



## wwPDB EM Validation Summary Report ⓘ

Jun 10, 2025 – 04:43 pm BST

PDB ID : 9G9T / pdb\_00009g9t  
EMDB ID : EMD-51157  
Title : Cryo-EM structure of the Toxoplasma gondii respiratory chain complex III inhibited by ELQ-300  
Authors : MacLean, A.; Muhleip, A.  
Deposited on : 2024-07-25  
Resolution : 1.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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) : 2.43.1

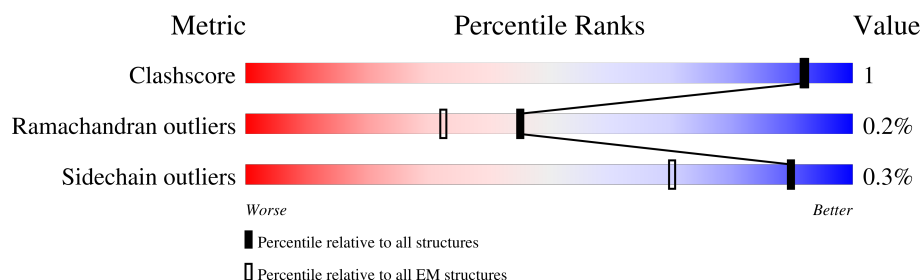
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 1.80 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  $\geq 3$ , 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	360	<div> <div>91%</div> <div>95%</div> <div>5%</div> </div>
1	a	360	<div> <div>90%</div> <div>95%</div> <div>.</div> </div>
2	B	398	<div> <div>54%</div> <div>59%</div> <div>39%</div> </div>
2	b	398	<div> <div>55%</div> <div>60%</div> <div>39%</div> </div>
3	C	487	<div> <div>34%</div> <div>40%</div> <div>58%</div> </div>
3	c	487	<div> <div>37%</div> <div>41%</div> <div>58%</div> </div>
4	D	509	<div> <div>80%</div> <div>89%</div> <div>9%</div> </div>
4	d	509	<div> <div>81%</div> <div>89%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	563	
5	e	563	
6	F	89	
6	f	89	
7	G	234	
7	g	234	
8	H	122	
8	h	122	
9	I	128	
9	i	128	
10	J	80	
10	j	80	
11	K	141	
11	k	141	
12	L	109	
12	l	109	

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 82791 atoms, of which 41180 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 Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	360	Total	C	H	N	O	S	0	0
			5840	1941	2958	452	470	19		
1	a	360	Total	C	H	N	O	S	0	0
			5840	1941	2958	452	470	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PHE	-	expression tag	UNP O20672
a	9	PHE	-	expression tag	UNP O20672

- Molecule 2 is a protein called Cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	243	Total	C	H	N	O	S	0	0
			3842	1270	1880	327	352	13		
2	b	243	Total	C	H	N	O	S	0	0
			3842	1270	1880	327	352	13		

- Molecule 3 is a protein called Putative ubiquinol cytochrome c oxidoreductase.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	205	Total	C	H	N	O	S	0	0
			3258	1071	1572	297	313	5		
3	c	205	Total	C	H	N	O	S	0	0
			3258	1071	1572	297	313	5		

- Molecule 4 is a protein called Putative peptidase M16 family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	462	Total	C	H	N	O	S	0	0
			7263	2305	3610	636	689	23		

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Mol	Chain	Residues	Atoms						AltConf	Trace
4	d	462	Total	C	H	N	O	S	0	0
			7263	2305	3610	636	689	23		

- Molecule 5 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	485	Total	C	H	N	O	S	0	0
			7579	2417	3773	659	701	29		
5	e	485	Total	C	H	N	O	S	0	0
			7579	2417	3773	659	701	29		

- Molecule 6 is a protein called Putative ubiquinol-cytochrome c reductase hinge protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	88	Total	C	H	N	O	S	0	0
			1429	462	702	126	132	7		
6	f	88	Total	C	H	N	O	S	0	0
			1429	462	702	126	132	7		

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	192	Total	C	H	N	O	S	0	0
			3093	1022	1525	266	273	7		
7	g	192	Total	C	H	N	O	S	0	0
			3093	1022	1525	266	273	7		

- Molecule 8 is a protein called QCR8/TGGT1\_227910.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	96	Total	C	H	N	O	S	0	0
			1606	552	778	136	134	6		
8	h	96	Total	C	H	N	O	S	0	0
			1606	552	778	136	134	6		

- Molecule 9 is a protein called Ubiquinol-cytochrome C family reductase UQCRX/QCR9-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	92	Total	C	H	N	O	S	0	0
			1597	537	786	138	130	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
9	i	92	Total	C	H	N	O	S	0	0
			1597	537	786	138	130	6		

- Molecule 10 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	74	Total	C	H	N	O	S	0	0
			1226	418	600	108	97	3		
10	j	74	Total	C	H	N	O	S	0	0
			1226	418	600	108	97	3		

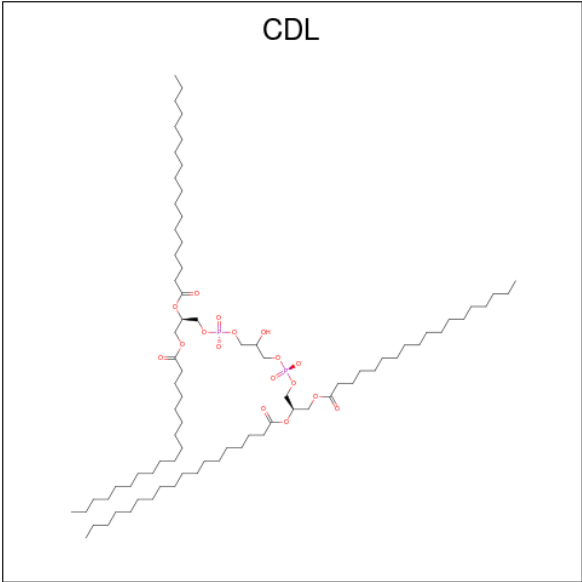
- Molecule 11 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	77	Total	C	H	N	O	S	0	0
			1232	397	625	107	99	4		
11	k	77	Total	C	H	N	O	S	0	0
			1232	397	625	107	99	4		

- Molecule 12 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	33	Total	C	H	N	O	S	0	0
			504	163	258	40	42	1		
12	l	33	Total	C	H	N	O	S	0	0
			504	163	258	40	42	1		

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



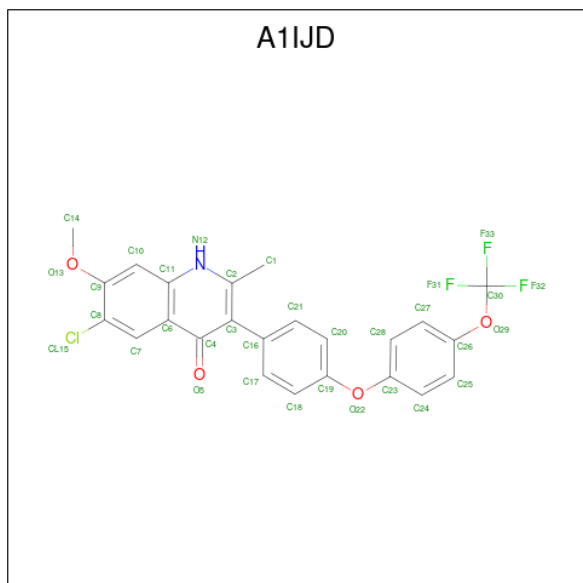
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	C	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	C	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	D	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	G	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	H	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	H	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	I	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	L	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	d	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	g	1	Total	C	H	O	P	0
			256	81	156	17	2	

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Mol	Chain	Residues	Atoms					AltConf
13	g	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	h	1	Total	C	H	O	P	0
			256	81	156	17	2	

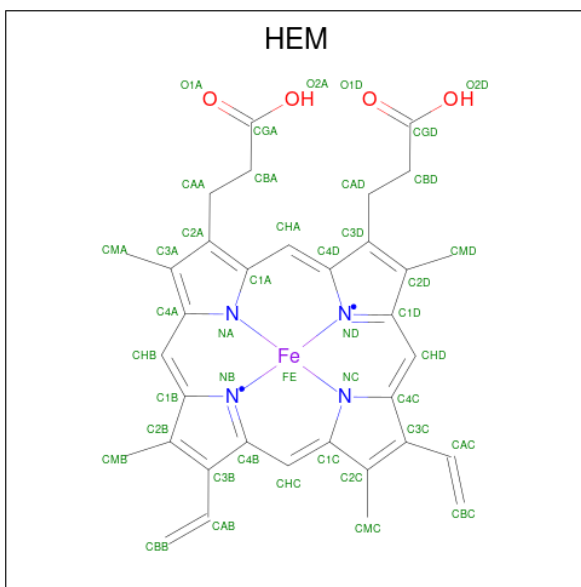
- Molecule 14 is 6-chloranyl-7-methoxy-2-methyl-3-[4-[4-(trifluoromethoxy)phenoxy]phenyl]-1 {H}-quinolin-4-one (CCD ID: A1IJD) (formula: C<sub>24</sub>H<sub>17</sub>ClF<sub>3</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms							AltConf
14	A	1	Total	C	Cl	F	H	N	O	1
			65	31	1	6	21	1	5	
14	A	1	Total	C	Cl	F	H	N	O	0
			50	24	1	3	17	1	4	
14	a	1	Total	C	Cl	F	H	N	O	1
			65	31	1	6	21	1	5	
14	a	1	Total	C	Cl	F	H	N	O	0
			50	24	1	3	17	1	4	

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



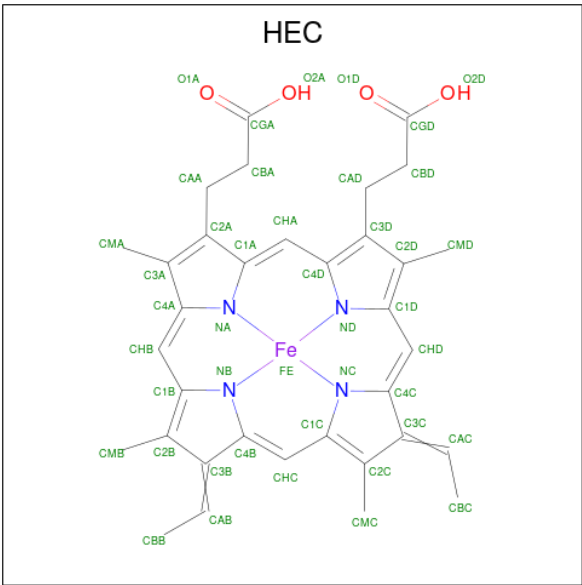


Mol	Chain	Residues	Atoms						AltConf
15	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
15	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
15	a	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
15	a	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

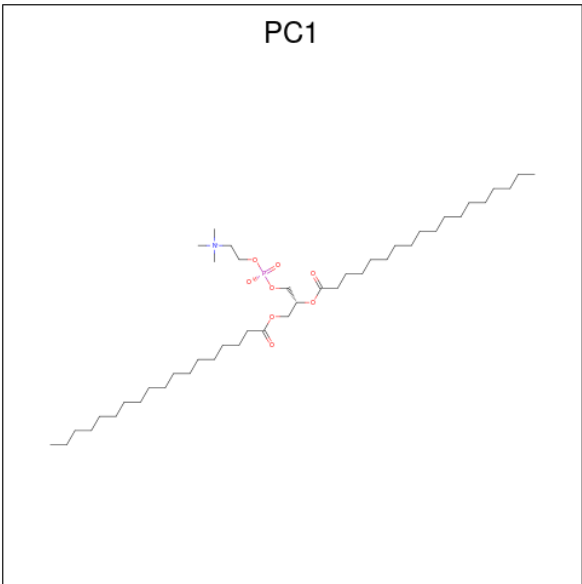
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	
16	a	1	Total	Mg	0
			1	1	

- Molecule 17 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
17	B	1	Total	C	Fe	H	N	O	0
			74	34	1	31	4	4	
17	b	1	Total	C	Fe	H	N	O	0
			74	34	1	31	4	4	

- Molecule 18 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms						AltConf
18	C	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
18	i	1	Total	C	H	N	O	P
			142	44	88	1	8	1
								0

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	D	1	Total	Zn	0
			1	1	
19	d	1	Total	Zn	0
			1	1	

- Molecule 20 is water.

Mol	Chain	Residues	Atoms			AltConf
20	A	59	Total	H	O	0
			89	30	59	
20	B	36	Total	H	O	0
			42	6	36	
20	C	40	Total	O		0
			40	40		
20	D	67	Total	H	O	0
			69	2	67	
20	E	26	Total	O		0
			26	26		
20	F	2	Total	O		0
			2	2		
20	G	65	Total	H	O	0
			77	12	65	
20	H	30	Total	H	O	0
			38	8	30	
20	I	7	Total	O		0
			7	7		
20	J	6	Total	O		0
			6	6		
20	K	3	Total	O		0
			3	3		
20	L	2	Total	O		0
			2	2		
20	a	61	Total	H	O	0
			91	30	61	
20	b	36	Total	H	O	0
			42	6	36	

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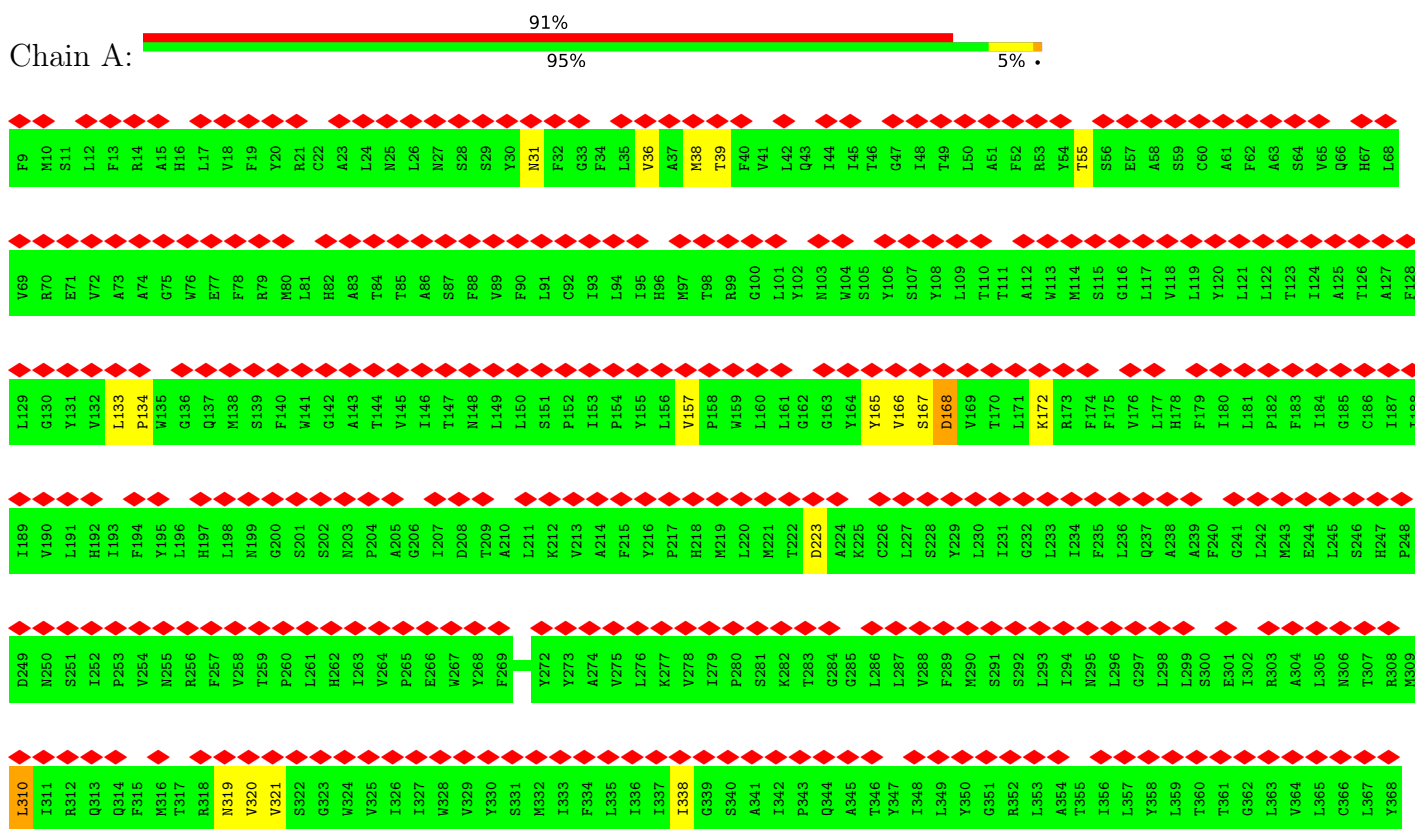
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Mol	Chain	Residues	Atoms	AltConf
20	c	39	Total O 39 39	0
20	d	68	Total H O 70 2 68	0
20	e	26	Total O 26 26	0
20	f	2	Total O 2 2	0
20	g	61	Total H O 73 12 61	0
20	h	27	Total H O 35 8 27	0
20	i	8	Total O 8 8	0
20	j	6	Total O 6 6	0
20	k	3	Total O 3 3	0
20	l	3	Total O 3 3	0

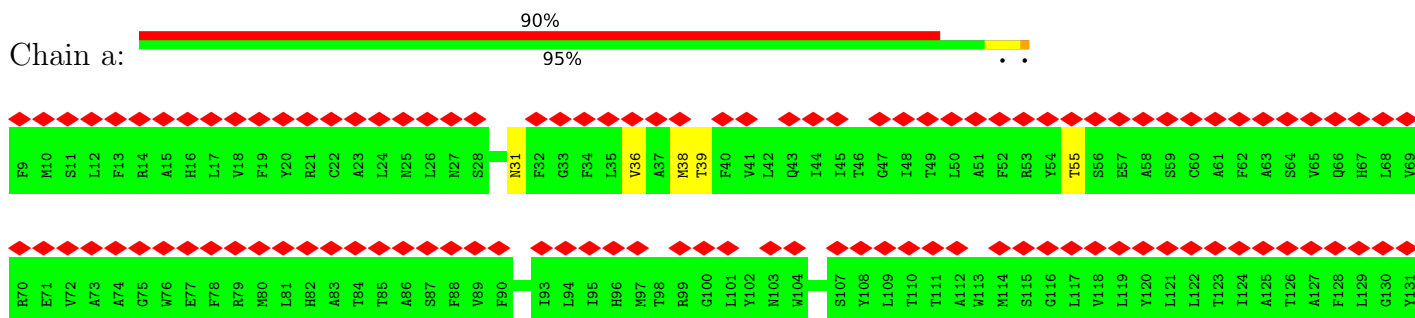
### 3 Residue-property plots

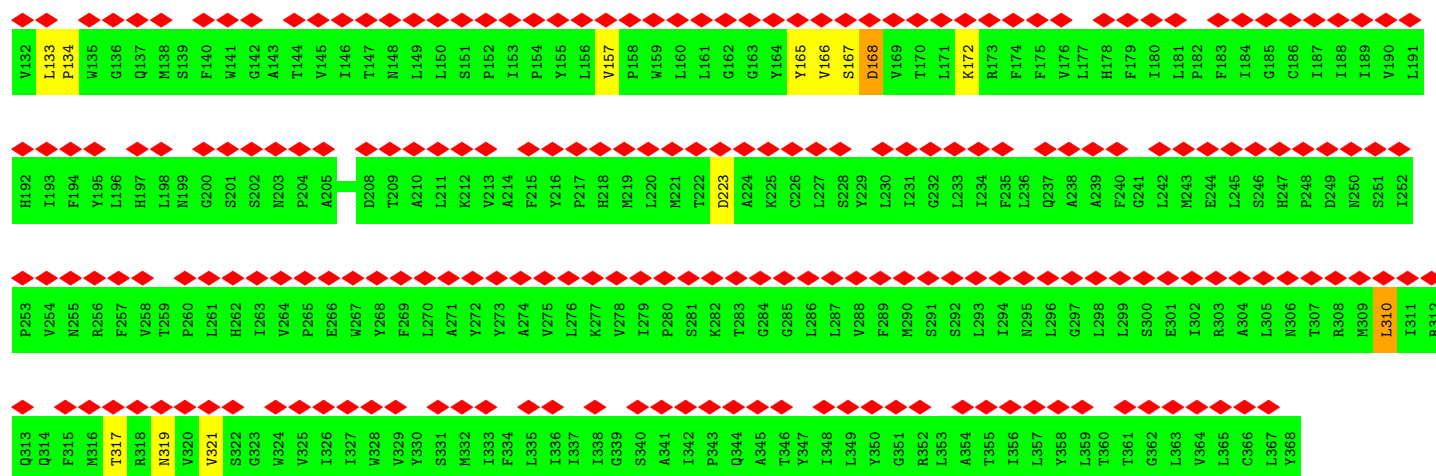
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cytochrome b

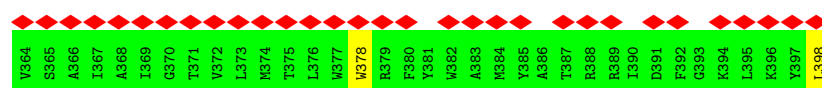
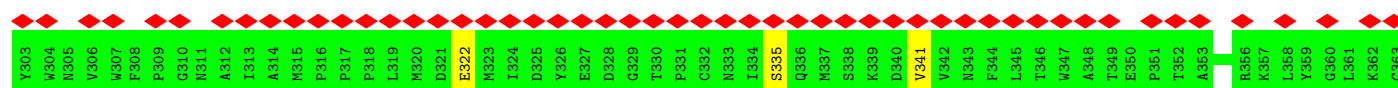
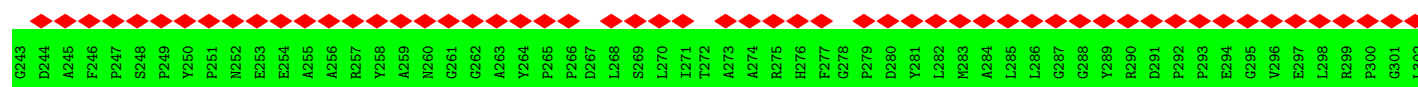
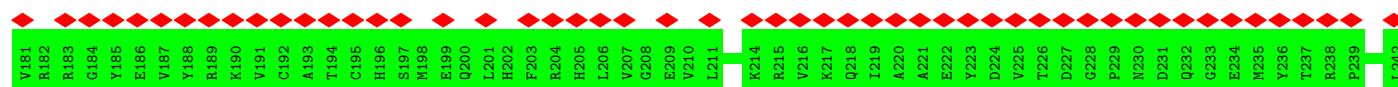
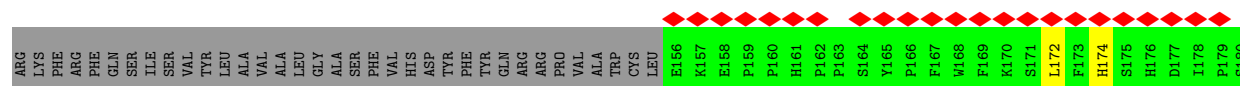
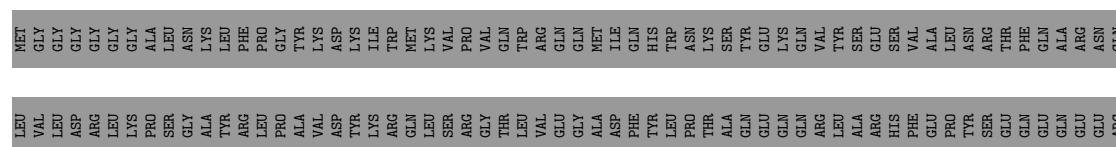


#### • Molecule 1: Cytochrome b

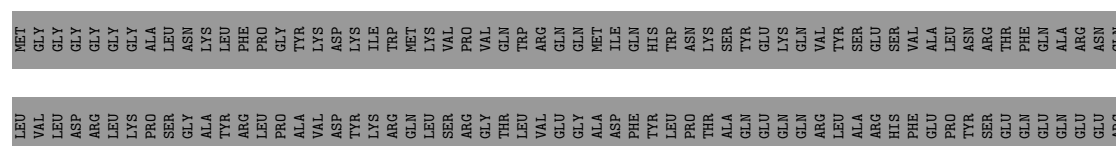


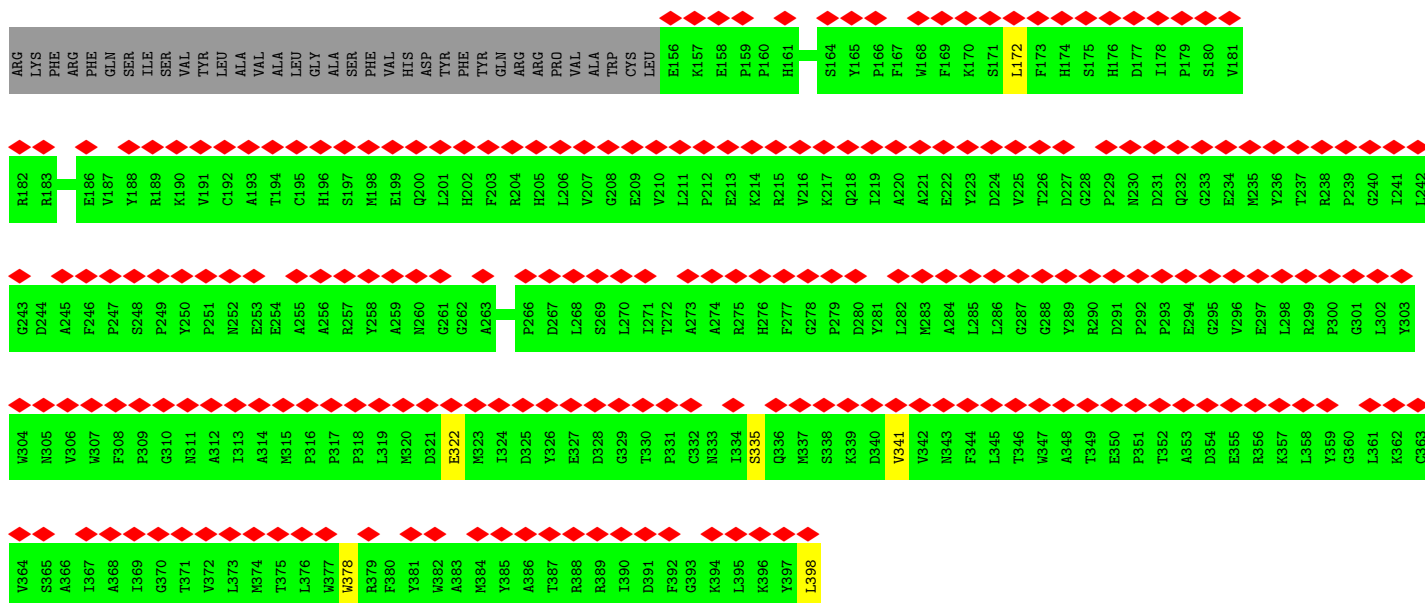


• Molecule 2: Cytochrome c1, heme protein

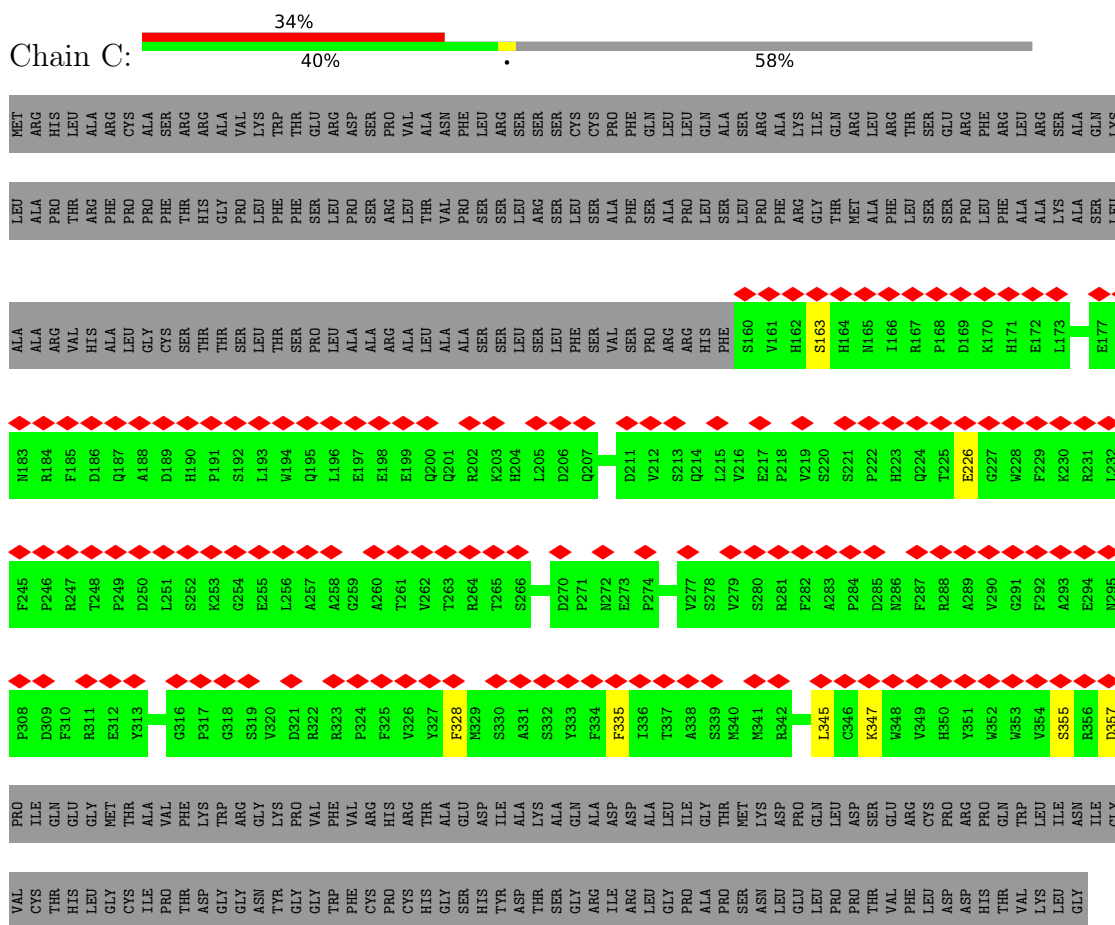


• Molecule 2: Cytochrome c1, heme protein





- Molecule 3: Putative ubiquinol cytochrome c oxidoreductase



- Molecule 3: Putative ubiquinol cytochrome c oxidoreductase

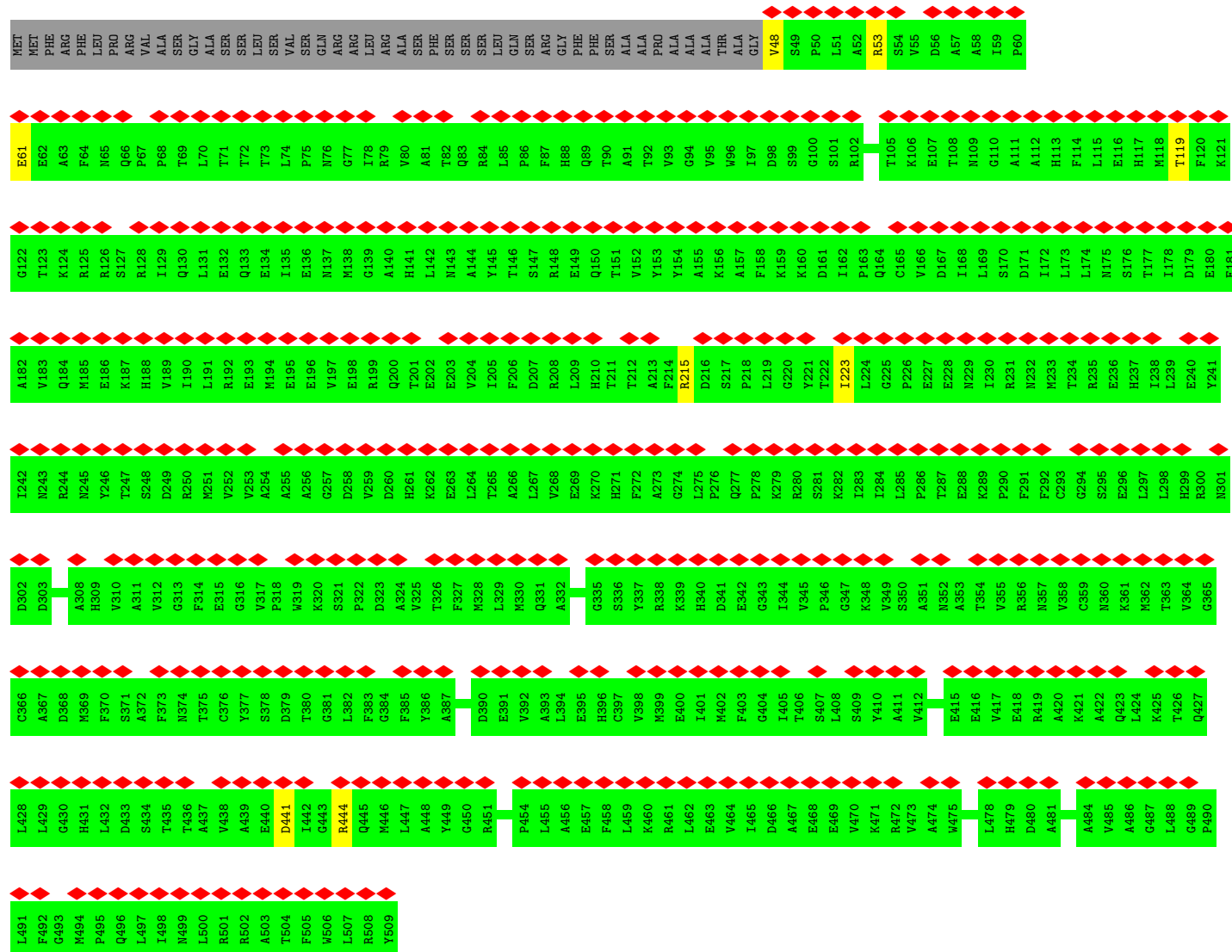
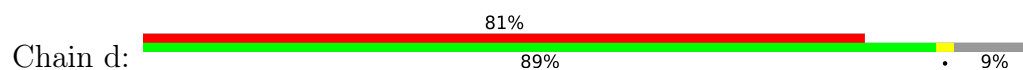






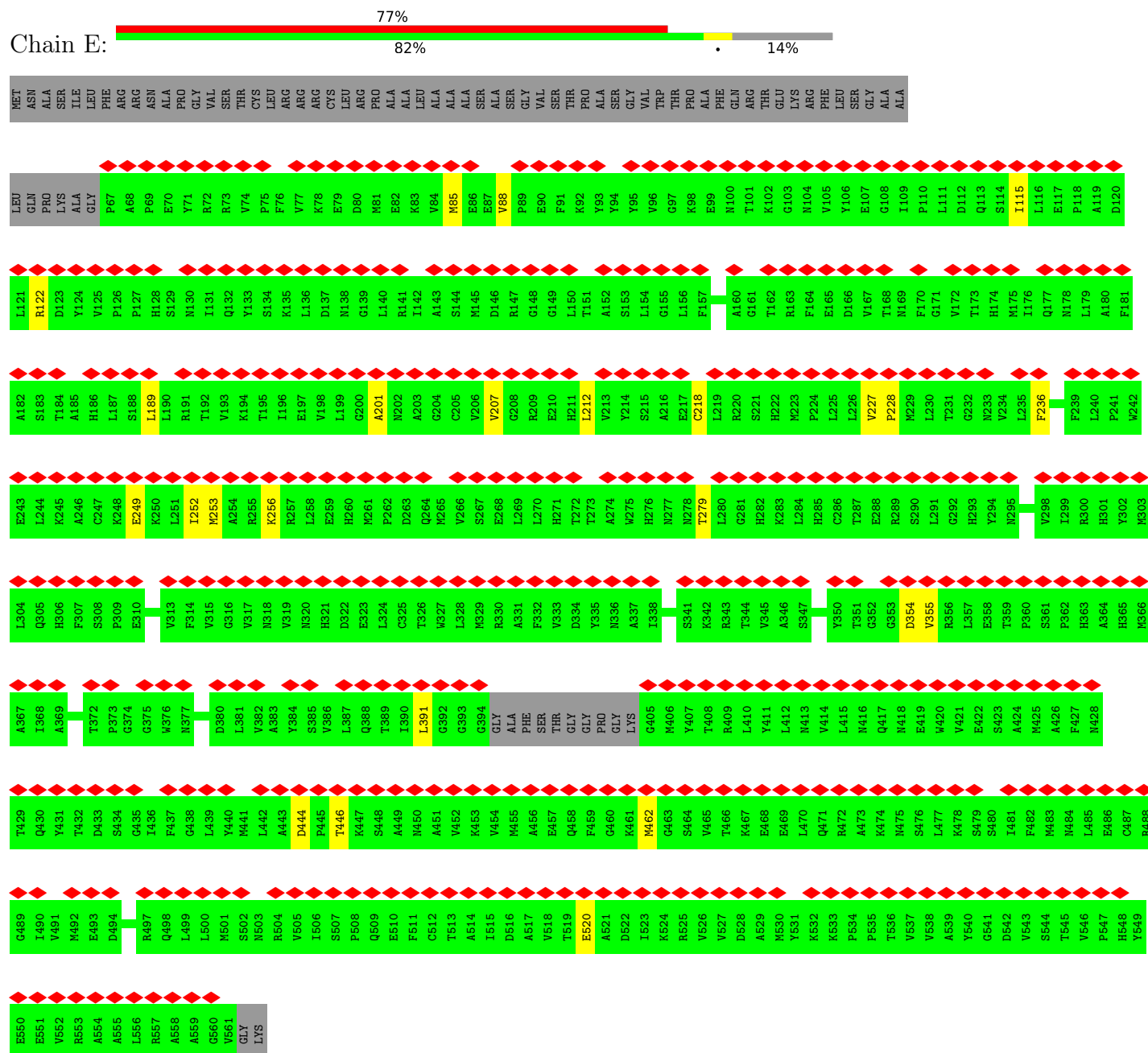


• Molecule 4: Putative peptidase M16 family protein



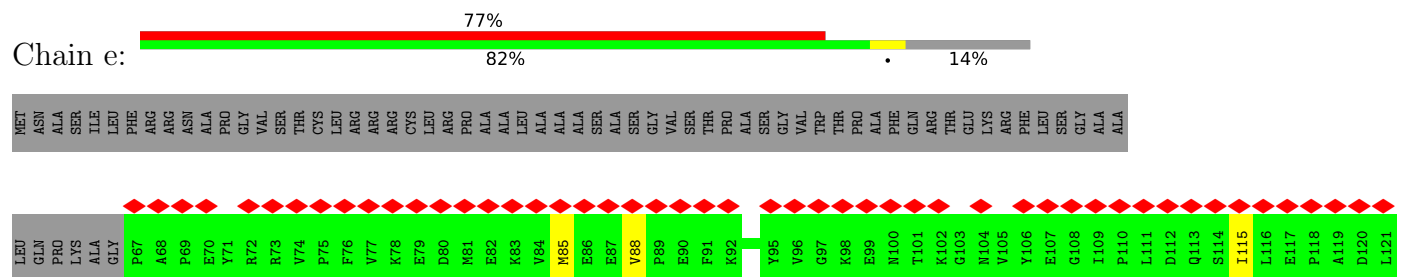
- Molecule 5: Alpha-MPP

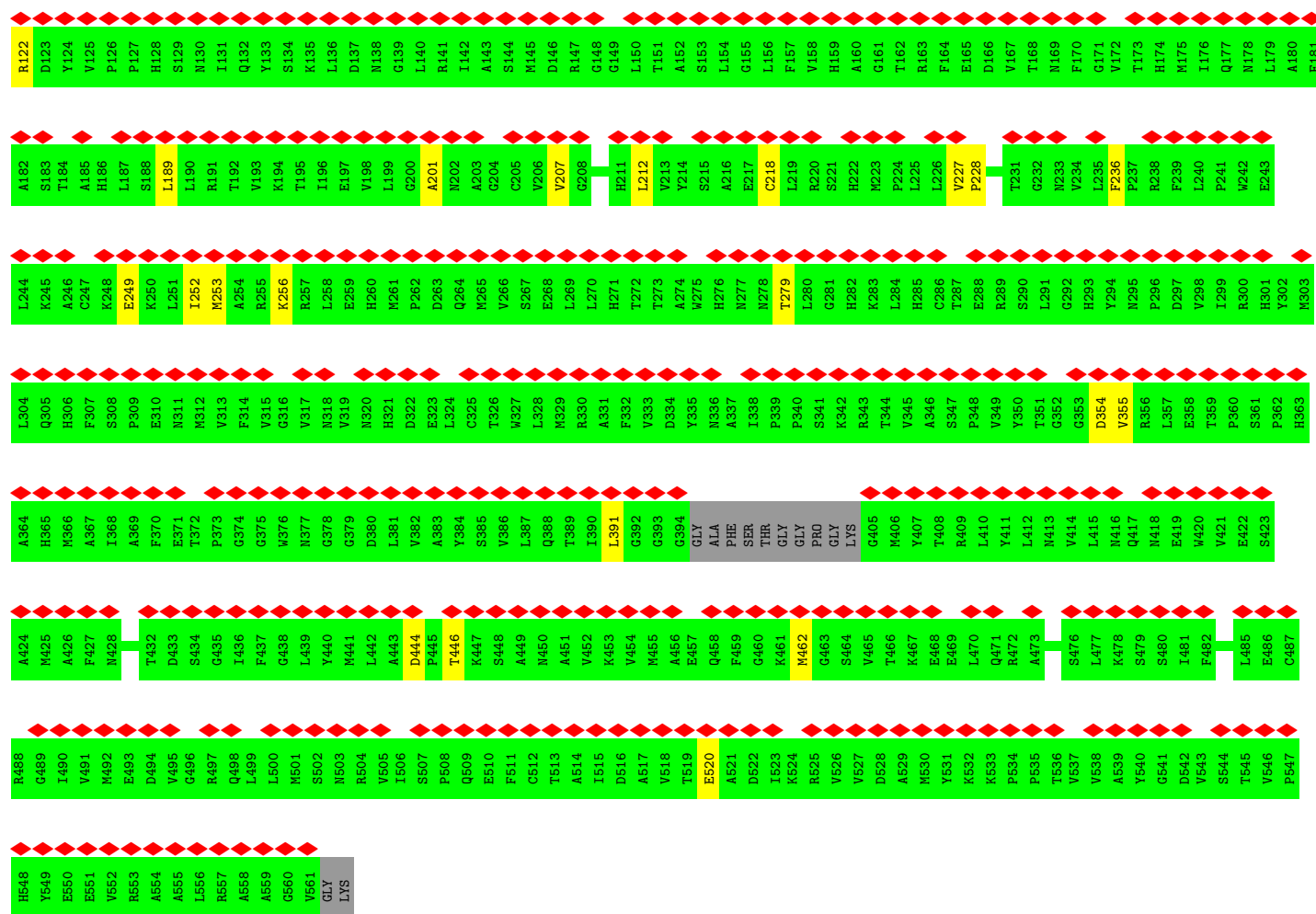
Chain E:



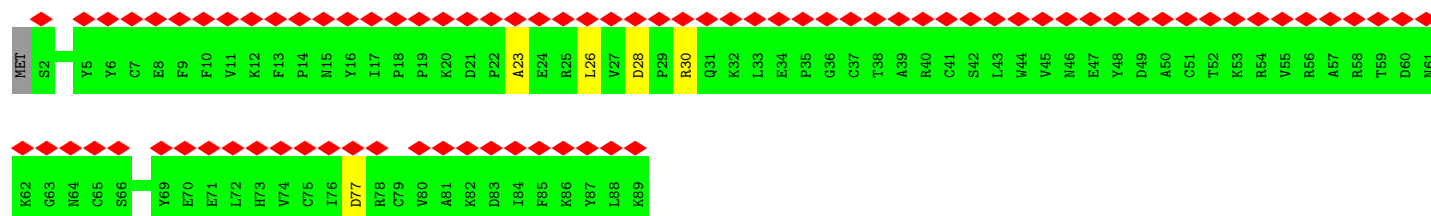
- Molecule 5: Alpha-MPP

Chain e:

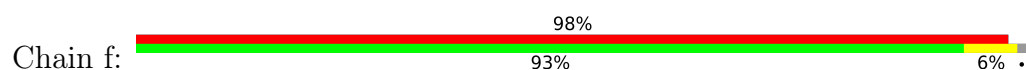




• Molecule 6: Putative ubiquinol-cytochrome c reductase hinge protein

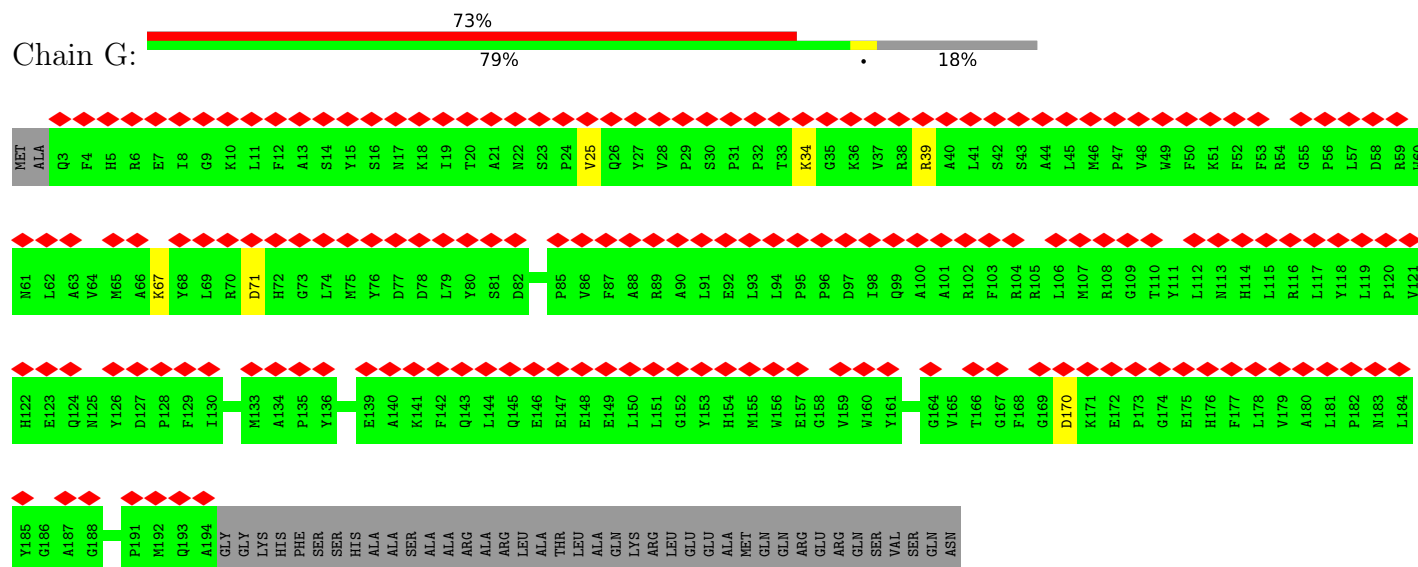


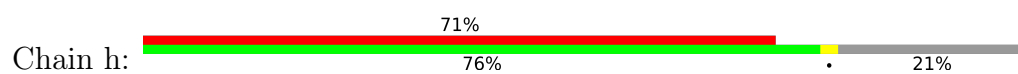
• Molecule 6: Putative ubiquinol-cytochrome c reductase hinge protein



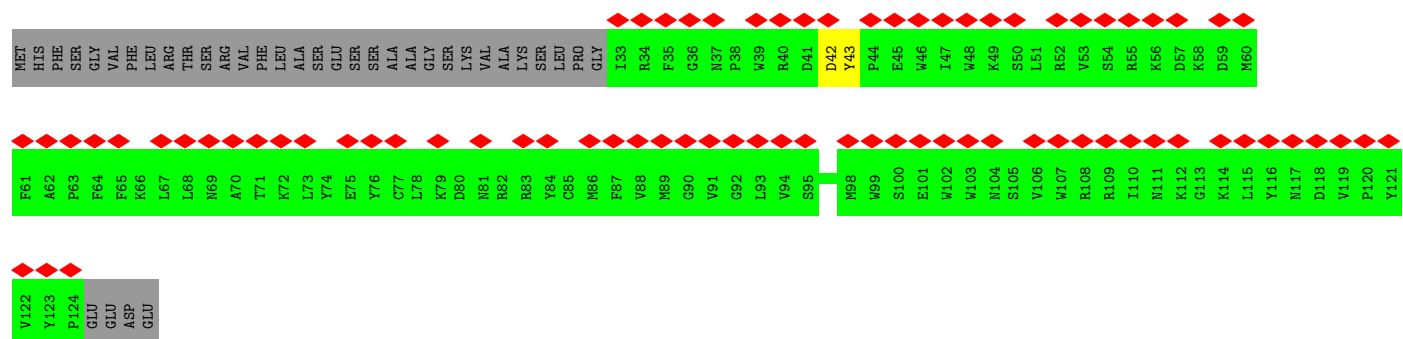
- Molecule 7: Ubiquinol-cytochrome c reductase

Chain G:

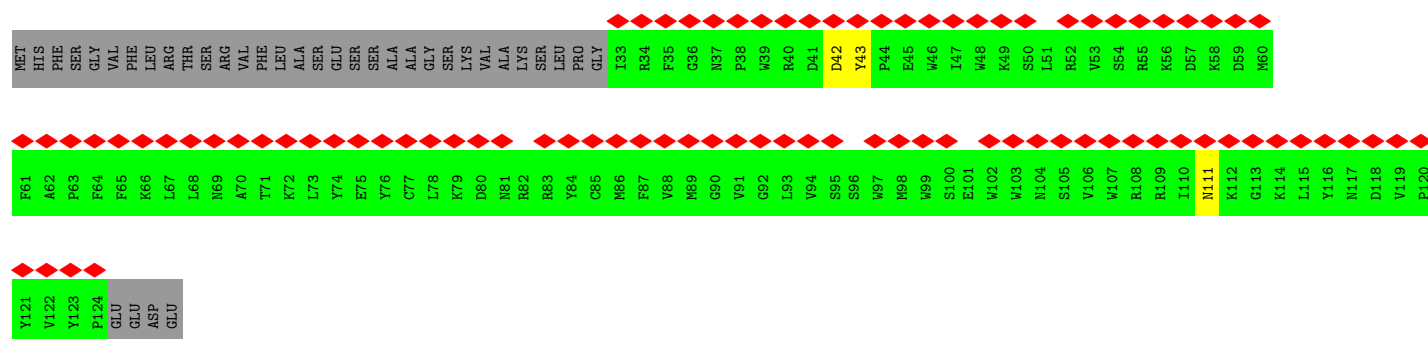




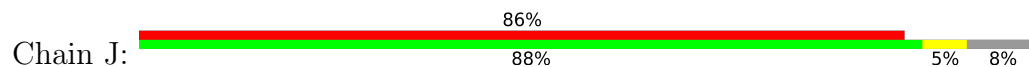
- Molecule 9: Ubiquinol-cytochrome C family reductase UQCRX/QCR9-like protein

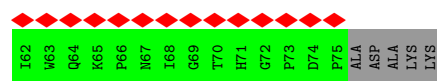


- Molecule 9: Ubiquinol-cytochrome C family reductase UQCRX/QCR9-like protein

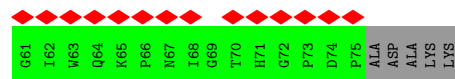
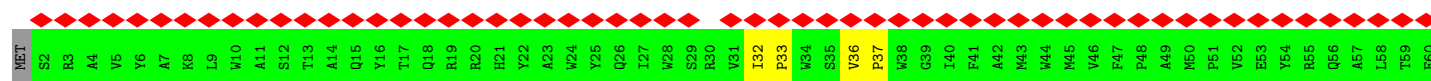
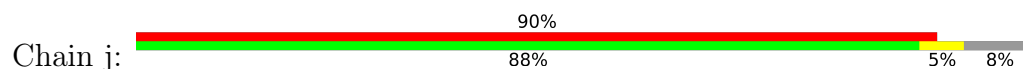


- Molecule 10: Transmembrane protein

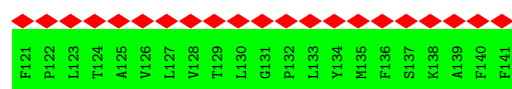
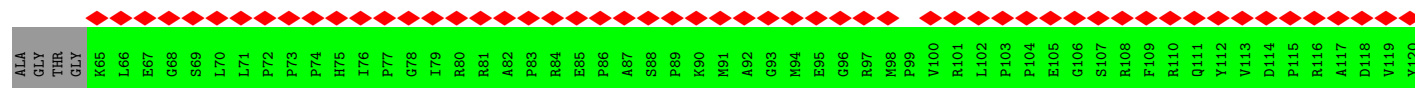




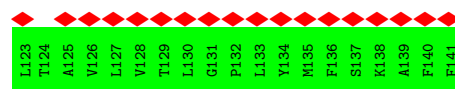
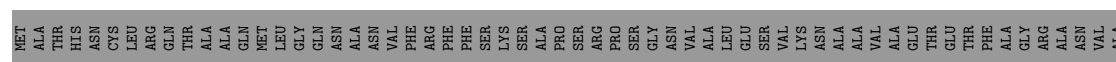
• Molecule 10: Transmembrane protein



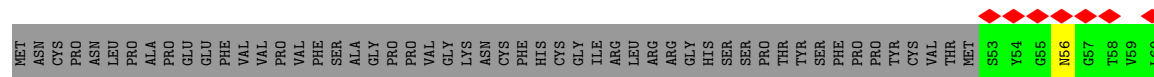
• Molecule 11: Transmembrane protein

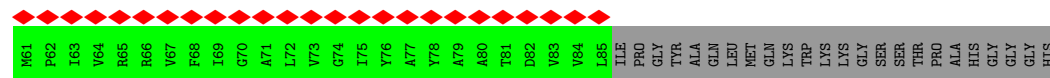


• Molecule 11: Transmembrane protein



• Molecule 12: Transmembrane protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2056878	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 ( $e^-/\text{\AA}^2$ )	36	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	9.712	Depositor
Minimum map value	-4.441	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	398.4, 398.4, 398.4	wwPDB
Map dimensions	480, 480, 480	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: HEC, HEM, CDL, A1IJD, MG, PC1, ZN

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	0.14	0/2970	0.28	0/4057
1	a	0.14	0/2970	0.28	0/4057
2	B	0.14	0/2032	0.28	0/2771
2	b	0.14	0/2032	0.28	0/2771
3	C	0.16	0/1746	0.31	0/2383
3	c	0.17	0/1746	0.31	0/2383
4	D	0.14	0/3729	0.30	0/5051
4	d	0.14	0/3729	0.30	0/5051
5	E	0.13	0/3895	0.28	0/5284
5	e	0.13	0/3895	0.28	0/5284
6	F	0.12	0/747	0.24	0/1009
6	f	0.12	0/747	0.24	0/1009
7	G	0.15	0/1621	0.30	0/2200
7	g	0.15	0/1621	0.30	0/2200
8	H	0.16	0/866	0.29	0/1178
8	h	0.16	0/866	0.29	0/1178
9	I	0.14	0/843	0.30	0/1143
9	i	0.14	0/843	0.30	0/1143
10	J	0.14	0/656	0.28	0/901
10	j	0.14	0/656	0.29	0/901
11	K	0.13	0/628	0.27	0/853
11	k	0.13	0/628	0.27	0/853
12	L	0.11	0/250	0.25	0/341
12	l	0.11	0/250	0.25	0/341
All	All	0.14	0/39966	0.29	0/54342

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	2882	2958	2959	12	0
1	a	2882	2958	2959	11	0
2	B	1962	1880	1880	3	0
2	b	1962	1880	1880	2	0
3	C	1686	1572	1572	7	0
3	c	1686	1572	1572	5	0
4	D	3653	3610	3610	6	0
4	d	3653	3610	3610	6	0
5	E	3806	3773	3772	15	0
5	e	3806	3773	3772	16	0
6	F	727	702	702	3	0
6	f	727	702	702	3	0
7	G	1568	1525	1525	4	0
7	g	1568	1525	1525	4	0
8	H	828	778	779	2	0
8	h	828	778	779	2	0
9	I	811	786	786	1	0
9	i	811	786	786	2	0
10	J	626	600	600	2	0
10	j	626	600	600	2	0
11	K	607	625	625	0	0
11	k	607	625	625	0	0
12	L	246	258	258	1	0
12	l	246	258	258	1	0
13	A	100	156	156	0	0
13	C	200	312	312	3	0
13	D	100	156	156	2	0
13	G	100	156	156	0	0
13	H	200	312	312	0	0
13	I	100	156	156	0	0
13	L	100	156	156	3	0
13	a	100	156	156	0	0
13	c	200	312	312	1	0
13	d	100	156	156	2	0
13	g	200	312	312	3	0
13	h	100	156	156	0	0
14	A	77	38	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	a	77	38	0	0	0
15	A	86	60	60	6	0
15	a	86	60	60	6	0
16	A	1	0	0	0	0
16	a	1	0	0	0	0
17	B	43	31	30	0	0
17	b	43	31	30	0	0
18	C	54	88	88	1	0
18	i	54	88	88	1	0
19	D	1	0	0	0	0
19	d	1	0	0	0	0
20	A	59	30	0	0	0
20	B	36	6	0	0	0
20	C	40	0	0	0	0
20	D	67	2	0	0	0
20	E	26	0	0	0	0
20	F	2	0	0	0	0
20	G	65	12	0	0	0
20	H	30	8	0	0	0
20	I	7	0	0	0	0
20	J	6	0	0	0	0
20	K	3	0	0	0	0
20	L	2	0	0	0	0
20	a	61	30	0	0	0
20	b	36	6	0	0	0
20	c	39	0	0	0	0
20	d	68	2	0	0	0
20	e	26	0	0	0	0
20	f	2	0	0	0	0
20	g	61	12	0	0	0
20	h	27	8	0	0	0
20	i	8	0	0	0	0
20	j	6	0	0	0	0
20	k	3	0	0	0	0
20	l	3	0	0	0	0
All	All	41611	41180	40988	117	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 1.

The worst 5 of 117 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)
4:D:48:VAL:O	4:D:53:ARG:NH2	2.12	0.82
4:d:48:VAL:O	4:d:53:ARG:NH2	2.12	0.82
7:G:34:LYS:O	7:G:39:ARG:NH1	2.16	0.79
7:g:34:LYS:O	7:g:39:ARG:NH1	2.16	0.77
5:E:249:GLU:N	5:E:249:GLU:OE1	2.18	0.77

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	358/360 (99%)	347 (97%)	9 (2%)	2 (1%)	22	11
1	a	358/360 (99%)	347 (97%)	9 (2%)	2 (1%)	22	11
2	B	241/398 (61%)	231 (96%)	9 (4%)	1 (0%)	30	19
2	b	241/398 (61%)	231 (96%)	9 (4%)	1 (0%)	30	19
3	C	203/487 (42%)	197 (97%)	6 (3%)	0	100	100
3	c	203/487 (42%)	197 (97%)	6 (3%)	0	100	100
4	D	460/509 (90%)	444 (96%)	16 (4%)	0	100	100
4	d	460/509 (90%)	444 (96%)	16 (4%)	0	100	100
5	E	481/563 (85%)	464 (96%)	16 (3%)	1 (0%)	44	31
5	e	481/563 (85%)	464 (96%)	16 (3%)	1 (0%)	44	31
6	F	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
6	f	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
7	G	190/234 (81%)	187 (98%)	3 (2%)	0	100	100
7	g	190/234 (81%)	187 (98%)	3 (2%)	0	100	100
8	H	94/122 (77%)	93 (99%)	1 (1%)	0	100	100
8	h	94/122 (77%)	93 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	90/128 (70%)	87 (97%)	3 (3%)	0	100	100
9	i	90/128 (70%)	87 (97%)	3 (3%)	0	100	100
10	J	72/80 (90%)	69 (96%)	3 (4%)	0	100	100
10	j	72/80 (90%)	69 (96%)	3 (4%)	0	100	100
11	K	75/141 (53%)	73 (97%)	2 (3%)	0	100	100
11	k	75/141 (53%)	73 (97%)	2 (3%)	0	100	100
12	L	31/109 (28%)	30 (97%)	1 (3%)	0	100	100
12	l	31/109 (28%)	30 (97%)	1 (3%)	0	100	100
All	All	4762/6440 (74%)	4612 (97%)	142 (3%)	8 (0%)	45	31

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	VAL
1	a	166	VAL
2	B	322	GLU
2	b	322	GLU
1	A	157	VAL

### 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	311/311 (100%)	309 (99%)	2 (1%)	84	82
1	a	311/311 (100%)	309 (99%)	2 (1%)	84	82
2	B	206/338 (61%)	203 (98%)	3 (2%)	60	53
2	b	206/338 (61%)	203 (98%)	3 (2%)	60	53
3	C	184/421 (44%)	183 (100%)	1 (0%)	86	86
3	c	184/421 (44%)	183 (100%)	1 (0%)	86	86
4	D	393/428 (92%)	393 (100%)	0	100	100
4	d	393/428 (92%)	393 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	414/468 (88%)	413 (100%)	1 (0%)	92	91
5	e	414/468 (88%)	413 (100%)	1 (0%)	92	91
6	F	80/81 (99%)	80 (100%)	0	100	100
6	f	80/81 (99%)	80 (100%)	0	100	100
7	G	162/193 (84%)	162 (100%)	0	100	100
7	g	162/193 (84%)	162 (100%)	0	100	100
8	H	85/104 (82%)	85 (100%)	0	100	100
8	h	85/104 (82%)	85 (100%)	0	100	100
9	I	86/115 (75%)	86 (100%)	0	100	100
9	i	86/115 (75%)	86 (100%)	0	100	100
10	J	62/66 (94%)	62 (100%)	0	100	100
10	j	62/66 (94%)	62 (100%)	0	100	100
11	K	65/111 (59%)	65 (100%)	0	100	100
11	k	65/111 (59%)	65 (100%)	0	100	100
12	L	25/88 (28%)	25 (100%)	0	100	100
12	l	25/88 (28%)	25 (100%)	0	100	100
All	All	4146/5448 (76%)	4132 (100%)	14 (0%)	90	90

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	168	ASP
1	a	310	LEU
5	e	236	PHE
2	b	378	TRP
3	c	347	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	314	GLN
3	c	195	GLN
9	i	111	ASN
3	c	165	ASN
4	d	261	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
13	CDL	c	501	-	99,99,99	0.29	0	105,111,111	0.24	0
14	A1IJD	A	402[A]	-	35,36,36	0.33	0	50,53,53	0.28	0
14	A1IJD	a	402[A]	-	35,36,36	0.33	0	50,53,53	0.28	0
13	CDL	C	503	-	99,99,99	0.29	0	105,111,111	0.24	0
13	CDL	C	502	-	99,99,99	0.29	0	105,111,111	0.26	0
13	CDL	d	601	-	99,99,99	0.31	0	105,111,111	0.28	0
15	HEM	A	404	1	41,50,50	1.47	4 (9%)	45,82,82	1.34	7 (15%)
13	CDL	L	201	-	99,99,99	0.30	0	105,111,111	0.26	0
18	PC1	i	501	-	53,53,53	0.30	0	59,61,61	0.26	0
13	CDL	c	502	-	99,99,99	0.29	0	105,111,111	0.26	0
13	CDL	I	201	-	99,99,99	0.31	0	105,111,111	0.28	0
15	HEM	A	405	1	41,50,50	1.50	3 (7%)	45,82,82	1.31	5 (11%)
15	HEM	a	405	1	41,50,50	1.49	3 (7%)	45,82,82	1.30	5 (11%)
13	CDL	H	201	-	99,99,99	0.30	0	105,111,111	0.25	0
13	CDL	g	302	-	99,99,99	0.29	0	105,111,111	0.25	0
18	PC1	C	501	-	53,53,53	0.30	0	59,61,61	0.26	0
13	CDL	D	601	-	99,99,99	0.31	0	105,111,111	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	A1IJD	A	402[B]	-	35,36,36	0.33	0	50,53,53	0.30	0
14	A1IJD	a	402[B]	-	35,36,36	0.33	0	50,53,53	0.30	0
13	CDL	h	201	-	99,99,99	0.30	0	105,111,111	0.25	0
13	CDL	G	301	-	99,99,99	0.29	0	105,111,111	0.25	0
13	CDL	g	301	-	99,99,99	0.30	0	105,111,111	0.26	0
17	HEC	B	401	2	32,50,50	2.27	4 (12%)	24,82,82	1.19	0
13	CDL	a	401	-	99,99,99	0.29	0	105,111,111	0.25	0
13	CDL	A	401	-	99,99,99	0.29	0	105,111,111	0.24	0
17	HEC	b	401	2	32,50,50	2.27	4 (12%)	24,82,82	1.18	0
13	CDL	H	202	-	99,99,99	0.30	0	105,111,111	0.28	0
14	A1IJD	A	403	-	35,36,36	0.33	0	50,53,53	0.32	0
14	A1IJD	a	403	-	35,36,36	0.32	0	50,53,53	0.32	0
15	HEM	a	404	1	41,50,50	1.46	4 (9%)	45,82,82	1.33	7 (15%)

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
13	CDL	c	501	-	-	18/110/110/110	-
14	A1IJD	A	402[A]	-	-	3/15/15/15	0/4/4/4
14	A1IJD	a	402[A]	-	-	3/15/15/15	0/4/4/4
13	CDL	C	503	-	-	18/110/110/110	-
13	CDL	C	502	-	-	22/110/110/110	-
13	CDL	d	601	-	-	42/110/110/110	-
15	HEM	A	404	1	-	3/12/54/54	-
13	CDL	L	201	-	-	27/110/110/110	-
18	PC1	i	501	-	-	27/57/57/57	-
13	CDL	c	502	-	-	22/110/110/110	-
13	CDL	I	201	-	-	38/110/110/110	-
15	HEM	A	405	1	-	4/12/54/54	-
15	HEM	a	405	1	-	4/12/54/54	-
13	CDL	H	201	-	-	18/110/110/110	-
13	CDL	g	302	-	-	21/110/110/110	-
18	PC1	C	501	-	-	27/57/57/57	-
13	CDL	D	601	-	-	42/110/110/110	-
14	A1IJD	A	402[B]	-	-	0/15/15/15	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	A1IJD	a	402[B]	-	-	0/15/15/15	0/4/4/4
13	CDL	h	201	-	-	18/110/110/110	-
13	CDL	G	301	-	-	21/110/110/110	-
13	CDL	g	301	-	-	27/110/110/110	-
17	HEC	B	401	2	-	2/10/54/54	-
13	CDL	a	401	-	-	21/110/110/110	-
13	CDL	A	401	-	-	21/110/110/110	-
17	HEC	b	401	2	-	2/10/54/54	-
13	CDL	H	202	-	-	38/110/110/110	-
14	A1IJD	A	403	-	-	2/15/15/15	0/4/4/4
14	A1IJD	a	403	-	-	2/15/15/15	0/4/4/4
15	HEM	a	404	1	-	3/12/54/54	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	401	HEC	C2B-C3B	-6.81	1.33	1.40
17	b	401	HEC	C2B-C3B	-6.81	1.33	1.40
17	B	401	HEC	C3C-C2C	-6.77	1.33	1.40
17	b	401	HEC	C3C-C2C	-6.77	1.33	1.40
17	b	401	HEC	C3D-C2D	5.40	1.53	1.37

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	405	HEM	C1B-NB-C4B	3.18	108.36	105.07
15	A	405	HEM	C1B-NB-C4B	3.15	108.33	105.07
15	A	404	HEM	C4B-CHC-C1C	2.86	126.33	122.56
15	A	404	HEM	C4C-CHD-C1D	2.86	126.33	122.56
15	a	404	HEM	C4C-CHD-C1D	2.86	126.33	122.56

There are no chirality outliers.

5 of 496 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	401	CDL	CA3-OA5-PA1-OA3
13	C	502	CDL	CB2-C1-CA2-OA2
13	C	502	CDL	CA2-OA2-PA1-OA4
13	C	502	CDL	CB3-OB5-PB2-OB2

*Continued on next page...*

*Continued from previous page...*

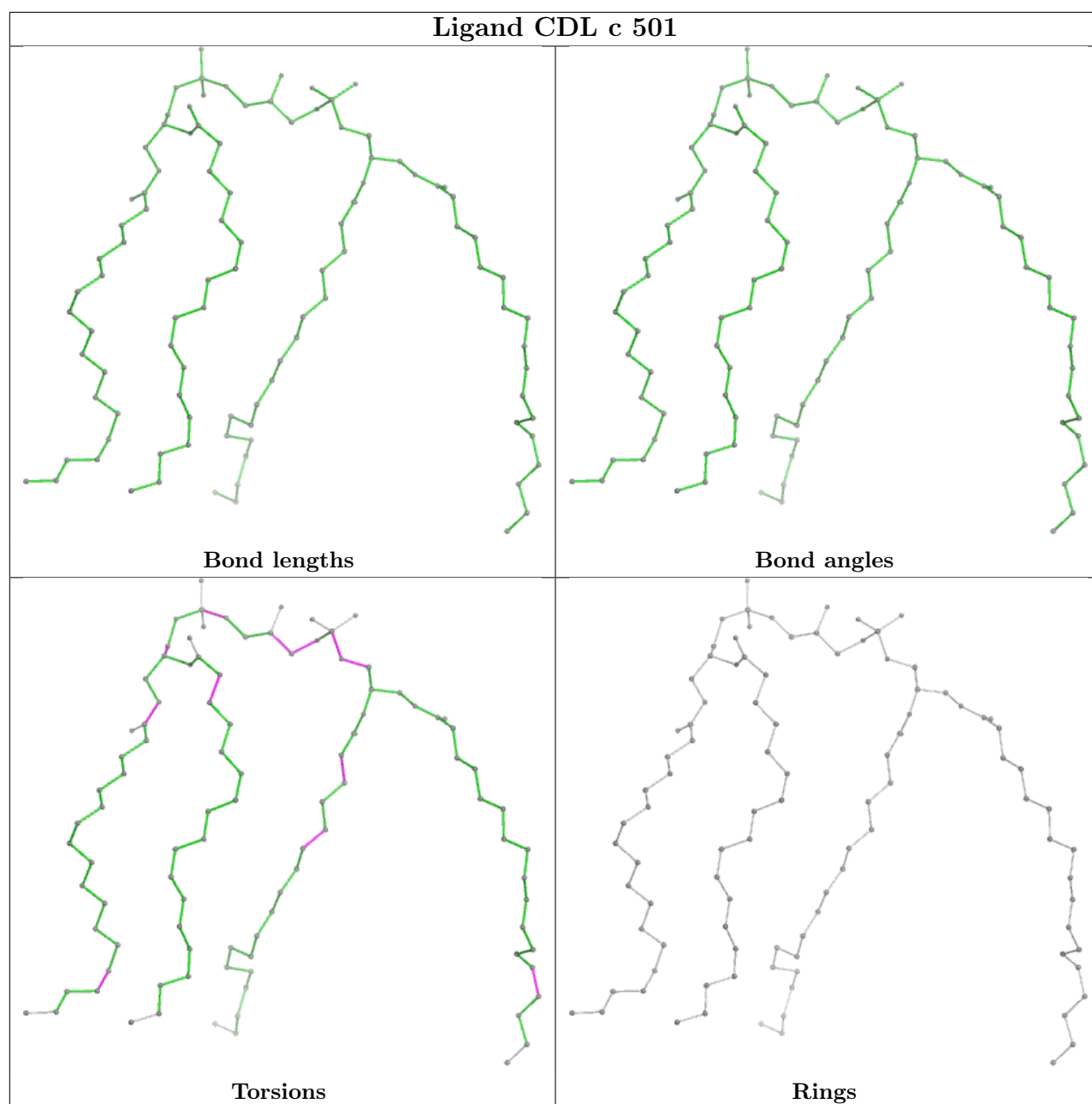
Mol	Chain	Res	Type	Atoms
13	C	503	CDL	O1-C1-CA2-OA2

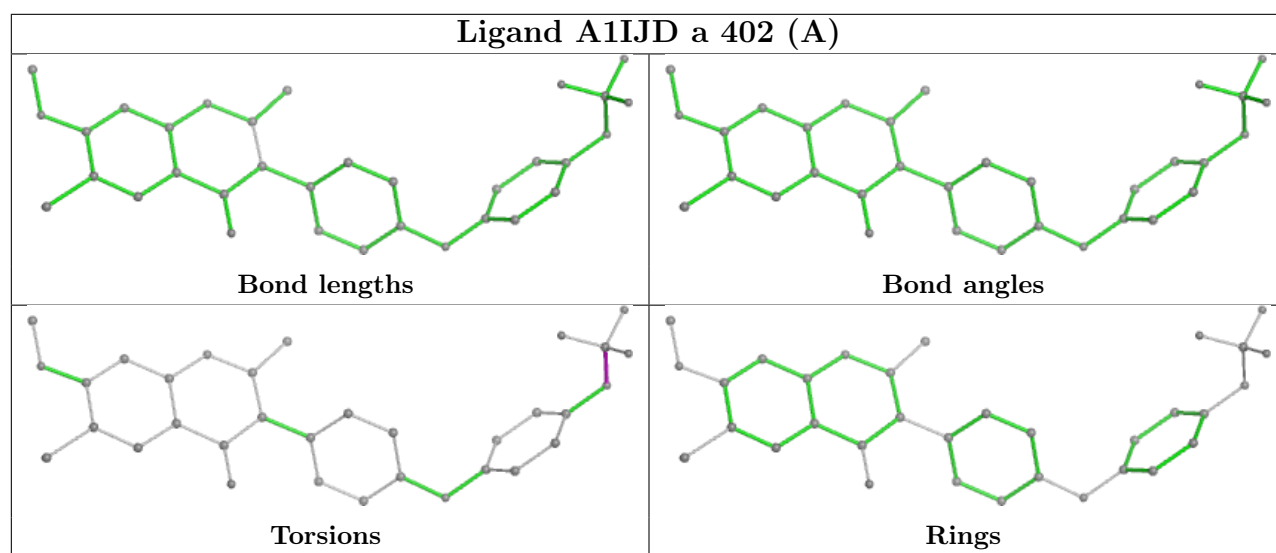
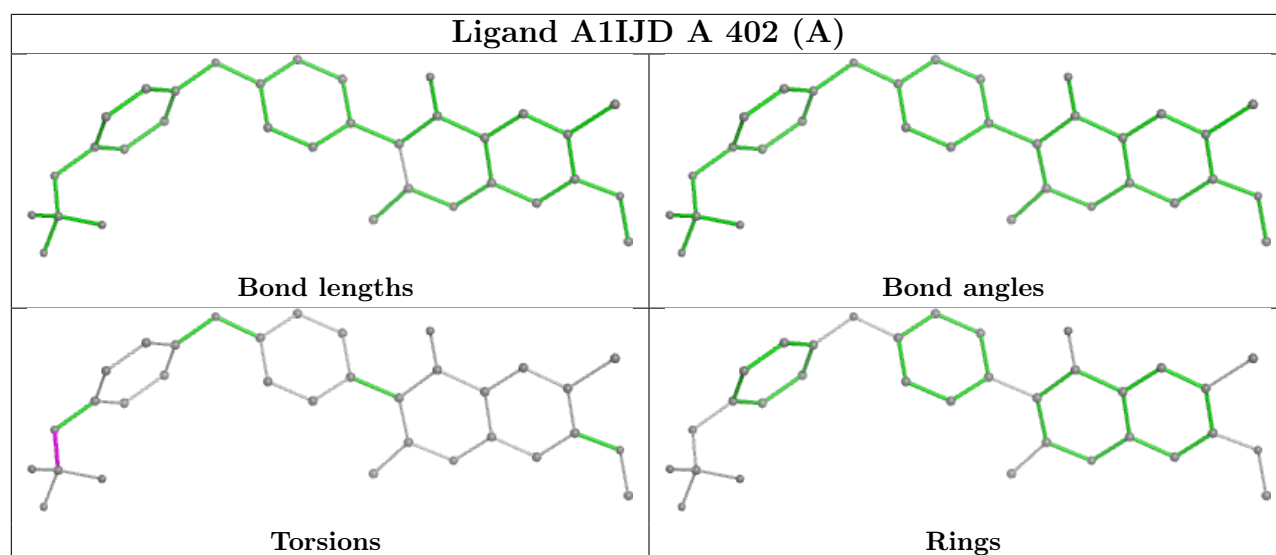
There are no ring outliers.

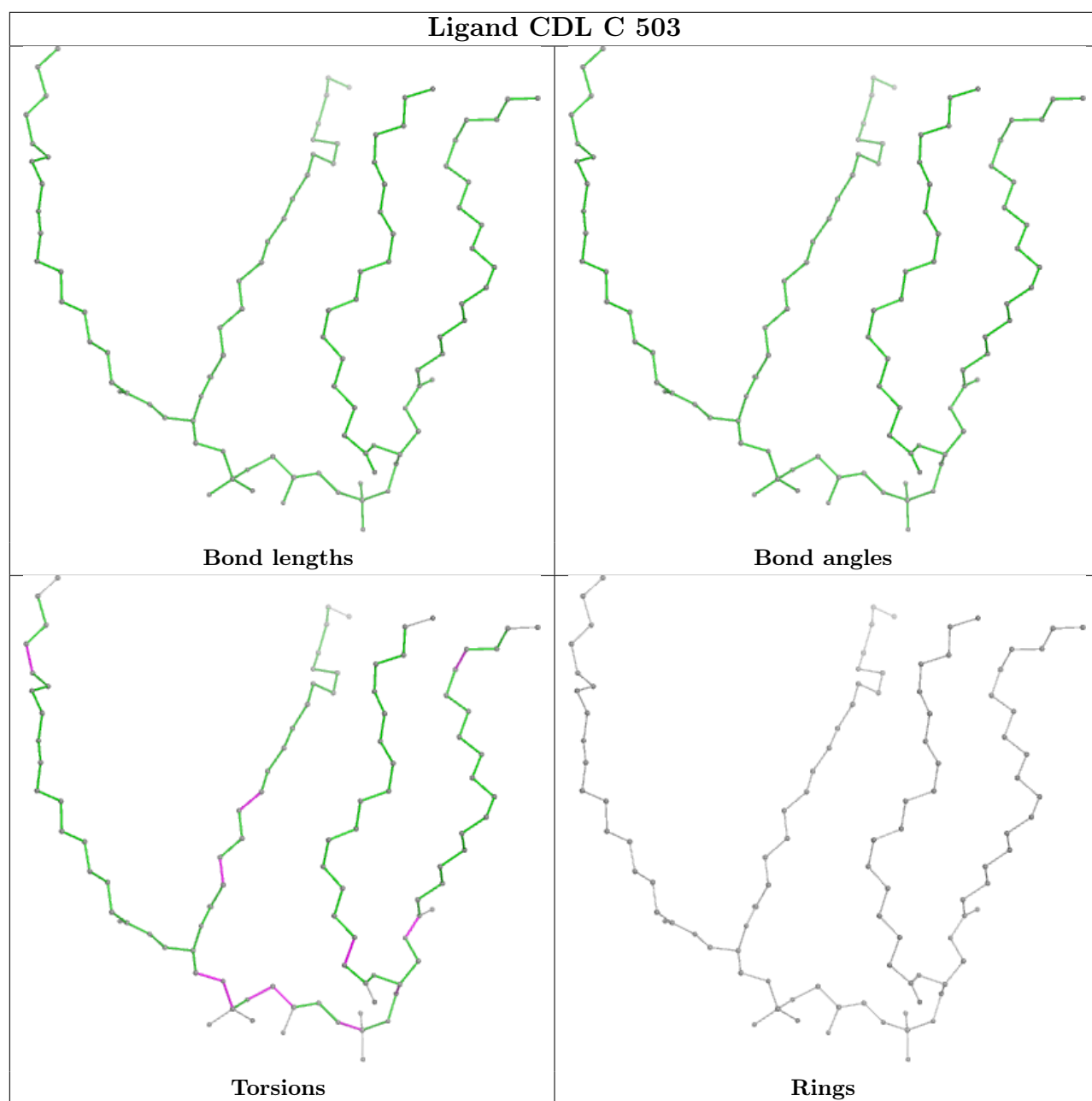
13 monomers are involved in 26 short contacts:

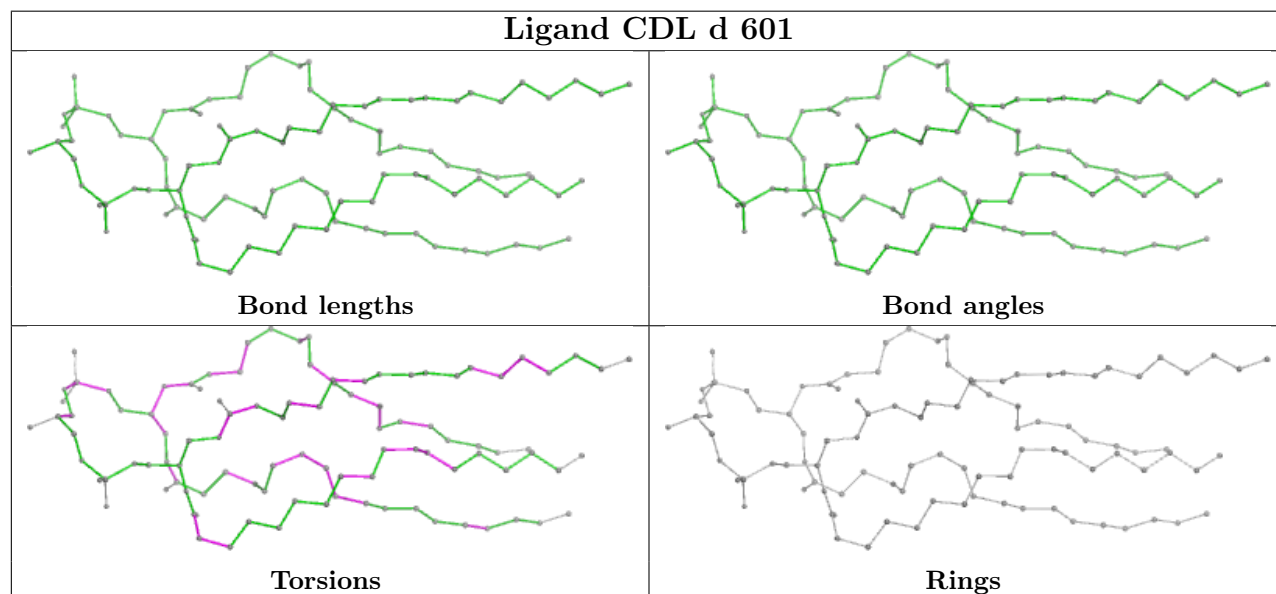
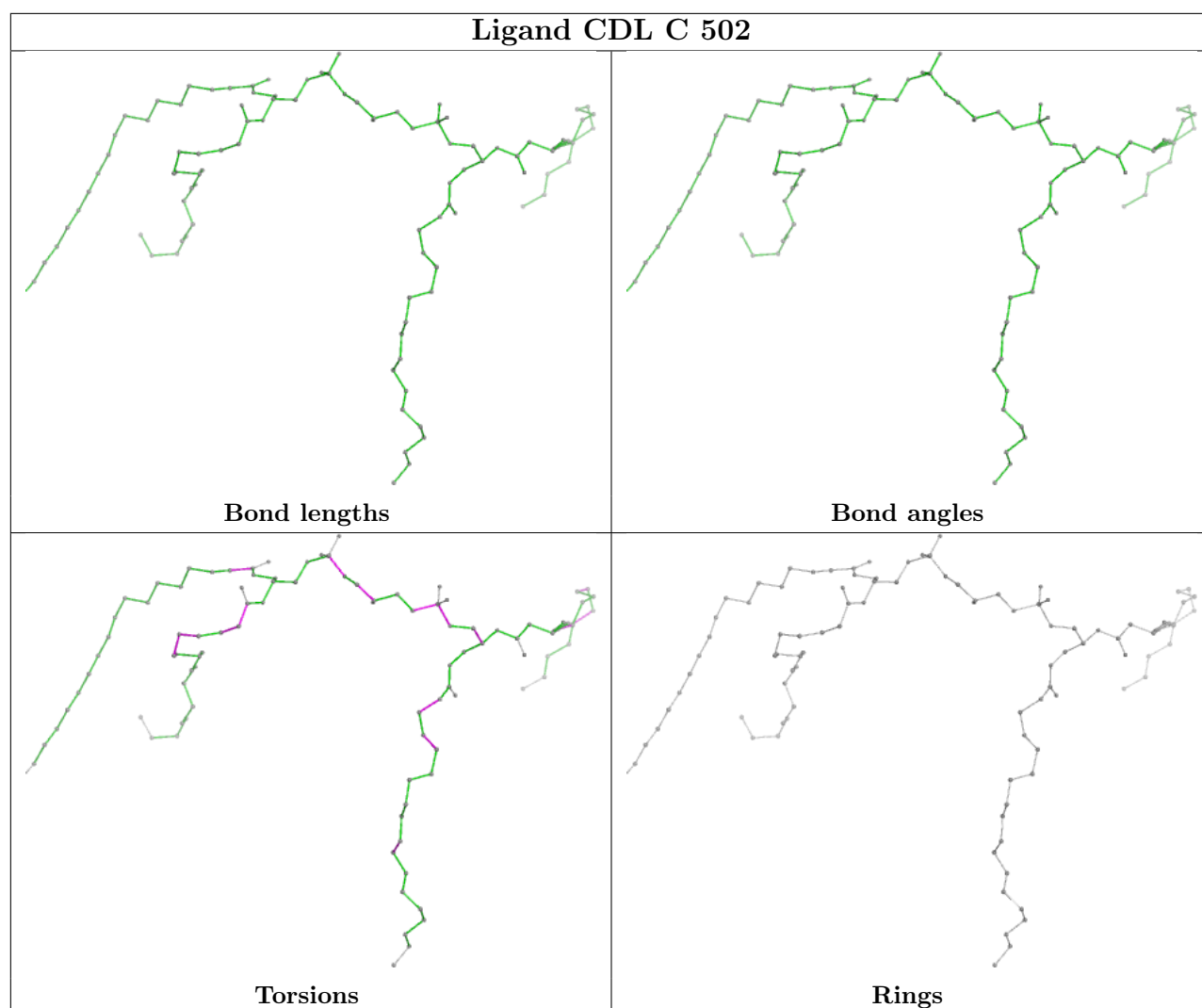
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	503	CDL	1	0
13	C	502	CDL	2	0
13	d	601	CDL	2	0
15	A	404	HEM	4	0
13	L	201	CDL	3	0
18	i	501	PC1	1	0
13	c	502	CDL	1	0
15	A	405	HEM	2	0
15	a	405	HEM	2	0
18	C	501	PC1	1	0
13	D	601	CDL	2	0
13	g	301	CDL	3	0
15	a	404	HEM	4	0

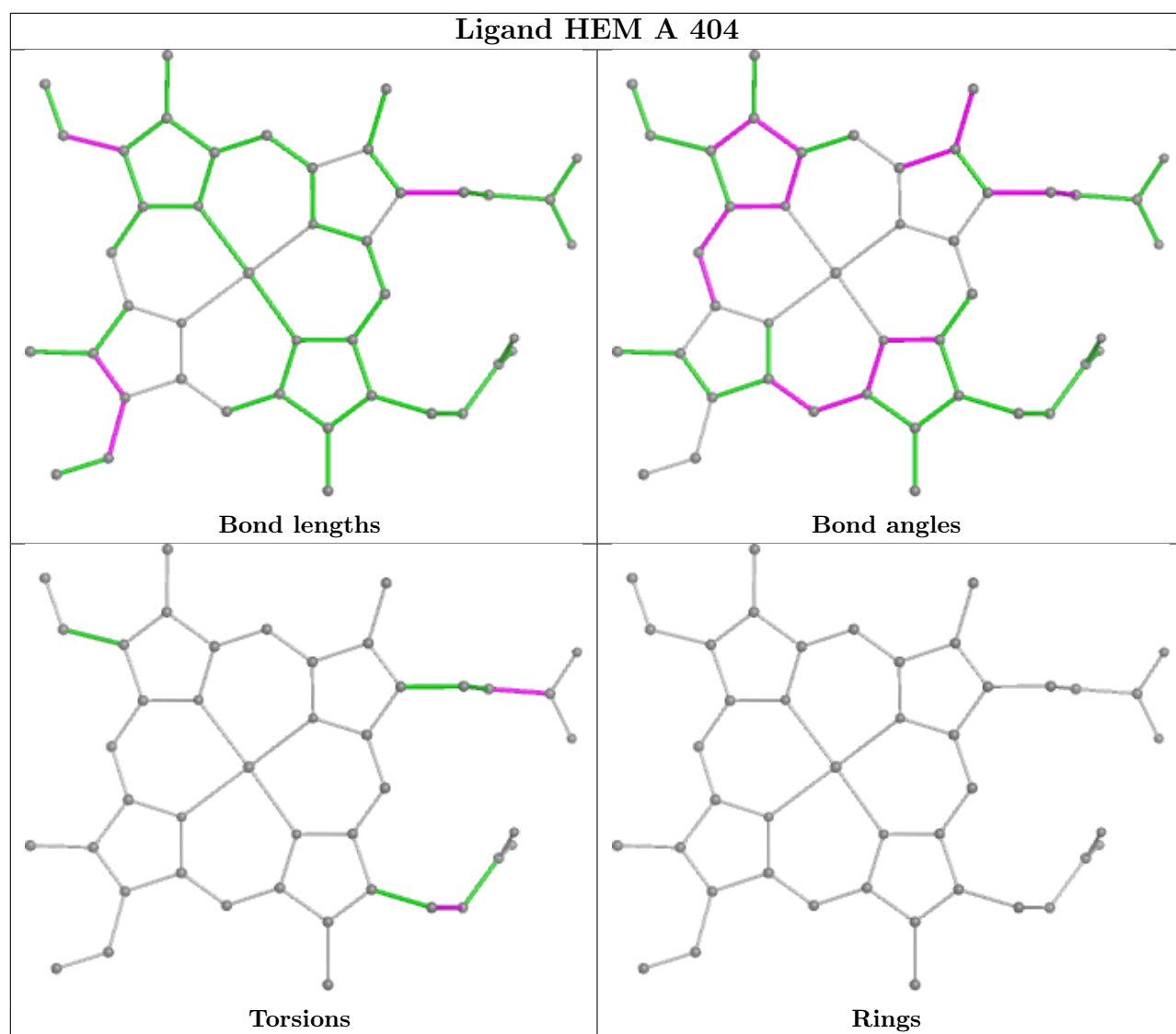
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

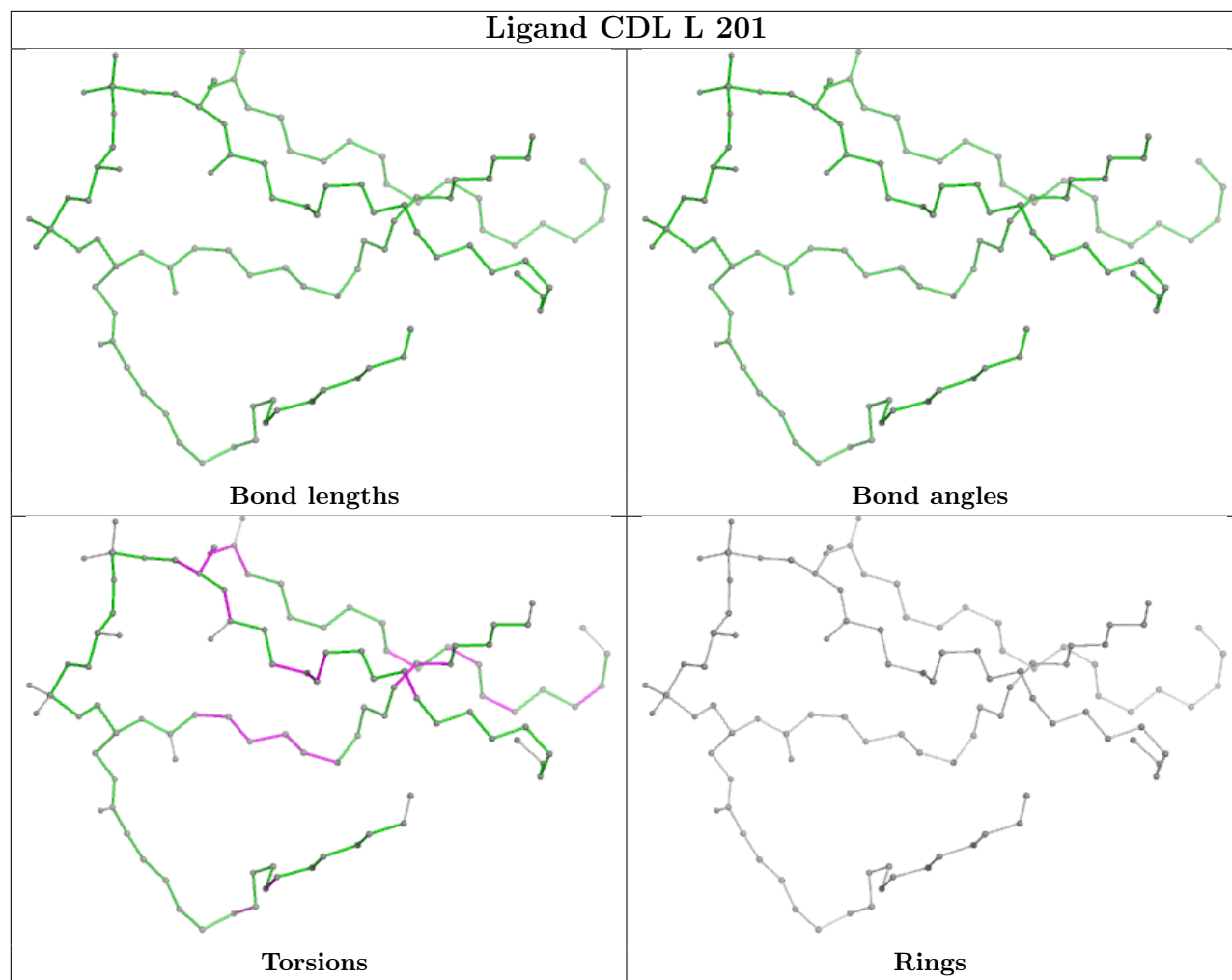




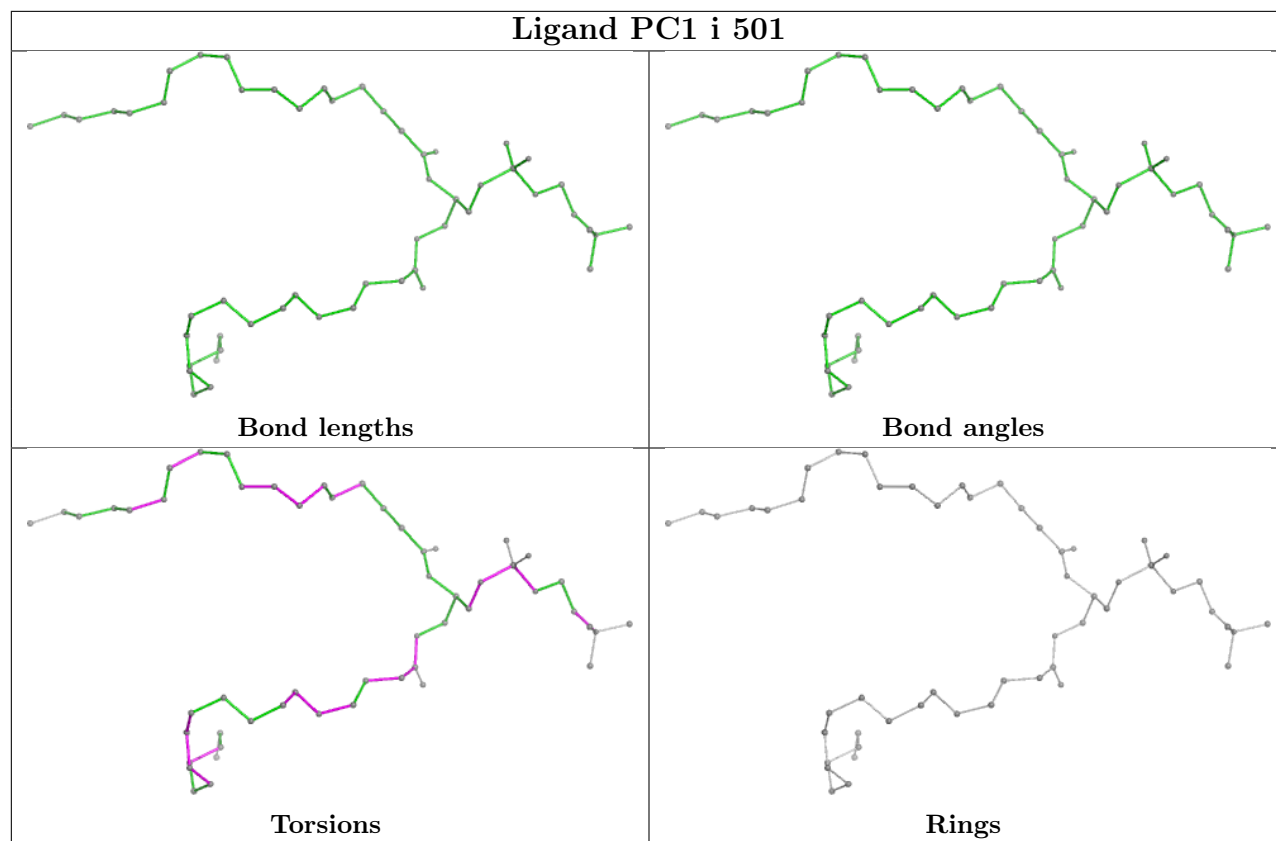


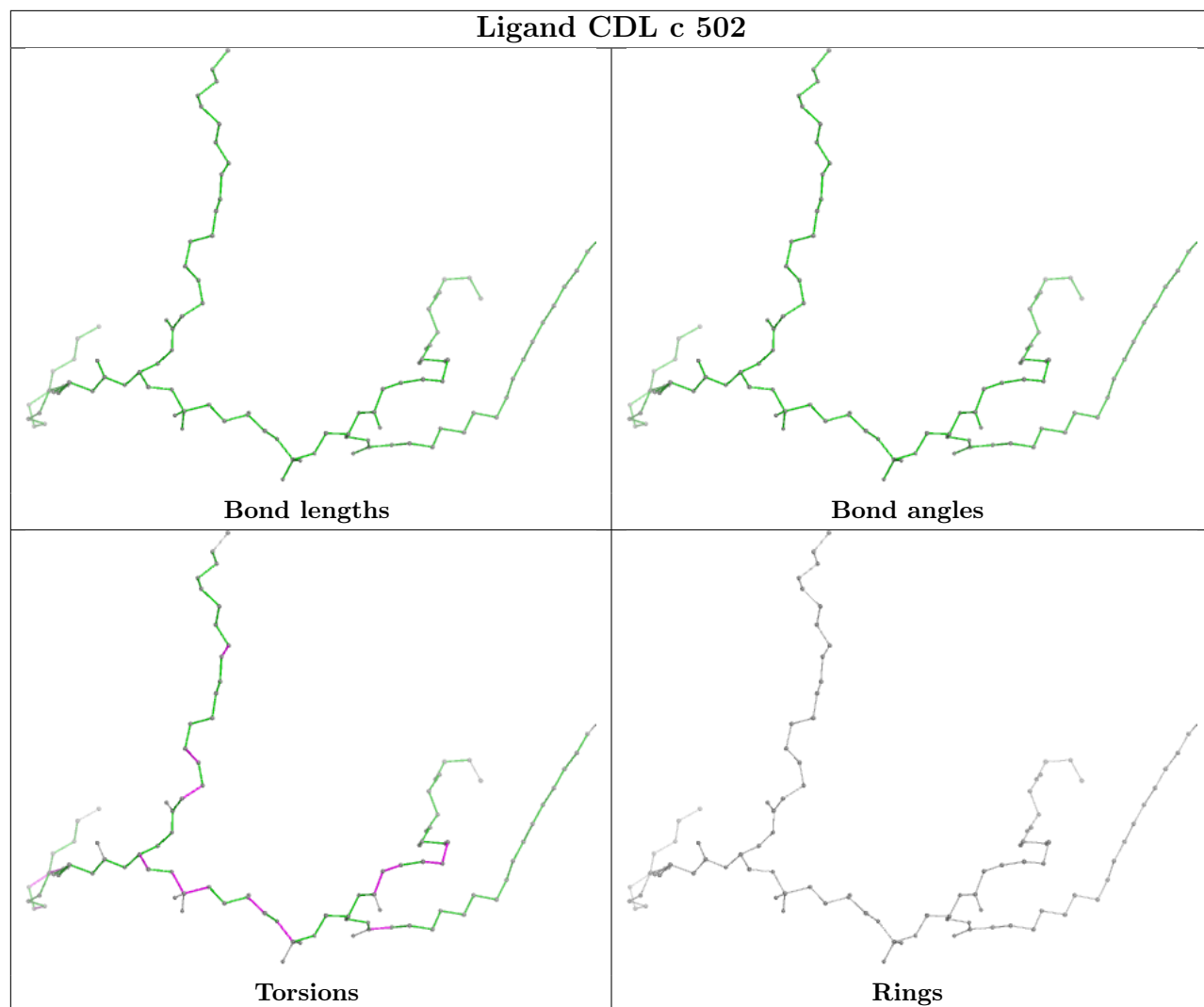


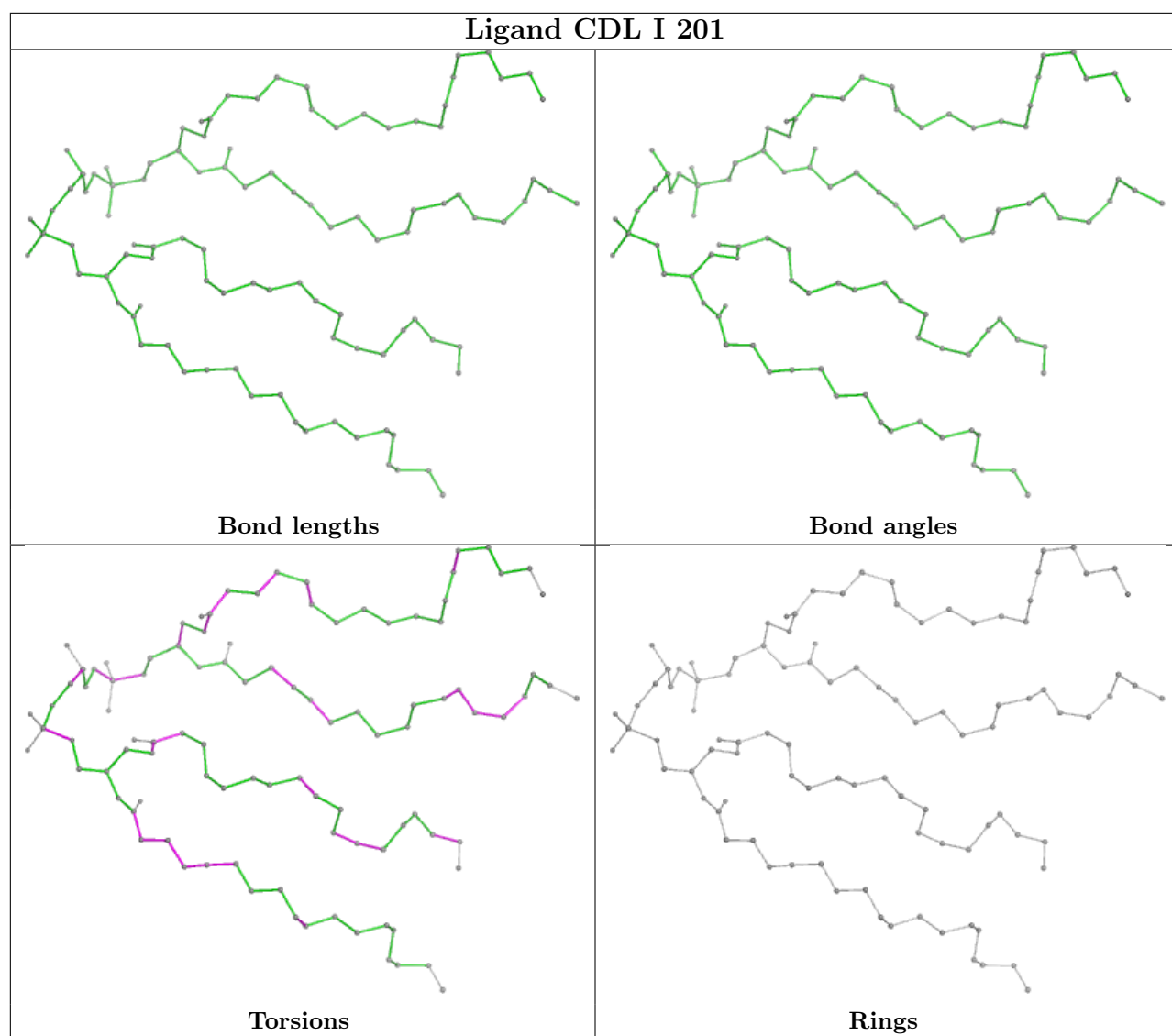


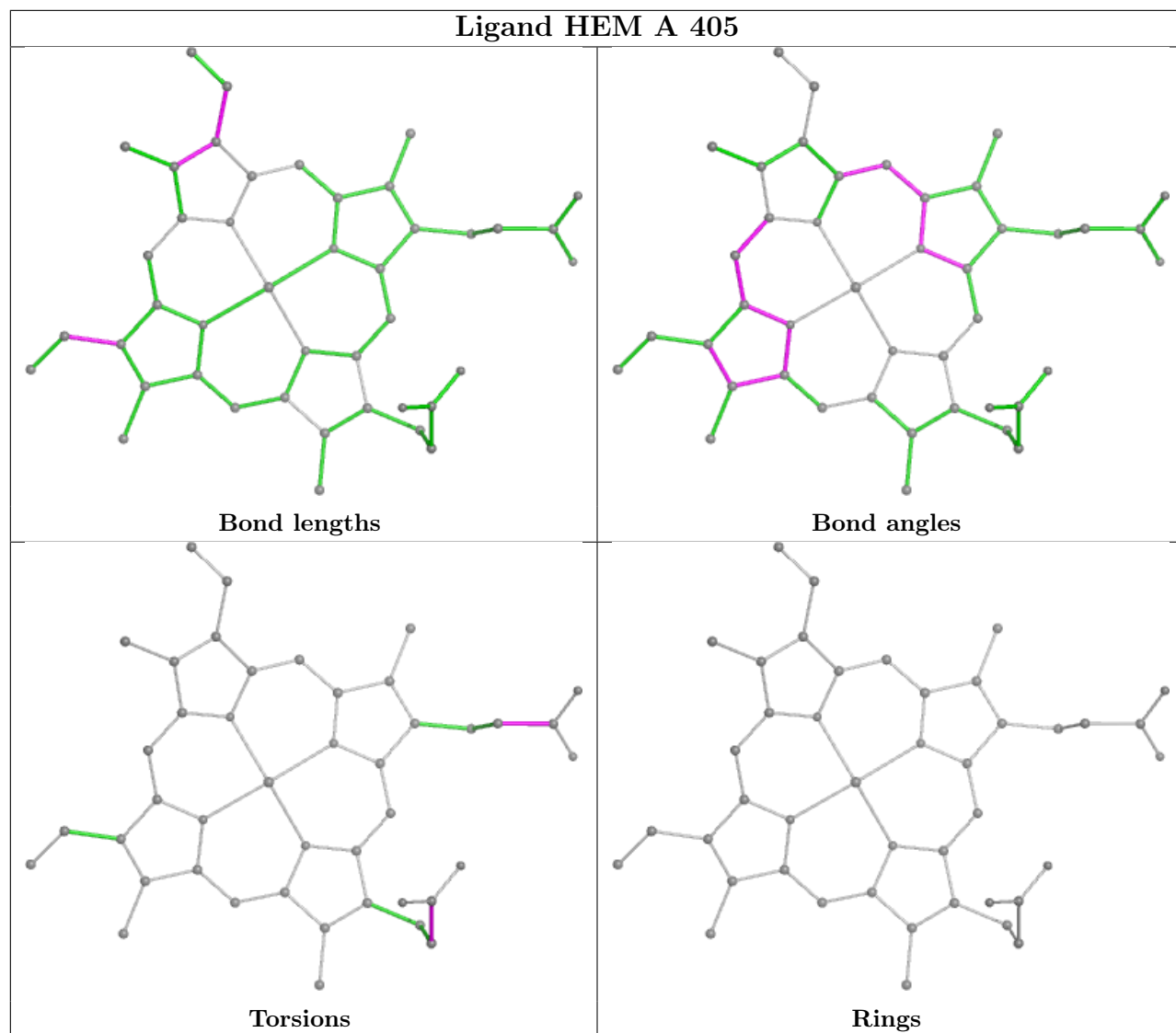


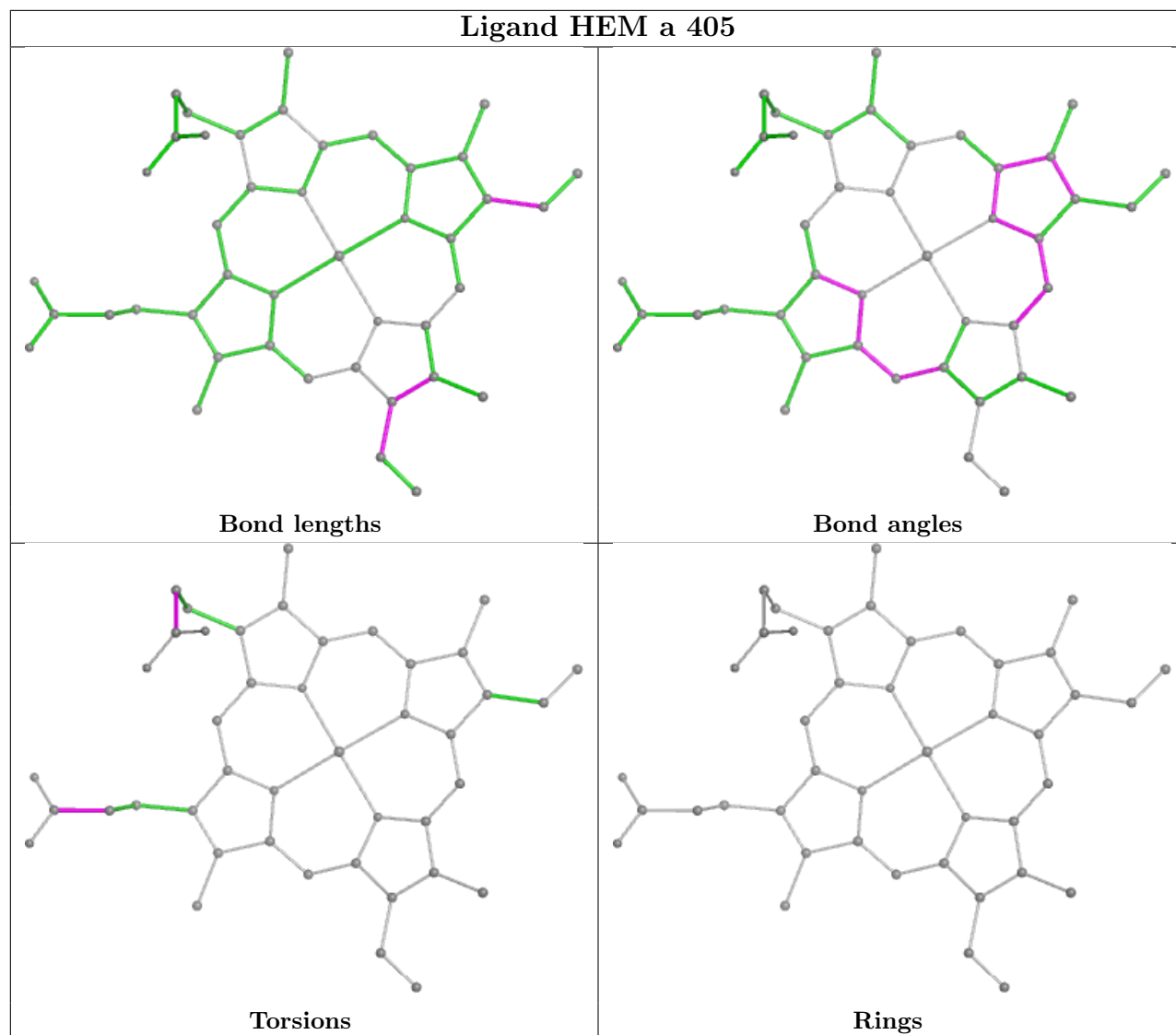


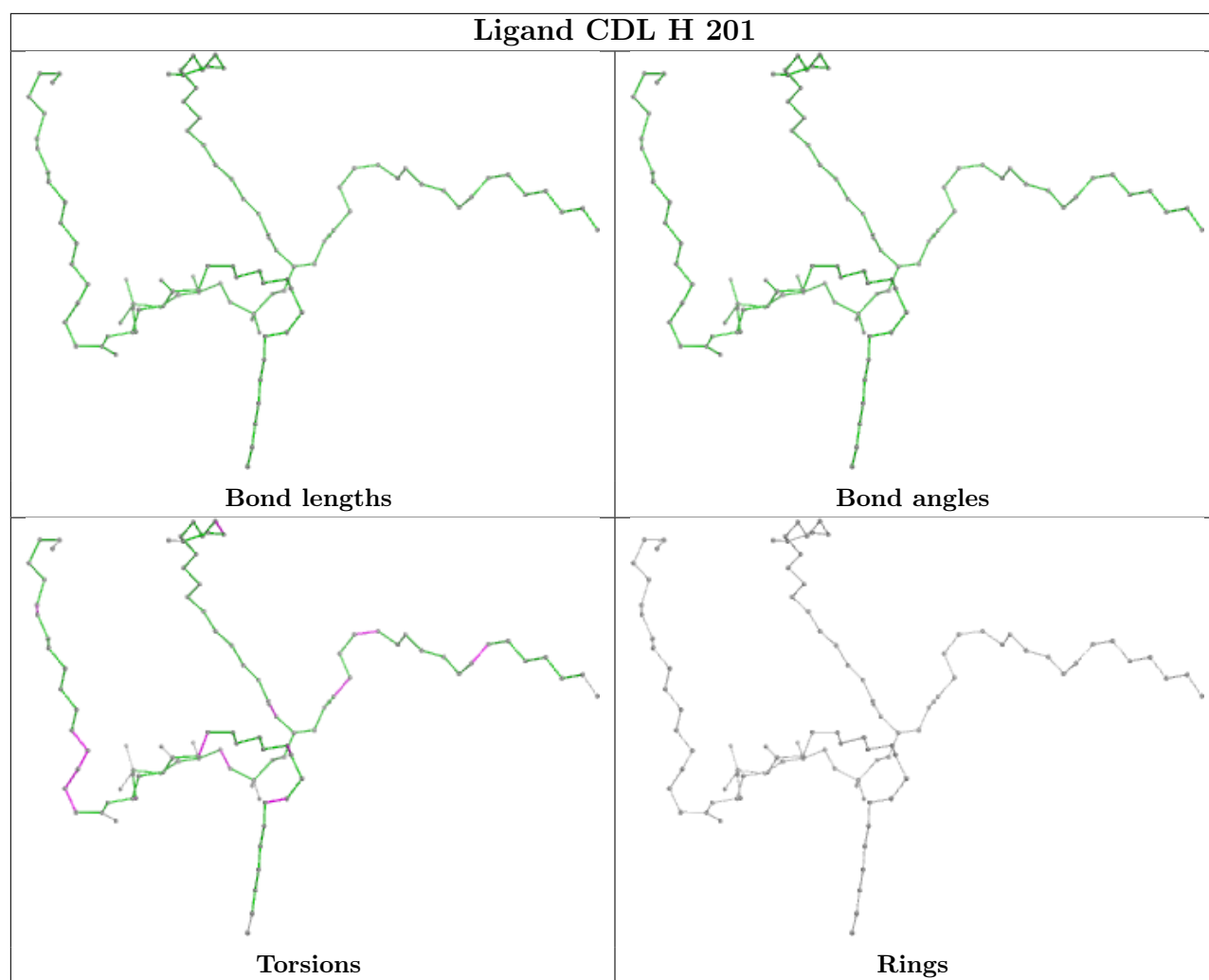


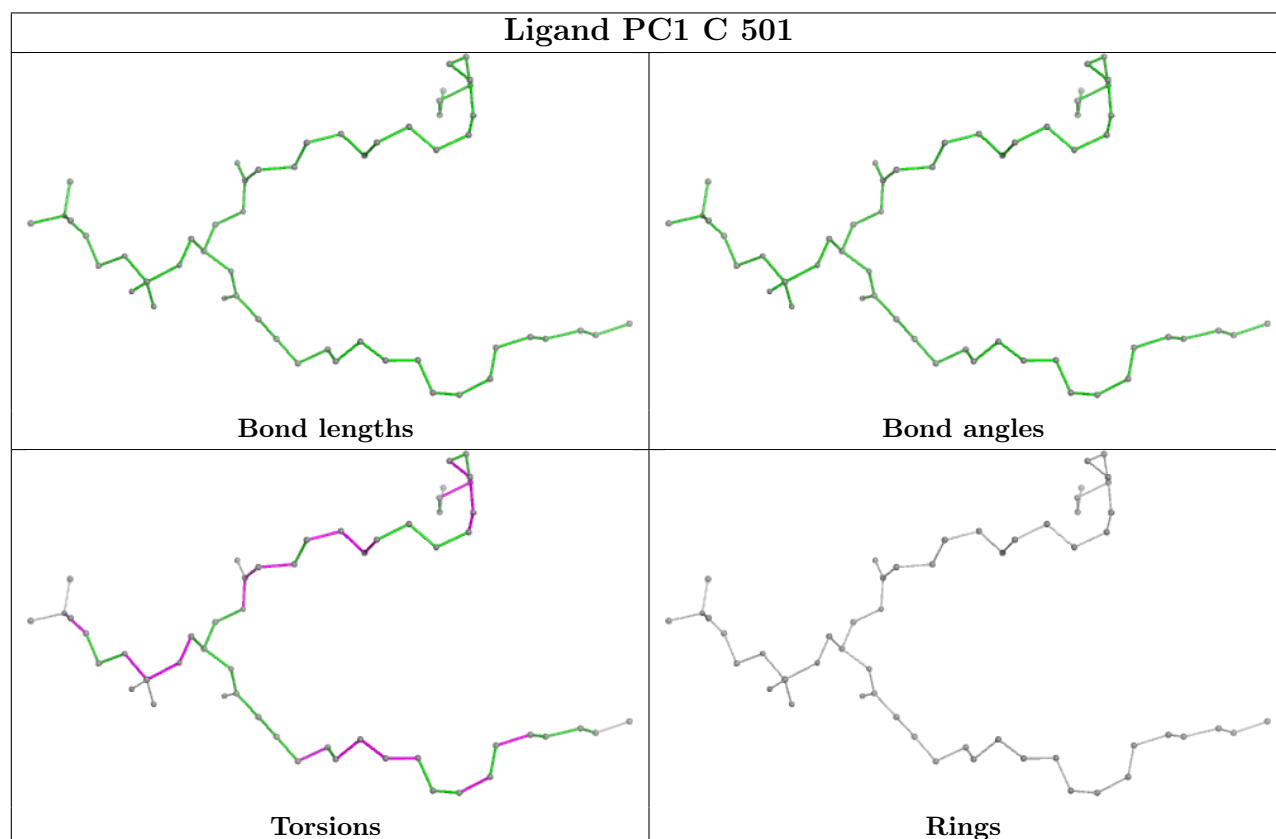
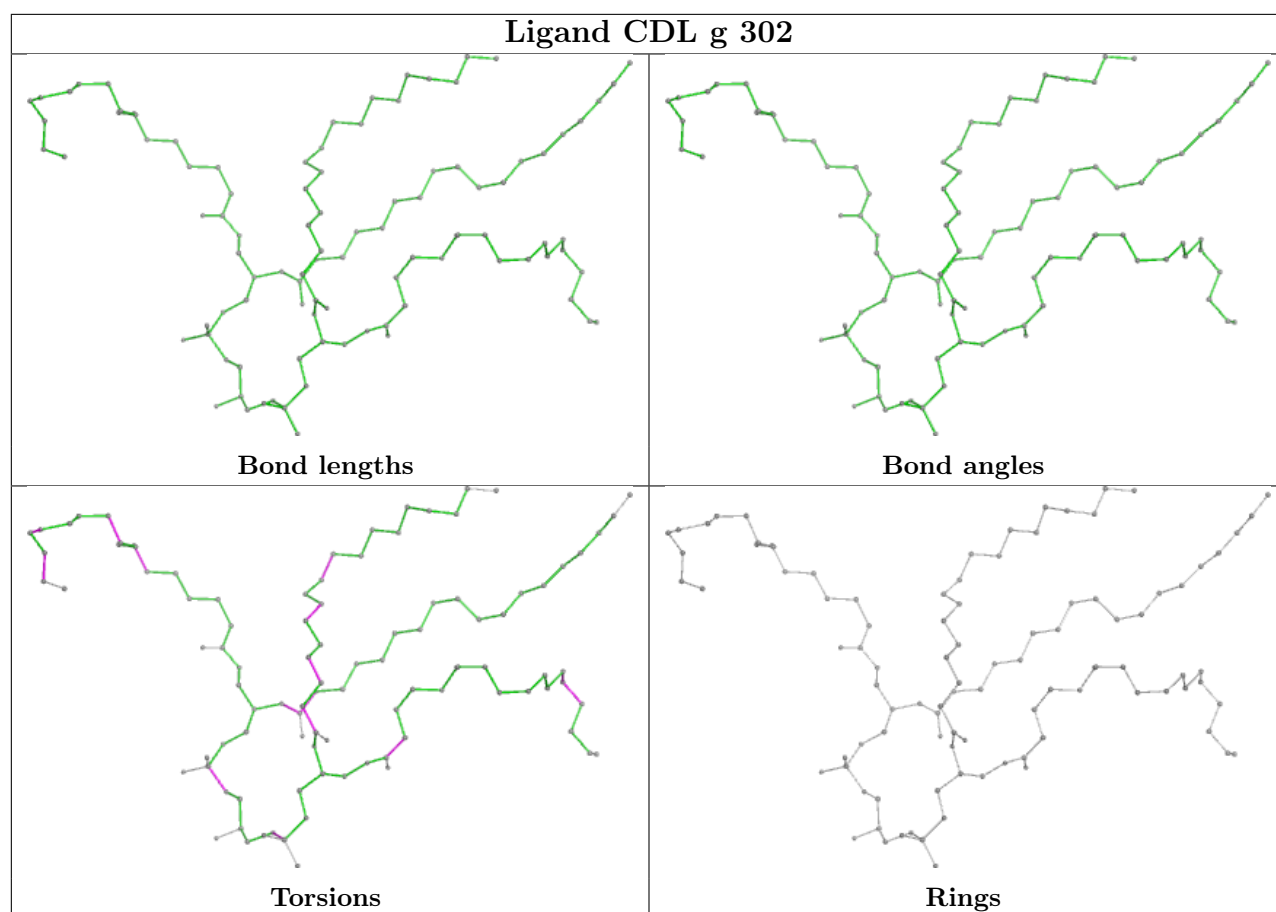


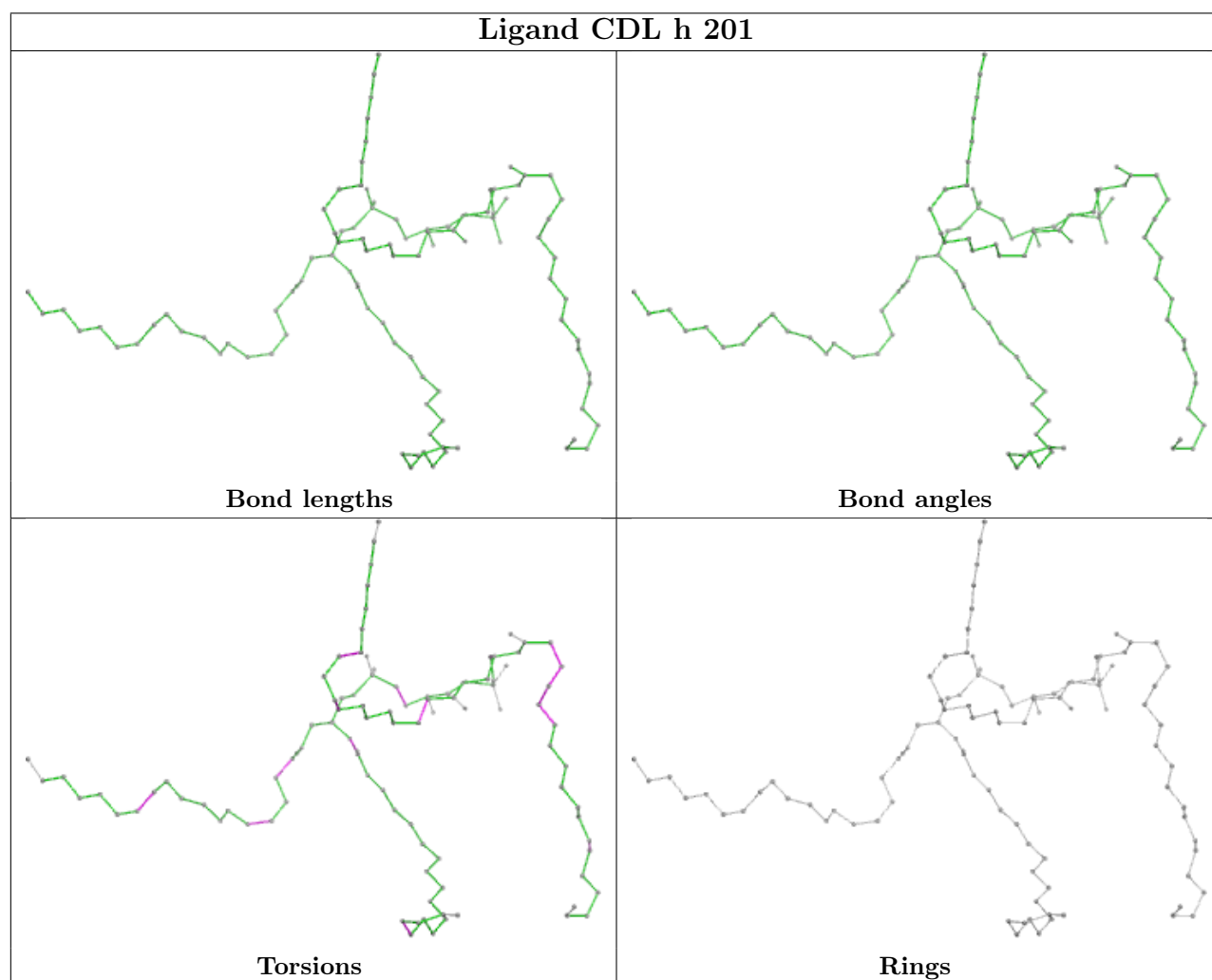
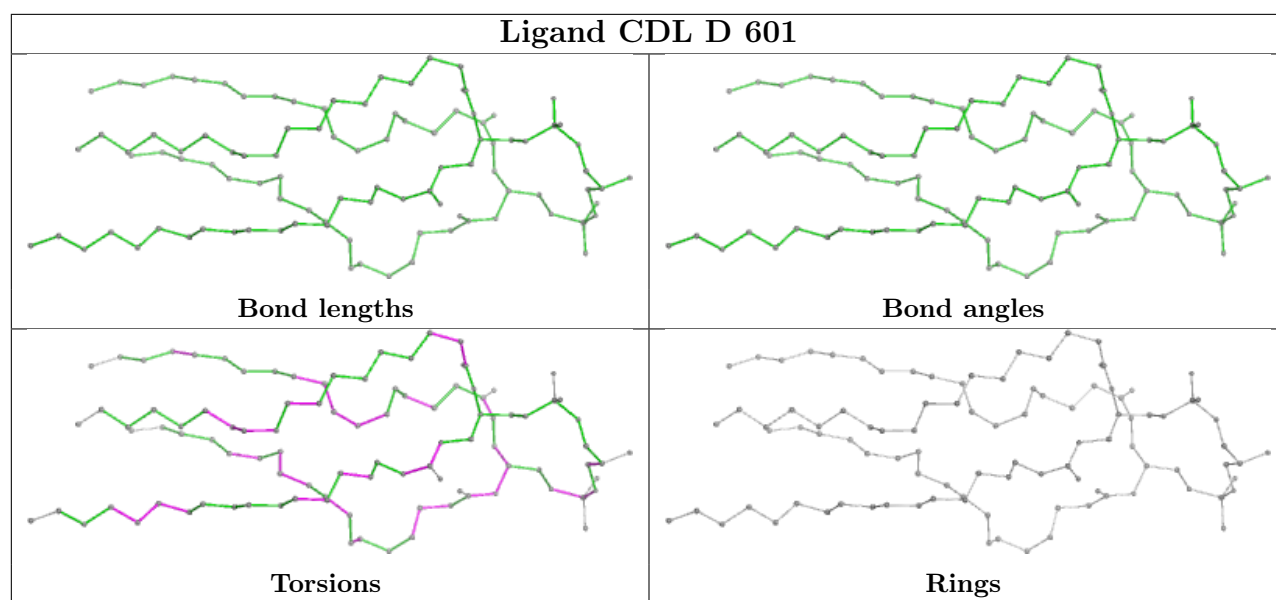




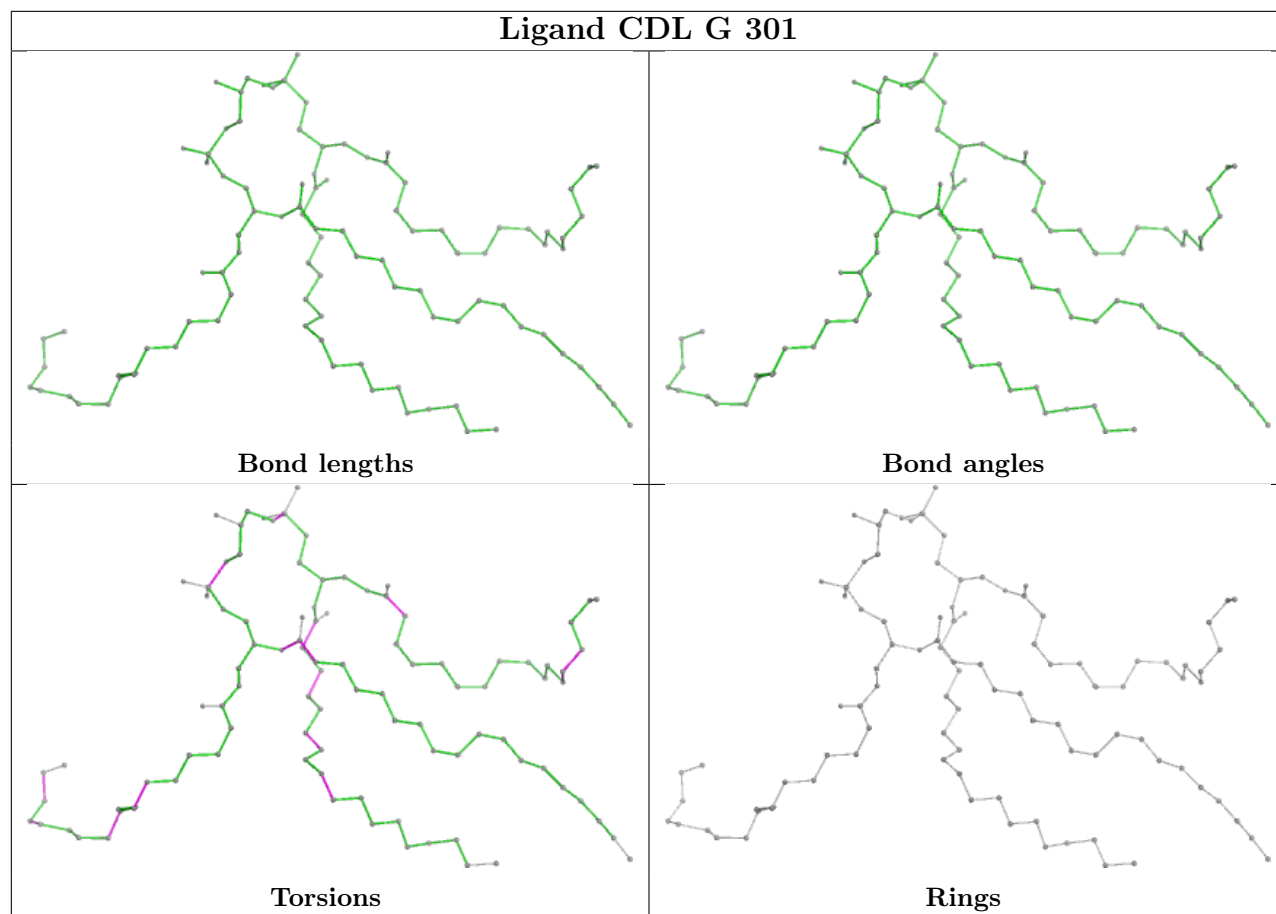


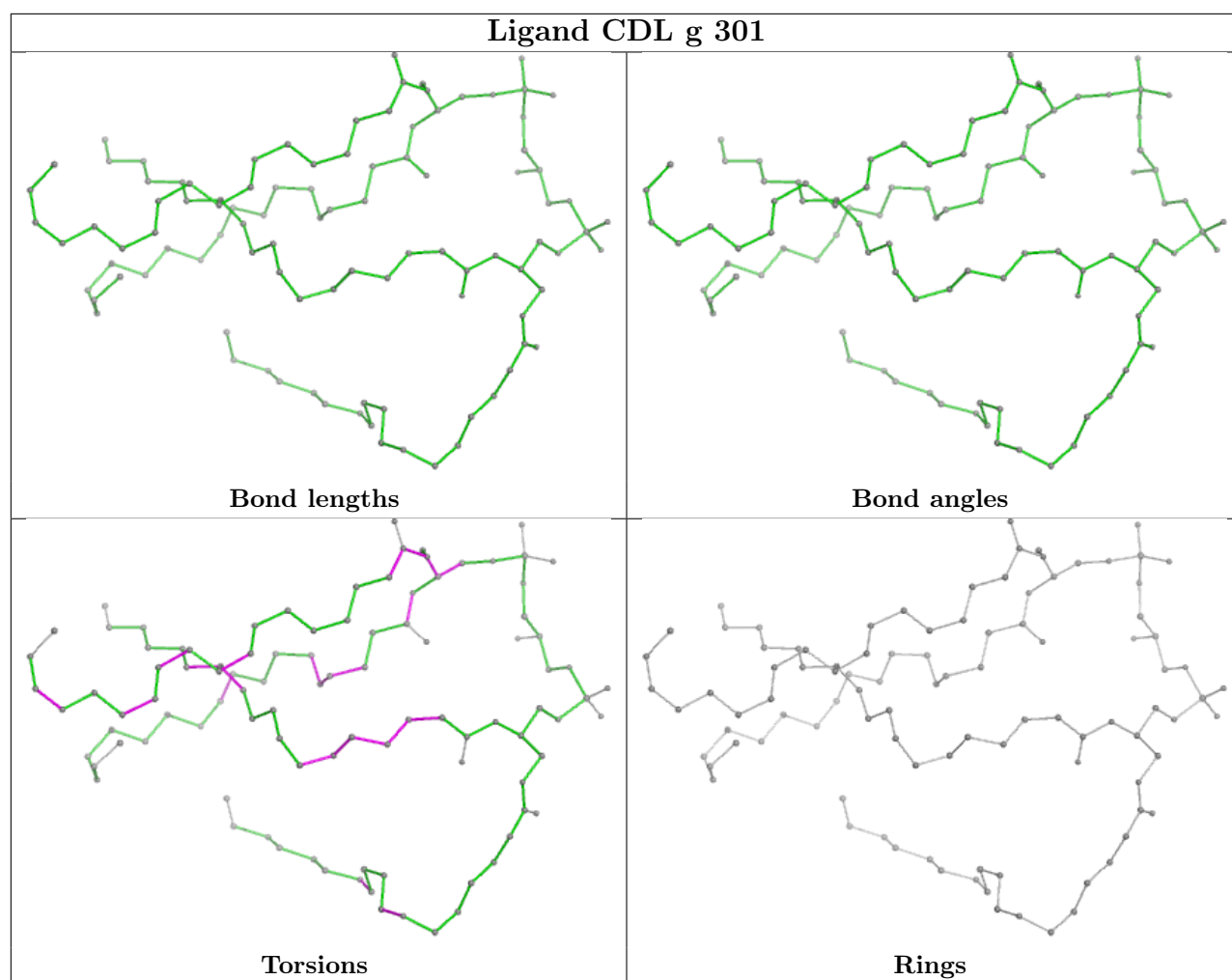


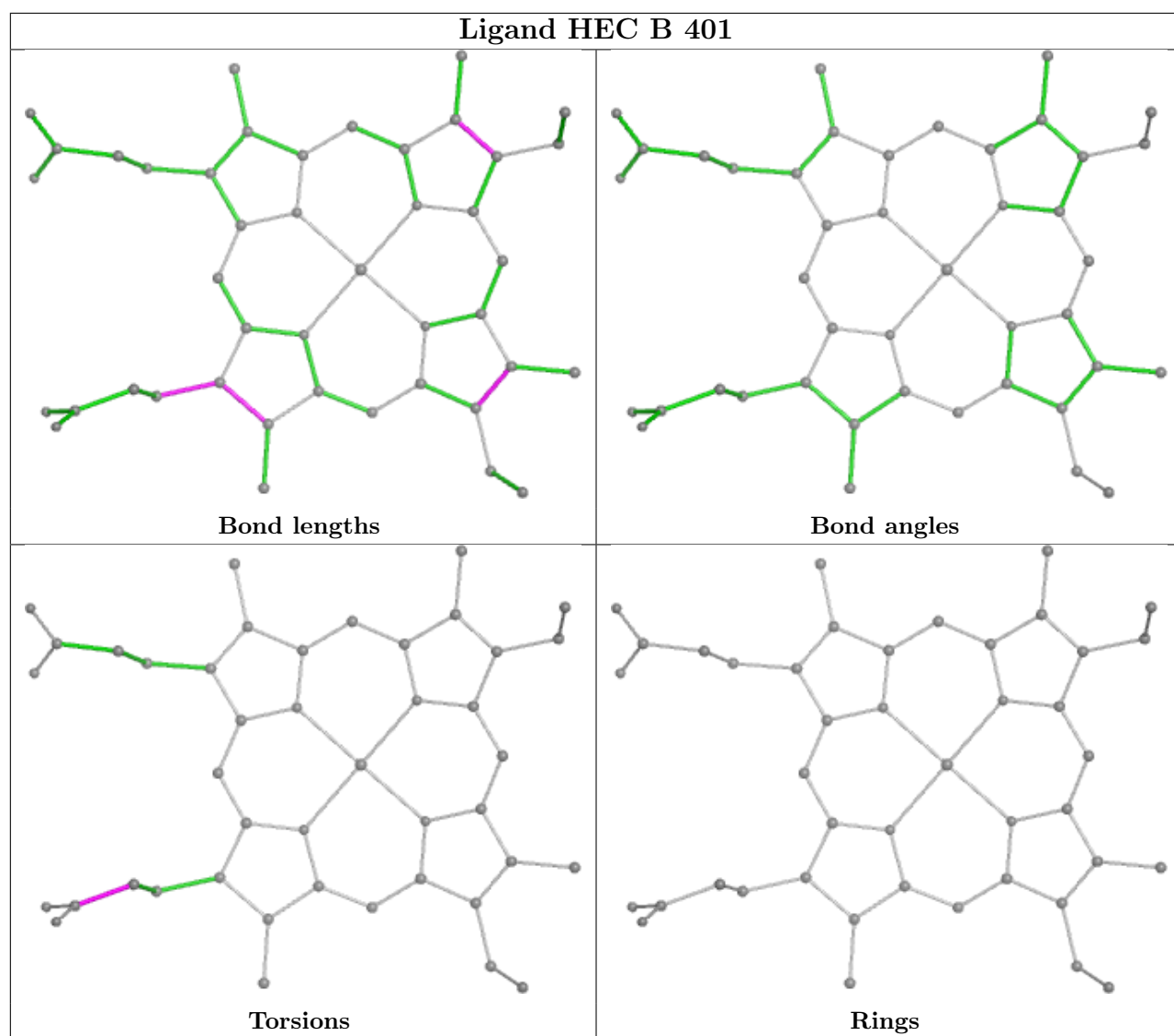


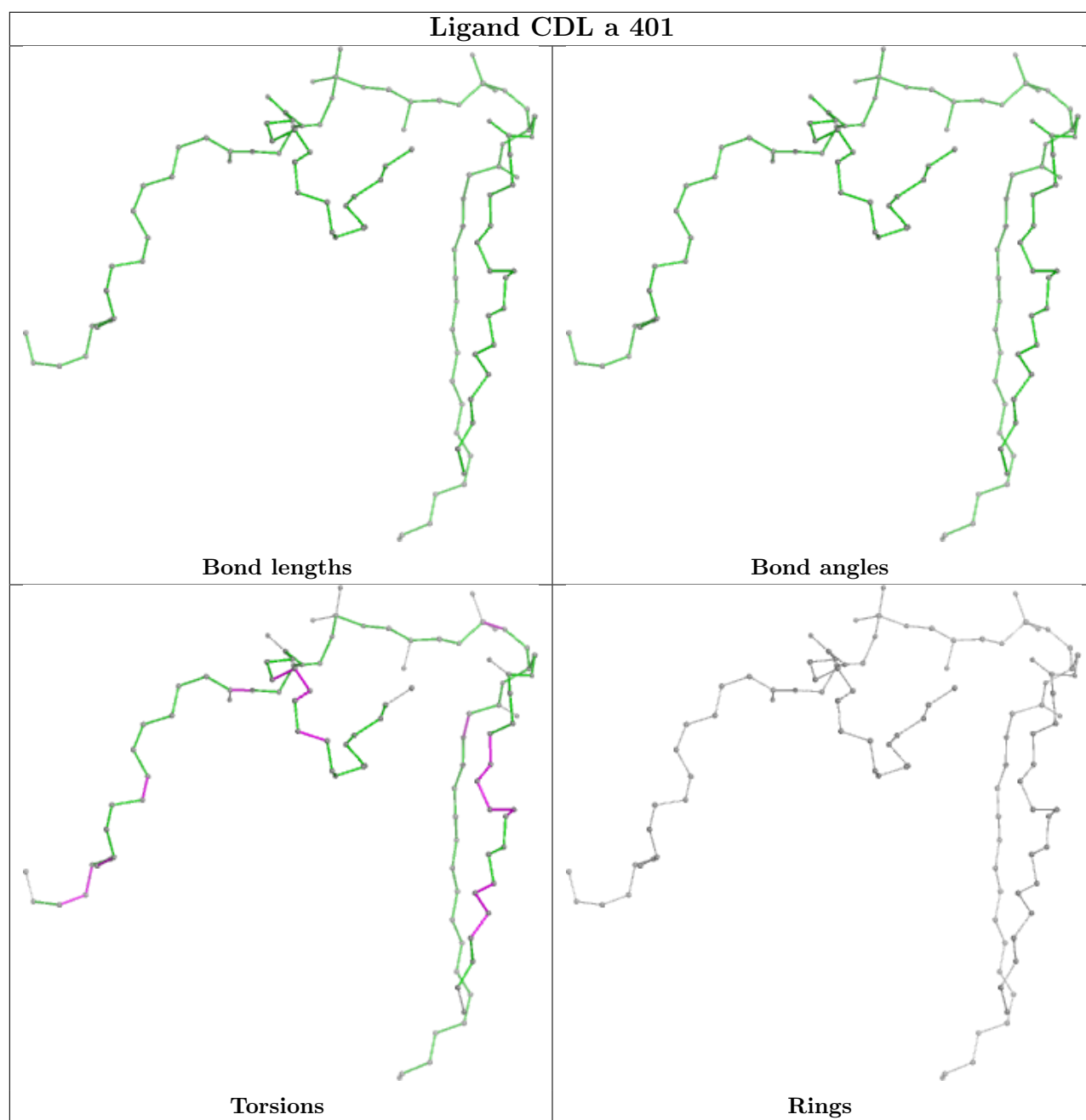


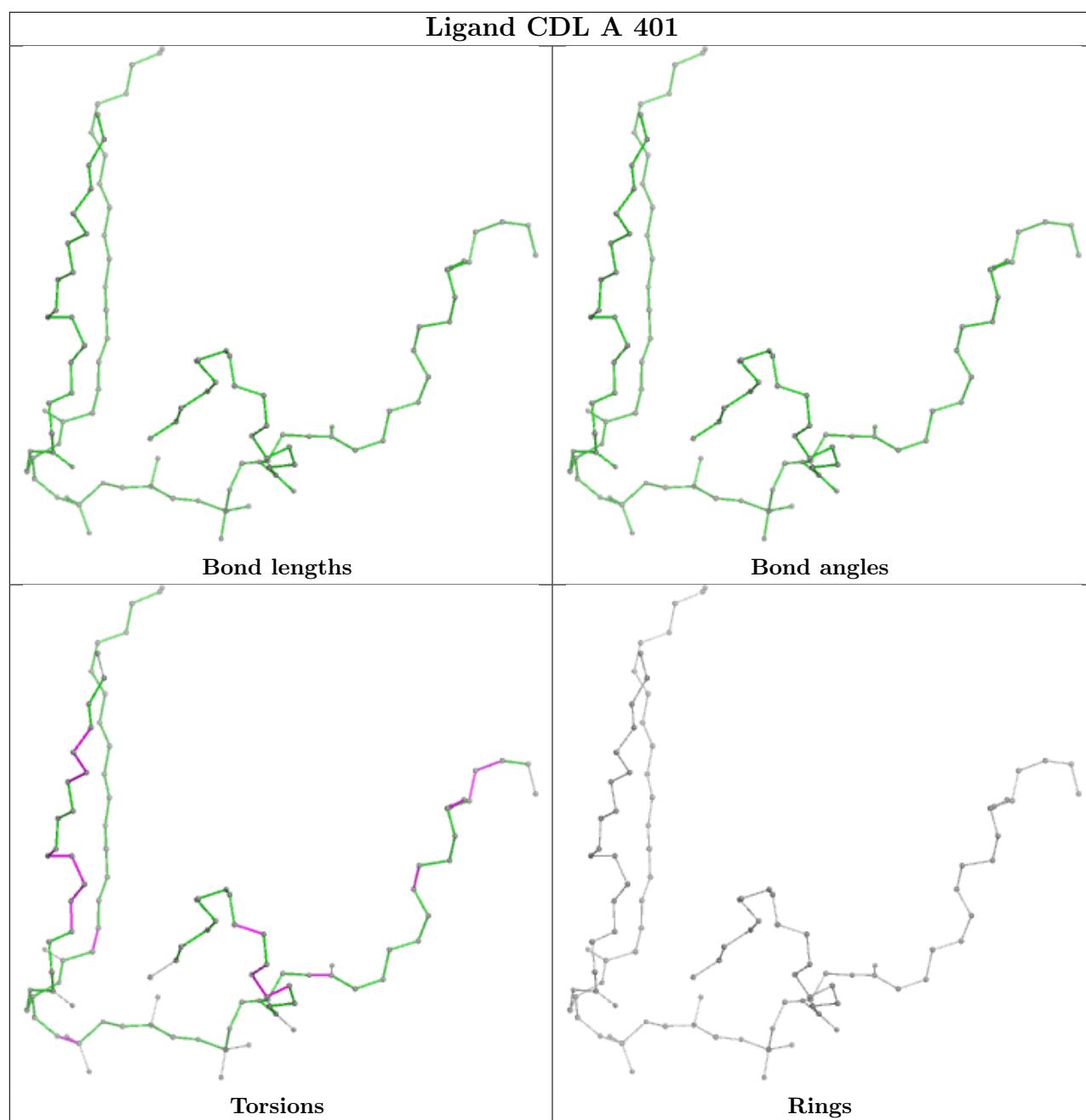


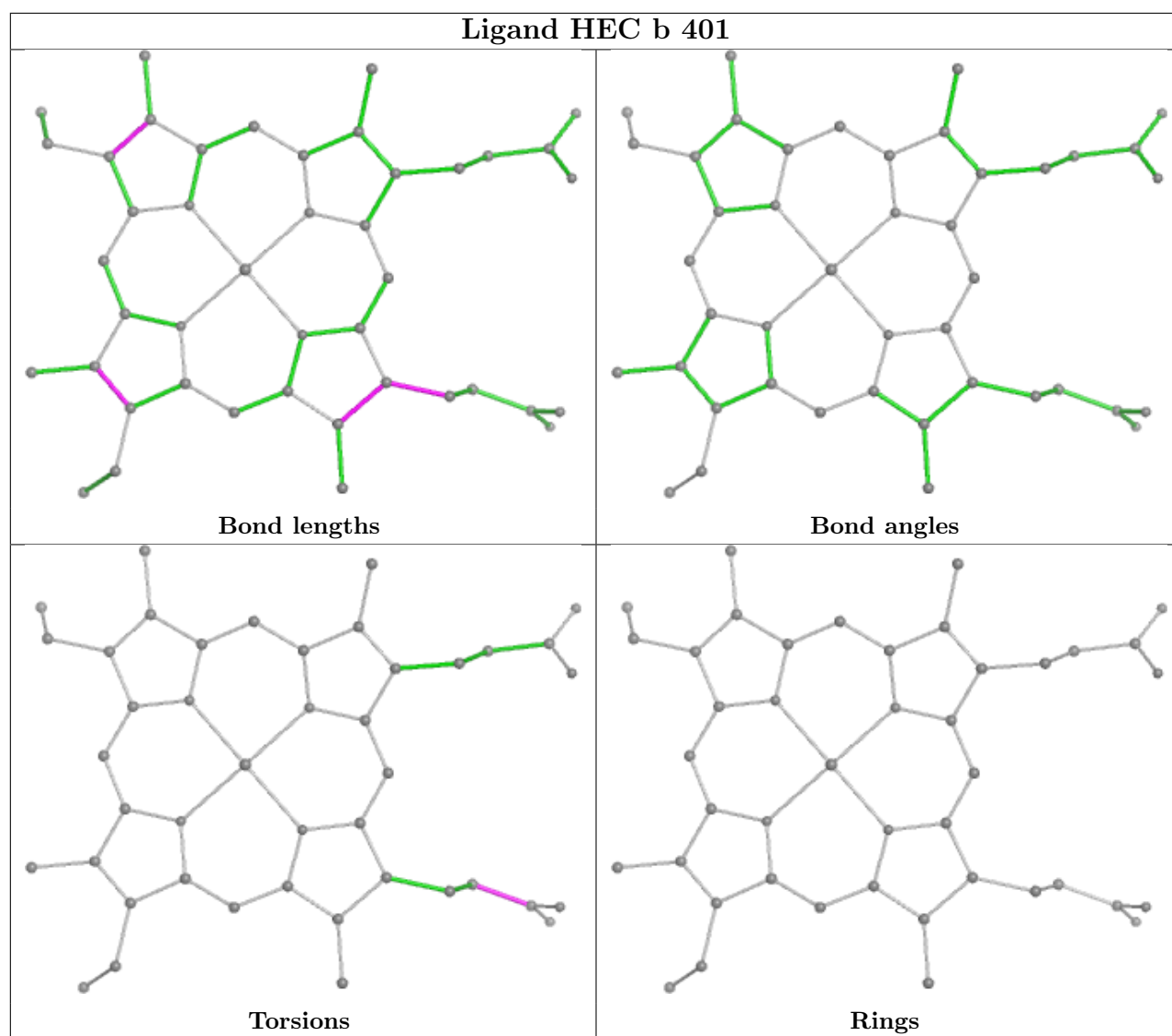


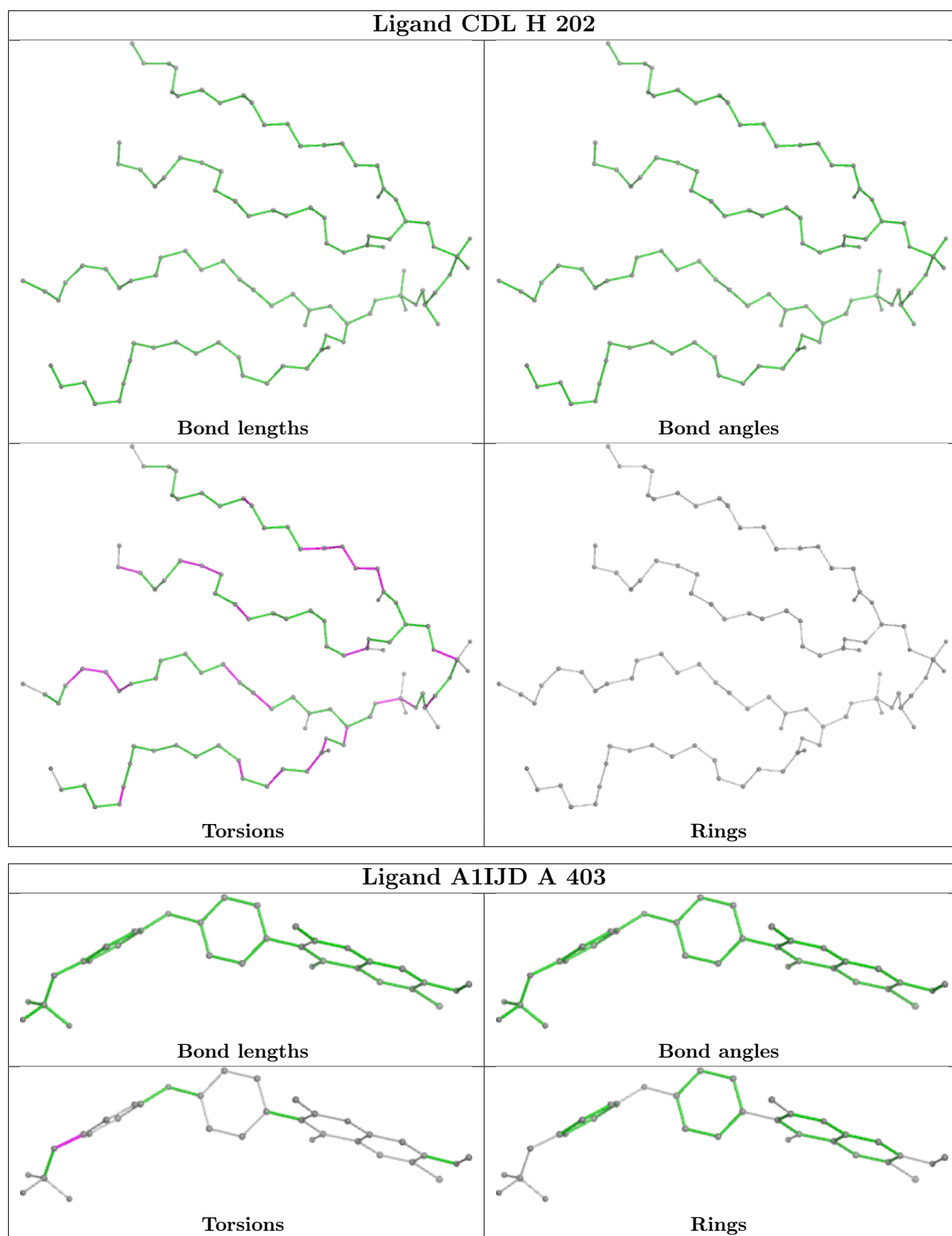




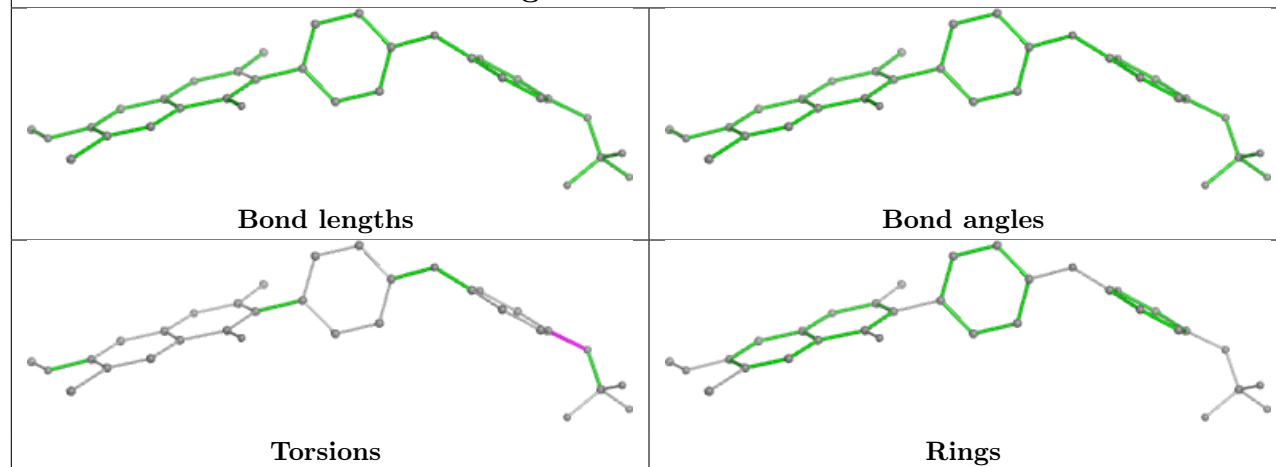




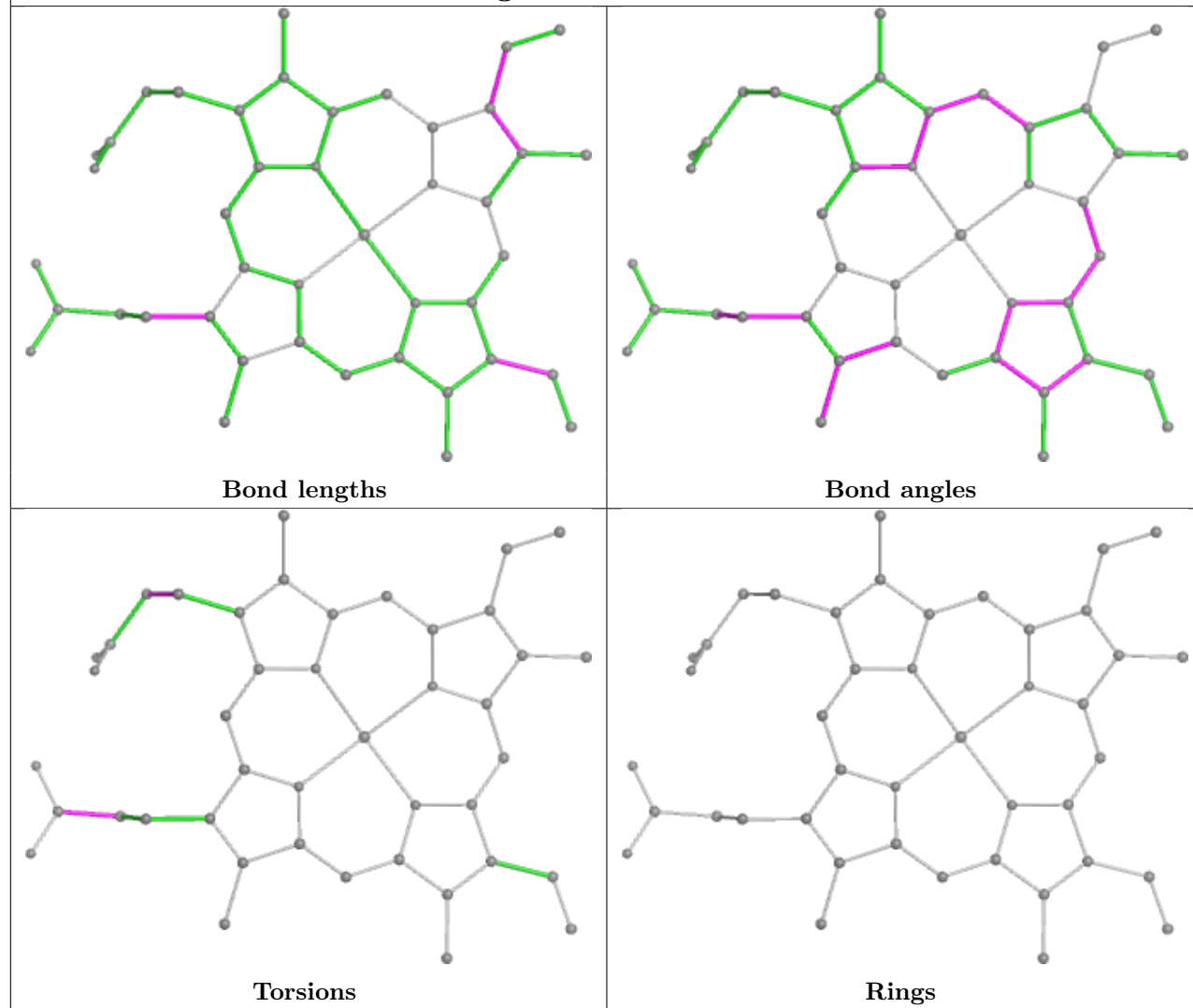




## Ligand A1IJD a 403



## Ligand HEM a 404





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

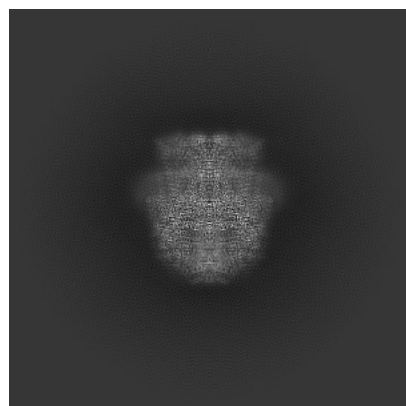
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51157. These allow visual inspection of the internal detail of the map and identification of artifacts.

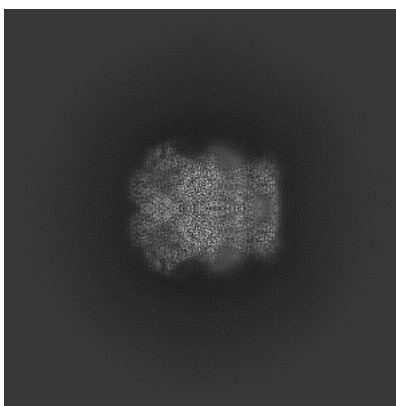
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

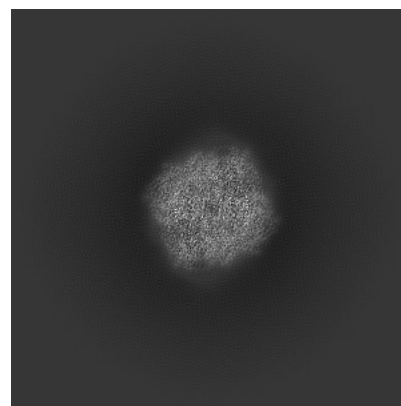
#### 6.1.1 Primary map



X

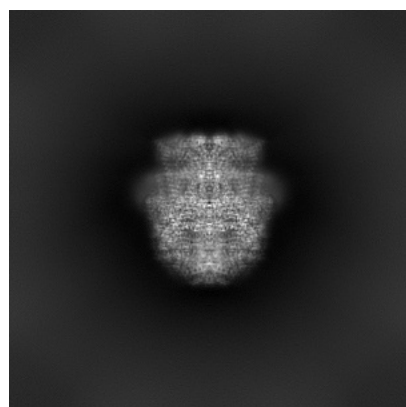


Y

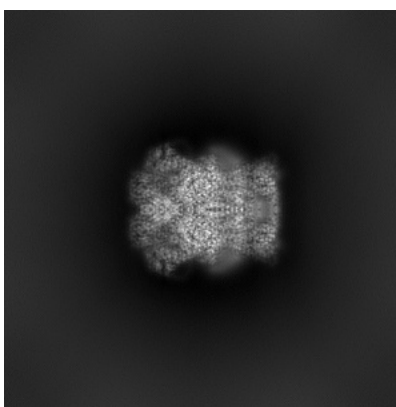


Z

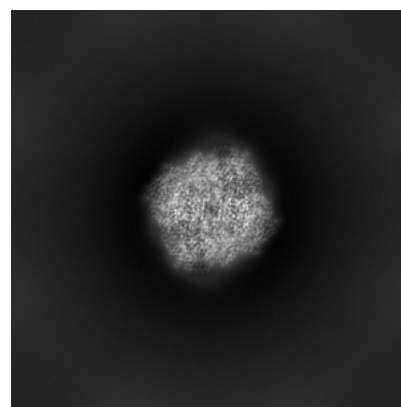
#### 6.1.2 Raw map



X



Y

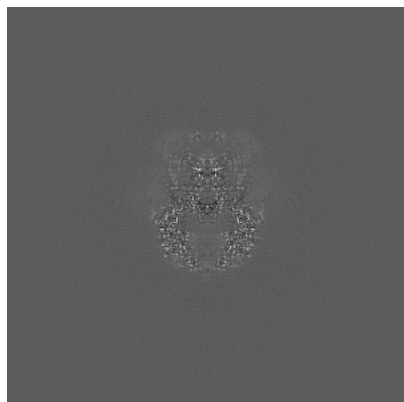


Z

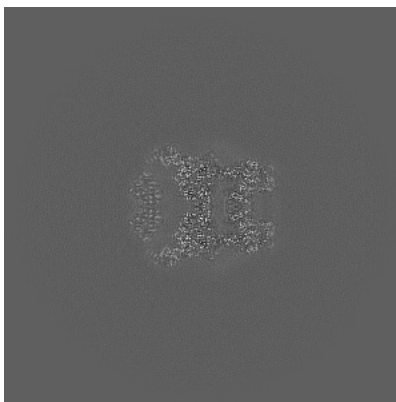
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

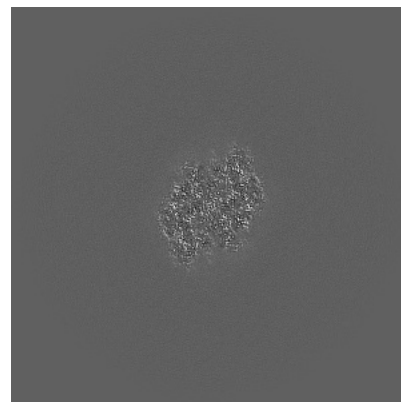
### 6.2.1 Primary map



X Index: 240

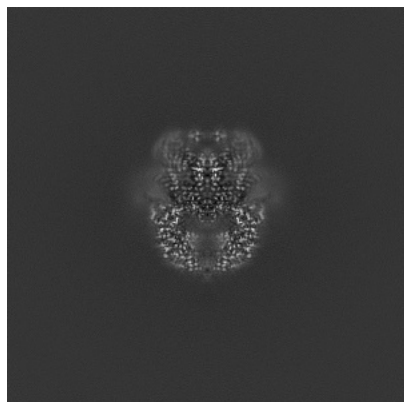


Y Index: 240

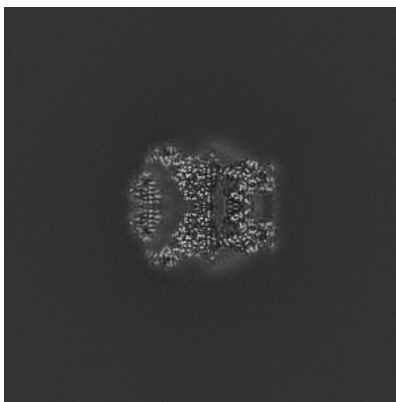


Z Index: 240

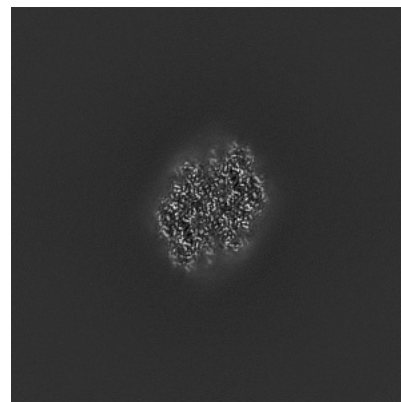
### 6.2.2 Raw map



X Index: 240



Y Index: 240

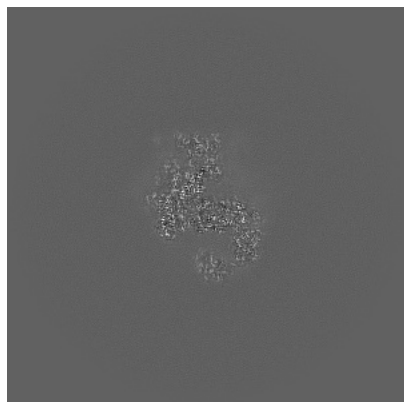


Z Index: 240

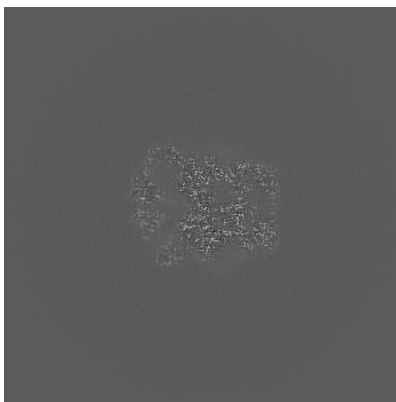
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

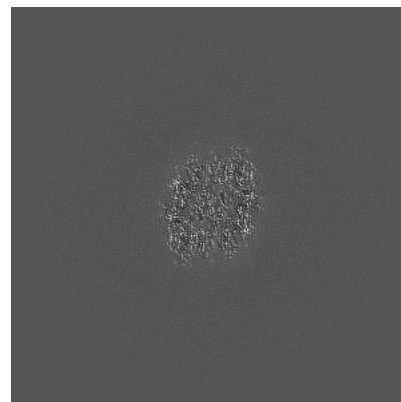
### 6.3.1 Primary map



X Index: 219

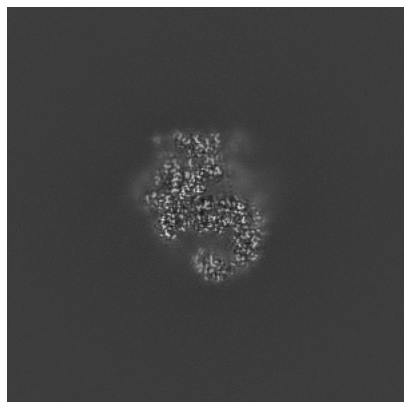


Y Index: 233

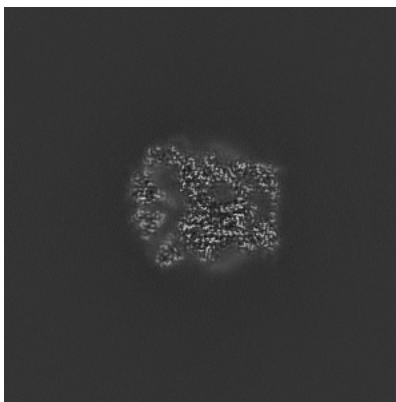


Z Index: 234

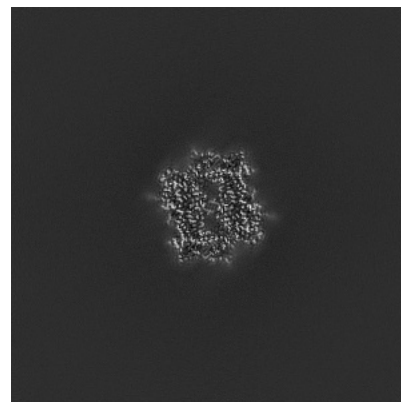
### 6.3.2 Raw map



X Index: 219



Y Index: 233

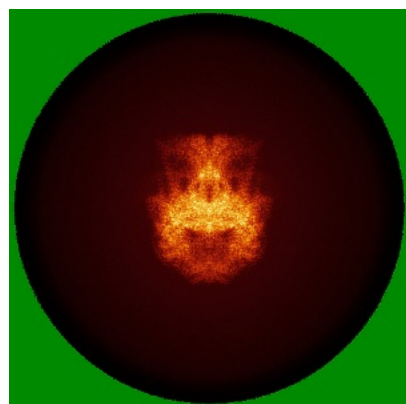


Z Index: 222

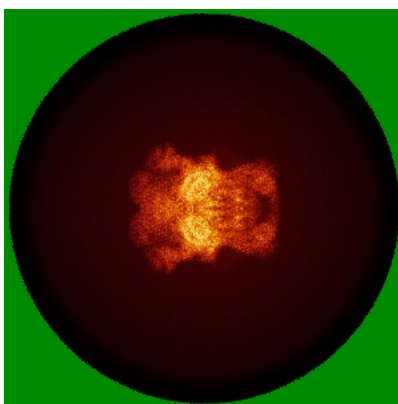
The images above show the largest variance slices of the map in three orthogonal directions.

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

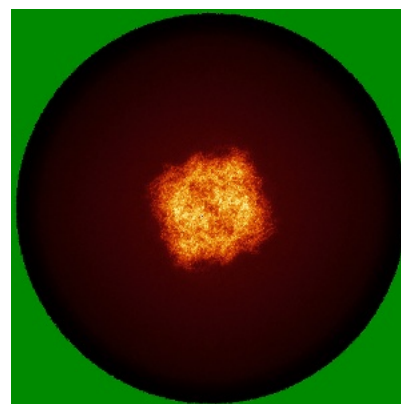
### 6.4.1 Primary map



X

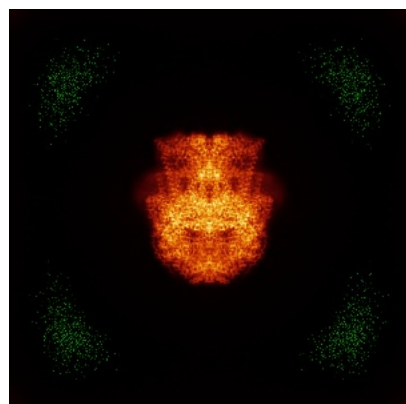


Y

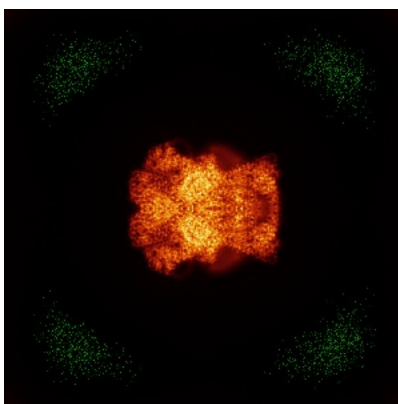


Z

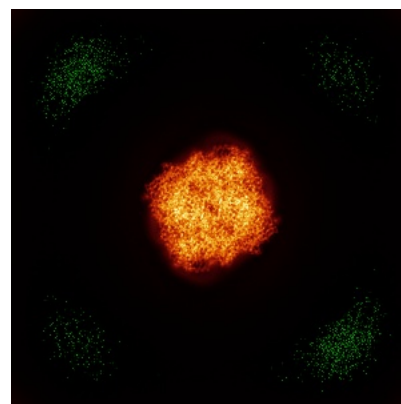
### 6.4.2 Raw map



X



Y

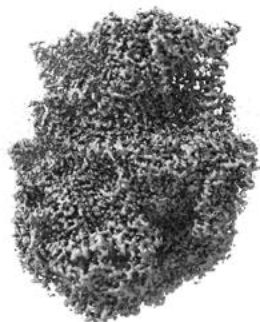


Z

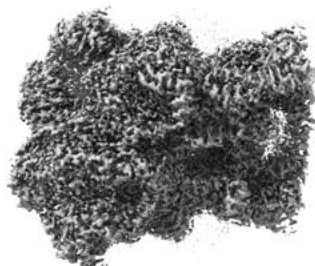
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

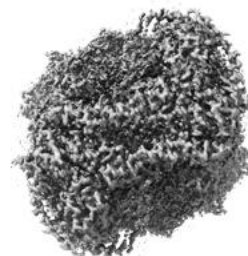
### 6.5.1 Primary map



X



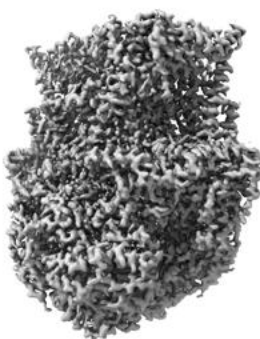
Y



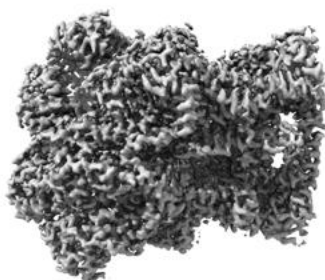
Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

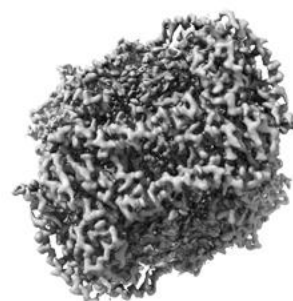
### 6.5.2 Raw map



X



Y



Z

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.



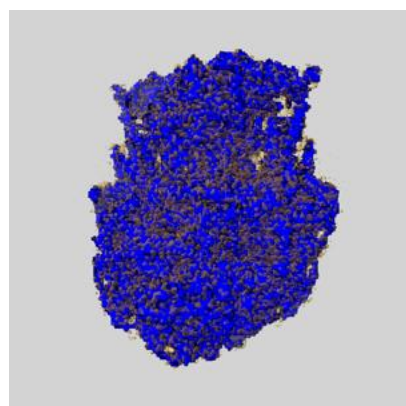
## 6.6 Mask visualisation [i](#)

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

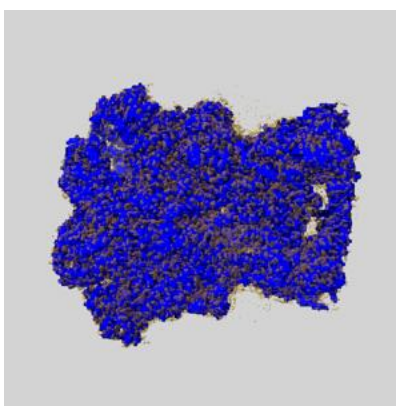
A mask typically either:

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

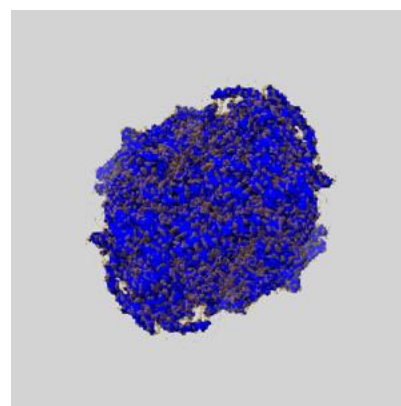
### 6.6.1 emd\_51157\_msk\_1.map [i](#)



X



Y

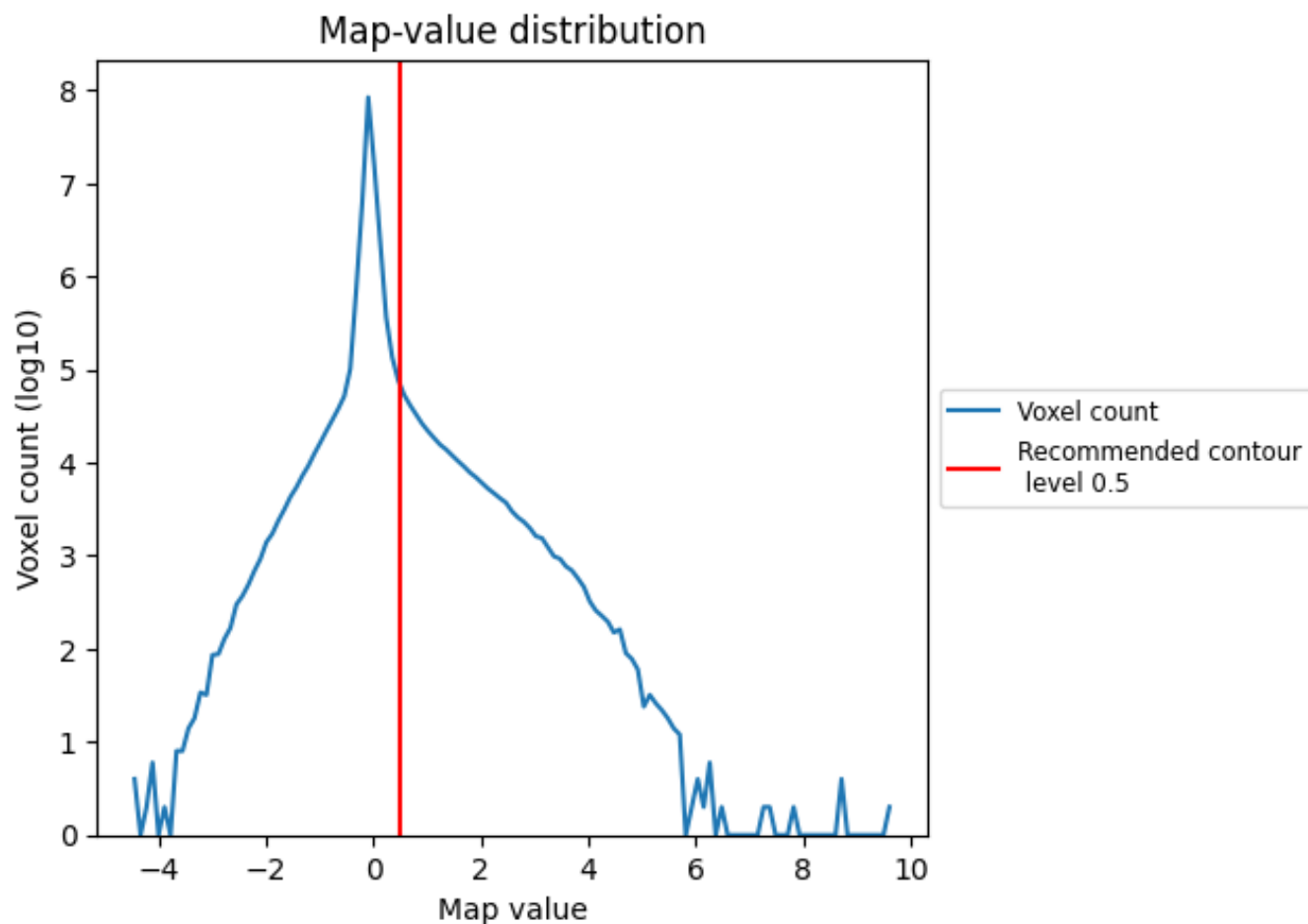


Z

## 7 Map analysis [i](#)

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

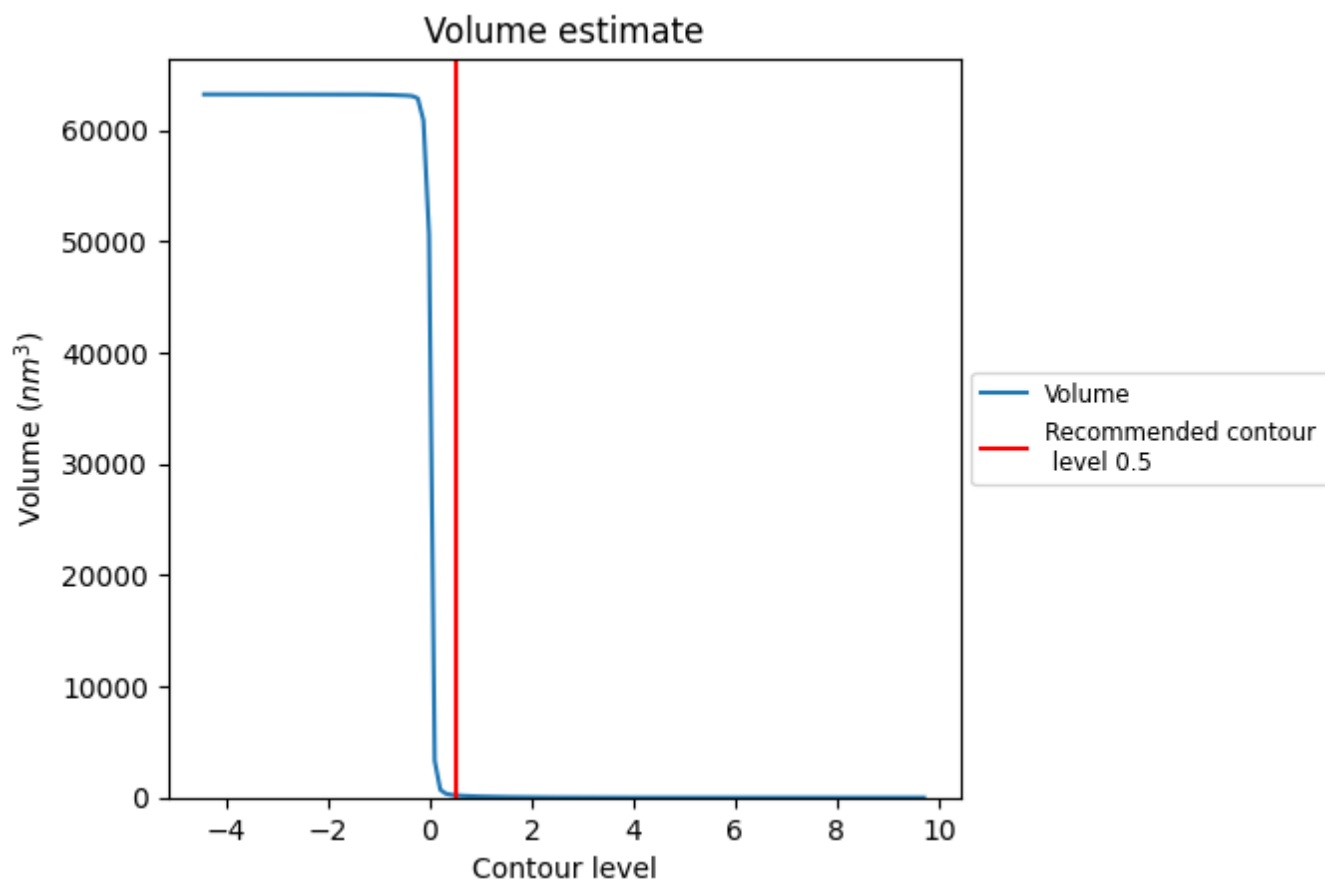
### 7.1 Map-value distribution [i](#)



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.



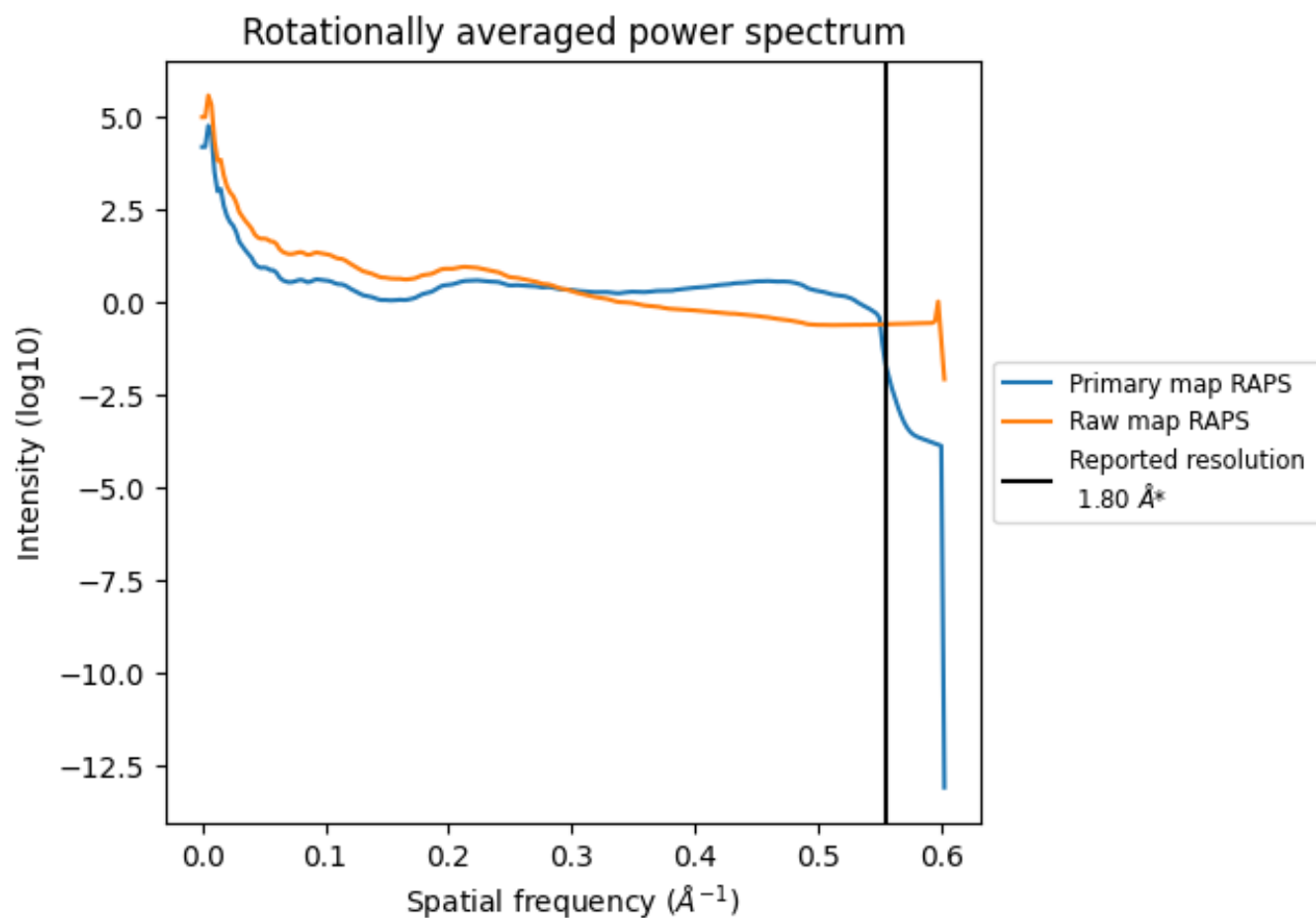
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 209 nm<sup>3</sup>; this corresponds to an approximate mass of 189 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 ⓘ

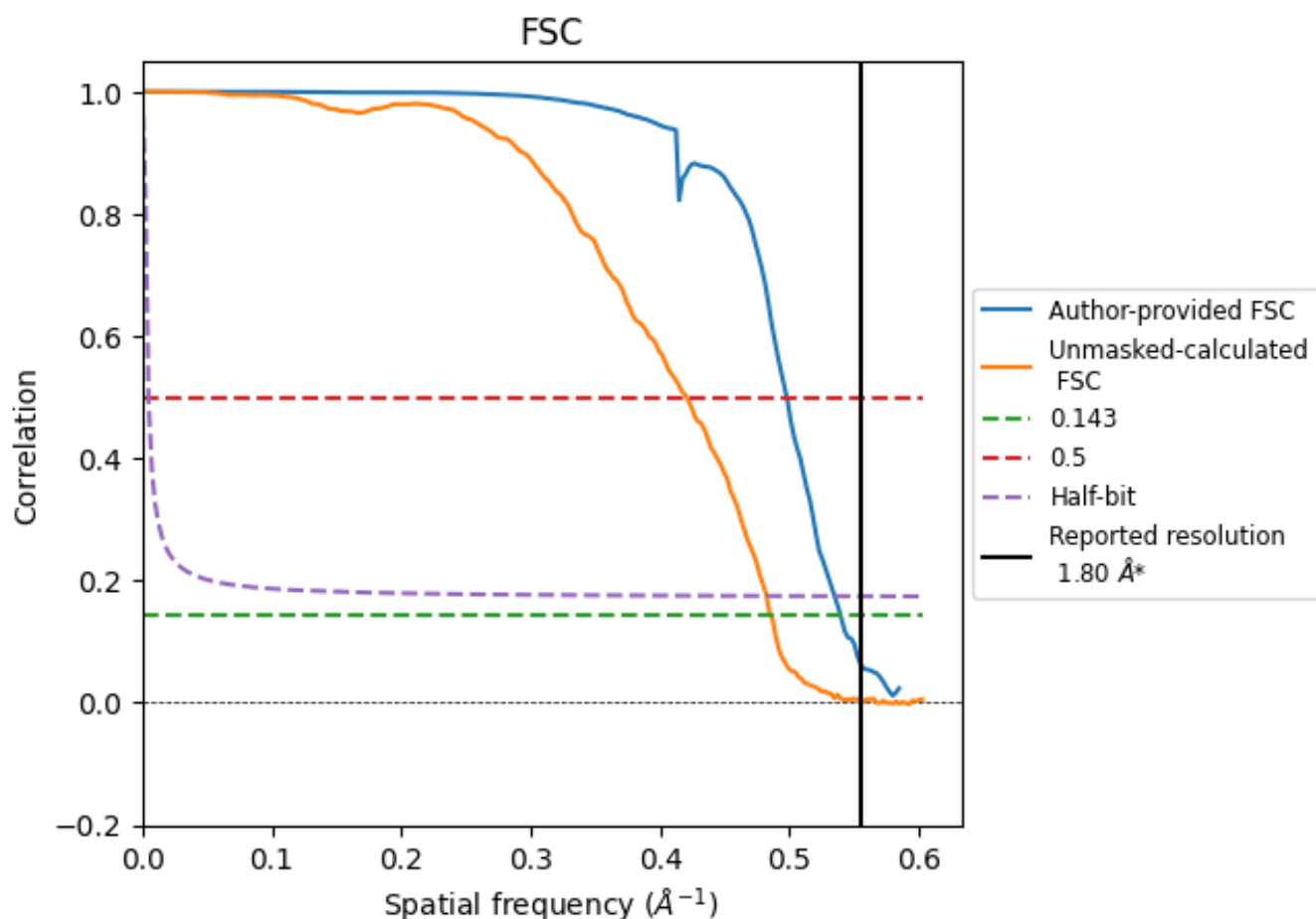


\*Reported resolution corresponds to spatial frequency of 0.556 Å<sup>-1</sup>

## 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  $0.556 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

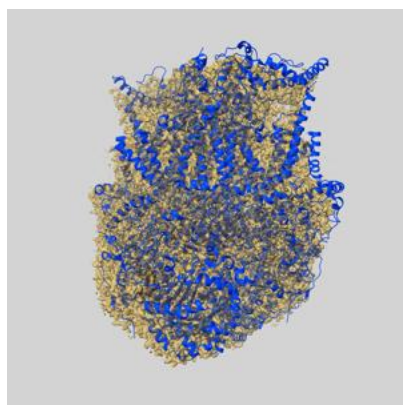
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.80	-	-
Author-provided FSC curve	1.85	2.01	1.87
Unmasked-calculated*	2.06	2.38	2.07

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.06 differs from the reported value 1.8 by more than 10 %

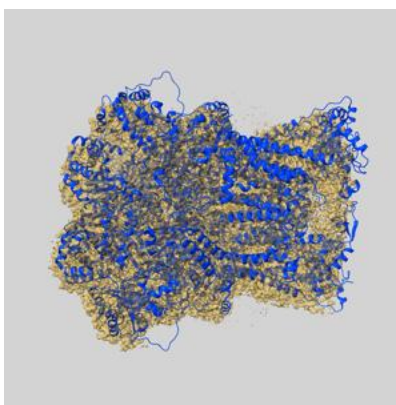
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51157 and PDB model 9G9T. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

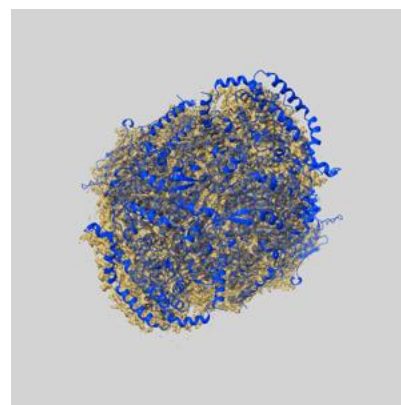
### 9.1 Map-model overlay [i](#)



X



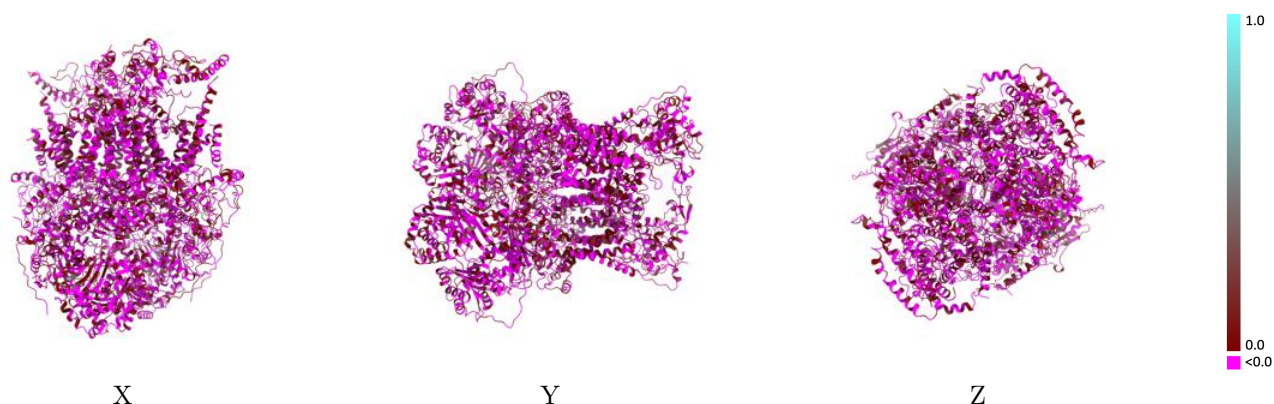
Y



Z

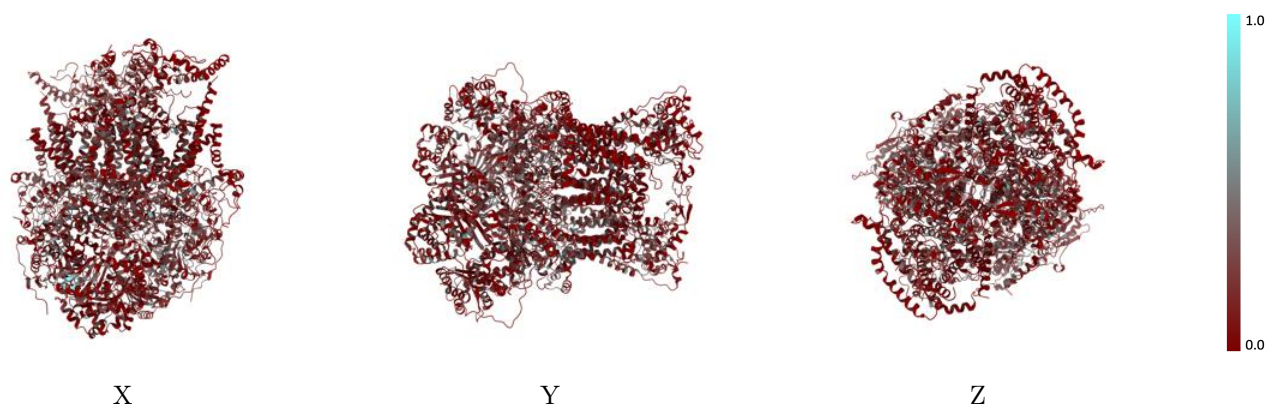
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



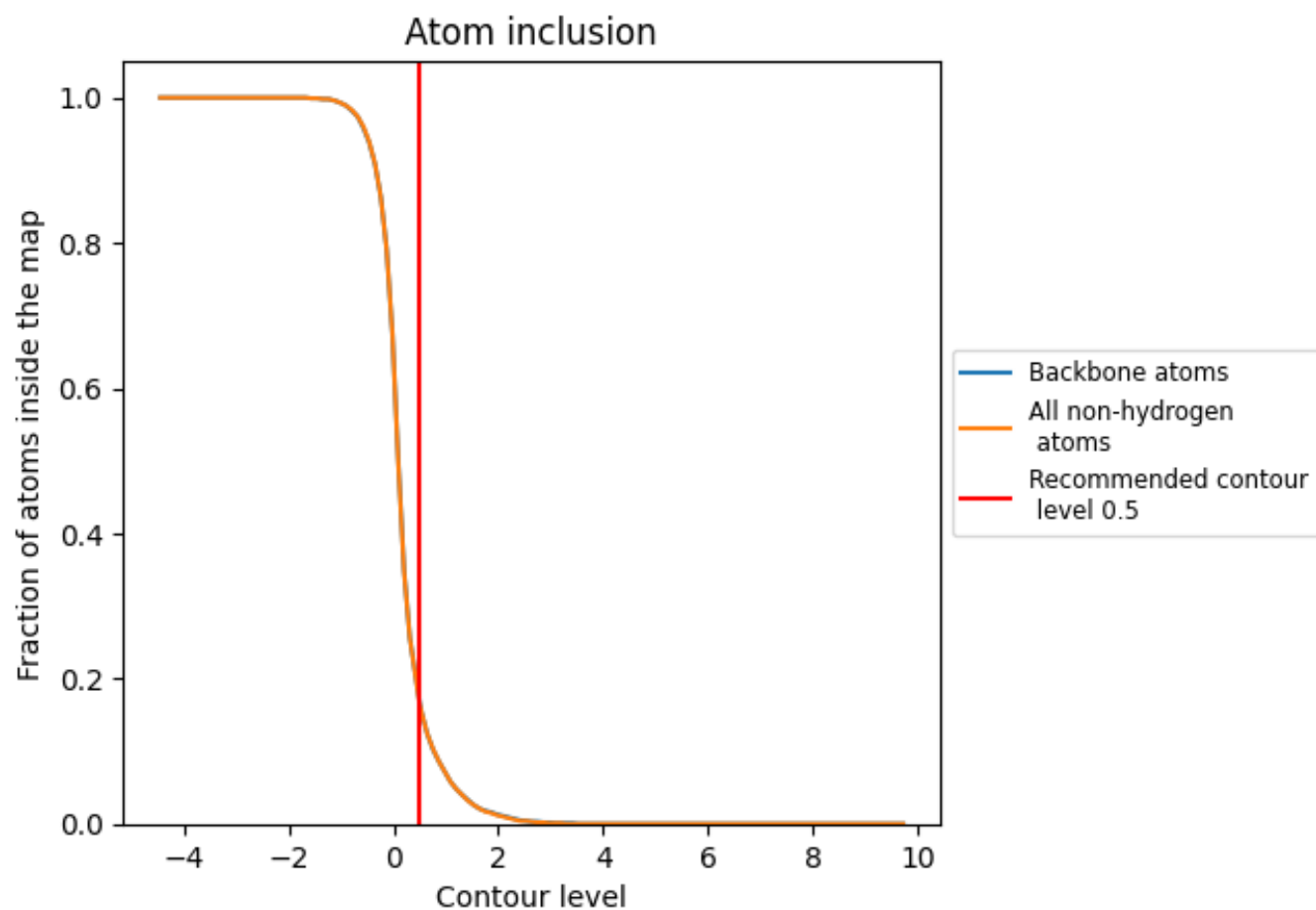
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 17% of all backbone atoms, 16% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1650	 -0.0150
A	 0.1680	 -0.0160
B	 0.1550	 -0.0150
C	 0.2090	 -0.0130
D	 0.1720	 -0.0120
E	 0.1640	 -0.0180
F	 0.0640	 0.0010
G	 0.1860	 -0.0260
H	 0.1210	 -0.0160
I	 0.2000	 -0.0140
J	 0.1870	 -0.0120
K	 0.0480	 -0.0250
L	 0.0770	 -0.0410
a	 0.1730	 -0.0040
b	 0.1570	 -0.0070
c	 0.1680	 -0.0070
d	 0.1820	 -0.0170
e	 0.1750	 -0.0170
f	 0.1120	 -0.0220
g	 0.1890	 -0.0230
h	 0.1730	 -0.0350
i	 0.1190	 -0.0140
j	 0.0700	 0.0060
k	 0.1850	 -0.0320
l	 0.0460	 -0.0150

