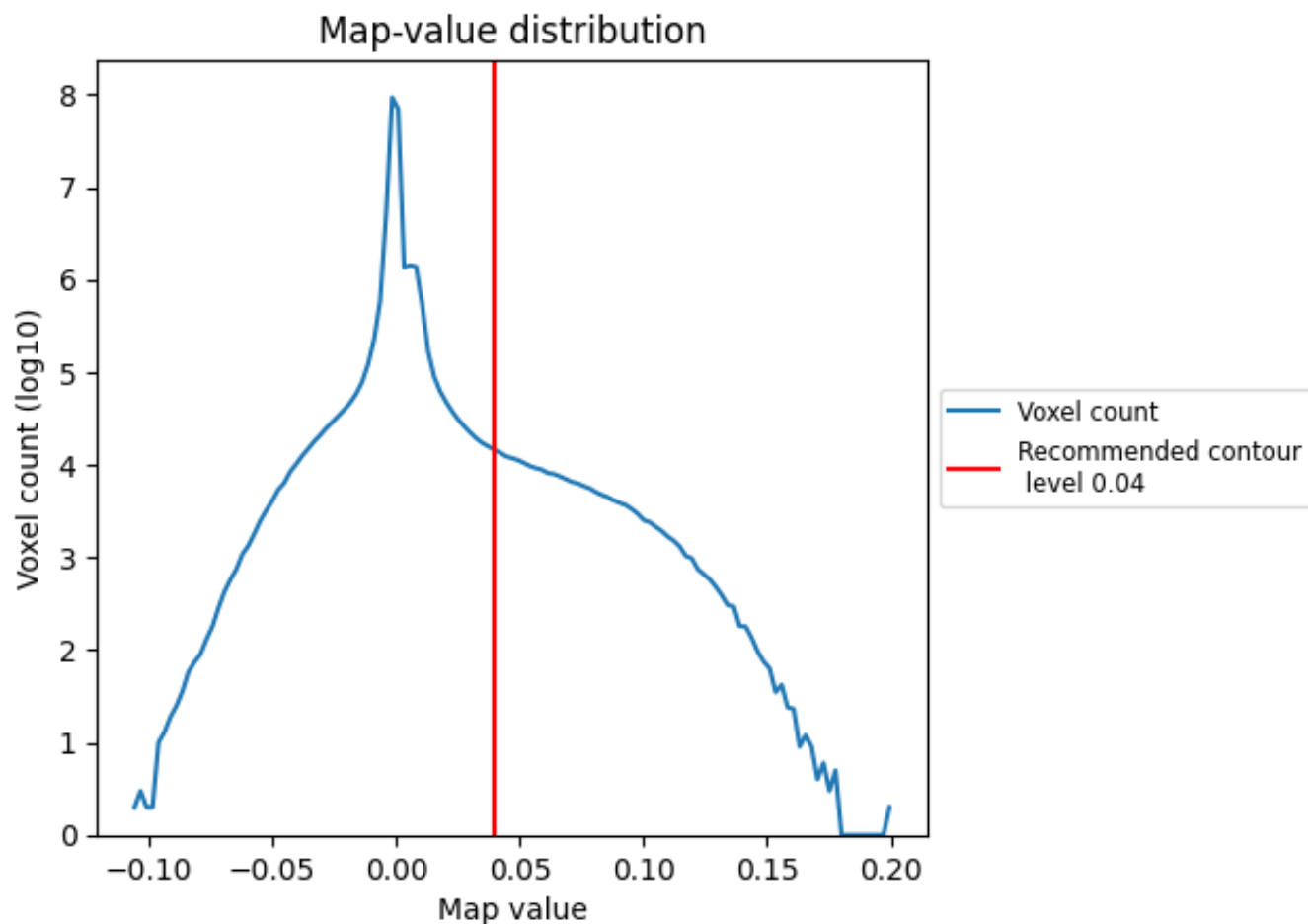


Z

7 Map analysis [i](#)

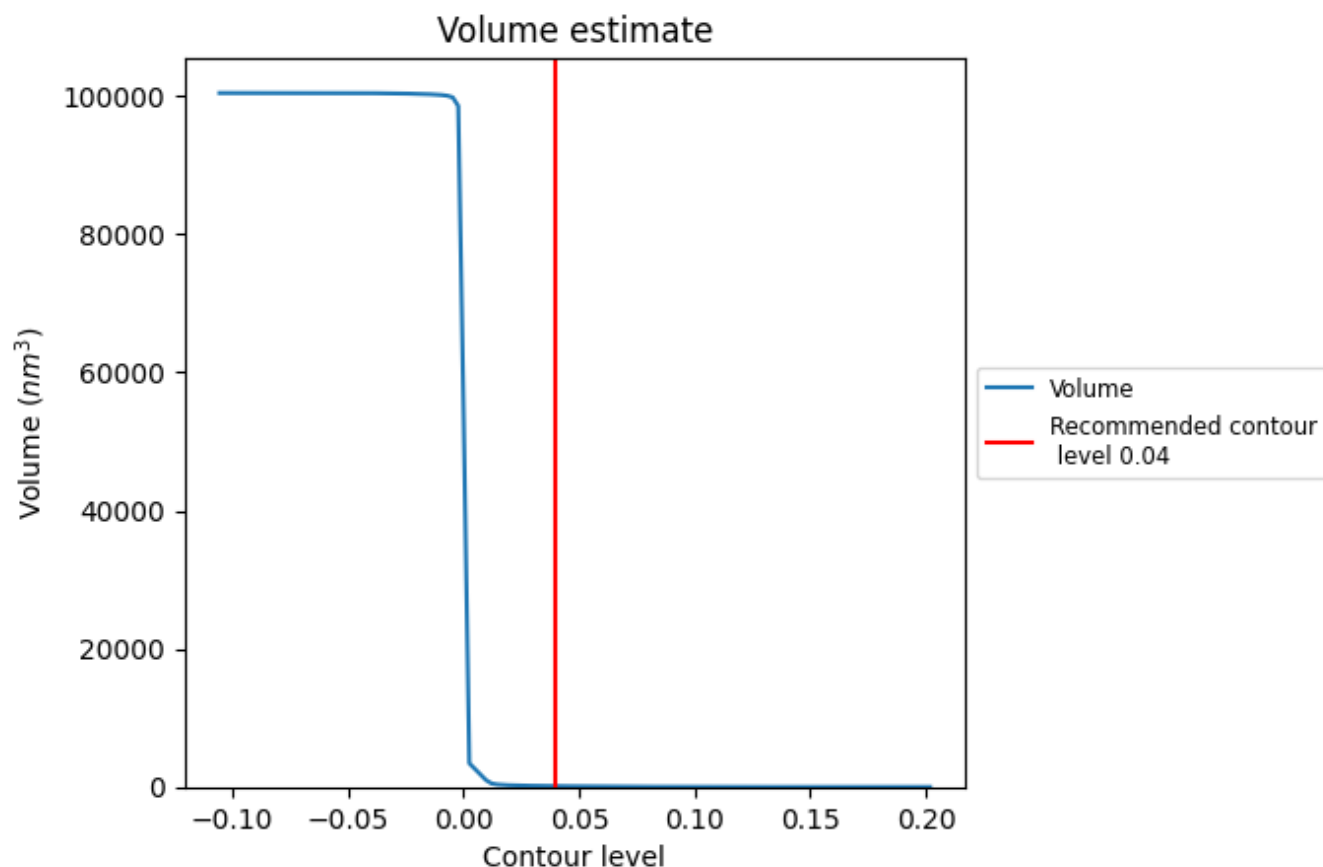
This section contains the results of statistical analysis of the map.

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.

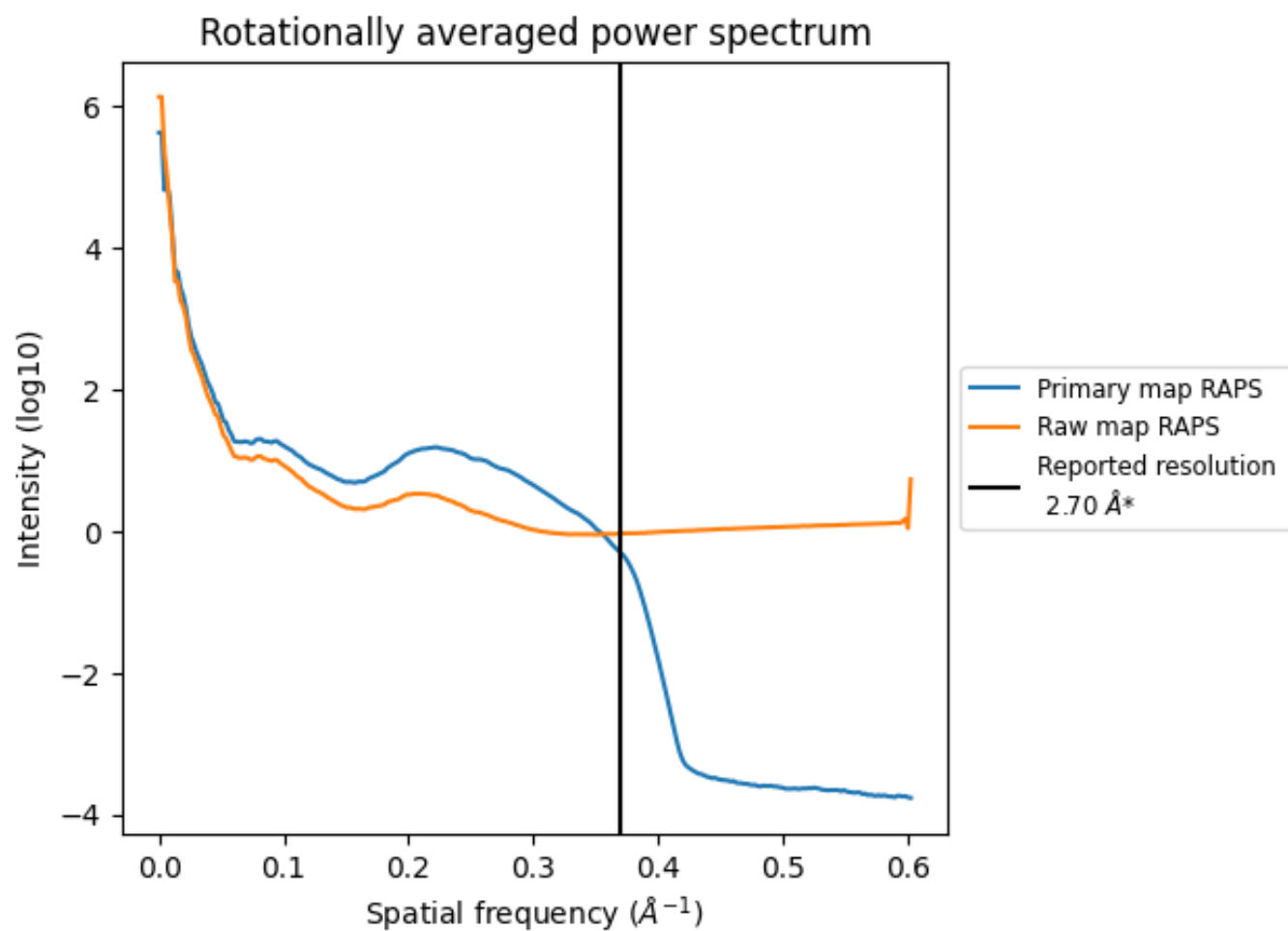
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm^3 ; this corresponds to an approximate mass of 107 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 ⓘ

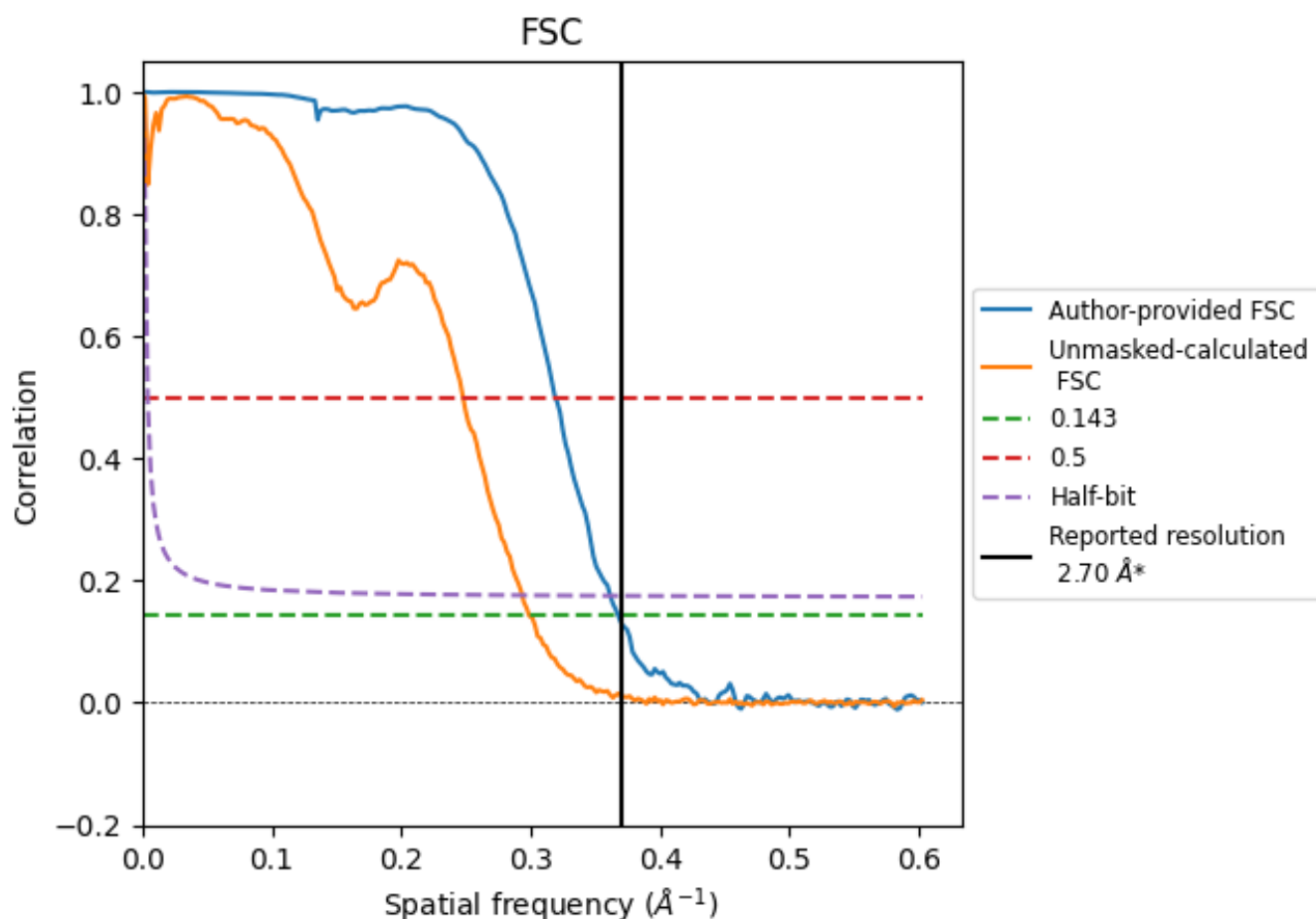


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

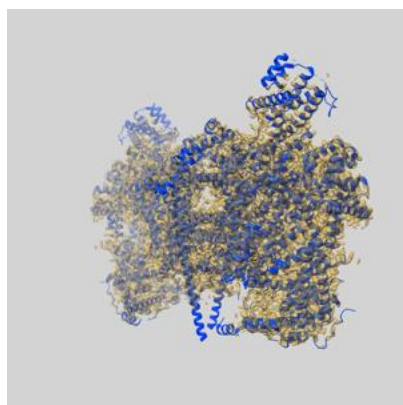
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	3.13	2.77
Unmasked-calculated*	3.35	4.04	3.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 2.7 by more than 10 %

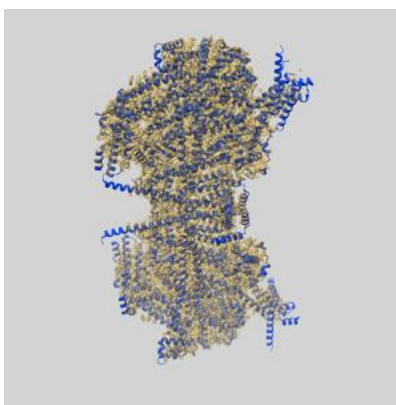
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15560 and PDB model 8AP7. Per-residue inclusion information can be found in section [3](#) on page [14](#).

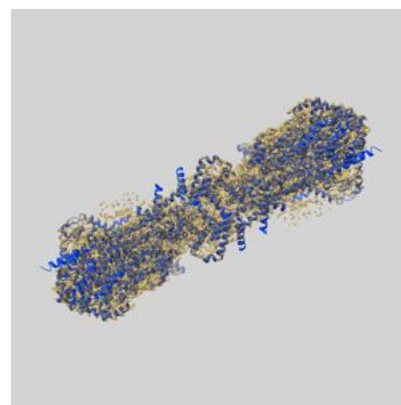
9.1 Map-model overlay [i](#)



X



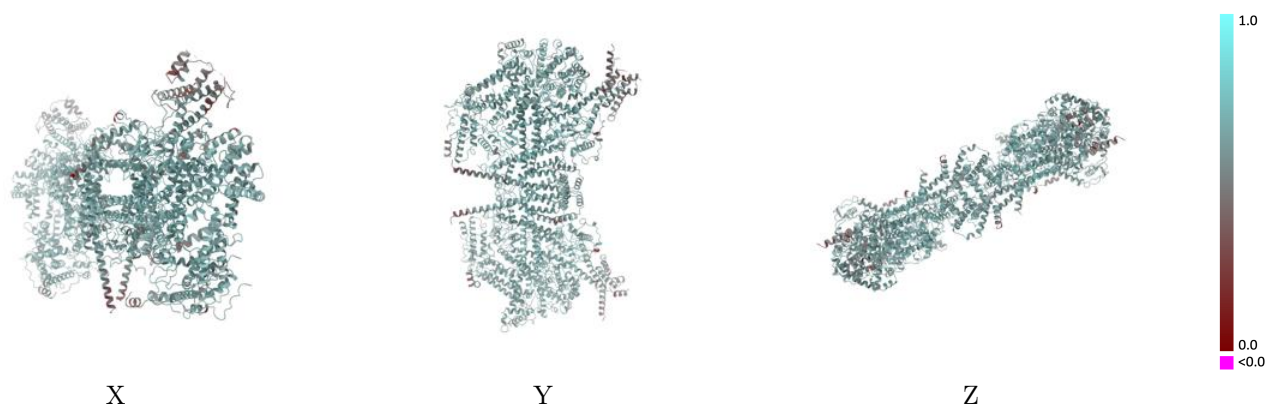
Y



Z

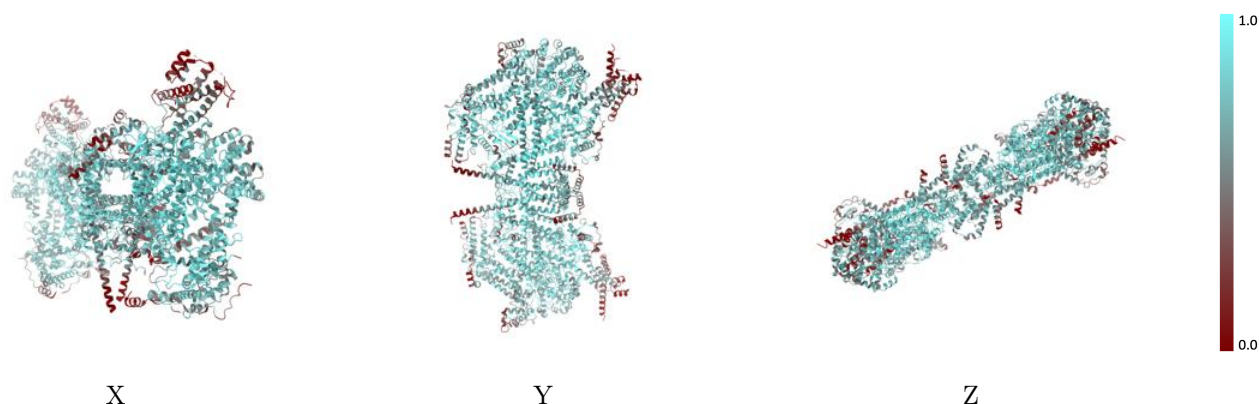
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



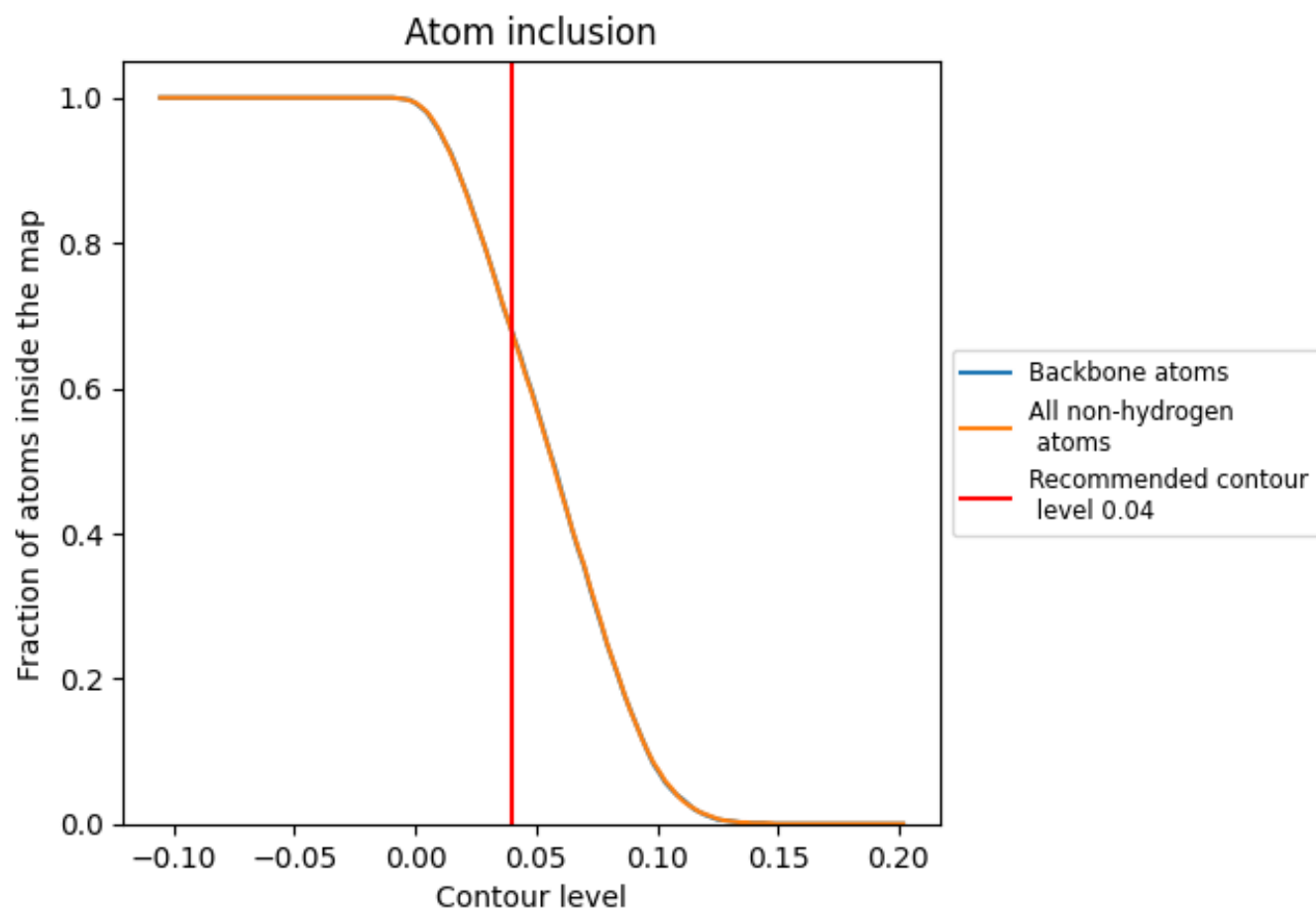
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6770	 0.6130
A	 0.7960	 0.6510
C	 0.7600	 0.6340
D	 0.4580	 0.5390
E	 0.7150	 0.6200
F	 0.7310	 0.6260
I	 0.7790	 0.6410
J	 0.6420	 0.5950
K	 0.5750	 0.5950
L	 0.4990	 0.5740
M	 0.6000	 0.5970
N	 0.8030	 0.6500
O	 0.5920	 0.5880
P	 0.7350	 0.6260
Q	 0.7470	 0.6250
R	 0.7850	 0.6420
a	 0.7960	 0.6500
c	 0.7520	 0.6310
d	 0.4560	 0.5390
e	 0.7150	 0.6190
f	 0.7290	 0.6230
i	 0.7830	 0.6400
j	 0.6430	 0.5940
k	 0.5690	 0.5950
l	 0.4990	 0.5680
m	 0.6040	 0.5970
n	 0.7940	 0.6460
o	 0.5880	 0.5870
p	 0.7340	 0.6240
q	 0.7460	 0.6240
r	 0.7810	 0.6400

