



wwPDB EM Validation Summary Report ⓘ

May 27, 2025 – 01:51 PM JST

PDB ID : 8ZOM / pdb_00008zom
EMDB ID : EMD-60307
Title : Cryo-EM structure of pyraclostrobin-bound *Arachis hypogaea* bc1 complex
Authors : Cui, G.R.; Wang, Y.X.; Yang, G.F.
Deposited on : 2024-05-28
Resolution : 2.74 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

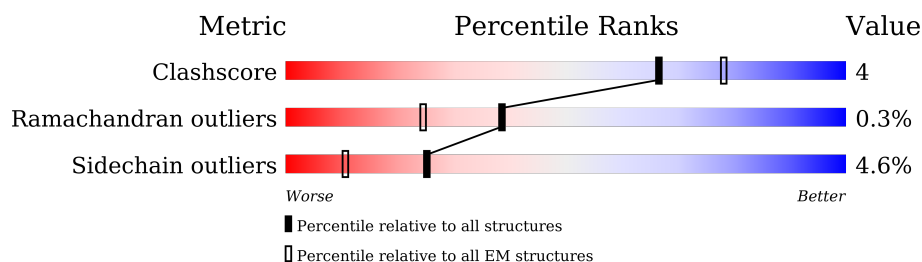
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 Å.

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





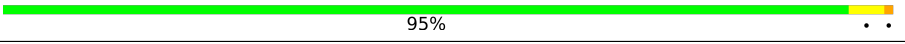
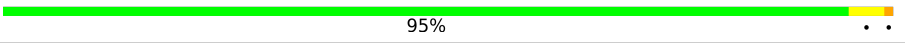
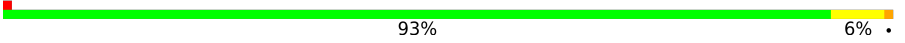



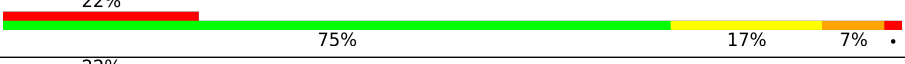



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	460	 85% 12% .
1	M	460	 86% 10% ..
2	B	487	 91% 8% .
2	N	487	 91% 7% .
3	C	386	 95% ..
3	O	386	 94% 5% .
4	D	242	 95% 5%
4	P	242	 94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	196	
5	Q	196	
6	F	117	
6	R	117	
7	G	70	
7	S	70	
8	H	64	
8	T	64	
9	J	60	
9	V	60	
10	K	29	
10	W	29	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 34466 atoms, of which 0 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 Mitochondrial-processing peptidase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	460	Total	C	N	O	S	0	0
			3502	2220	591	679	12		
1	M	460	Total	C	N	O	S	0	0
			3502	2220	591	679	12		

- Molecule 2 is a protein called Mitochondrial-processing peptidase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	487	Total	C	N	O	S	0	0
			3855	2426	676	738	15		
2	N	487	Total	C	N	O	S	0	0
			3855	2426	676	738	15		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	386	Total	C	N	O	S	0	0
			3076	2059	501	502	14		
3	O	385	Total	C	N	O	S	0	0
			3068	2055	500	499	14		

- Molecule 4 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	242	Total	C	N	O	S	0	0
			1893	1205	323	354	11		
4	P	242	Total	C	N	O	S	0	0
			1893	1205	323	354	11		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	81	GLN	ASN	conflict	UNP A0A445B1W5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	125	GLU	ASP	conflict	UNP A0A445B1W5
D	186	PRO	ARG	conflict	UNP A0A445B1W5
D	246	SER	ALA	conflict	UNP A0A445B1W5
P	81	GLN	ASN	conflict	UNP A0A445B1W5
P	125	GLU	ASP	conflict	UNP A0A445B1W5
P	186	PRO	ARG	conflict	UNP A0A445B1W5
P	246	SER	ALA	conflict	UNP A0A445B1W5

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	196	Total	C	N	O	S	0	0
			1536	986	265	280	5		
5	Q	196	Total	C	N	O	S	0	0
			1536	986	265	280	5		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	117	Total	C	N	O	S	0	0
			986	628	179	174	5		
6	R	117	Total	C	N	O	S	0	0
			986	628	179	174	5		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	70	Total	C	N	O	S	0	0
			573	378	95	98	2		
7	S	70	Total	C	N	O	S	0	0
			573	378	95	98	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	64	Total	C	N	O	S	0	0
			519	330	87	96	6		
8	T	64	Total	C	N	O	S	0	0
			519	330	87	96	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	60	Total	C	N	O	S	0	0
			486	312	88	85	1		
9	V	60	Total	C	N	O	S	0	0
			486	312	88	85	1		

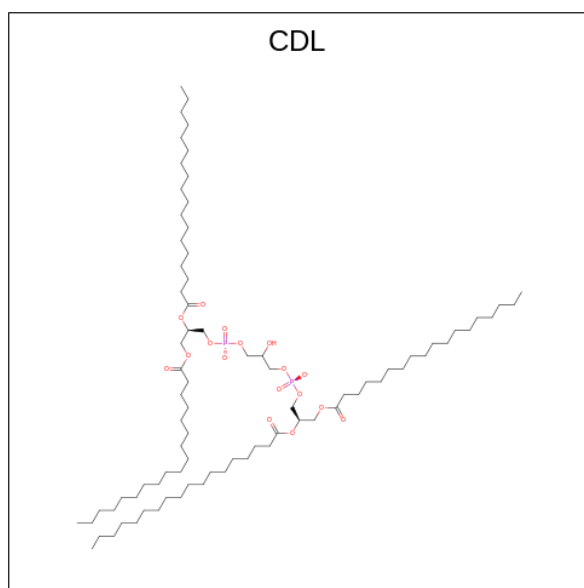
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 6.7 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	29	Total	C	N	O	S	0	0
			218	145	35	37	1		
10	W	29	Total	C	N	O	S	0	0
			218	145	35	37	1		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

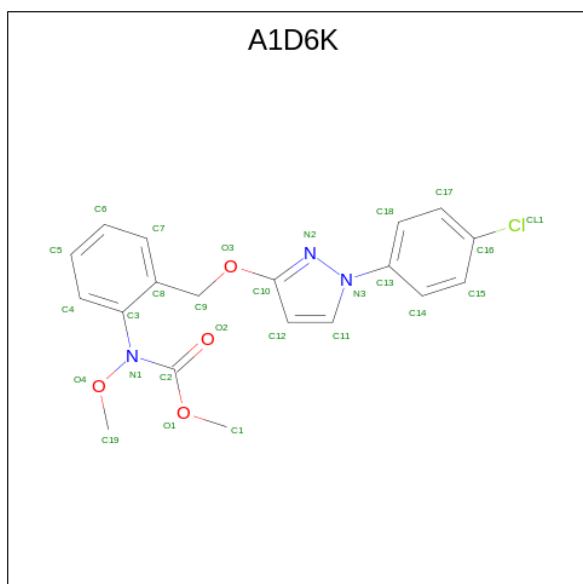
Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total	Zn	0
			1	1	
11	N	1	Total	Zn	0
			1	1	

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



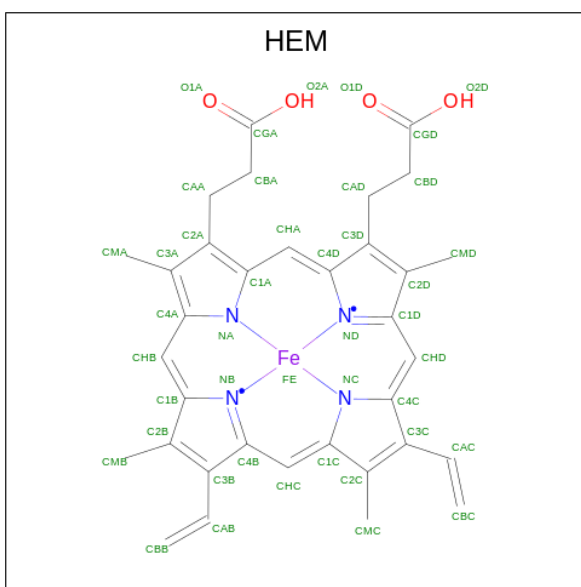
Mol	Chain	Residues	Atoms				AltConf
12	B	1	Total	C	O	P	0
			64	45	17	2	
12	C	1	Total	C	O	P	0
			64	45	17	2	
12	N	1	Total	C	O	P	0
			81	62	17	2	
12	N	1	Total	C	O	P	0
			70	51	17	2	
12	O	1	Total	C	O	P	0
			58	39	17	2	
12	O	1	Total	C	O	P	0
			63	44	17	2	

- Molecule 13 is methyl {N}-[2-[[1-(4-chlorophenyl)pyrazol-3-yl]oxymethyl]phenyl]- {N}-methoxy-carbamate (CCD ID: A1D6K) (formula: C₁₉H₁₈ClN₃O₄).



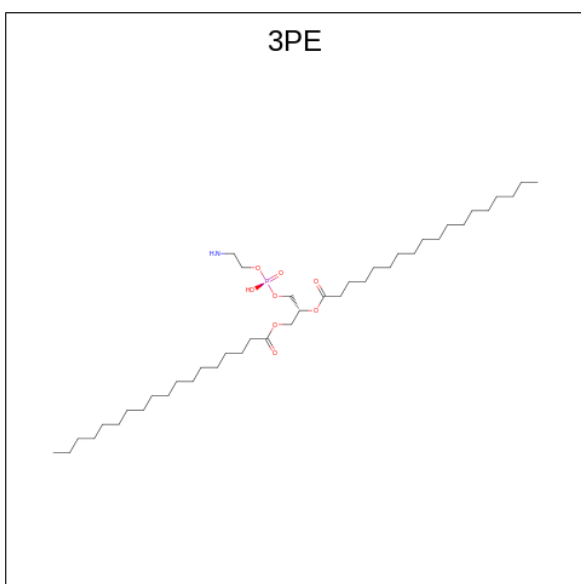
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	Cl	N	O	0
			27	19	1	3	4	
13	O	1	Total	C	Cl	N	O	0
			27	19	1	3	4	

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



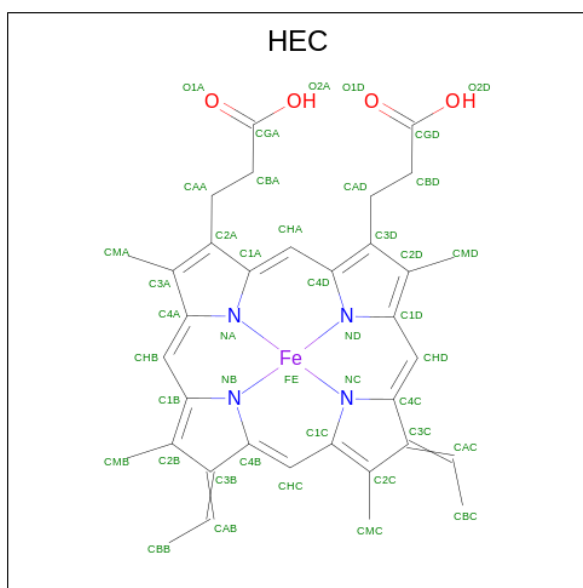
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 15 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



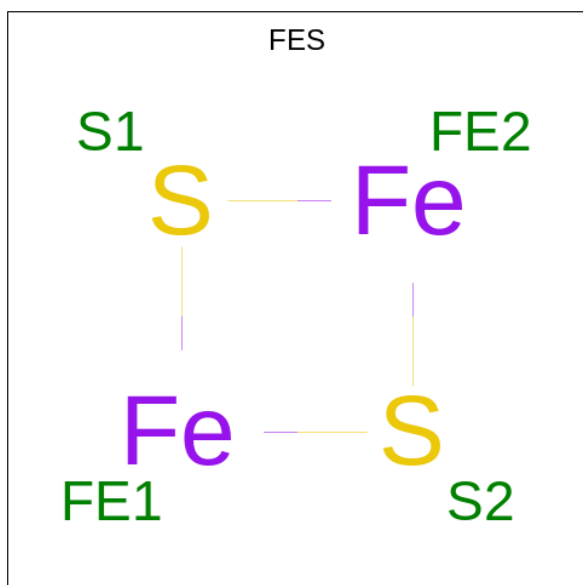
Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	C	N	O	P	0
			28	18	1	8	1	
15	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
15	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
15	C	1	Total	C	N	O	P	0
			37	27	1	8	1	
15	C	1	Total	C	N	O	P	0
			33	23	1	8	1	
15	C	1	Total	C	N	O	P	0
			34	24	1	8	1	
15	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
15	K	1	Total	C	N	O	P	0
			30	20	1	8	1	
15	O	1	Total	C	N	O	P	0
			39	29	1	8	1	
15	O	1	Total	C	N	O	P	0
			33	23	1	8	1	
15	R	1	Total	C	N	O	P	0
			38	28	1	8	1	
15	R	1	Total	C	N	O	P	0
			48	38	1	8	1	

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



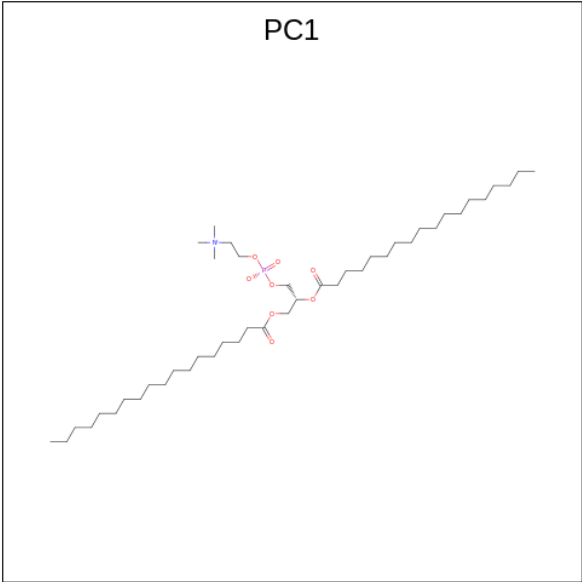
Mol	Chain	Residues	Atoms					AltConf
16	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	E	1	Total	Fe	S	0
			4	2	2	
17	Q	1	Total	Fe	S	0
			4	2	2	

- Molecule 18 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $\text{C}_{44}\text{H}_{88}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).

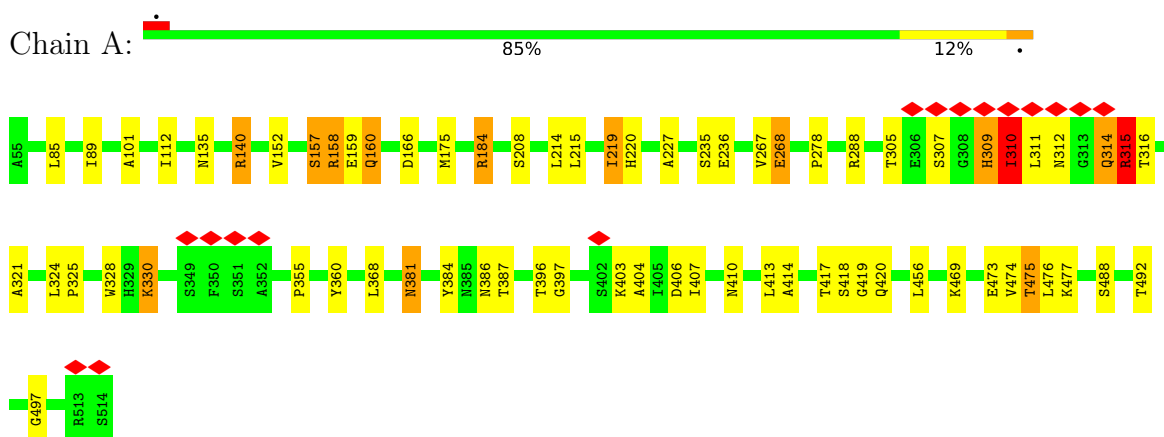


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	Q	1	25	17	1	6	1	0

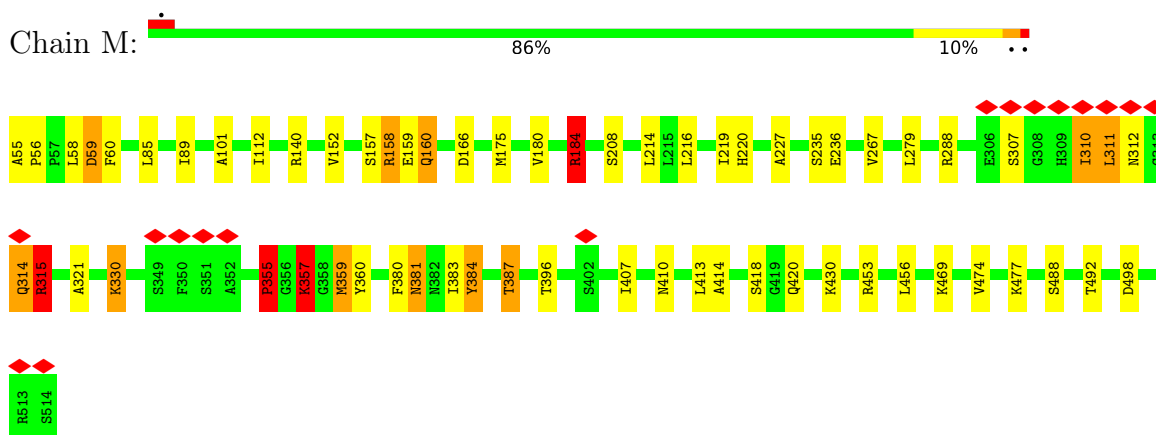
3 Residue-property plots

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

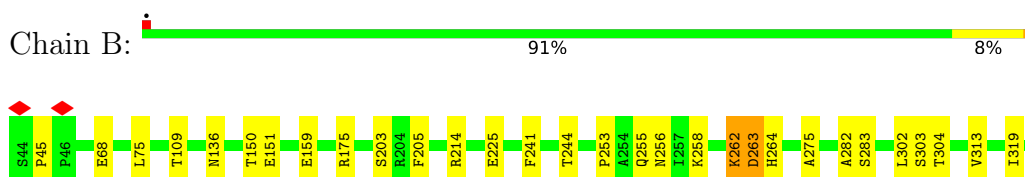
- Molecule 1: Mitochondrial-processing peptidase subunit alpha



- Molecule 1: Mitochondrial-processing peptidase subunit alpha



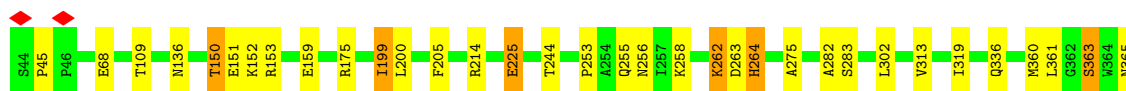
- Molecule 2: Mitochondrial-processing peptidase subunit beta





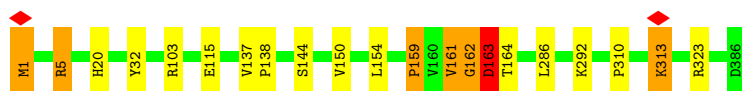
- Molecule 2: Mitochondrial-processing peptidase subunit beta

Chain N: 91% 7% .



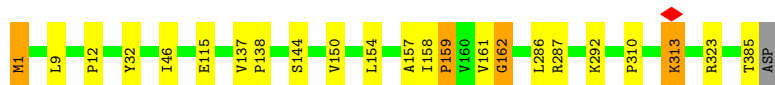
- Molecule 3: Cytochrome b

Chain C: 95% . .



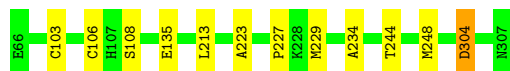
- Molecule 3: Cytochrome b

Chain O: 94% 5% .



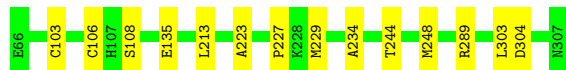
- Molecule 4: Cytochrome c domain-containing protein

Chain D: 95% 5%



- Molecule 4: Cytochrome c domain-containing protein

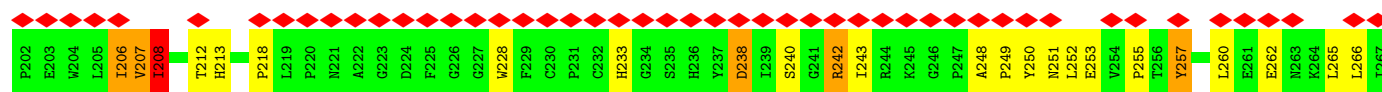
Chain P: 94% 6%



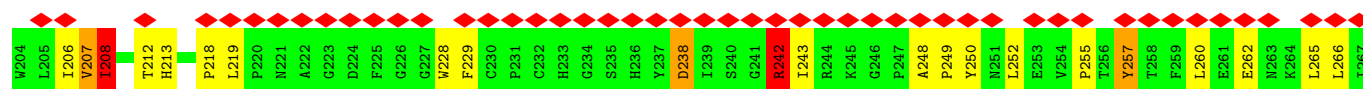
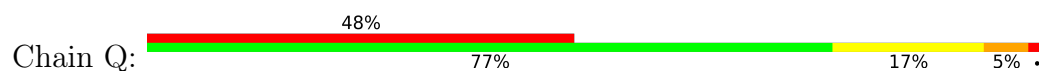
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 47% 79% 16% 5% .

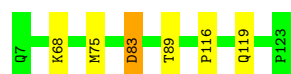




- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 6: Cytochrome b-c1 complex subunit 7



- Molecule 6: Cytochrome b-c1 complex subunit 7



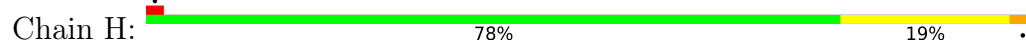
- Molecule 7: Cytochrome b-c1 complex subunit 8

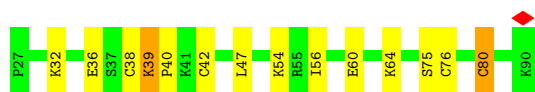


- Molecule 7: Cytochrome b-c1 complex subunit 8

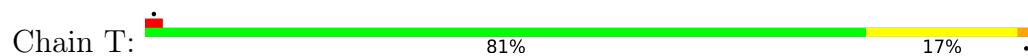


- Molecule 8: Cytochrome b-c1 complex subunit 6

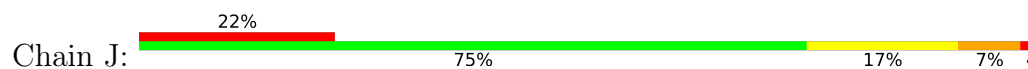




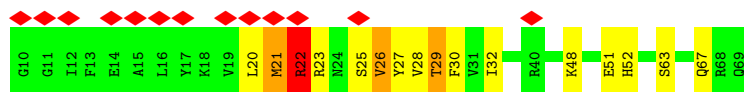
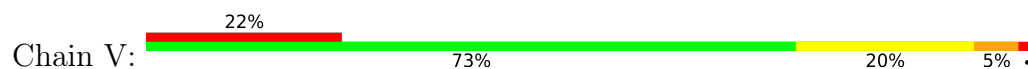
- Molecule 8: Cytochrome b-c1 complex subunit 6



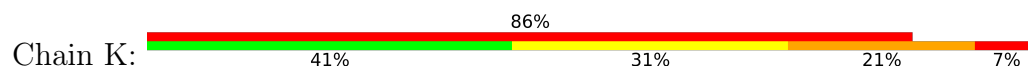
- Molecule 9: Complex III subunit 9



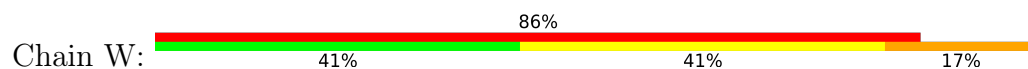
- Molecule 9: Complex III subunit 9



- Molecule 10: Ubiquinol-cytochrome c reductase complex 6.7 kDa protein



- Molecule 10: Ubiquinol-cytochrome c reductase complex 6.7 kDa protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95092	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 ($e^-/\text{\AA}^2$)	49.48	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	8.780	Depositor
Minimum map value	-4.329	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.230	Depositor
Recommended contour level	0.586	Depositor
Map size (Å)	307.19998, 307.19998, 307.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9599999, 0.9599999, 0.9599999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, CDL, HEM, FES, PC1, ZN, 3PE, A1D6K

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	0.59	7/3574 (0.2%)	0.85	5/4860 (0.1%)
1	M	0.65	13/3574 (0.4%)	0.92	14/4860 (0.3%)
2	B	0.56	6/3933 (0.2%)	0.74	10/5332 (0.2%)
2	N	0.57	6/3933 (0.2%)	0.80	12/5332 (0.2%)
3	C	0.51	2/3194 (0.1%)	0.80	8/4379 (0.2%)
3	O	0.51	1/3186 (0.0%)	0.77	5/4368 (0.1%)
4	D	0.47	0/1946	0.62	1/2644 (0.0%)
4	P	0.52	3/1946 (0.2%)	0.70	7/2644 (0.3%)
5	E	0.48	1/1576 (0.1%)	0.84	6/2144 (0.3%)
5	Q	0.56	1/1576 (0.1%)	0.94	7/2144 (0.3%)
6	F	0.49	0/1008	0.69	1/1352 (0.1%)
6	R	0.49	0/1008	0.72	1/1352 (0.1%)
7	G	0.56	0/591	0.87	3/799 (0.4%)
7	S	0.56	0/591	0.87	3/799 (0.4%)
8	H	0.44	0/529	0.79	2/705 (0.3%)
8	T	0.41	0/529	0.73	1/705 (0.1%)
9	J	0.58	0/496	1.20	4/666 (0.6%)
9	V	0.60	0/496	1.27	9/666 (1.4%)
10	K	0.99	0/226	2.02	9/310 (2.9%)
10	W	0.67	0/226	1.80	7/310 (2.3%)
All	All	0.55	40/34138 (0.1%)	0.84	115/46371 (0.2%)

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	5
1	M	0	5
2	B	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	4
3	C	0	2
3	O	0	1
5	E	0	2
5	Q	0	4
9	J	0	2
9	V	0	1
All	All	0	29

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	303	LEU	C-N	11.20	1.48	1.33
1	M	384	TYR	CA-C	-9.97	1.43	1.53
1	A	386	ASN	C-O	-9.35	1.12	1.24
2	N	363	SER	C-O	-9.22	1.12	1.23
2	B	363	SER	C-O	-9.13	1.12	1.24

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	22	ARG	N-CA-C	-12.63	96.58	112.88
2	N	225	GLU	N-CA-C	-12.51	95.64	114.16
6	R	83	ASP	CB-CA-C	-11.73	91.08	110.79
10	K	33	ILE	CA-C-N	-10.50	112.61	122.37
10	K	33	ILE	C-N-CA	-10.50	112.61	122.37

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	ARG	Sidechain
1	A	184	ARG	Sidechain
1	A	288	ARG	Sidechain
1	A	315	ARG	Sidechain
1	A	355	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3502	0	3495	38	0
1	M	3502	0	3495	29	0
2	B	3855	0	3817	20	0
2	N	3855	0	3817	24	0
3	C	3076	0	3058	8	0
3	O	3068	0	3054	14	0
4	D	1893	0	1827	5	0
4	P	1893	0	1827	6	0
5	E	1536	0	1541	24	0
5	Q	1536	0	1540	27	0
6	F	986	0	997	5	0
6	R	986	0	997	5	0
7	G	573	0	585	1	0
7	S	573	0	585	3	0
8	H	519	0	519	3	0
8	T	519	0	521	3	0
9	J	486	0	481	8	0
9	V	486	0	481	6	0
10	K	218	0	212	16	0
10	W	218	0	212	15	0
11	B	1	0	0	0	0
11	N	1	0	0	0	0
12	B	64	0	72	3	0
12	C	64	0	72	3	0
12	N	151	0	199	6	0
12	O	121	0	130	6	0
13	C	27	0	0	0	0
13	O	27	0	0	0	0
14	C	86	0	60	1	0
14	O	86	0	60	0	0
15	C	251	0	326	12	0
15	K	30	0	34	1	0
15	O	72	0	92	0	0
15	R	86	0	123	5	0
16	D	43	0	32	2	0
16	P	43	0	32	2	0
17	E	4	0	0	0	0
17	Q	4	0	0	0	0
18	Q	25	0	31	3	0
All	All	34466	0	34324	254	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 4.

The worst 5 of 254 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)
9:V:20:LEU:HG	9:V:26:VAL:HB	1.42	0.97
5:Q:207:VAL:HG12	5:Q:255:PRO:HD2	1.54	0.90
5:E:207:VAL:HG12	5:E:255:PRO:HD2	1.55	0.89
9:J:36:PHE:HZ	10:K:36:TRP:HA	1.39	0.87
2:N:205:PHE:HB2	2:N:262:LYS:HG3	1.64	0.79

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	458/460 (100%)	420 (92%)	36 (8%)	2 (0%)	30	48
1	M	458/460 (100%)	422 (92%)	36 (8%)	0	100	100
2	B	485/487 (100%)	463 (96%)	21 (4%)	1 (0%)	44	63
2	N	485/487 (100%)	463 (96%)	21 (4%)	1 (0%)	44	63
3	C	384/386 (100%)	368 (96%)	13 (3%)	3 (1%)	16	30
3	O	383/386 (99%)	369 (96%)	12 (3%)	2 (0%)	25	41
4	D	240/242 (99%)	230 (96%)	9 (4%)	1 (0%)	30	48
4	P	240/242 (99%)	230 (96%)	10 (4%)	0	100	100
5	E	194/196 (99%)	173 (89%)	20 (10%)	1 (0%)	25	41
5	Q	194/196 (99%)	172 (89%)	20 (10%)	2 (1%)	13	23
6	F	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
6	R	115/117 (98%)	111 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
7	S	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
8	H	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
8	T	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
9	J	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
9	V	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	7	13
10	K	27/29 (93%)	22 (82%)	5 (18%)	0	100	100
10	W	27/29 (93%)	23 (85%)	4 (15%)	0	100	100
All	All	4181/4222 (99%)	3919 (94%)	248 (6%)	14 (0%)	38	55

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	159	PRO
3	C	163	ASP
3	O	159	PRO
3	O	162	GLY
5	Q	169	PHE

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	384/384 (100%)	364 (95%)	20 (5%)	19	35
1	M	384/384 (100%)	363 (94%)	21 (6%)	18	32
2	B	409/409 (100%)	402 (98%)	7 (2%)	56	73
2	N	409/409 (100%)	398 (97%)	11 (3%)	40	60
3	C	331/331 (100%)	327 (99%)	4 (1%)	67	82
3	O	330/331 (100%)	327 (99%)	3 (1%)	75	86
4	D	197/197 (100%)	194 (98%)	3 (2%)	60	76
4	P	197/197 (100%)	194 (98%)	3 (2%)	60	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	169/169 (100%)	153 (90%)	16 (10%)	7	13
5	Q	169/169 (100%)	151 (89%)	18 (11%)	5	9
6	F	104/104 (100%)	103 (99%)	1 (1%)	73	84
6	R	104/104 (100%)	103 (99%)	1 (1%)	73	84
7	G	63/63 (100%)	61 (97%)	2 (3%)	34	55
7	S	63/63 (100%)	61 (97%)	2 (3%)	34	55
8	H	58/58 (100%)	50 (86%)	8 (14%)	3	4
8	T	58/58 (100%)	50 (86%)	8 (14%)	3	4
9	J	49/49 (100%)	39 (80%)	10 (20%)	1	1
9	V	49/49 (100%)	41 (84%)	8 (16%)	2	2
10	K	19/19 (100%)	9 (47%)	10 (53%)	0	0
10	W	19/19 (100%)	11 (58%)	8 (42%)	0	0
All	All	3565/3566 (100%)	3401 (95%)	164 (5%)	25	40

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	O	313	LYS
8	T	43	VAL
5	Q	146	LEU
5	Q	208	ILE
9	V	23	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	212	GLN
2	N	136	ASN
9	V	24	ASN
1	M	220	HIS
1	M	369	ASN

5.3.3 RNA ⓘ

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 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	$\# Z > 2$
15	3PE	C	404	-	27,27,50	1.12	4 (14%)	30,32,55	1.24	2 (6%)
15	3PE	K	101	-	29,29,50	1.12	3 (10%)	32,34,55	1.17	2 (6%)
13	A1D6K	C	401	-	26,29,29	0.87	2 (7%)	27,39,39	1.90	1 (3%)
15	3PE	C	405	-	31,31,50	1.06	3 (9%)	34,36,55	1.23	2 (5%)
15	3PE	C	407	-	36,36,50	1.00	4 (11%)	39,41,55	1.25	3 (7%)
14	HEM	O	403	3	41,50,50	1.51	4 (9%)	45,82,82	2.04	14 (31%)
12	CDL	N	602	-	80,80,99	0.32	0	86,92,111	0.49	1 (1%)
15	3PE	C	408	-	32,32,50	1.06	4 (12%)	35,37,55	1.18	2 (5%)
14	HEM	O	402	3	41,50,50	1.41	4 (9%)	45,82,82	1.55	7 (15%)
12	CDL	O	404	-	57,57,99	1.13	8 (14%)	63,69,111	1.25	5 (7%)
18	PC1	Q	302	-	24,24,53	1.09	1 (4%)	29,30,61	0.92	1 (3%)
14	HEM	C	403	3	41,50,50	1.47	4 (9%)	45,82,82	1.57	10 (22%)
13	A1D6K	O	401	-	26,29,29	0.86	1 (3%)	27,39,39	1.91	1 (3%)
12	CDL	C	410	-	63,63,99	1.09	6 (9%)	69,75,111	1.29	5 (7%)
15	3PE	C	409	-	33,33,50	1.03	4 (12%)	36,38,55	1.11	2 (5%)
15	3PE	O	405	-	38,38,50	0.97	3 (7%)	41,43,55	1.16	2 (4%)
14	HEM	C	402	3	41,50,50	1.40	4 (9%)	45,82,82	1.55	7 (15%)
17	FES	Q	301	-	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	HEC	D	501	4	32,50,50	2.20	3 (9%)	24,82,82	1.64	4 (16%)
15	3PE	C	411	-	35,35,50	1.04	4 (11%)	38,40,55	1.21	2 (5%)
12	CDL	N	603	-	69,69,99	1.05	8 (11%)	75,81,111	1.14	4 (5%)
15	3PE	R	201	-	37,37,50	1.00	4 (10%)	40,42,55	1.14	2 (5%)
12	CDL	B	602	-	63,63,99	1.09	8 (12%)	69,75,111	1.13	4 (5%)
15	3PE	C	406	-	50,50,50	0.86	2 (4%)	53,55,55	0.95	2 (3%)
15	3PE	O	406	-	32,32,50	1.05	4 (12%)	35,37,55	1.20	1 (2%)
16	HEC	P	401	4	32,50,50	2.18	3 (9%)	24,82,82	1.61	4 (16%)
15	3PE	R	202	-	47,47,50	0.88	3 (6%)	50,52,55	1.11	2 (4%)
17	FES	E	301	-	0,4,4	-	-	-	-	-
12	CDL	O	407	-	62,62,99	0.40	0	68,74,111	0.61	1 (1%)

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
15	3PE	C	404	-	-	21/31/31/54	-
15	3PE	K	101	-	-	12/33/33/54	-
13	A1D6K	C	401	-	-	4/16/21/21	0/3/3/3
15	3PE	C	405	-	-	21/35/35/54	-
15	3PE	C	407	-	-	20/40/40/54	-
14	HEM	O	403	3	-	5/12/54/54	-
12	CDL	N	602	-	-	62/91/91/110	-
15	3PE	C	408	-	-	22/36/36/54	-
14	HEM	O	402	3	-	5/12/54/54	-
12	CDL	O	404	-	-	37/68/68/110	-
18	PC1	Q	302	-	-	14/25/25/57	-
14	HEM	C	403	3	-	3/12/54/54	-
13	A1D6K	O	401	-	-	4/16/21/21	0/3/3/3
12	CDL	C	410	-	-	34/74/74/110	-
15	3PE	C	409	-	-	27/37/37/54	-
15	3PE	O	405	-	-	30/42/42/54	-
14	HEM	C	402	3	-	5/12/54/54	-
17	FES	Q	301	-	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	HEC	D	501	4	-	0/10/54/54	-
15	3PE	C	411	-	-	24/39/39/54	-
12	CDL	N	603	-	-	51/80/80/110	-
15	3PE	R	201	-	-	23/41/41/54	-
12	CDL	B	602	-	-	33/74/74/110	-
15	3PE	C	406	-	-	32/54/54/54	-
15	3PE	O	406	-	-	19/36/36/54	-
16	HEC	P	401	4	-	0/10/54/54	-
15	3PE	R	202	-	-	27/51/51/54	-
17	FES	E	301	-	-	-	0/1/1/1
12	CDL	O	407	-	-	31/73/73/110	-

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	501	HEC	C2B-C3B	-6.94	1.33	1.40
16	P	401	HEC	C2B-C3B	-6.77	1.33	1.40
16	D	501	HEC	C3C-C2C	-6.66	1.33	1.40
16	P	401	HEC	C3C-C2C	-6.64	1.33	1.40
16	D	501	HEC	C3D-C2D	4.95	1.52	1.37

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	401	A1D6K	C19-O4-N1	9.23	119.98	109.99
13	C	401	A1D6K	C19-O4-N1	9.20	119.95	109.99
14	O	403	HEM	CAD-C3D-C4D	5.72	134.65	124.66
14	O	403	HEM	CAD-C3D-C2D	-5.27	118.07	127.88
12	C	410	CDL	OB6-CB5-C51	4.89	122.04	111.50

There are no chirality outliers.

5 of 566 torsion outliers are listed below:

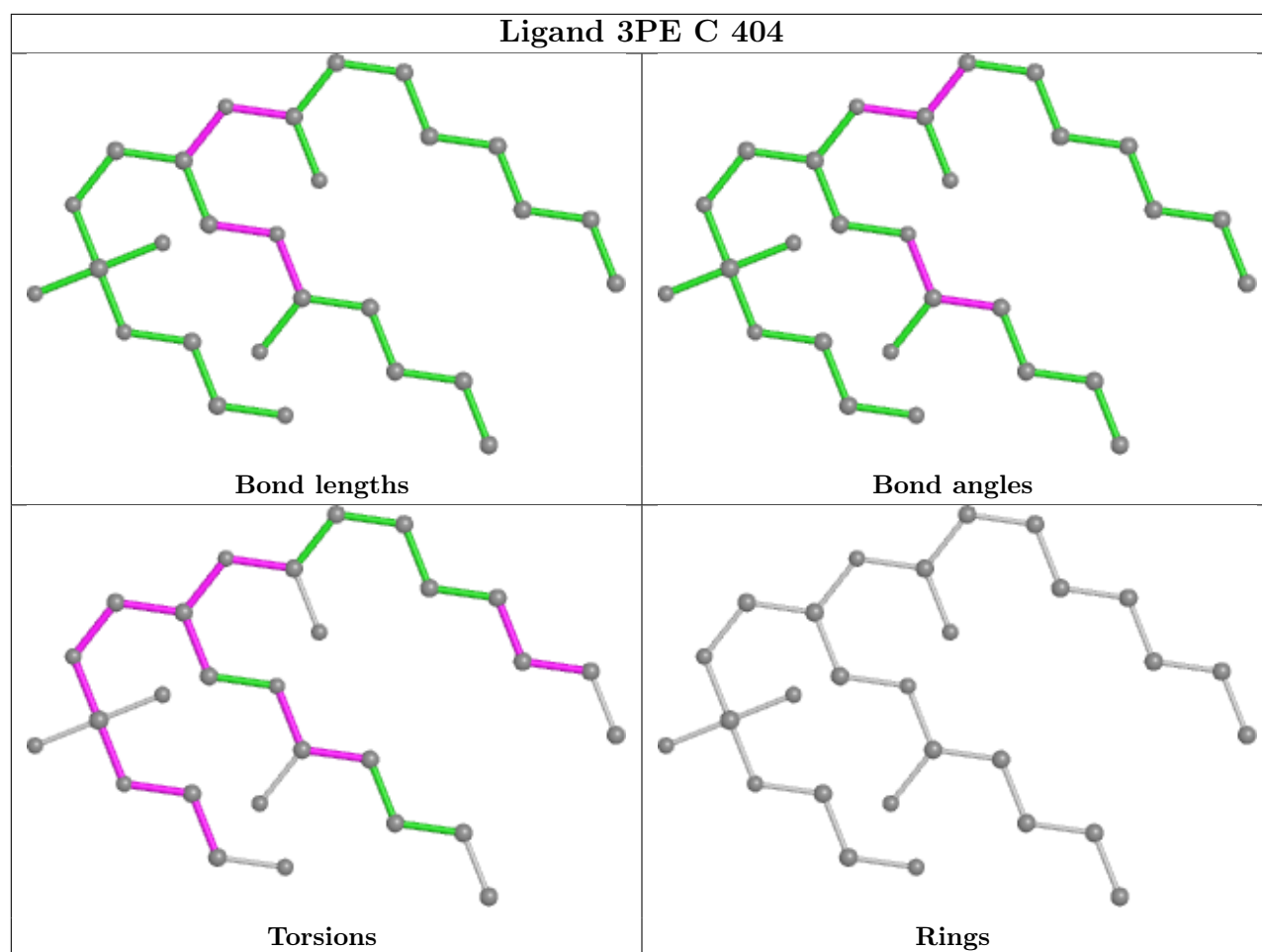
Mol	Chain	Res	Type	Atoms
12	B	602	CDL	O1-C1-CB2-OB2
12	C	410	CDL	C11-CA5-OA6-CA4
12	C	410	CDL	C51-CB5-OB6-CB4
12	N	602	CDL	CB2-C1-CA2-OA2
12	N	602	CDL	CA2-OA2-PA1-OA4

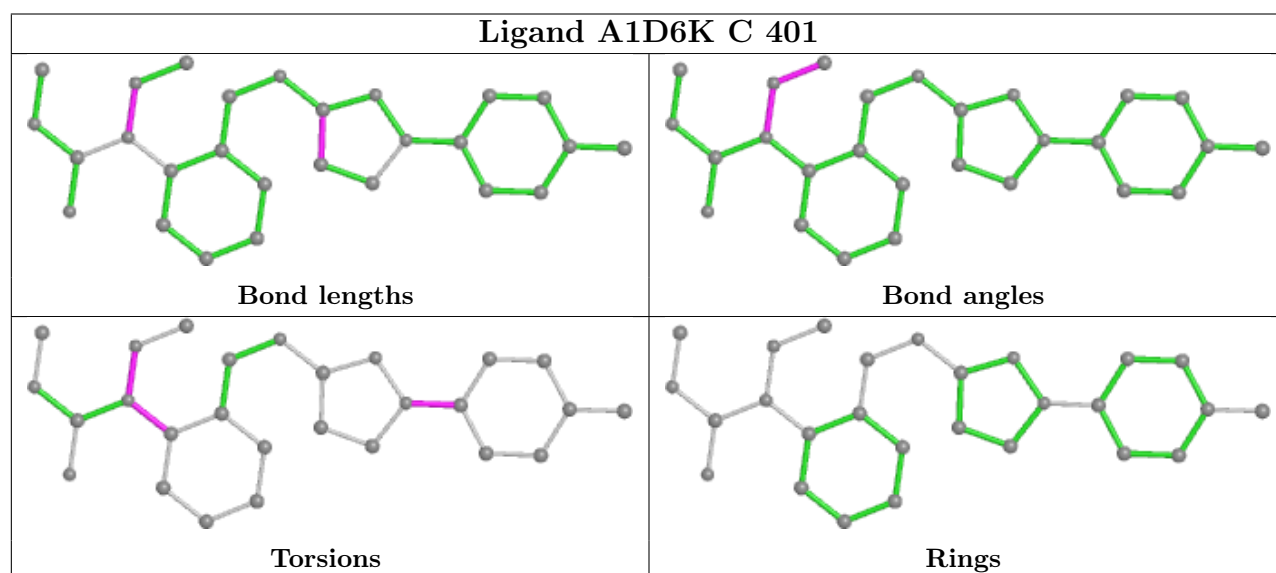
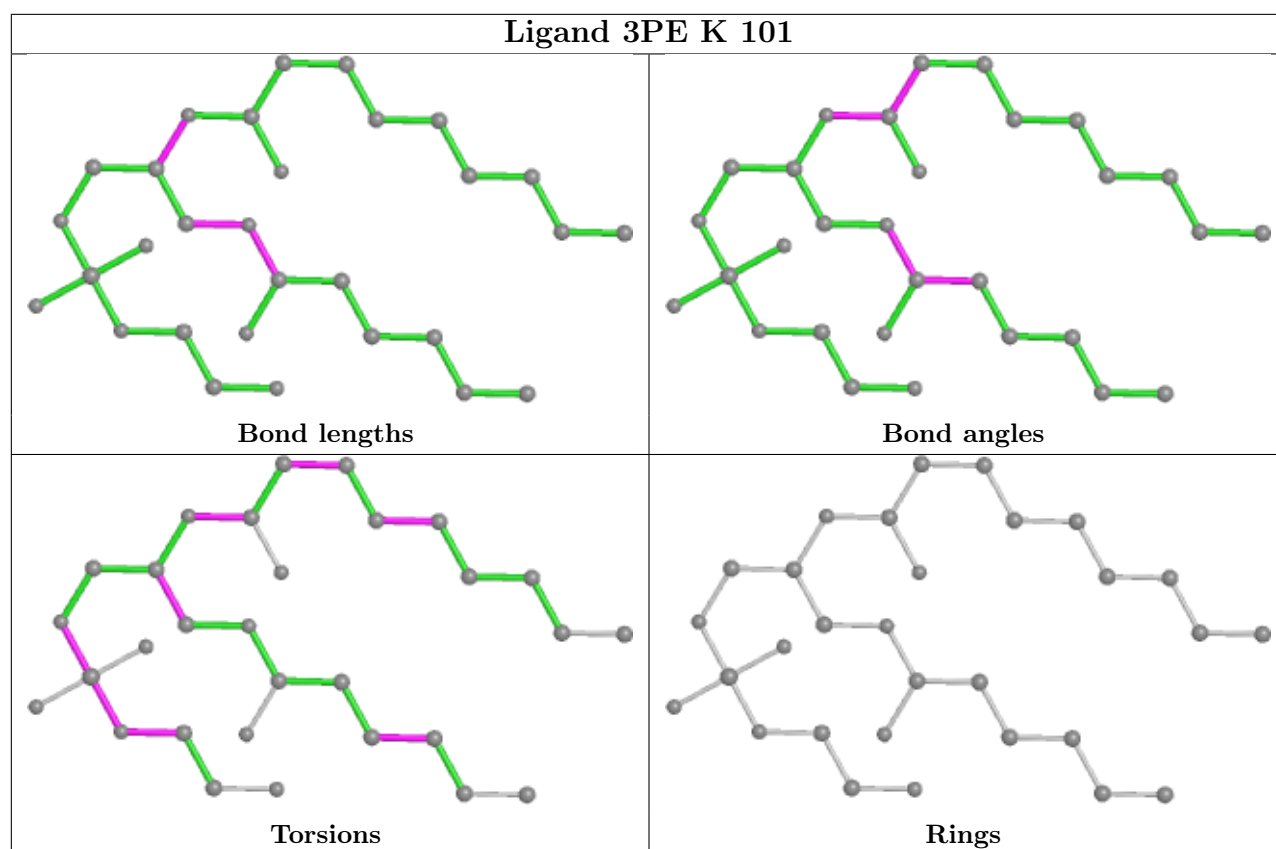
There are no ring outliers.

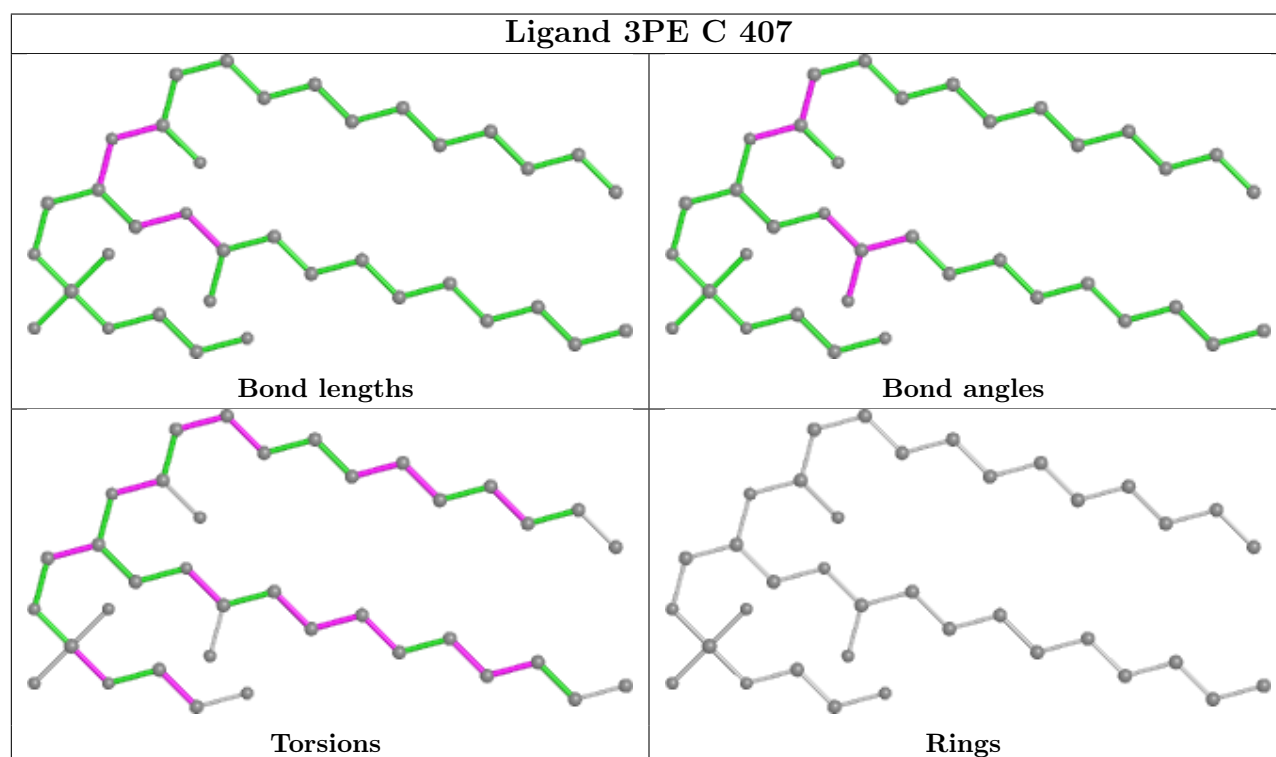
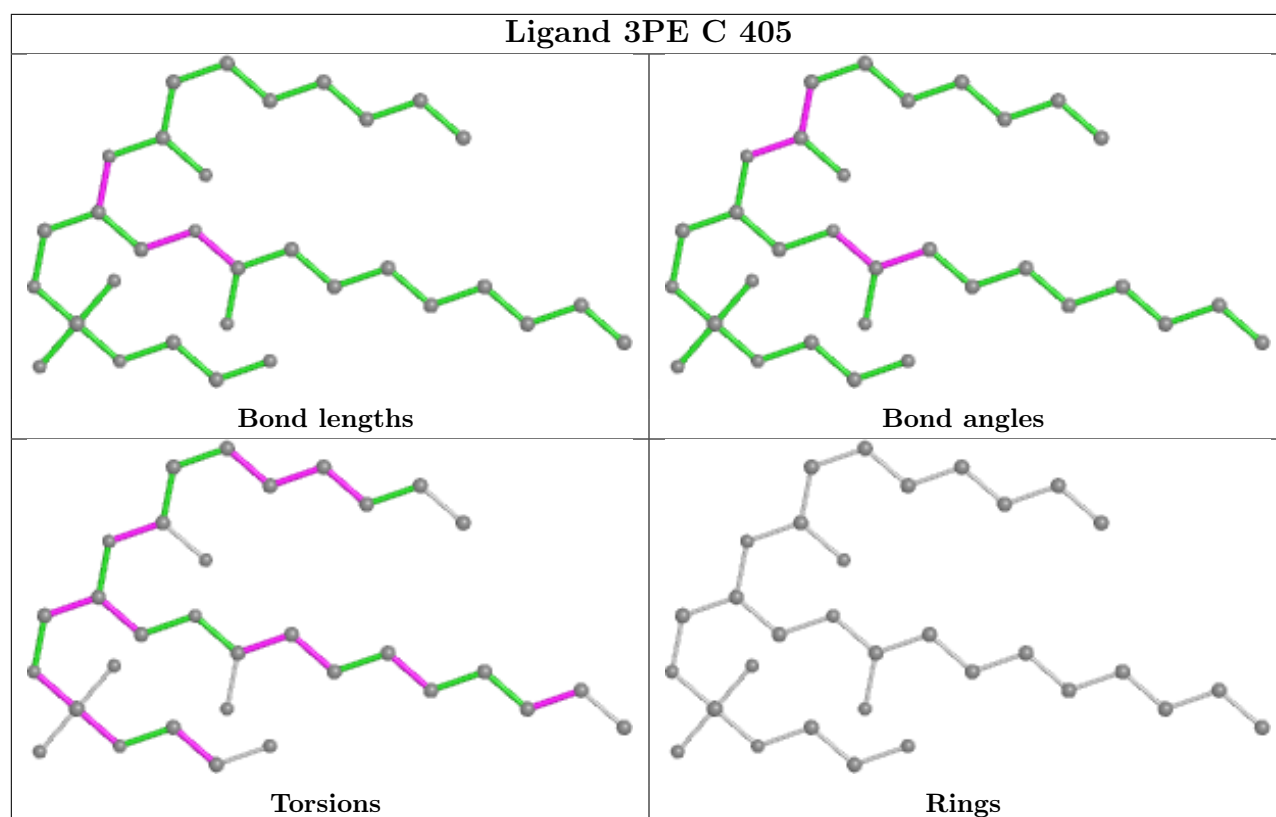
15 monomers are involved in 43 short contacts:

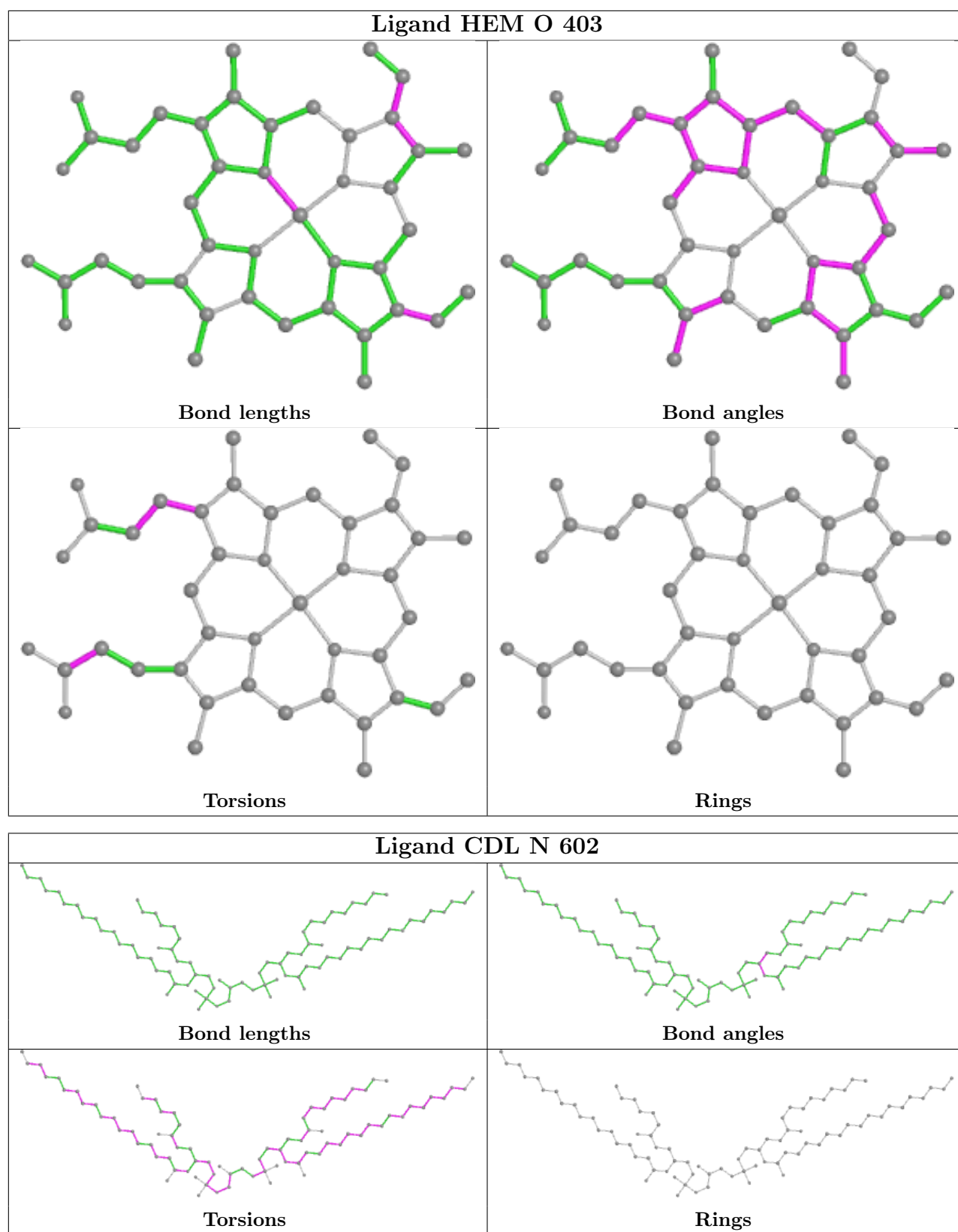
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	404	3PE	3	0
15	K	101	3PE	1	0
15	C	407	3PE	1	0
12	N	602	CDL	4	0
18	Q	302	PC1	3	0
14	C	403	HEM	1	0
12	C	410	CDL	3	0
16	D	501	HEC	2	0
15	C	411	3PE	5	0
12	N	603	CDL	3	0
12	B	602	CDL	3	0
15	C	406	3PE	3	0
16	P	401	HEC	2	0
15	R	202	3PE	5	0
12	O	407	CDL	6	0

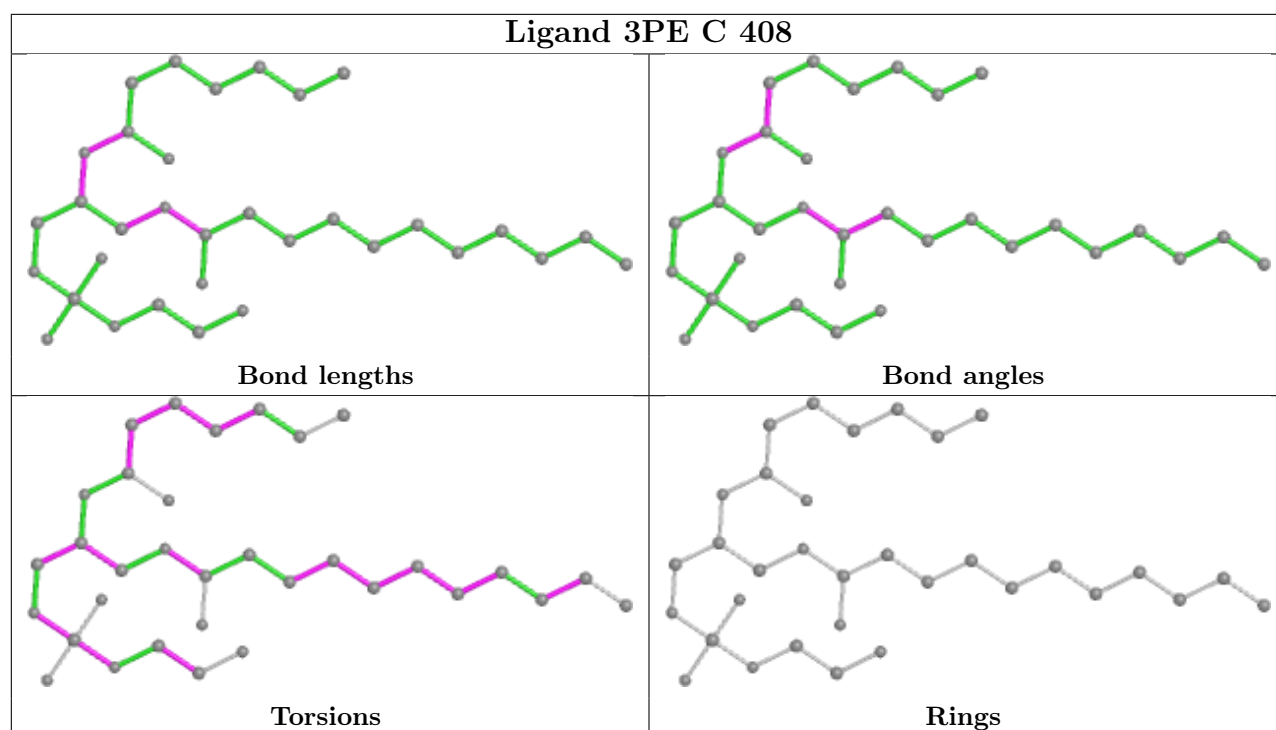
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

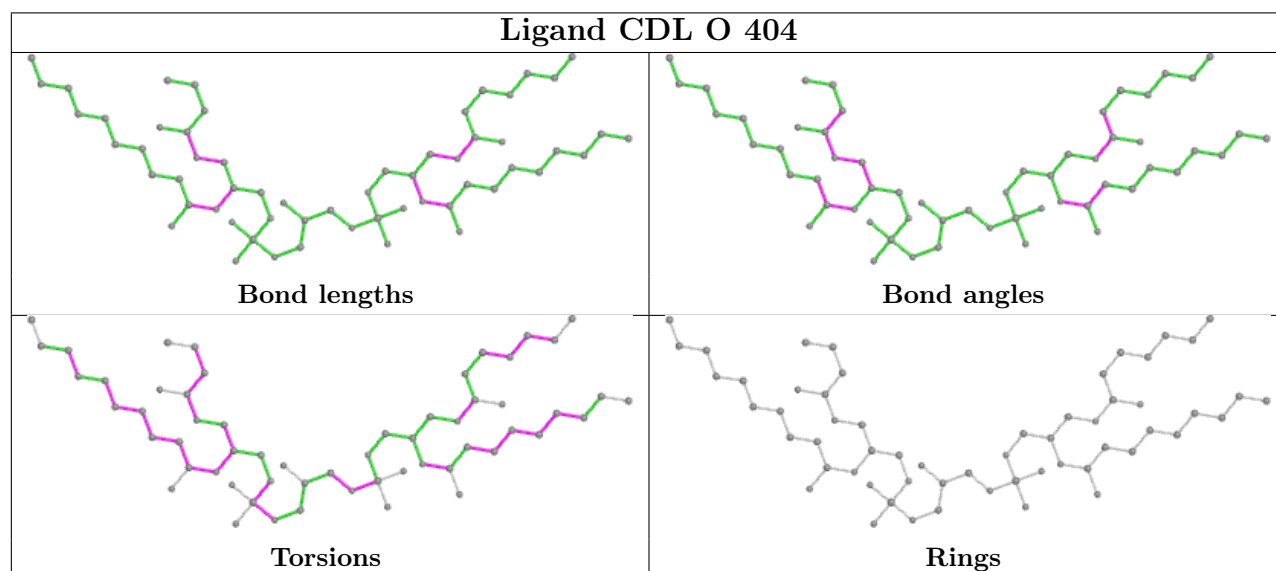
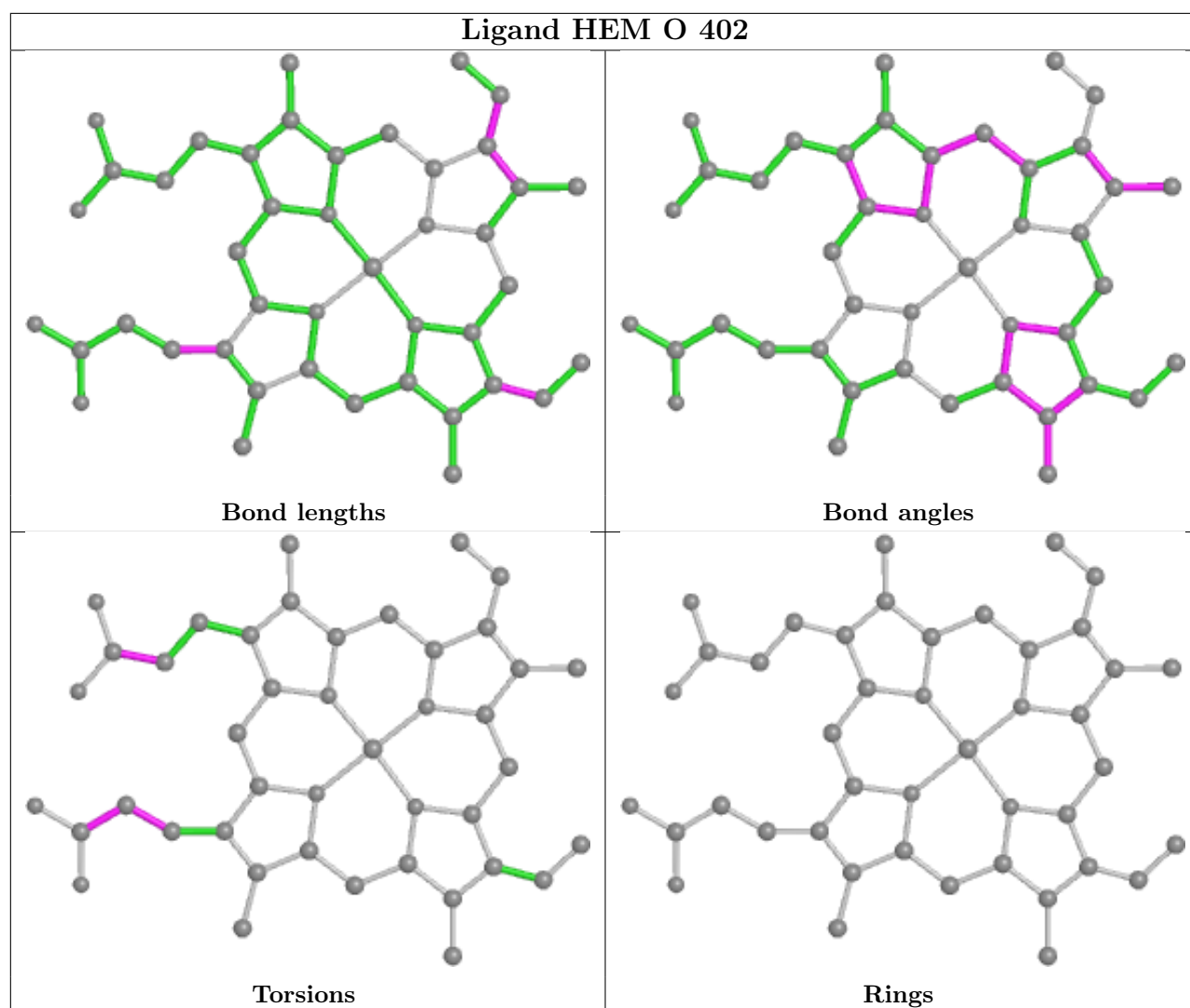




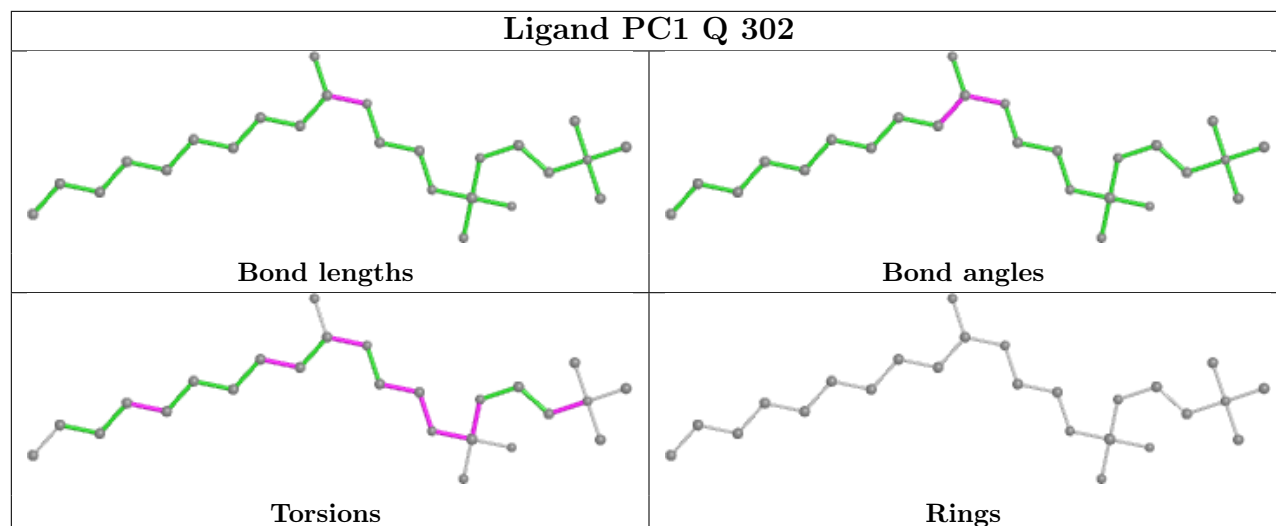




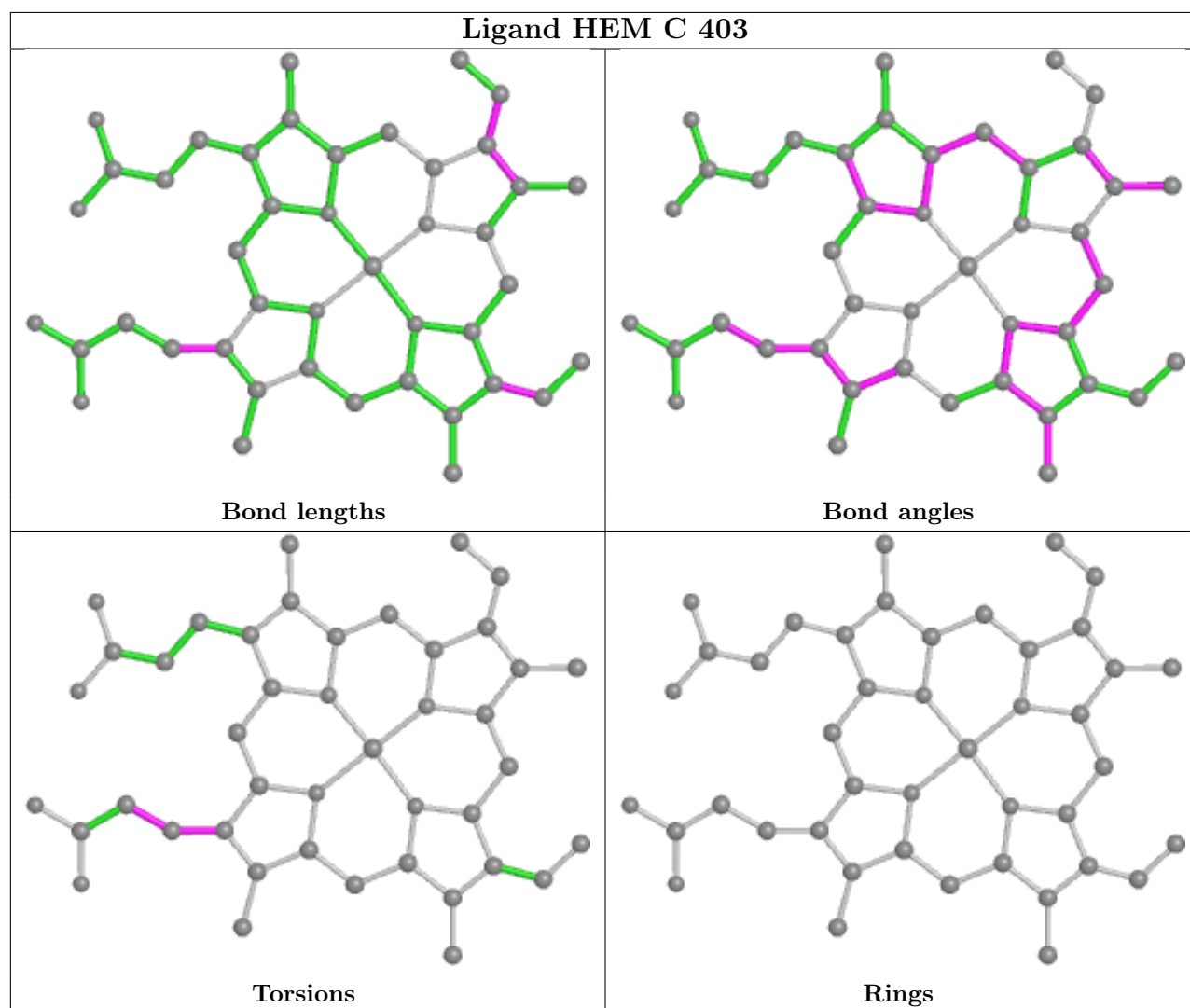


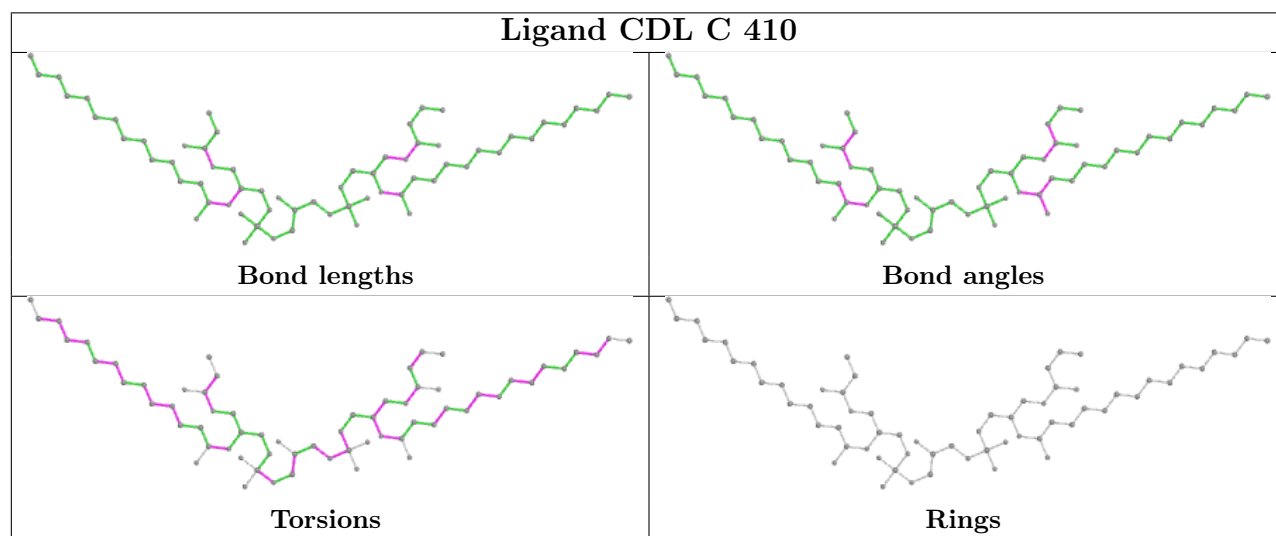
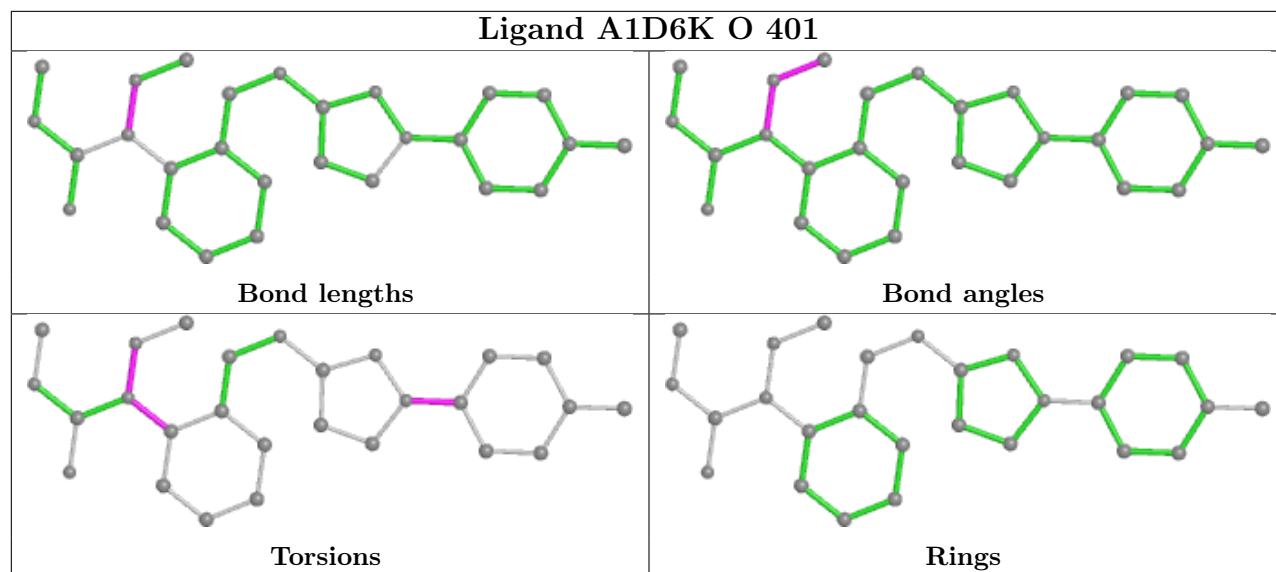


Ligand PC1 Q 302

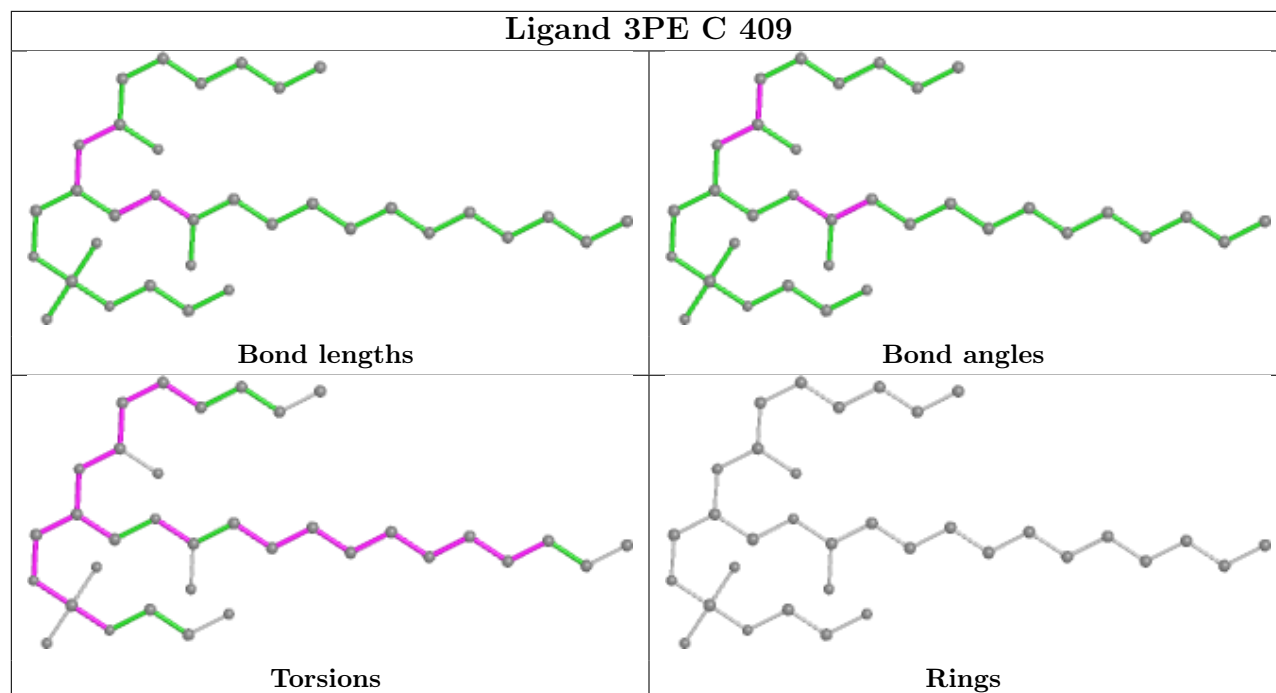


Ligand HEM C 403

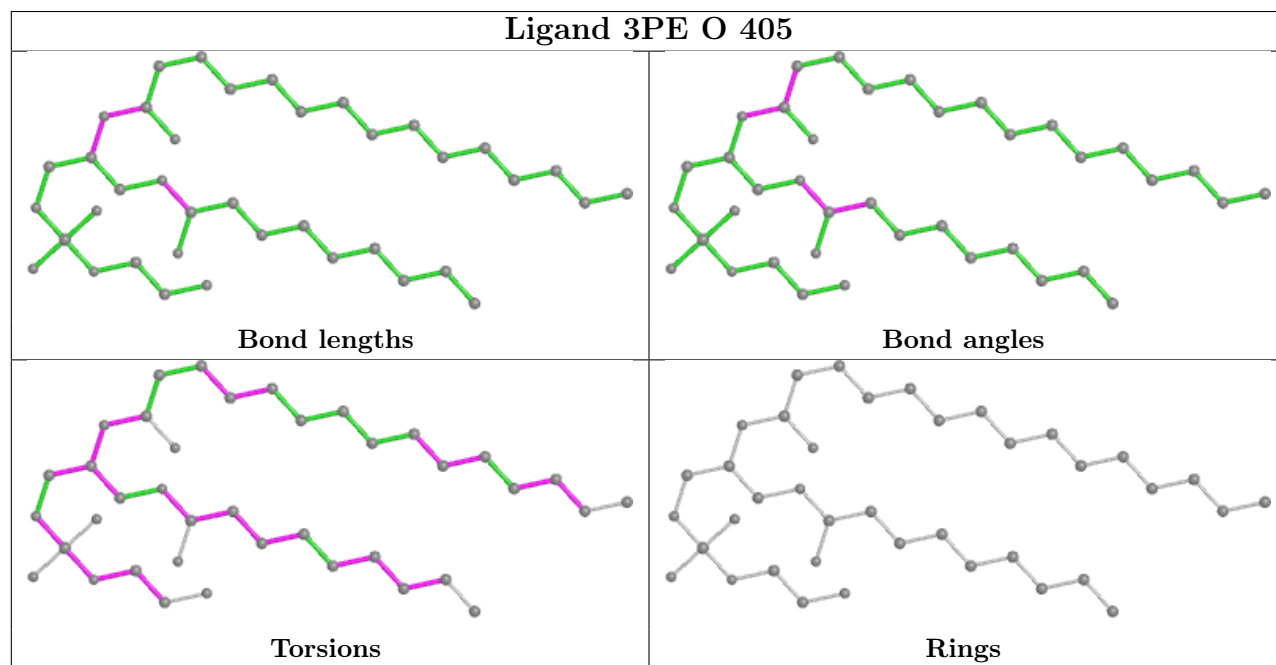


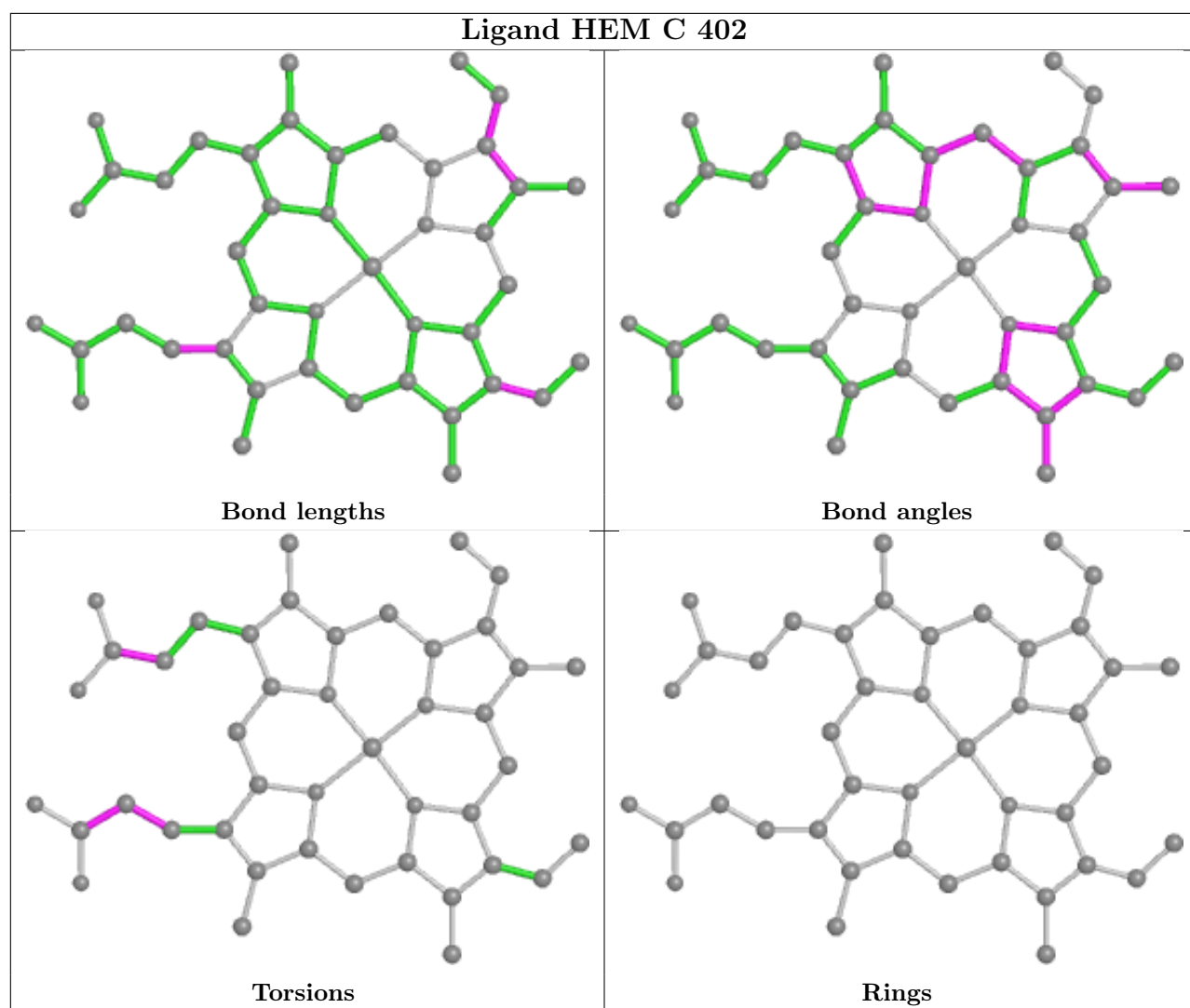


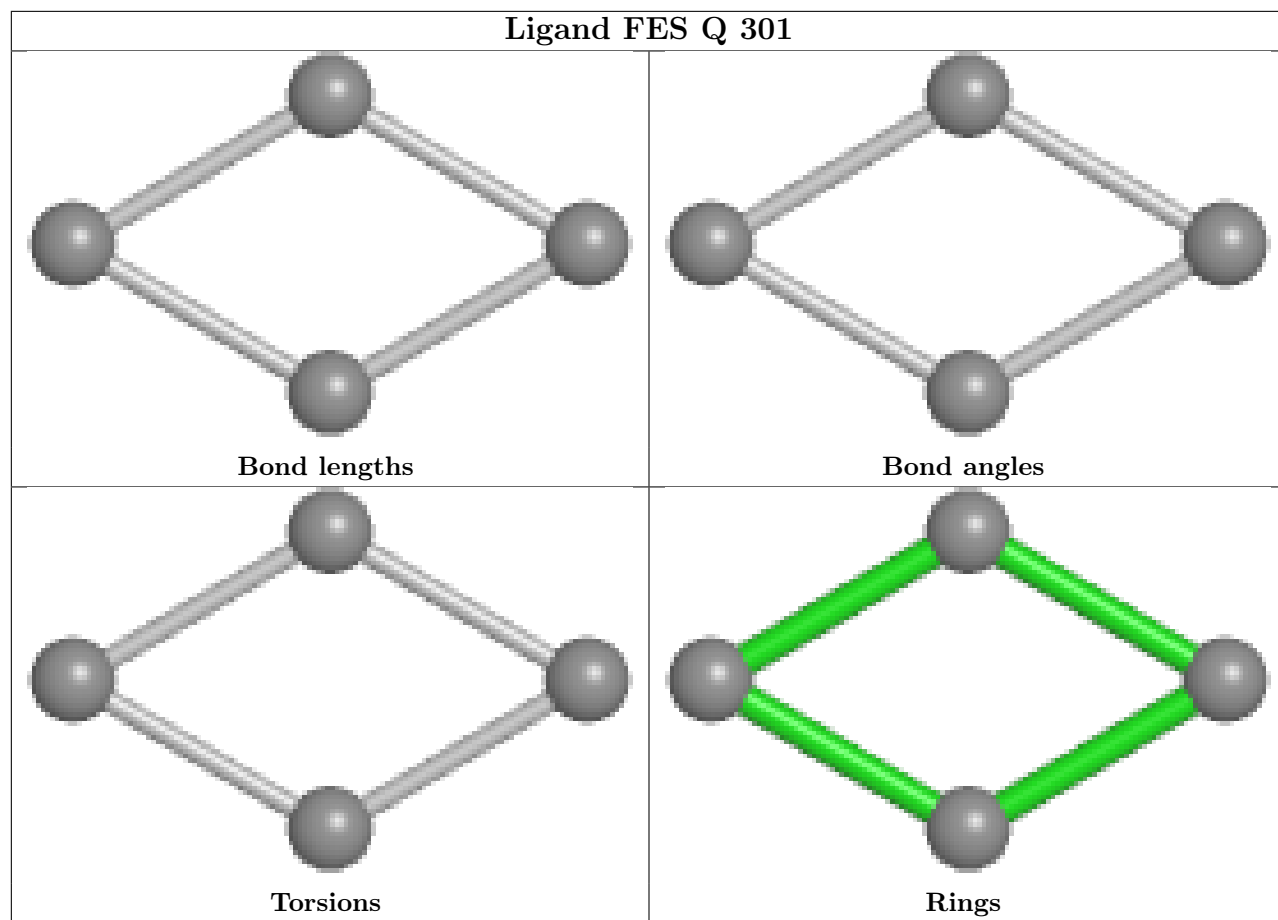
Ligand 3PE C 409

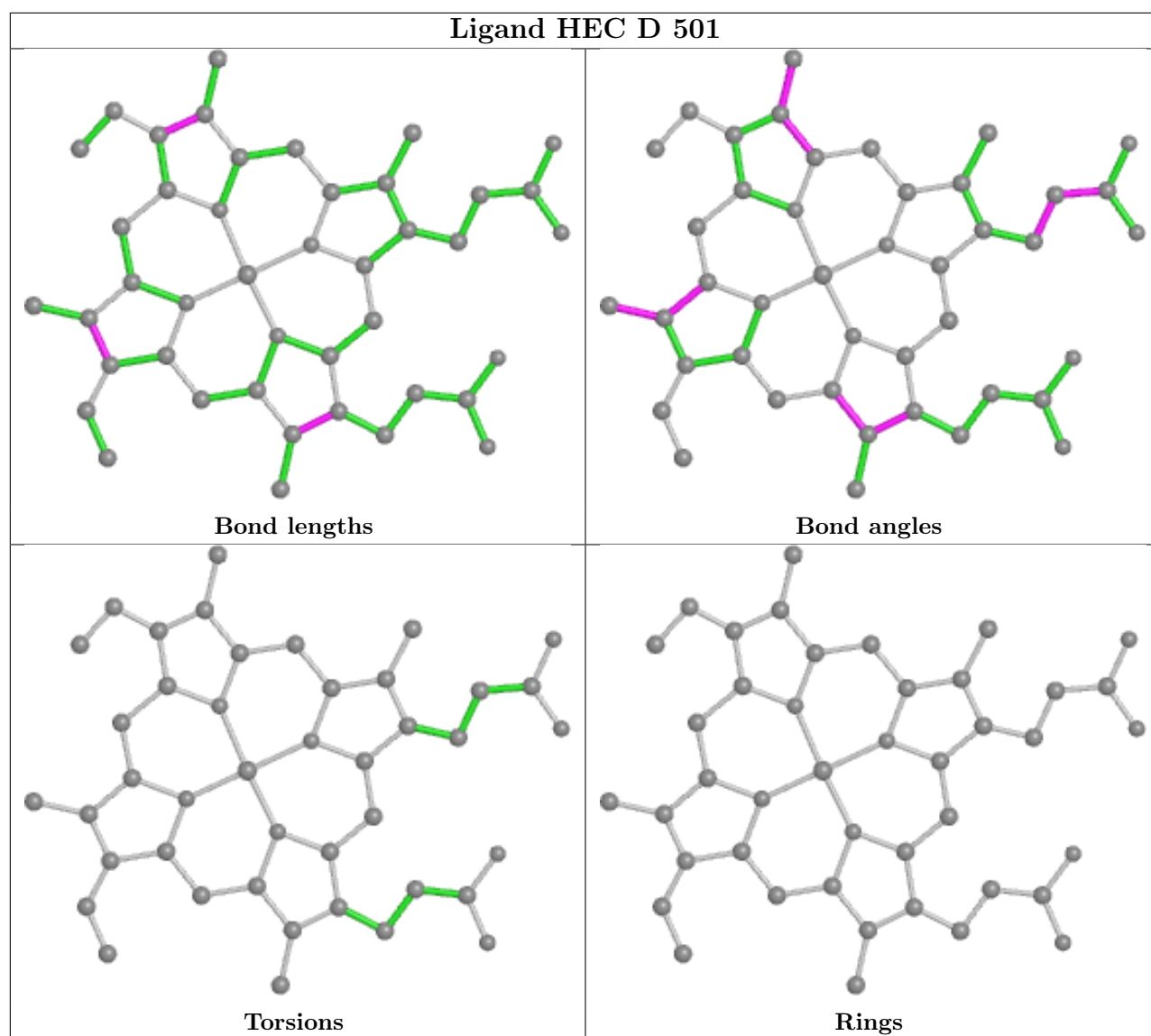


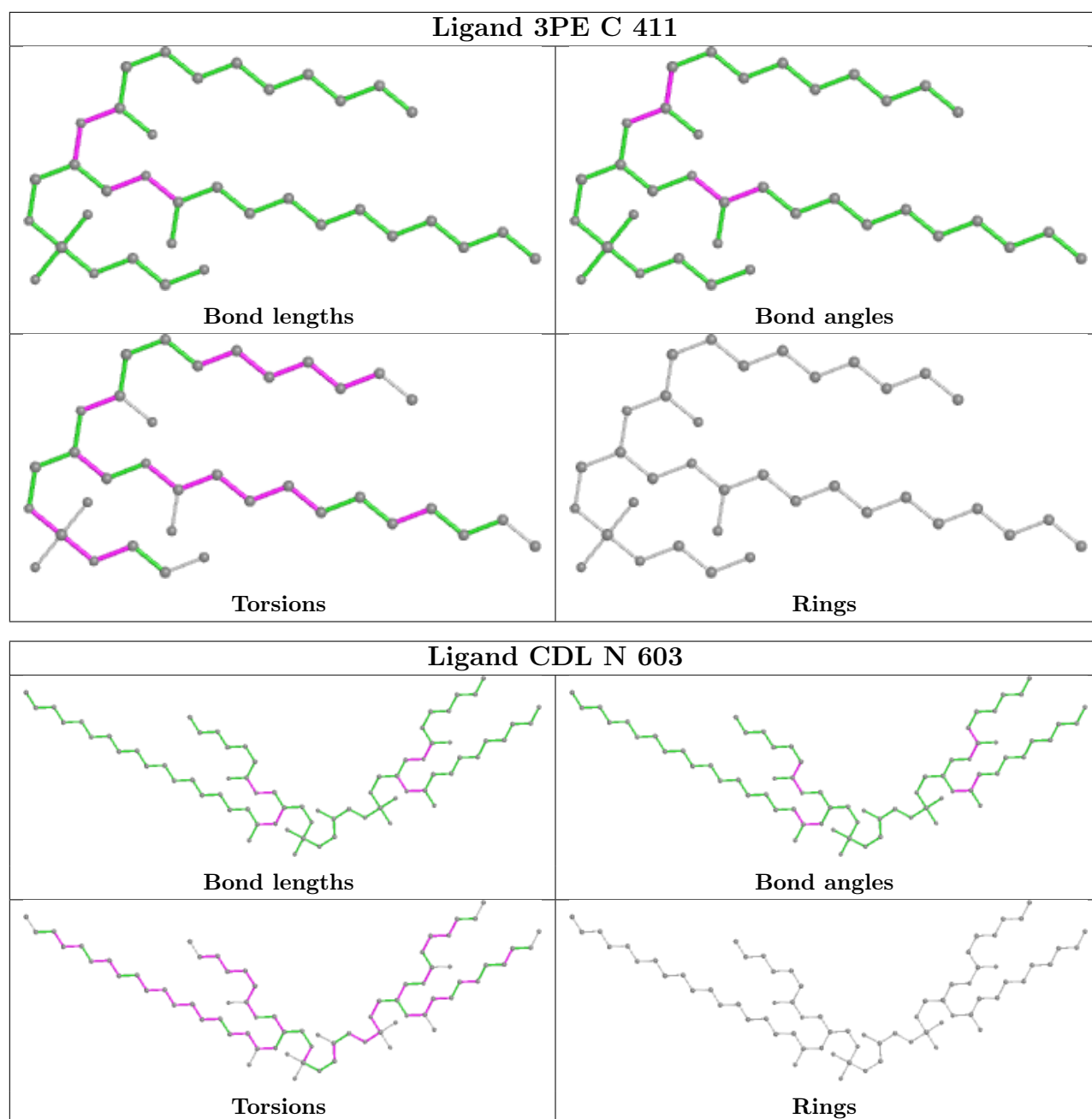
Ligand 3PE O 405

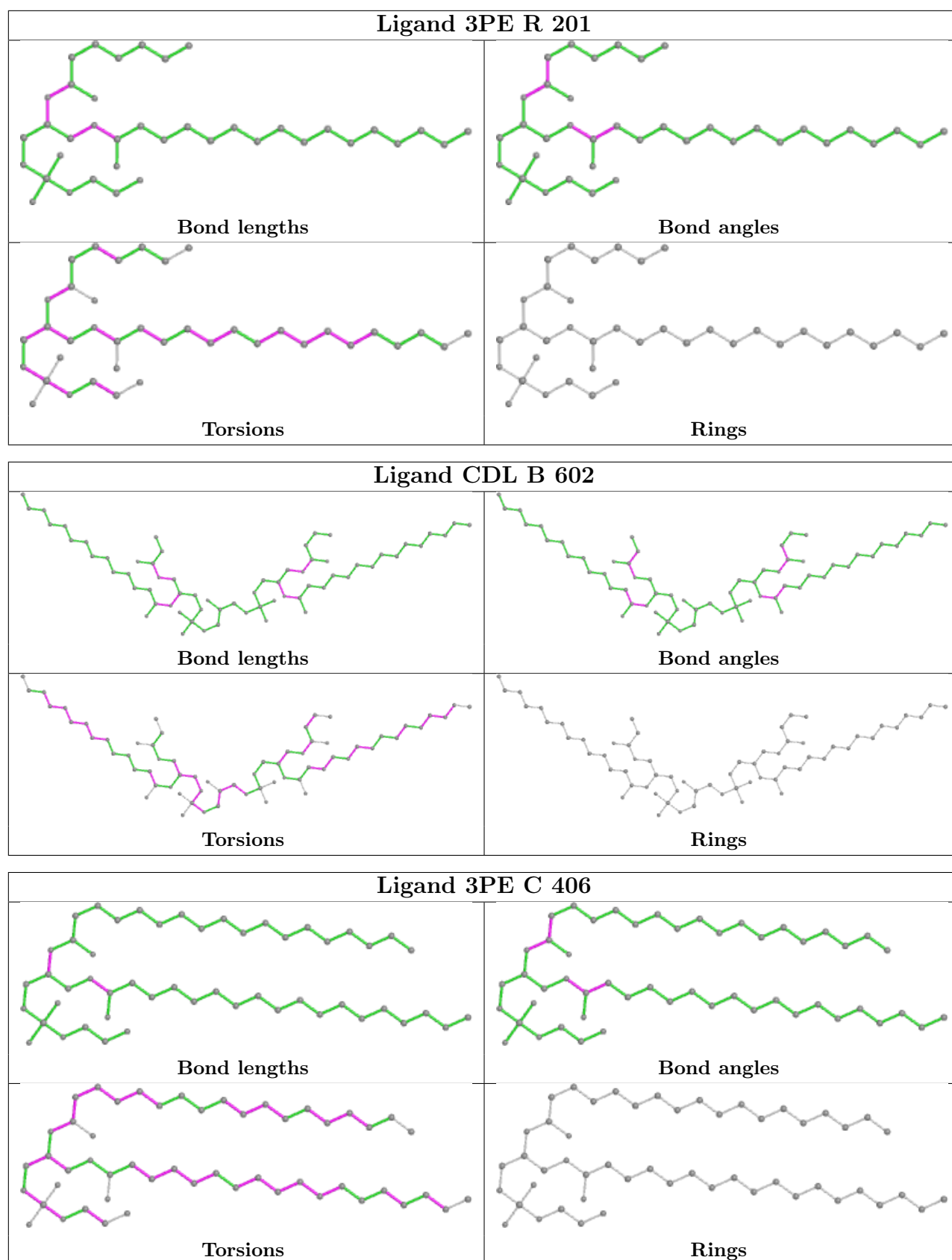


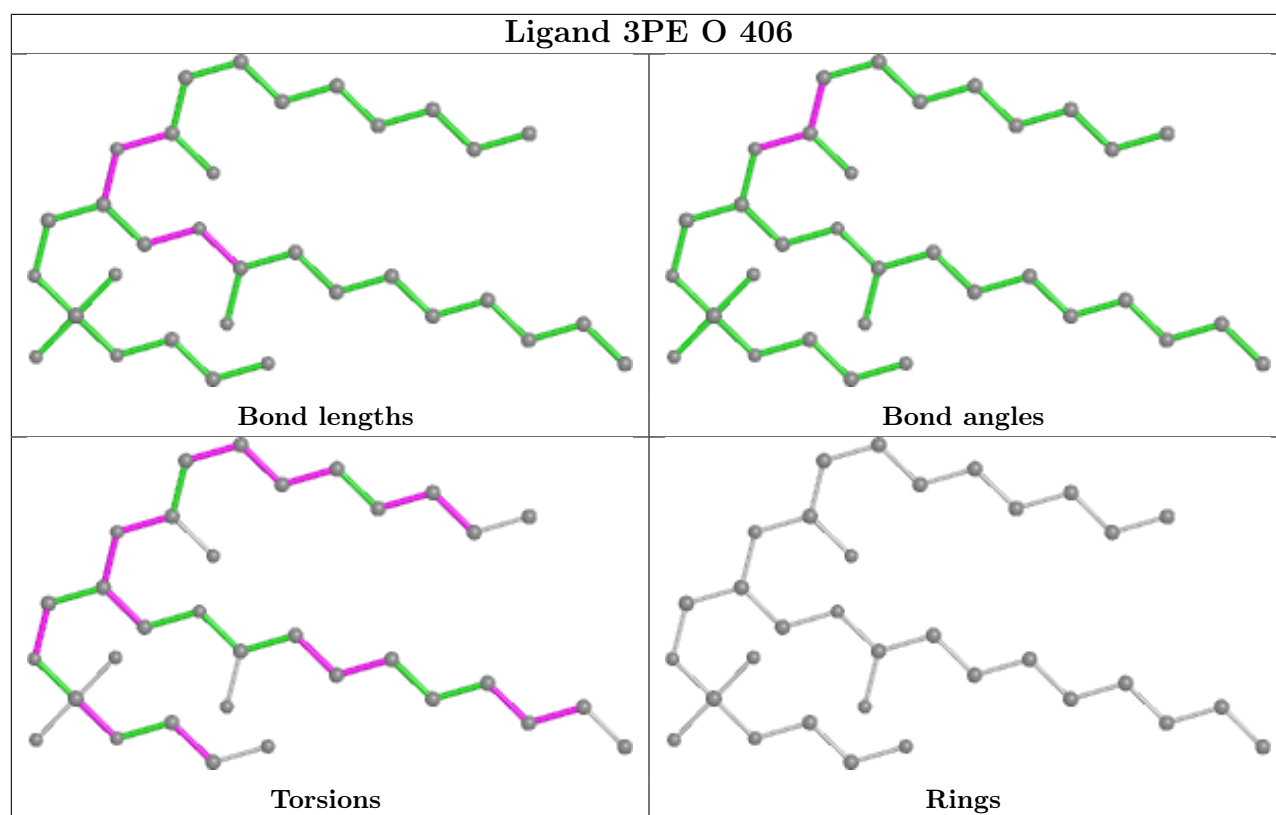


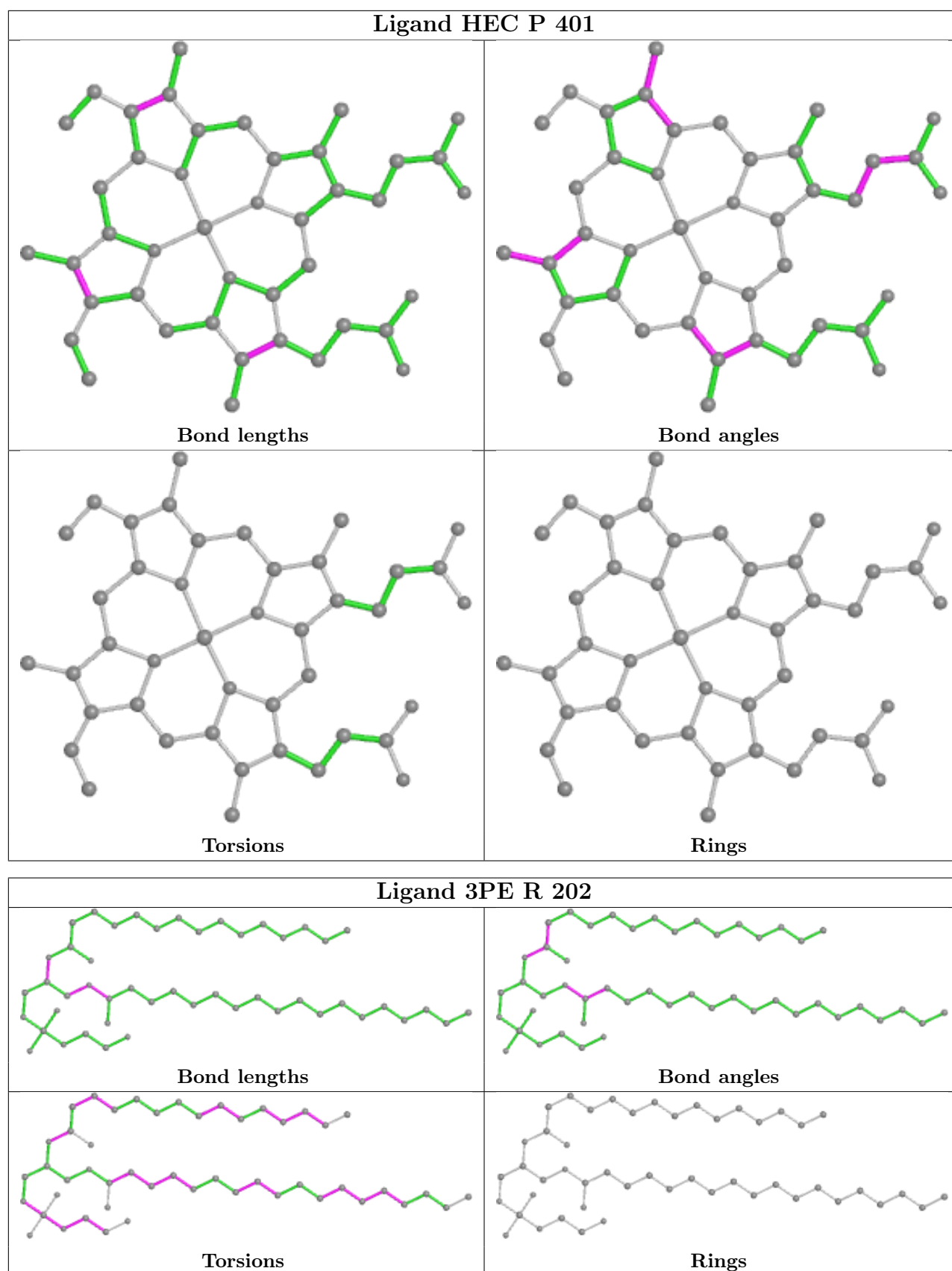


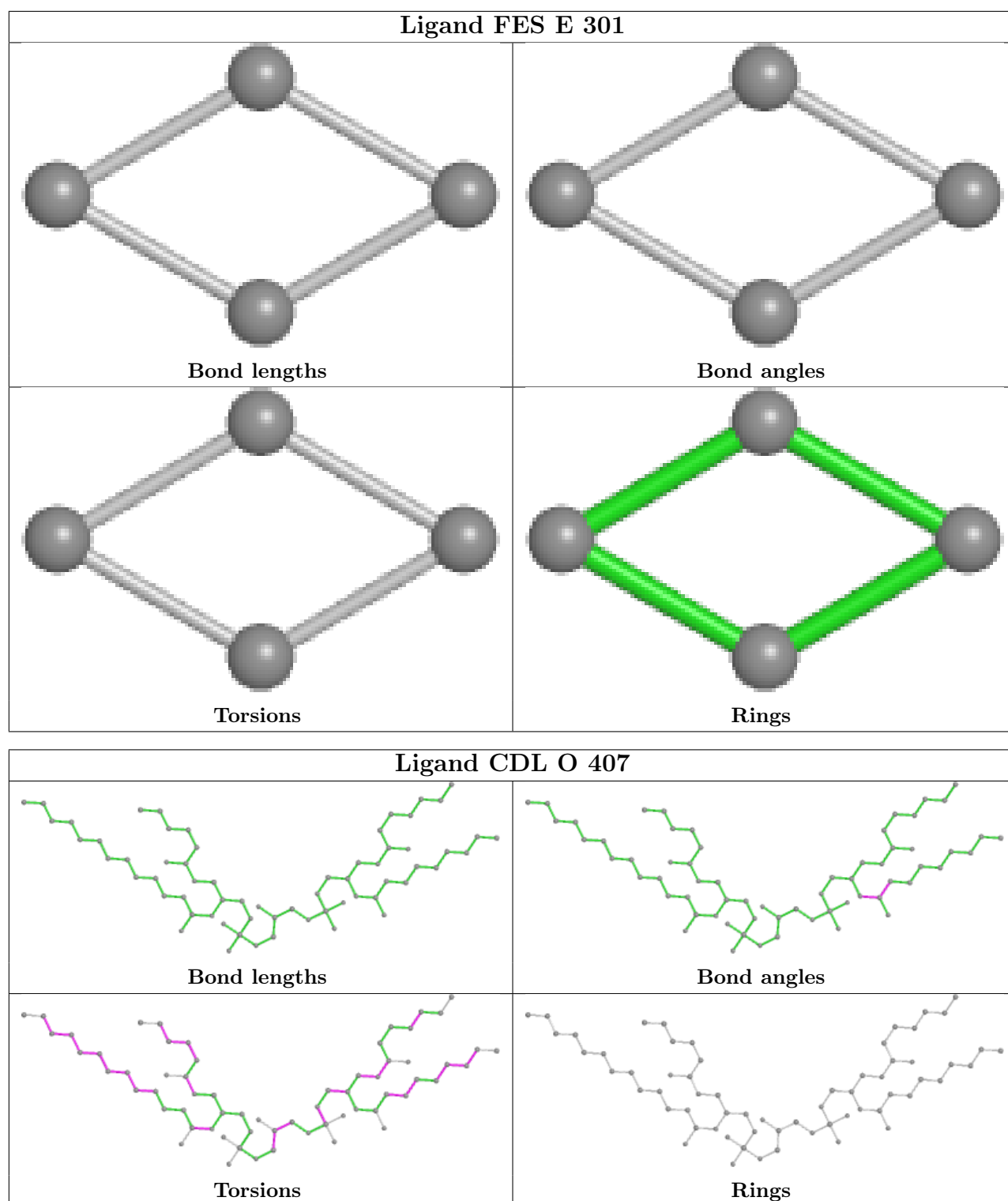












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

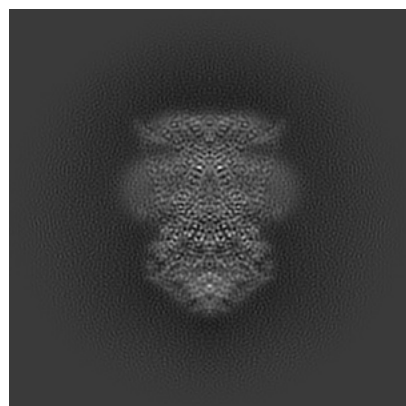
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60307. These allow visual inspection of the internal detail of the map and identification of artifacts.

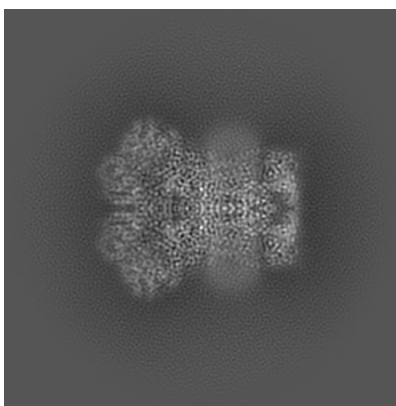
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

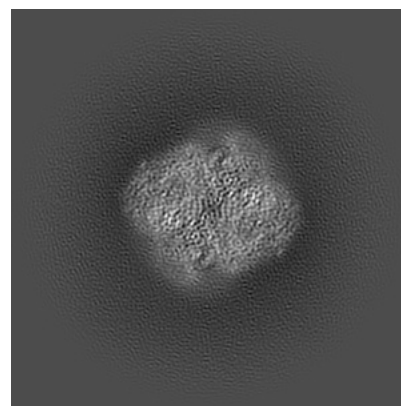
6.1.1 Primary map



X

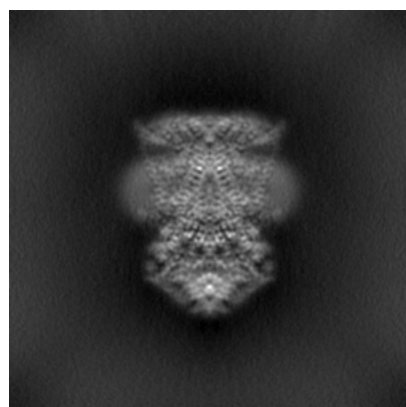


Y

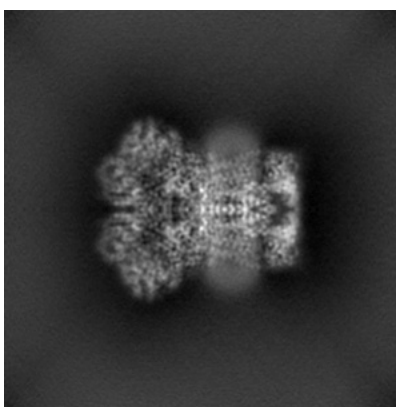


Z

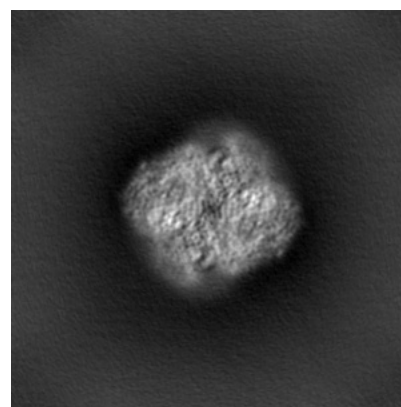
6.1.2 Raw map



X



Y

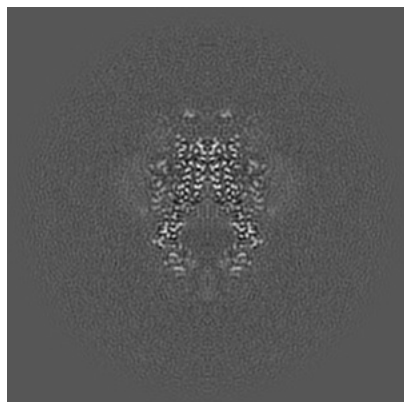


Z

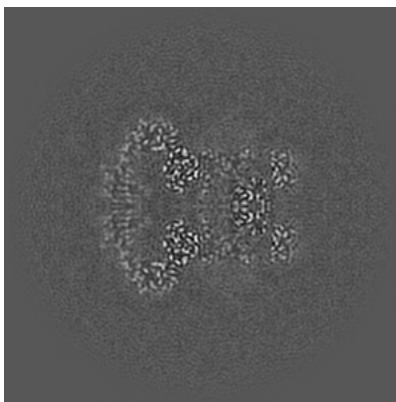
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

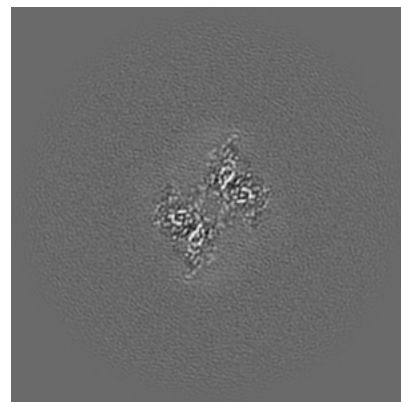
6.2.1 Primary map



X Index: 160

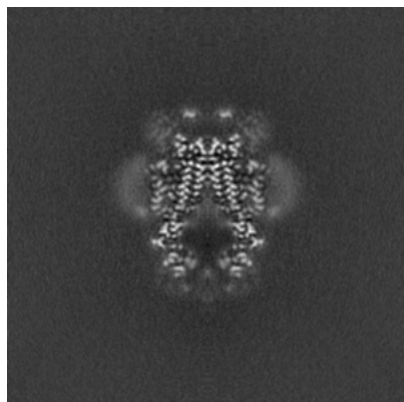


Y Index: 160

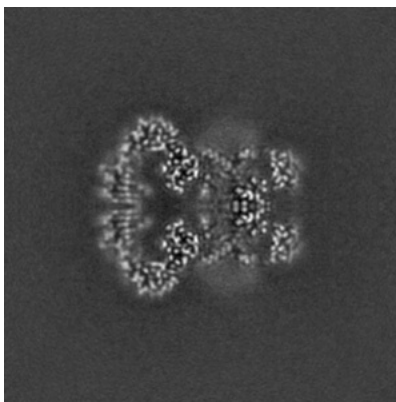


Z Index: 160

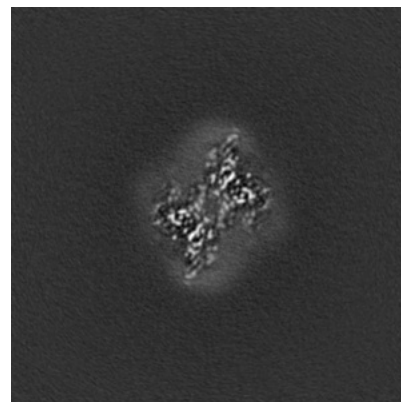
6.2.2 Raw map



X Index: 160



Y Index: 160

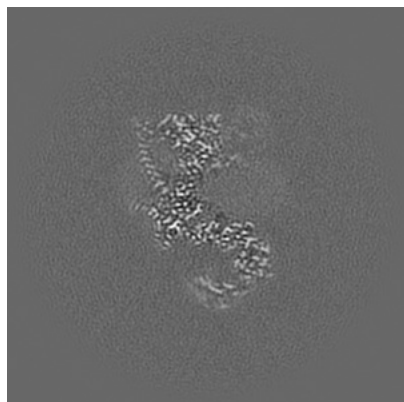


Z Index: 160

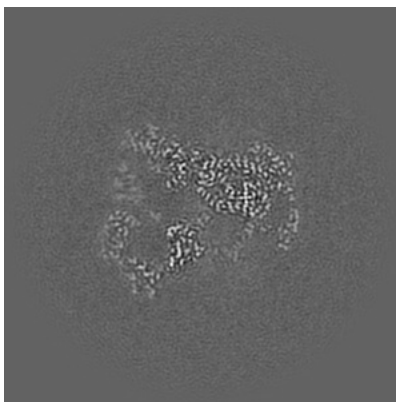
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

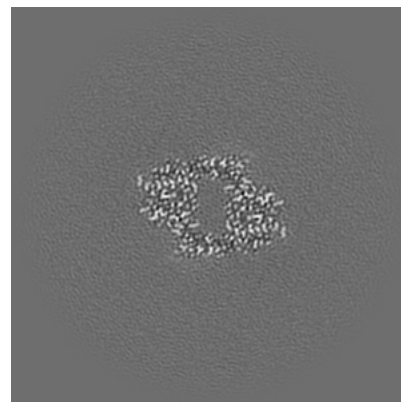
6.3.1 Primary map



X Index: 141

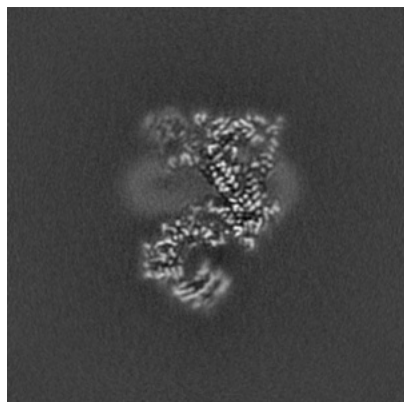


Y Index: 168

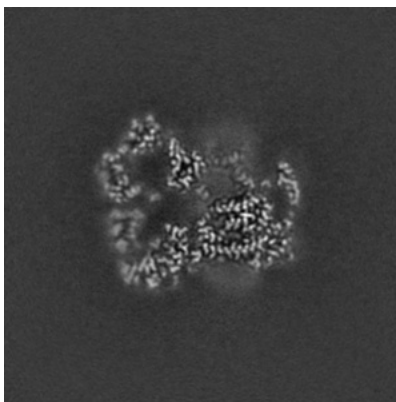


Z Index: 140

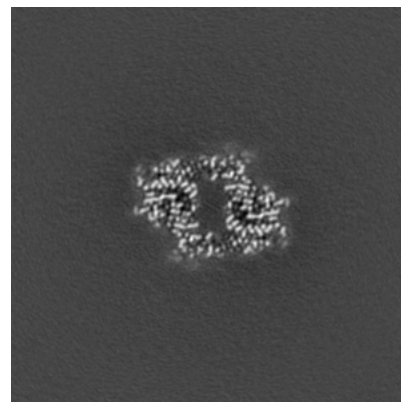
6.3.2 Raw map



X Index: 175



Y Index: 153

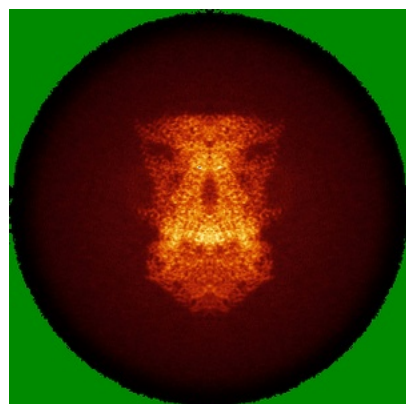


Z Index: 139

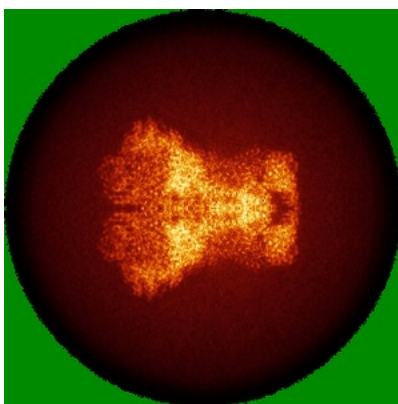
The images above show the largest variance slices of the map in three orthogonal directions.

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

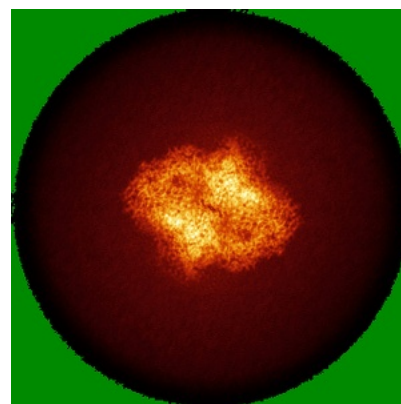
6.4.1 Primary map



X

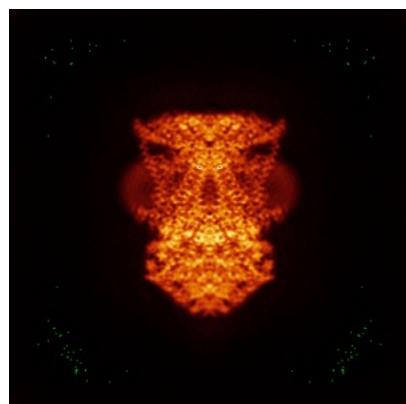


Y

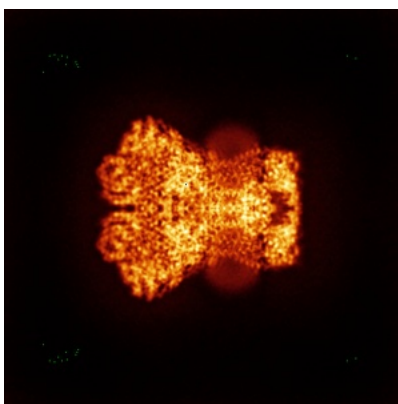


Z

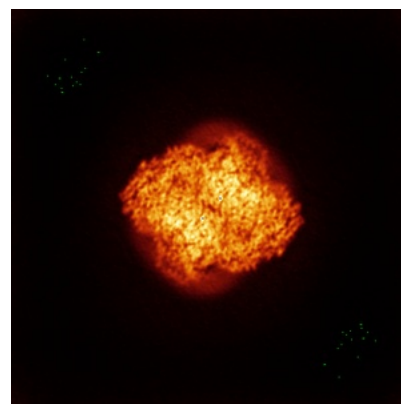
6.4.2 Raw map



X



Y

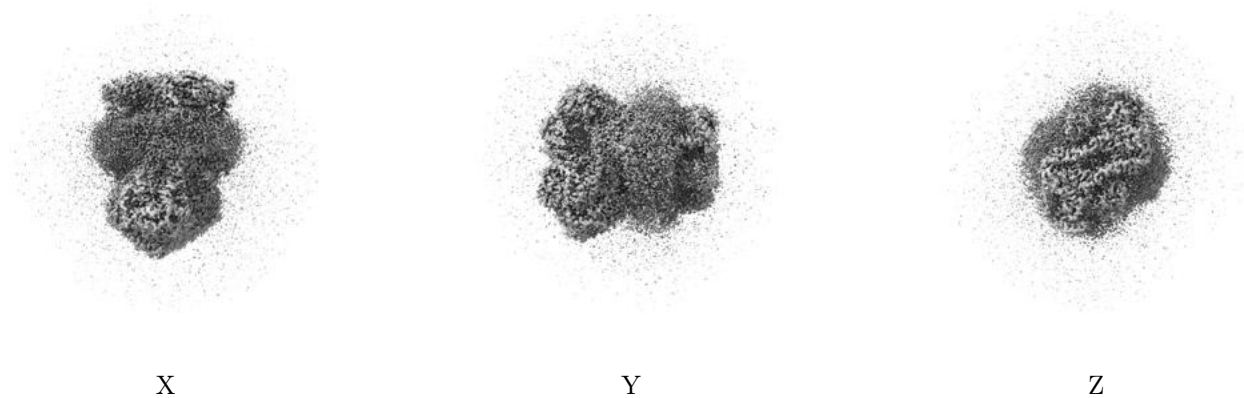


Z

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.

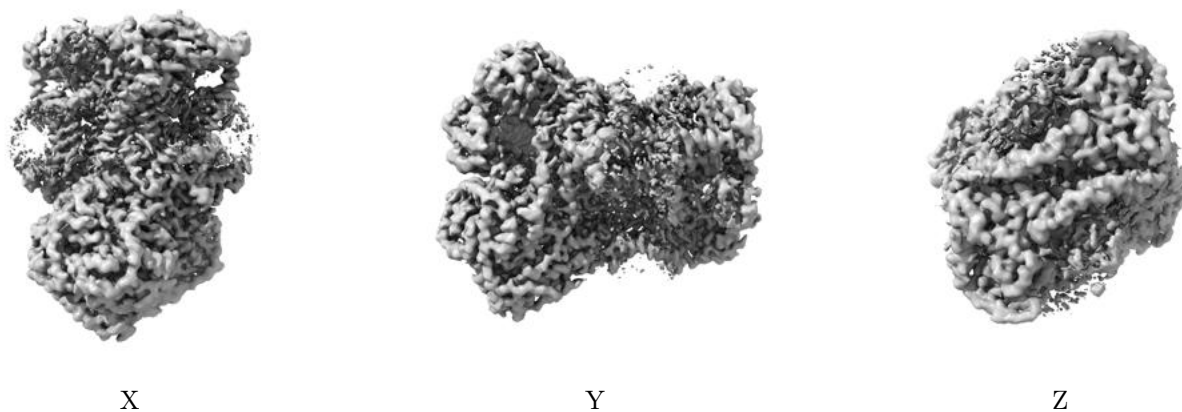
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.586. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

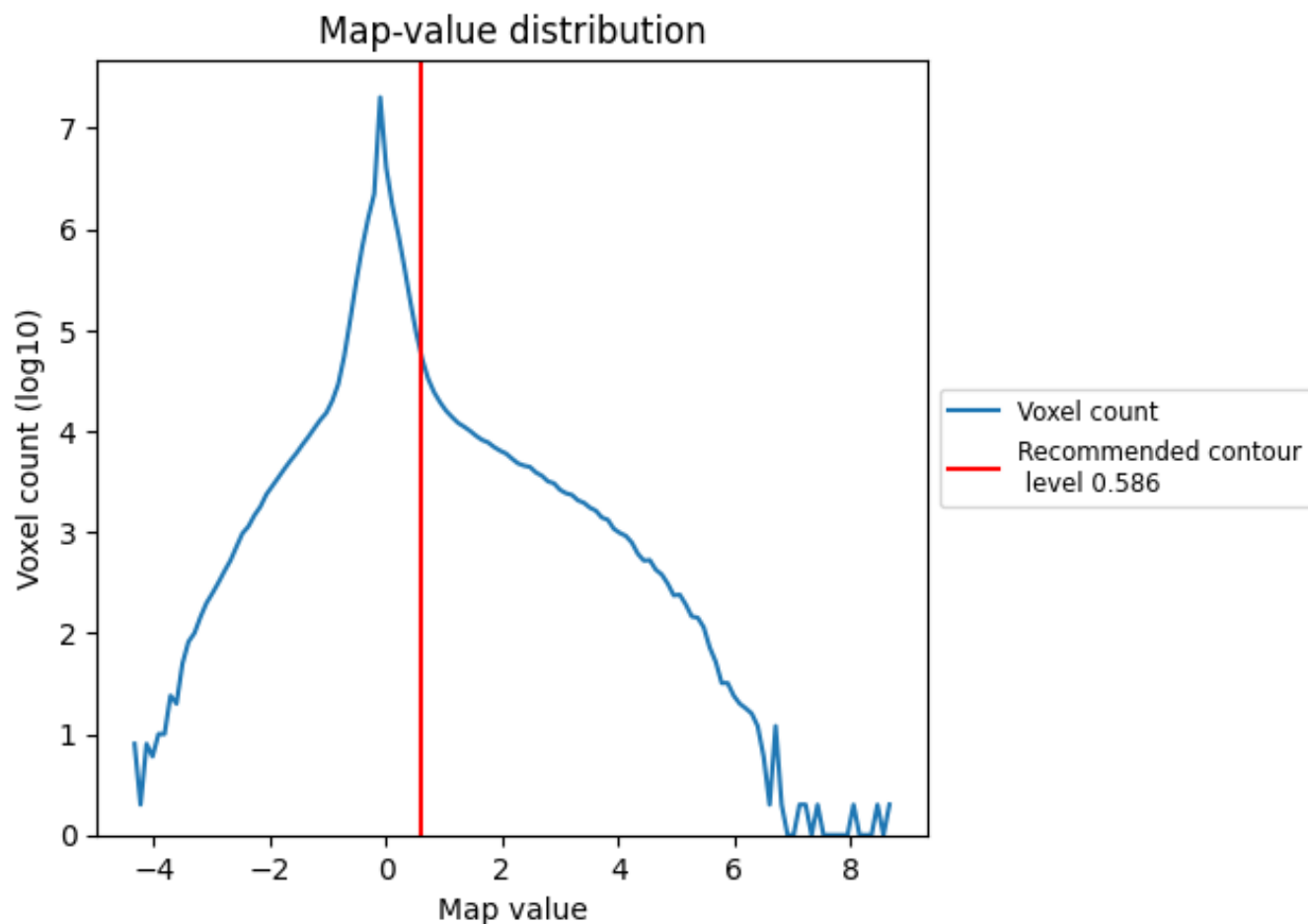
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

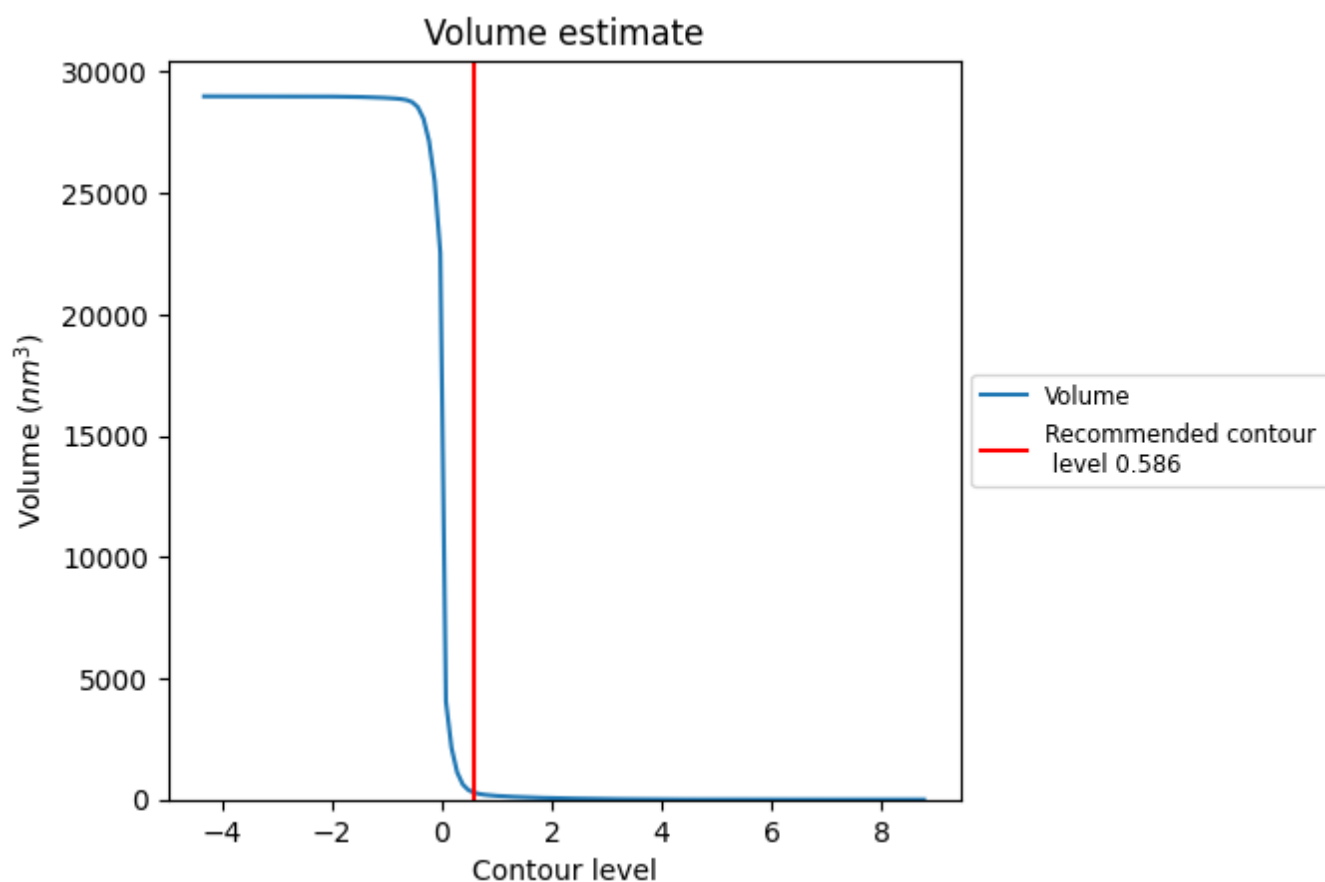
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

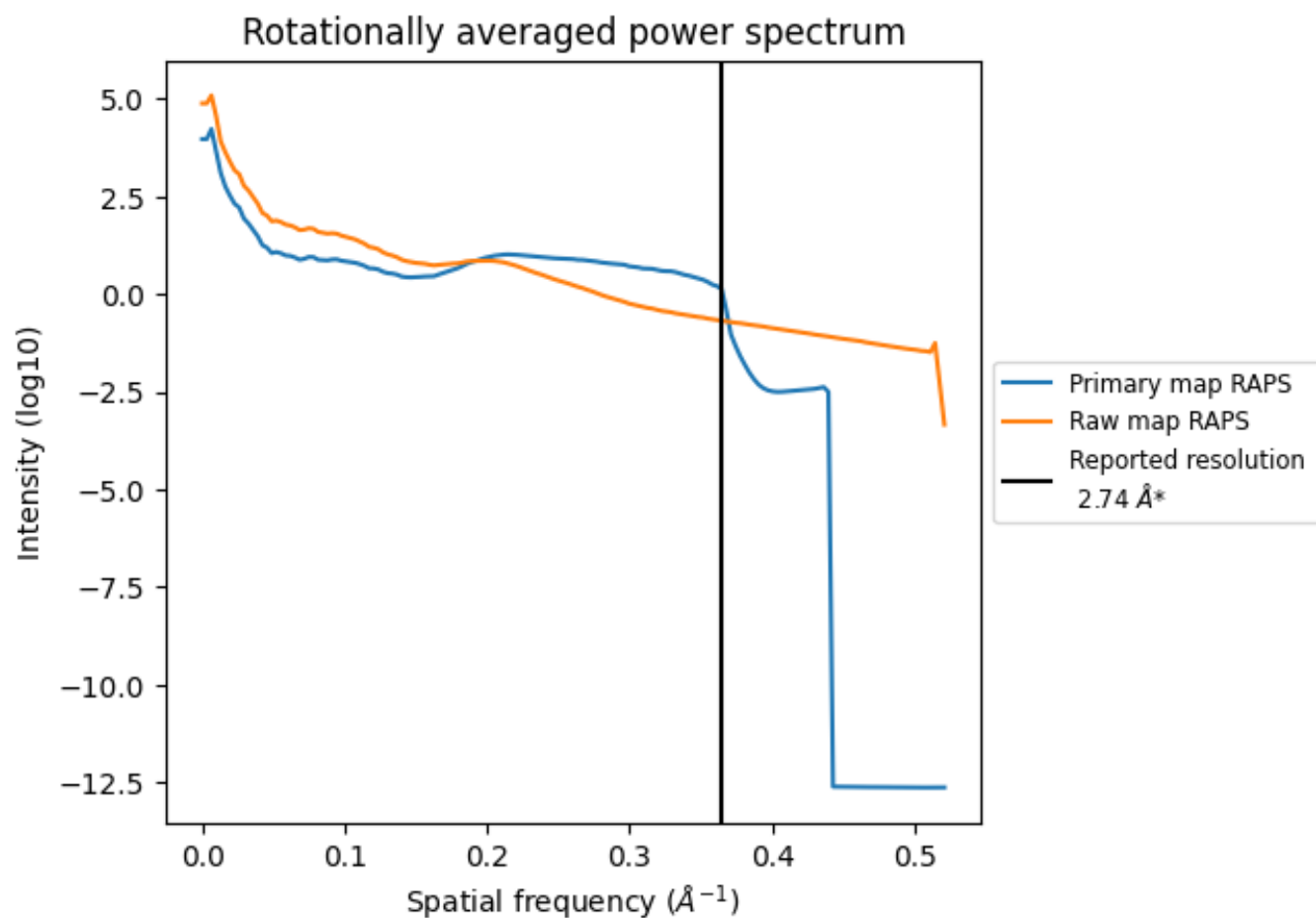
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 286 nm³; this corresponds to an approximate mass of 259 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 ⓘ

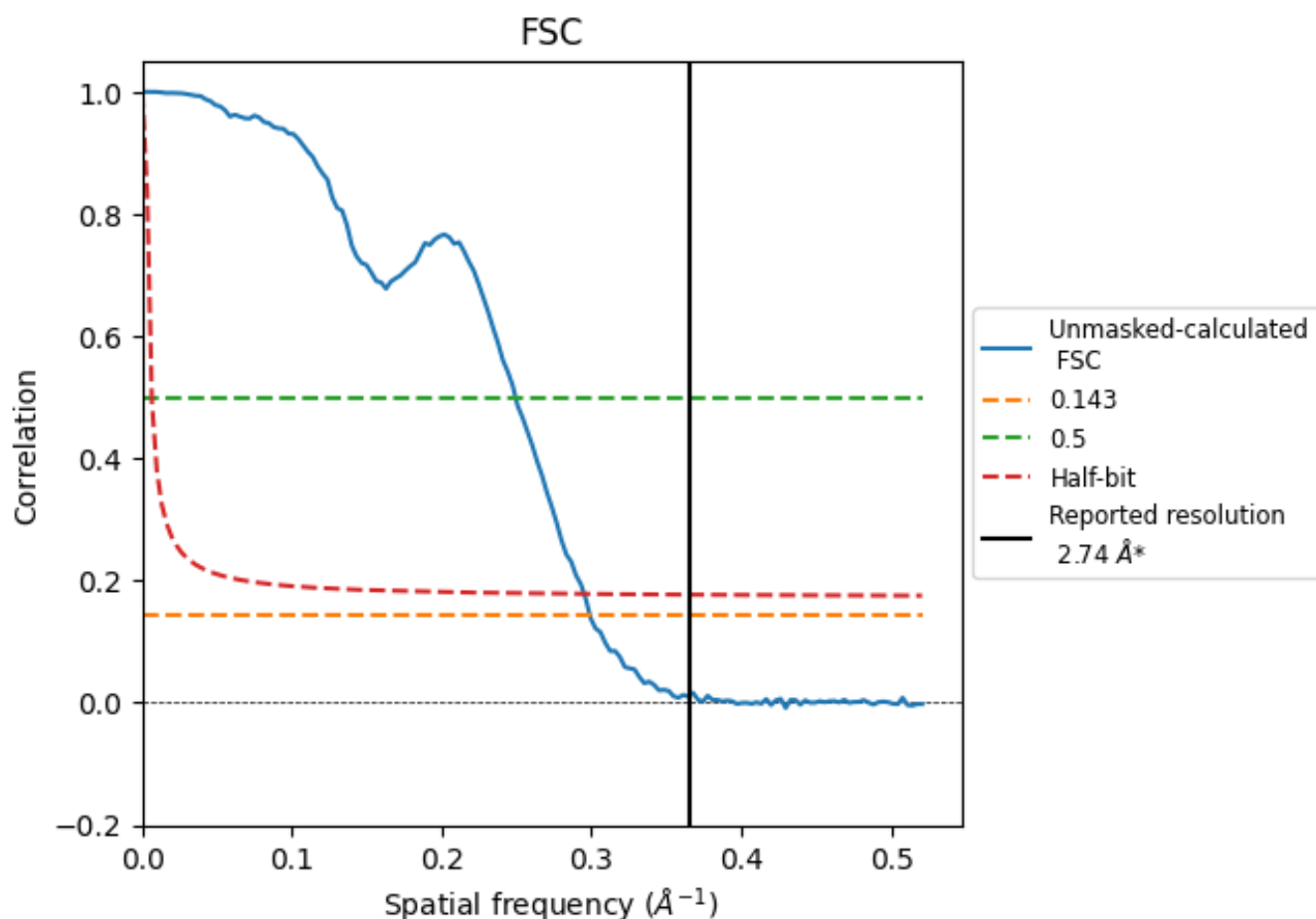


*Reported resolution corresponds to spatial frequency of 0.365 \AA^{-1}

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 0.365 \AA^{-1}

8.2 Resolution estimates [i](#)

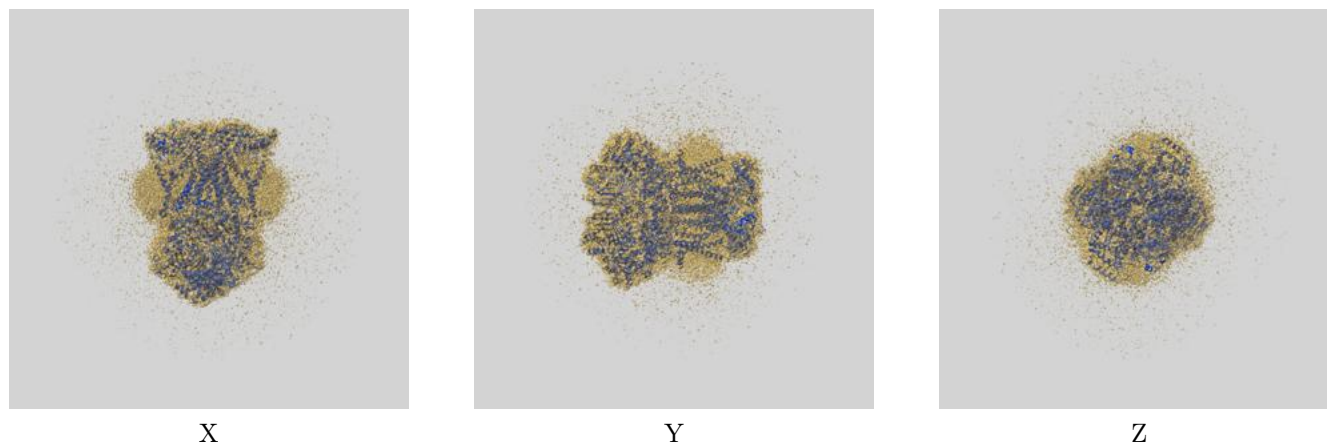
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	4.01	3.39

*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 3.34 differs from the reported value 2.74 by more than 10 %

9 Map-model fit [i](#)

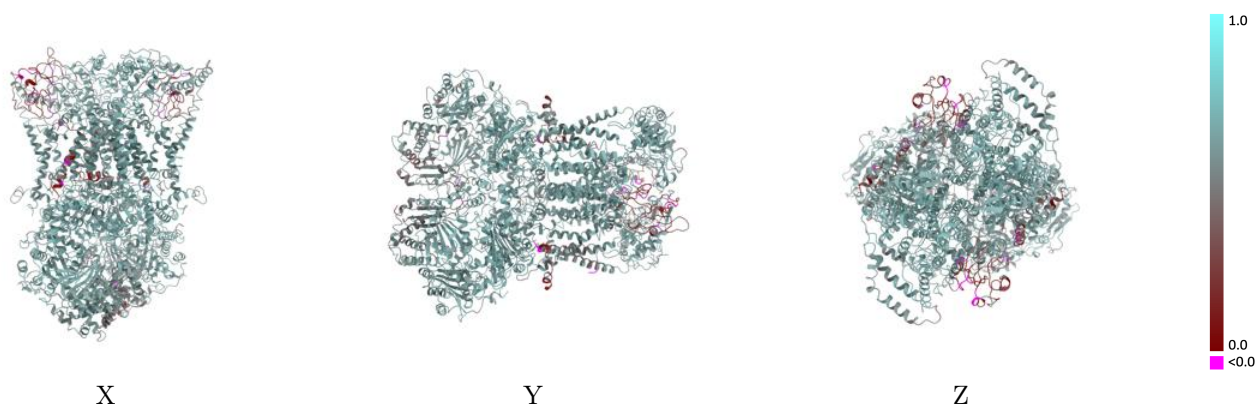
This section contains information regarding the fit between EMDB map EMD-60307 and PDB model 8ZOM. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



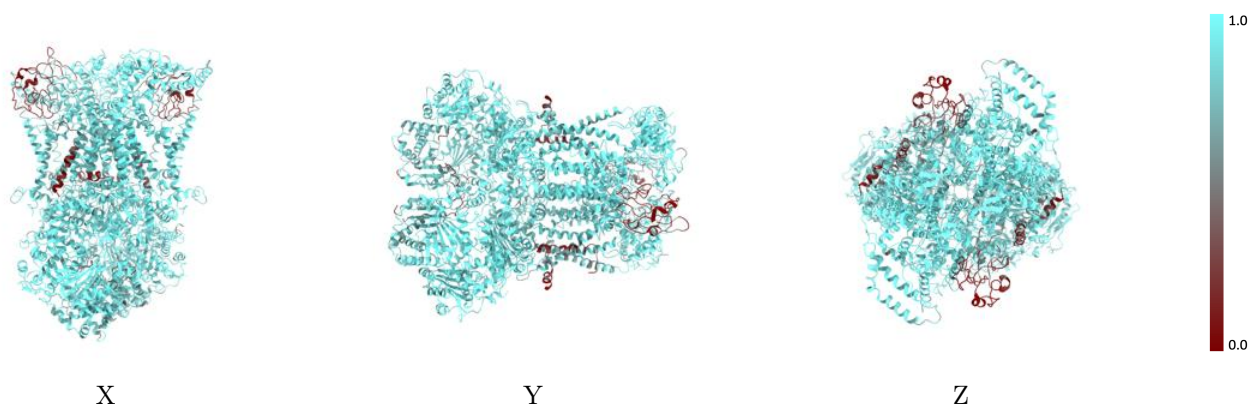
The images above show the 3D surface view of the map at the recommended contour level 0.586 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



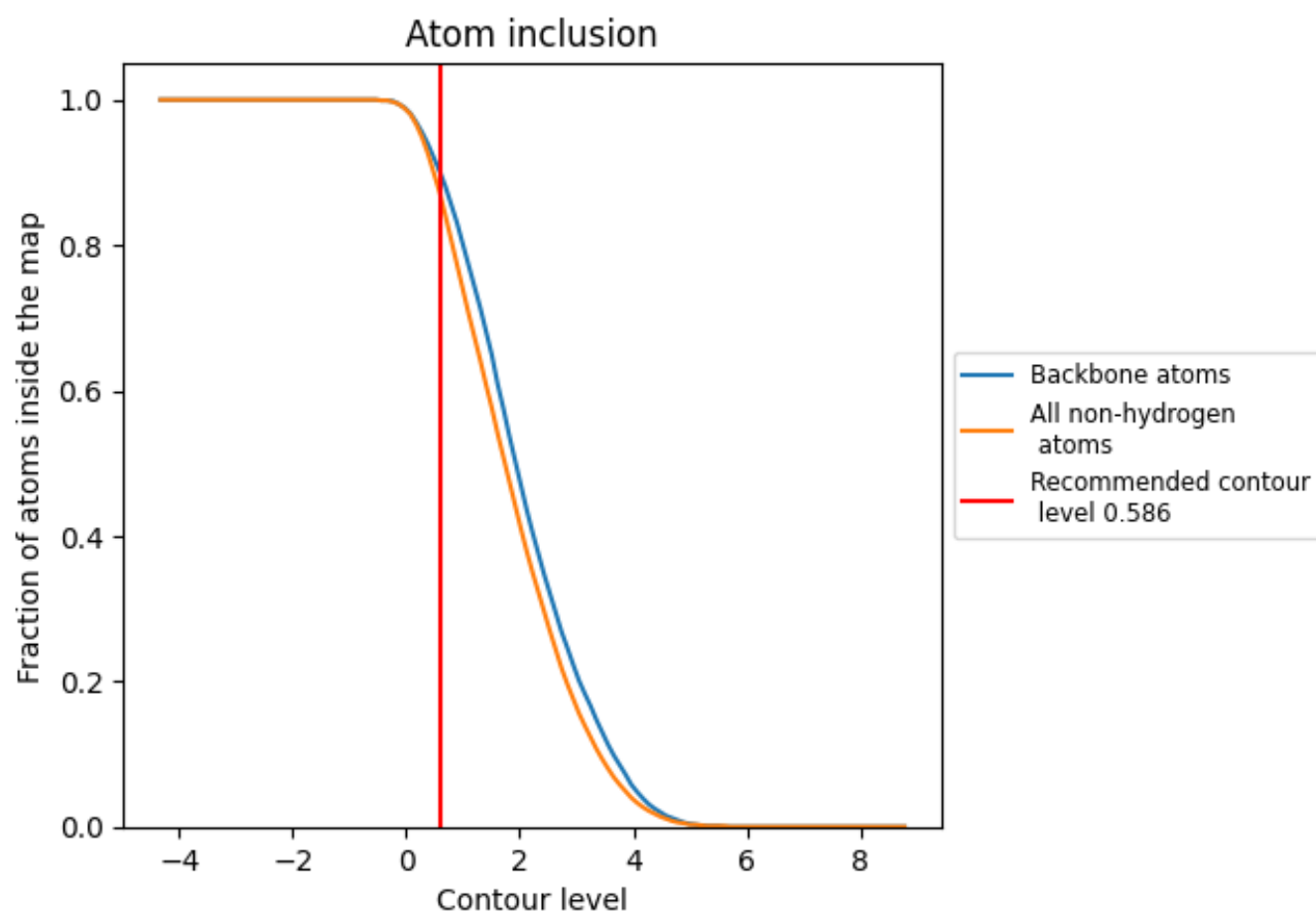
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.586).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.586) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.5780
A	 0.8730	 0.5630
B	 0.9450	 0.6170
C	 0.9530	 0.6290
D	 0.9740	 0.6310
E	 0.4790	 0.3750
F	 0.9680	 0.6350
G	 0.8810	 0.5880
H	 0.8910	 0.5660
J	 0.7010	 0.5000
K	 0.2300	 0.2620
M	 0.8720	 0.5620
N	 0.9370	 0.6180
O	 0.9610	 0.6330
P	 0.9720	 0.6300
Q	 0.4830	 0.3740
R	 0.9380	 0.6270
S	 0.8850	 0.5890
T	 0.8830	 0.5650
V	 0.6900	 0.4890
W	 0.2150	 0.2390

