



wwPDB EM Validation Summary Report ⓘ

Aug 26, 2026 – 09:42 am BST

PDB ID : 9I4X / pdb_00009i4x
EMDB ID : EMD-52621
Title : Toxoplasma gondii cytochrome bc1 complex from the respiratory supercomplex III2-IV inhibited by atovaquone and ELQ-300
Authors : Maclean, A.; Muhleip, A.
Deposited on : 2025-01-27
Resolution : 2.79 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

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

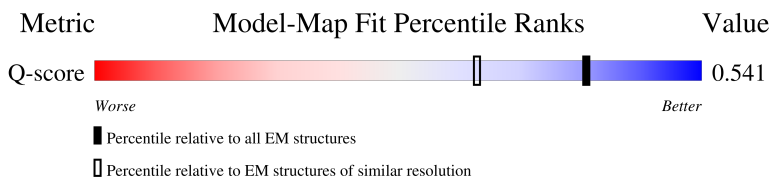
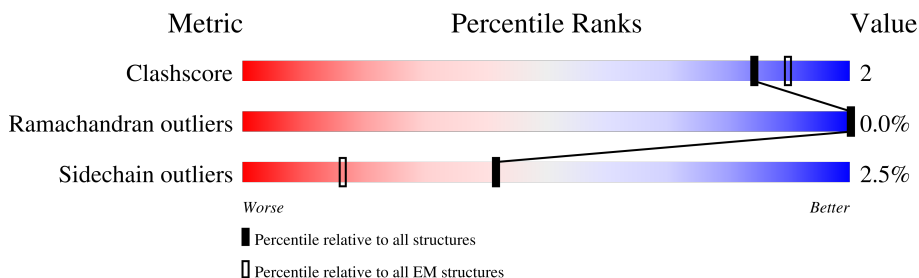
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10811 (2.29 - 3.29)

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	368	 86% 10% . .
1	a	368	 86% 9% . .
2	B	398	 57% . 39%
2	b	398	 58% . 39%

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Mol	Chain	Length	Quality of chain
3	C	487	
3	c	487	
4	D	509	
4	d	509	
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	

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
17	HEC	B	402	X	-	-	-
17	HEC	b	402	X	-	-	-

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 85458 atoms, of which 42742 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
			5841	1941	2959	452	470	19		
1	a	360	Total	C	H	N	O	S	0	0
			5841	1941	2959	452	470	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PHE	SER	engineered mutation	UNP O20672
a	9	PHE	SER	engineered mutation	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
			3834	1268	1876	327	350	13		
2	b	243	Total	C	H	N	O	S	0	0
			3834	1268	1876	327	350	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	328	Total	C	H	N	O	S	0	0
			5136	1671	2496	469	488	12		
3	c	328	Total	C	H	N	O	S	0	0
			5136	1671	2496	469	488	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	456	Total	C	H	N	O	S	0	0
			7147	2272	3544	626	682	23		

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Mol	Chain	Residues	Atoms						AltConf	Trace
4	d	456	Total	C	H	N	O	S	0	0
			7147	2272	3544	626	682	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
			1427	462	700	126	132	7		
6	f	88	Total	C	H	N	O	S	0	0
			1427	462	700	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
			1607	552	779	136	134	6		
8	h	96	Total	C	H	N	O	S	0	0
			1607	552	779	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
			1598	537	787	138	130	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
9	i	92	Total	C	H	N	O	S	0	0
			1598	537	787	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		

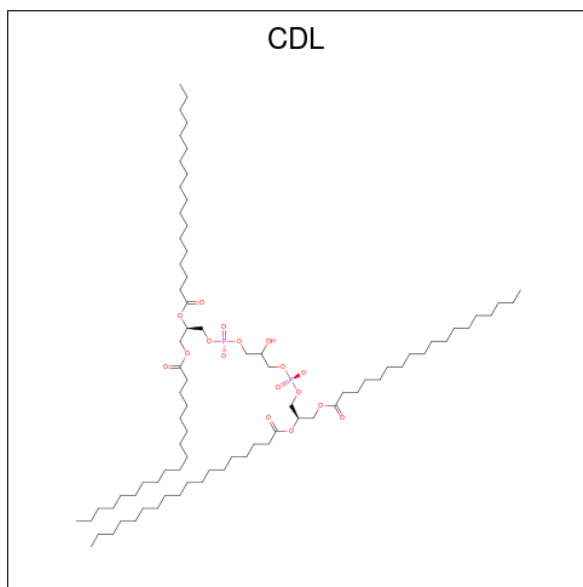
- Molecule 11 is a protein called Transmembrane protein.

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.

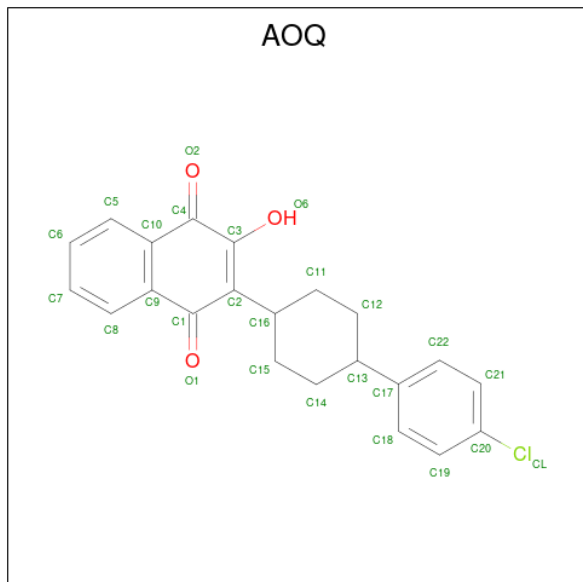
Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	40	Total	C	H	N	O	S	0	0
			611	199	312	48	51	1		
12	l	40	Total	C	H	N	O	S	0	0
			611	199	312	48	51	1		

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



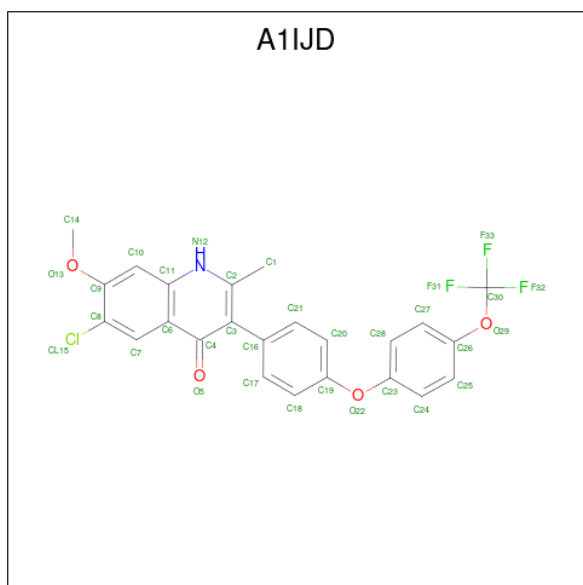
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	B	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	C	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	D	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	G	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	I	1	Total	C	H	O	P	0
			256	81	156	17	2	
13	J	1	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	b	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	l	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 14 is 2-[trans-4-(4-chlorophenyl)cyclohexyl]-3-hydroxynaphthalene-1,4-dione (CCD ID: AOQ) (formula: $C_{22}H_{19}ClO_3$) (labeled as "Ligand of Interest" by depositor).



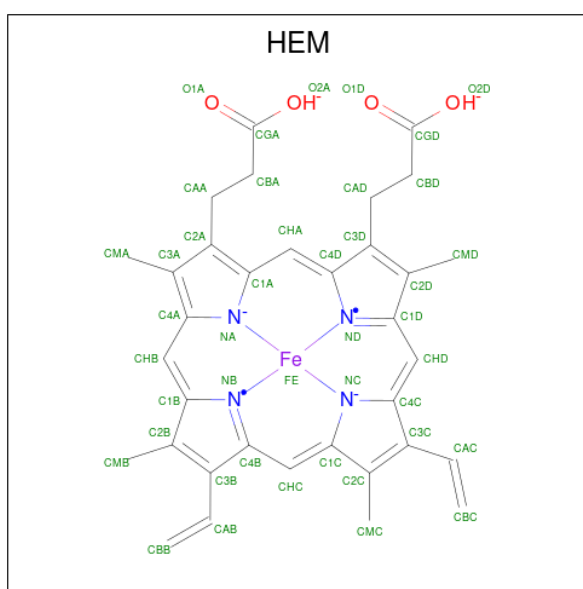
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	H	O	
14	A	1	44	22	1	18	3	0
14	a	1	44	22	1	18	3	0

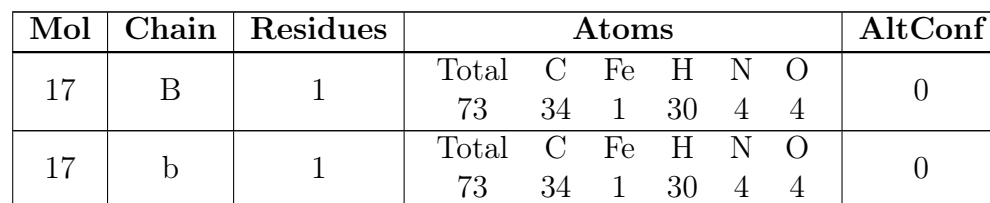
- Molecule 15 is 6-chloranyl-7-methoxy-2-methyl-3-[4-[4-(trifluoromethoxy)phenoxy]phenyl]-1 {H}-quinolin-4-one (CCD ID: A1IJD) (formula: $C_{24}H_{17}ClF_3NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
15	A	1	Total	C	Cl	F	H	N	O	0
			50	24	1	3	17	1	4	
15	A	1	Total C							0
			1 1							
15	a	1	Total	C	Cl	F	H	N	O	0
			50	24	1	3	17	1	4	
15	a	1	Total C							0
			1 1							

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

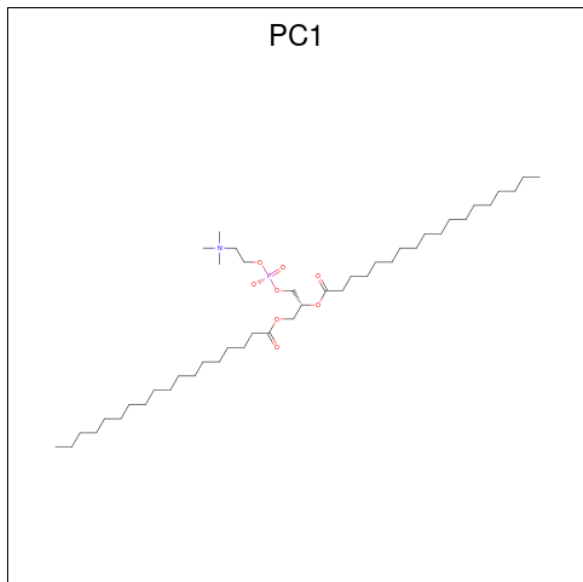




- FES
-
- S1 S⁻² Fe FE2
- Fe S⁻² S2
- FE1

Mol	Chain	Residues	Atoms			AltConf
18	C	1	Total 4	Fe 2	S 2	0
18	c	1	Total 4	Fe 2	S 2	0

- Molecule 19 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



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

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

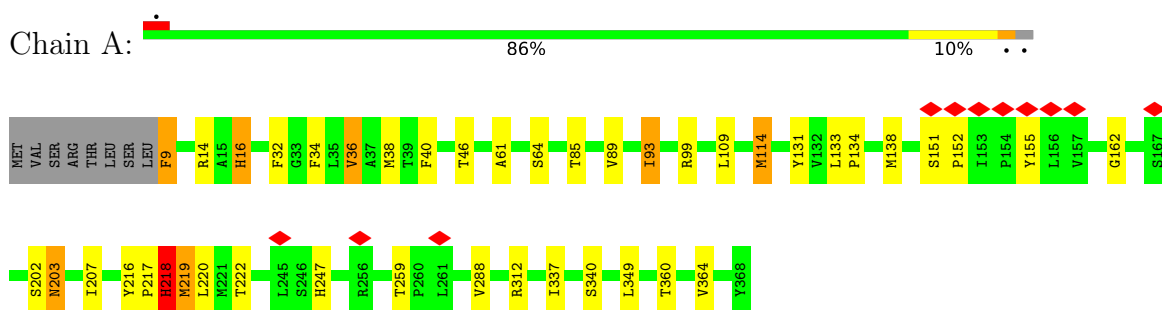
- Molecule 21 is water.

Mol	Chain	Residues	Atoms			AltConf
21	D	1	Total	H	O	0
			3	2	1	
21	d	1	Total	H	O	0
			3	2	1	

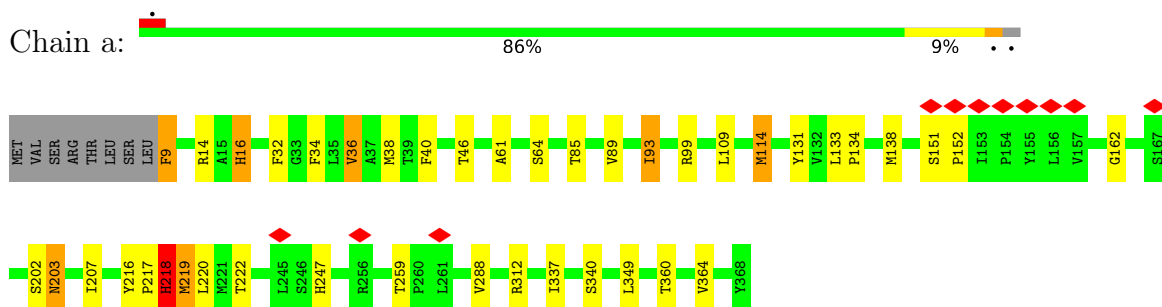
3 Residue-property plots

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.

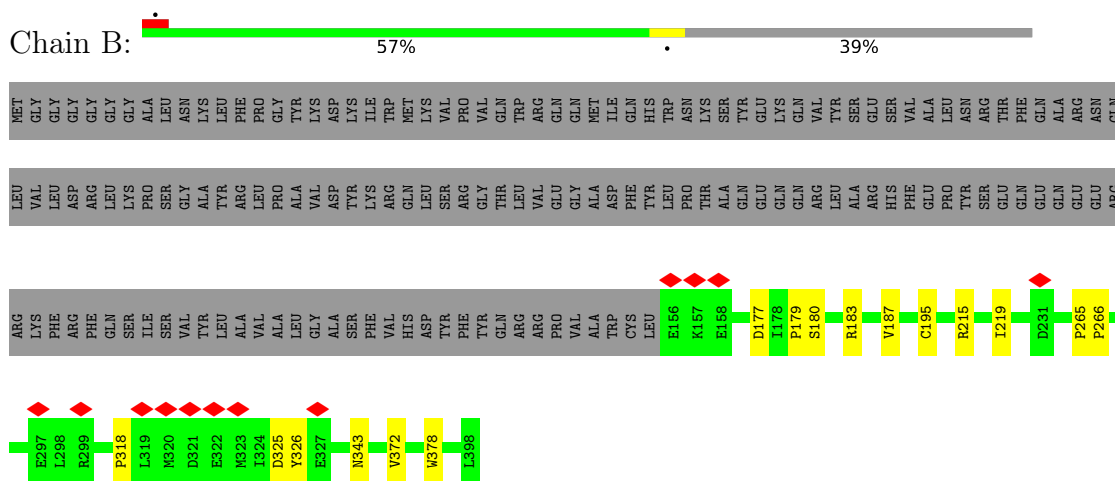
- Molecule 1: Cytochrome b



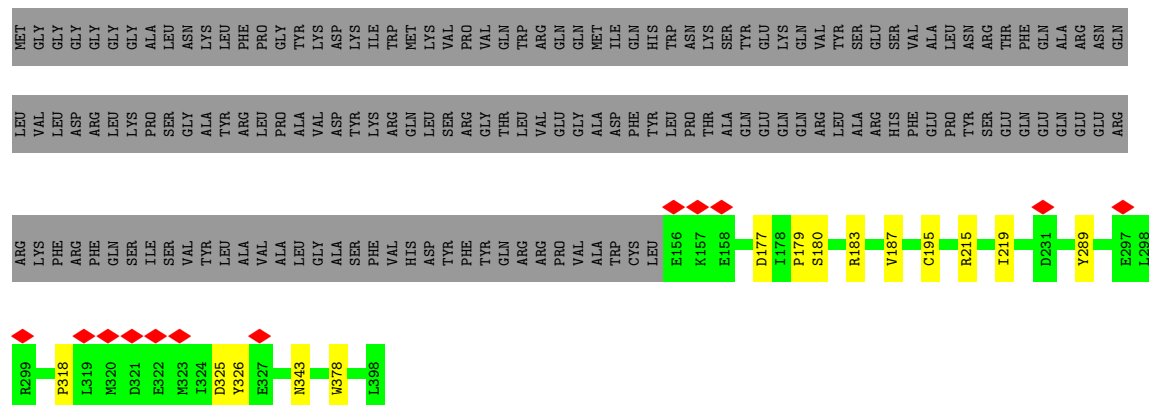
- Molecule 1: Cytochrome b



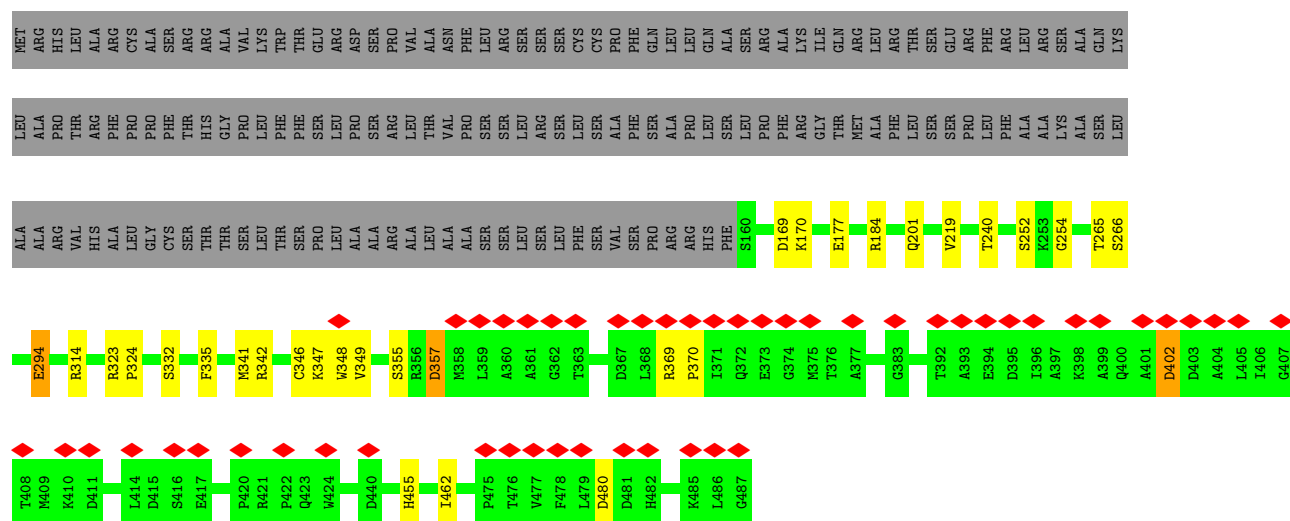
- Molecule 2: Cytochrome c1, heme protein



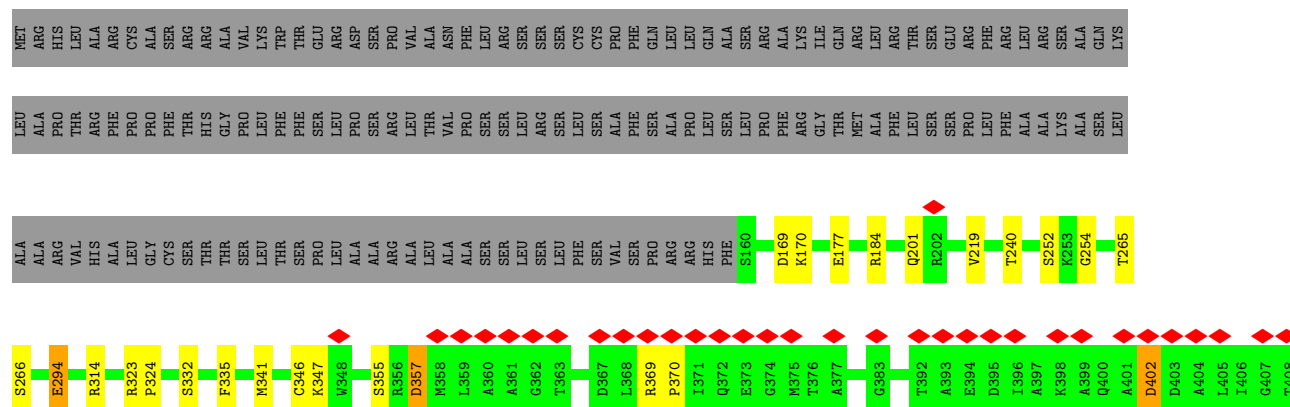
Chain b: 58% 39%



Chain C: 10% 61% 6% 23%



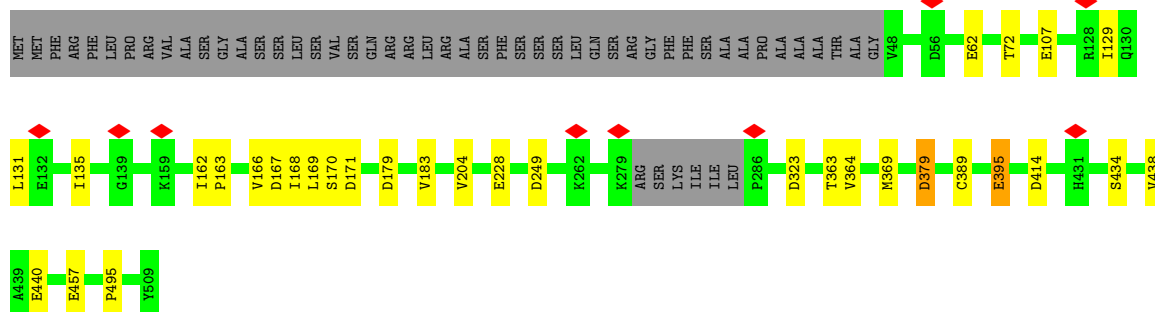
Chain c:





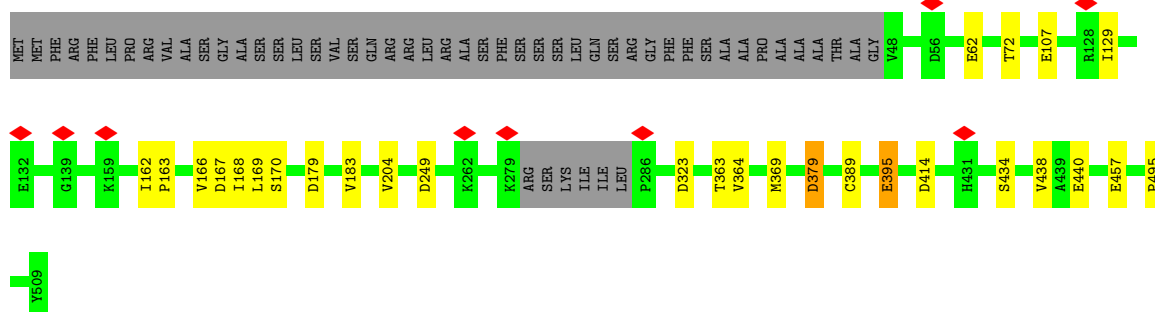
- Molecule 4: Putative peptidase M16 family protein

Chain D: 83% 6% 10%



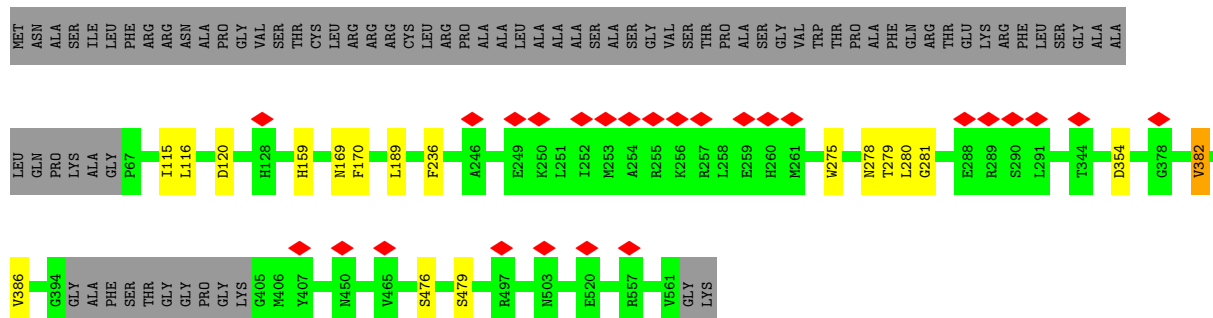
- Molecule 4: Putative peptidase M16 family protein

Chain d: 84% 5% 10%



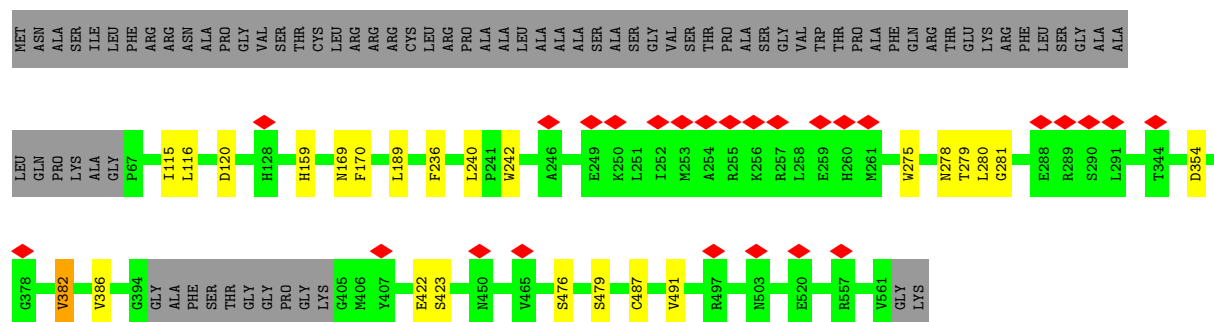
- Molecule 5: Alpha-MPP

Chain E: 5% 83% 14%



- Molecule 5: Alpha-MPP

Chain e: 5% 82% 14%



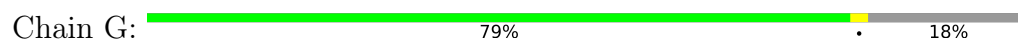
- Molecule 6: Putative ubiquinol-cytochrome c reductase hinge protein



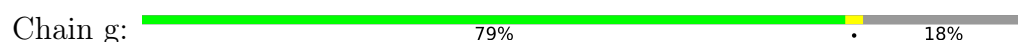
- Molecule 6: Putative ubiquinol-cytochrome c reductase hinge protein



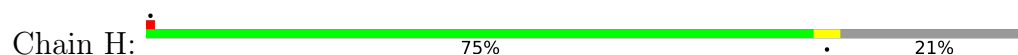
- Molecule 7: Ubiquinol-cytochrome c reductase



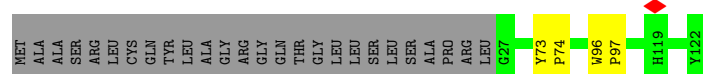
- Molecule 7: Ubiquinol-cytochrome c reductase

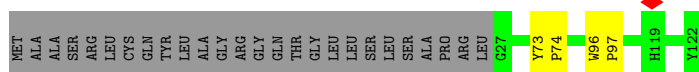
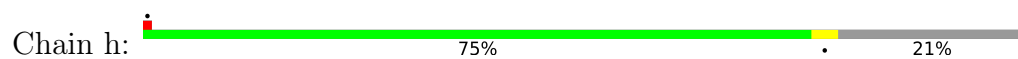


- Molecule 8: QCR8, TGGT1_227910

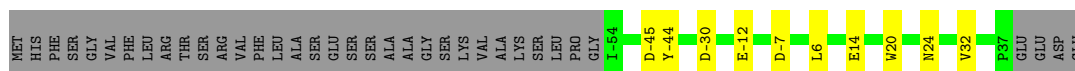


- Molecule 8: QCR8, TGGT1_227910

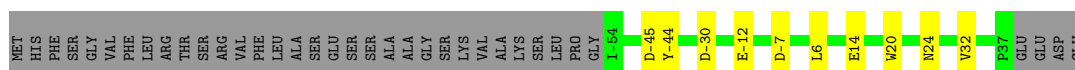




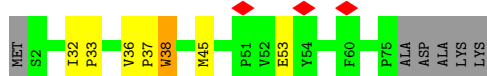
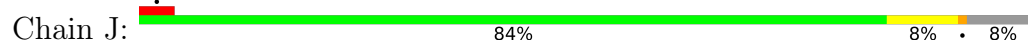
- Molecule 9: Ubiquinol-cytochrome C family reductase UQCRX/QCR9-like protein



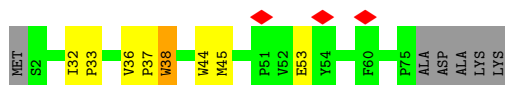
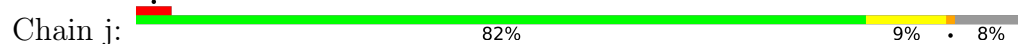
- Molecule 9: Ubiquinol-cytochrome C family reductase UQCRX/QCR9-like protein



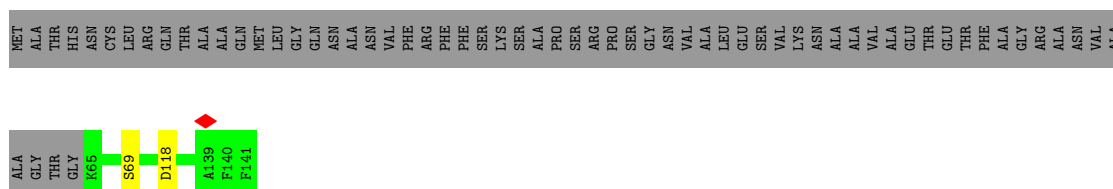
- Molecule 10: Transmembrane protein



- Molecule 10: Transmembrane protein



- Molecule 11: Transmembrane protein



- Molecule 11: Transmembrane protein



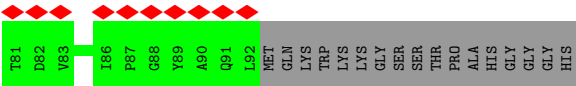
MET ALA THR HIS ASN CYS LEU ARG GLN THR ALA ALA GLN MET LEU GLY GLN ASN ALA ASN VAL PHE ARG PHE PHE SER LYS THR ALA PRO SER ARG PRO GLY VAL ASN ALA LEU GLY SER VAL LYS ASN ALA THR GLU THR GLU THR PHE ALA GLY



• Molecule 12: Transmembrane protein



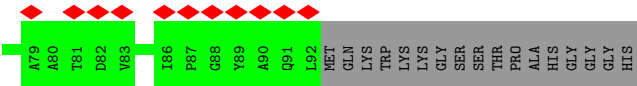
MET ASN CYS PRO LEU PRO ALA GLU PHE VAL VAL PRO PHE TRP SER ALA GLY PRO PRO VAL GLY LYS ASN CYS PHE HIS CYS GLY ILE ARG LEU ARG ARG GLY HIS SER SER PRO THR TYR SER PHE PRO PRO TYR CYS VAL THR THR MET SS3 TS8 M61 A79 A80



• Molecule 12: Transmembrane protein



MET ASN CYS PRO LEU PRO ALA GLU PHE VAL VAL PRO PHE TRP SER ALA GLY PRO PRO VAL GLY LYS ASN CYS PHE HIS CYS GLY ILE ARG LEU ARG ARG GLY HIS SER SER PRO THR TYR SER PHE PRO PRO TYR CYS VAL THR THR MET SS3 TS8 V63 L60 M61 V64



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	3.227	Depositor
Minimum map value	-1.909	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	507.84003, 507.84003, 507.84003	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8464, 0.8464, 0.8464	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, HEM, HEC, FES, PC1, AOQ, A1IJD, 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	0.30	1/2970 (0.0%)	0.53	4/4057 (0.1%)
1	a	0.30	1/2970 (0.0%)	0.53	4/4057 (0.1%)
2	B	0.18	0/2028	0.38	0/2766
2	b	0.18	0/2028	0.38	0/2766
3	C	0.18	0/2728	0.40	0/3720
3	c	0.18	0/2728	0.40	0/3720
4	D	0.19	0/3678	0.46	0/4981
4	d	0.19	0/3678	0.46	0/4981
5	E	0.19	0/3895	0.44	0/5284
5	e	0.19	0/3895	0.44	0/5284
6	F	0.19	0/747	0.43	0/1009
6	f	0.18	0/747	0.43	0/1009
7	G	0.22	0/1621	0.43	0/2200
7	g	0.22	0/1621	0.43	0/2200
8	H	0.21	0/866	0.41	0/1178
8	h	0.21	0/866	0.41	0/1178
9	I	0.19	0/843	0.42	0/1143
9	i	0.19	0/843	0.42	0/1143
10	J	0.18	0/656	0.44	0/901
10	j	0.18	0/656	0.44	0/901
11	K	0.16	0/628	0.41	0/853
11	k	0.16	0/628	0.41	0/853
12	L	0.21	0/305	0.43	0/417
12	l	0.21	0/305	0.42	0/417
All	All	0.21	2/41930 (0.0%)	0.44	8/57018 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	a	0	4
3	C	0	1
3	c	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	HIS	CE1-NE2	-5.12	1.27	1.32
1	a	16	HIS	CE1-NE2	-5.11	1.27	1.32

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	218	HIS	ND1-CG-CD2	-6.77	99.33	106.10
1	A	218	HIS	ND1-CG-CD2	-6.76	99.34	106.10
1	A	16	HIS	ND1-CG-CD2	-6.25	99.86	106.10
1	a	16	HIS	ND1-CG-CD2	-6.23	99.87	106.10
1	A	16	HIS	CE1-NE2-CD2	-5.80	103.20	109.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	16	HIS	Sidechain
1	A	162	GLY	Peptide
1	A	218	HIS	Sidechain
3	C	314	ARG	Sidechain

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	2959	2959	22	0
1	a	2882	2959	2959	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1958	1876	1874	8	0
2	b	1958	1876	1874	6	0
3	C	2640	2496	2496	15	0
3	c	2640	2496	2496	13	0
4	D	3603	3544	3544	17	0
4	d	3603	3544	3544	15	0
5	E	3806	3773	3772	9	0
5	e	3806	3773	3772	13	0
6	F	727	700	700	2	0
6	f	727	700	700	3	0
7	G	1568	1525	1525	4	0
7	g	1568	1525	1525	3	0
8	H	828	779	779	2	0
8	h	828	779	779	2	0
9	I	811	787	789	7	0
9	i	811	787	789	7	0
10	J	626	600	600	5	0
10	j	626	600	600	6	0
11	K	607	625	625	1	0
11	k	607	625	625	1	0
12	L	299	312	312	1	0
12	l	299	312	312	2	0
13	A	100	156	156	0	0
13	B	100	156	156	1	0
13	C	100	156	156	0	0
13	D	100	156	156	1	0
13	G	100	156	156	1	0
13	I	100	156	156	1	0
13	J	100	156	156	1	0
13	L	100	156	156	0	0
13	a	100	156	156	0	0
13	b	100	156	156	0	0
13	c	100	156	156	0	0
13	d	100	156	156	0	0
13	g	100	156	156	1	0
13	l	100	156	156	0	0
14	A	26	18	18	0	0
14	a	26	18	18	0	0
15	A	34	17	0	0	0
15	a	34	17	0	0	0
16	A	86	60	60	12	0
16	a	86	60	60	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	B	43	30	30	0	0
17	b	43	30	30	0	0
18	C	4	0	0	0	0
18	c	4	0	0	0	0
19	C	108	176	176	3	0
19	c	108	176	176	2	0
20	D	1	0	0	0	0
20	d	1	0	0	0	0
21	D	1	2	0	0	0
21	d	1	2	0	0	0
All	All	42716	42742	42702	196	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.

The worst 5 of 196 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:107:GLU:N	4:d:107:GLU:OE1	2.20	0.74
4:D:107:GLU:N	4:D:107:GLU:OE1	2.20	0.73
7:G:91:LEU:HD23	7:G:94:LEU:HD11	1.69	0.73
7:g:91:LEU:HD23	7:g:94:LEU:HD11	1.69	0.73
1:a:202:SER:OG	16:a:406:HEM:O1D	2.10	0.69

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	358/368 (97%)	342 (96%)	15 (4%)	1 (0%)	36 66
1	a	358/368 (97%)	342 (96%)	15 (4%)	1 (0%)	36 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	241/398 (61%)	226 (94%)	15 (6%)	0	100	100
2	b	241/398 (61%)	226 (94%)	15 (6%)	0	100	100
3	C	326/487 (67%)	312 (96%)	14 (4%)	0	100	100
3	c	326/487 (67%)	312 (96%)	14 (4%)	0	100	100
4	D	452/509 (89%)	437 (97%)	15 (3%)	0	100	100
4	d	452/509 (89%)	437 (97%)	15 (3%)	0	100	100
5	E	481/563 (85%)	464 (96%)	17 (4%)	0	100	100
5	e	481/563 (85%)	464 (96%)	17 (4%)	0	100	100
6	F	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
6	f	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
7	G	190/234 (81%)	185 (97%)	5 (3%)	0	100	100
7	g	190/234 (81%)	185 (97%)	5 (3%)	0	100	100
8	H	94/122 (77%)	92 (98%)	2 (2%)	0	100	100
8	h	94/122 (77%)	92 (98%)	2 (2%)	0	100	100
9	I	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
9	i	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
10	J	72/80 (90%)	68 (94%)	4 (6%)	0	100	100
10	j	72/80 (90%)	68 (94%)	4 (6%)	0	100	100
11	K	75/141 (53%)	75 (100%)	0	0	100	100
11	k	75/141 (53%)	75 (100%)	0	0	100	100
12	L	38/109 (35%)	35 (92%)	3 (8%)	0	100	100
12	l	38/109 (35%)	35 (92%)	3 (8%)	0	100	100
All	All	5006/6456 (78%)	4816 (96%)	188 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	PRO
1	a	217	PRO

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	311/319 (98%)	297 (96%)	14 (4%)	24	58
1	a	311/319 (98%)	297 (96%)	14 (4%)	24	58
2	B	205/338 (61%)	202 (98%)	3 (2%)	57	84
2	b	205/338 (61%)	202 (98%)	3 (2%)	57	84
3	C	287/421 (68%)	277 (96%)	10 (4%)	32	67
3	c	287/421 (68%)	277 (96%)	10 (4%)	32	67
4	D	387/428 (90%)	377 (97%)	10 (3%)	40	75
4	d	387/428 (90%)	377 (97%)	10 (3%)	40	75
5	E	414/468 (88%)	407 (98%)	7 (2%)	53	83
5	e	414/468 (88%)	407 (98%)	7 (2%)	53	83
6	F	80/81 (99%)	79 (99%)	1 (1%)	61	86
6	f	80/81 (99%)	79 (99%)	1 (1%)	61	86
7	G	162/193 (84%)	159 (98%)	3 (2%)	50	81
7	g	162/193 (84%)	159 (98%)	3 (2%)	50	81
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%)	84 (98%)	2 (2%)	44	78
9	i	86/115 (75%)	84 (98%)	2 (2%)	44	78
10	J	62/66 (94%)	61 (98%)	1 (2%)	55	83
10	j	62/66 (94%)	61 (98%)	1 (2%)	55	83
11	K	65/111 (59%)	64 (98%)	1 (2%)	57	84
11	k	65/111 (59%)	64 (98%)	1 (2%)	57	84
12	L	30/88 (34%)	28 (93%)	2 (7%)	15	42
12	l	30/88 (34%)	28 (93%)	2 (7%)	15	42
All	All	4348/5464 (80%)	4240 (98%)	108 (2%)	42	76

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	46	THR
3	c	177	GLU

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Mol	Chain	Res	Type
7	g	25	VAL
1	a	99	ARG
1	a	259	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	193	GLN
7	g	5	HIS
3	c	195	GLN
5	e	130	ASN
2	b	311	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 2 are modelled with single atom and 2 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
16	HEM	A	406	1	50,50,50	1.28	6 (12%)	66,82,82	1.08	5 (7%)
14	AOQ	a	402	-	29,29,29	0.17	0	40,42,42	0.27	0
18	FES	c	503	3	0,4,4	-	-	-	-	-
15	A1IJD	A	403	-	35,36,36	0.34	0	50,53,53	0.26	0
16	HEM	a	405	1	50,50,50	1.34	6 (12%)	66,82,82	1.16	5 (7%)
13	CDL	I	101	-	99,99,99	0.29	0	105,111,111	0.27	0
13	CDL	D	601	-	99,99,99	0.29	0	105,111,111	0.28	0
19	PC1	c	504	-	53,53,53	0.27	0	59,61,61	0.28	0
13	CDL	J	101	-	99,99,99	0.29	0	105,111,111	0.27	0
17	HEC	B	402	2	50,50,50	1.77	5 (10%)	68,82,82	1.39	6 (8%)
14	AOQ	A	402	-	29,29,29	0.17	0	40,42,42	0.27	0
13	CDL	C	503	-	99,99,99	0.30	0	105,111,111	0.25	0
13	CDL	b	401	2	99,99,99	0.30	0	105,111,111	0.31	0
15	A1IJD	a	403	-	35,36,36	0.33	0	50,53,53	0.26	0
19	PC1	C	502	-	53,53,53	0.27	0	59,61,61	0.29	0
13	CDL	L	201	-	99,99,99	0.29	0	105,111,111	0.27	0
19	PC1	C	504	-	53,53,53	0.26	0	59,61,61	0.30	0
13	CDL	B	401	2	99,99,99	0.30	0	105,111,111	0.31	0
16	HEM	A	405	1	50,50,50	1.34	6 (12%)	66,82,82	1.16	5 (7%)
13	CDL	A	401	-	99,99,99	0.30	0	105,111,111	0.27	0
13	CDL	c	501	-	99,99,99	0.30	0	105,111,111	0.25	0
18	FES	C	501	3	0,4,4	-	-	-	-	-
16	HEM	a	406	1	50,50,50	1.29	6 (12%)	66,82,82	1.09	5 (7%)
13	CDL	a	401	-	99,99,99	0.30	0	105,111,111	0.27	0
19	PC1	c	502	-	53,53,53	0.27	0	59,61,61	0.30	0
13	CDL	g	301	-	99,99,99	0.28	0	105,111,111	0.28	0
13	CDL	d	601	-	99,99,99	0.28	0	105,111,111	0.28	0
17	HEC	b	402	2	50,50,50	1.77	5 (10%)	68,82,82	1.39	6 (8%)
13	CDL	l	201	-	99,99,99	0.30	0	105,111,111	0.27	0
13	CDL	G	301	-	99,99,99	0.28	0	105,111,111	0.28	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	HEM	A	406	1	-	5/14/54/54	-
14	AOQ	a	402	-	-	0/8/38/38	0/4/4/4
18	FES	c	503	3	-	-	0/1/1/1
15	A1IJD	A	403	-	-	3/15/15/15	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	HEM	a	405	1	-	2/14/54/54	-
13	CDL	I	101	-	-	53/110/110/110	-
13	CDL	D	601	-	-	43/110/110/110	-
19	PC1	c	504	-	-	25/57/57/57	-
13	CDL	J	101	-	-	53/110/110/110	-
17	HEC	B	402	2	1/1/7/7	7/14/54/54	-
14	AOQ	A	402	-	-	0/8/38/38	0/4/4/4
13	CDL	C	503	-	-	18/110/110/110	-
13	CDL	b	401	2	-	16/110/110/110	-
15	A1IJD	a	403	-	-	3/15/15/15	0/4/4/4
19	PC1	C	502	-	-	25/57/57/57	-
13	CDL	L	201	-	-	21/110/110/110	-
19	PC1	C	504	-	-	21/57/57/57	-
13	CDL	B	401	2	-	16/110/110/110	-
16	HEM	A	405	1	-	2/14/54/54	-
13	CDL	A	401	-	-	14/110/110/110	-
13	CDL	c	501	-	-	18/110/110/110	-
18	FES	C	501	3	-	-	0/1/1/1
16	HEM	a	406	1	-	5/14/54/54	-
13	CDL	a	401	-	-	14/110/110/110	-
19	PC1	c	502	-	-	21/57/57/57	-
13	CDL	g	301	-	-	44/110/110/110	-
13	CDL	d	601	-	-	43/110/110/110	-
17	HEC	b	402	2	1/1/7/7	7/14/54/54	-
13	CDL	l	201	-	-	21/110/110/110	-
13	CDL	G	301	-	-	44/110/110/110	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	402	HEC	C3D-C2D	7.94	1.53	1.36
17	b	402	HEC	C3D-C2D	7.91	1.53	1.36
17	B	402	HEC	FE-ND	4.30	2.08	1.94
17	b	402	HEC	FE-ND	4.29	2.08	1.94
17	B	402	HEC	FE-NB	4.21	2.07	1.94

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	402	HEC	C1D-ND-C4D	6.36	111.64	105.07
17	B	402	HEC	C1D-ND-C4D	6.34	111.62	105.07
16	a	406	HEM	C4D-ND-C1D	2.72	107.89	105.07
16	A	405	HEM	C4D-ND-C1D	2.69	107.85	105.07
16	A	406	HEM	C4D-ND-C1D	2.68	107.84	105.07

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	B	402	HEC	NA
17	b	402	HEC	NA

5 of 544 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	401	CDL	CA2-OA2-PA1-OA3
13	B	401	CDL	O1-C1-CA2-OA2
13	B	401	CDL	CA3-OA5-PA1-OA4
13	B	401	CDL	CB3-CB4-OB6-CB5
13	B	401	CDL	C51-CB5-OB6-CB4

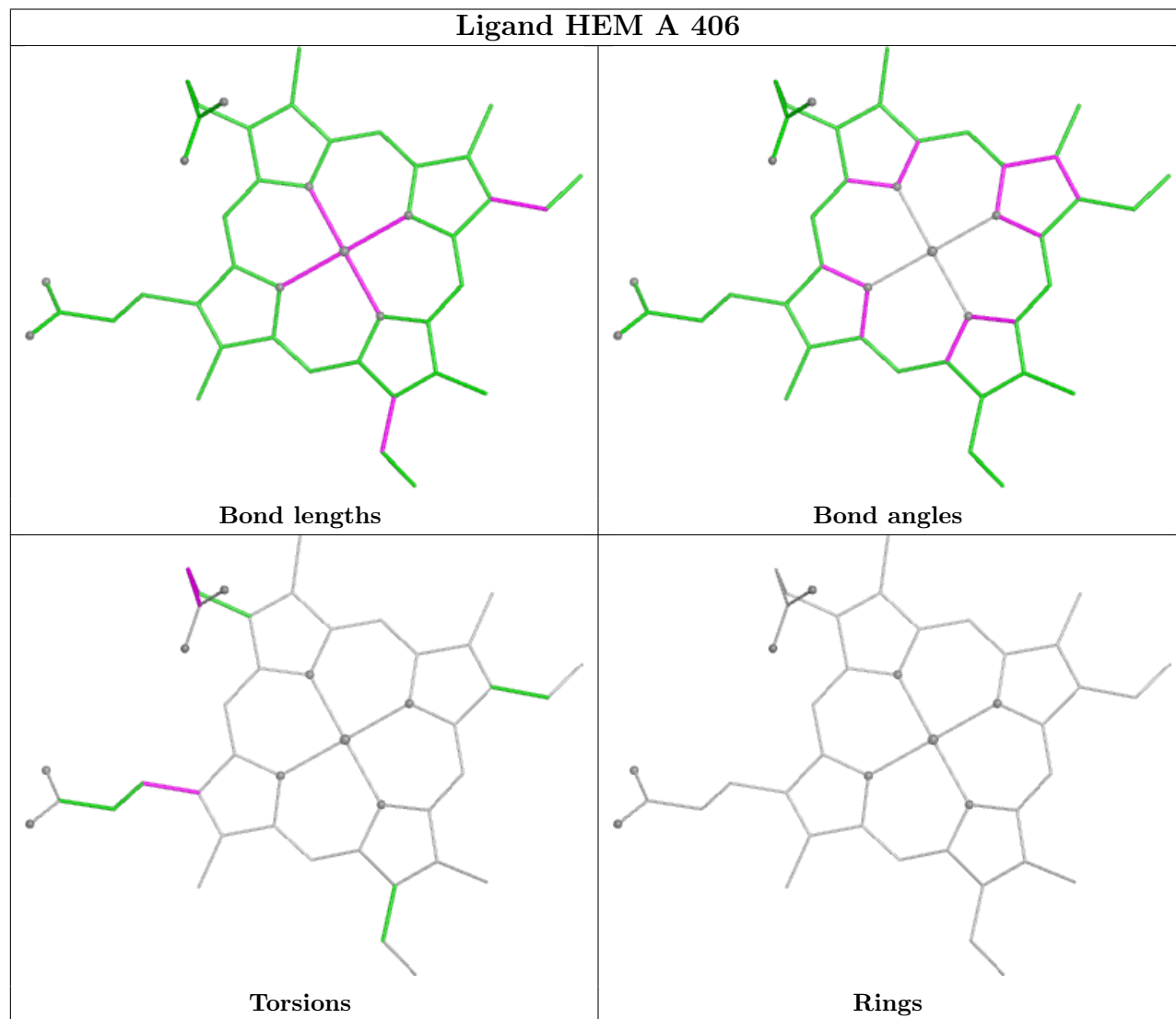
There are no ring outliers.

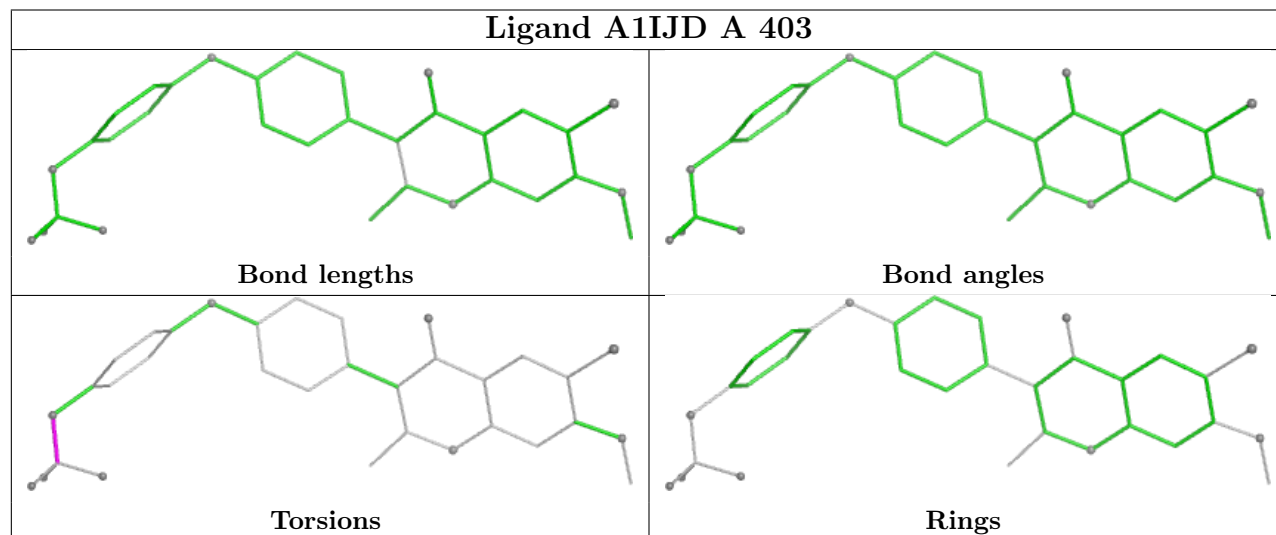
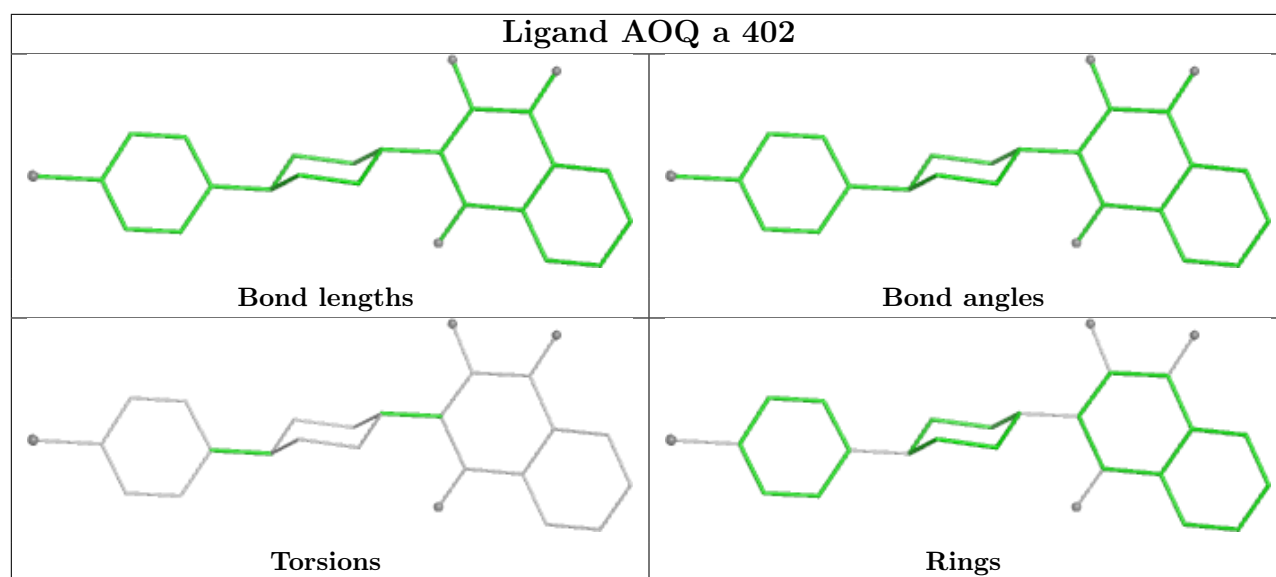
13 monomers are involved in 34 short contacts:

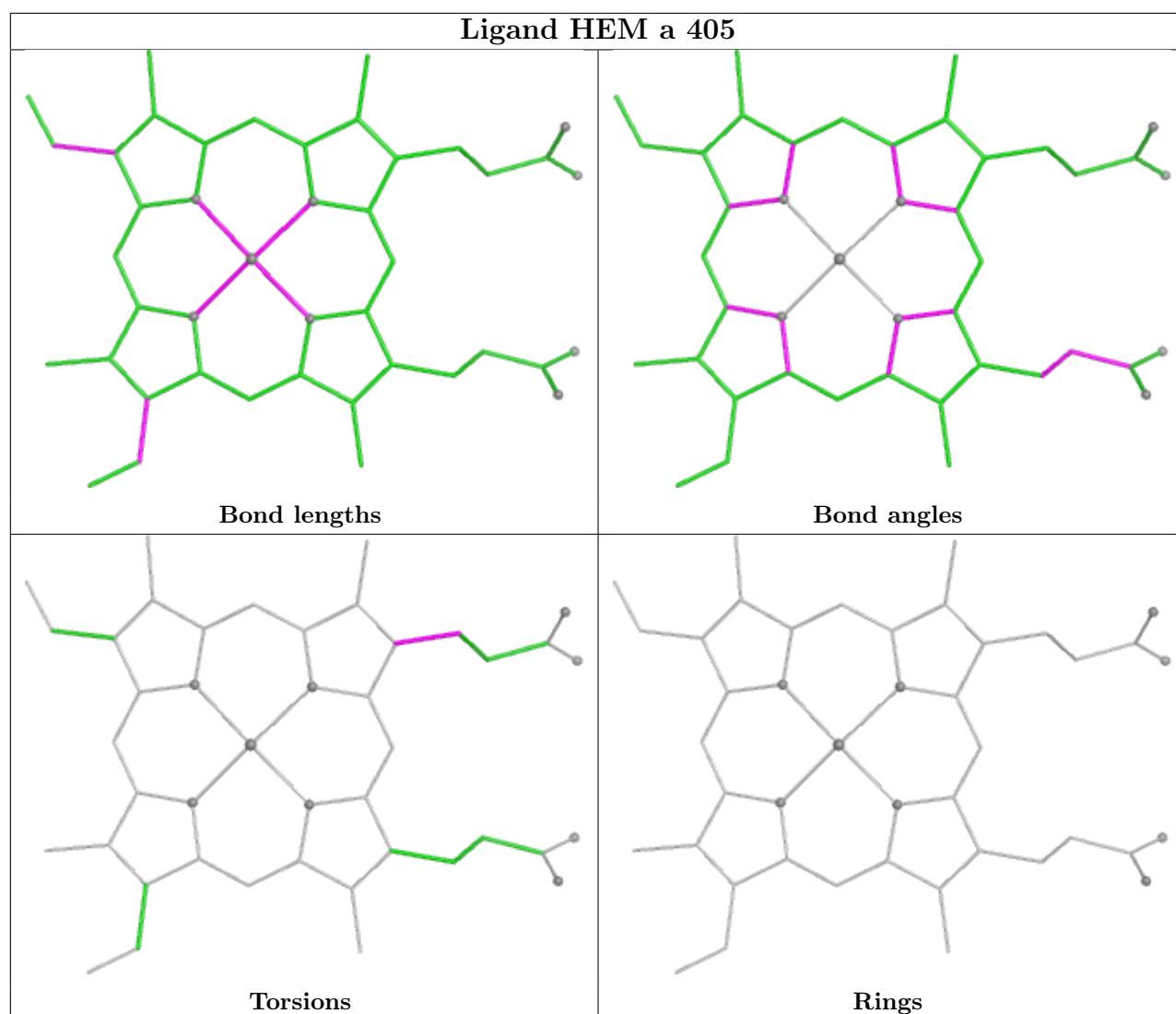
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	406	HEM	6	0
16	a	405	HEM	6	0
13	I	101	CDL	1	0
13	D	601	CDL	1	0
19	c	504	PC1	1	0
13	J	101	CDL	1	0
19	C	504	PC1	3	0
13	B	401	CDL	1	0
16	A	405	HEM	6	0
16	a	406	HEM	6	0
19	c	502	PC1	1	0
13	g	301	CDL	1	0
13	G	301	CDL	1	0

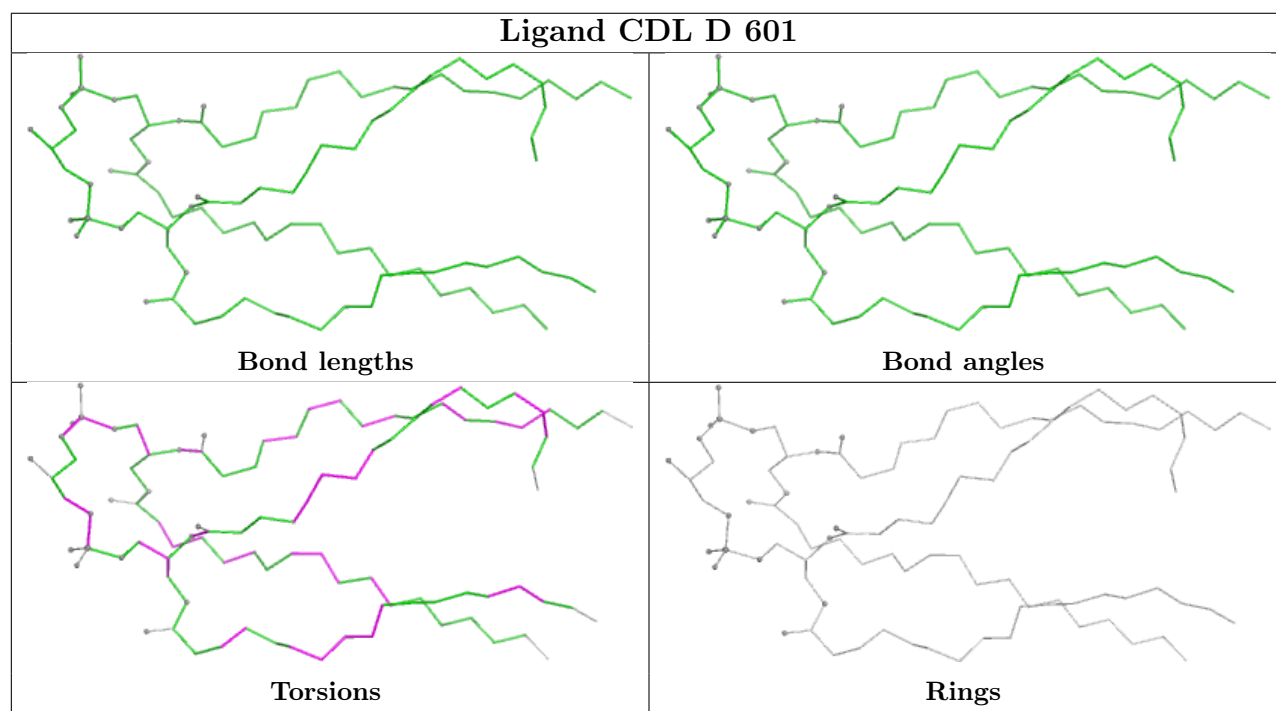
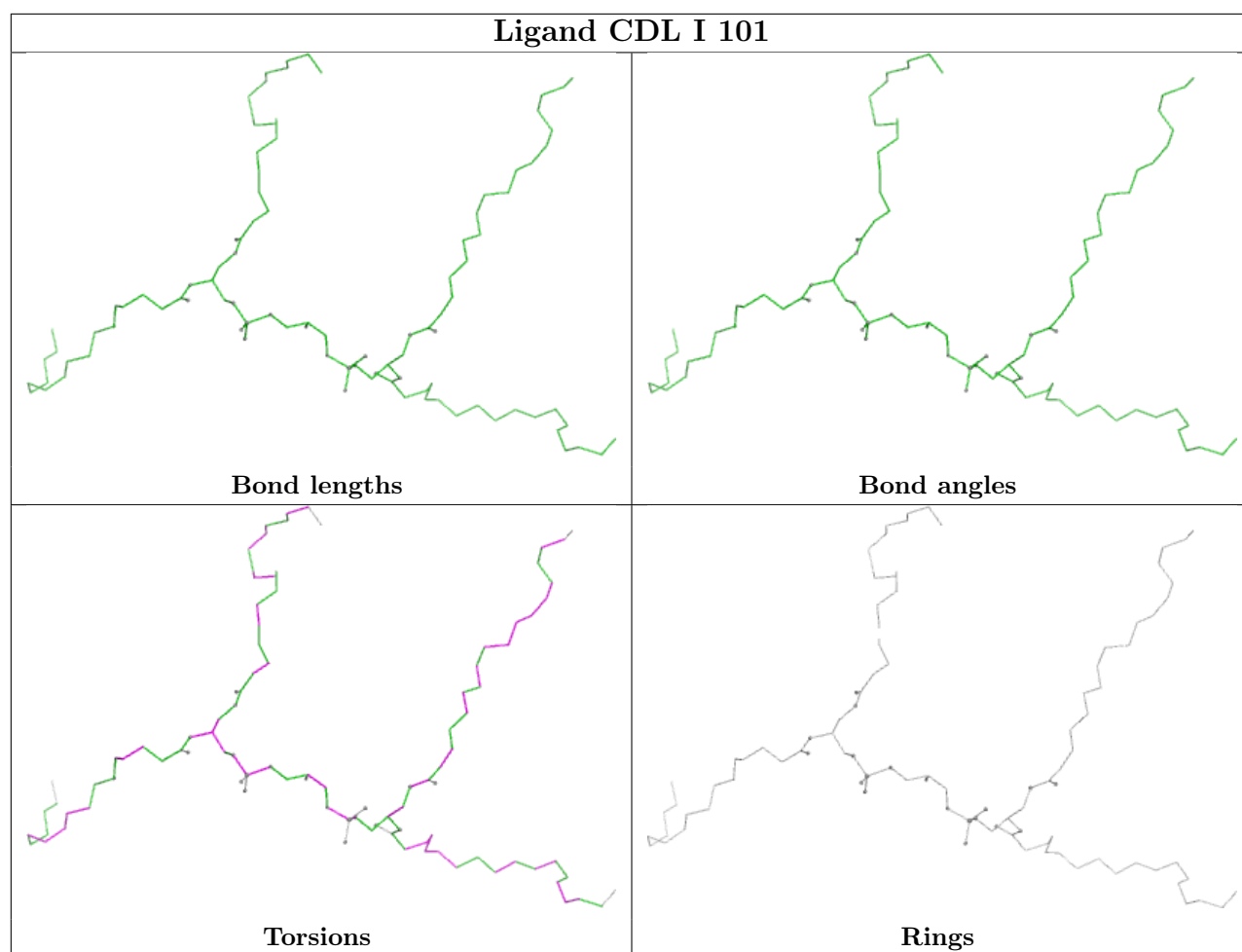
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

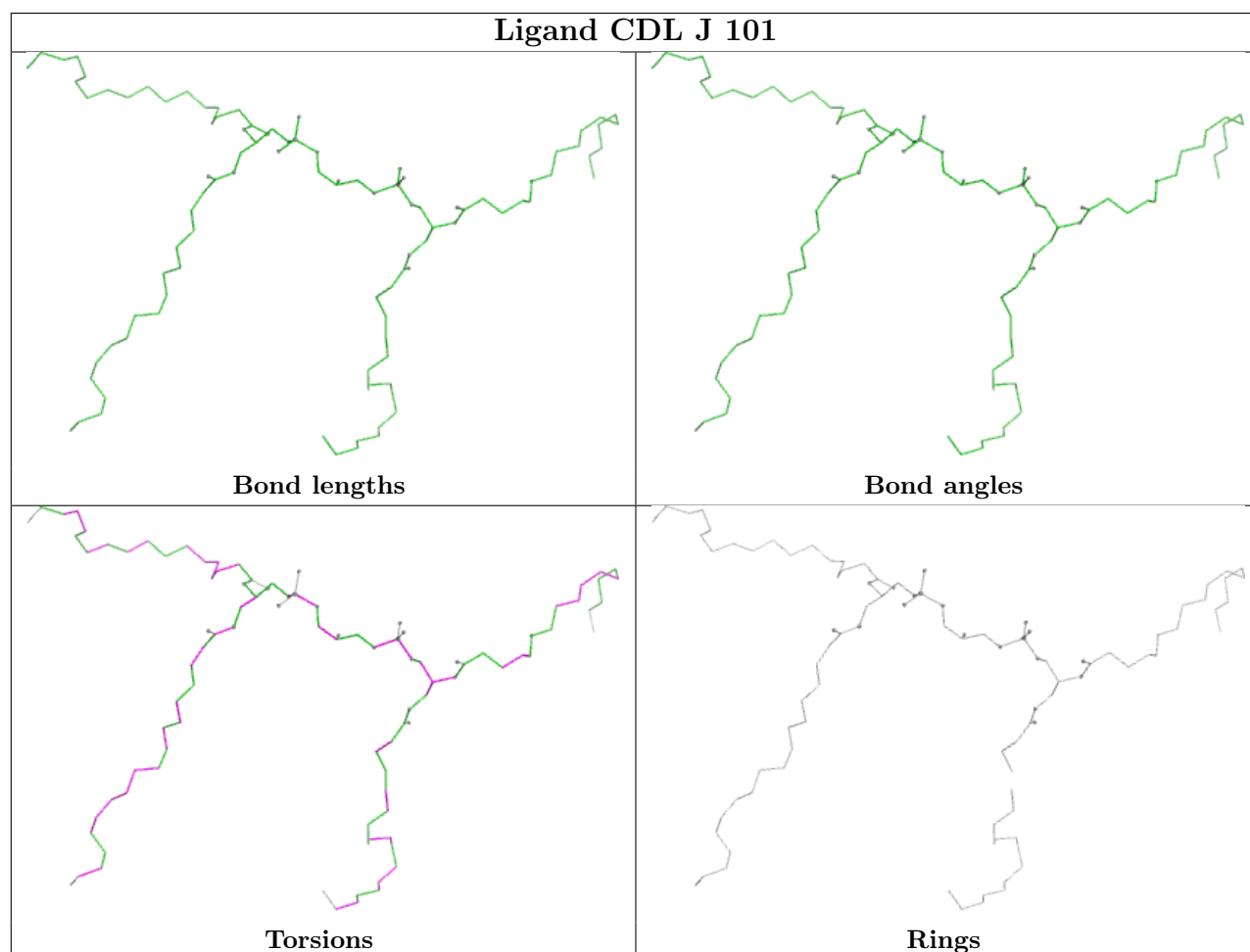
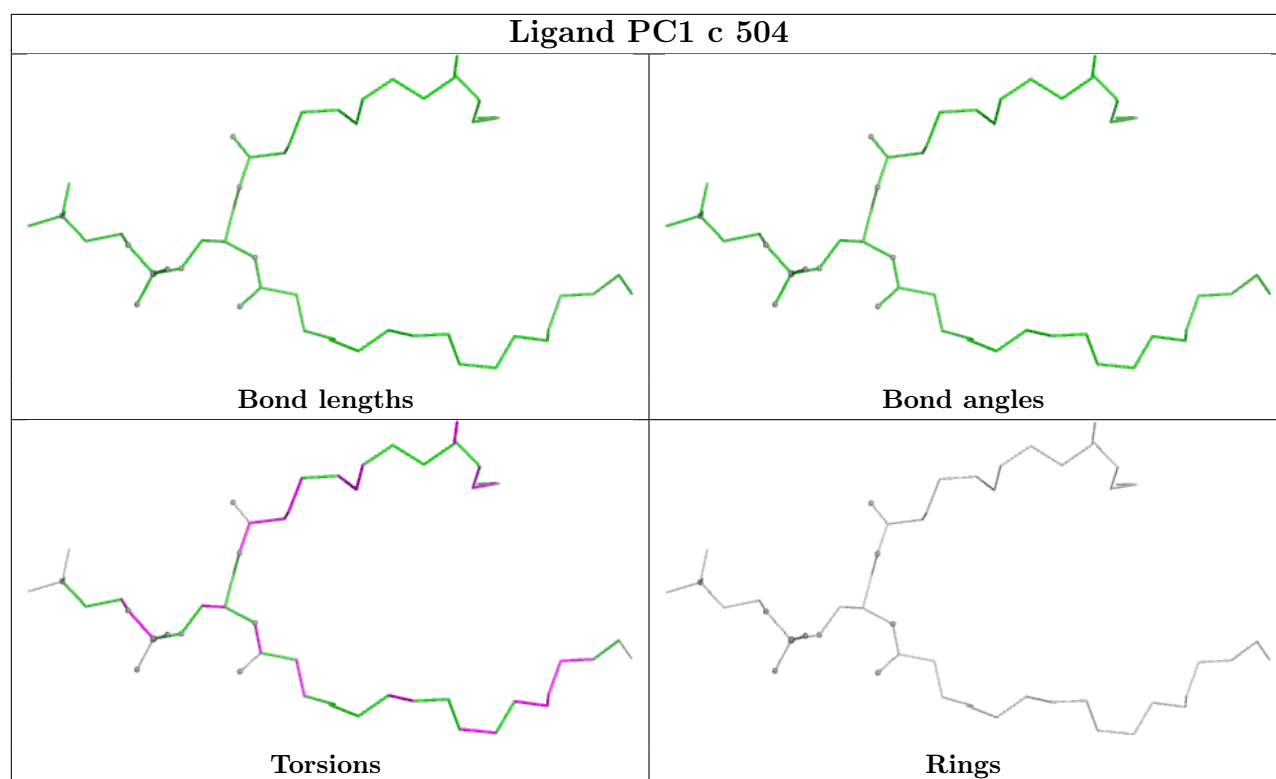
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

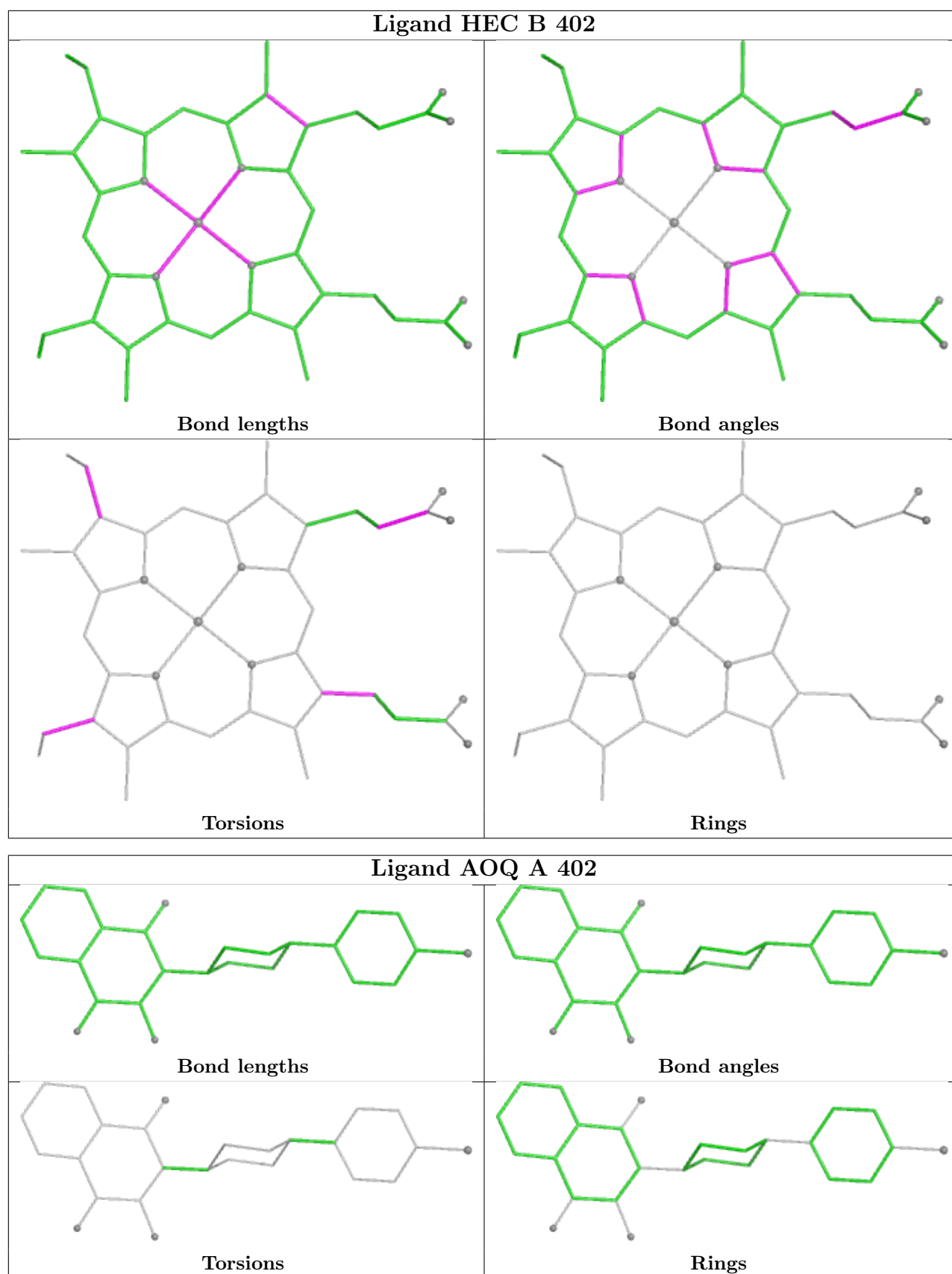


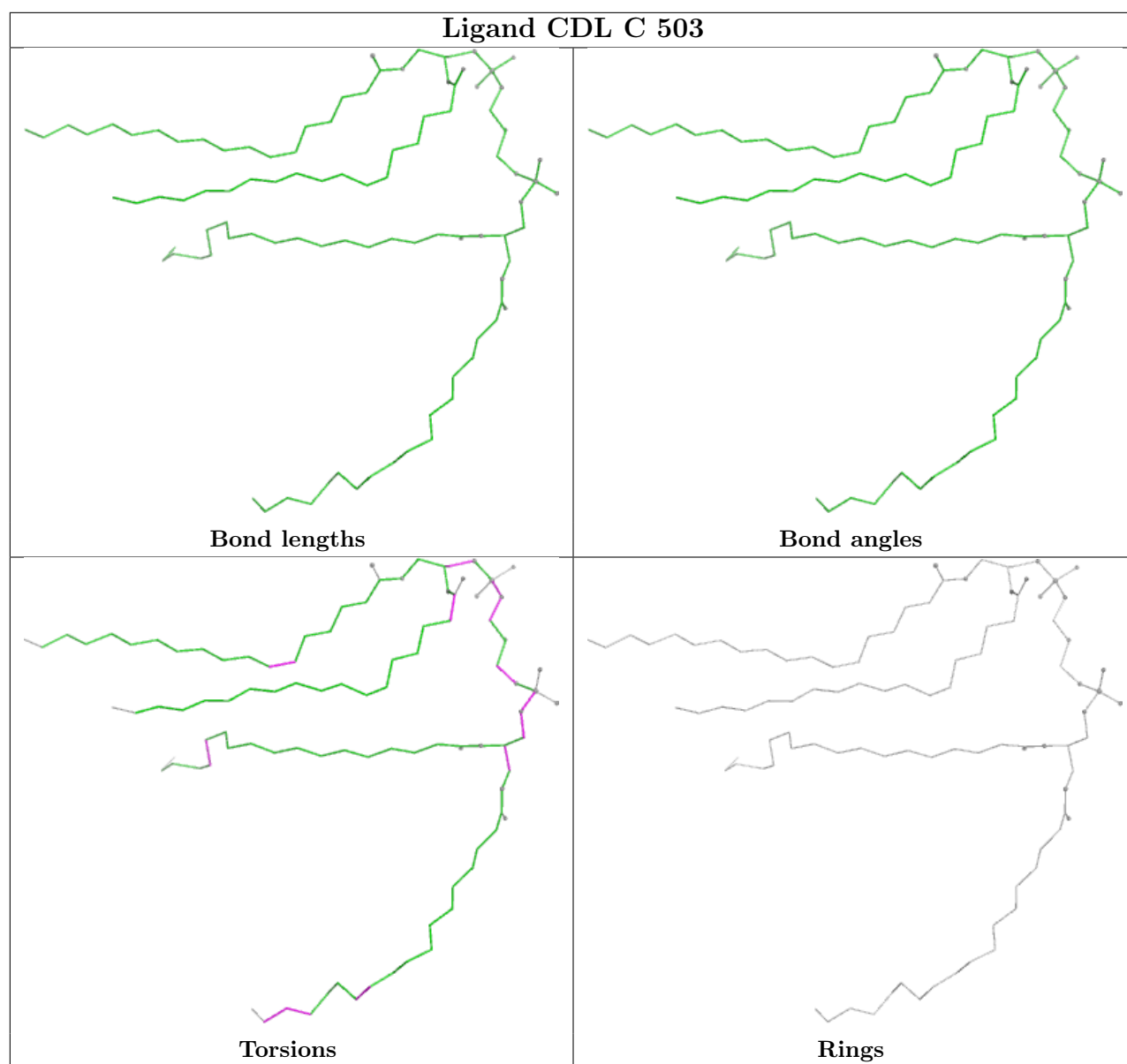


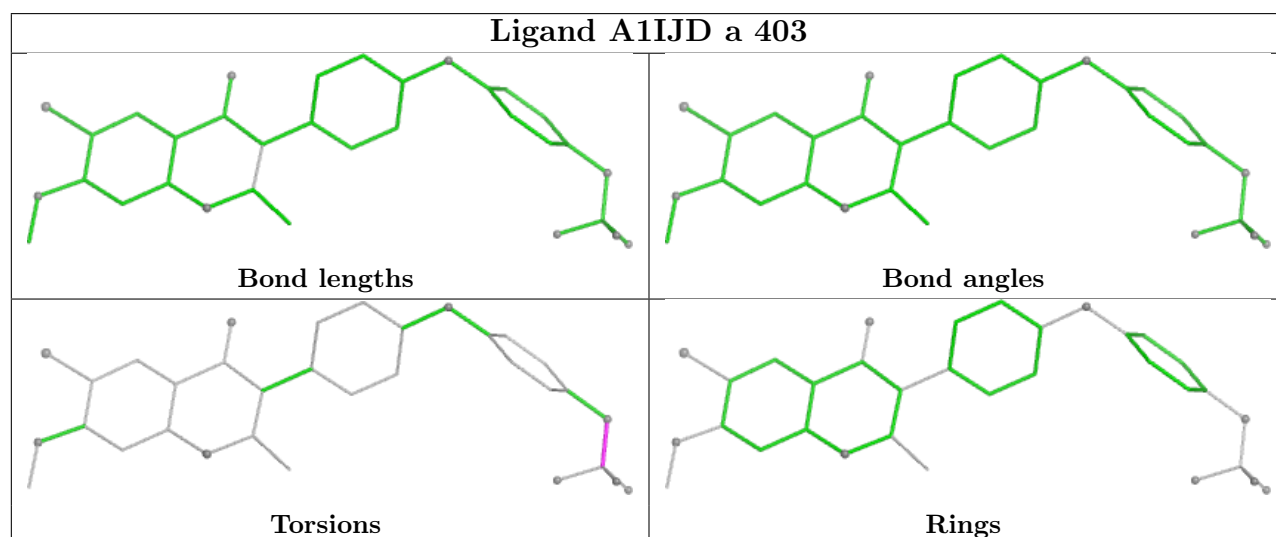
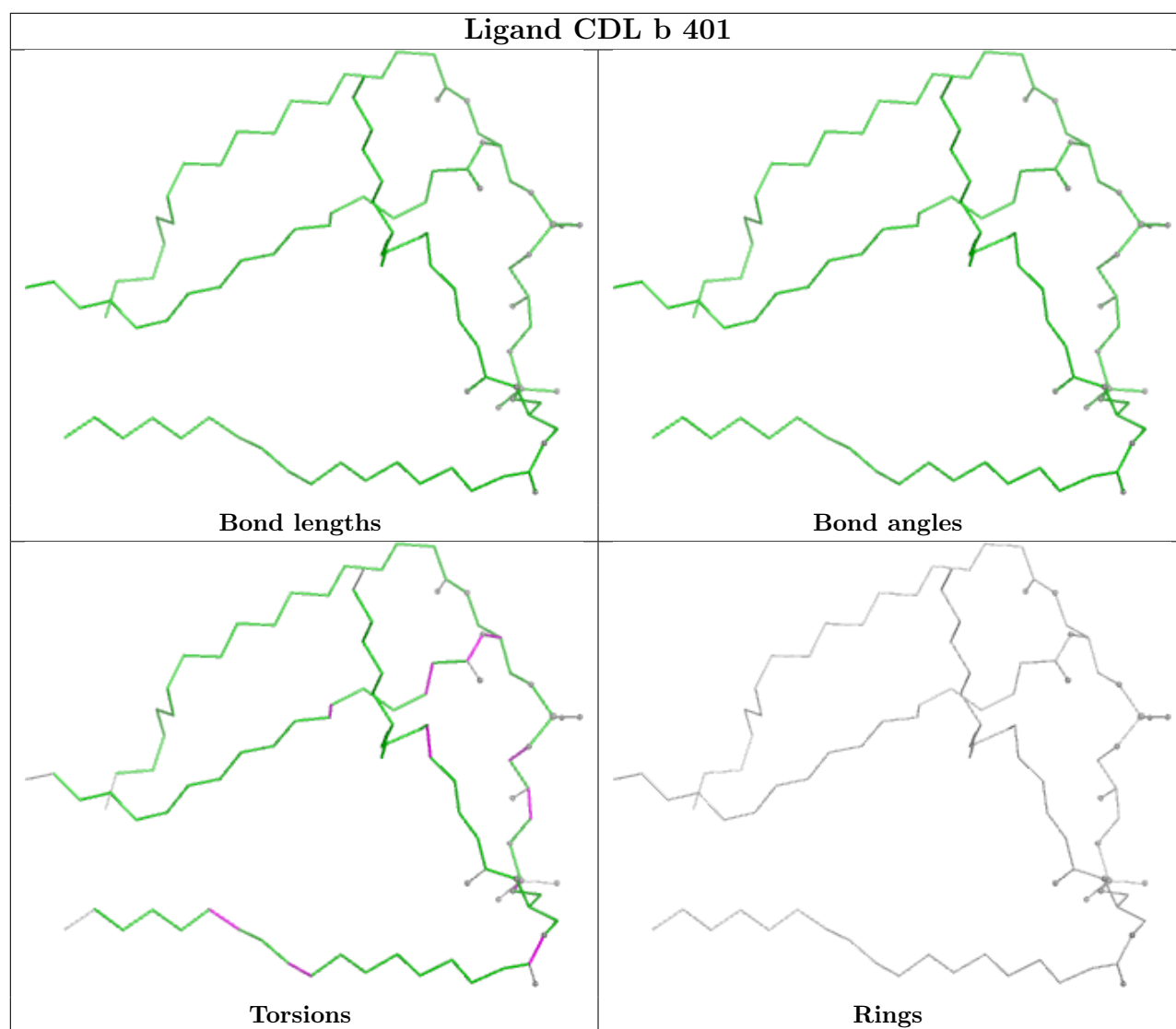


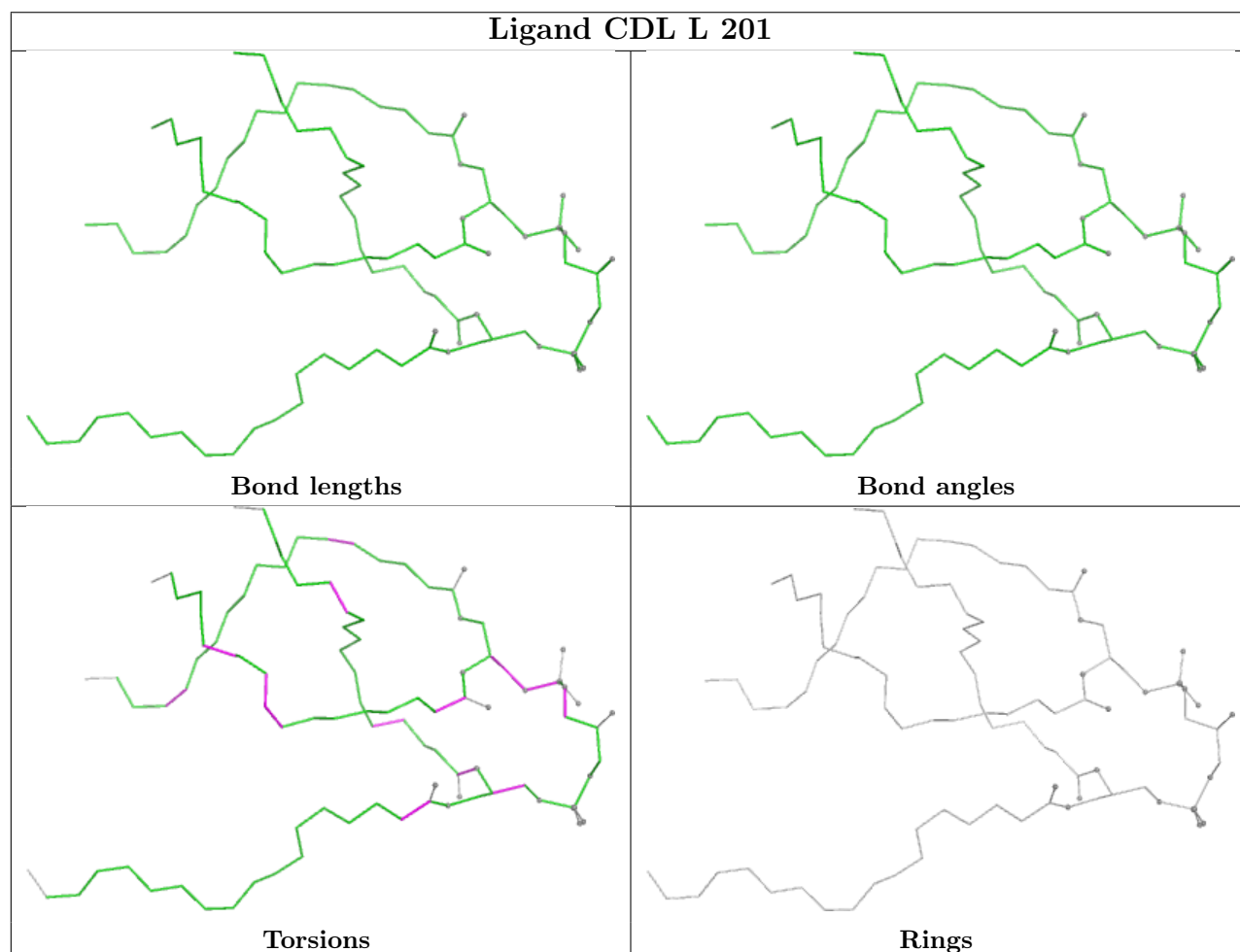
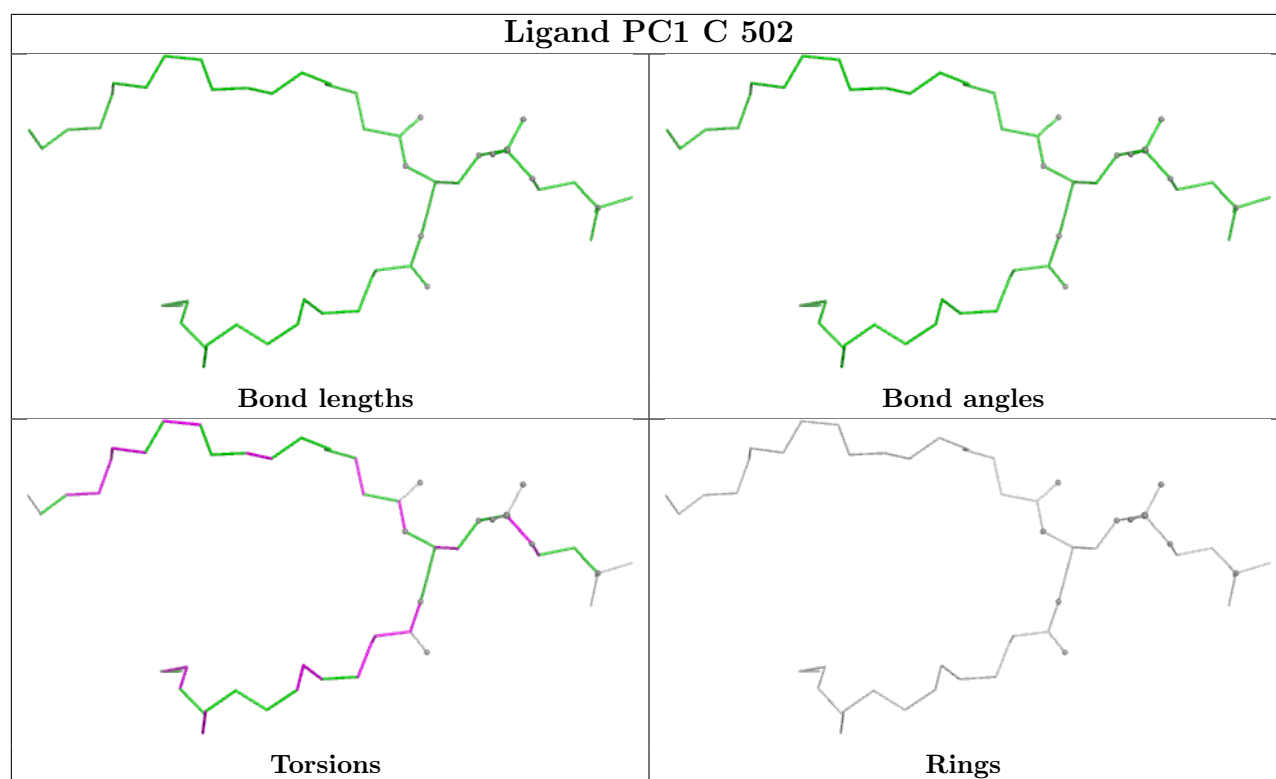


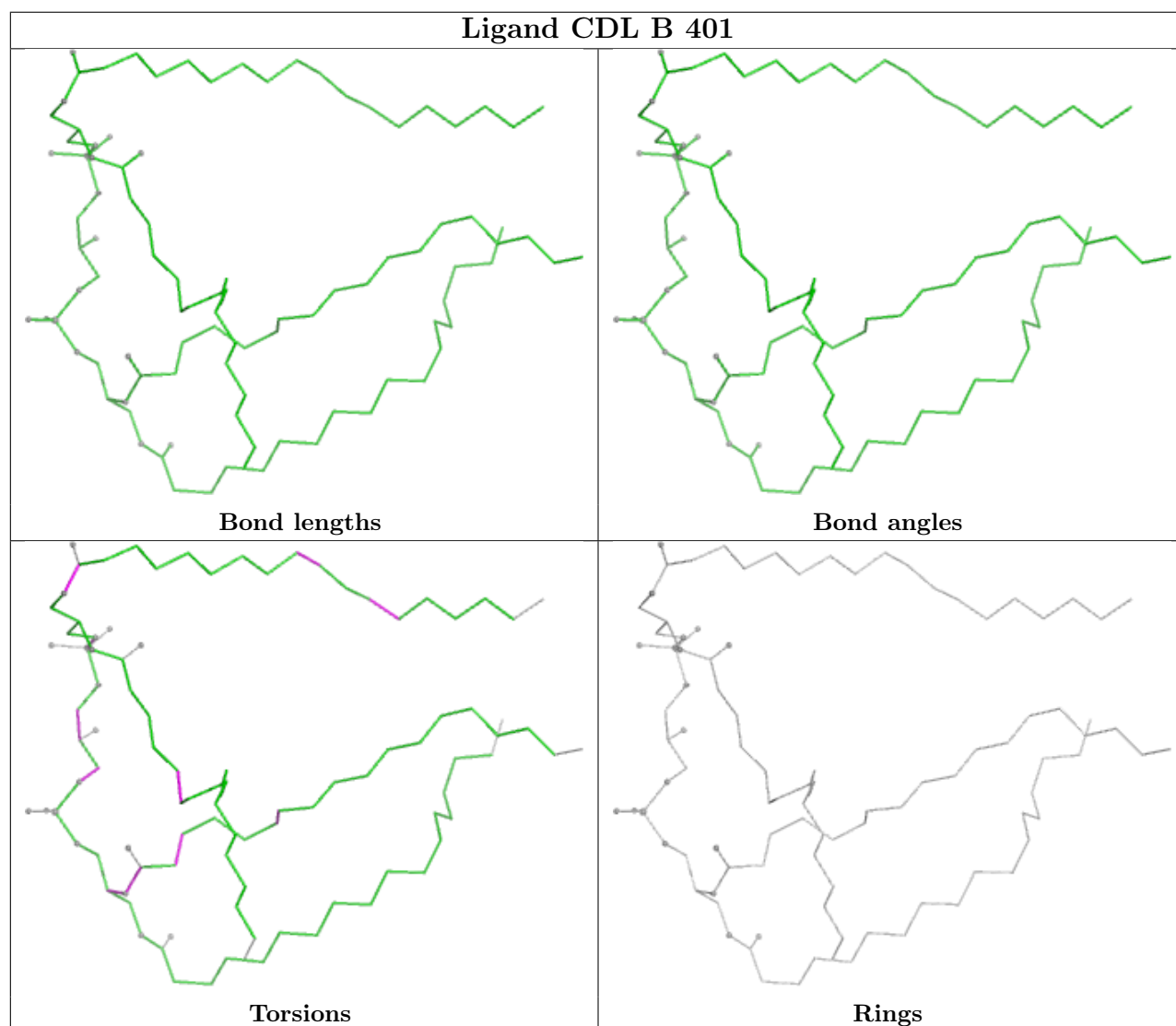
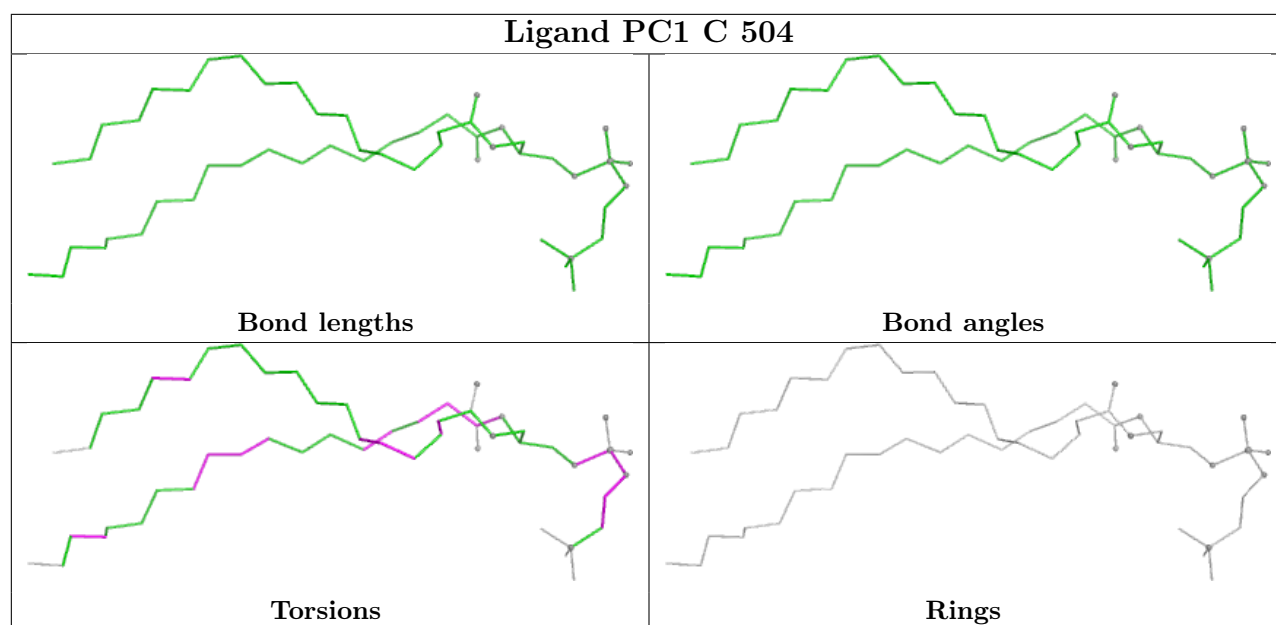


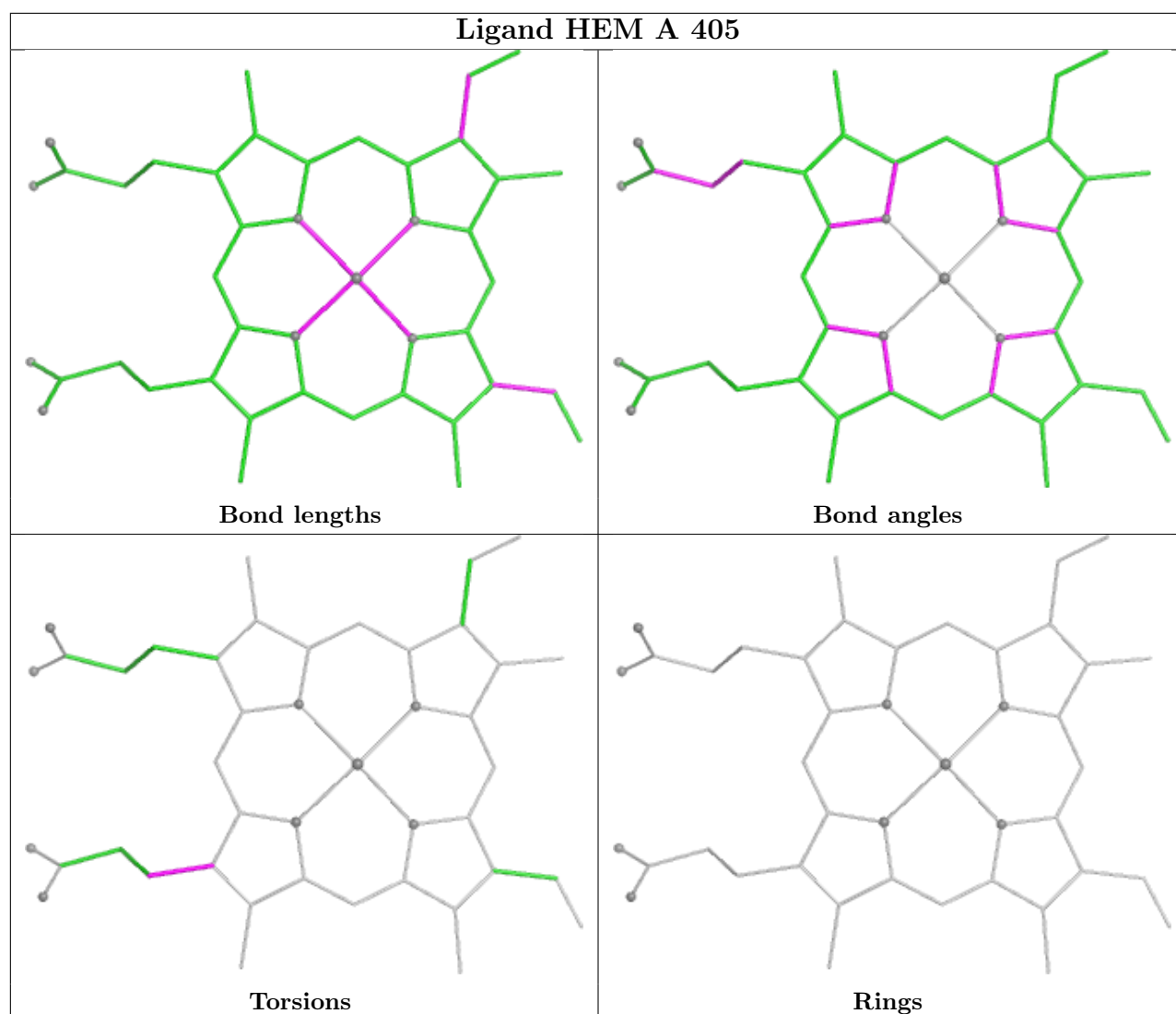


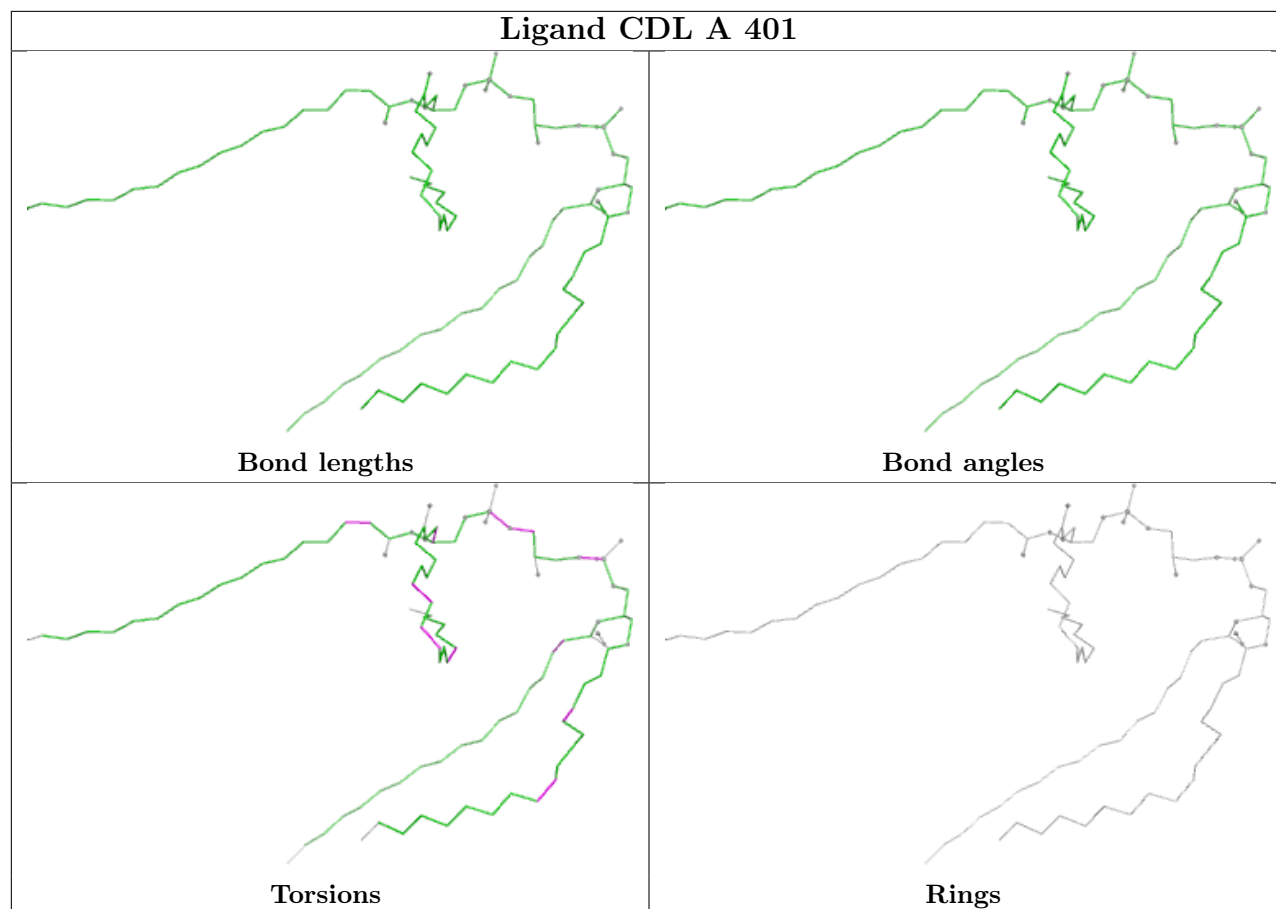


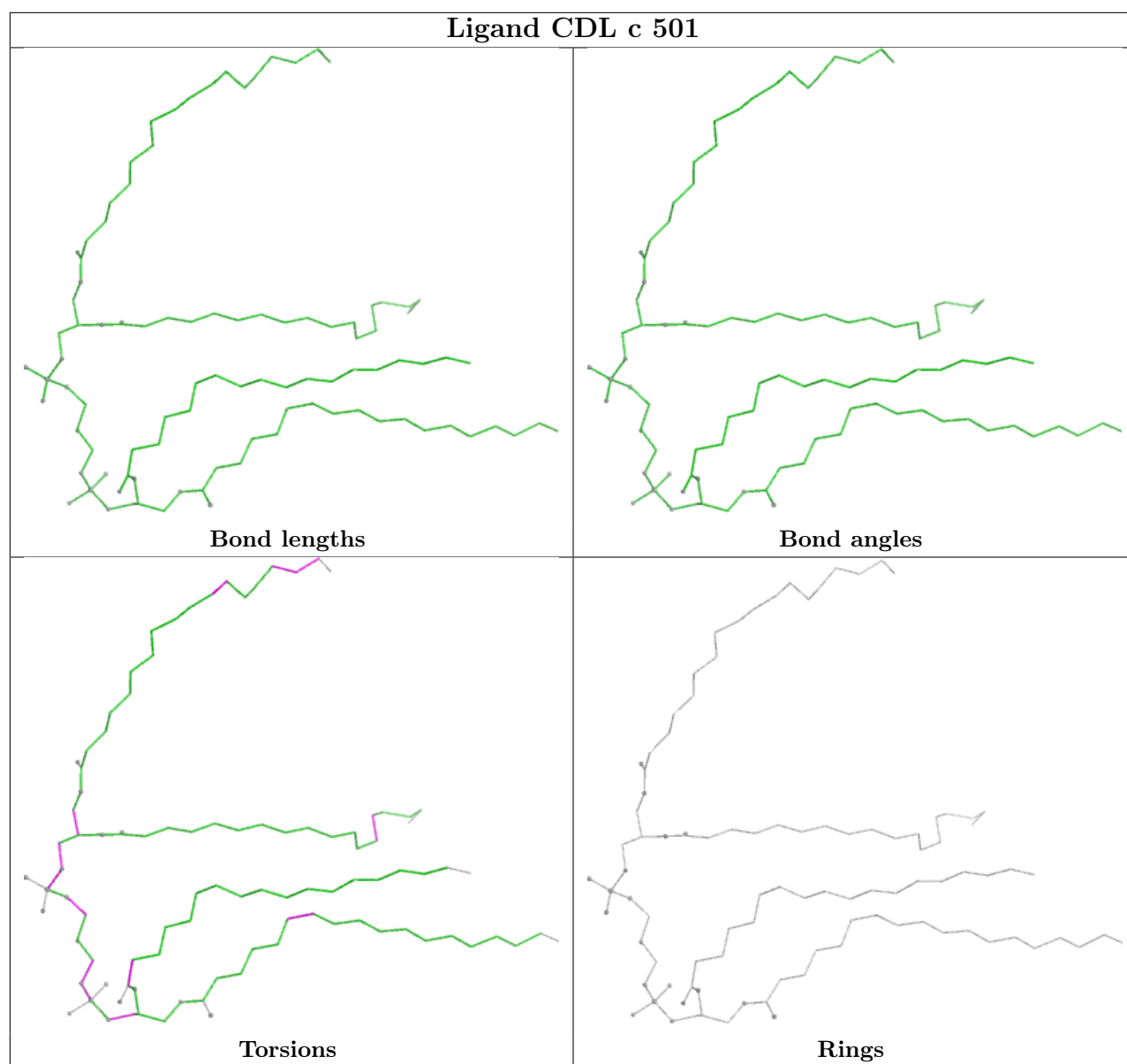


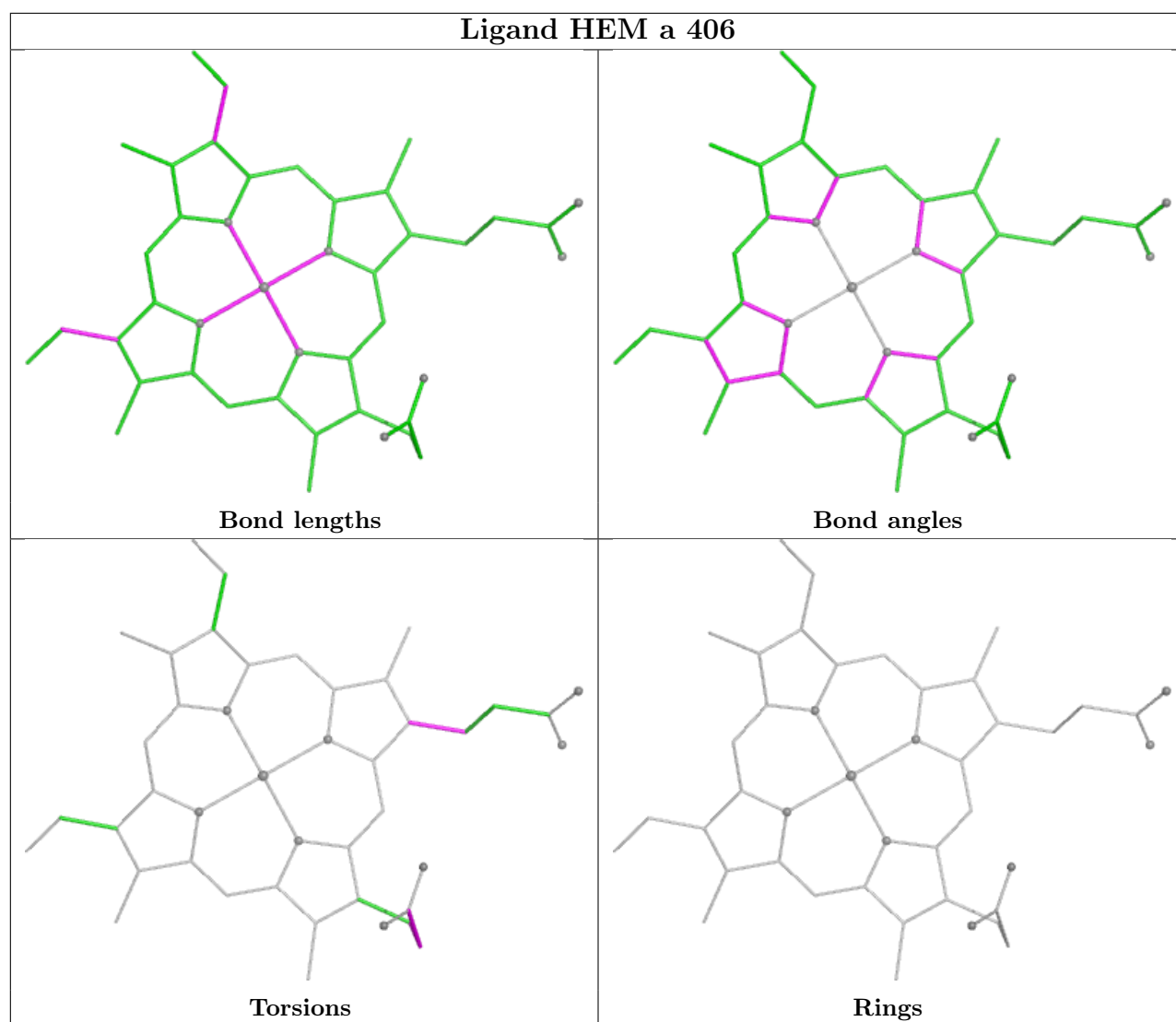


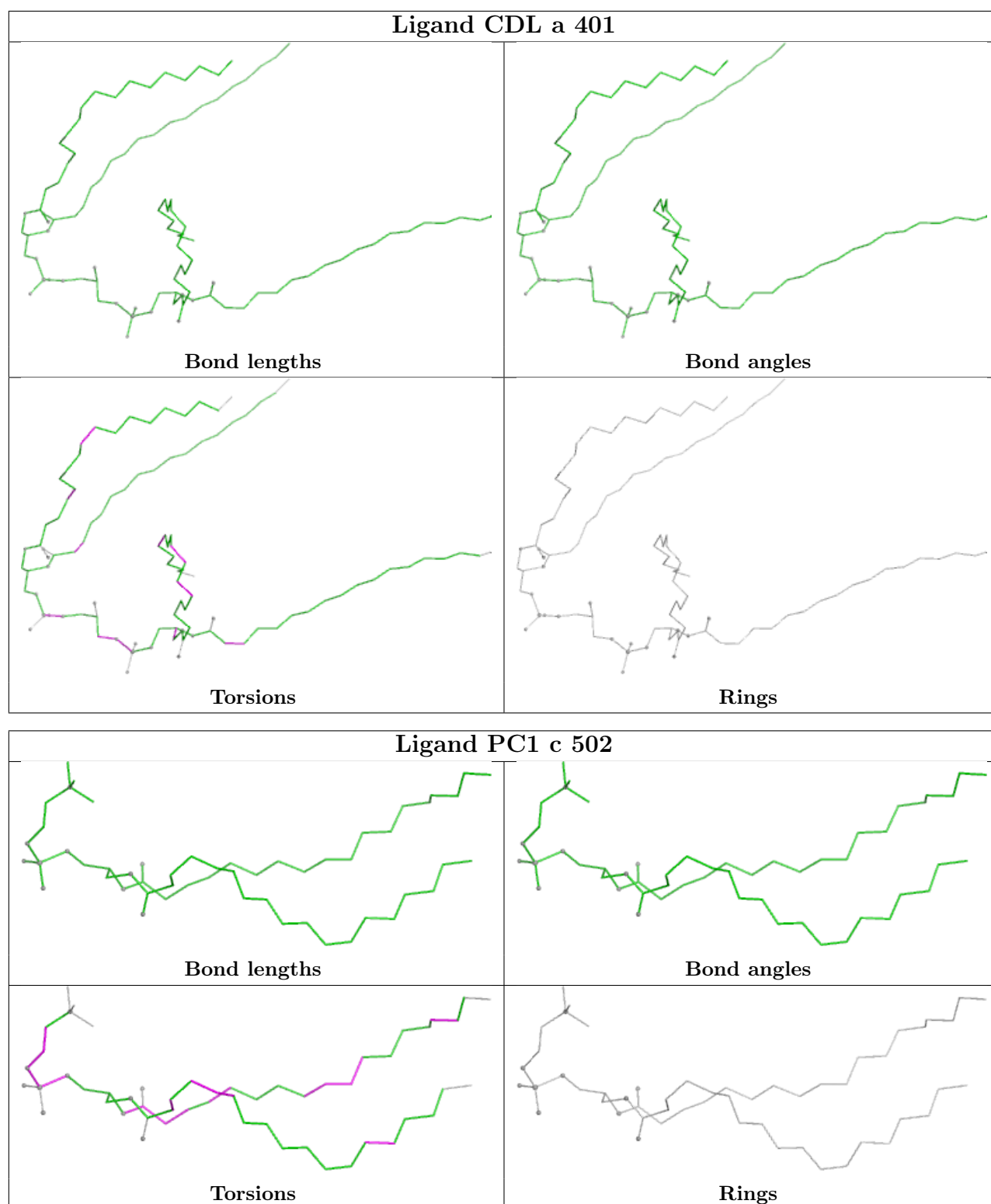


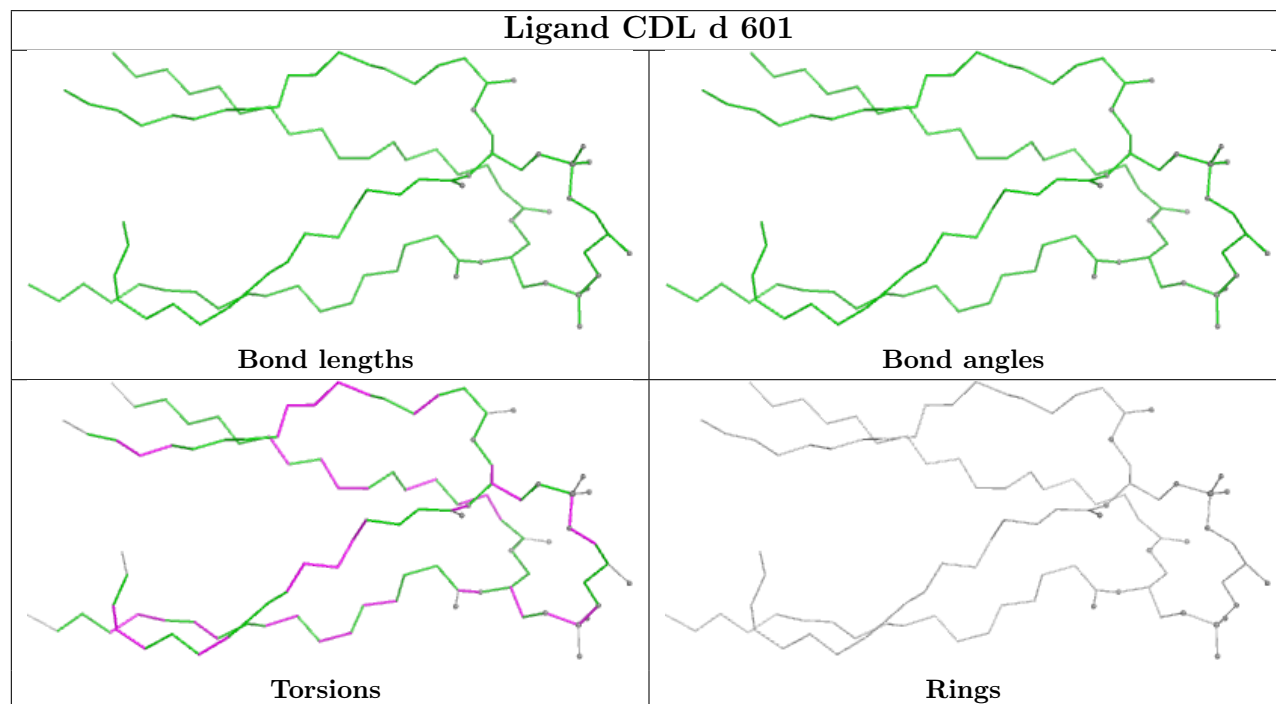
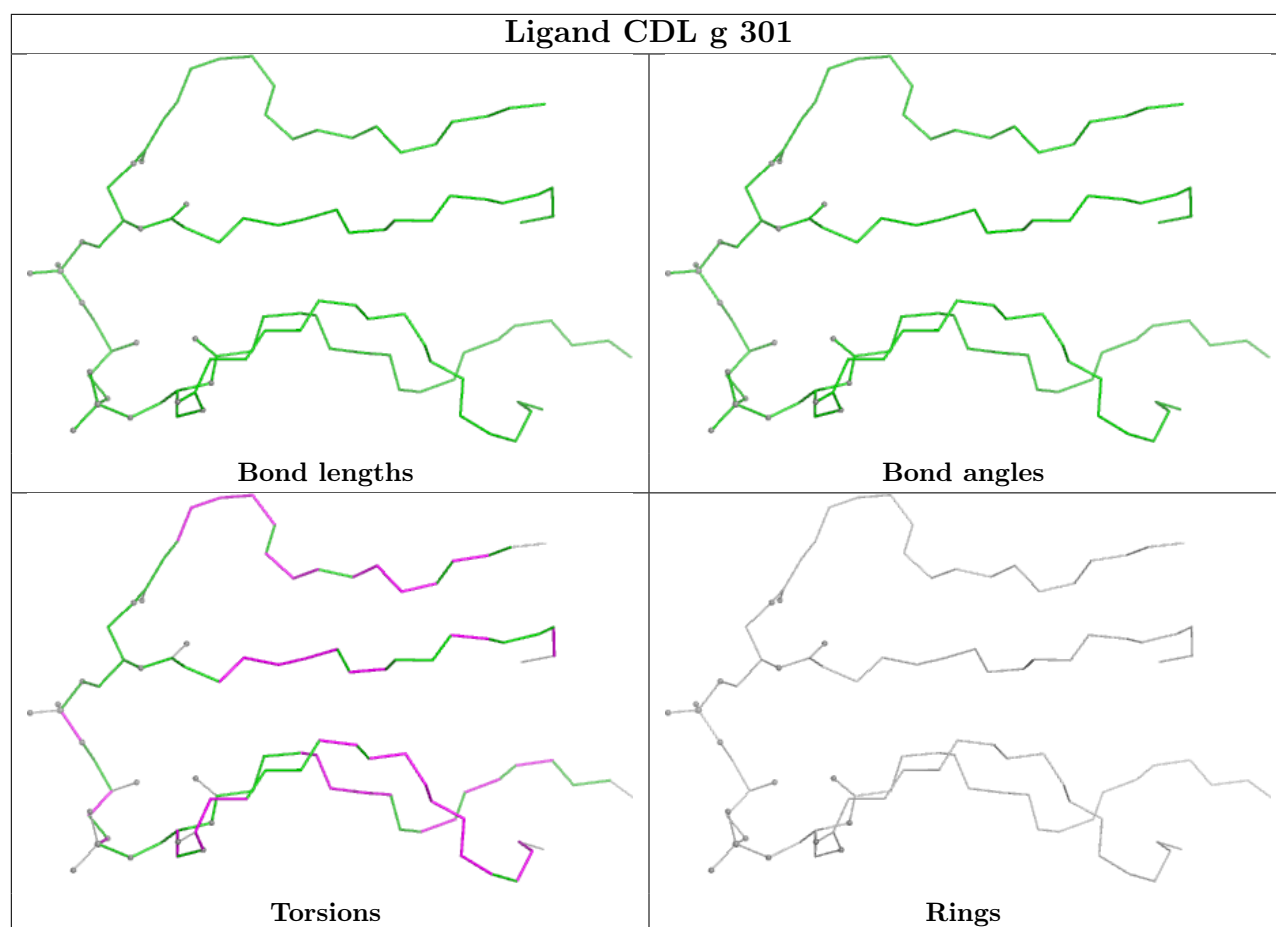


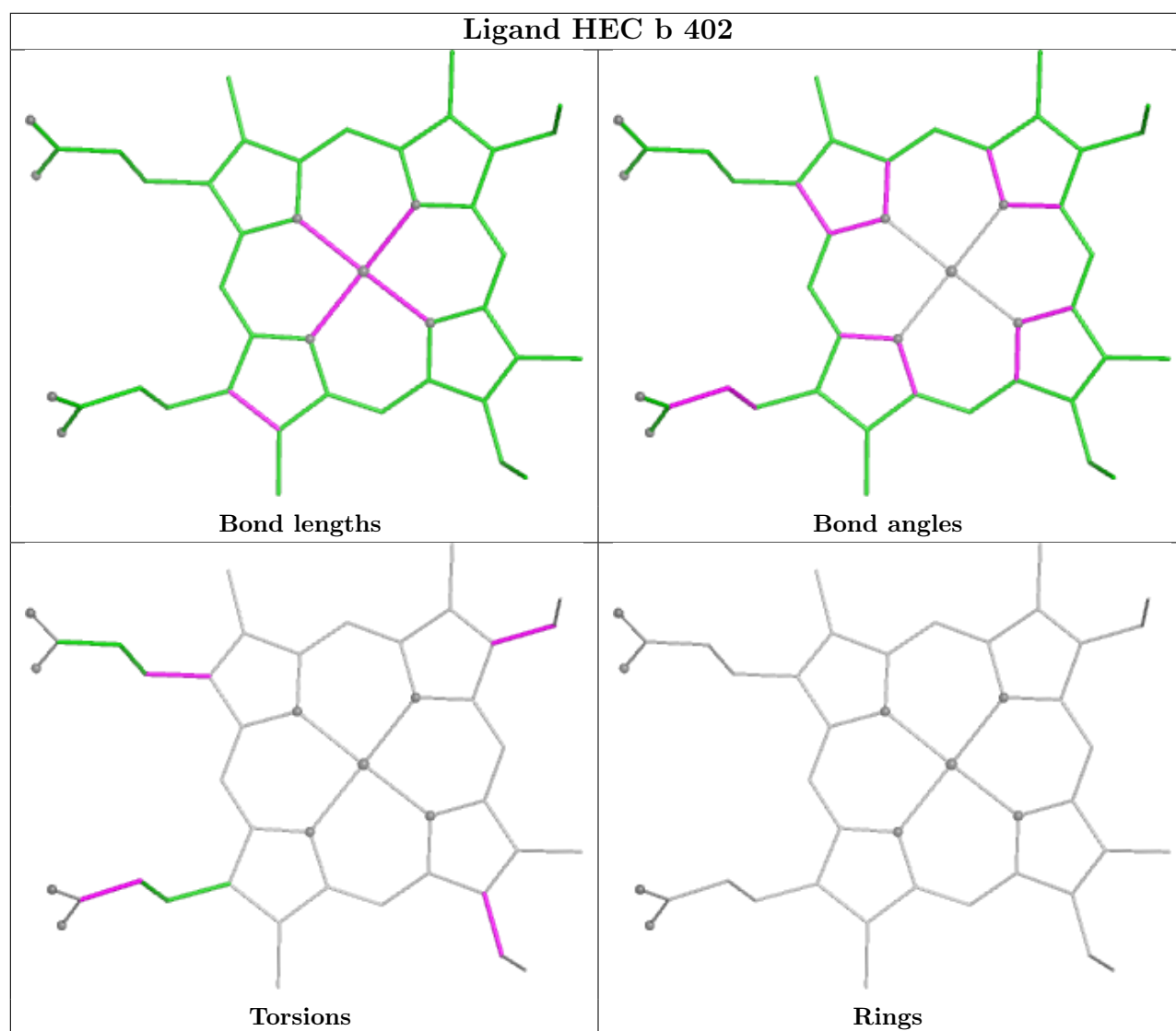


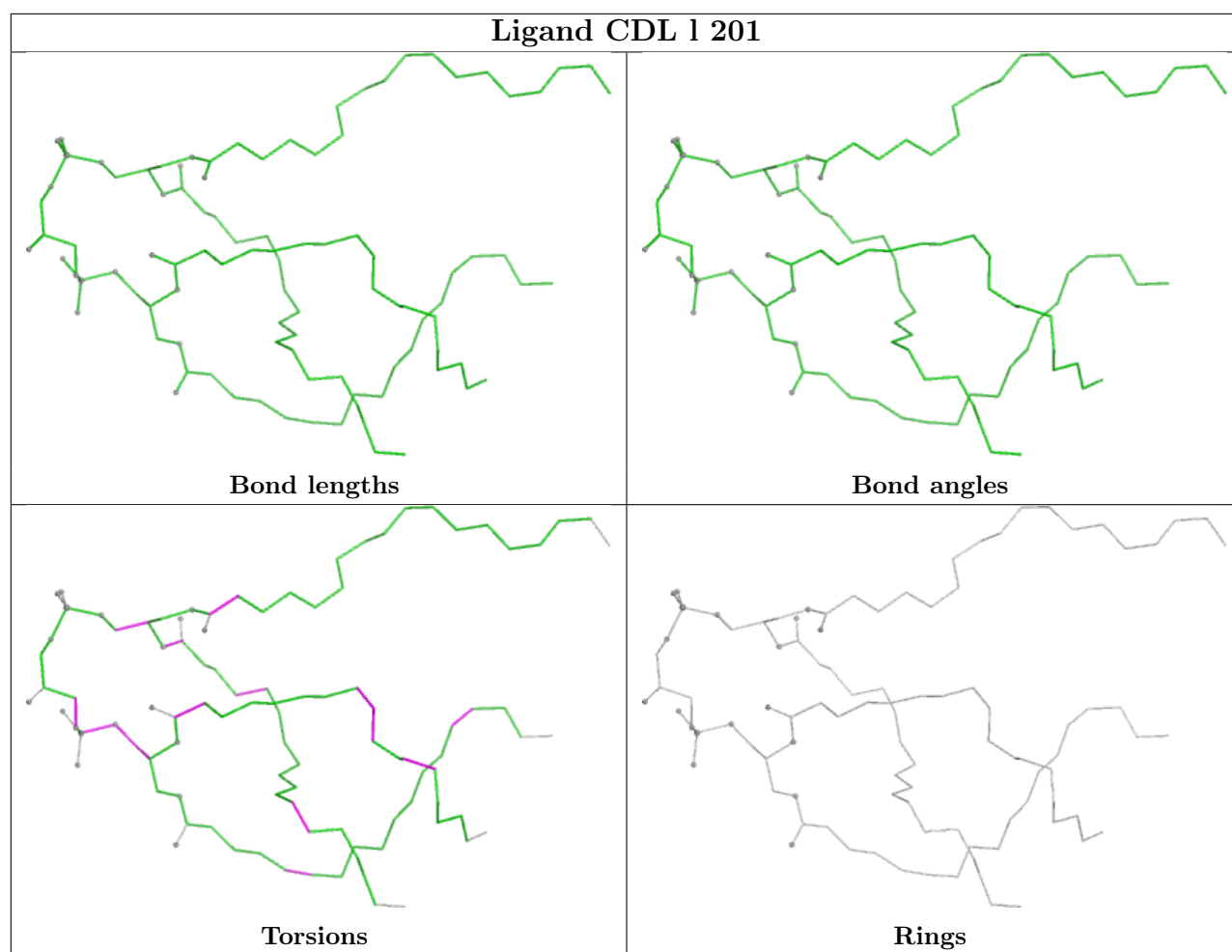


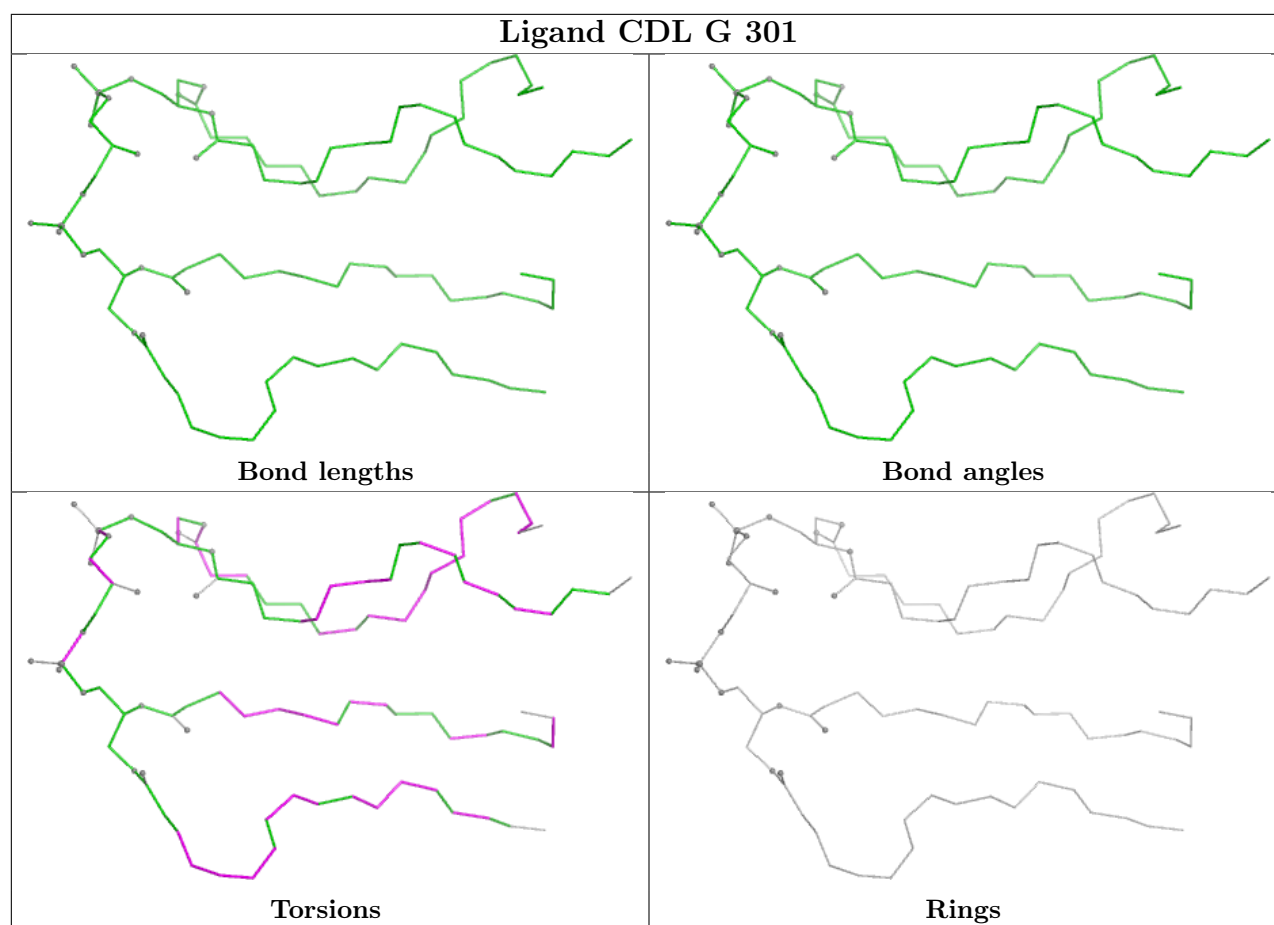












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

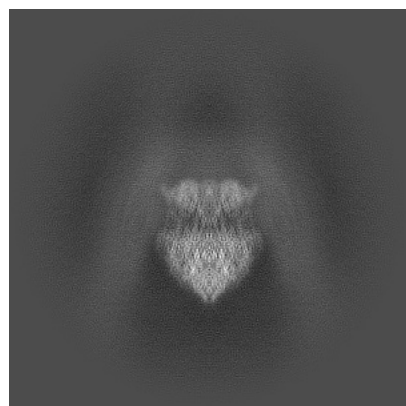
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52621. These allow visual inspection of the internal detail of the map and identification of artifacts.

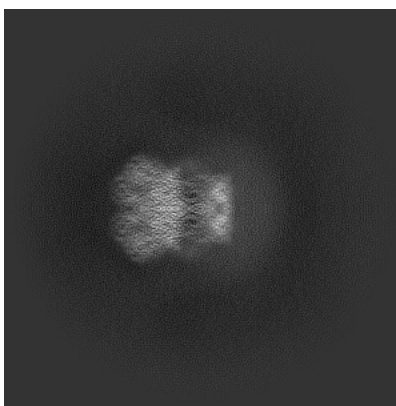
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

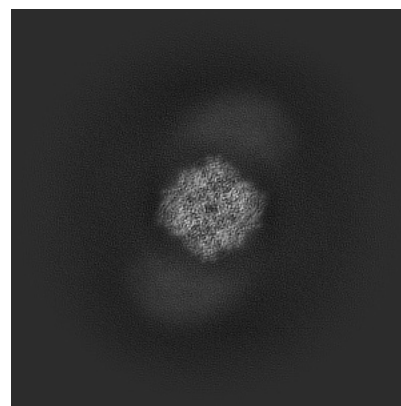
6.1.1 Primary map



X

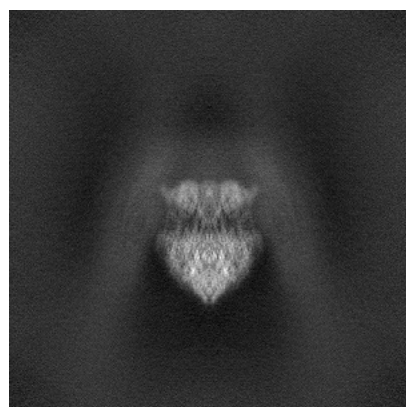


Y

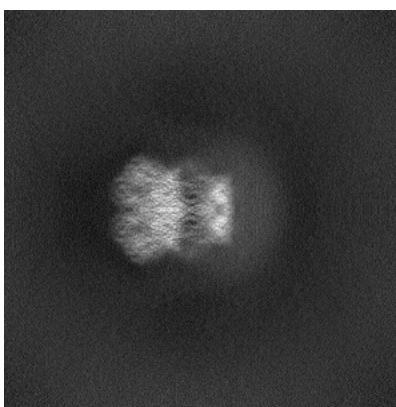


Z

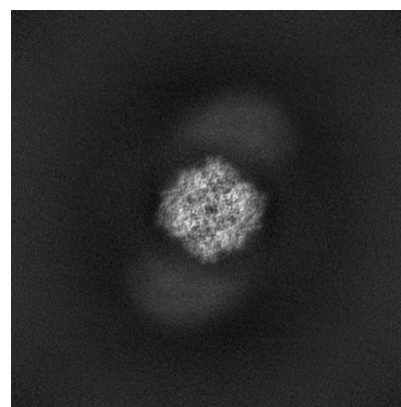
6.1.2 Raw map



X



Y

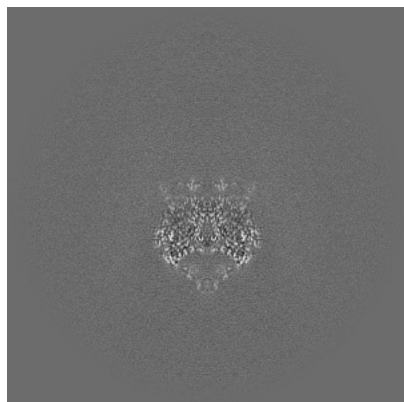


Z

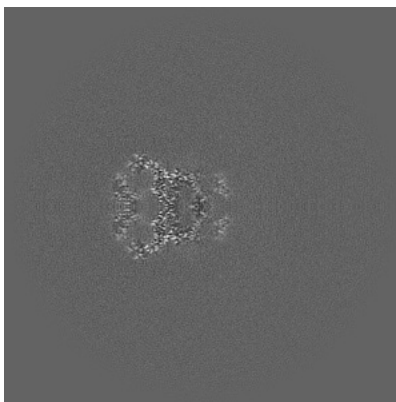
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

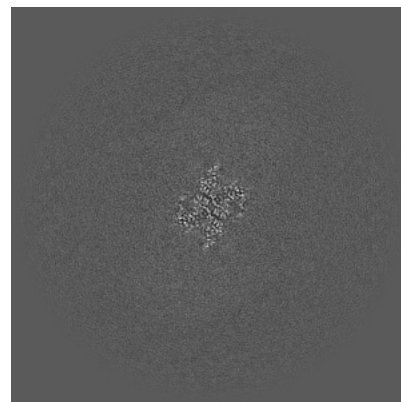
6.2.1 Primary map



X Index: 300

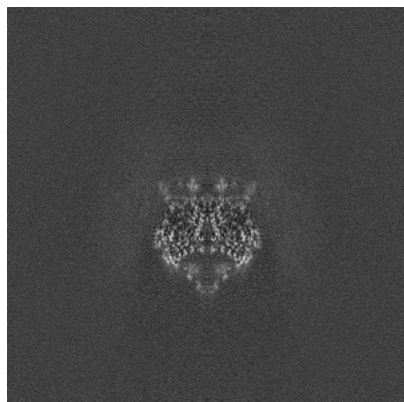


Y Index: 300

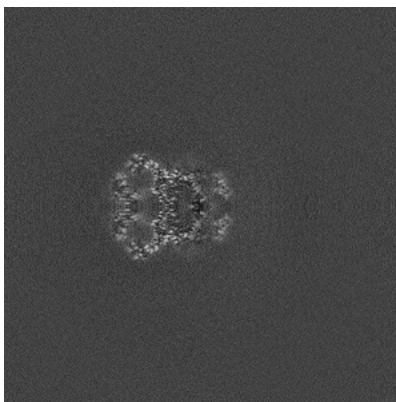


Z Index: 300

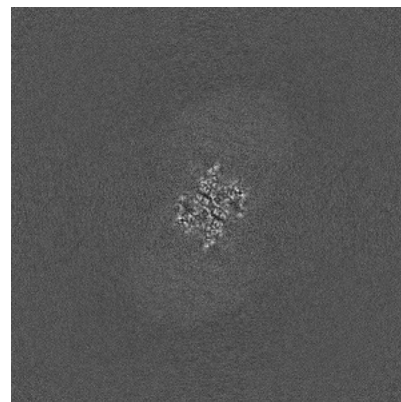
6.2.2 Raw map



X Index: 300



Y Index: 300

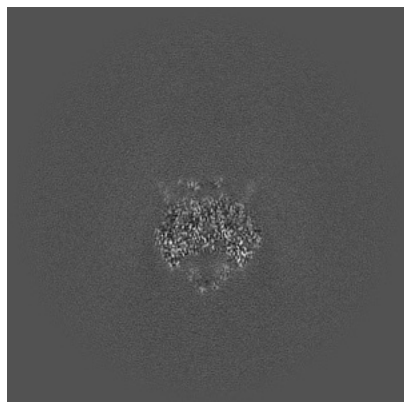


Z Index: 300

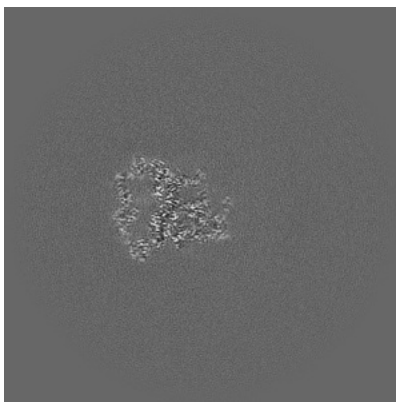
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

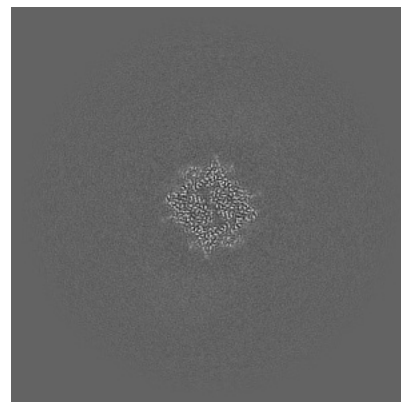
6.3.1 Primary map



X Index: 298

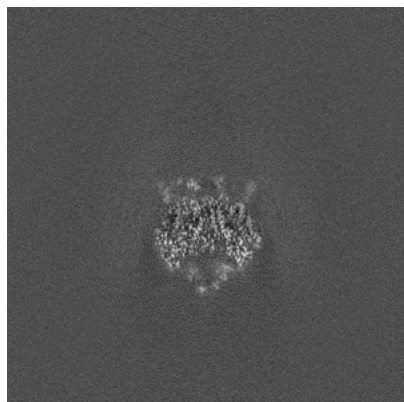


Y Index: 290

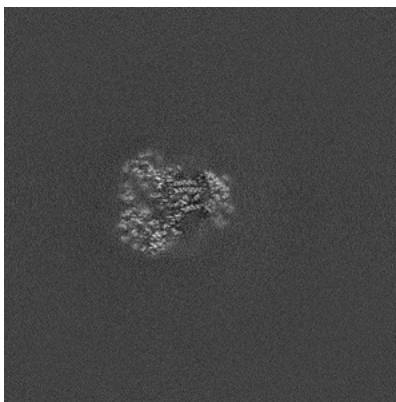


Z Index: 235

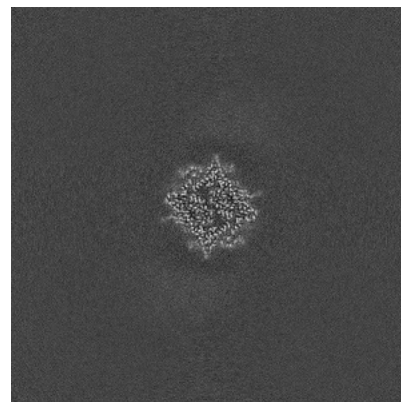
6.3.2 Raw map



X Index: 298



Y Index: 320

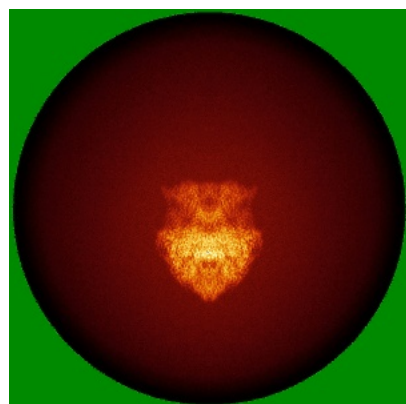


Z Index: 235

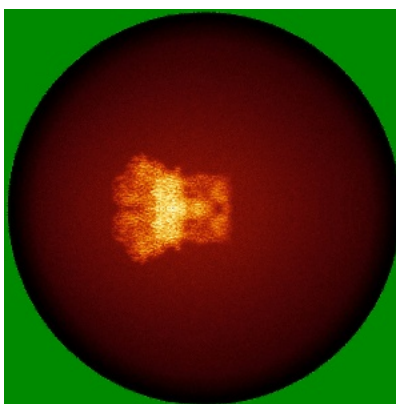
The images above show the largest variance slices of the map in three orthogonal directions.

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

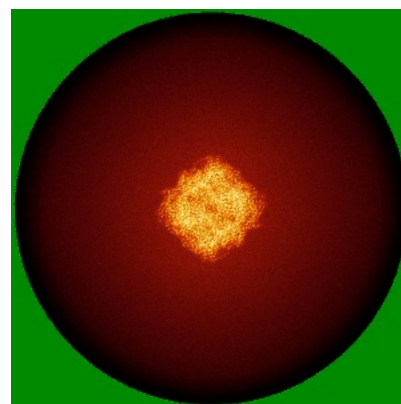
6.4.1 Primary map



X

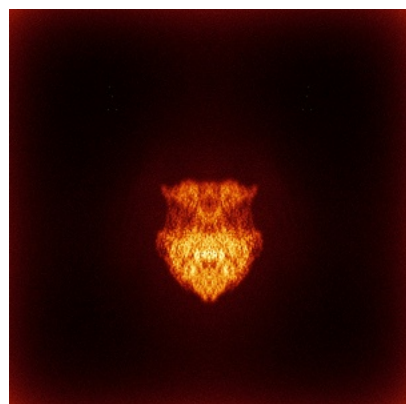


Y

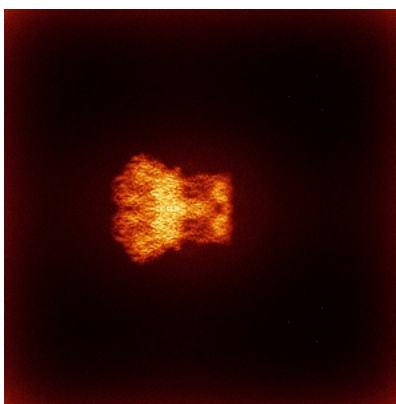


Z

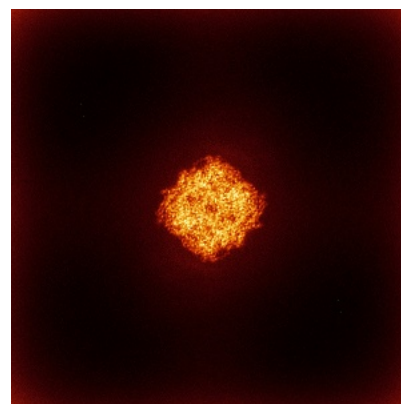
6.4.2 Raw map



X



Y

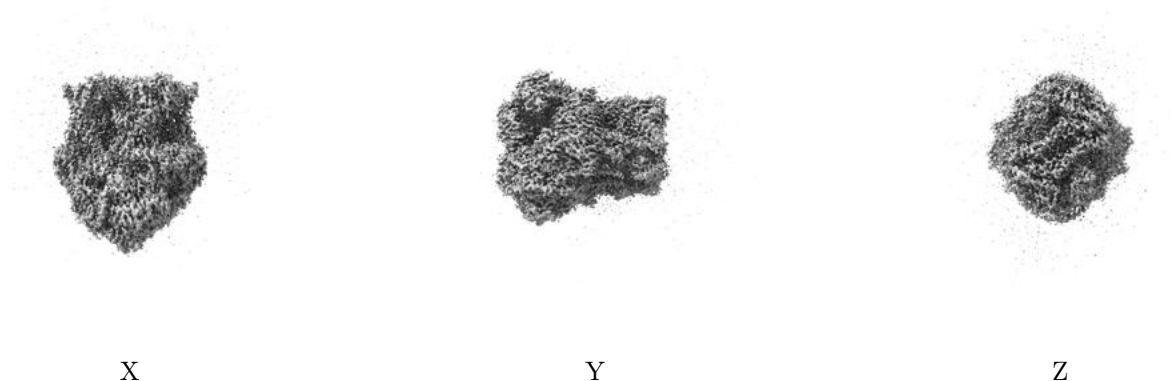


Z

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.

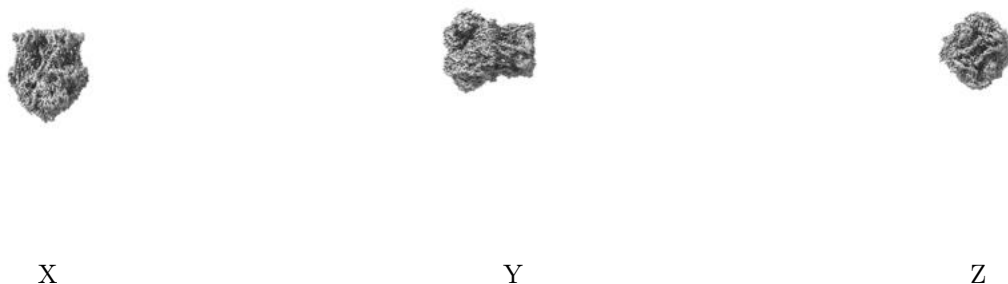
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

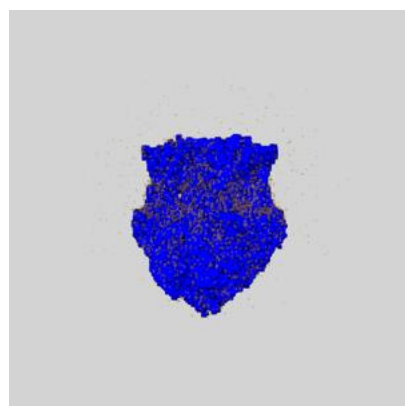
6.6 Mask visualisation [i](#)

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

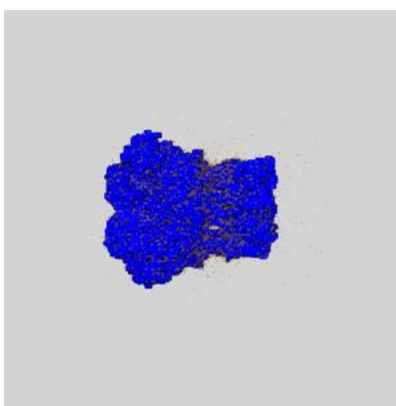
A mask typically either:

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

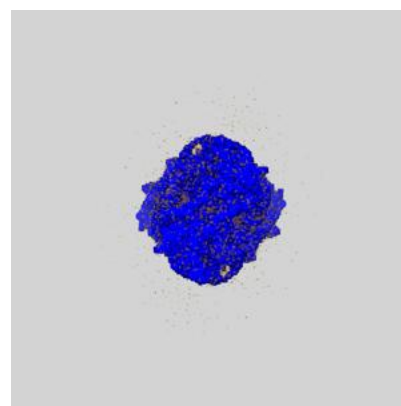
6.6.1 emd_52621_msk_1.map [i](#)



X



Y

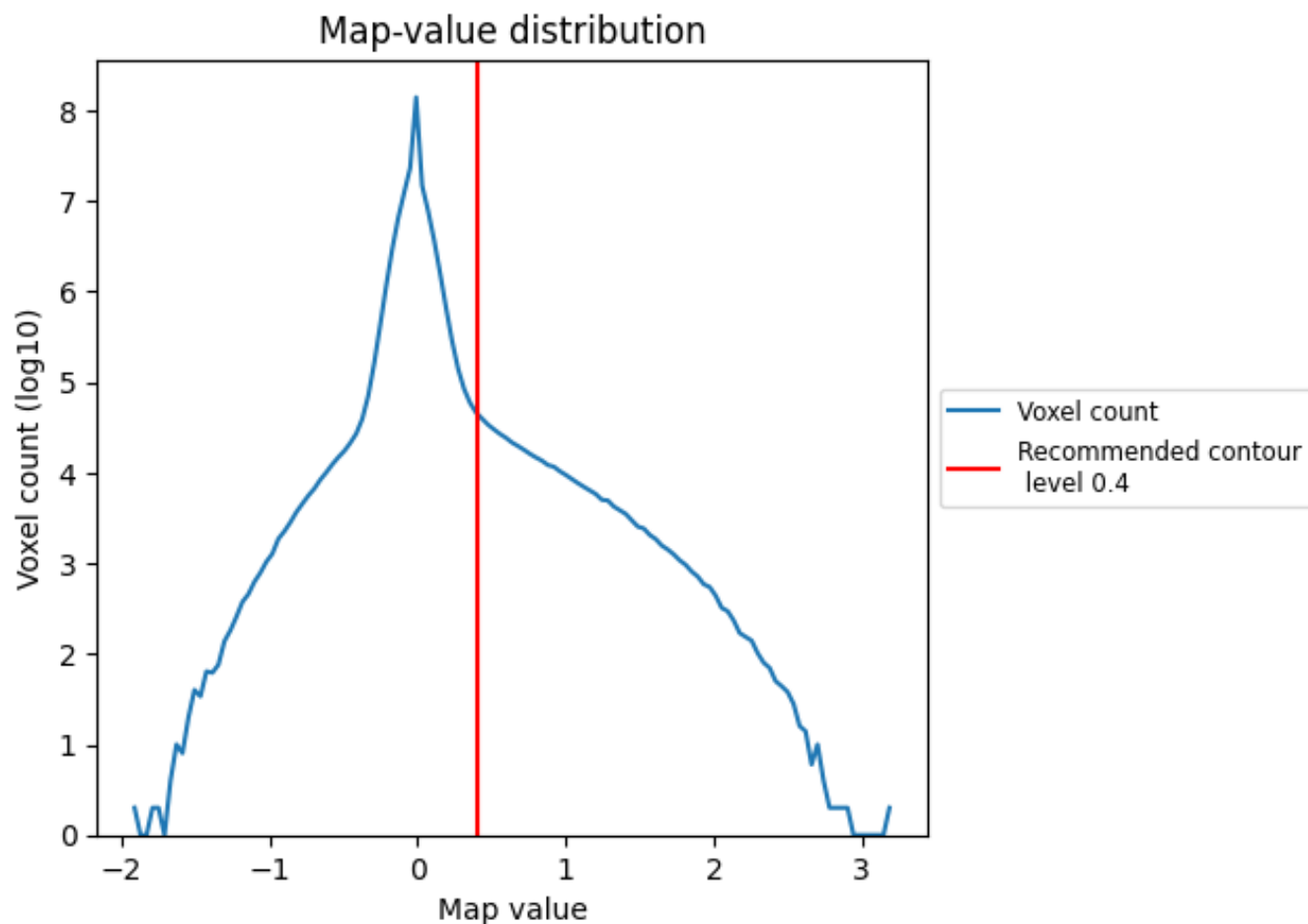


Z

7 Map analysis [i](#)

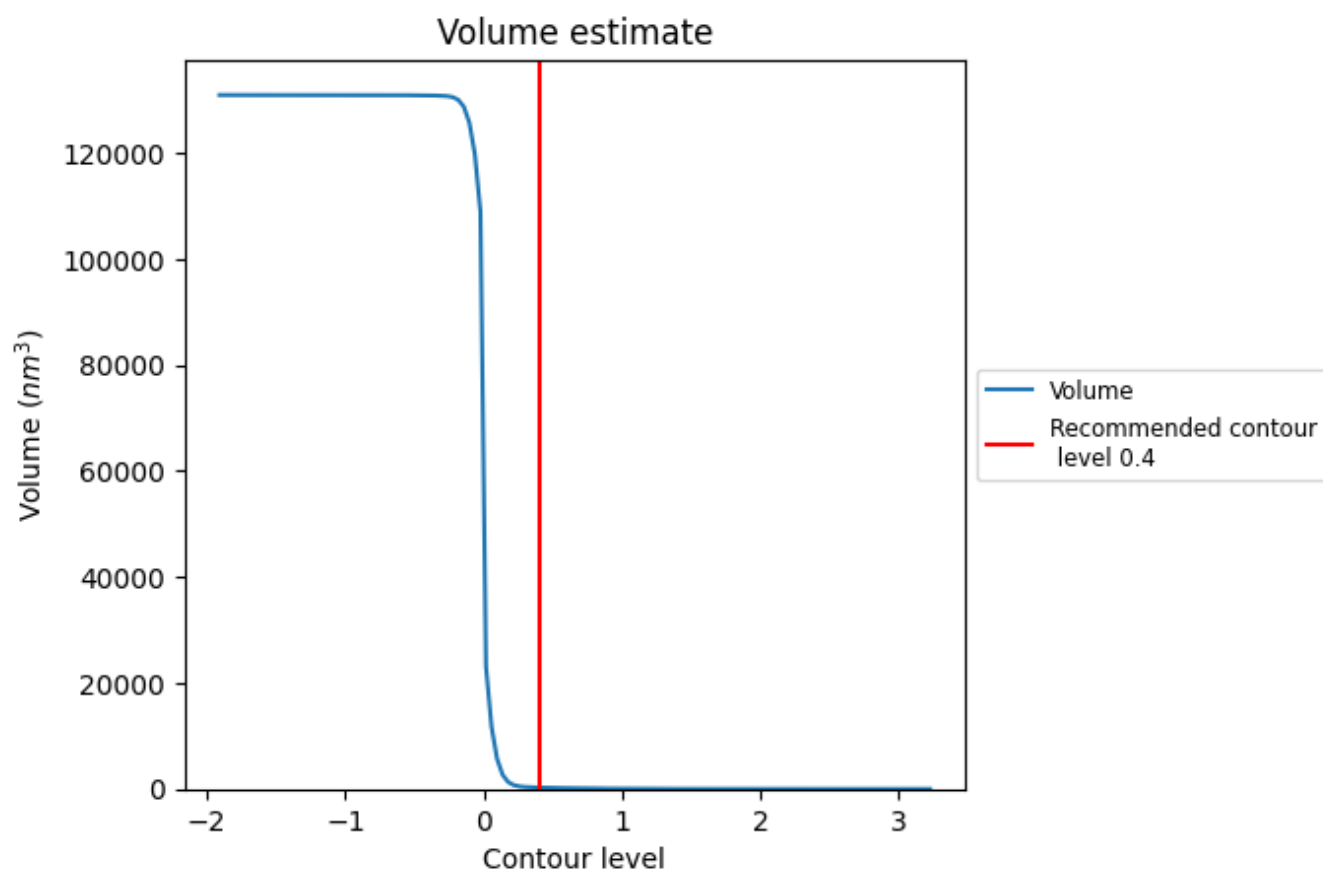
This section contains the results of statistical analysis of the map.

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.

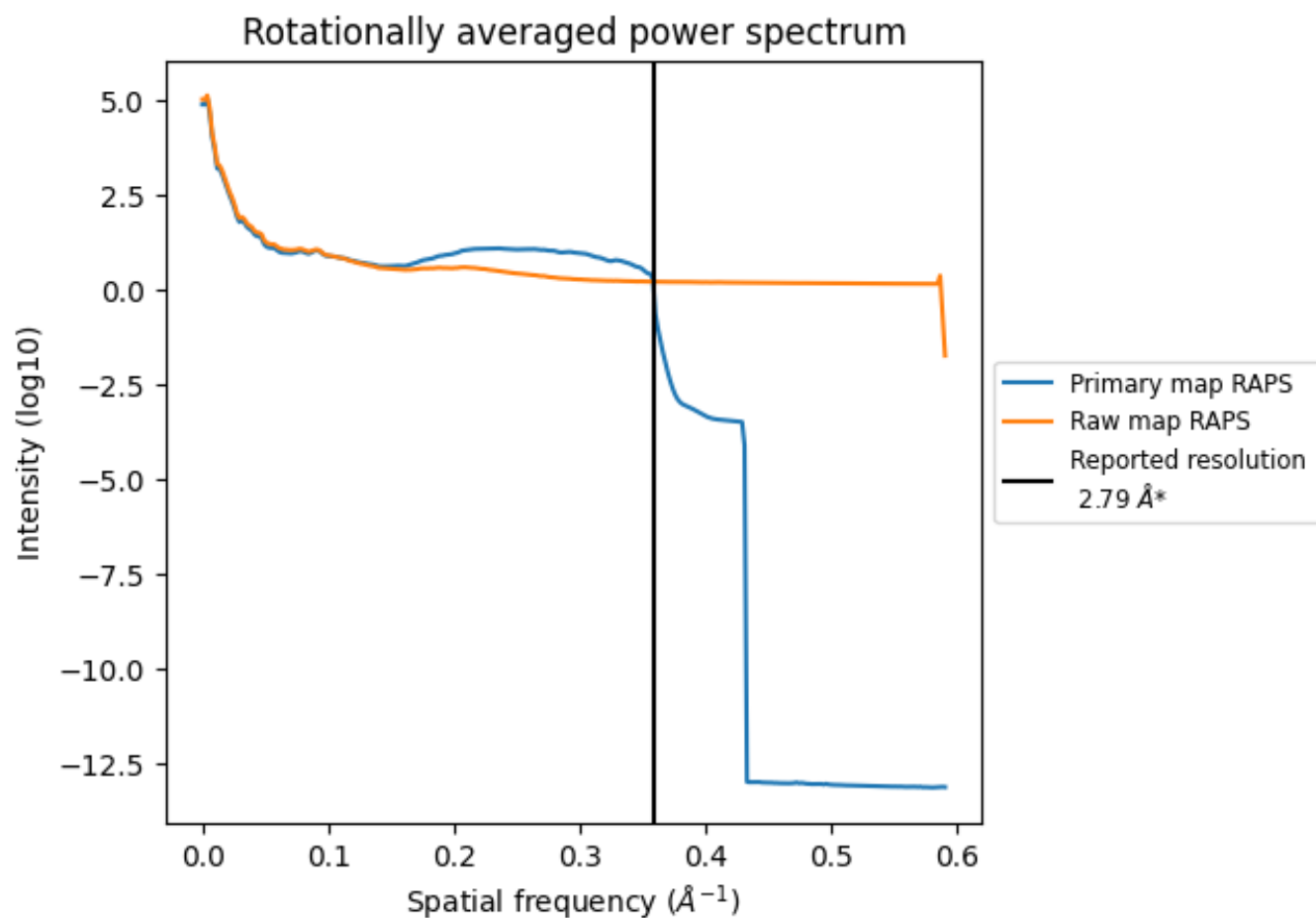
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm³; this corresponds to an approximate mass of 232 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 ⓘ

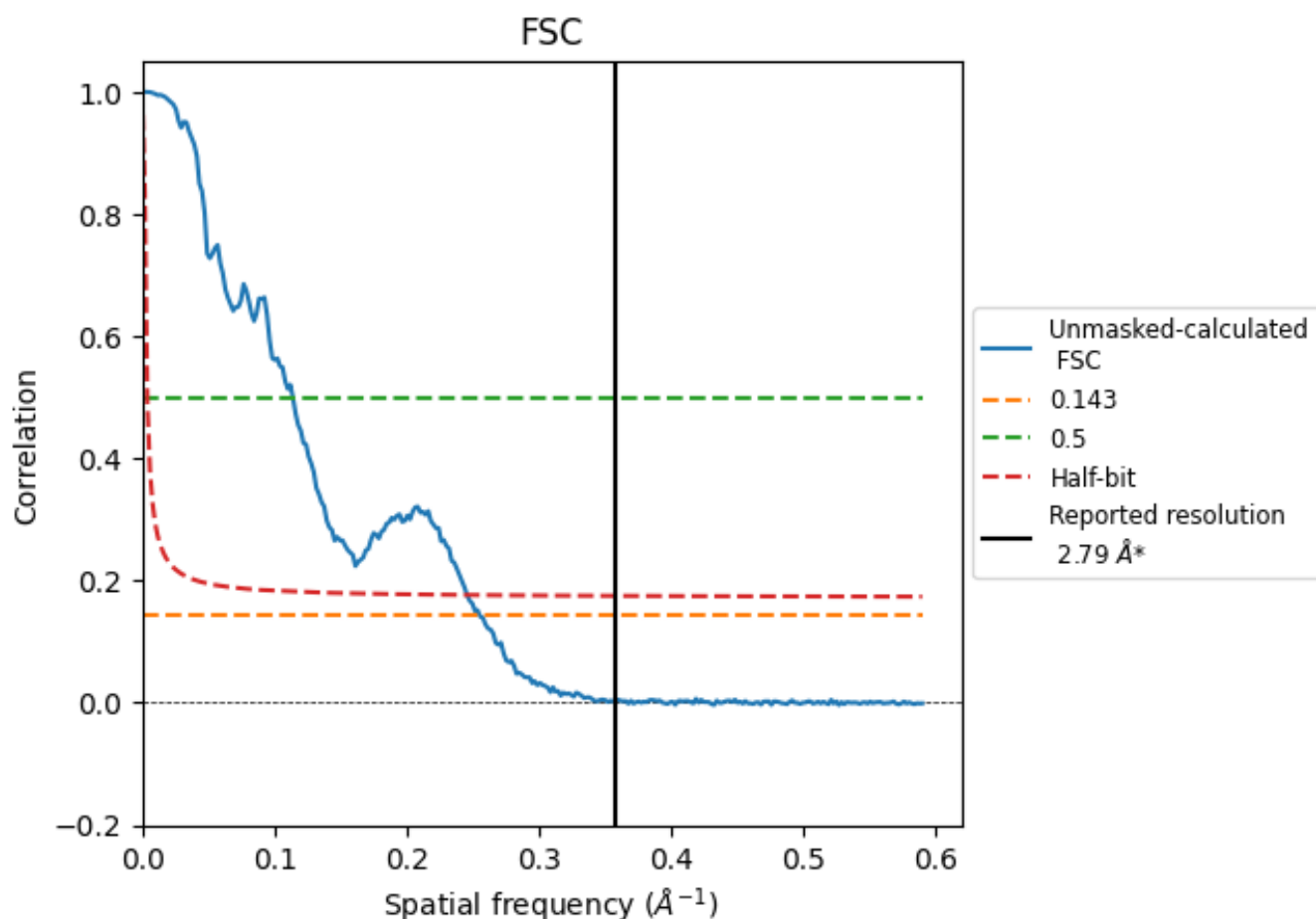


*Reported resolution corresponds to spatial frequency of 0.358 $\text{\AA}^{-1}$

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 0.358 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

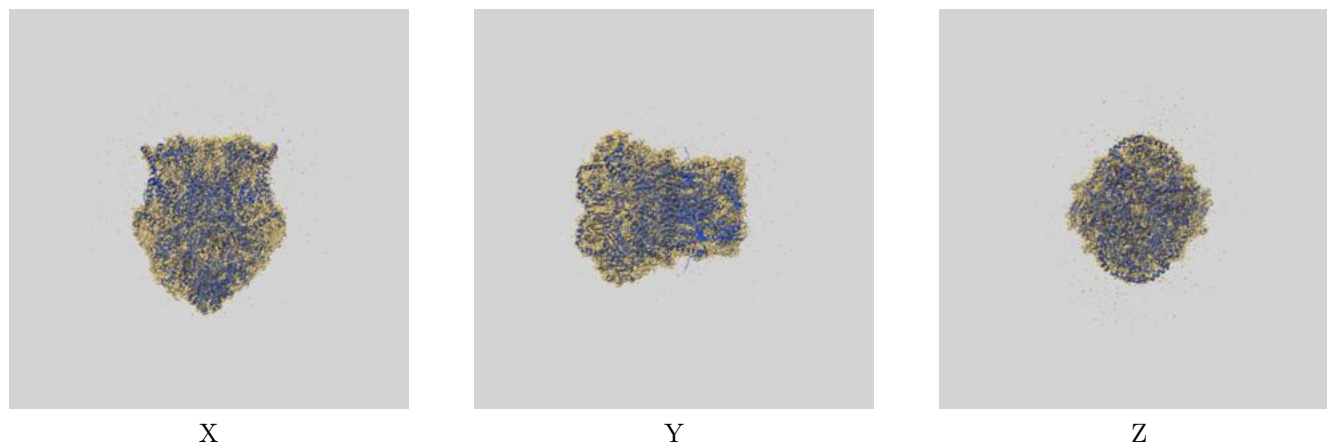
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	8.76	4.07

*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 3.91 differs from the reported value 2.79 by more than 10 %

9 Map-model fit [i](#)

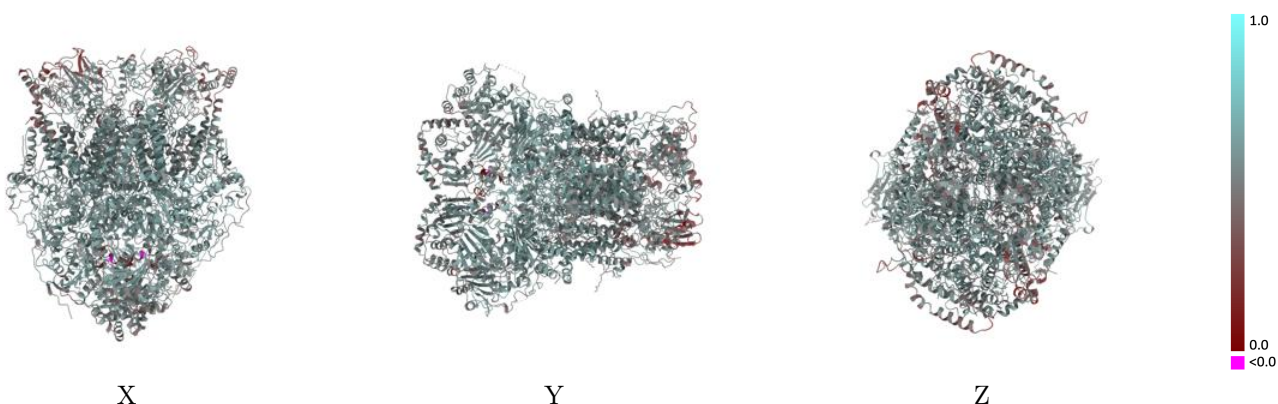
This section contains information regarding the fit between EMDB map EMD-52621 and PDB model 9I4X. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



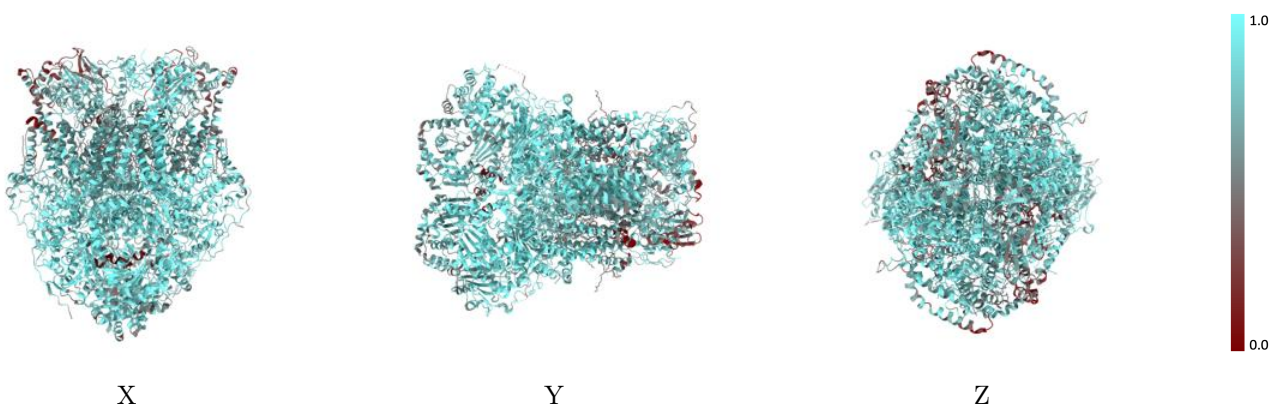
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



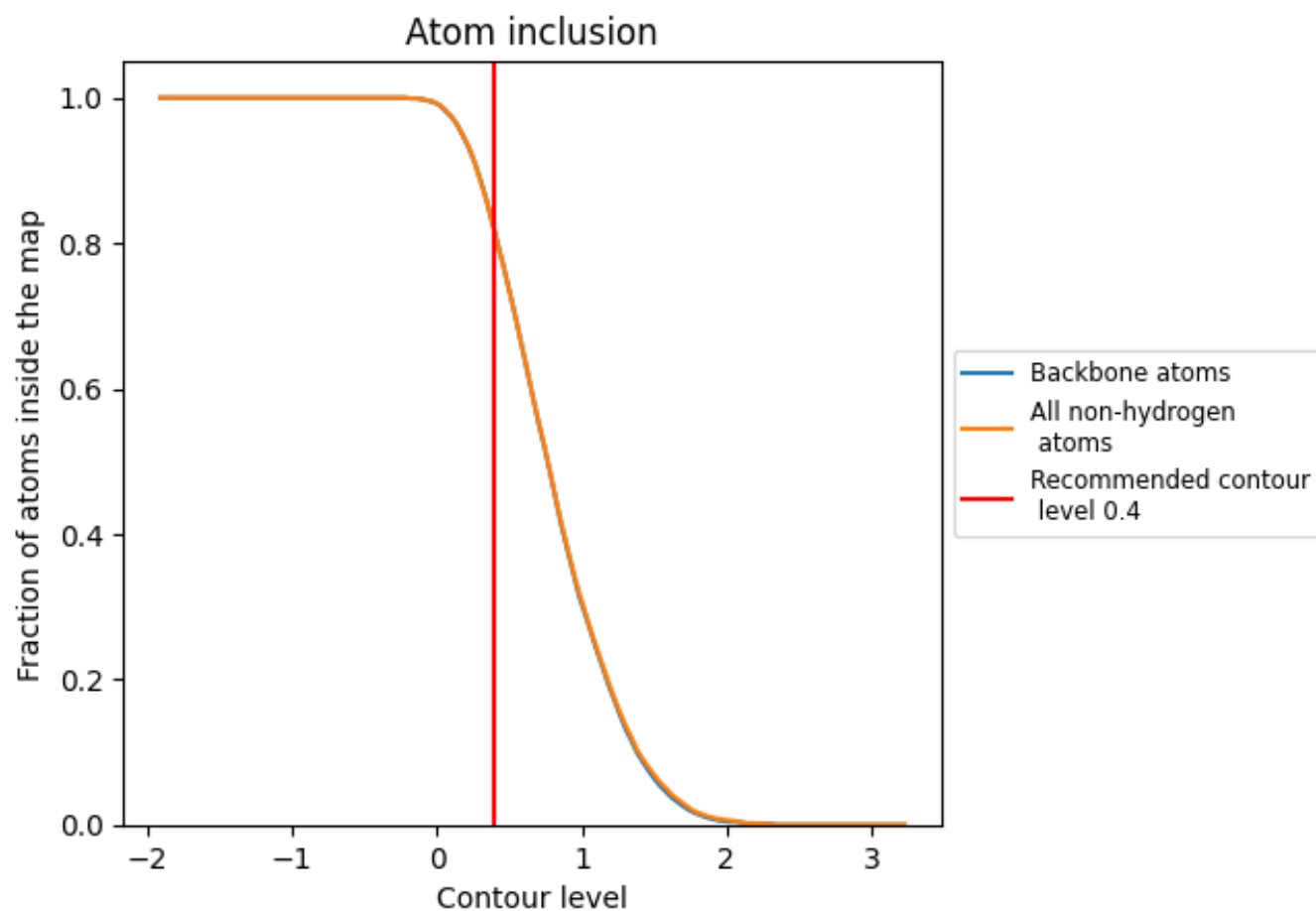
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8130	 0.5410
A	 0.8390	 0.5680
B	 0.8220	 0.5270
C	 0.7280	 0.5130
D	 0.8590	 0.5530
E	 0.8150	 0.5240
F	 0.6380	 0.4580
G	 0.8990	 0.5760
H	 0.8670	 0.5690
I	 0.8300	 0.5590
J	 0.7830	 0.5650
K	 0.7700	 0.5360
L	 0.6090	 0.5100
a	 0.8400	 0.5680
b	 0.8220	 0.5280
c	 0.7270	 0.5120
d	 0.8610	 0.5520
e	 0.8140	 0.5230
f	 0.6340	 0.4560
g	 0.8970	 0.5780
h	 0.8670	 0.5700
i	 0.8830	 0.5640
j	 0.8340	 0.5740
k	 0.7640	 0.5370
l	 0.6090	 0.5050

