



Full wwPDB EM Validation Report ⓘ

Jun 26, 2025 – 02:36 pm BST

PDB ID : 9H8T / pdb_00009h8t
EMDB ID : EMD-51939
Title : Cryo-EM structure of the atovaquone-inhibited Complex III from the *Chloro-
cebus sabaeus* respirasome
Authors : Maclean, A.; Muhleip, A.
Deposited on : 2024-10-29
Resolution : 2.67 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

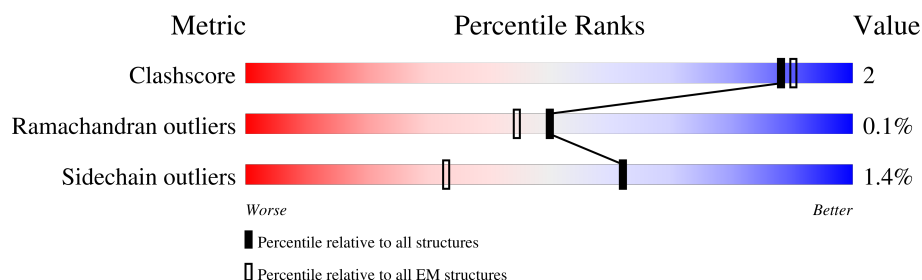
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.67 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	D	325	
1	d	325	
2	A	274	
2	T	274	
2	a	274	
3	G	111	
3	g	111	
4	C	82	

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Mol	Chain	Length	Quality of chain
4	c	82	
5	E	63	
5	e	63	
6	F	91	
6	f	91	
7	K	453	
7	k	453	
8	J	380	
8	j	380	
9	L	480	
9	l	480	
10	H	56	
10	h	56	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 67324 atoms, of which 33779 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 c1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	239	Total	C	H	N	O	S	0	0
			3757	1219	1856	326	341	15		
1	d	239	Total	C	H	N	O	S	0	0
			3757	1219	1856	326	341	15		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	196	Total	C	H	N	O	S	0	0
			3044	968	1512	267	289	8		
2	T	77	Total	C	H	N	O	S	0	0
			1142	349	591	102	98	2		
2	a	196	Total	C	H	N	O	S	0	0
			3044	968	1512	267	289	8		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	104	Total	C	H	N	O	S	0	0
			1803	580	895	160	166	2		
3	g	104	Total	C	H	N	O	S	0	0
			1803	580	895	160	166	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	43	ASP	GLU	conflict	UNP A0A0D9RJ49
g	43	ASP	GLU	conflict	UNP A0A0D9RJ49

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	81	Total	C	H	N	O	S	0	0
			1367	439	686	124	117	1		
4	c	81	Total	C	H	N	O	S	0	0
			1367	439	686	124	117	1		

- Molecule 5 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	56	Total	C	H	N	O		0	0
			911	300	458	76	77			
5	e	56	Total	C	H	N	O		0	0
			911	300	458	76	77			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	67	Total	C	H	N	O	S	0	0
			1093	338	539	99	111	6		
6	f	67	Total	C	H	N	O	S	0	0
			1093	338	539	99	111	6		

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase core protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	K	418	Total	C	H	N	O	S	0	0
			6326	1993	3161	554	610	8		
7	k	418	Total	C	H	N	O	S	0	0
			6326	1993	3161	554	610	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	100	THR	ILE	conflict	UNP A0A0D9R493
K	439	VAL	ALA	conflict	UNP A0A0D9R493
k	100	THR	ILE	conflict	UNP A0A0D9R493
k	439	VAL	ALA	conflict	UNP A0A0D9R493

- Molecule 8 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	378	Total	C	H	N	O	S	0	0
			6117	2030	3090	472	507	18		

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Mol	Chain	Residues	Atoms						AltConf	Trace
8	j	378	Total	C	H	N	O	S	0	0
			6117	2030	3090	472	507	18		

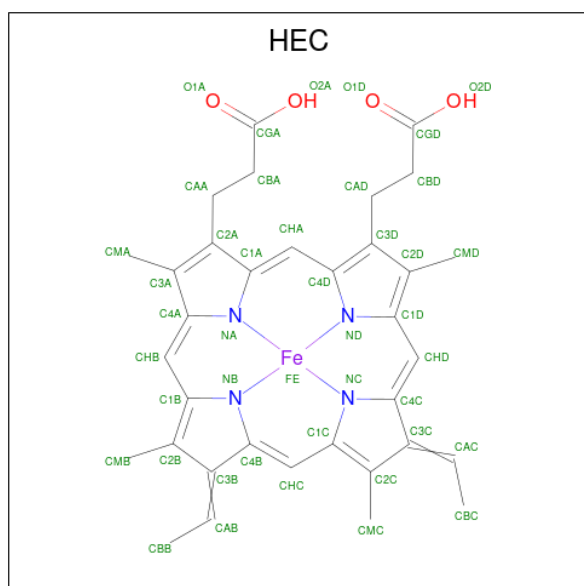
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase core protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	L	423	Total	C	H	N	O	S	0	0
			6533	2075	3231	574	633	20		
9	l	423	Total	C	H	N	O	S	0	0
			6533	2075	3231	574	633	20		

- Molecule 10 is a protein called UQCRB.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	H	45	Total	C	H	N	O	S	0	0
			748	251	374	65	57	1		
10	h	45	Total	C	H	N	O	S	0	0
			748	251	374	65	57	1		

- Molecule 11 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
11	D	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

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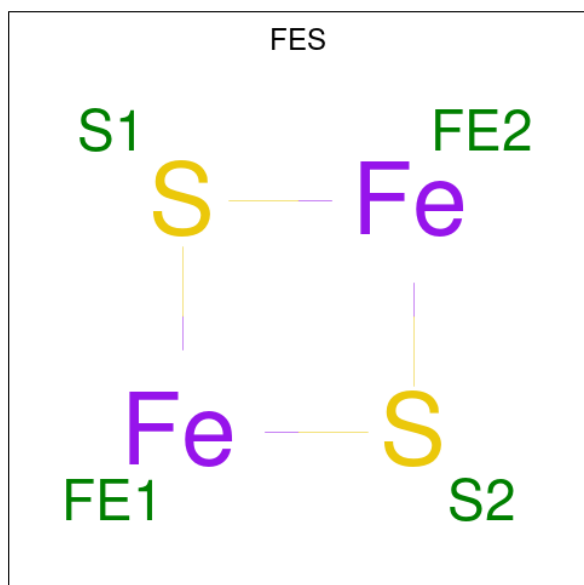
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Mol	Chain	Residues	Atoms						AltConf
11	d	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

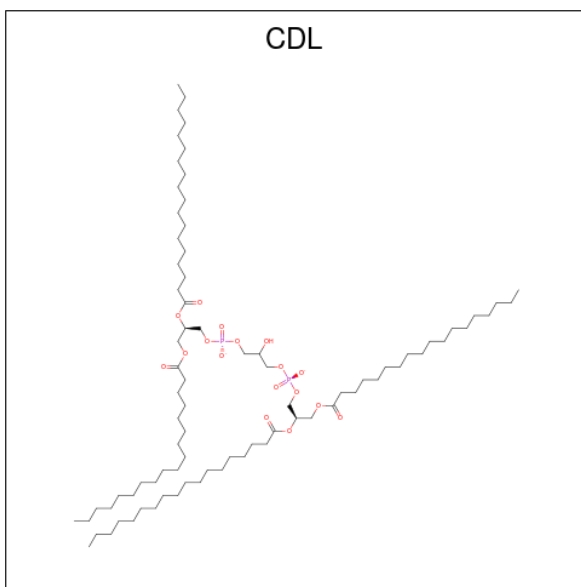
Mol	Chain	Residues	Atoms		AltConf
12	D	1	Total	Zn	0
			1	1	
12	d	1	Total	Zn	0
			1	1	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



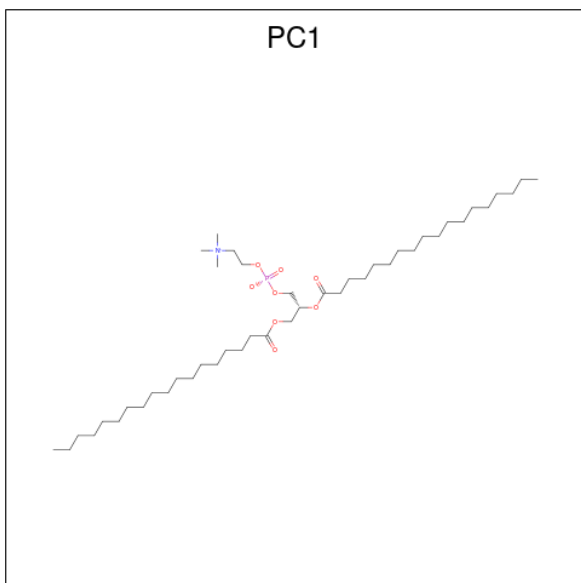
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	Fe	S	0
			4	2	2	
13	a	1	Total	Fe	S	0
			4	2	2	

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



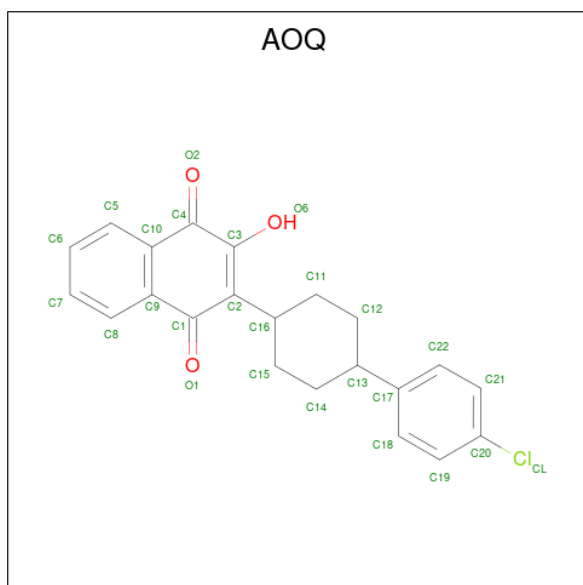
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	H	O	P	0
			256	81	156	17	2	
14	L	1	Total	C	H	O	P	0
			256	81	156	17	2	
14	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
14	l	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 15 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



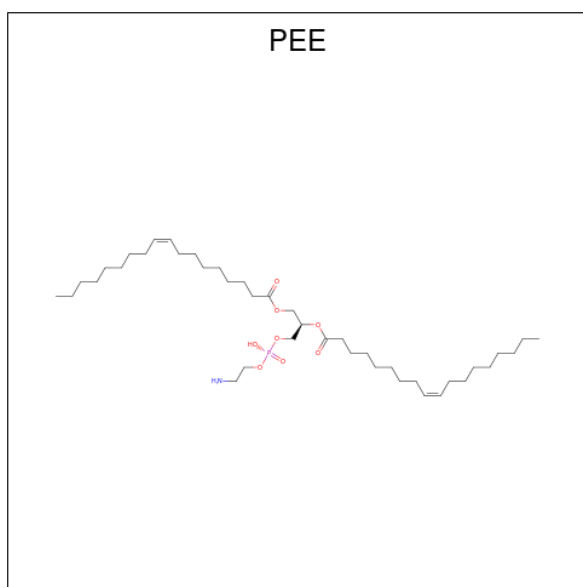
Mol	Chain	Residues	Atoms						AltConf
15	E	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
15	e	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

- Molecule 16 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
16	J	1	Total	C	Cl	H	O	0
			44	22	1	18	3	
16	j	1	Total	C	Cl	H	O	0
			44	22	1	18	3	

- Molecule 17 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
17	J	1	Total	C	H	N	O	P	0
			134	41	83	1	8	1	
17	J	1	Total	C	H	N	O	P	0
			134	41	83	1	8	1	
17	L	1	Total	C	H	N	O	P	0
			134	41	83	1	8	1	
17	j	1	Total	C	H	N	O	P	0
			134	41	83	1	8	1	
17	j	1	Total	C	H	N	O	P	0
			134	41	83	1	8	1	
17	l	1	Total	C	H	N	O	P	0
			134	41	83	1	8	1	

- Molecule 18 is 2-[4-(4-CHLOROPHENYL)CYCLOHEXYLIDENE]-3,4-DIHYDROXY-1 (2H)-NAPHTHALENONE (CCD ID: AFI) (formula: C₂₂H₁₉ClO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltCon
18	J	1	Total 45	C 22	Cl 1	H 19	O 3	0
18	j	1	Total 45	C 22	Cl 1	H 19	O 3	0

- Molecule 19 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltCon
19	J	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

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Mol	Chain	Residues	Atoms						AltConf
19	J	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
19	j	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
19	j	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

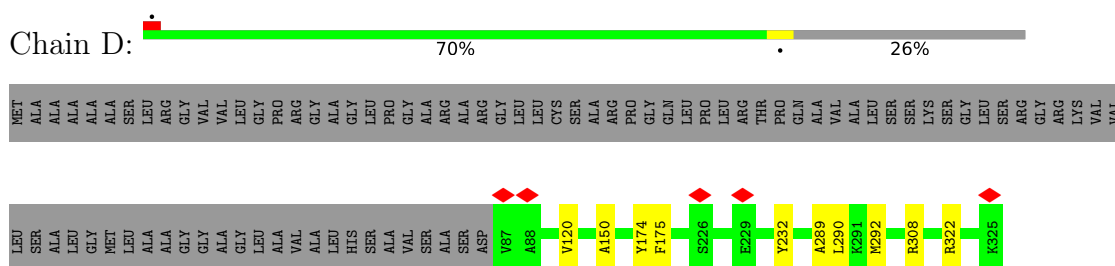
- Molecule 20 is water.

Mol	Chain	Residues	Atoms			AltConf
20	J	7	Total	H	O	0
			21	14	7	
20	j	7	Total	H	O	0
			21	14	7	

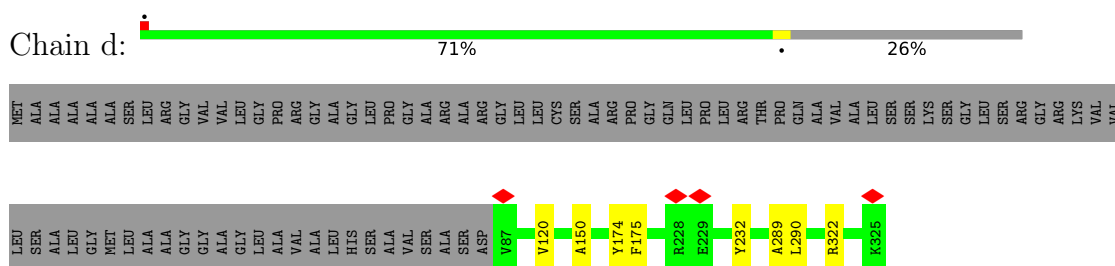
3 Residue-property plots

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.

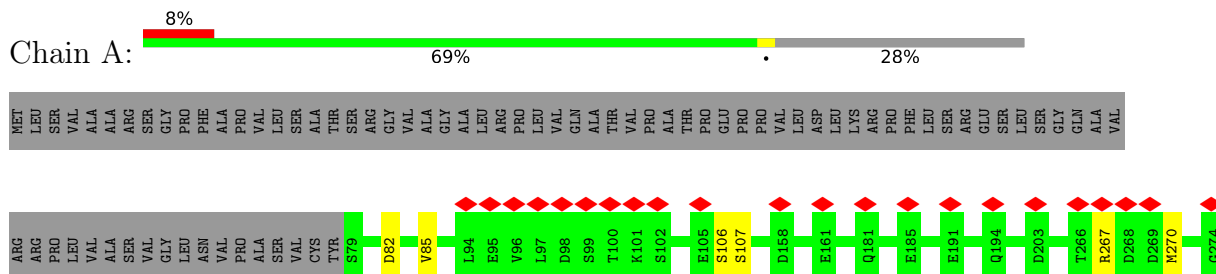
- Molecule 1: Cytochrome c1



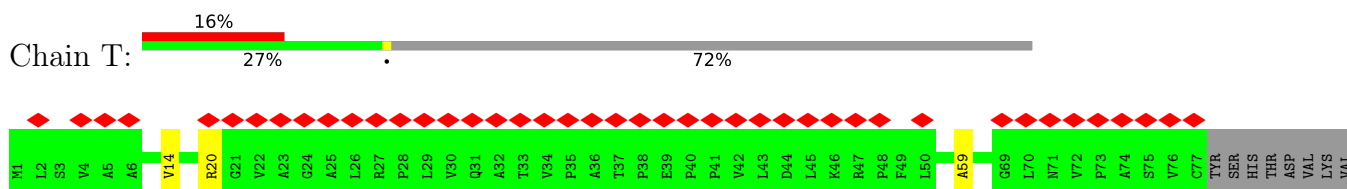
- Molecule 1: Cytochrome c1

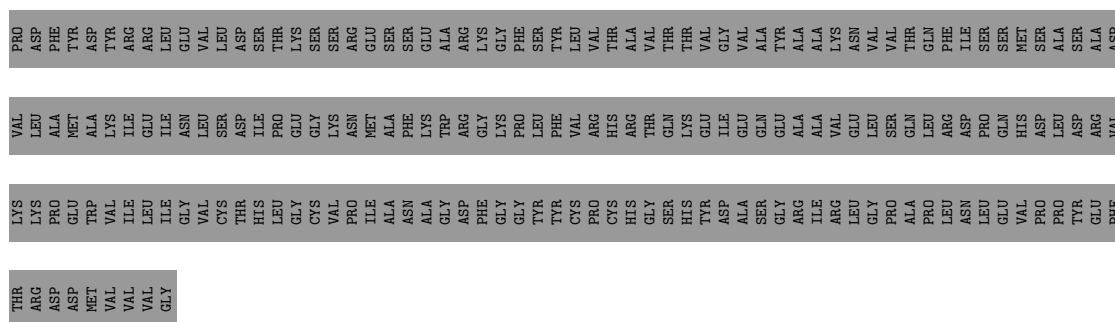


- Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

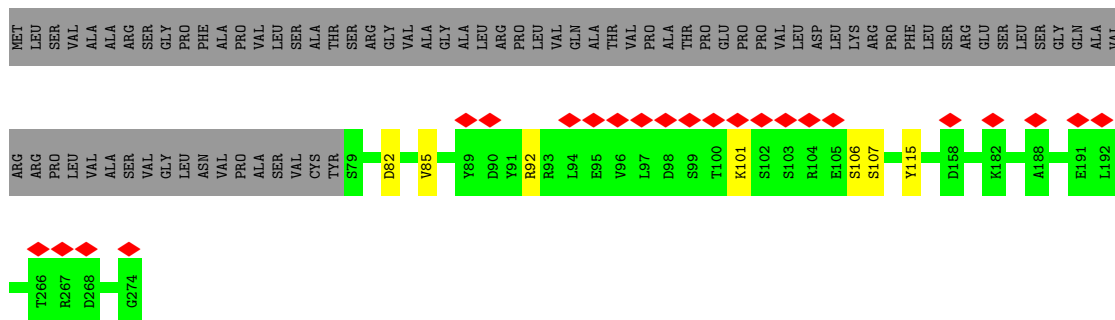


- Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

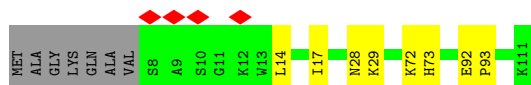




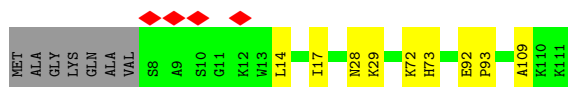
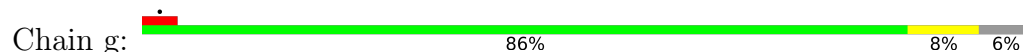
- Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial



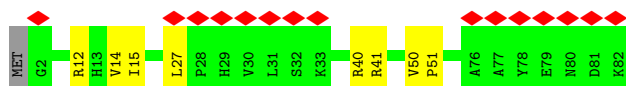
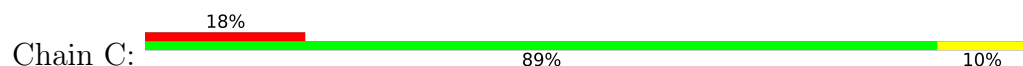
- Molecule 3: Cytochrome b-c1 complex subunit 7



- Molecule 3: Cytochrome b-c1 complex subunit 7



- Molecule 4: Cytochrome b-c1 complex subunit 8

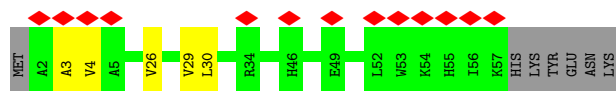
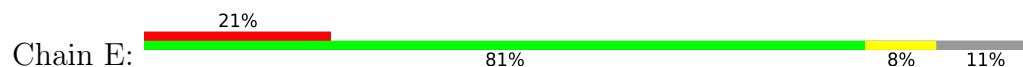


- Molecule 4: Cytochrome b-c1 complex subunit 8

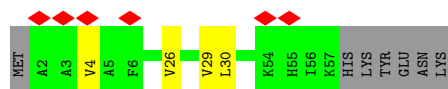
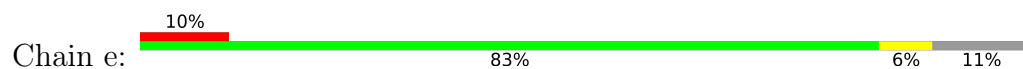




- Molecule 5: Complex III subunit 9



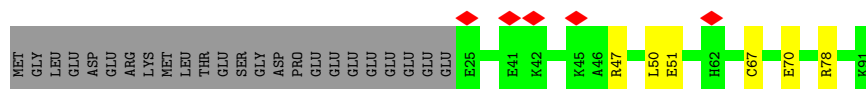
- Molecule 5: Complex III subunit 9



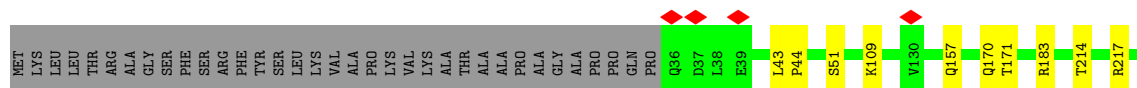
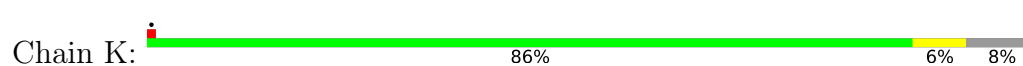
- Molecule 6: Cytochrome b-c1 complex subunit 6



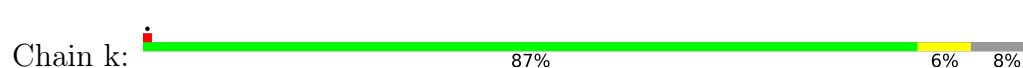
- Molecule 6: Cytochrome b-c1 complex subunit 6

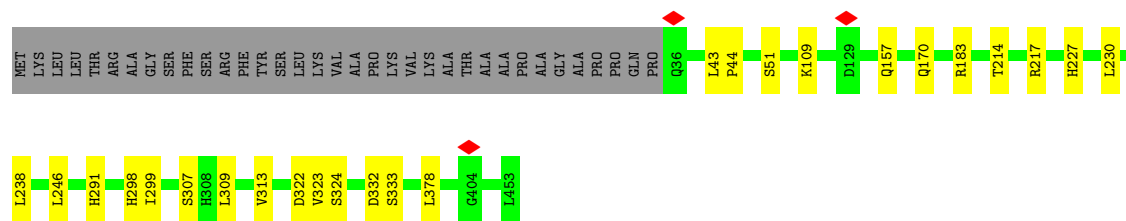


- Molecule 7: Ubiquinol-cytochrome c reductase core protein 2

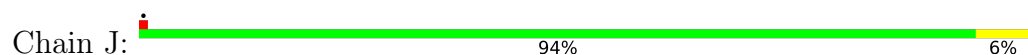


- Molecule 7: Ubiquinol-cytochrome c reductase core protein 2

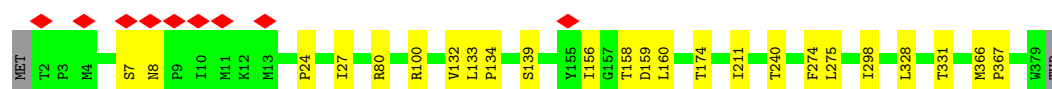
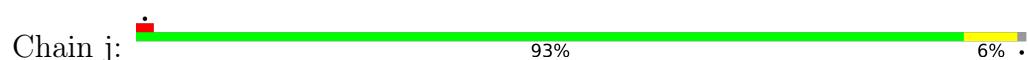




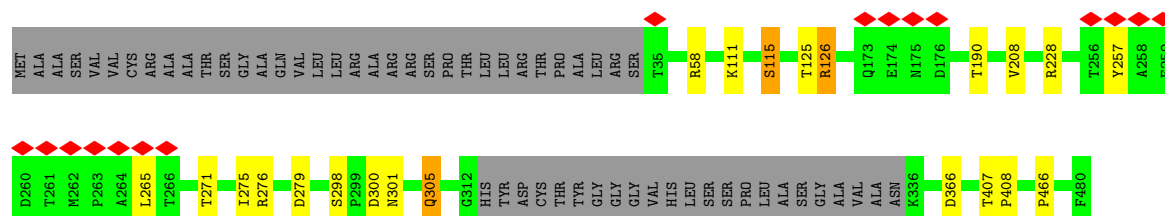
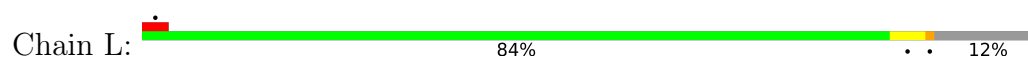
- Molecule 8: Cytochrome b



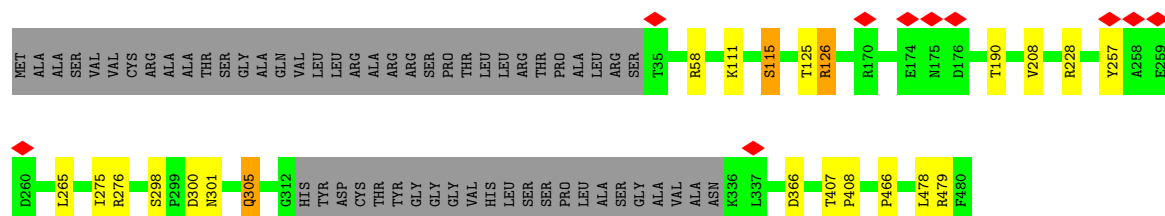
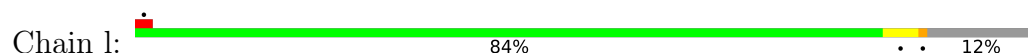
- Molecule 8: Cytochrome b



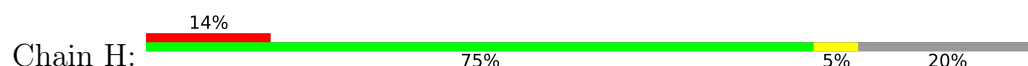
- Molecule 9: Ubiquinol-cytochrome c reductase core protein 1

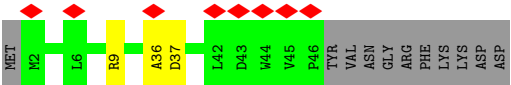


- Molecule 9: Ubiquinol-cytochrome c reductase core protein 1

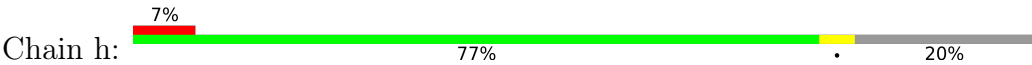


- Molecule 10: UQCRB





• Molecule 10: UQCRB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	637526	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)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	8.553	Depositor
Minimum map value	-4.276	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	592.482, 592.482, 592.482	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98747, 0.98747, 0.98747	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CDL, PC1, FES, HEC, ZN, AFI, PEE, AOQ

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	D	0.21	0/1961	0.47	0/2662
1	d	0.21	0/1961	0.47	0/2662
2	A	0.20	0/1567	0.48	0/2124
2	T	0.19	0/562	0.41	0/770
2	a	0.21	0/1567	0.48	0/2124
3	G	0.29	0/929	0.52	0/1245
3	g	0.29	0/929	0.52	0/1245
4	C	0.23	0/699	0.51	0/941
4	c	0.24	0/699	0.52	0/941
5	E	0.22	0/464	0.53	0/626
5	e	0.22	0/464	0.54	0/626
6	F	0.19	0/560	0.47	0/750
6	f	0.19	0/560	0.47	0/750
7	K	0.22	0/3221	0.54	0/4366
7	k	0.22	0/3221	0.54	0/4366
8	J	0.25	0/3128	0.52	0/4281
8	j	0.25	0/3128	0.52	0/4281
9	L	0.24	0/3370	0.54	0/4571
9	l	0.24	0/3370	0.54	0/4571
10	H	0.24	0/389	0.51	0/535
10	h	0.24	0/389	0.51	0/535
All	All	0.23	0/33138	0.52	0/44972

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
7	K	0	1
7	k	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	L	0	2
9	l	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	K	183	ARG	Sidechain
9	L	228	ARG	Sidechain
9	L	276	ARG	Sidechain
7	k	183	ARG	Sidechain
9	l	228	ARG	Sidechain
9	l	276	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1901	1856	1853	5	0
1	d	1901	1856	1853	3	0
2	A	1532	1512	1508	4	0
2	T	551	591	591	2	0
2	a	1532	1512	1508	7	0
3	G	908	895	894	4	0
3	g	908	895	894	5	0
4	C	681	686	685	6	0
4	c	681	686	685	4	0
5	E	453	458	457	4	0
5	e	453	458	457	2	0
6	F	554	539	538	3	0
6	f	554	539	538	3	0
7	K	3165	3161	3157	13	0
7	k	3165	3161	3157	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	3027	3090	3088	10	0
8	j	3027	3090	3088	11	0
9	L	3302	3231	3227	11	0
9	l	3302	3231	3227	11	0
10	H	374	374	373	2	0
10	h	374	374	373	1	0
11	D	43	32	30	0	0
11	d	43	32	30	0	0
12	D	1	0	0	0	0
12	d	1	0	0	0	0
13	A	4	0	0	0	0
13	a	4	0	0	0	0
14	C	100	156	156	0	0
14	L	100	156	156	0	0
14	c	100	156	156	0	0
14	l	100	156	156	1	0
15	E	54	88	88	1	0
15	e	54	88	88	1	0
16	J	26	18	18	1	0
16	j	26	18	18	1	0
17	J	102	166	164	0	0
17	L	51	83	82	0	0
17	j	102	166	164	0	0
17	l	51	83	82	0	0
18	J	26	19	17	0	0
18	j	26	19	17	0	0
19	J	86	60	60	8	0
19	j	86	60	60	9	0
20	J	7	14	0	0	0
20	j	7	14	0	1	0
All	All	33545	33779	33693	124	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (124) 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)
19:j:406:HEM:O2D	20:j:501:HOH:O	2.05	0.75
19:J:405:HEM:HBC2	19:J:405:HEM:HHD	1.70	0.74
19:j:405:HEM:HBC2	19:j:405:HEM:HHD	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:59:ALA:N	7:k:322:ASP:OD2	2.26	0.69
8:J:7:SER:OG	8:J:8:ASN:ND2	2.22	0.68
8:J:100:ARG:NH1	19:J:406:HEM:O2A	2.26	0.68
8:j:7:SER:OG	8:j:8:ASN:ND2	2.22	0.66
5:E:3:ALA:HB3	2:a:101:LYS:HD3	1.80	0.63
9:L:275:ILE:HD11	2:a:85:VAL:CG2	2.29	0.63
9:L:407:THR:HB	9:L:408:PRO:HD3	1.82	0.61
9:l:407:THR:HB	9:l:408:PRO:HD3	1.82	0.61
9:L:275:ILE:HD11	2:a:85:VAL:HG22	1.82	0.60
19:J:406:HEM:HBA1	19:J:406:HEM:HHA	1.84	0.60
8:j:100:ARG:NH1	19:j:406:HEM:O2A	2.35	0.60
19:j:406:HEM:HBB2	19:j:406:HEM:HMB1	1.85	0.59
9:l:305:GLN:HA	9:l:305:GLN:OE1	2.03	0.58
19:J:406:HEM:HMB1	19:J:406:HEM:HBB2	1.84	0.58
5:e:4:VAL:HG23	5:e:4:VAL:O	2.04	0.58
19:j:406:HEM:HHA	19:j:406:HEM:HBA1	1.84	0.58
5:E:4:VAL:HG23	5:E:4:VAL:O	2.04	0.58
9:l:111:LYS:O	9:l:115:SER:OG	2.23	0.56
9:L:305:GLN:OE1	9:L:305:GLN:HA	2.03	0.56
9:l:479:ARG:NH1	14:l:501:CDL:OA3	2.37	0.56
1:D:308:ARG:NH2	4:C:27:LEU:HD23	2.22	0.55
19:J:405:HEM:HMB1	19:J:405:HEM:HBB2	1.91	0.53
6:f:70:GLU:OE1	6:f:70:GLU:N	2.40	0.52
19:j:405:HEM:HBB2	19:j:405:HEM:HMB1	1.91	0.52
6:F:70:GLU:OE1	6:F:70:GLU:N	2.40	0.52
19:J:406:HEM:HBB2	19:J:406:HEM:CMB	2.40	0.51
9:l:125:THR:HG22	9:l:126:ARG:N	2.26	0.51
9:L:125:THR:HG22	9:L:126:ARG:N	2.26	0.51
19:j:406:HEM:HBB2	19:j:406:HEM:CMB	2.40	0.50
9:L:111:LYS:O	9:L:115:SER:OG	2.23	0.50
10:H:9:ARG:NE	3:g:109:ALA:O	2.35	0.49
1:D:292:MET:SD	8:J:244:LEU:HD11	2.52	0.49
15:e:101:PC1:O32	9:l:478:LEU:HD22	2.12	0.49
7:K:217:ARG:NH2	7:K:246:LEU:O	2.45	0.49
7:k:217:ARG:NH2	7:k:246:LEU:O	2.45	0.49
4:C:15:ILE:N	4:C:15:ILE:HD12	2.29	0.48
8:J:156:ILE:HD12	8:J:160:LEU:HD11	1.94	0.48
5:E:3:ALA:HB3	2:a:101:LYS:CD	2.44	0.48
8:j:156:ILE:HD12	8:j:160:LEU:HD11	1.94	0.48
7:K:171:THR:HG22	2:T:14:VAL:HG12	1.96	0.48
19:J:405:HEM:HBB2	19:J:405:HEM:CMB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:15:ILE:HD12	4:c:15:ILE:N	2.29	0.47
9:L:366:ASP:OD1	9:L:466:PRO:HG3	2.15	0.47
3:G:92:GLU:HB3	3:G:93:PRO:HD3	1.96	0.47
19:j:405:HEM:HBB2	19:j:405:HEM:CMB	2.44	0.47
1:D:289:ALA:O	1:D:290:LEU:C	2.58	0.46
1:d:289:ALA:O	1:d:290:LEU:C	2.58	0.46
19:J:406:HEM:HBC2	19:J:406:HEM:HMC2	1.97	0.46
19:j:406:HEM:HBC2	19:j:406:HEM:HMC2	1.97	0.46
9:l:366:ASP:OD1	9:l:466:PRO:HG3	2.15	0.46
3:g:92:GLU:HB3	3:g:93:PRO:HD3	1.96	0.46
7:k:170:GLN:N	7:k:170:GLN:OE1	2.49	0.46
15:E:101:PC1:H153	2:a:115:TYR:CE2	2.51	0.46
7:k:309:LEU:O	7:k:313:VAL:HG23	2.15	0.46
7:K:170:GLN:N	7:K:170:GLN:OE1	2.49	0.46
7:K:309:LEU:O	7:K:313:VAL:HG23	2.15	0.46
7:K:298:HIS:C	7:K:299:ILE:HD12	2.42	0.45
8:J:132:VAL:HA	8:J:139:SER:HB3	1.99	0.45
7:k:298:HIS:C	7:k:299:ILE:HD12	2.42	0.45
8:j:132:VAL:HA	8:j:139:SER:HB3	1.99	0.45
2:A:106:SER:O	2:A:107:SER:C	2.60	0.44
3:G:14:LEU:HD12	3:G:17:ILE:HD11	1.99	0.44
4:c:14:VAL:C	4:c:15:ILE:HD12	2.43	0.44
7:K:291:HIS:CE1	7:K:378:LEU:HD13	2.52	0.44
2:a:106:SER:O	2:a:107:SER:C	2.60	0.44
9:L:271:THR:HG23	2:a:92:ARG:NH2	2.32	0.44
3:g:14:LEU:HD12	3:g:17:ILE:HD11	1.99	0.44
8:j:328:LEU:O	8:j:331:THR:OG1	2.30	0.44
7:k:291:HIS:CE1	7:k:378:LEU:HD13	2.52	0.44
7:k:51:SER:HB2	7:k:230:LEU:HD22	2.01	0.43
7:K:51:SER:HB2	7:K:230:LEU:HD22	2.01	0.43
7:K:332:ASP:O	7:K:333:SER:HB2	2.18	0.43
4:C:14:VAL:C	4:C:15:ILE:HD12	2.43	0.43
7:k:332:ASP:O	7:k:333:SER:HB2	2.18	0.43
7:K:299:ILE:HD12	7:K:299:ILE:N	2.34	0.42
1:d:232:TYR:CD1	1:d:232:TYR:N	2.87	0.42
10:h:36:ALA:O	10:h:37:ASP:C	2.62	0.42
6:F:28:ASP:O	6:F:31:THR:OG1	2.30	0.42
4:c:50:VAL:N	4:c:51:PRO:HD2	2.34	0.42
10:H:36:ALA:O	10:H:37:ASP:C	2.62	0.42
3:g:28:ASN:OD1	3:g:29:LYS:N	2.52	0.42
2:A:85:VAL:CG2	9:l:275:ILE:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:VAL:HG22	9:l:275:ILE:HD11	2.01	0.42
3:G:28:ASN:OD1	3:G:29:LYS:N	2.52	0.42
3:G:72:LYS:O	3:G:73:HIS:C	2.62	0.42
6:F:67:CYS:O	6:F:67:CYS:SG	2.77	0.42
3:g:72:LYS:O	3:g:73:HIS:C	2.62	0.42
4:C:12:ARG:HG2	9:L:279:ASP:OD1	2.20	0.42
6:f:67:CYS:SG	6:f:67:CYS:O	2.77	0.42
5:E:26:VAL:O	5:E:29:VAL:HG12	2.19	0.42
1:d:174:TYR:O	1:d:175:PHE:C	2.63	0.42
4:c:40:ARG:HG3	4:c:41:ARG:N	2.35	0.41
5:e:26:VAL:O	5:e:29:VAL:HG12	2.19	0.41
7:k:299:ILE:HD12	7:k:299:ILE:N	2.34	0.41
4:C:50:VAL:N	4:C:51:PRO:HD2	2.34	0.41
7:k:323:VAL:HG22	7:k:324:SER:N	2.35	0.41
4:C:40:ARG:HG3	4:C:41:ARG:N	2.35	0.41
7:K:43:LEU:HB3	7:K:44:PRO:HD2	2.02	0.41
7:k:43:LEU:HB3	7:k:44:PRO:HD2	2.02	0.41
9:l:300:ASP:O	9:l:301:ASN:C	2.63	0.41
7:K:323:VAL:HG22	7:K:324:SER:N	2.35	0.41
8:j:158:THR:HG23	8:j:159:ASP:N	2.36	0.41
1:D:232:TYR:CD1	1:D:232:TYR:N	2.87	0.41
1:D:174:TYR:O	1:D:175:PHE:C	2.63	0.41
2:A:267:ARG:HB2	2:A:270:MET:HB2	2.03	0.41
7:K:319:GLN:HB3	7:K:320:PRO:CD	2.51	0.41
8:J:274:PHE:O	8:J:275:LEU:C	2.64	0.41
8:J:298:ILE:HD13	16:J:401:AOQ:CL	2.58	0.41
8:J:328:LEU:O	8:J:331:THR:OG1	2.30	0.41
9:L:125:THR:CG2	9:L:126:ARG:N	2.84	0.41
8:j:274:PHE:O	8:j:275:LEU:C	2.64	0.41
8:j:298:ILE:HD13	16:j:401:AOQ:CL	2.58	0.41
8:j:366:MET:HB2	8:j:367:PRO:HD3	2.03	0.41
8:J:158:THR:HG23	8:J:159:ASP:N	2.36	0.41
9:l:125:THR:CG2	9:l:126:ARG:N	2.83	0.41
6:f:47:ARG:NH1	6:f:51:GLU:OE2	2.52	0.40
7:K:382:TYR:O	7:K:385:SER:OG	2.37	0.40
8:J:24:PRO:HB2	8:J:27:ILE:HG23	2.03	0.40
8:j:24:PRO:HB2	8:j:27:ILE:HG23	2.03	0.40
8:j:133:LEU:N	8:j:134:PRO:CD	2.84	0.40
9:L:300:ASP:O	9:L:301:ASN:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	237/325 (73%)	223 (94%)	13 (6%)	1 (0%)	30	52
1	d	237/325 (73%)	223 (94%)	13 (6%)	1 (0%)	30	52
2	A	194/274 (71%)	180 (93%)	13 (7%)	1 (0%)	25	46
2	T	75/274 (27%)	72 (96%)	3 (4%)	0	100	100
2	a	194/274 (71%)	180 (93%)	13 (7%)	1 (0%)	25	46
3	G	102/111 (92%)	99 (97%)	3 (3%)	0	100	100
3	g	102/111 (92%)	99 (97%)	3 (3%)	0	100	100
4	C	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
4	c	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
5	E	54/63 (86%)	51 (94%)	3 (6%)	0	100	100
5	e	54/63 (86%)	51 (94%)	3 (6%)	0	100	100
6	F	65/91 (71%)	63 (97%)	2 (3%)	0	100	100
6	f	65/91 (71%)	63 (97%)	2 (3%)	0	100	100
7	K	416/453 (92%)	404 (97%)	12 (3%)	0	100	100
7	k	416/453 (92%)	404 (97%)	12 (3%)	0	100	100
8	J	376/380 (99%)	354 (94%)	22 (6%)	0	100	100
8	j	376/380 (99%)	354 (94%)	22 (6%)	0	100	100
9	L	419/480 (87%)	404 (96%)	15 (4%)	0	100	100
9	l	419/480 (87%)	404 (96%)	15 (4%)	0	100	100
10	H	43/56 (77%)	41 (95%)	2 (5%)	0	100	100
10	h	43/56 (77%)	41 (95%)	2 (5%)	0	100	100
All	All	4045/4904 (82%)	3856 (95%)	185 (5%)	4 (0%)	50	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	150	ALA
1	d	150	ALA
2	A	82	ASP
2	a	82	ASP

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	D	203/257 (79%)	201 (99%)	2 (1%)	73	88
1	d	203/257 (79%)	201 (99%)	2 (1%)	73	88
2	A	167/229 (73%)	167 (100%)	0	100	100
2	T	61/229 (27%)	60 (98%)	1 (2%)	58	80
2	a	167/229 (73%)	167 (100%)	0	100	100
3	G	94/98 (96%)	94 (100%)	0	100	100
3	g	94/98 (96%)	94 (100%)	0	100	100
4	C	74/75 (99%)	74 (100%)	0	100	100
4	c	74/75 (99%)	74 (100%)	0	100	100
5	E	46/53 (87%)	45 (98%)	1 (2%)	47	73
5	e	46/53 (87%)	45 (98%)	1 (2%)	47	73
6	F	64/86 (74%)	62 (97%)	2 (3%)	35	61
6	f	64/86 (74%)	62 (97%)	2 (3%)	35	61
7	K	335/361 (93%)	329 (98%)	6 (2%)	54	78
7	k	335/361 (93%)	329 (98%)	6 (2%)	54	78
8	J	340/342 (99%)	336 (99%)	4 (1%)	67	85
8	j	340/342 (99%)	336 (99%)	4 (1%)	67	85
9	L	354/396 (89%)	345 (98%)	9 (2%)	42	69
9	l	354/396 (89%)	345 (98%)	9 (2%)	42	69
10	H	36/46 (78%)	36 (100%)	0	100	100
10	h	36/46 (78%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3487/4115 (85%)	3438 (99%)	49 (1%)	62 82

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	120	VAL
1	D	322	ARG
5	E	30	LEU
6	F	50	LEU
6	F	78	ARG
7	K	109	LYS
7	K	157	GLN
7	K	214	THR
7	K	227	HIS
7	K	238	LEU
7	K	307	SER
8	J	80	ARG
8	J	174	THR
8	J	211	ILE
8	J	240	THR
9	L	58	ARG
9	L	115	SER
9	L	126	ARG
9	L	190	THR
9	L	208	VAL
9	L	257	TYR
9	L	265	LEU
9	L	298	SER
9	L	305	GLN
2	T	20	ARG
1	d	120	VAL
1	d	322	ARG
5	e	30	LEU
6	f	50	LEU
6	f	78	ARG
7	k	109	LYS
7	k	157	GLN
7	k	214	THR
7	k	227	HIS
7	k	238	LEU
7	k	307	SER
8	j	80	ARG

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Mol	Chain	Res	Type
8	j	174	THR
8	j	211	ILE
8	j	240	THR
9	l	58	ARG
9	l	115	SER
9	l	126	ARG
9	l	190	THR
9	l	208	VAL
9	l	257	TYR
9	l	265	LEU
9	l	298	SER
9	l	305	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	48	ASN
6	F	84	HIS
7	K	212	HIS
7	K	291	HIS
7	K	304	ASN
7	K	343	GLN
7	K	365	ASN
8	J	8	ASN
8	J	85	ASN
9	L	152	GLN
9	L	188	HIS
9	L	286	HIS
9	L	357	HIS
9	L	375	GLN
2	T	31	GLN
1	d	309	HIS
5	e	48	ASN
6	f	84	HIS
7	k	167	GLN
7	k	212	HIS
7	k	291	HIS
7	k	304	ASN
7	k	365	ASN
8	j	85	ASN
8	j	255	ASN
8	j	375	ASN

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Mol	Chain	Res	Type
9	1	152	GLN
9	1	188	HIS
9	1	286	HIS
9	1	375	GLN

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 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	$\# Z > 2$
17	PEE	J	403	-	50,50,50	0.76	2 (4%)	53,55,55	0.47	0
18	AFI	j	404	-	29,29,29	3.85	7 (24%)	38,42,42	1.83	6 (15%)
16	AOQ	J	401	-	29,29,29	0.18	0	40,42,42	0.30	0
19	HEM	j	406	8	41,50,50	1.43	4 (9%)	45,82,82	1.34	6 (13%)
17	PEE	j	403	-	50,50,50	0.77	2 (4%)	53,55,55	0.47	0
11	HEC	d	401	1	32,50,50	2.28	3 (9%)	24,82,82	1.54	1 (4%)
11	HEC	D	401	1	32,50,50	2.29	3 (9%)	24,82,82	1.53	1 (4%)
17	PEE	J	402	-	50,50,50	0.76	2 (4%)	53,55,55	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PEE	L	502	-	50,50,50	0.77	2 (4%)	53,55,55	0.44	0
18	AFI	J	404	-	29,29,29	3.87	7 (24%)	38,42,42	1.82	6 (15%)
15	PC1	E	101	-	53,53,53	0.28	0	59,61,61	0.27	0
14	CDL	l	501	-	99,99,99	0.31	0	105,111,111	0.33	0
19	HEM	J	406	8	41,50,50	1.44	4 (9%)	45,82,82	1.34	6 (13%)
19	HEM	j	405	8	41,50,50	1.51	3 (7%)	45,82,82	1.30	4 (8%)
17	PEE	j	402	-	50,50,50	0.76	2 (4%)	53,55,55	0.45	0
14	CDL	C	101	-	99,99,99	0.31	0	105,111,111	0.28	0
13	FES	a	300	2	0,4,4	-	-	-	-	-
14	CDL	L	501	-	99,99,99	0.31	0	105,111,111	0.33	0
15	PC1	e	101	-	53,53,53	0.28	0	59,61,61	0.27	0
16	AOQ	j	401	-	29,29,29	0.18	0	40,42,42	0.29	0
13	FES	A	300	2	0,4,4	-	-	-	-	-
14	CDL	c	101	-	99,99,99	0.31	0	105,111,111	0.28	0
19	HEM	J	405	8	41,50,50	1.50	3 (7%)	45,82,82	1.30	4 (8%)
17	PEE	l	502	-	50,50,50	0.76	2 (4%)	53,55,55	0.44	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
17	PEE	J	403	-	-	14/54/54/54	-
18	AFI	j	404	-	-	6/8/38/38	0/4/4/4
16	AOQ	J	401	-	-	2/8/38/38	0/4/4/4
19	HEM	j	406	8	-	4/12/54/54	-
17	PEE	j	403	-	-	14/54/54/54	-
11	HEC	d	401	1	-	0/10/54/54	-
11	HEC	D	401	1	-	0/10/54/54	-
17	PEE	J	402	-	-	16/54/54/54	-
17	PEE	L	502	-	-	18/54/54/54	-
18	AFI	J	404	-	-	6/8/38/38	0/4/4/4
15	PC1	E	101	-	-	14/57/57/57	-
14	CDL	l	501	-	-	26/110/110/110	-
19	HEM	J	406	8	-	4/12/54/54	-
19	HEM	j	405	8	-	2/12/54/54	-
17	PEE	j	402	-	-	16/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	C	101	-	-	14/110/110/110	-
14	CDL	L	501	-	-	26/110/110/110	-
13	FES	a	300	2	-	-	0/1/1/1
15	PC1	e	101	-	-	14/57/57/57	-
16	AOQ	j	401	-	-	2/8/38/38	0/4/4/4
13	FES	A	300	2	-	-	0/1/1/1
14	CDL	c	101	-	-	14/110/110/110	-
19	HEM	J	405	8	-	2/12/54/54	-
17	PEE	l	502	-	-	18/54/54/54	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	404	AFI	C3-C4	18.18	1.53	1.36
18	j	404	AFI	C3-C4	18.09	1.53	1.36
11	D	401	HEC	C2B-C3B	-7.07	1.33	1.40
11	d	401	HEC	C2B-C3B	-7.02	1.33	1.40
11	D	401	HEC	C3C-C2C	-6.72	1.33	1.40
11	d	401	HEC	C3C-C2C	-6.71	1.33	1.40
18	J	404	AFI	C16-C2	5.80	1.50	1.35
18	j	404	AFI	C16-C2	5.80	1.50	1.35
11	D	401	HEC	C3D-C2D	5.33	1.53	1.37
11	d	401	HEC	C3D-C2D	5.30	1.53	1.37
19	j	405	HEM	C3C-C2C	-5.00	1.33	1.40
18	j	404	AFI	O1-C1	4.95	1.33	1.23
18	J	404	AFI	O1-C1	4.95	1.33	1.23
19	J	405	HEM	C3C-C2C	-4.95	1.33	1.40
19	J	406	HEM	C3C-C2C	-3.79	1.35	1.40
18	J	404	AFI	C2-C1	-3.77	1.37	1.46
18	j	404	AFI	C2-C1	-3.77	1.37	1.46
19	J	406	HEM	C3C-CAC	3.76	1.55	1.47
19	j	406	HEM	C3C-CAC	3.76	1.55	1.47
19	j	406	HEM	C3C-C2C	-3.75	1.35	1.40
18	j	404	AFI	O2-C4	-3.69	1.23	1.33
18	J	404	AFI	O2-C4	-3.67	1.23	1.33
17	J	402	PEE	C39-C38	3.59	1.52	1.31
17	j	402	PEE	C39-C38	3.59	1.52	1.31
17	j	403	PEE	C18-C19	3.57	1.52	1.31
17	L	502	PEE	C18-C19	3.57	1.52	1.31
19	j	405	HEM	C3C-CAC	3.56	1.55	1.47
17	j	403	PEE	C39-C38	3.56	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	502	PEE	C39-C38	3.55	1.52	1.31
17	J	403	PEE	C18-C19	3.55	1.52	1.31
17	l	502	PEE	C18-C19	3.55	1.52	1.31
17	J	403	PEE	C39-C38	3.55	1.52	1.31
17	l	502	PEE	C39-C38	3.53	1.52	1.31
19	J	405	HEM	C3C-CAC	3.51	1.55	1.47
17	j	402	PEE	C18-C19	3.42	1.51	1.31
17	J	402	PEE	C18-C19	3.42	1.51	1.31
18	J	404	AFI	O6-C3	-3.14	1.23	1.33
18	j	404	AFI	O6-C3	-3.13	1.23	1.33
19	j	405	HEM	CAB-C3B	2.80	1.55	1.47
19	J	405	HEM	CAB-C3B	2.79	1.55	1.47
19	J	406	HEM	CAB-C3B	2.78	1.55	1.47
19	j	406	HEM	CAB-C3B	2.77	1.55	1.47
19	J	406	HEM	CAA-C2A	2.33	1.55	1.52
19	j	406	HEM	CAA-C2A	2.32	1.55	1.52
18	j	404	AFI	C2-C3	2.05	1.48	1.41
18	J	404	AFI	C2-C3	2.05	1.48	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	404	AFI	C15-C16-C2	-5.84	113.17	123.06
18	j	404	AFI	C15-C16-C2	-5.83	113.19	123.06
18	j	404	AFI	C11-C16-C2	-5.82	113.20	123.06
18	J	404	AFI	C11-C16-C2	-5.82	113.21	123.06
11	d	401	HEC	CMB-C2B-C3B	-4.47	120.56	125.82
11	D	401	HEC	CMB-C2B-C3B	-4.45	120.59	125.82
18	j	404	AFI	O2-C4-C10	4.16	122.80	115.53
18	J	404	AFI	O2-C4-C10	4.13	122.75	115.53
18	j	404	AFI	C9-C1-C2	3.33	123.07	116.74
18	J	404	AFI	C9-C1-C2	3.33	123.06	116.74
19	J	406	HEM	CMC-C2C-C3C	3.24	130.75	124.68
19	j	406	HEM	CMC-C2C-C3C	3.22	130.69	124.68
18	J	404	AFI	O1-C1-C9	-2.97	116.75	121.56
18	j	404	AFI	O1-C1-C9	-2.97	116.75	121.56
19	j	406	HEM	C4A-C3A-C2A	2.82	108.96	107.00
19	J	406	HEM	C4A-C3A-C2A	2.82	108.96	107.00
19	J	405	HEM	C4C-CHD-C1D	2.58	125.96	122.56
19	j	405	HEM	C4D-ND-C1D	2.57	107.73	105.07
19	J	405	HEM	C1B-NB-C4B	2.56	107.71	105.07
19	J	406	HEM	C1B-NB-C4B	2.55	107.71	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	j	405	HEM	C4C-CHD-C1D	2.54	125.92	122.56
19	j	405	HEM	C1B-NB-C4B	2.54	107.70	105.07
19	j	406	HEM	C1B-NB-C4B	2.53	107.69	105.07
19	J	405	HEM	C4D-ND-C1D	2.52	107.68	105.07
19	j	406	HEM	C4D-ND-C1D	2.50	107.66	105.07
19	J	406	HEM	C4D-ND-C1D	2.50	107.66	105.07
19	J	405	HEM	C4B-CHC-C1C	2.45	125.80	122.56
19	j	405	HEM	C4B-CHC-C1C	2.44	125.78	122.56
19	J	406	HEM	C4B-CHC-C1C	2.36	125.68	122.56
19	j	406	HEM	C4B-CHC-C1C	2.32	125.62	122.56
19	J	406	HEM	C3B-C2B-C1B	2.08	108.03	106.49
18	J	404	AFI	O6-C3-C2	2.06	122.45	118.10
18	j	404	AFI	O6-C3-C2	2.04	122.41	118.10
19	j	406	HEM	C3B-C2B-C1B	2.04	108.00	106.49

There are no chirality outliers.

All (232) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	101	CDL	CA3-OA5-PA1-OA4
14	C	101	CDL	CB3-OB5-PB2-OB2
14	L	501	CDL	O1-C1-CA2-OA2
14	L	501	CDL	OB5-CB3-CB4-OB6
14	L	501	CDL	OB7-CB5-OB6-CB4
14	L	501	CDL	C51-CB5-OB6-CB4
14	c	101	CDL	CA3-OA5-PA1-OA4
14	c	101	CDL	CB3-OB5-PB2-OB2
14	l	501	CDL	O1-C1-CA2-OA2
14	l	501	CDL	OB5-CB3-CB4-OB6
14	l	501	CDL	OB7-CB5-OB6-CB4
14	l	501	CDL	C51-CB5-OB6-CB4
15	E	101	PC1	C11-O13-P-O14
15	E	101	PC1	C1-O11-P-O14
15	E	101	PC1	O13-C11-C12-N
15	E	101	PC1	C22-C21-O21-C2
15	e	101	PC1	C11-O13-P-O14
15	e	101	PC1	C1-O11-P-O14
15	e	101	PC1	O13-C11-C12-N
15	e	101	PC1	C22-C21-O21-C2
17	J	402	PEE	C1-O3P-P-O1P
17	J	402	PEE	O4P-C4-C5-N
17	J	403	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
17	L	502	PEE	C1-O3P-P-O1P
17	j	402	PEE	C1-O3P-P-O1P
17	j	402	PEE	O4P-C4-C5-N
17	j	403	PEE	C11-C10-O2-C2
17	l	502	PEE	C1-O3P-P-O1P
18	J	404	AFI	C11-C16-C2-C1
18	J	404	AFI	C15-C16-C2-C1
18	J	404	AFI	C11-C16-C2-C3
18	J	404	AFI	C15-C16-C2-C3
18	j	404	AFI	C11-C16-C2-C1
18	j	404	AFI	C15-C16-C2-C1
18	j	404	AFI	C11-C16-C2-C3
18	j	404	AFI	C15-C16-C2-C3
19	J	406	HEM	C1A-C2A-CAA-CBA
19	J	406	HEM	C3A-C2A-CAA-CBA
19	j	406	HEM	C1A-C2A-CAA-CBA
19	j	406	HEM	C3A-C2A-CAA-CBA
17	L	502	PEE	O5-C30-O3-C3
17	l	502	PEE	O5-C30-O3-C3
15	E	101	PC1	O22-C21-O21-C2
15	e	101	PC1	O22-C21-O21-C2
17	L	502	PEE	O4-C10-O2-C2
17	l	502	PEE	O4-C10-O2-C2
17	L	502	PEE	C31-C30-O3-C3
17	l	502	PEE	C31-C30-O3-C3
17	L	502	PEE	C11-C10-O2-C2
17	l	502	PEE	C11-C10-O2-C2
17	J	403	PEE	C31-C30-O3-C3
17	j	403	PEE	C31-C30-O3-C3
17	L	502	PEE	C37-C38-C39-C40
17	l	502	PEE	C37-C38-C39-C40
17	J	403	PEE	O4-C10-O2-C2
17	j	403	PEE	O4-C10-O2-C2
17	J	403	PEE	O5-C30-O3-C3
17	j	403	PEE	O5-C30-O3-C3
14	C	101	CDL	CA3-OA5-PA1-OA2
14	c	101	CDL	CA3-OA5-PA1-OA2
15	E	101	PC1	C1-O11-P-O13
15	e	101	PC1	C11-O13-P-O11
15	e	101	PC1	C1-O11-P-O13
17	J	402	PEE	C1-O3P-P-O4P
17	J	402	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
17	L	502	PEE	C1-O3P-P-O4P
17	j	402	PEE	C1-O3P-P-O4P
17	j	402	PEE	C4-O4P-P-O3P
17	l	502	PEE	C1-O3P-P-O4P
14	l	501	CDL	C31-C32-C33-C34
19	J	405	HEM	C3D-CAD-CBD-CGD
19	j	405	HEM	C3D-CAD-CBD-CGD
14	L	501	CDL	C31-C32-C33-C34
14	L	501	CDL	C39-C40-C41-C42
14	l	501	CDL	C39-C40-C41-C42
14	L	501	CDL	CB2-C1-CA2-OA2
14	l	501	CDL	CB2-C1-CA2-OA2
14	L	501	CDL	C13-C14-C15-C16
14	l	501	CDL	C13-C14-C15-C16
14	L	501	CDL	C42-C43-C44-C45
14	l	501	CDL	C42-C43-C44-C45
17	L	502	PEE	C17-C18-C19-C20
17	l	502	PEE	C17-C18-C19-C20
17	J	402	PEE	C16-C17-C18-C19
17	j	402	PEE	C16-C17-C18-C19
15	E	101	PC1	C11-O13-P-O11
14	L	501	CDL	OA5-CA3-CA4-CA6
14	l	501	CDL	OA5-CA3-CA4-CA6
17	L	502	PEE	O3P-C1-C2-C3
17	l	502	PEE	O3P-C1-C2-C3
14	C	101	CDL	CB3-CB4-CB6-OB8
14	L	501	CDL	CB3-CB4-CB6-OB8
14	l	501	CDL	CB3-CB4-CB6-OB8
17	J	403	PEE	C1-C2-O2-C10
17	j	403	PEE	C1-C2-O2-C10
17	J	403	PEE	O2-C2-C3-O3
17	j	403	PEE	O2-C2-C3-O3
17	L	502	PEE	C32-C33-C34-C35
17	l	502	PEE	C32-C33-C34-C35
17	L	502	PEE	C42-C43-C44-C45
17	l	502	PEE	C42-C43-C44-C45
19	J	406	HEM	C4D-C3D-CAD-CBD
19	j	406	HEM	C4D-C3D-CAD-CBD
14	L	501	CDL	C64-C65-C66-C67
14	l	501	CDL	C64-C65-C66-C67
14	c	101	CDL	CB3-CB4-CB6-OB8
17	J	403	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
17	j	403	PEE	C1-C2-C3-O3
14	l	501	CDL	CB5-C51-C52-C53
14	L	501	CDL	CB5-C51-C52-C53
16	J	401	AOQ	C14-C13-C17-C18
16	j	401	AOQ	C14-C13-C17-C18
17	j	403	PEE	C38-C39-C40-C41
15	e	101	PC1	C3C-C3D-C3E-C3F
19	J	406	HEM	C2D-C3D-CAD-CBD
19	j	406	HEM	C2D-C3D-CAD-CBD
15	E	101	PC1	C3C-C3D-C3E-C3F
14	L	501	CDL	OB5-CB3-CB4-CB6
14	l	501	CDL	OB5-CB3-CB4-CB6
16	J	401	AOQ	C14-C13-C17-C22
16	j	401	AOQ	C14-C13-C17-C22
17	J	402	PEE	C18-C19-C20-C21
17	J	403	PEE	C38-C39-C40-C41
17	j	402	PEE	C18-C19-C20-C21
14	L	501	CDL	CB6-CB4-OB6-CB5
14	l	501	CDL	CB6-CB4-OB6-CB5
14	L	501	CDL	OA5-CA3-CA4-OA6
14	l	501	CDL	OA5-CA3-CA4-OA6
14	L	501	CDL	OB6-CB4-CB6-OB8
14	l	501	CDL	OB6-CB4-CB6-OB8
14	C	101	CDL	CA3-OA5-PA1-OA3
14	c	101	CDL	CA3-OA5-PA1-OA3
15	E	101	PC1	C11-O13-P-O12
15	E	101	PC1	C1-O11-P-O12
15	e	101	PC1	C11-O13-P-O12
15	e	101	PC1	C1-O11-P-O12
17	J	402	PEE	C1-O3P-P-O2P
17	J	402	PEE	C4-O4P-P-O2P
17	J	402	PEE	C4-O4P-P-O1P
17	L	502	PEE	C1-O3P-P-O2P
17	j	402	PEE	C1-O3P-P-O2P
17	j	402	PEE	C4-O4P-P-O2P
17	j	402	PEE	C4-O4P-P-O1P
17	l	502	PEE	C1-O3P-P-O2P
17	L	502	PEE	C10-C11-C12-C13
18	J	404	AFI	C14-C13-C17-C18
18	j	404	AFI	C14-C13-C17-C18
17	L	502	PEE	O3P-C1-C2-O2
17	l	502	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	l	502	PEE	O3P-C1-C2-O2
17	L	502	PEE	C18-C19-C20-C21
17	l	502	PEE	C18-C19-C20-C21
18	J	404	AFI	C14-C13-C17-C22
18	j	404	AFI	C14-C13-C17-C22
14	C	101	CDL	OB6-CB4-CB6-OB8
14	c	101	CDL	OB6-CB4-CB6-OB8
15	e	101	PC1	C29-C2A-C2B-C2C
15	E	101	PC1	C29-C2A-C2B-C2C
17	J	402	PEE	C38-C39-C40-C41
17	j	402	PEE	C38-C39-C40-C41
14	C	101	CDL	CA6-CA4-OA6-CA5
14	c	101	CDL	CA6-CA4-OA6-CA5
14	l	501	CDL	C81-C82-C83-C84
14	L	501	CDL	C81-C82-C83-C84
17	J	403	PEE	C16-C17-C18-C19
17	j	403	PEE	C16-C17-C18-C19
14	L	501	CDL	CB3-OB5-PB2-OB2
14	l	501	CDL	CB3-OB5-PB2-OB2
17	J	403	PEE	C4-O4P-P-O3P
17	j	403	PEE	C4-O4P-P-O3P
14	C	101	CDL	CA7-C31-C32-C33
14	c	101	CDL	CA7-C31-C32-C33
17	J	403	PEE	C2-C1-O3P-P
17	j	403	PEE	C2-C1-O3P-P
17	L	502	PEE	C36-C37-C38-C39
17	l	502	PEE	C36-C37-C38-C39
17	J	402	PEE	O5-C30-O3-C3
17	j	402	PEE	O5-C30-O3-C3
17	J	402	PEE	C31-C30-O3-C3
17	j	402	PEE	C31-C30-O3-C3
14	C	101	CDL	CB5-C51-C52-C53
14	c	101	CDL	CB5-C51-C52-C53
17	J	402	PEE	C36-C37-C38-C39
17	j	402	PEE	C36-C37-C38-C39
14	L	501	CDL	C14-C15-C16-C17
14	l	501	CDL	C14-C15-C16-C17
14	C	101	CDL	OA6-CA4-CA6-OA8
14	c	101	CDL	OA6-CA4-CA6-OA8
17	J	403	PEE	C18-C19-C20-C21
17	j	403	PEE	C18-C19-C20-C21
15	E	101	PC1	C2A-C2B-C2C-C2D

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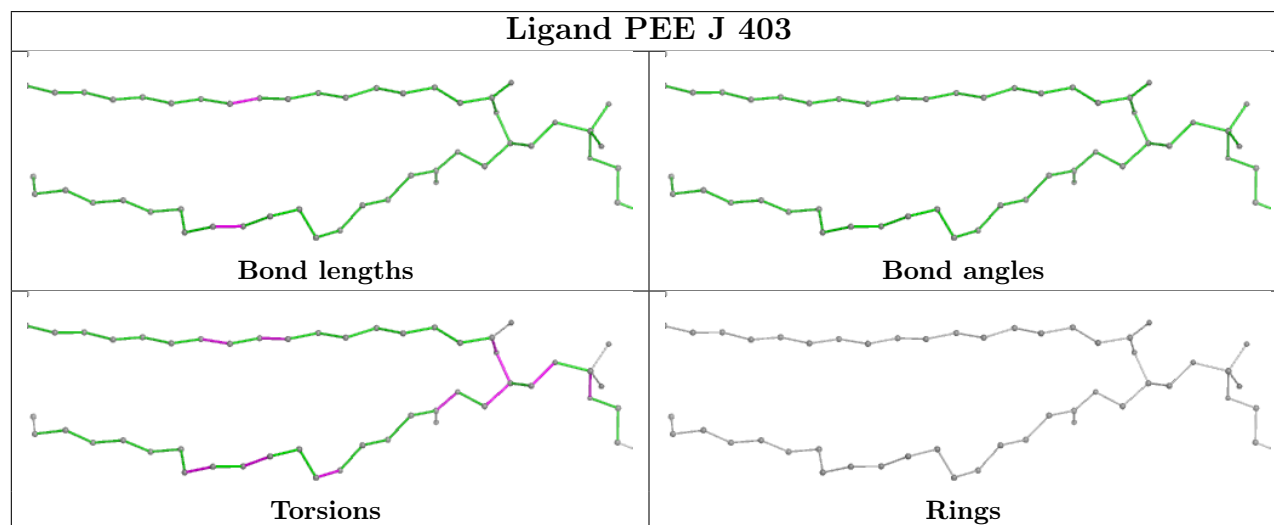
Mol	Chain	Res	Type	Atoms
15	e	101	PC1	C2A-C2B-C2C-C2D
17	L	502	PEE	C16-C17-C18-C19
17	l	502	PEE	C16-C17-C18-C19
17	J	402	PEE	C1-C2-O2-C10
17	j	402	PEE	C1-C2-O2-C10
15	E	101	PC1	C26-C27-C28-C29
15	e	101	PC1	C26-C27-C28-C29
14	L	501	CDL	C33-C34-C35-C36
14	l	501	CDL	C33-C34-C35-C36
17	J	403	PEE	C33-C34-C35-C36
17	j	403	PEE	C33-C34-C35-C36
15	E	101	PC1	O31-C31-C32-C33
15	e	101	PC1	O31-C31-C32-C33
14	L	501	CDL	C56-C57-C58-C59
17	J	402	PEE	C19-C20-C21-C22
17	j	402	PEE	C19-C20-C21-C22
14	l	501	CDL	C56-C57-C58-C59
17	J	403	PEE	C36-C37-C38-C39
17	j	403	PEE	C36-C37-C38-C39
14	c	101	CDL	OB7-CB5-OB6-CB4
14	L	501	CDL	C12-C11-CA5-OA6
14	l	501	CDL	C12-C11-CA5-OA6
17	L	502	PEE	C19-C20-C21-C22
17	l	502	PEE	C19-C20-C21-C22
14	C	101	CDL	OB7-CB5-OB6-CB4
14	C	101	CDL	C75-C76-C77-C78
14	c	101	CDL	C75-C76-C77-C78
14	C	101	CDL	C51-CB5-OB6-CB4
14	c	101	CDL	C51-CB5-OB6-CB4
14	L	501	CDL	C12-C11-CA5-OA7
14	l	501	CDL	C12-C11-CA5-OA7
14	L	501	CDL	CB4-CB3-OB5-PB2
14	l	501	CDL	CB4-CB3-OB5-PB2
14	C	101	CDL	CB3-OB5-PB2-OB4
14	c	101	CDL	CB3-OB5-PB2-OB4
17	J	402	PEE	C3-C2-O2-C10
17	j	402	PEE	C3-C2-O2-C10
14	L	501	CDL	C32-C31-CA7-OA8
14	l	501	CDL	C32-C31-CA7-OA8
19	J	405	HEM	CAD-CBD-CGD-O2D
19	j	405	HEM	CAD-CBD-CGD-O2D

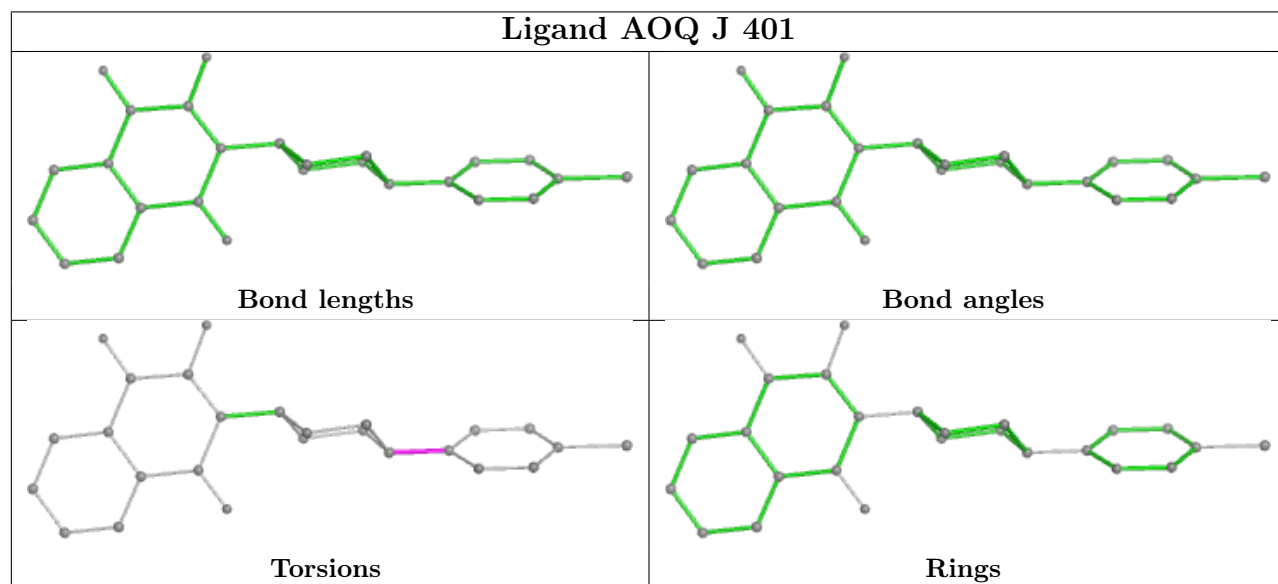
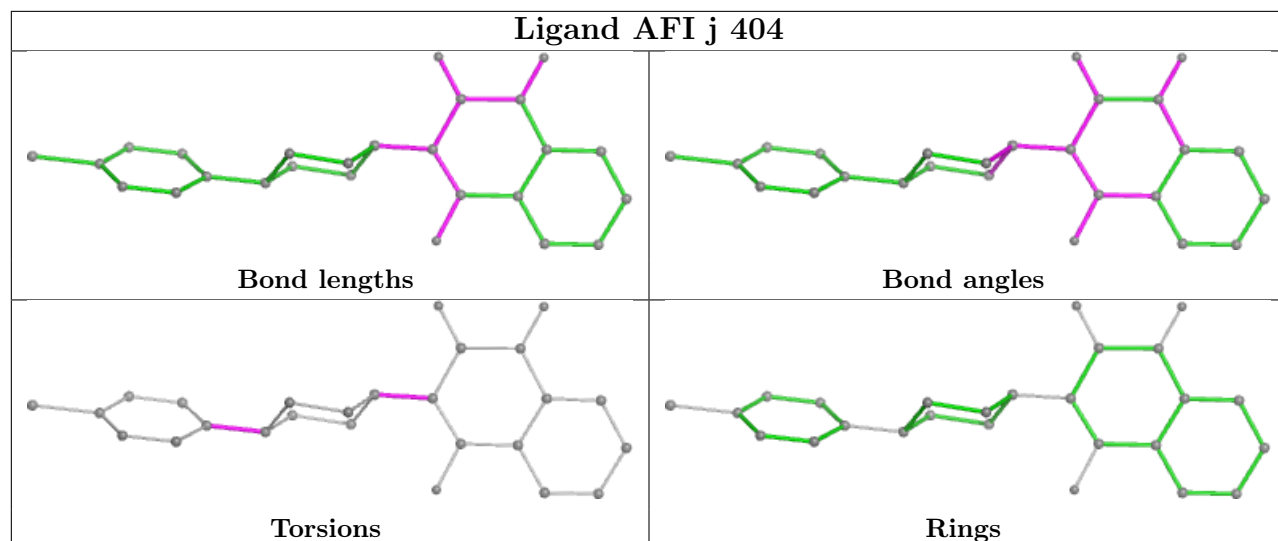
There are no ring outliers.

9 monomers are involved in 22 short contacts:

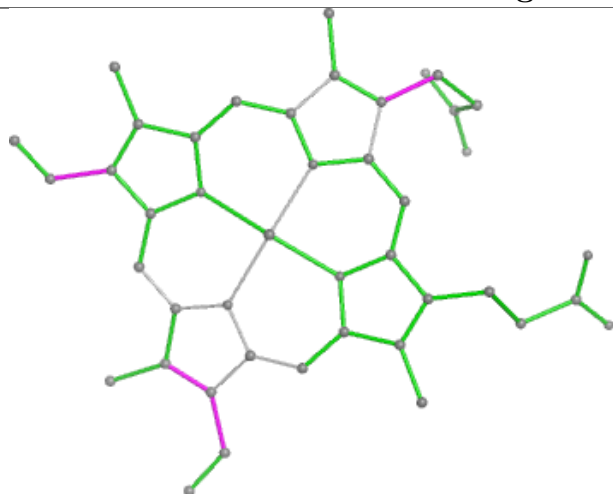
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	J	401	AOQ	1	0
19	j	406	HEM	6	0
15	E	101	PC1	1	0
14	l	501	CDL	1	0
19	J	406	HEM	5	0
19	j	405	HEM	3	0
15	e	101	PC1	1	0
16	j	401	AOQ	1	0
19	J	405	HEM	3	0

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

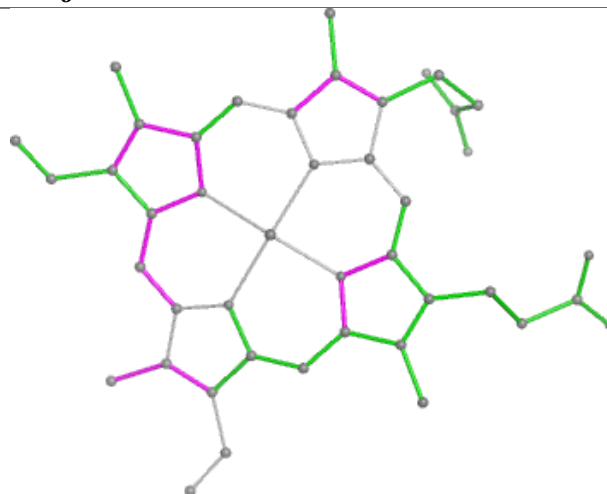




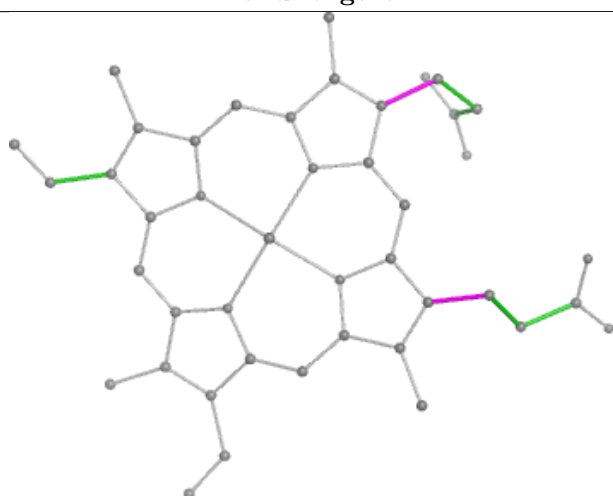
Ligand HEM j 406



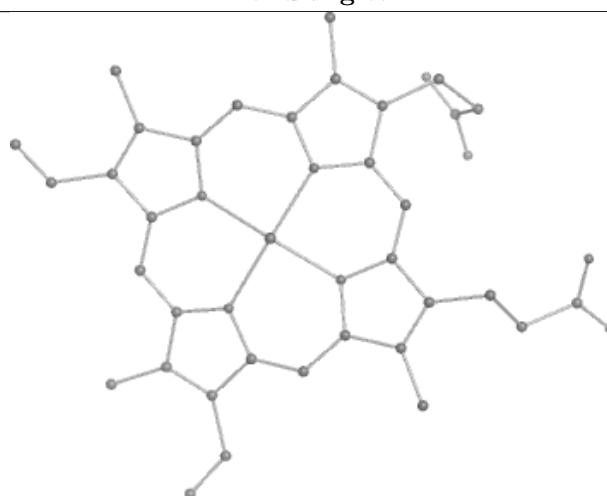
Bond lengths



Bond angles

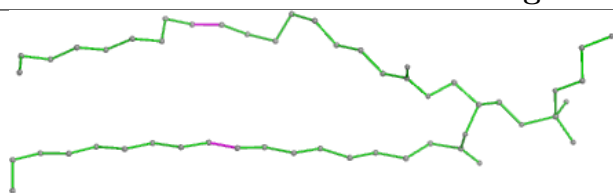


Torsions

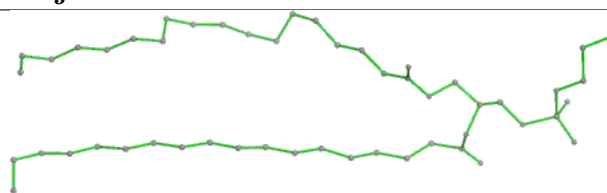


Rings

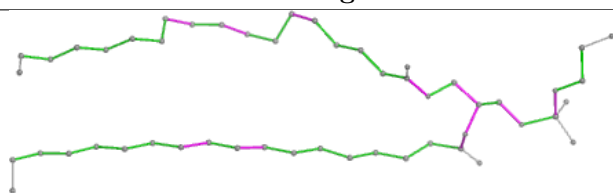
Ligand PEE j 403



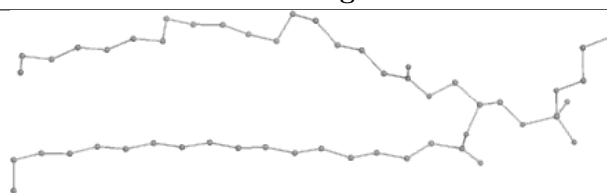
Bond lengths



Bond angles

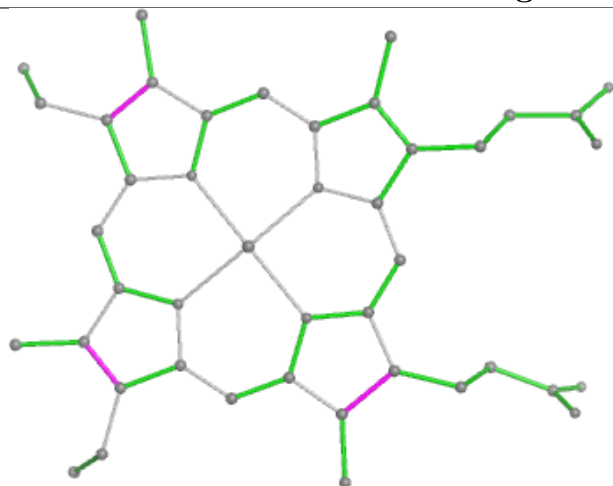


Torsions

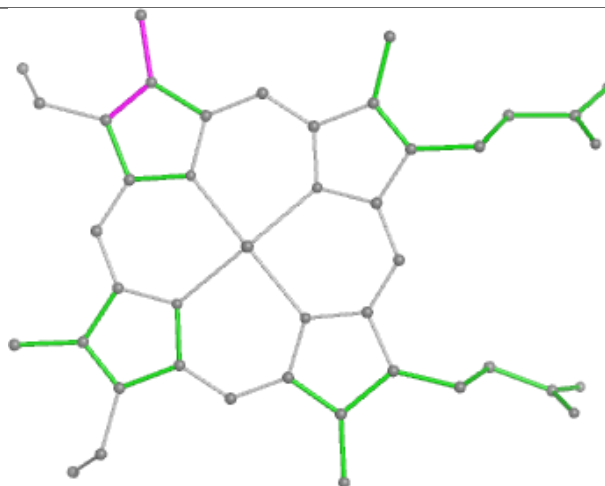


Rings

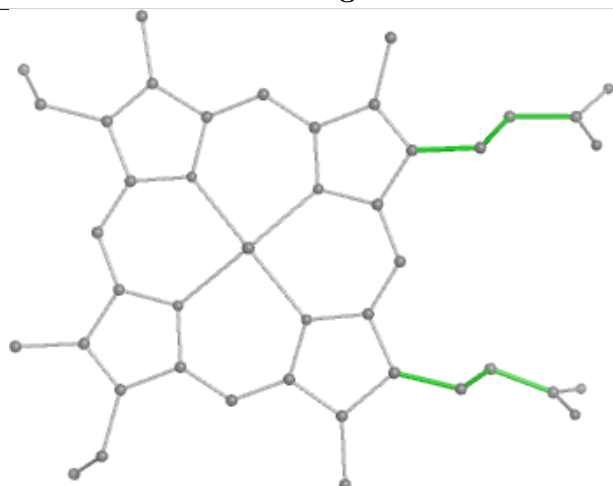
Ligand HEC d 401



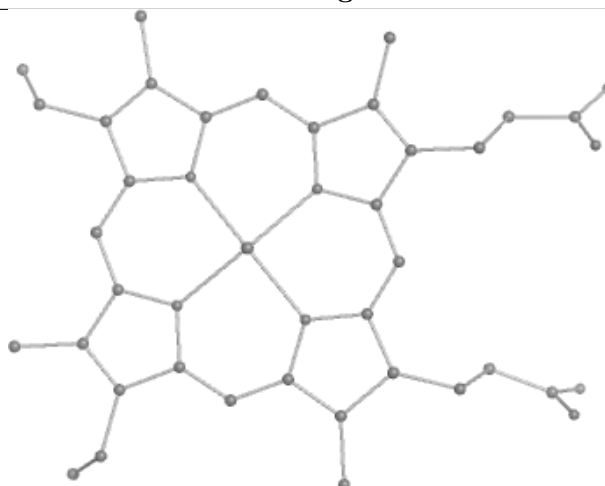
Bond lengths



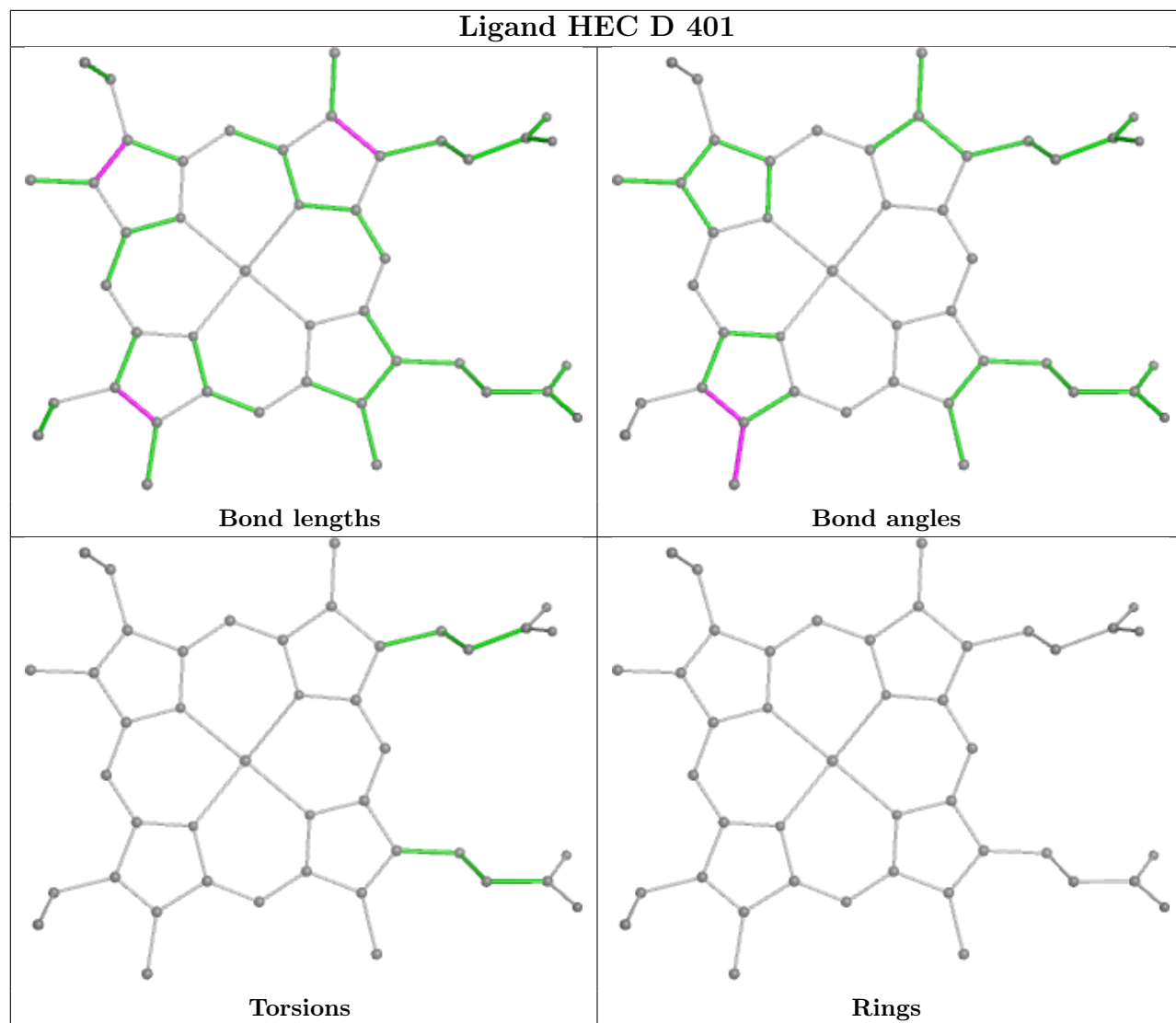
Bond angles

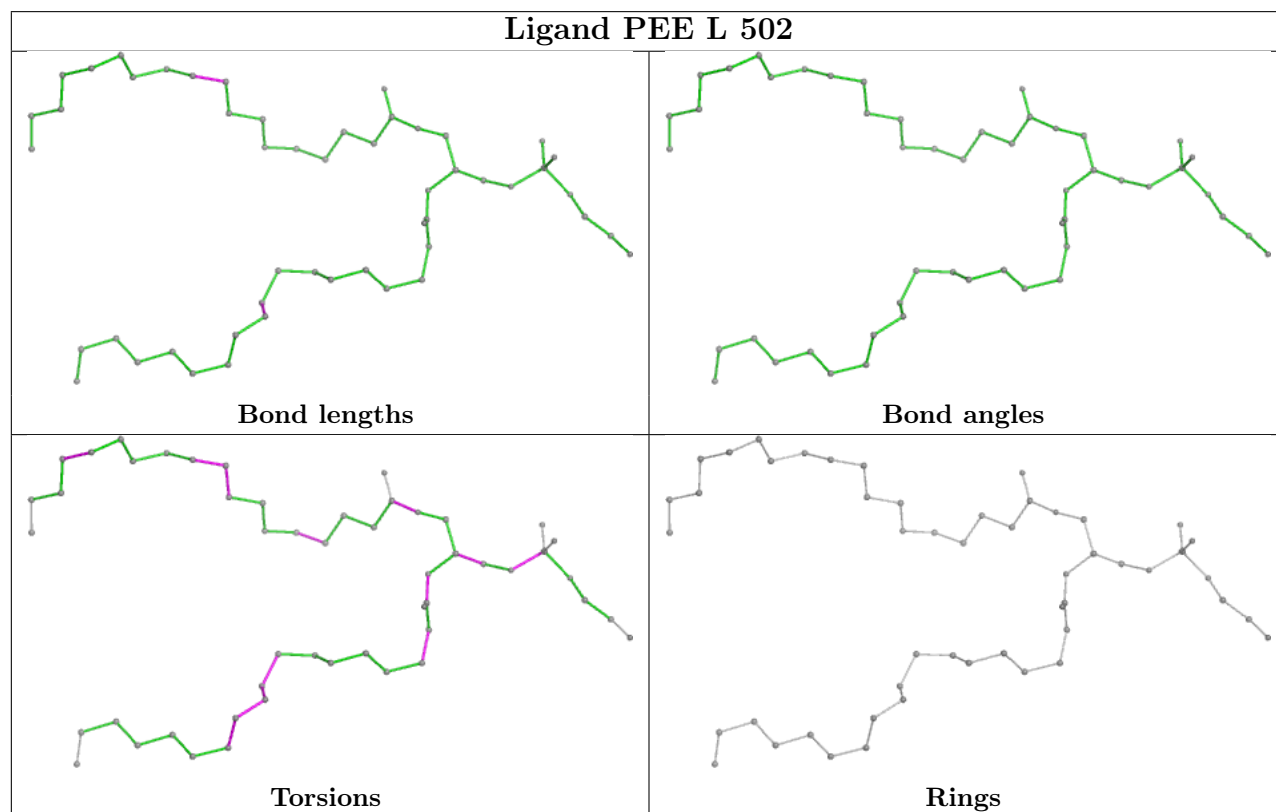
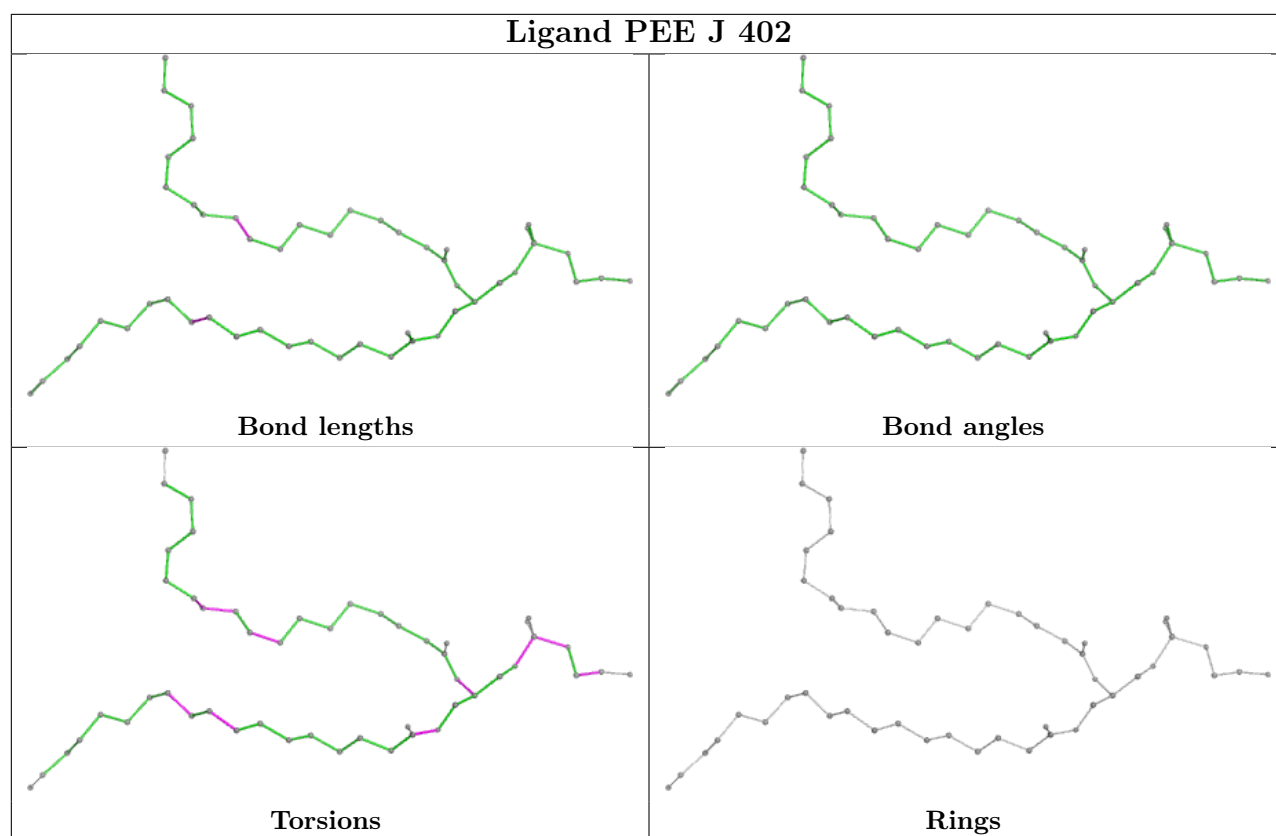


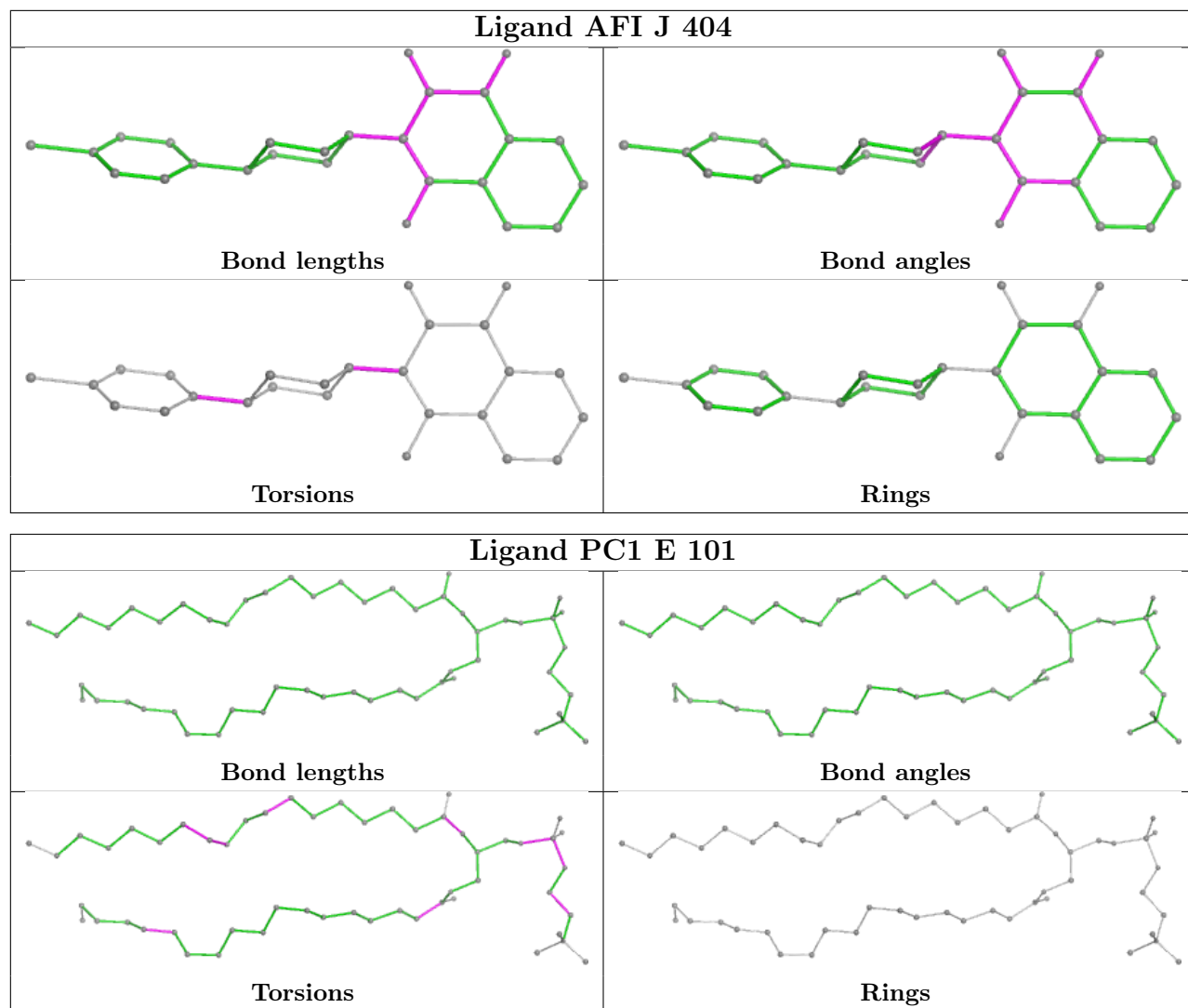
Torsions

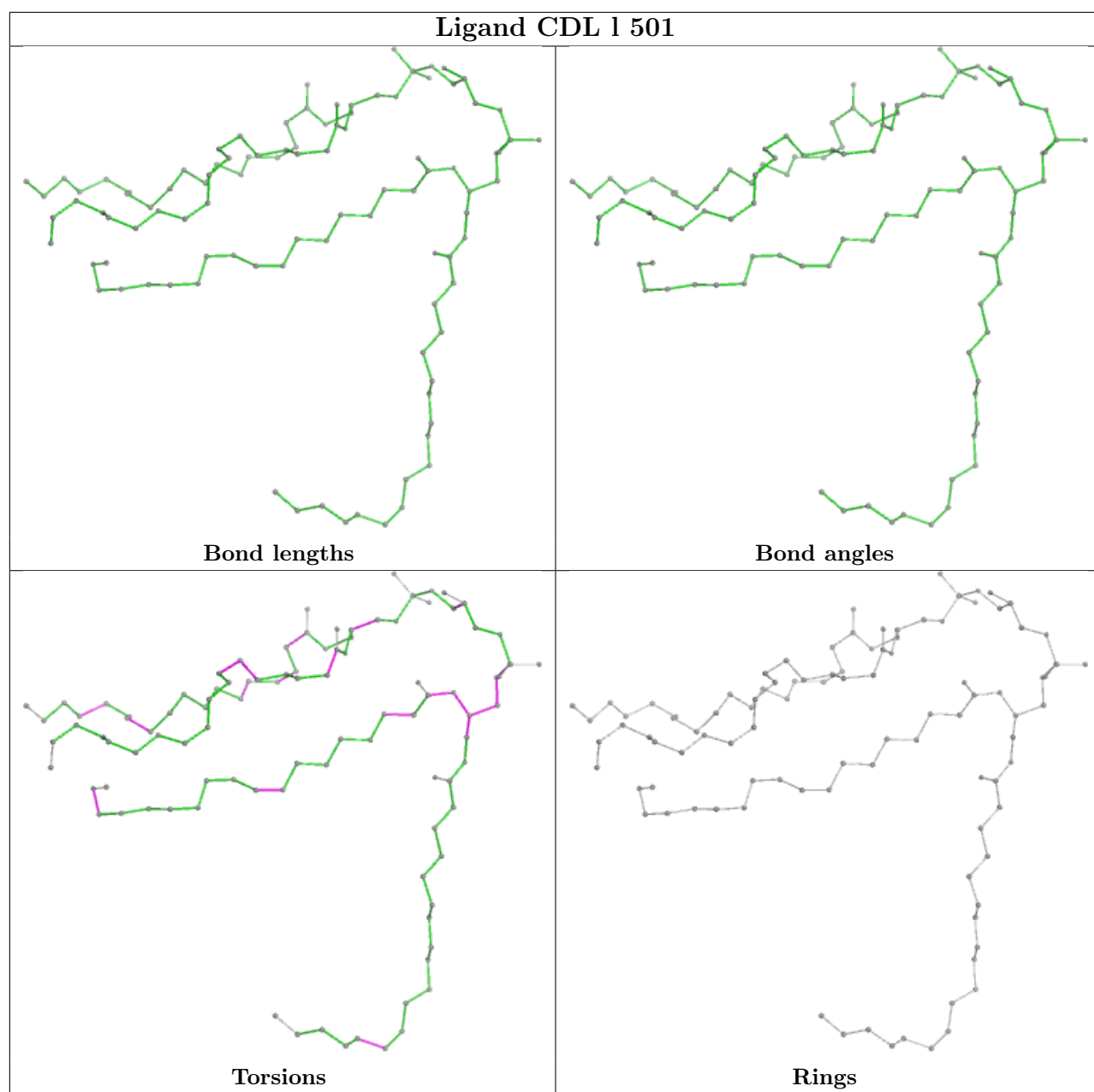


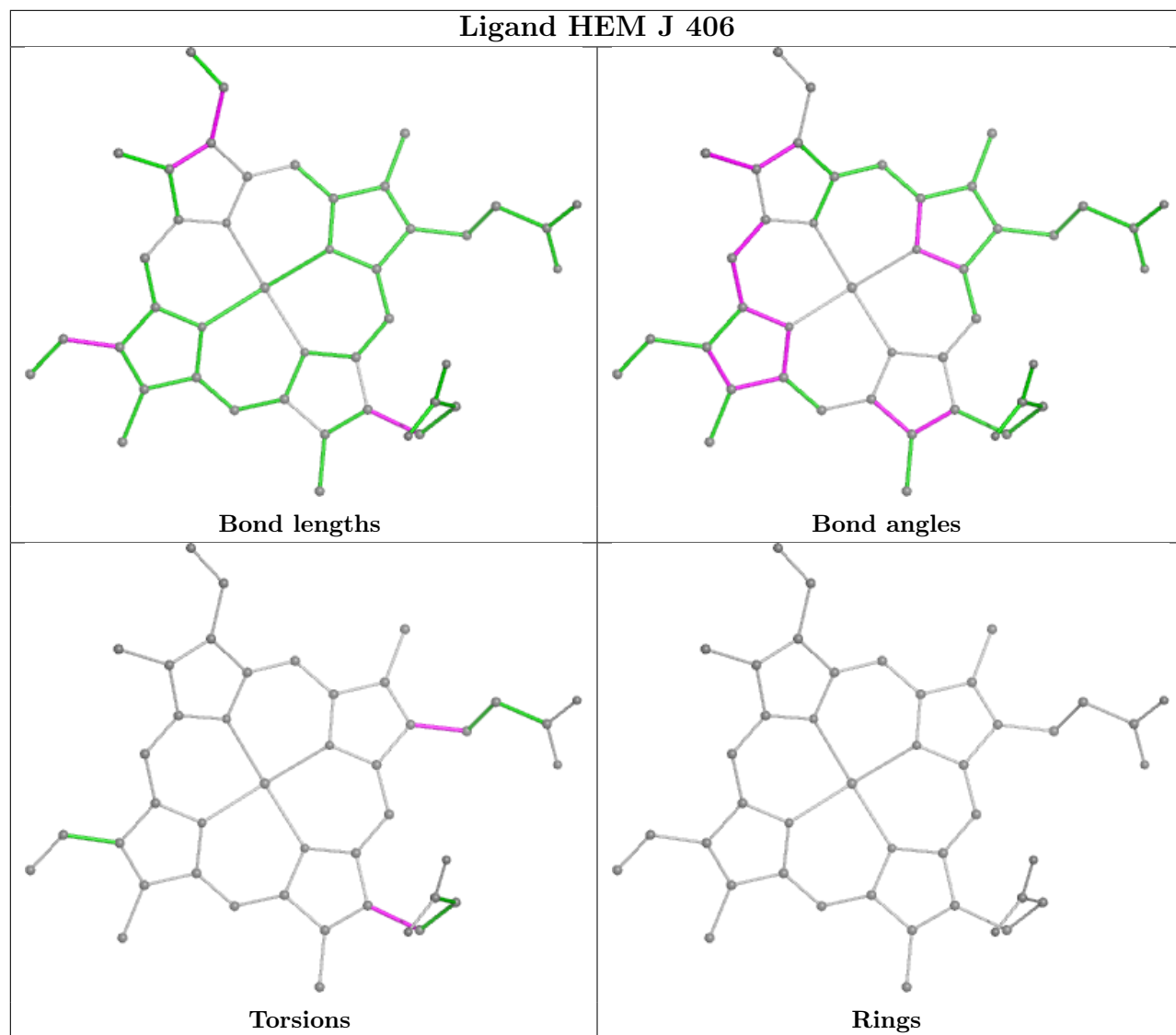
Rings

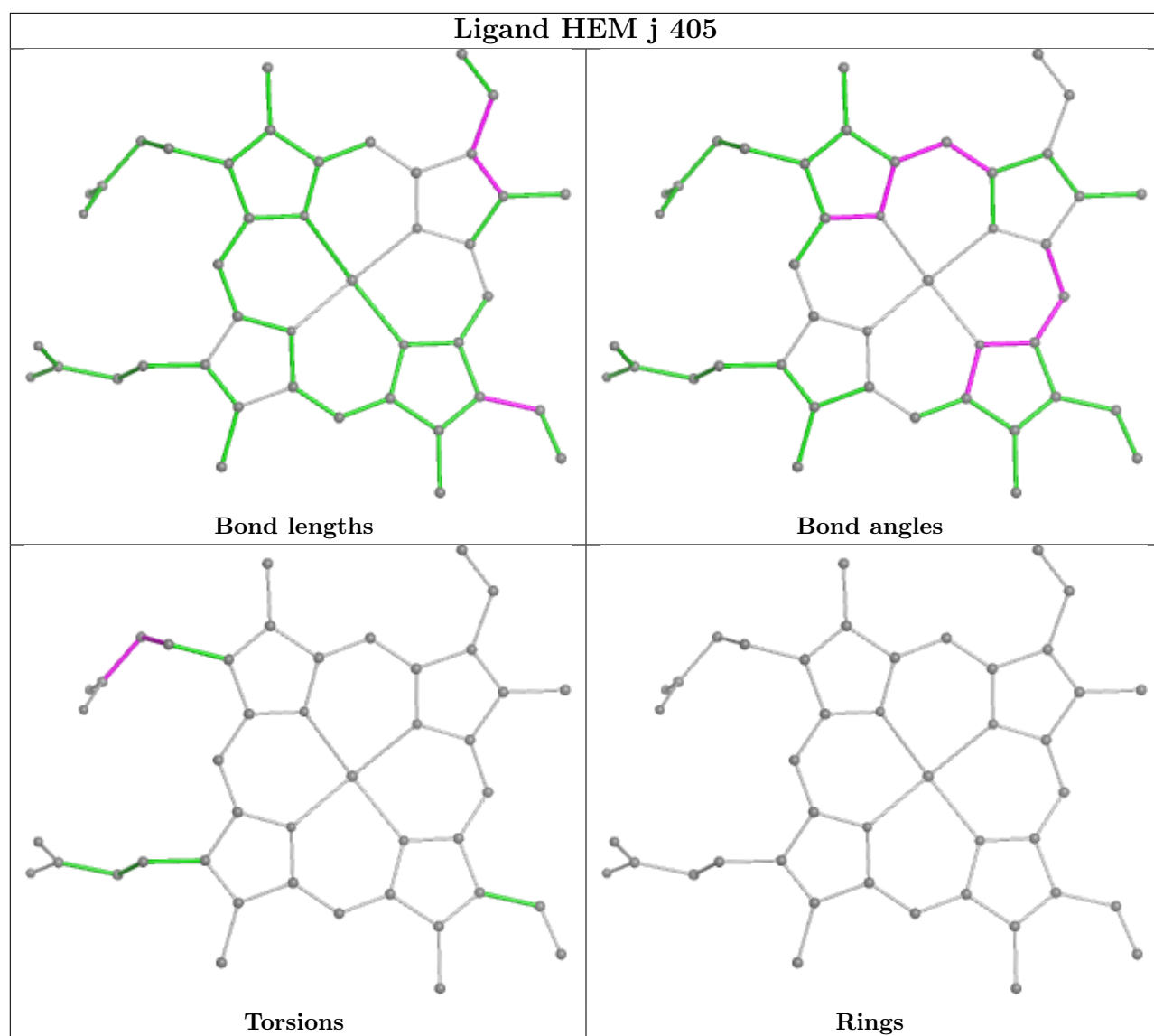


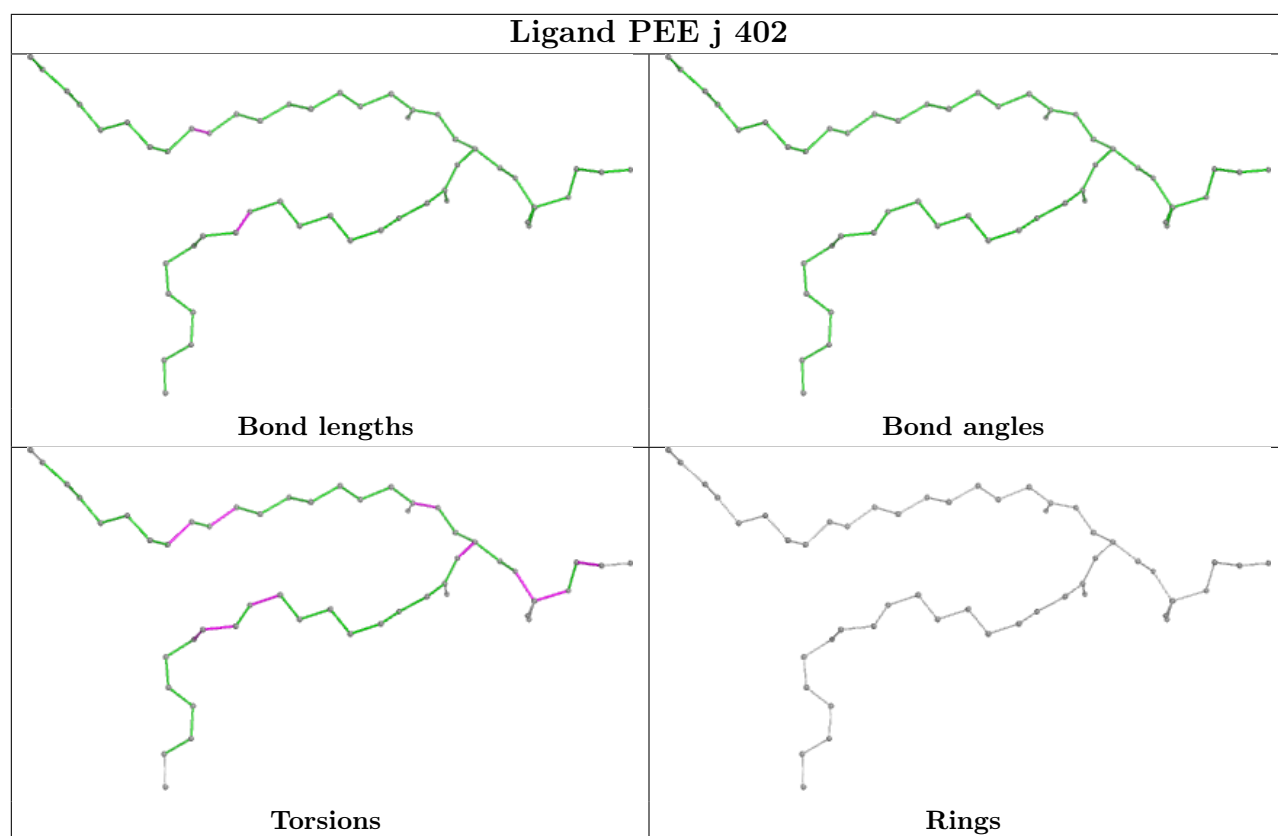


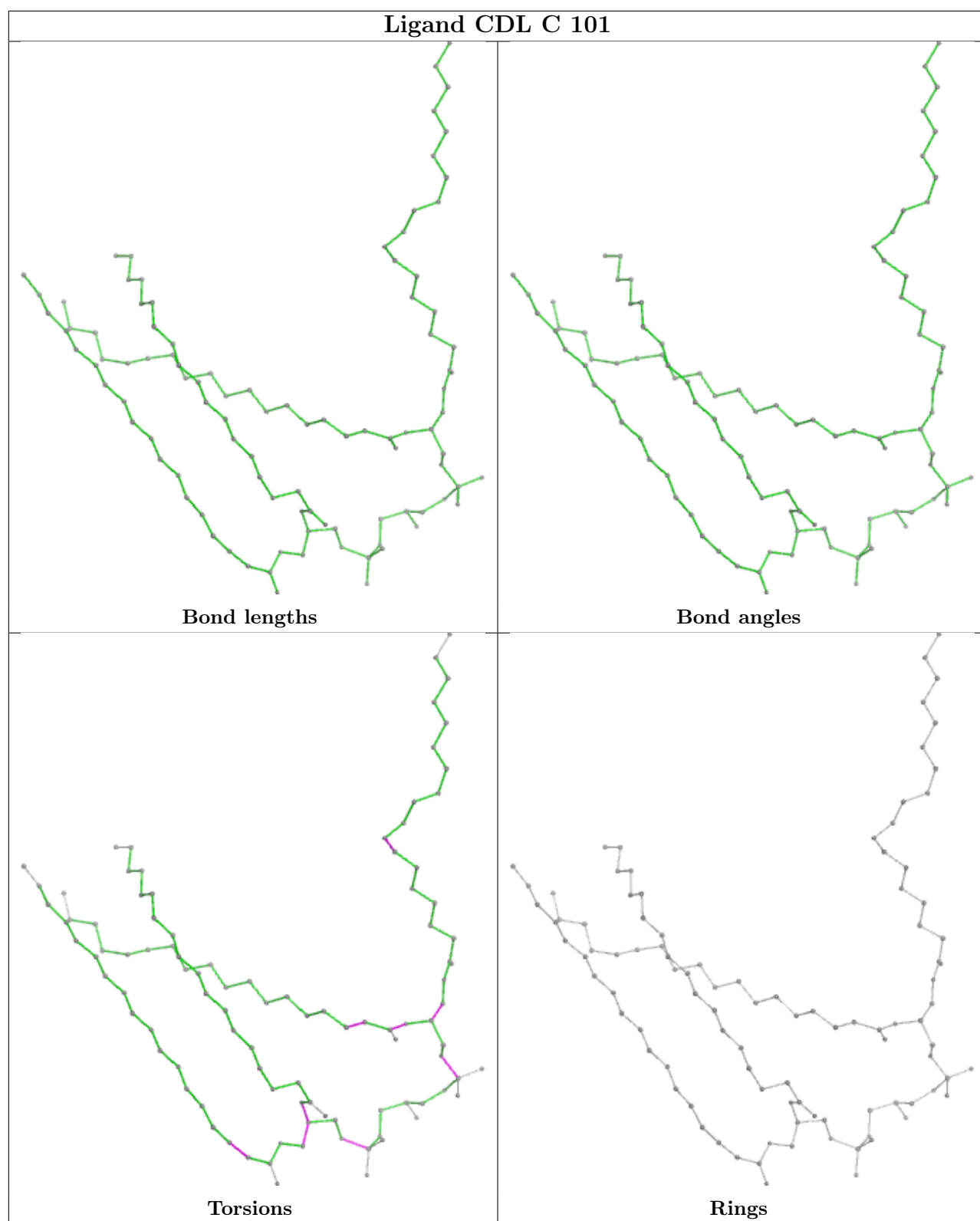


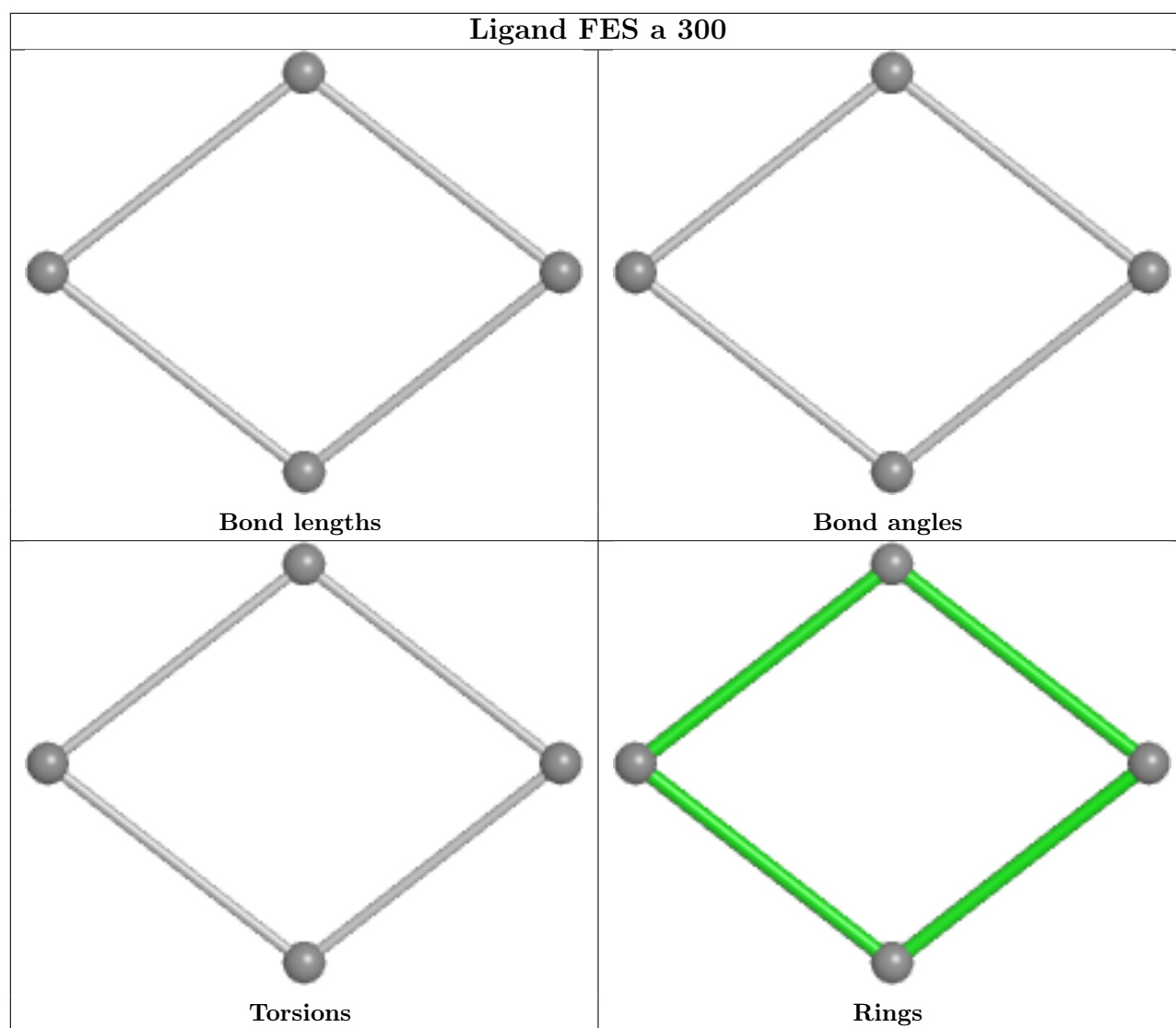


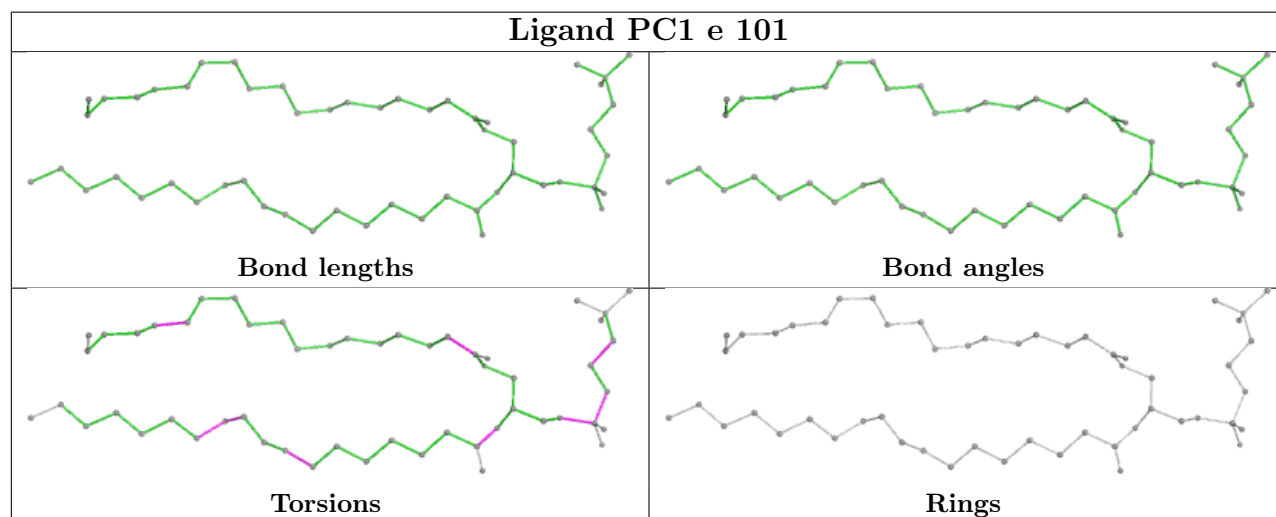
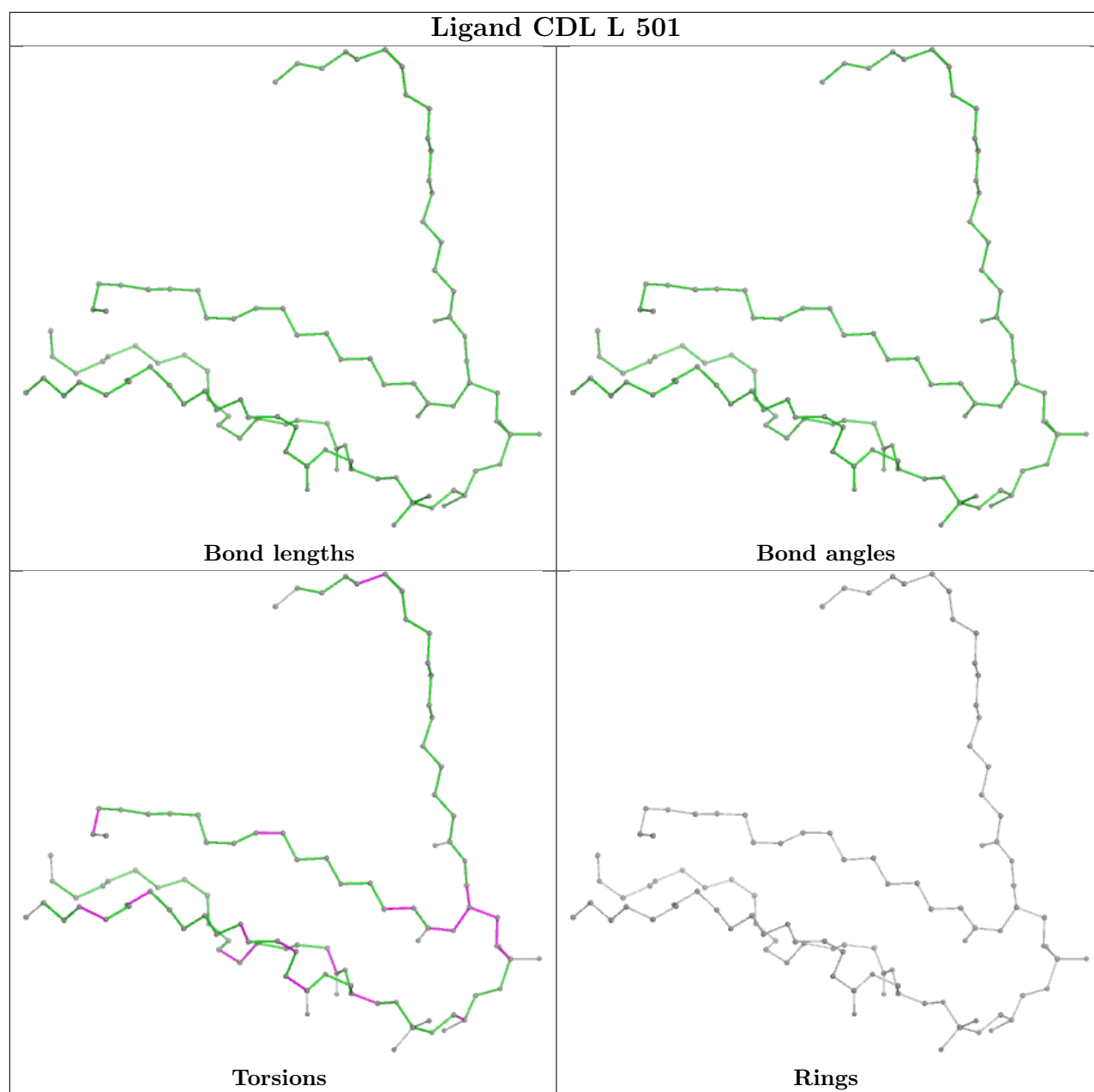


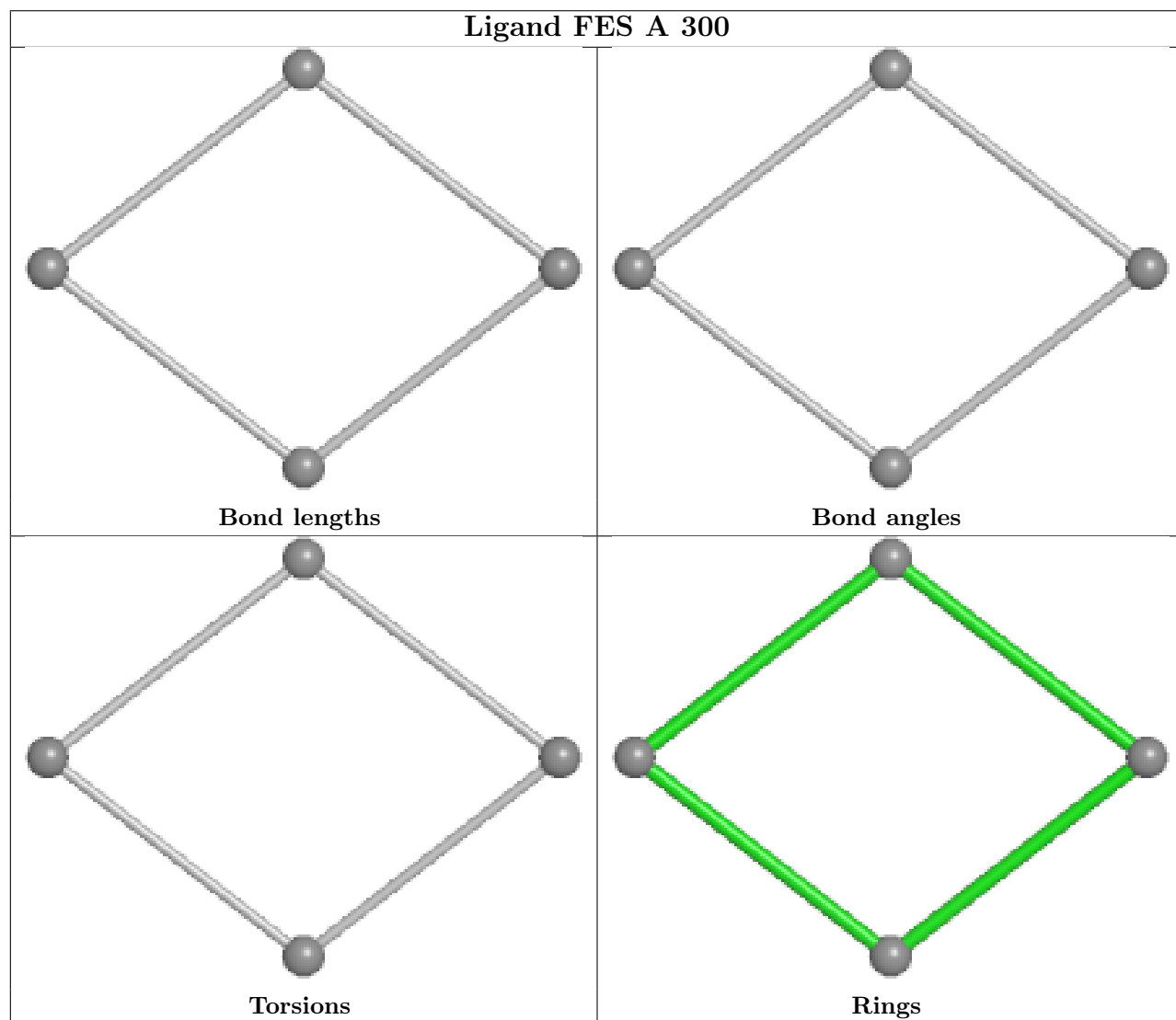
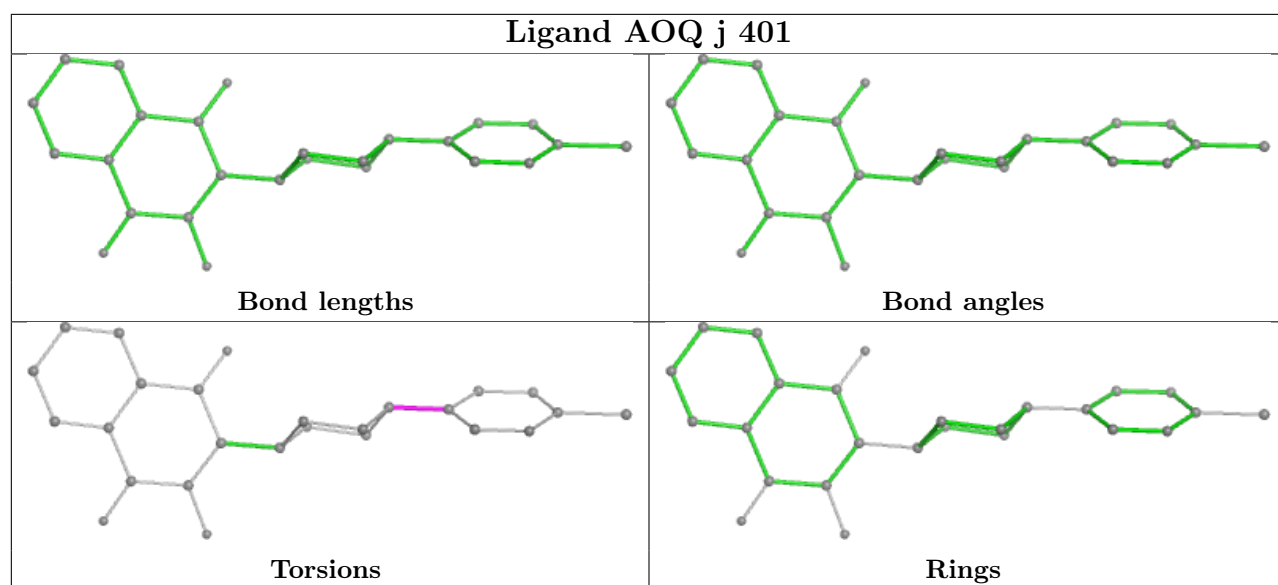


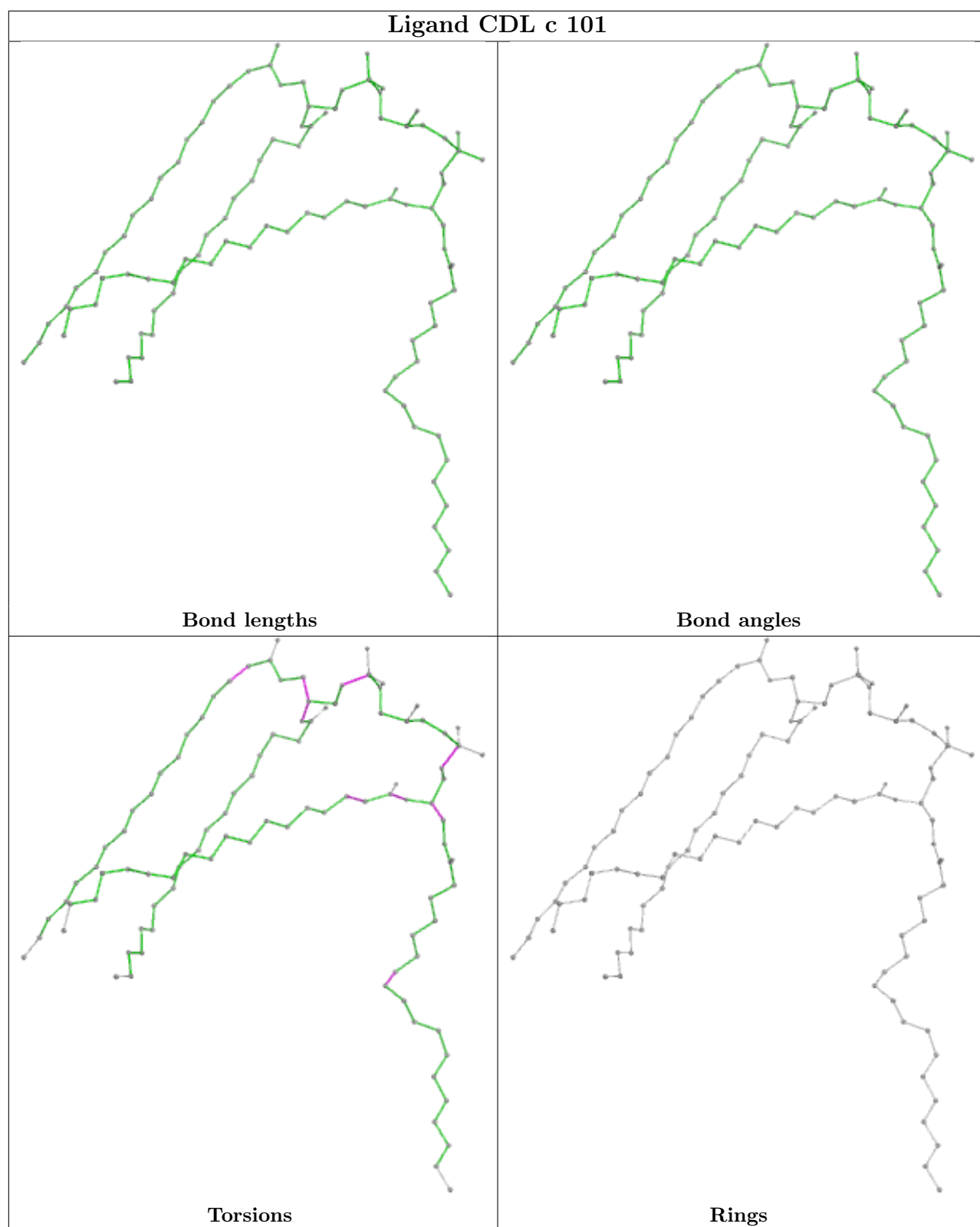


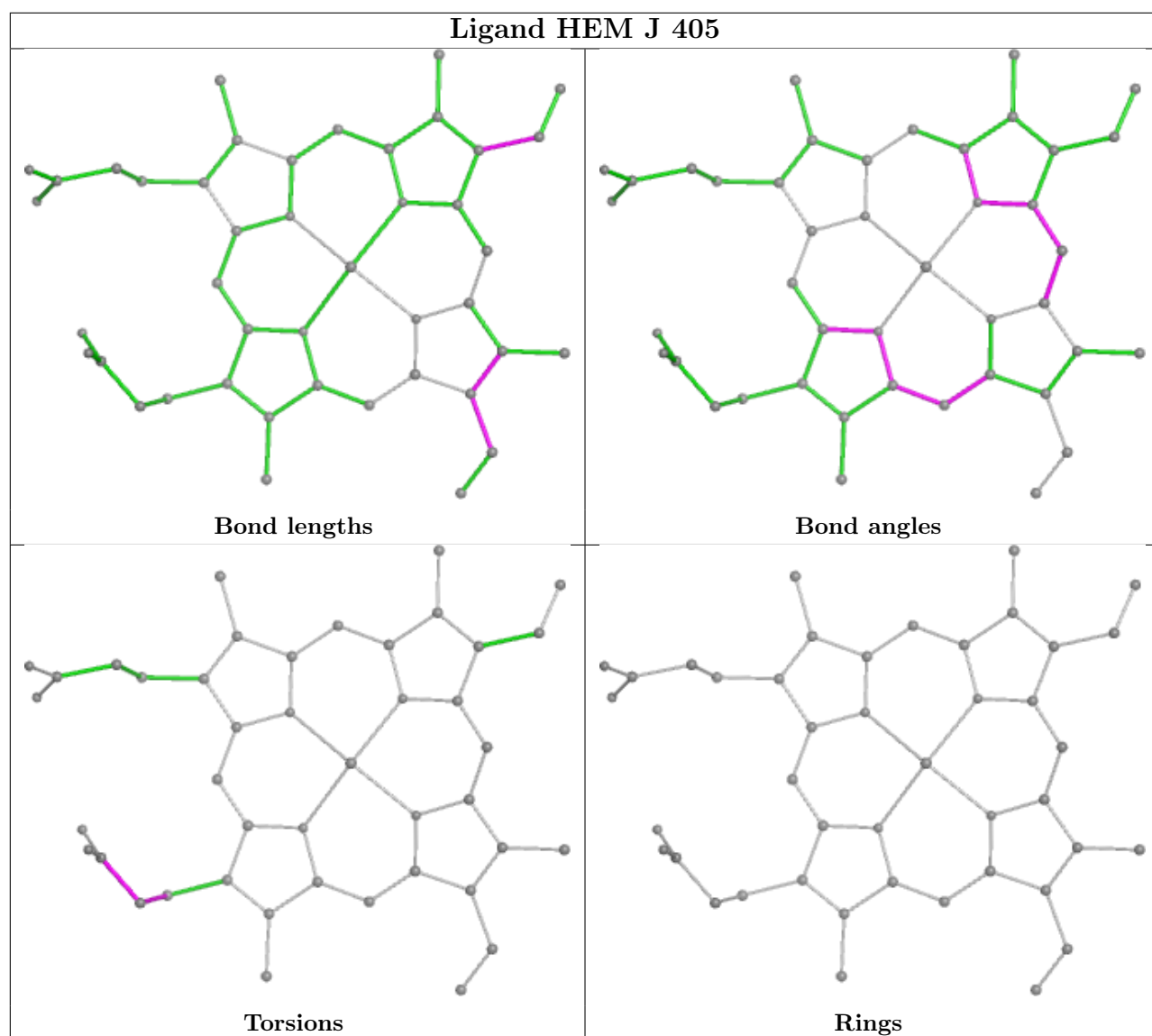


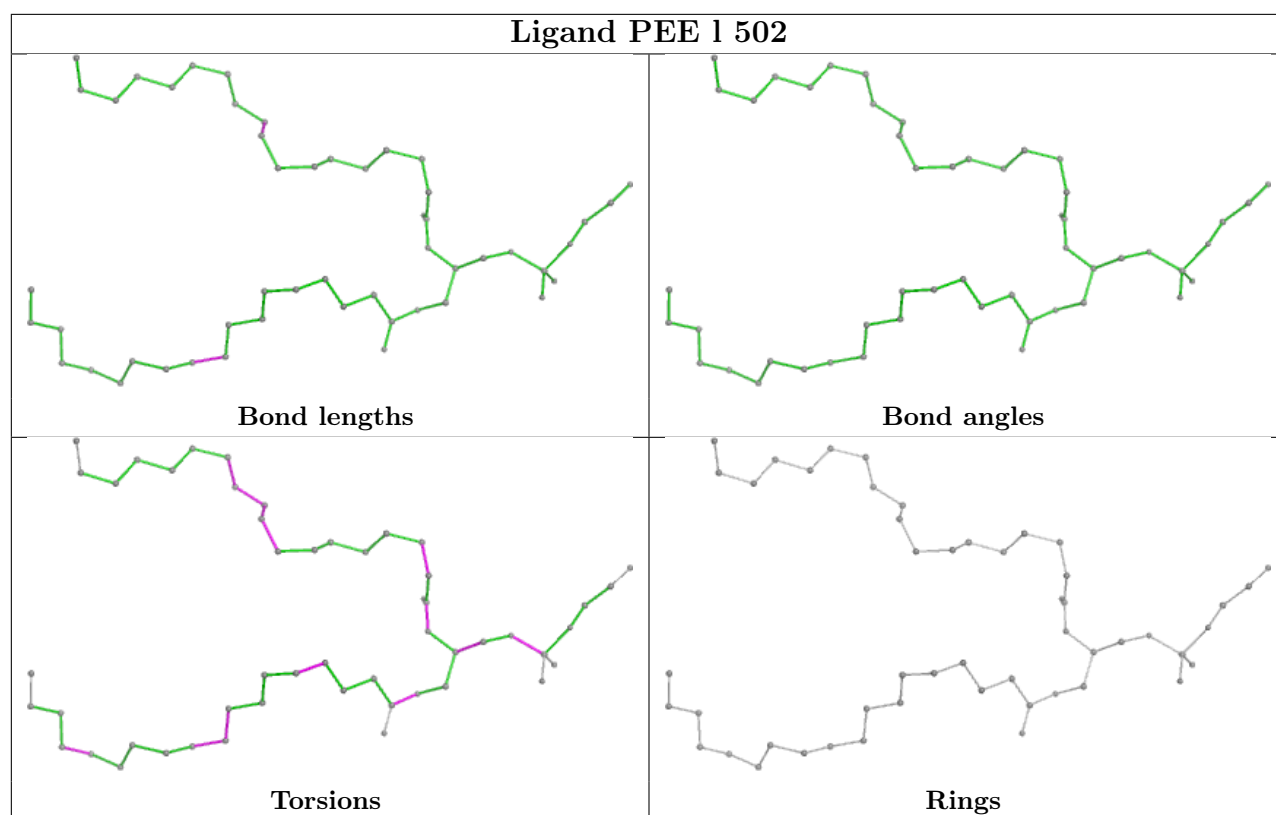












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

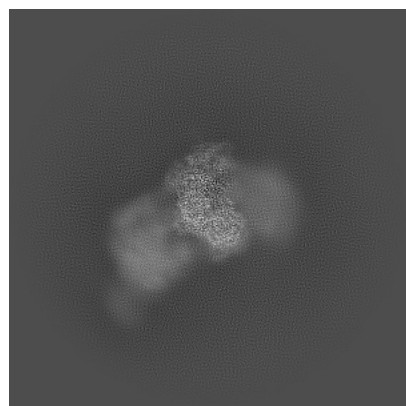
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51939. These allow visual inspection of the internal detail of the map and identification of artifacts.

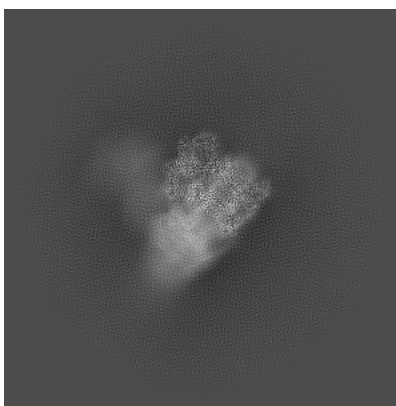
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

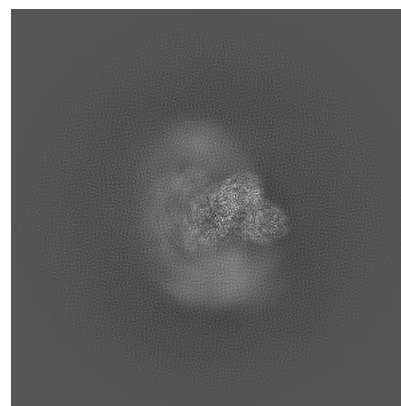
6.1.1 Primary map



X

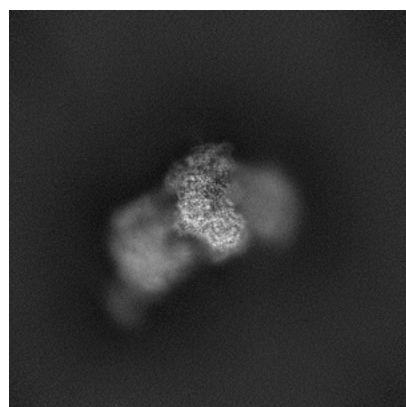


Y

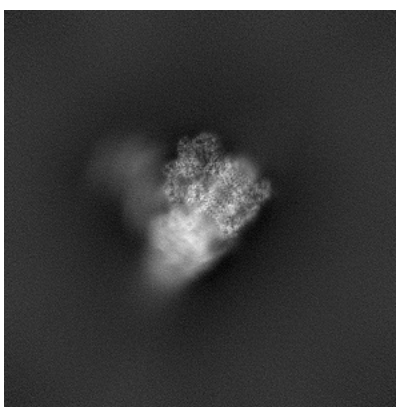


Z

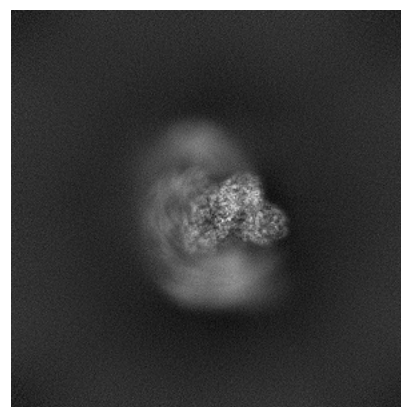
6.1.2 Raw map



X



Y

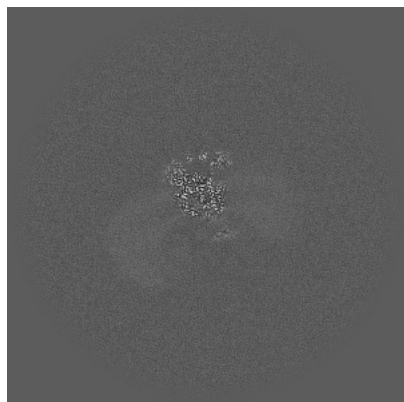


Z

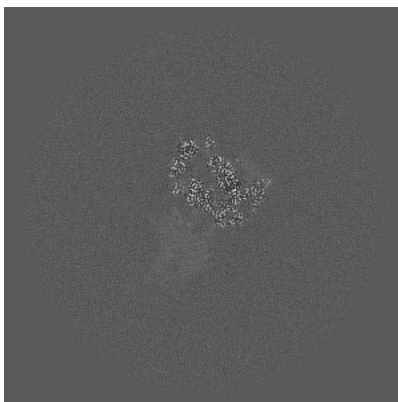
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

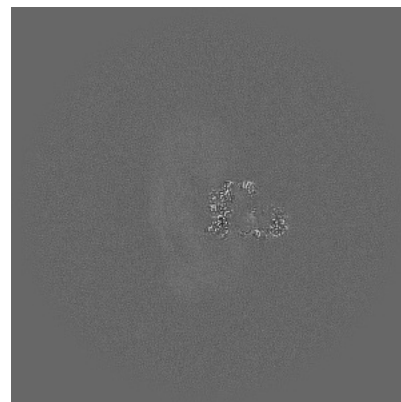
6.2.1 Primary map



X Index: 300

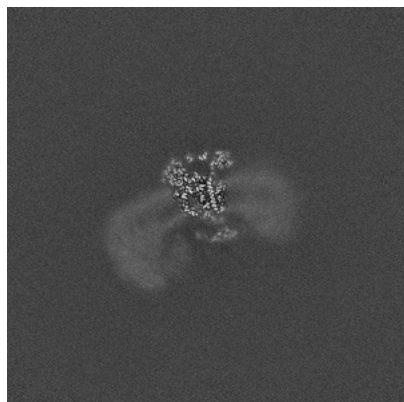


Y Index: 300

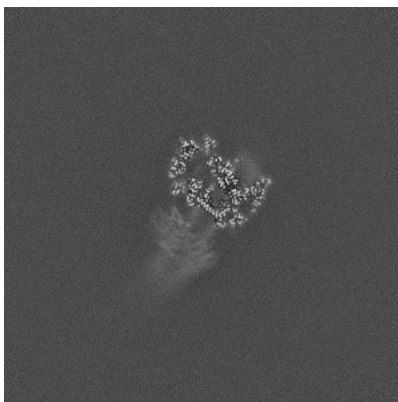


Z Index: 300

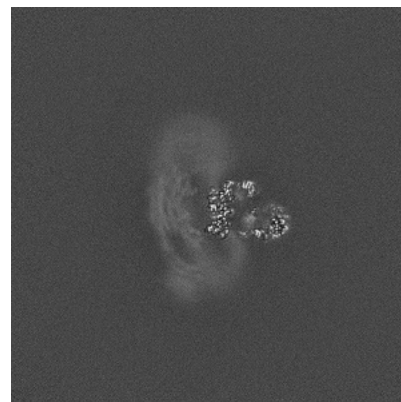
6.2.2 Raw map



X Index: 300



Y Index: 300

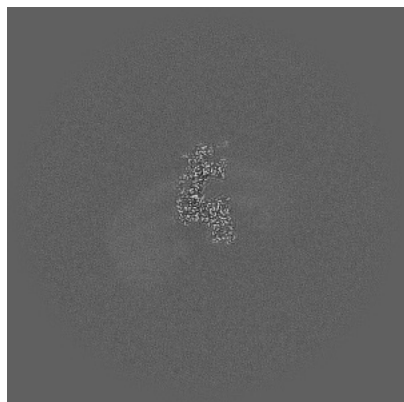


Z Index: 300

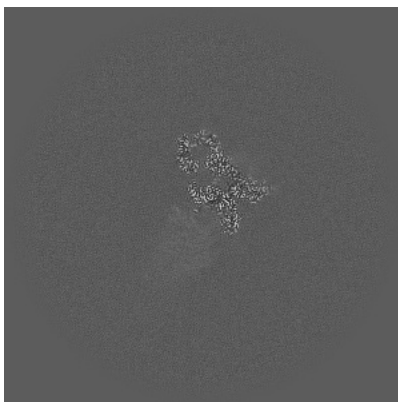
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

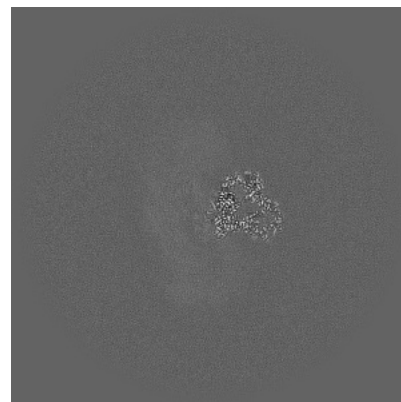
6.3.1 Primary map



X Index: 317



Y Index: 286

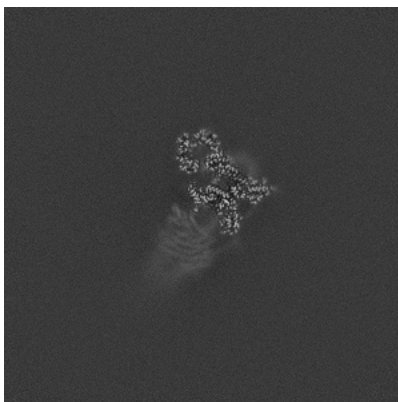


Z Index: 284

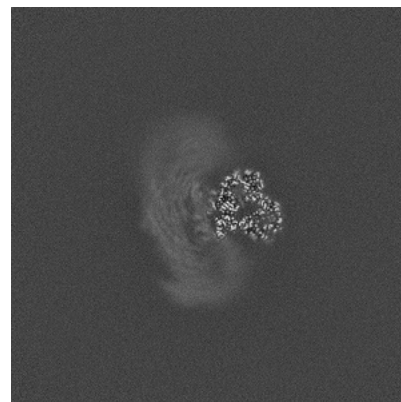
6.3.2 Raw map



X Index: 317



Y Index: 286

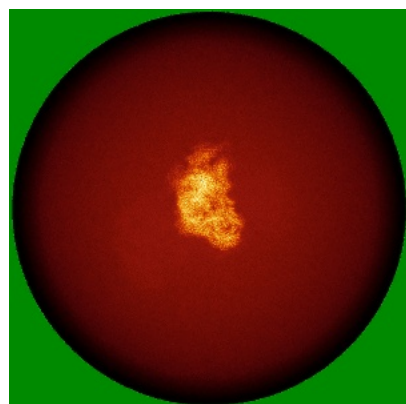


Z Index: 283

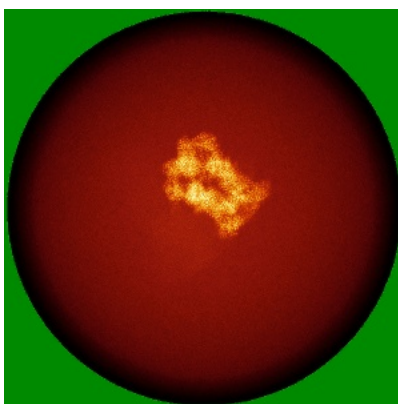
The images above show the largest variance slices of the map in three orthogonal directions.

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

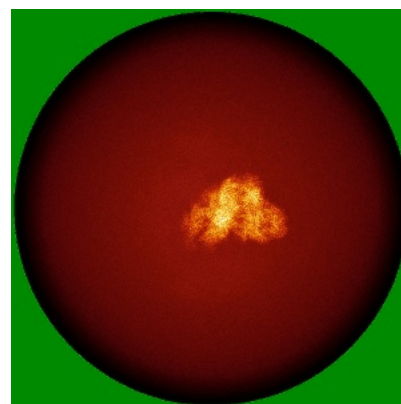
6.4.1 Primary map



X

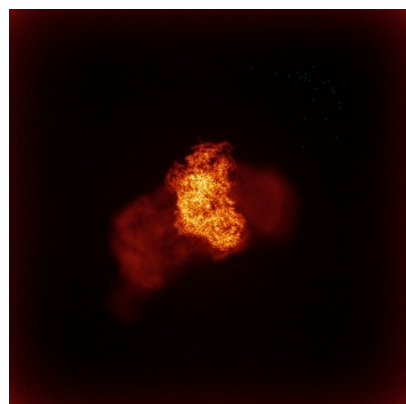


Y

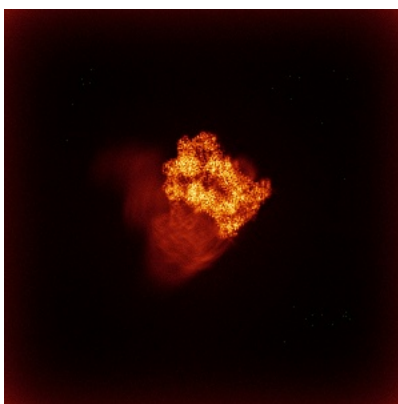


Z

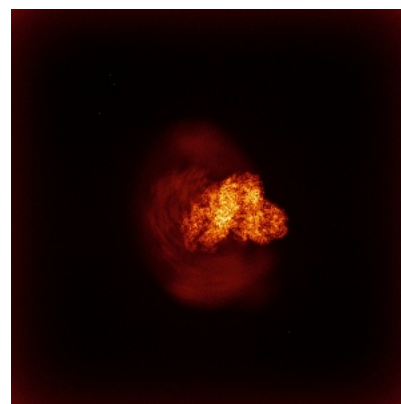
6.4.2 Raw map



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.

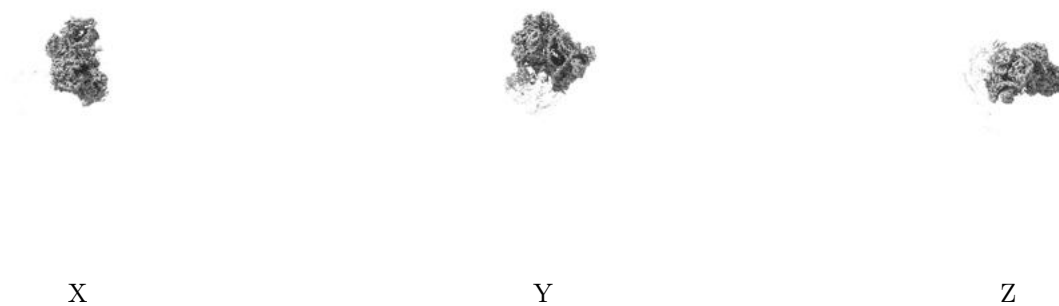
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

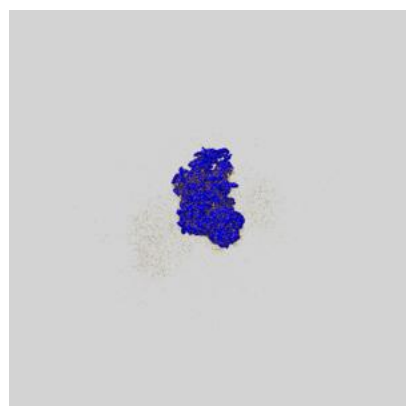
6.6 Mask visualisation [i](#)

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

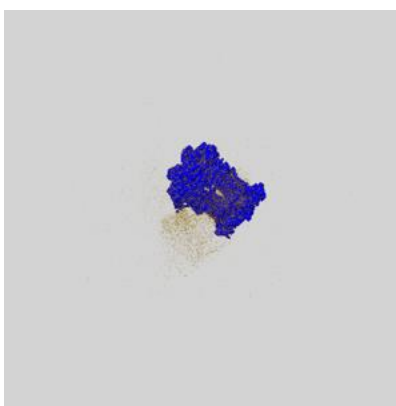
A mask typically either:

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

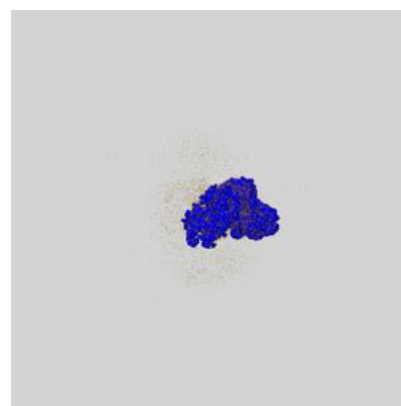
6.6.1 emd_51939_msk_1.map [i](#)



X



Y

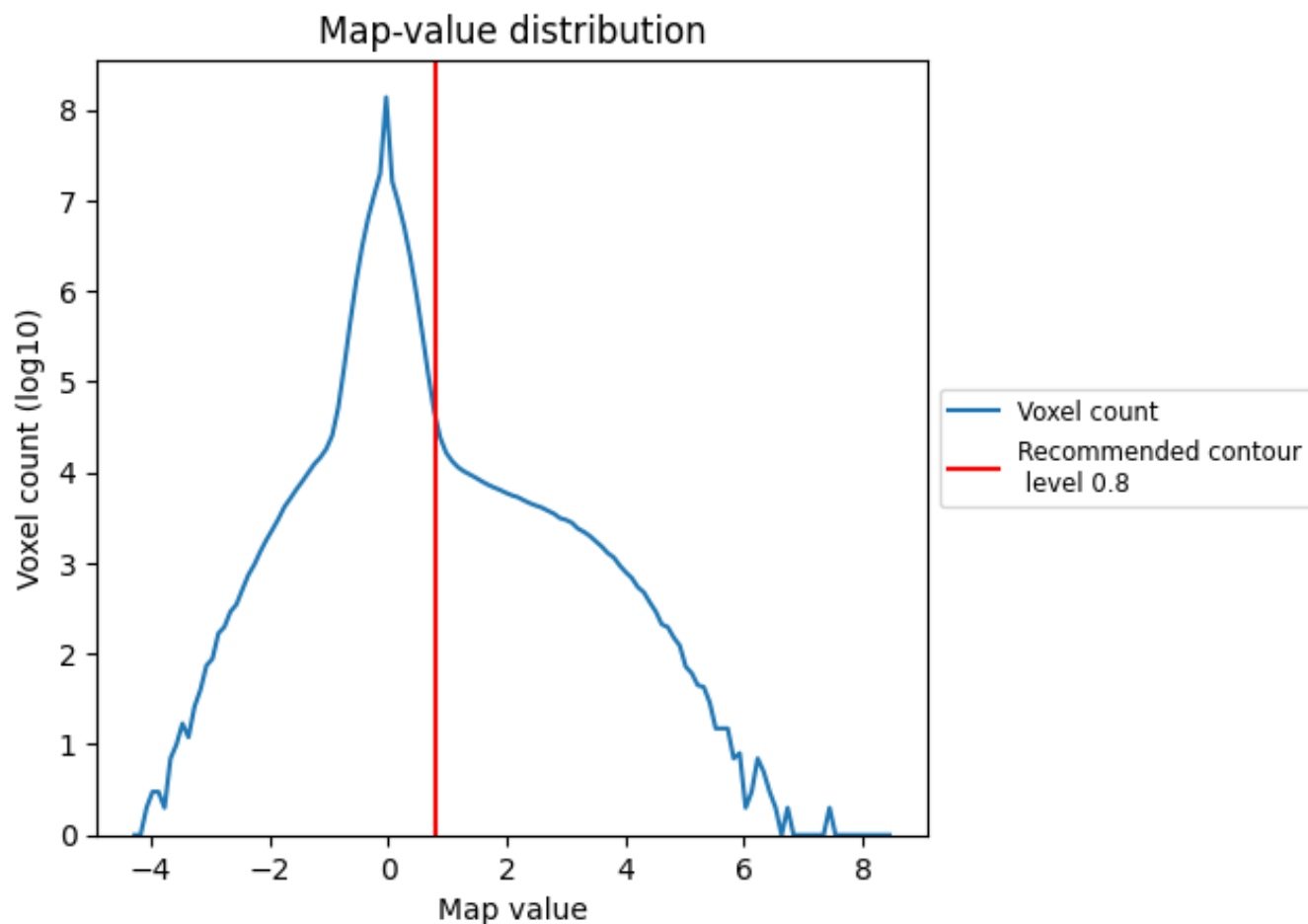


Z

7 Map analysis [i](#)

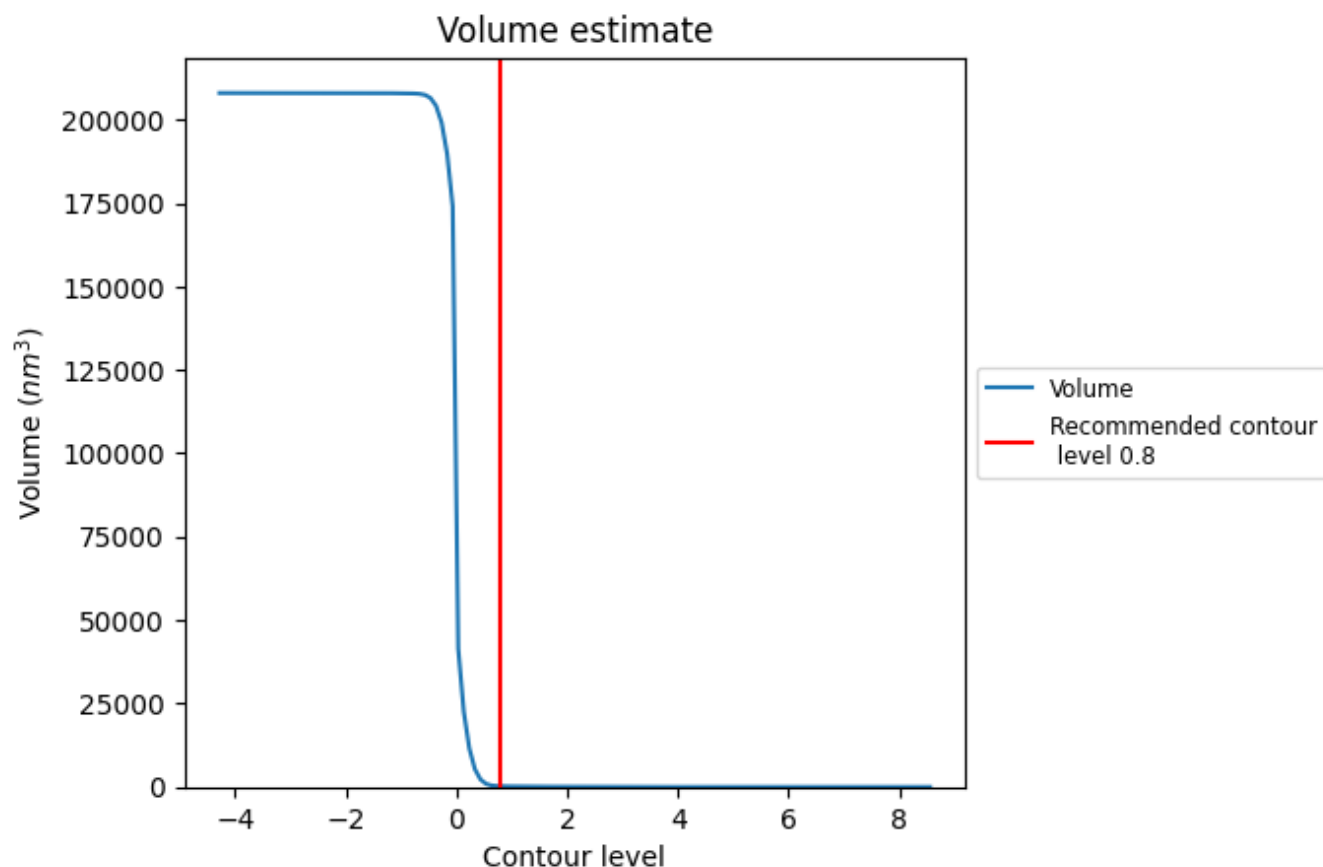
This section contains the results of statistical analysis of the map.

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.

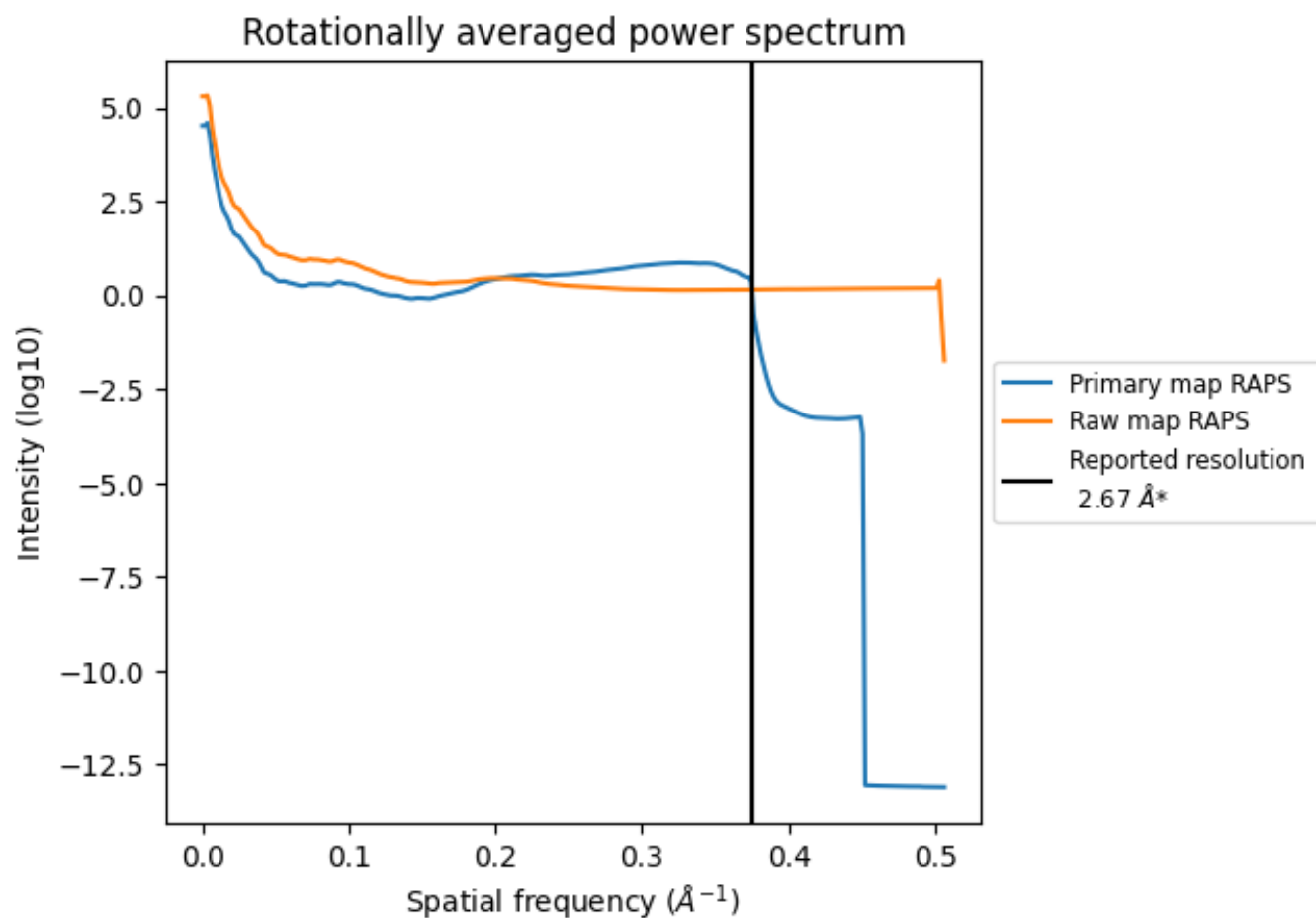
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 221 nm^3 ; this corresponds to an approximate mass of 199 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 ⓘ

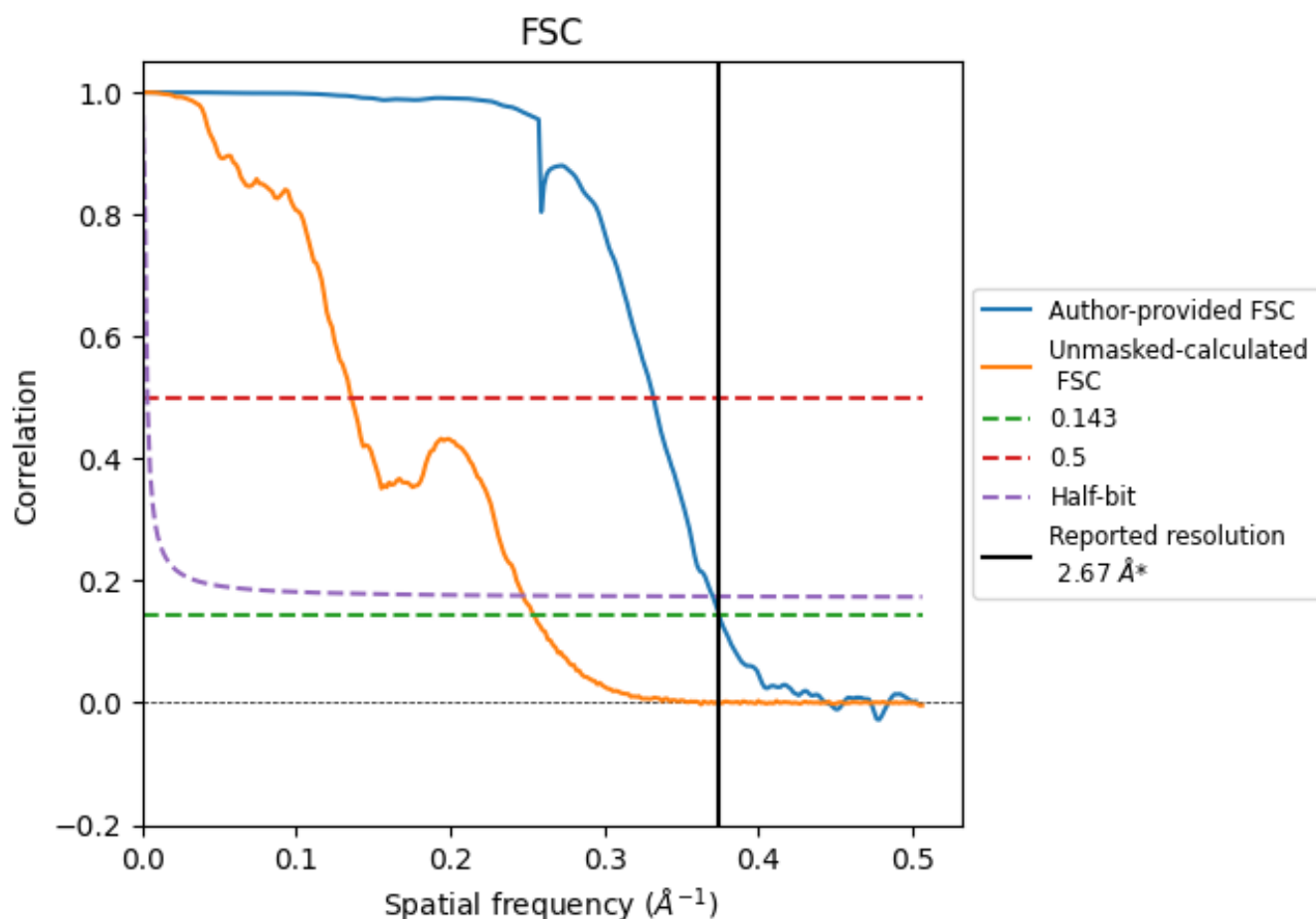


*Reported resolution corresponds to spatial frequency of 0.375 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.375 \AA^{-1}

8.2 Resolution estimates [i](#)

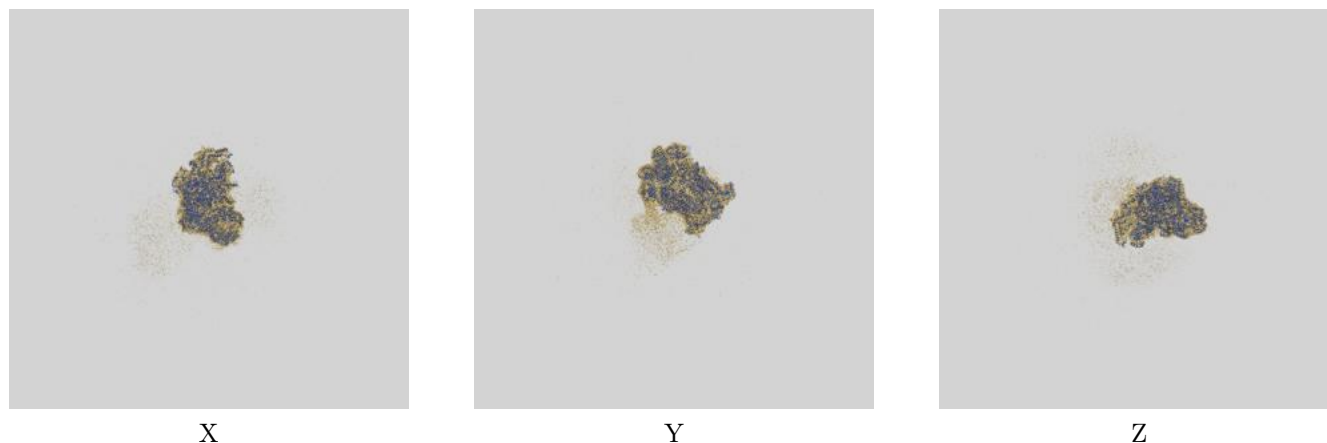
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.67	3.01	2.70
Unmasked-calculated*	3.93	7.36	4.05

*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 3.93 differs from the reported value 2.67 by more than 10 %

9 Map-model fit [i](#)

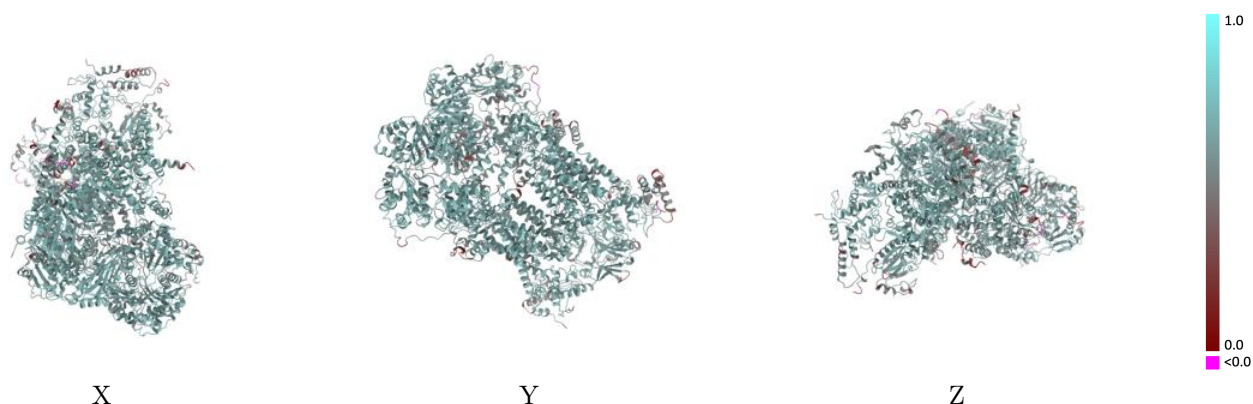
This section contains information regarding the fit between EMDB map EMD-51939 and PDB model 9H8T. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



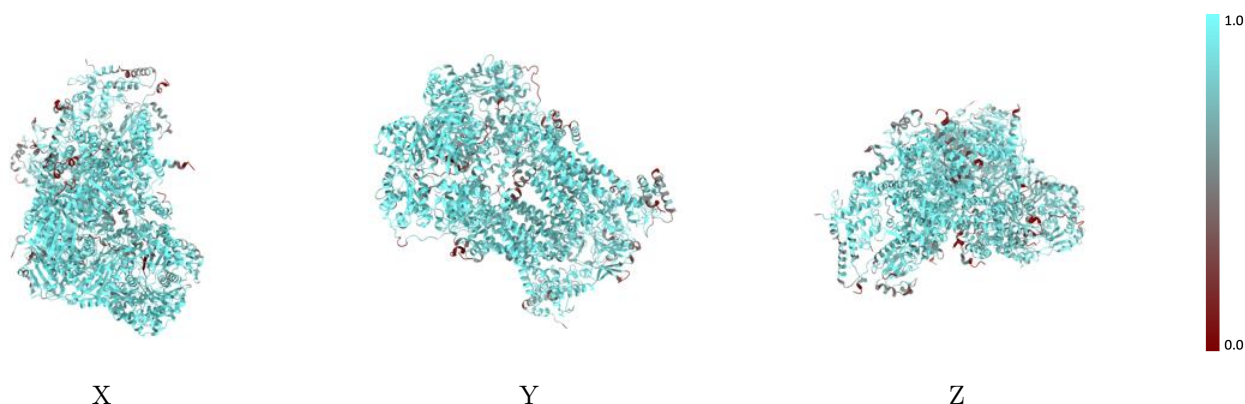
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



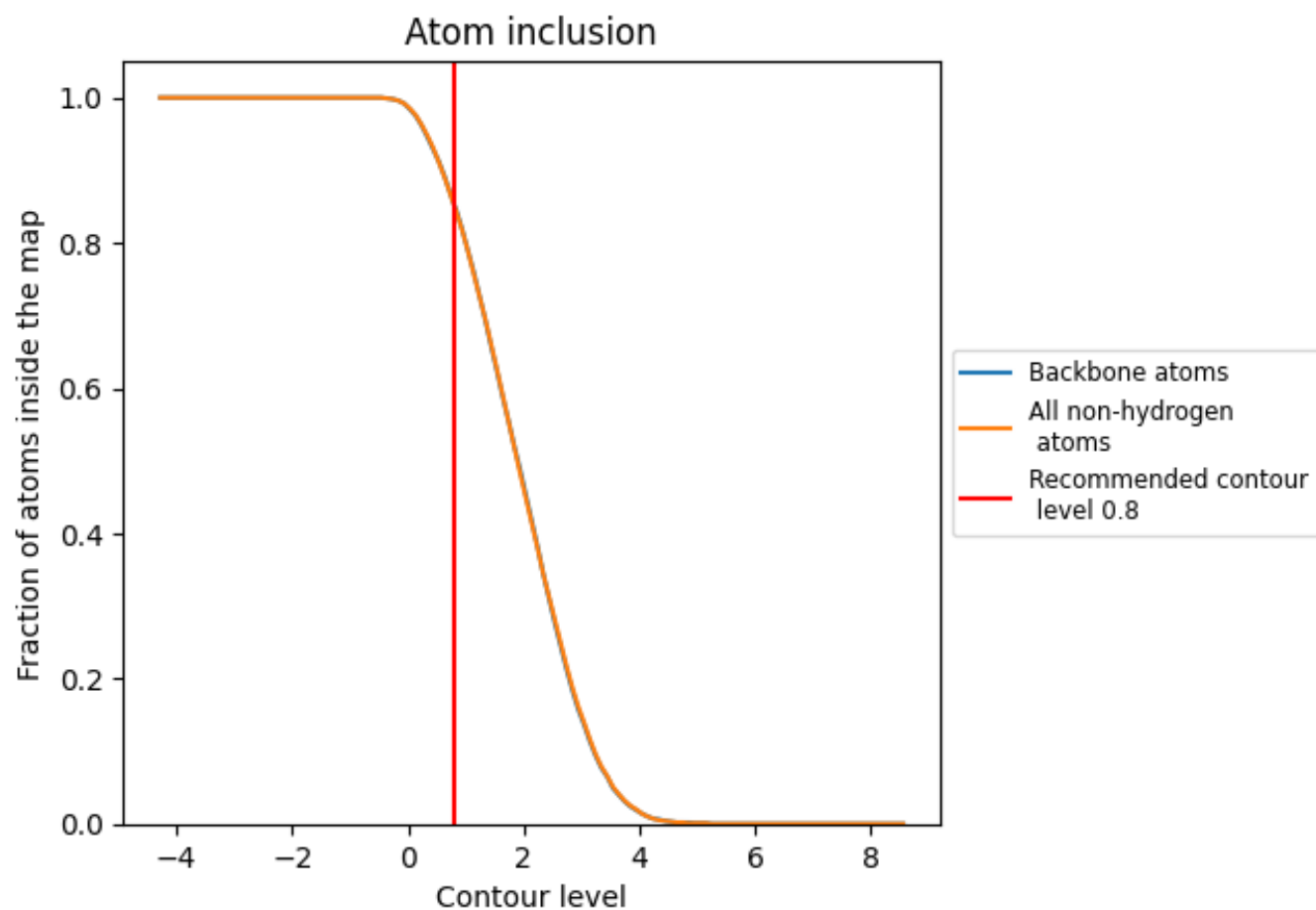
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8520	 0.5980
A	 0.7960	 0.5850
C	 0.6640	 0.5140
D	 0.9010	 0.6190
E	 0.6030	 0.5080
F	 0.6250	 0.4590
G	 0.8930	 0.6200
H	 0.6940	 0.4730
J	 0.9260	 0.6380
K	 0.9110	 0.6260
L	 0.8530	 0.5950
T	 0.4000	 0.4550
a	 0.7250	 0.5370
c	 0.7760	 0.5550
d	 0.9120	 0.6120
e	 0.8080	 0.5870
f	 0.7360	 0.5340
g	 0.9020	 0.6270
h	 0.8500	 0.5990
j	 0.9140	 0.6240
k	 0.9060	 0.6170
l	 0.8850	 0.6110

