



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 11:49 am GMT

PDB ID : 7O3H
EMDB ID : EMD-12706
Title : Murine CIII2 focus-refined from supercomplex CIIII2
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2021-04-01
Resolution : 2.60 Å(reported)
Based on initial models : 1NTZ, 3L75

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
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) : 2.39

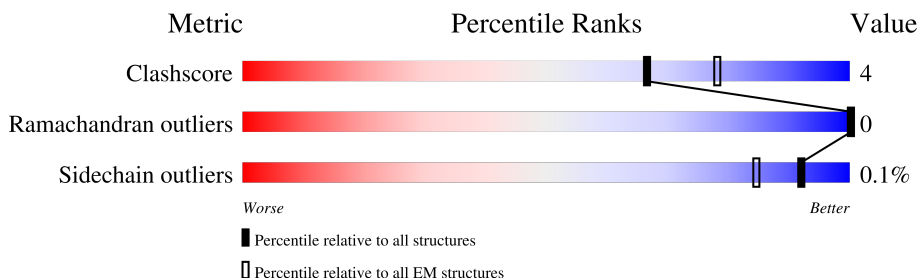
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	446	
1	L	446	
2	B	439	
2	M	439	
3	C	381	
3	N	381	
4	D	241	
4	O	241	

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Mol	Chain	Length	Quality of chain
5	E	196	
5	P	196	
6	F	110	
6	Q	110	
7	G	81	
7	R	81	
8	H	76	
8	S	76	
9	J	63	
9	U	63	
10	K	56	
10	V	56	
11	T	78	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 33700 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	446	Total	C	N	O	S	0	0
			3466	2167	611	671	17		
1	L	445	Total	C	N	O	S	0	0
			3460	2163	610	670	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		
2	M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		
3	N	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	241	Total	C	N	O	S	0	0
			1919	1224	329	352	14		
4	O	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		

- 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
			1512	952	263	290	7		
5	P	196	Total	C	N	O	S	0	0
			1512	952	263	290	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	102	Total	C	N	O	S	0	0
			900	575	160	162	3		
6	Q	101	Total	C	N	O	S	0	0
			894	572	159	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	80	Total	C	N	O	S	0	0
			674	434	124	115	1		
7	R	76	Total	C	N	O	S	0	0
			637	412	119	105	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	68	Total	C	N	O	S	0	0
			563	343	103	112	5		
8	S	68	Total	C	N	O	S	0	0
			563	343	103	112	5		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	60	Total	C	N	O	0	0
			495	323	86	86		
9	U	60	Total	C	N	O	0	0
			495	323	86	86		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

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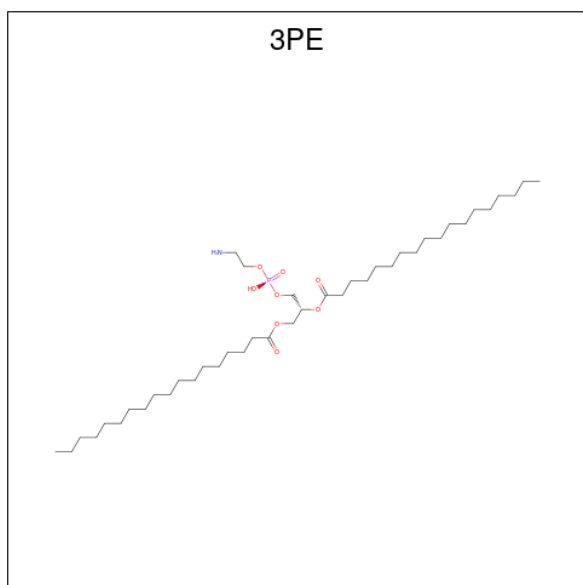
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Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	53	Total	C	N	O	S	0	0
			438	292	77	67	2		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	78	Total	C	N	O	S	0	0
			554	352	103	97	2		

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



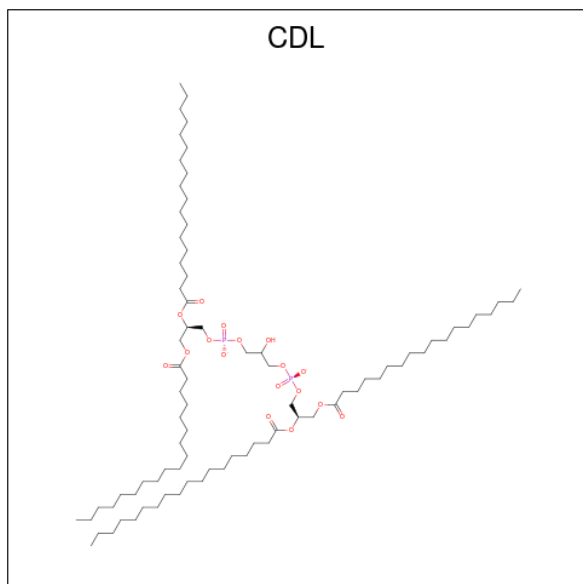
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			23	13	1	8	1	
12	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
12	G	1	Total	C	N	O	P	0
			51	41	1	8	1	
12	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
12	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
12	O	1	Total	C	N	O	P	0
			23	13	1	8	1	

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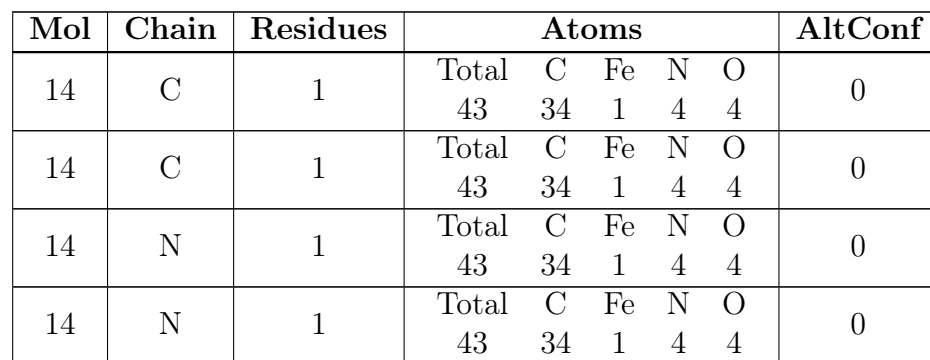
Mol	Chain	Residues	Atoms					AltConf
12	R	1	Total	C	N	O	P	0
			51	41	1	8	1	

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

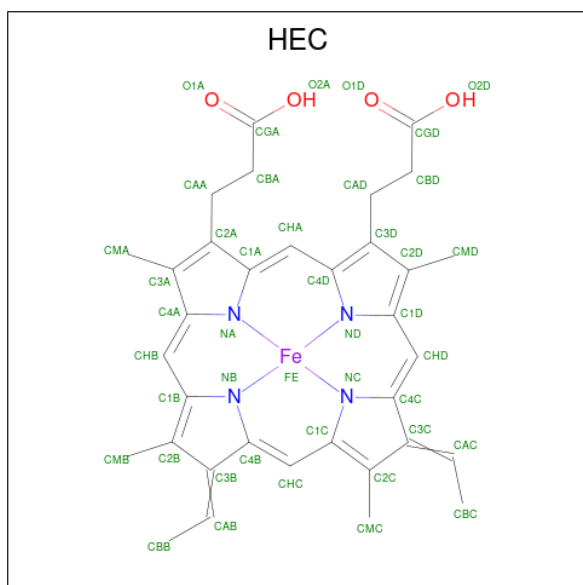


Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			46	27	17	2	
13	G	1	Total	C	O	P	0
			42	23	17	2	
13	G	1	Total	C	O	P	0
			56	37	17	2	
13	N	1	Total	C	O	P	0
			46	27	17	2	
13	O	1	Total	C	O	P	0
			57	38	17	2	
13	R	1	Total	C	O	P	0
			41	22	17	2	

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

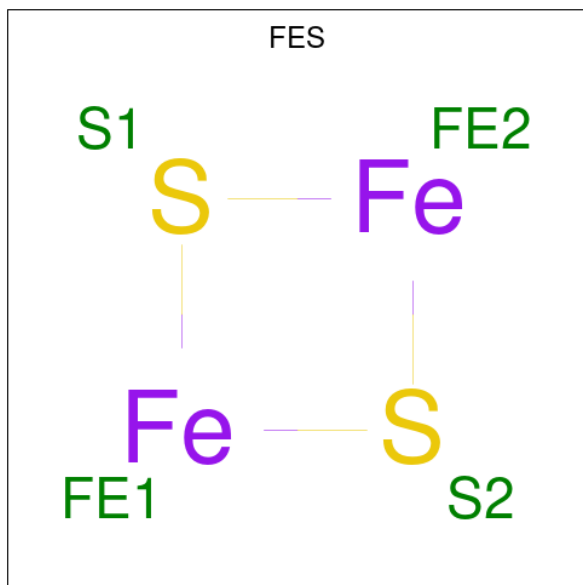


- Molecule 15 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



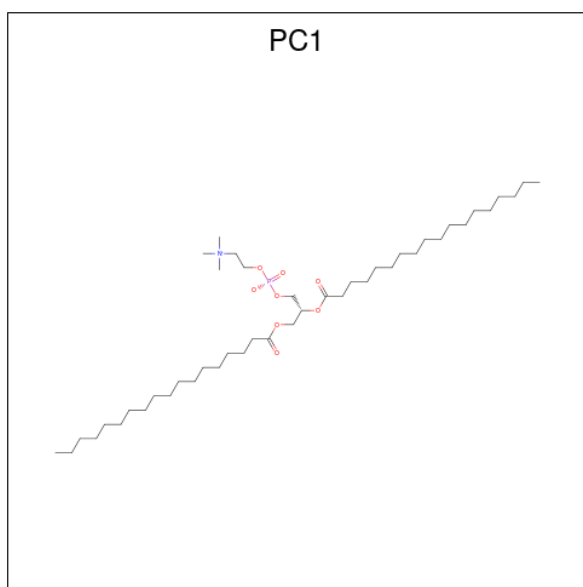
Mol	Chain	Residues	Atoms					AltConf
15	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
16	E	1	Total	Fe	S	0
			4	2	2	
16	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $\text{C}_{44}\text{H}_{88}\text{NO}_8\text{P}$).

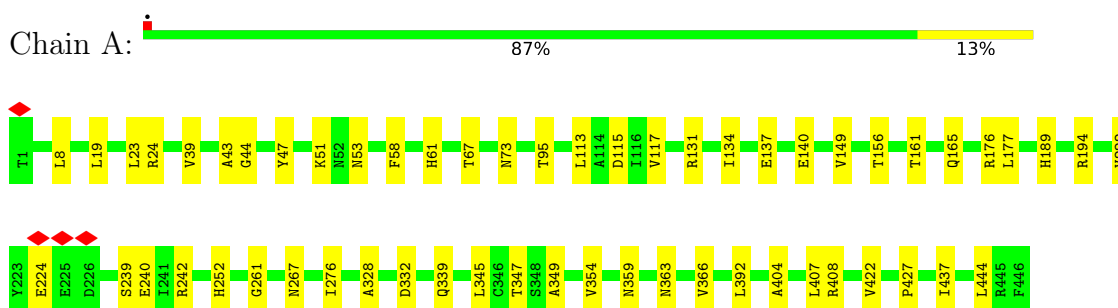


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	J	1	35	25	1	8	1	0
17	P	1	24	14	1	8	1	0

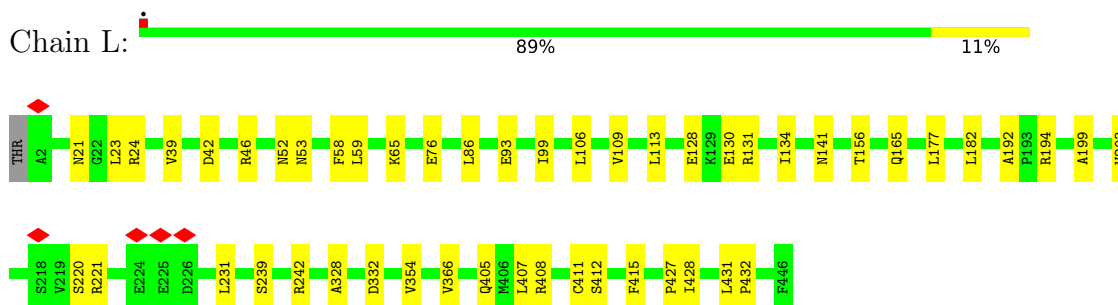
3 Residue-property plots [i](#)

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

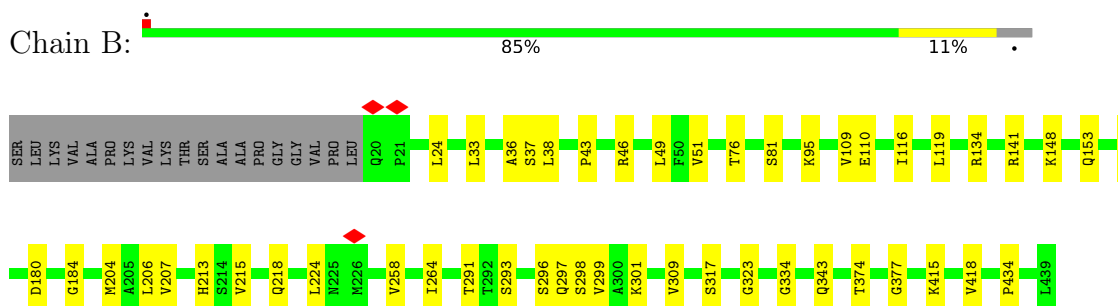
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



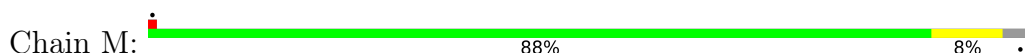
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



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



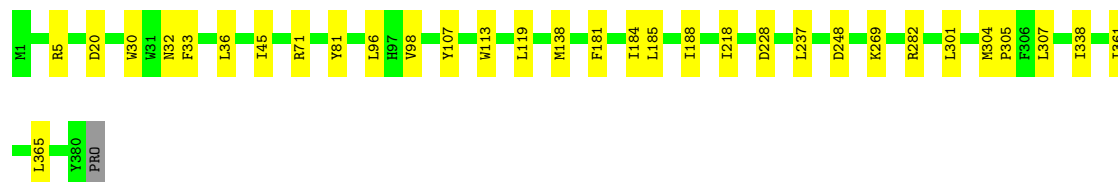
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





- Molecule 3: Cytochrome b

Chain C: 91% 8%



- Molecule 3: Cytochrome b

Chain N: 90% 9%



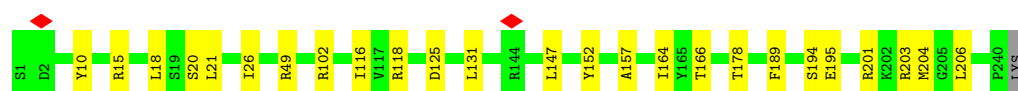
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 91% 9%



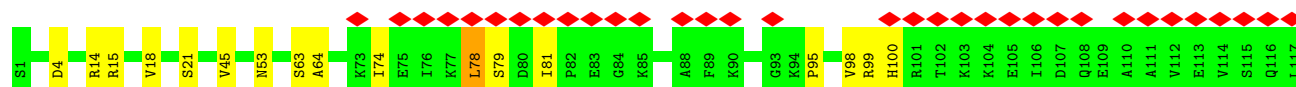
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

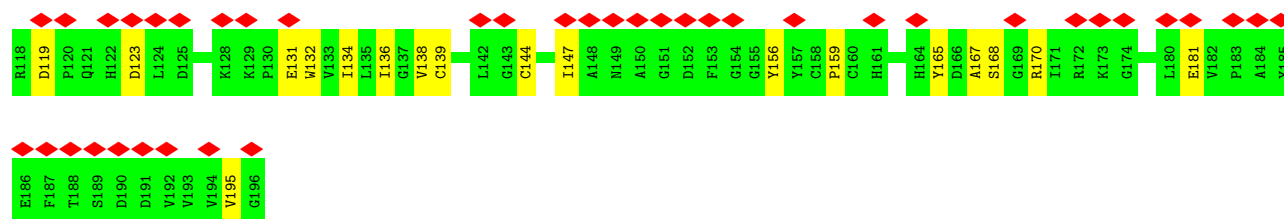
Chain O: 89% 10%



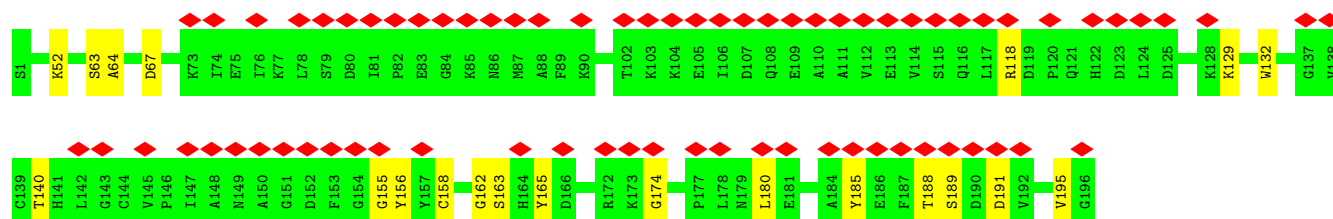
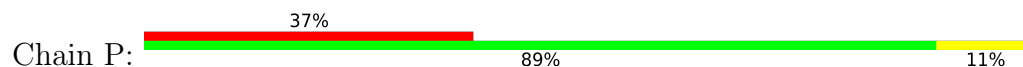
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 37% 82% 17%

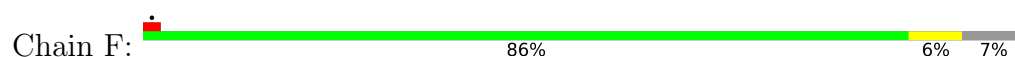




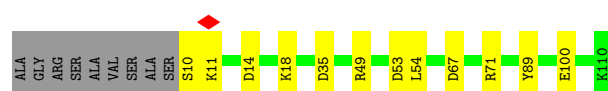
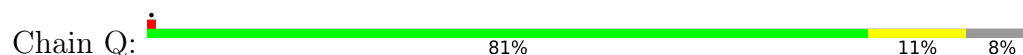
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



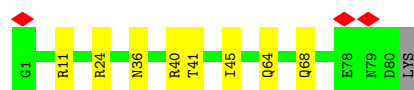
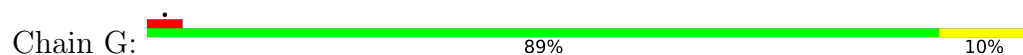
- Molecule 6: Cytochrome b-c1 complex subunit 7



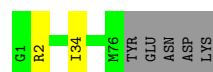
- Molecule 6: Cytochrome b-c1 complex subunit 7



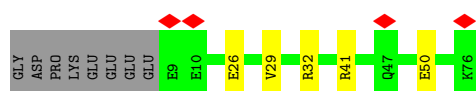
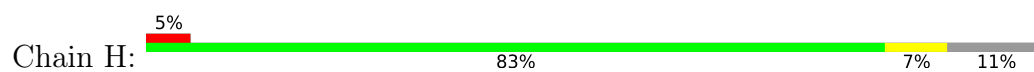
- Molecule 7: Cytochrome b-c1 complex subunit 8



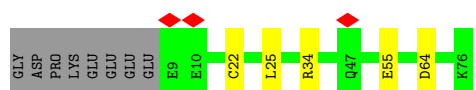
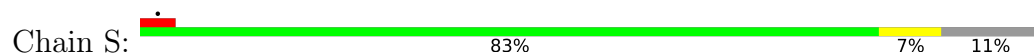
- Molecule 7: Cytochrome b-c1 complex subunit 8



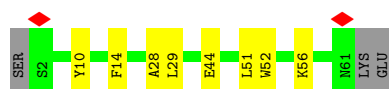
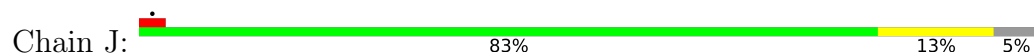
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



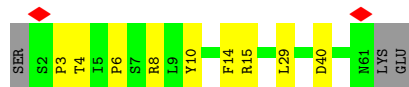
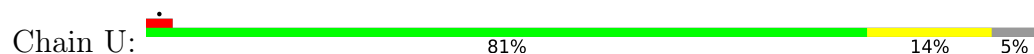
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



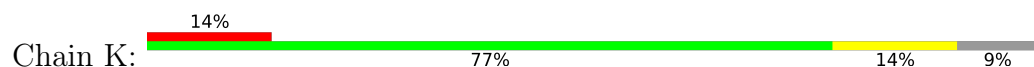
- Molecule 9: Cytochrome b-c1 complex subunit 9



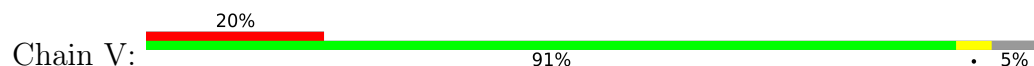
- Molecule 9: Cytochrome b-c1 complex subunit 9



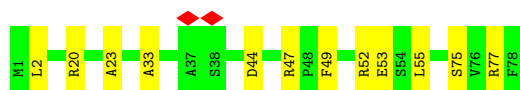
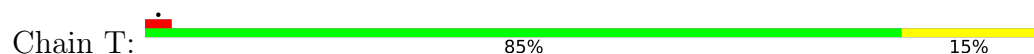
- Molecule 10: Cytochrome b-c1 complex subunit 10



- Molecule 10: Cytochrome b-c1 complex subunit 10



- Molecule 11: Cytochrome b-c1 complex subunit 9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	129	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 ($e^-/\text{\AA}^2$)	90.66	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.309	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	121.4548, 128.4522, 162.43954	wwPDB
Map dimensions	325, 257, 243	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.499814, 0.49981397, 0.49981397	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.29	0/3536	0.59	1/4803 (0.0%)
1	L	0.29	0/3530	0.61	2/4793 (0.0%)
2	B	0.28	0/3205	0.55	0/4332
2	M	0.30	0/3205	0.55	0/4332
3	C	0.30	0/3147	0.54	0/4297
3	N	0.30	0/3147	0.56	1/4297 (0.0%)
4	D	0.29	0/1978	0.53	0/2685
4	O	0.28	0/1968	0.53	0/2674
5	E	0.26	0/1545	0.58	1/2091 (0.0%)
5	P	0.28	0/1545	0.56	0/2091
6	F	0.27	0/922	0.55	0/1234
6	Q	0.28	0/916	0.57	0/1226
7	G	0.33	0/693	0.63	0/936
7	R	0.36	0/655	0.68	0/884
8	H	0.32	0/570	0.68	0/763
8	S	0.27	0/570	0.59	0/763
9	J	0.32	0/509	0.59	1/687 (0.1%)
9	U	0.29	0/509	0.59	1/687 (0.1%)
10	K	0.26	0/437	0.54	0/598
10	V	0.26	0/454	0.56	0/619
11	T	0.32	0/565	0.65	0/772
All	All	0.29	0/33606	0.57	7/45564 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ASP	CB-CG-OD1	9.51	126.86	118.30
1	L	332	ASP	CB-CG-OD1	8.58	126.02	118.30
5	E	78	LEU	CA-CB-CG	8.20	134.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	29	LEU	CA-CB-CG	6.10	129.33	115.30
3	N	377	LEU	CA-CB-CG	5.74	128.50	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3466	0	3377	33	0
1	L	3460	0	3367	30	0
2	B	3154	0	3158	29	0
2	M	3154	0	3158	23	0
3	C	3046	0	3112	20	0
3	N	3046	0	3112	23	0
4	D	1919	0	1867	17	0
4	O	1909	0	1854	18	0
5	E	1512	0	1495	21	0
5	P	1512	0	1495	13	0
6	F	900	0	887	5	0
6	Q	894	0	882	7	0
7	G	674	0	672	7	0
7	R	637	0	647	2	0
8	H	563	0	543	3	0
8	S	563	0	541	3	0
9	J	495	0	489	4	0
9	U	495	0	489	5	0
10	K	421	0	418	5	0
10	V	438	0	443	1	0
11	T	554	0	590	8	0
12	A	23	0	20	1	0
12	C	35	0	44	0	0
12	E	32	0	38	2	0
12	G	51	0	82	0	0
12	L	23	0	20	1	0
12	N	37	0	48	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	O	23	0	20	1	0
12	R	51	0	82	2	0
13	A	46	0	36	0	0
13	G	98	0	84	2	0
13	N	46	0	36	3	0
13	O	57	0	58	1	0
13	R	41	0	26	0	0
14	C	86	0	60	3	0
14	N	86	0	60	4	0
15	D	43	0	30	1	0
15	O	43	0	30	2	0
16	E	4	0	0	0	0
16	P	4	0	0	1	0
17	J	35	0	44	0	0
17	P	24	0	22	0	0
All	All	33700	0	33436	246	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 246 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)
3:N:98:VAL:HG22	14:N:402:HEM:HBC2	1.71	0.71
1:L:411:CYS:O	1:L:415:PHE:HB2	1.93	0.68
9:U:4:THR:HG22	9:U:6:PRO:HD2	1.76	0.67
3:C:98:VAL:HG22	14:C:402:HEM:HBC2	1.78	0.65
4:D:102:ARG:HE	4:D:109:LEU:HB2	1.62	0.64

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	444/446 (100%)	428 (96%)	16 (4%)	0	100	100
1	L	443/446 (99%)	432 (98%)	11 (2%)	0	100	100
2	B	418/439 (95%)	405 (97%)	13 (3%)	0	100	100
2	M	418/439 (95%)	402 (96%)	16 (4%)	0	100	100
3	C	378/381 (99%)	371 (98%)	7 (2%)	0	100	100
3	N	378/381 (99%)	370 (98%)	8 (2%)	0	100	100
4	D	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
4	O	238/241 (99%)	234 (98%)	4 (2%)	0	100	100
5	E	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
5	P	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
6	F	100/110 (91%)	100 (100%)	0	0	100	100
6	Q	99/110 (90%)	99 (100%)	0	0	100	100
7	G	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
7	R	74/81 (91%)	72 (97%)	2 (3%)	0	100	100
8	H	66/76 (87%)	65 (98%)	1 (2%)	0	100	100
8	S	66/76 (87%)	62 (94%)	4 (6%)	0	100	100
9	J	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
9	U	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
10	K	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
10	V	51/56 (91%)	51 (100%)	0	0	100	100
11	T	76/78 (97%)	69 (91%)	7 (9%)	0	100	100
All	All	4119/4256 (97%)	4004 (97%)	115 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/373 (100%)	372 (100%)	1 (0%)	91	97
1	L	372/373 (100%)	371 (100%)	1 (0%)	91	97
2	B	330/344 (96%)	330 (100%)	0	100	100
2	M	330/344 (96%)	330 (100%)	0	100	100
3	C	332/333 (100%)	332 (100%)	0	100	100
3	N	332/333 (100%)	331 (100%)	1 (0%)	91	97
4	D	206/206 (100%)	206 (100%)	0	100	100
4	O	205/206 (100%)	205 (100%)	0	100	100
5	E	166/166 (100%)	166 (100%)	0	100	100
5	P	166/166 (100%)	166 (100%)	0	100	100
6	F	94/98 (96%)	94 (100%)	0	100	100
6	Q	93/98 (95%)	93 (100%)	0	100	100
7	G	72/73 (99%)	72 (100%)	0	100	100
7	R	68/73 (93%)	68 (100%)	0	100	100
8	H	65/72 (90%)	65 (100%)	0	100	100
8	S	65/72 (90%)	65 (100%)	0	100	100
9	J	51/54 (94%)	51 (100%)	0	100	100
9	U	51/54 (94%)	51 (100%)	0	100	100
10	K	41/46 (89%)	41 (100%)	0	100	100
10	V	43/46 (94%)	42 (98%)	1 (2%)	45	71
11	T	58/58 (100%)	58 (100%)	0	100	100
All	All	3513/3588 (98%)	3509 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	L	24	ARG
3	N	331	ASN
10	V	39	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN

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Mol	Chain	Res	Type
1	A	53	ASN
7	G	36	ASN
7	G	68	GLN
1	L	53	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	HEC	O	303	4	32,50,50	2.17	3 (9%)	24,82,82	1.74	4 (16%)
14	HEM	C	402	3	41,50,50	1.26	3 (7%)	45,82,82	1.71	8 (17%)
15	HEC	D	301	4	32,50,50	2.18	3 (9%)	24,82,82	1.65	5 (20%)
12	3PE	N	403	-	36,36,50	0.35	0	39,41,55	0.32	0
13	CDL	G	102	-	55,55,99	0.39	0	61,67,111	0.33	0
16	FES	P	201	5	0,4,4	-	-	-	-	-
12	3PE	E	201	-	31,31,50	0.38	0	34,36,55	0.38	0
13	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.32	0
12	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEM	N	401	3	41,50,50	1.23	4 (9%)	45,82,82	1.71	8 (17%)
17	PC1	P	202	-	23,23,53	0.45	0	29,31,61	0.70	1 (3%)
13	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.37	0
12	3PE	R	102	-	50,50,50	0.33	0	53,55,55	0.59	1 (1%)
14	HEM	N	402	3	41,50,50	1.26	3 (7%)	45,82,82	1.70	9 (20%)
12	3PE	O	302	-	22,22,50	0.44	0	25,27,55	0.40	0
16	FES	E	202	5	0,4,4	-	-	-	-	-
12	3PE	L	501	-	22,22,50	0.43	0	25,27,55	0.40	0
12	3PE	A	501	-	22,22,50	0.46	0	25,27,55	0.73	1 (4%)
13	CDL	N	404	-	45,45,99	0.44	0	51,57,111	0.55	1 (1%)
12	3PE	G	103	-	50,50,50	0.31	0	53,55,55	0.29	0
13	CDL	G	101	-	41,41,99	0.45	0	47,53,111	0.35	0
14	HEM	C	401	3	41,50,50	1.24	4 (9%)	45,82,82	1.69	8 (17%)
17	PC1	J	101	-	34,34,53	0.35	0	40,42,61	0.37	0
13	CDL	R	101	-	40,40,99	0.47	0	46,52,111	0.58	1 (2%)

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	HEC	O	303	4	-	2/10/54/54	-
14	HEM	C	402	3	-	6/12/54/54	-
15	HEC	D	301	4	-	0/10/54/54	-
12	3PE	N	403	-	-	4/40/40/54	-
13	CDL	G	102	-	-	13/66/66/110	-
16	FES	P	201	5	-	-	0/1/1/1
12	3PE	E	201	-	-	8/35/35/54	-
13	CDL	O	301	-	-	19/67/67/110	-
12	3PE	C	403	-	-	2/38/38/54	-
14	HEM	N	401	3	-	7/12/54/54	-
17	PC1	P	202	-	-	12/27/27/57	-
13	CDL	A	502	-	-	17/56/56/110	-
12	3PE	R	102	-	-	10/54/54/54	-
14	HEM	N	402	3	-	6/12/54/54	-
12	3PE	O	302	-	-	10/26/26/54	-
16	FES	E	202	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	3PE	L	501	-	-	7/26/26/54	-
12	3PE	A	501	-	-	7/26/26/54	-
13	CDL	N	404	-	-	5/56/56/110	-
12	3PE	G	103	-	-	10/54/54/54	-
13	CDL	G	101	-	-	14/52/52/110	-
14	HEM	C	401	3	-	7/12/54/54	-
17	PC1	J	101	-	-	7/38/38/57	-
13	CDL	R	101	-	-	10/51/51/110	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	301	HEC	C3C-C2C	-6.35	1.34	1.40
15	O	303	HEC	C3C-C2C	-6.35	1.34	1.40
15	D	301	HEC	C2B-C3B	-6.31	1.34	1.40
15	O	303	HEC	C2B-C3B	-6.26	1.34	1.40
15	D	301	HEC	C3D-C2D	5.39	1.53	1.37

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	401	HEM	CHC-C4B-NB	4.80	129.65	124.43
14	C	401	HEM	CHC-C4B-NB	4.71	129.55	124.43
14	N	402	HEM	C4D-ND-C1D	4.43	109.65	105.07
14	C	402	HEM	CHC-C4B-NB	4.32	129.12	124.43
14	C	402	HEM	C4D-ND-C1D	4.31	109.53	105.07

There are no chirality outliers.

5 of 183 torsion outliers are listed below:

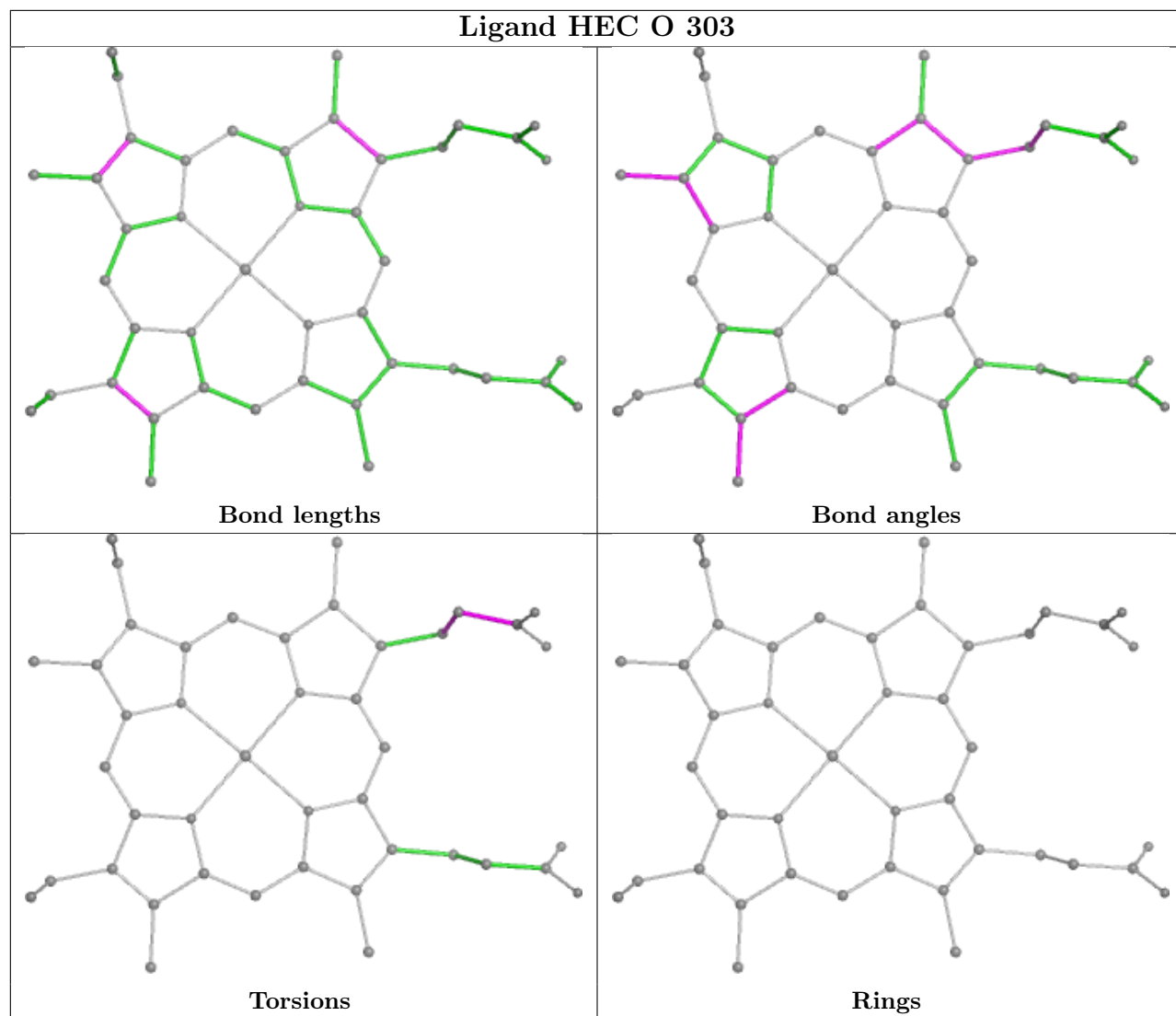
Mol	Chain	Res	Type	Atoms
12	A	501	3PE	C11-O13-P-O12
12	A	501	3PE	O13-C11-C12-N
12	C	403	3PE	C11-O13-P-O14
12	G	103	3PE	C1-O11-P-O12
12	G	103	3PE	C1-O11-P-O14

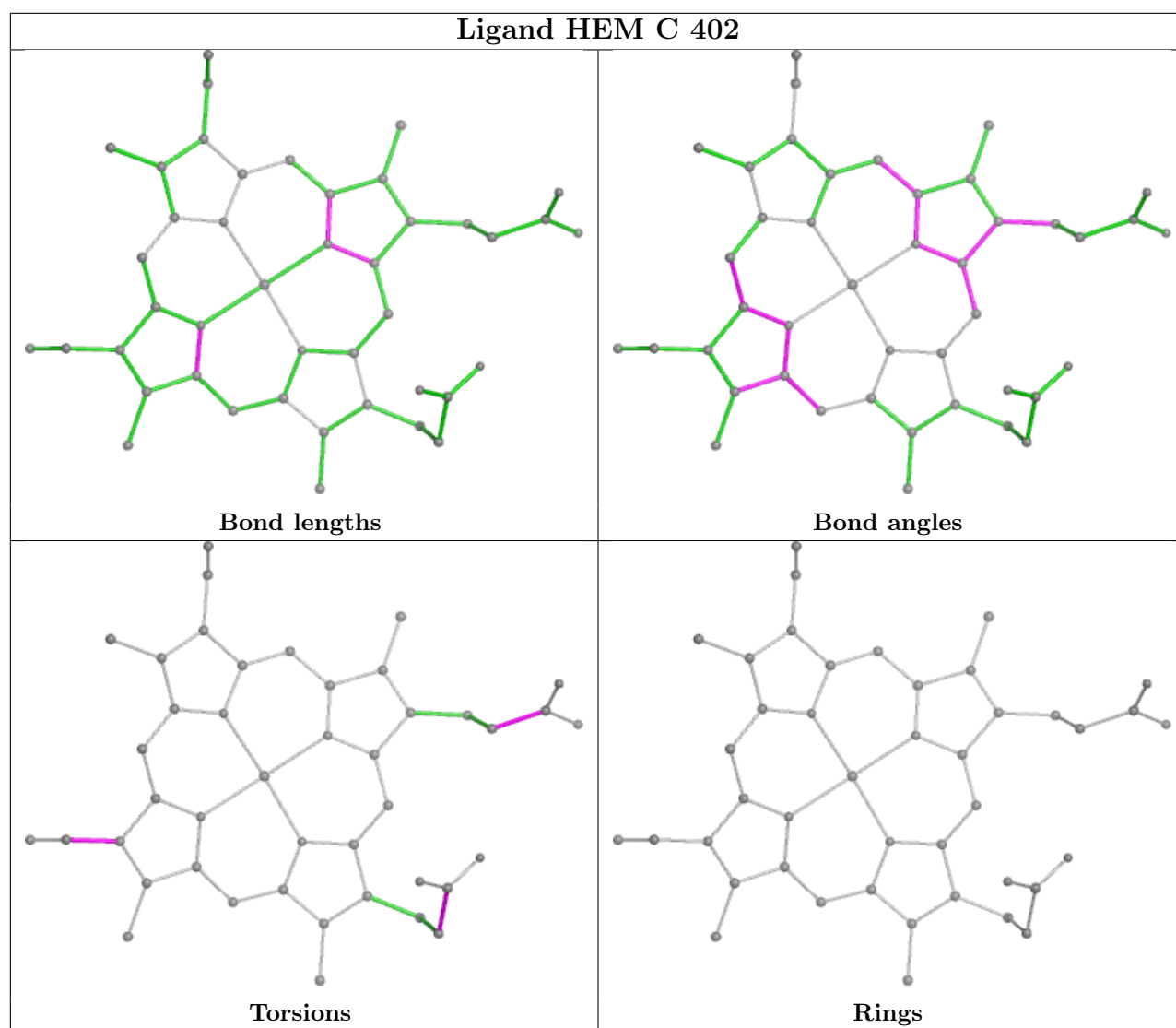
There are no ring outliers.

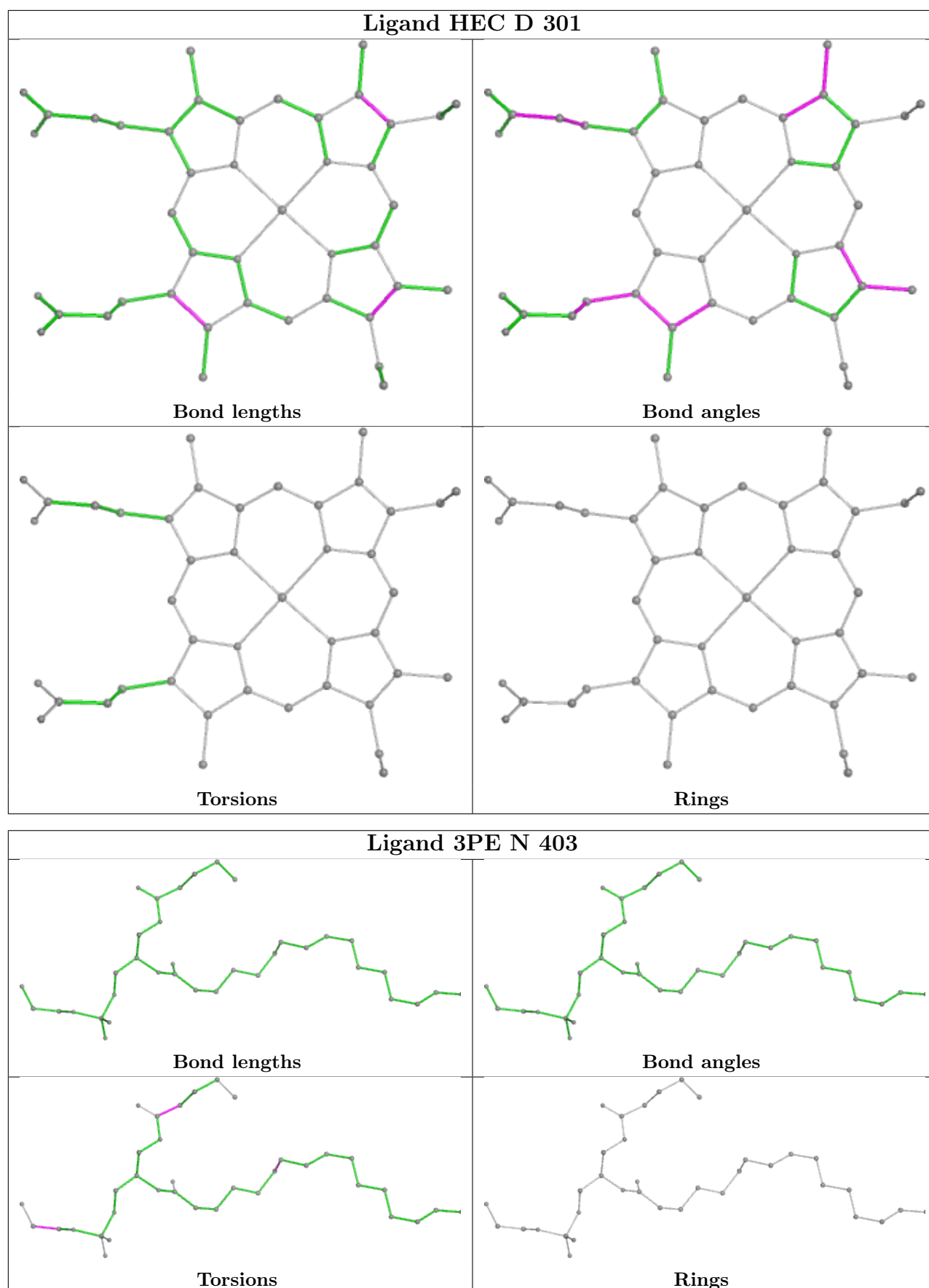
16 monomers are involved in 23 short contacts:

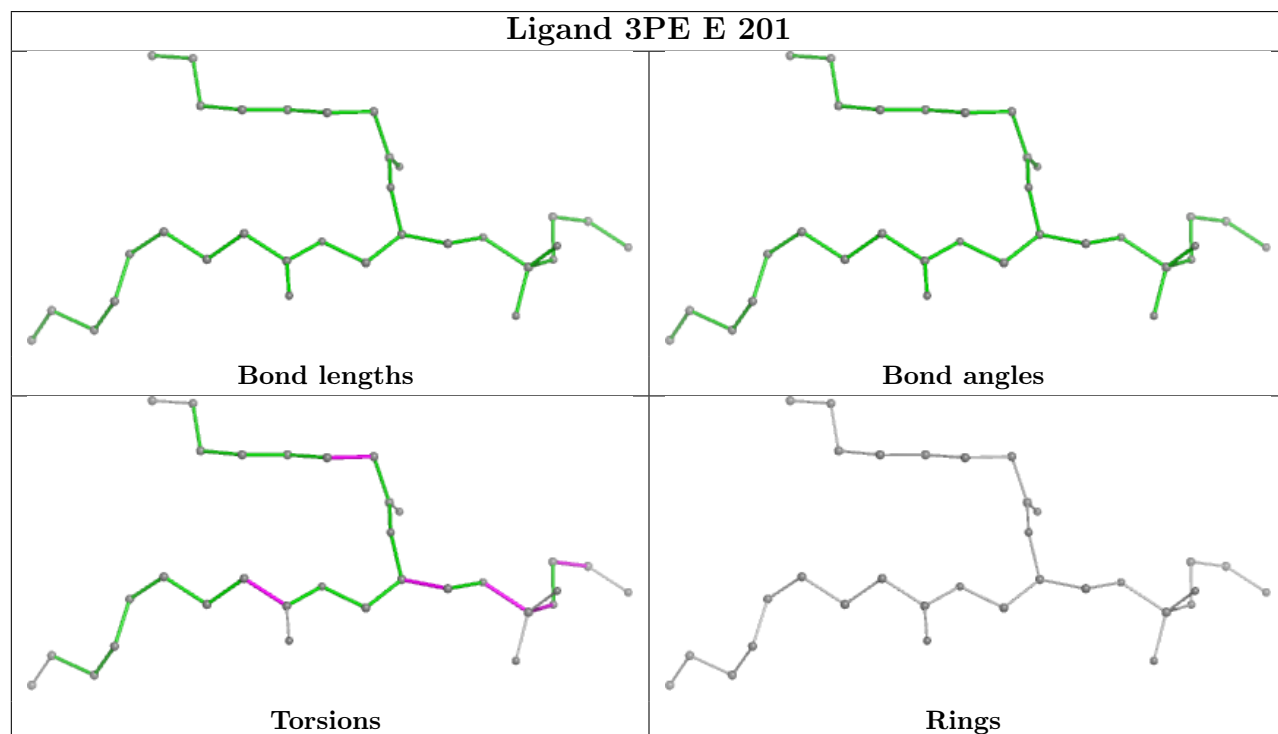
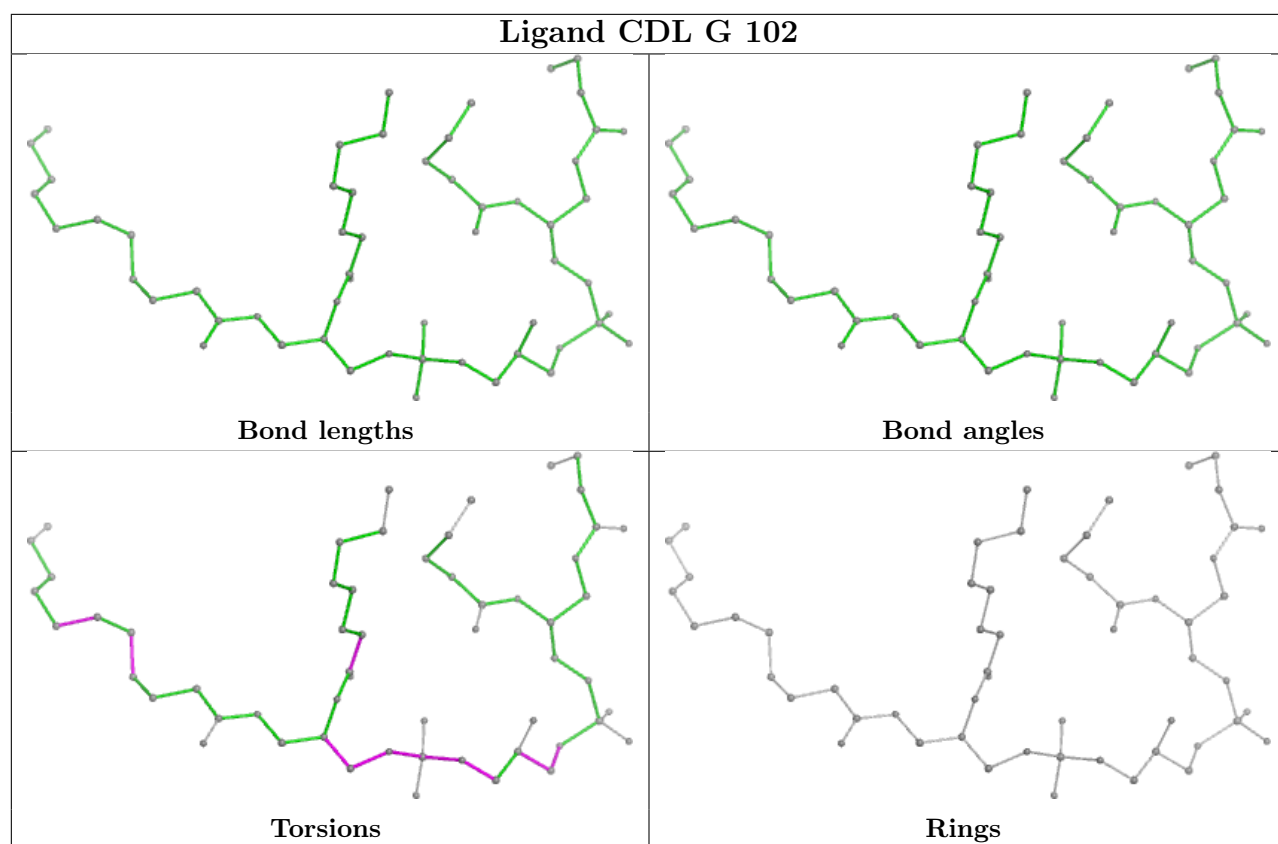
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	O	303	HEC	2	0
14	C	402	HEM	2	0
15	D	301	HEC	1	0
13	G	102	CDL	1	0
16	P	201	FES	1	0
12	E	201	3PE	2	0
13	O	301	CDL	1	0
14	N	401	HEM	2	0
12	R	102	3PE	2	0
14	N	402	HEM	2	0
12	O	302	3PE	1	0
12	L	501	3PE	1	0
12	A	501	3PE	1	0
13	N	404	CDL	3	0
13	G	101	CDL	1	0
14	C	401	HEM	1	0

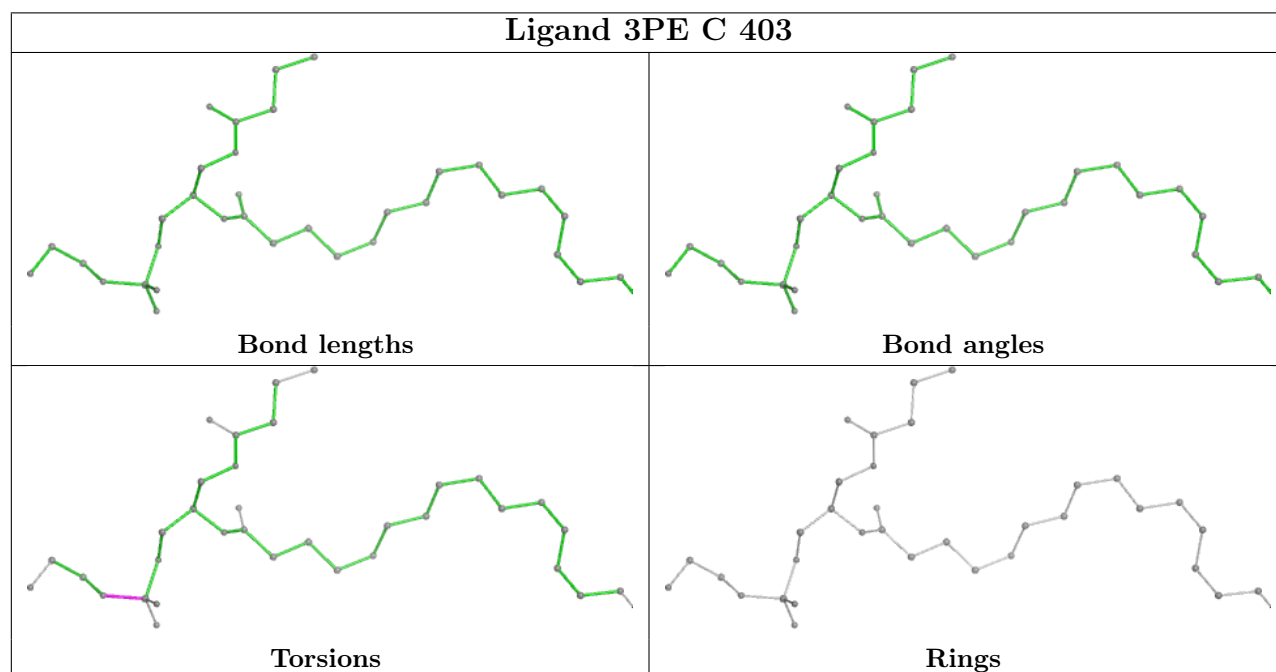
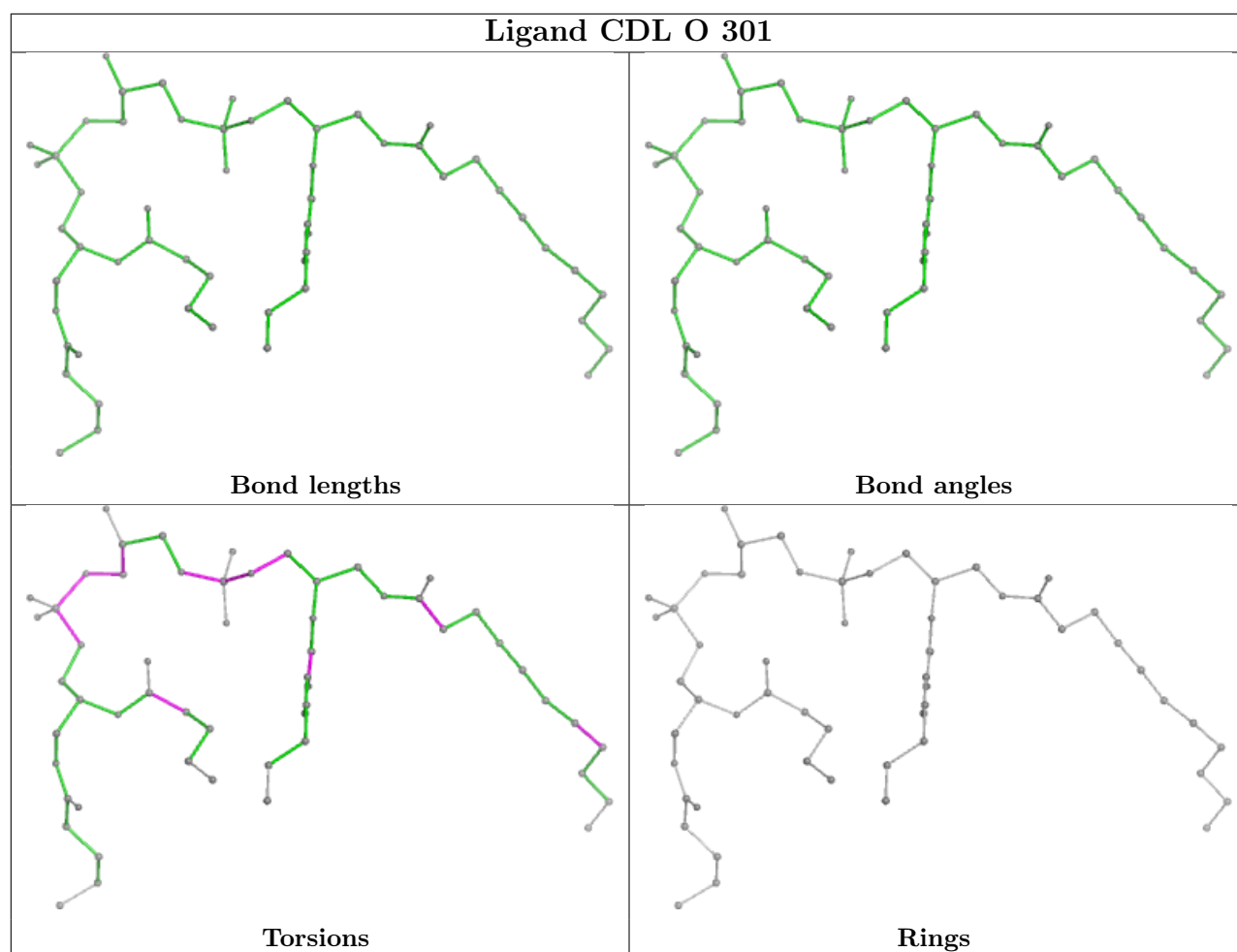
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

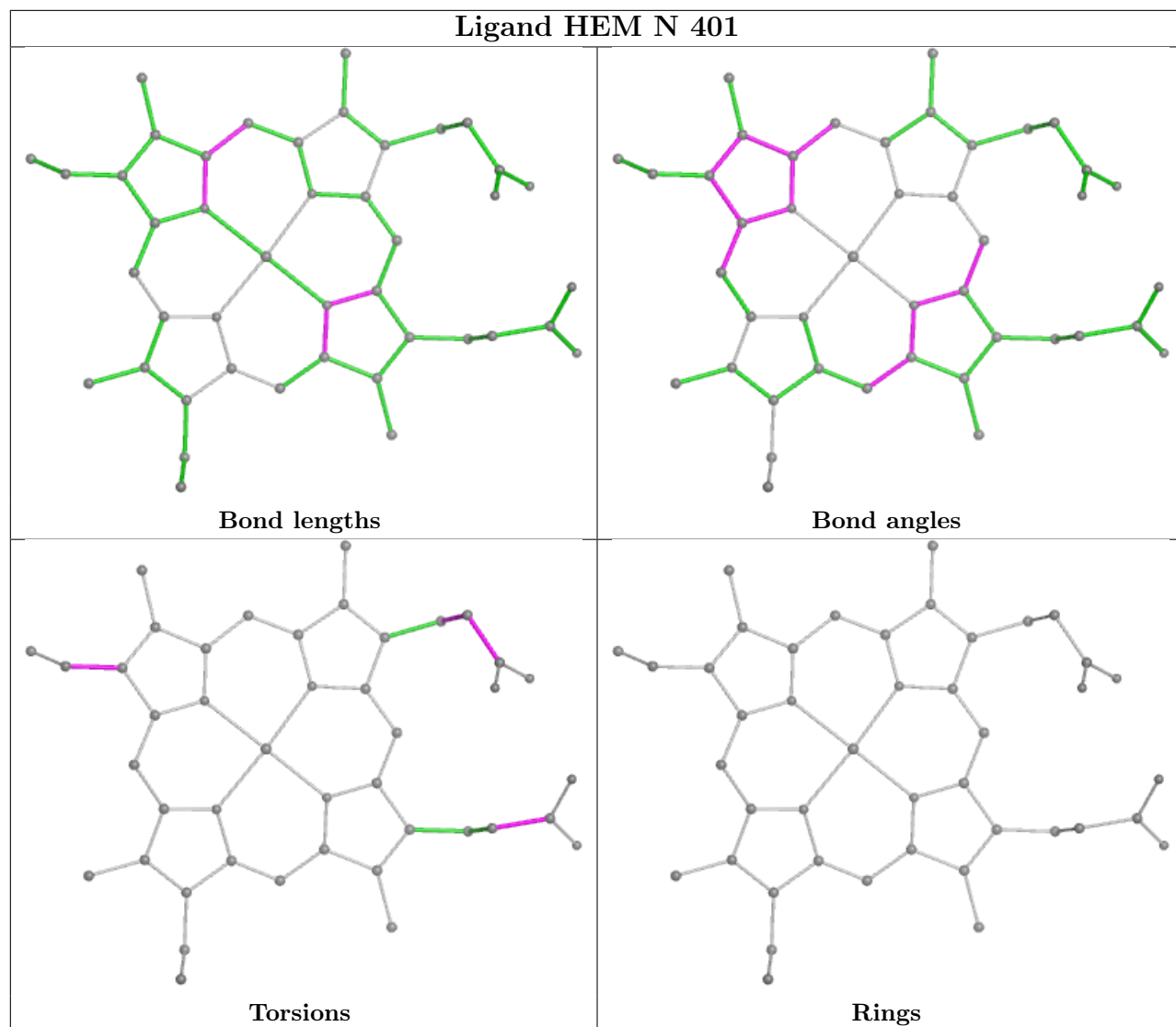


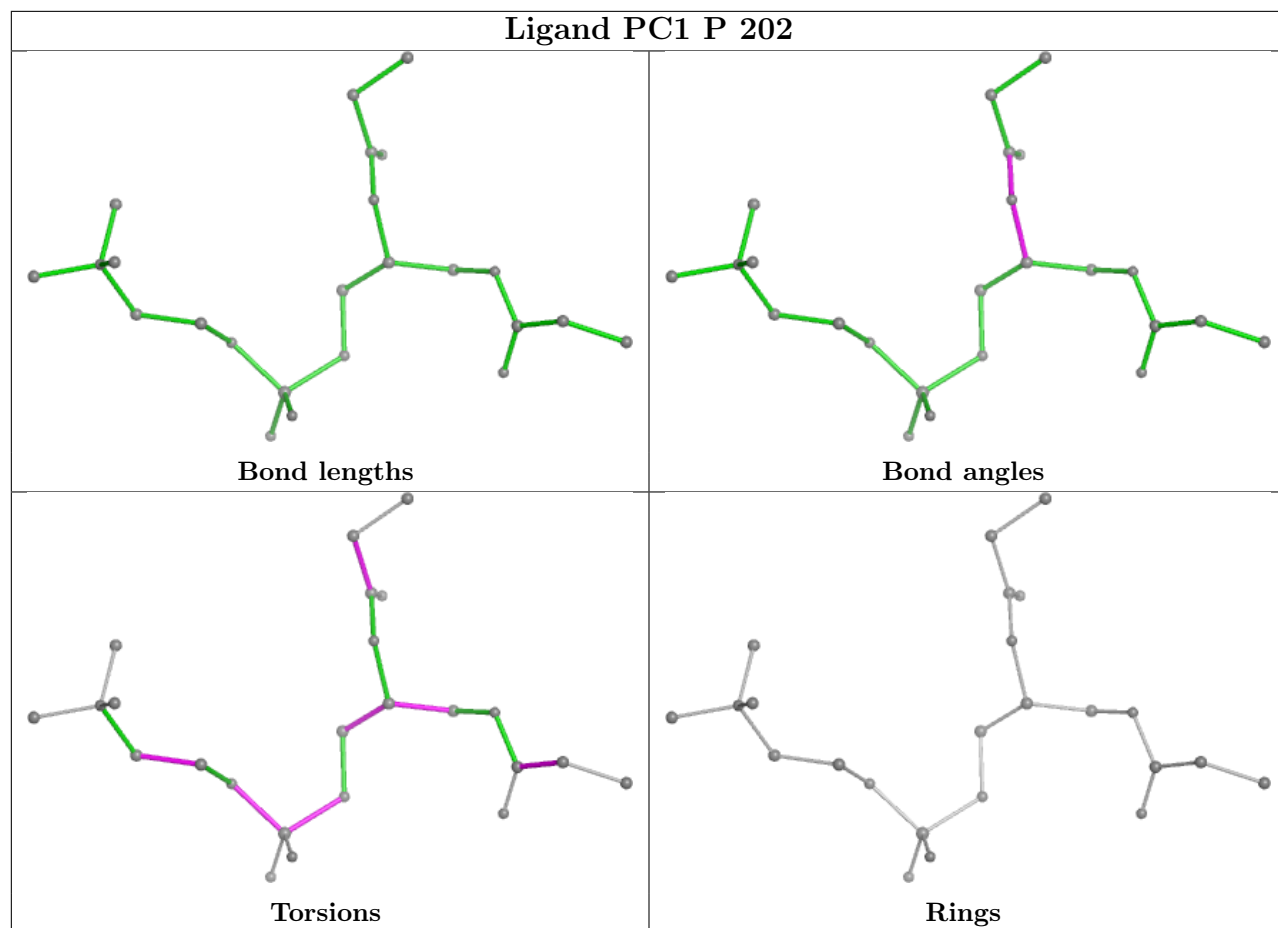


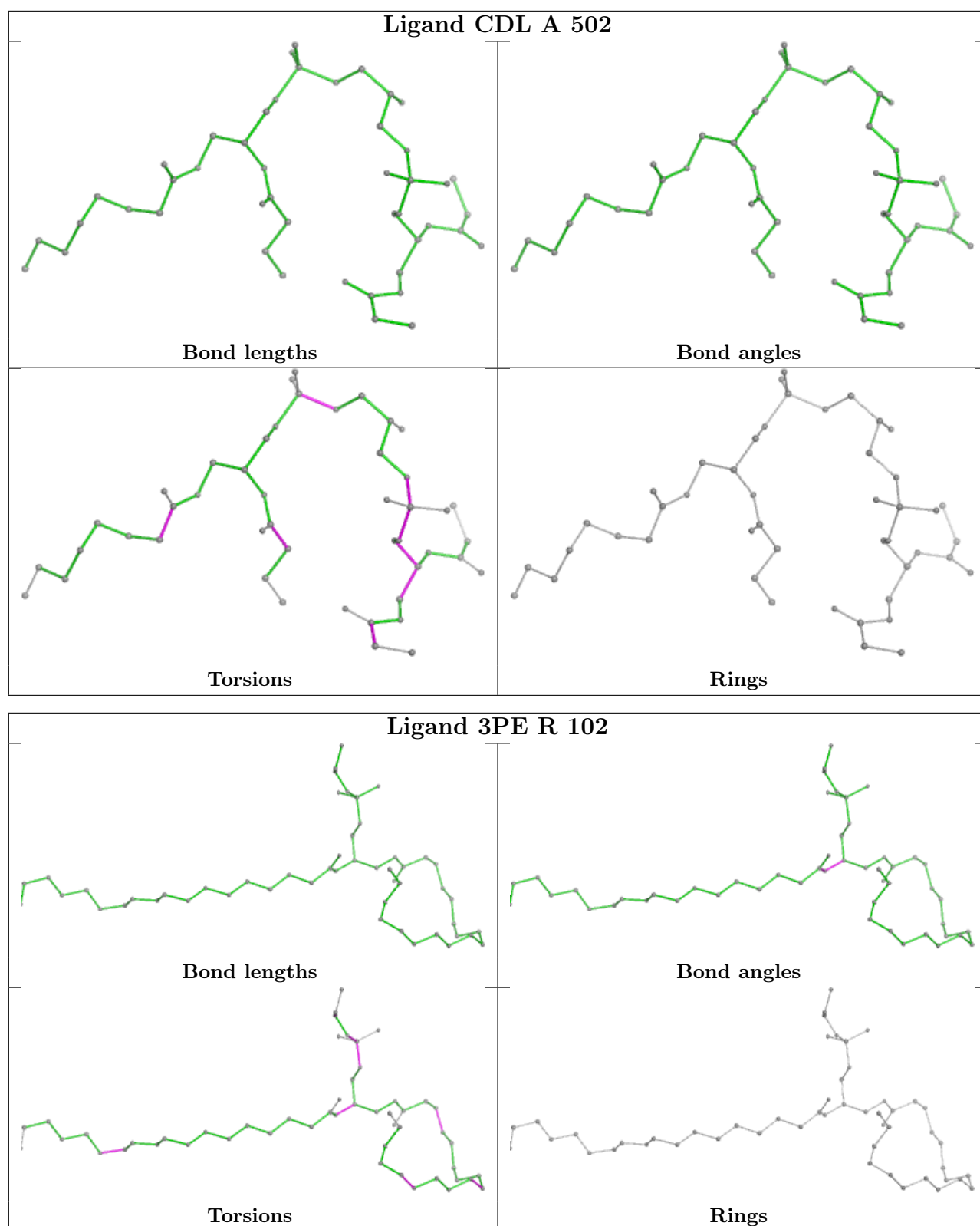


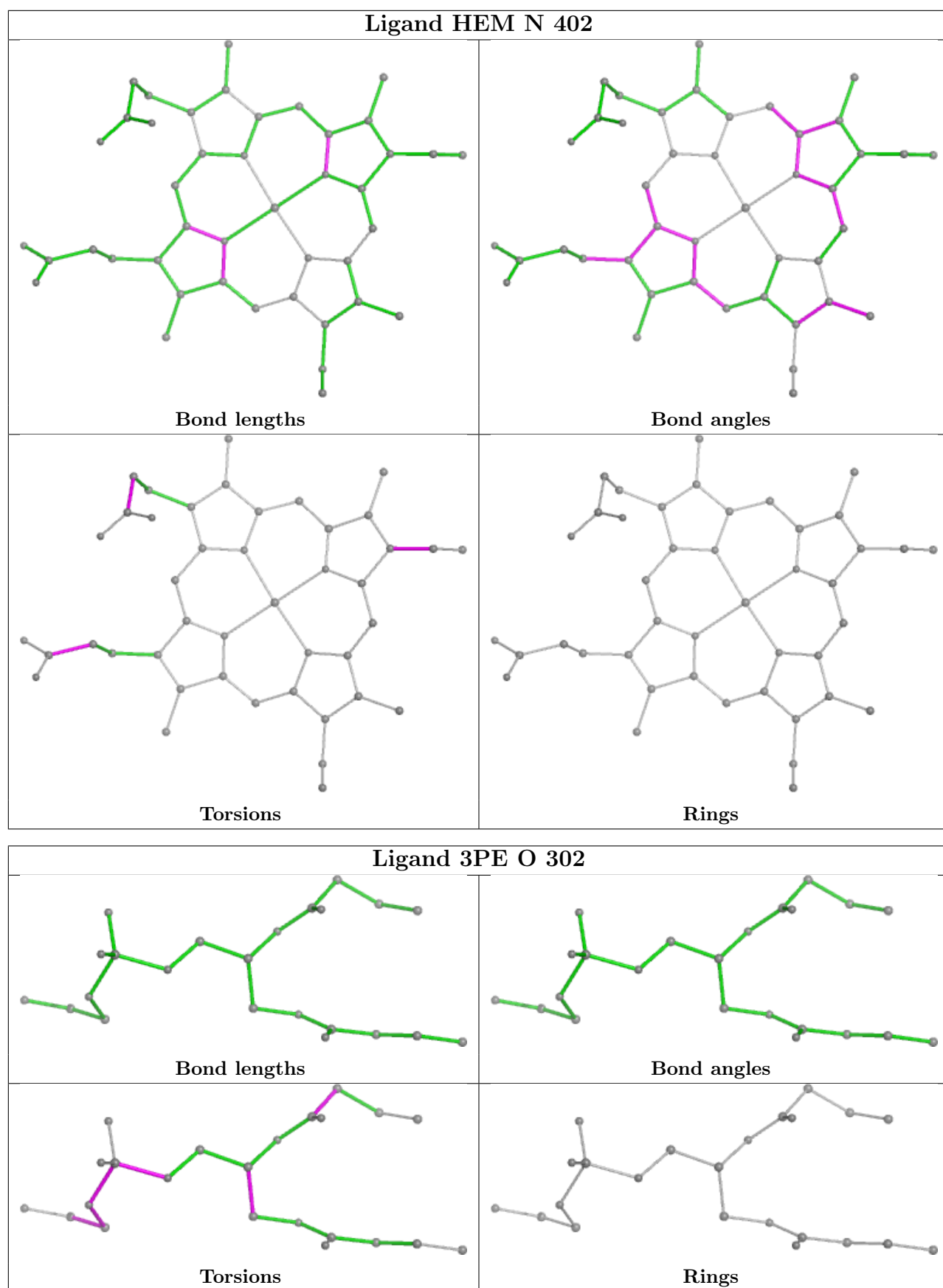




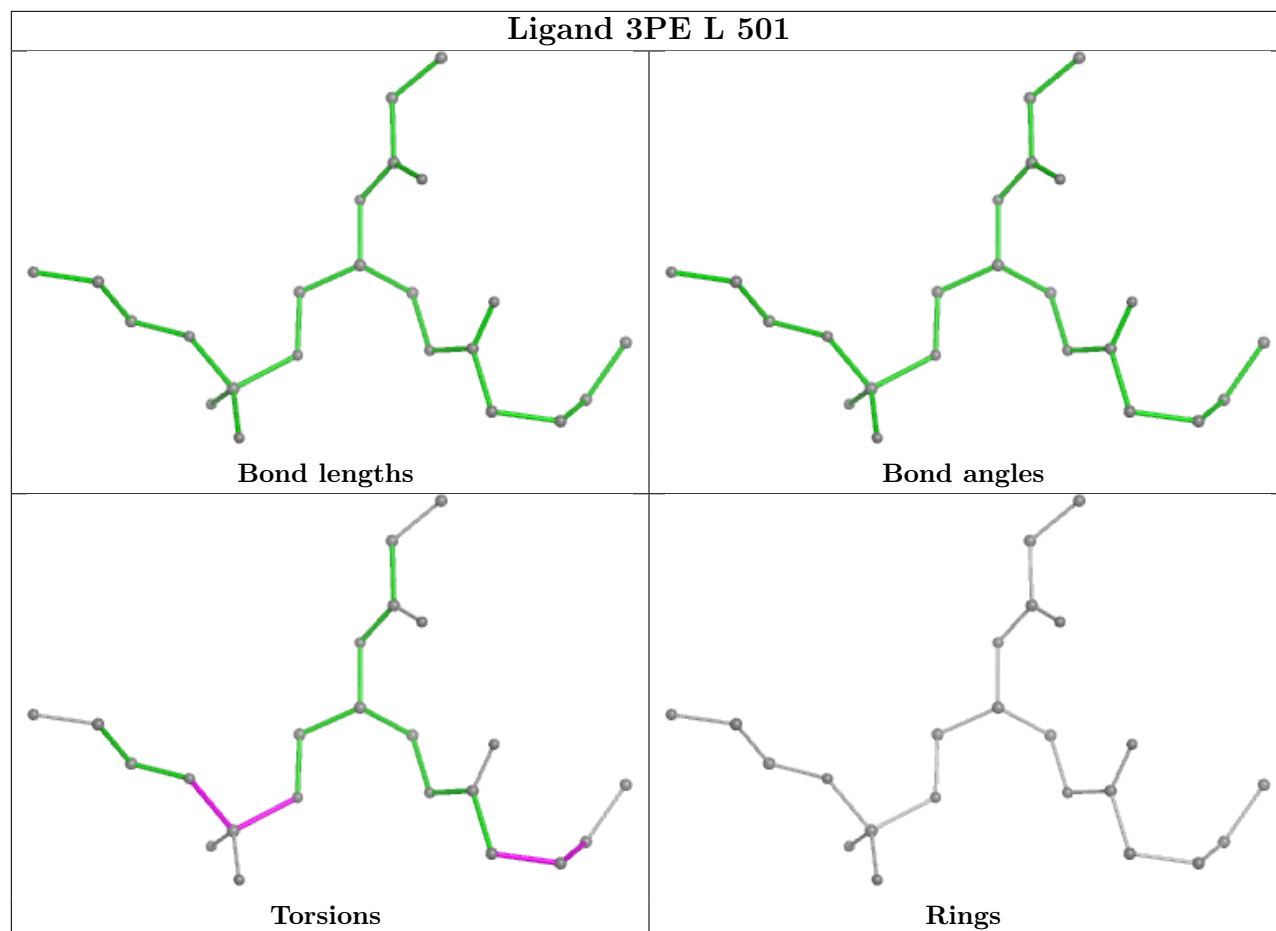




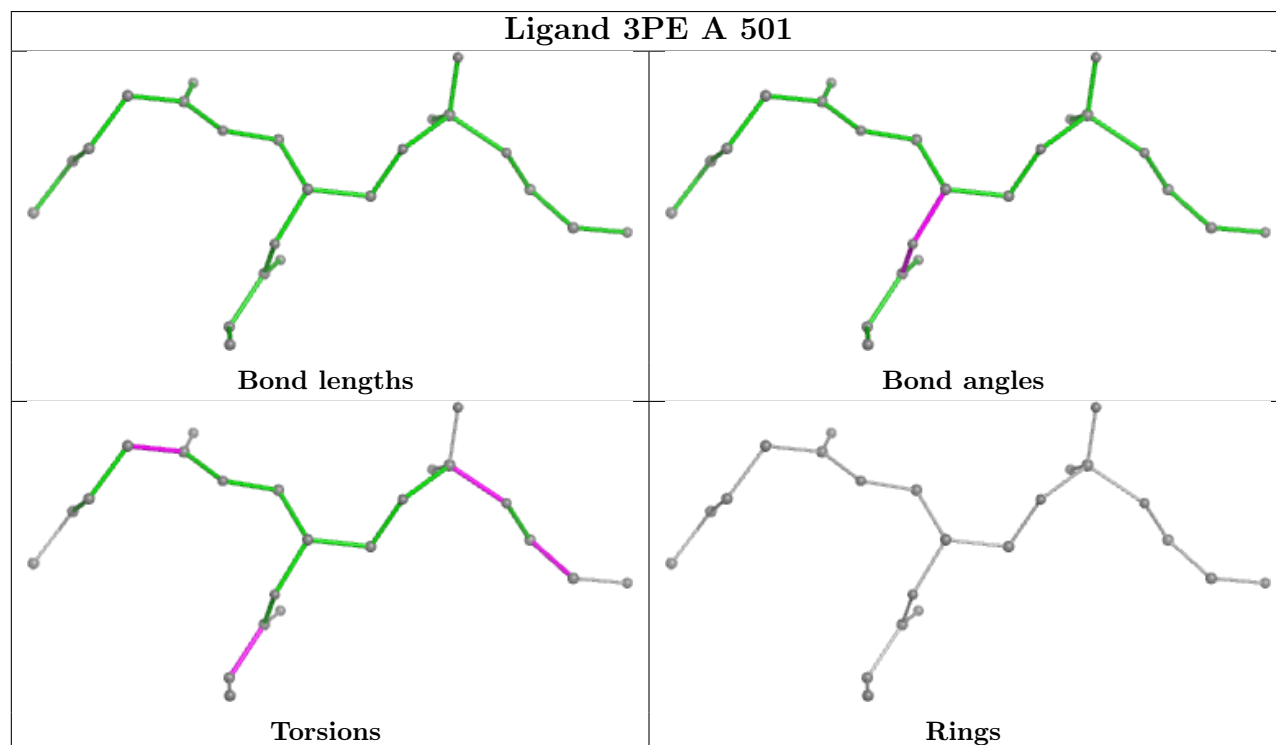


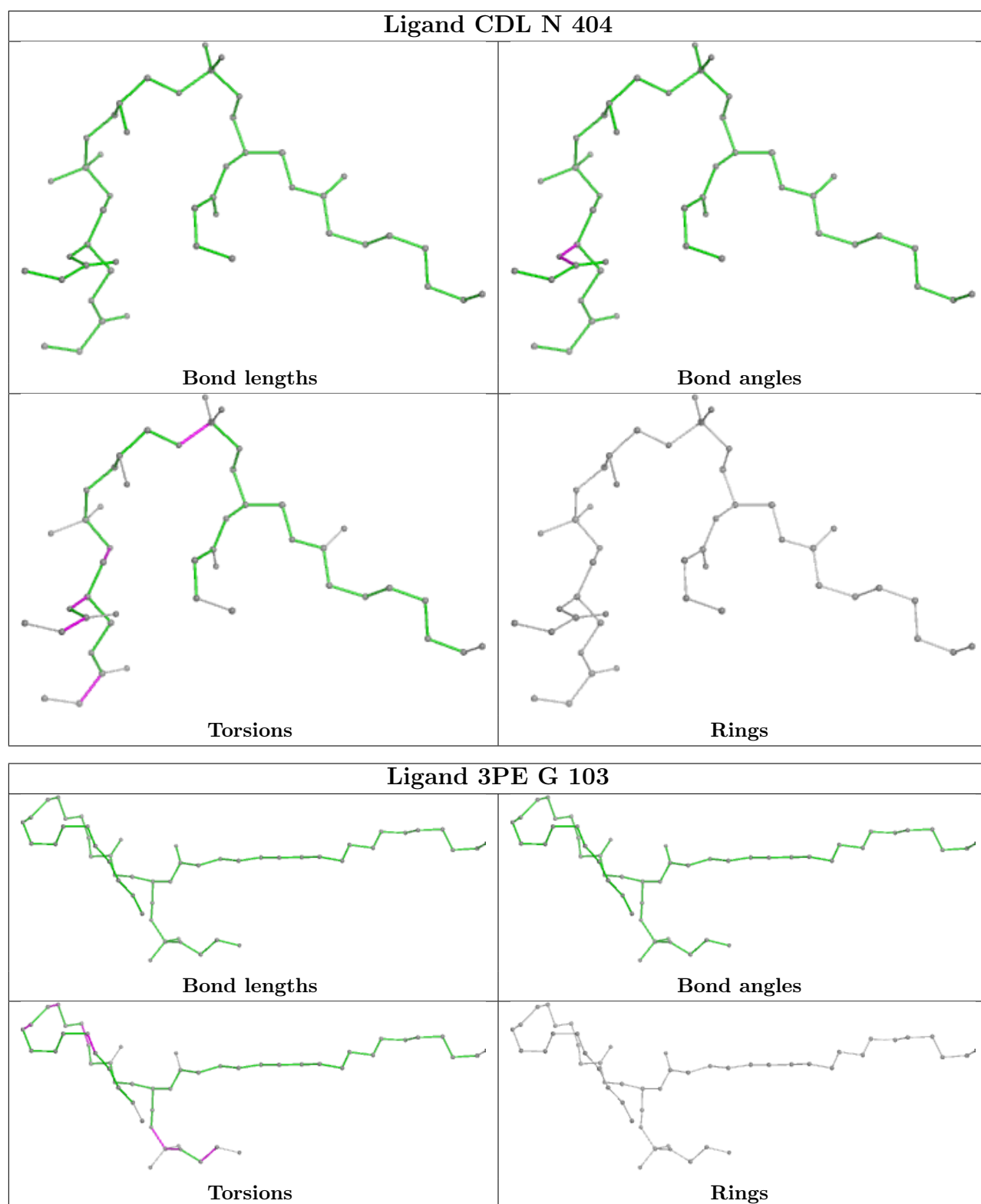


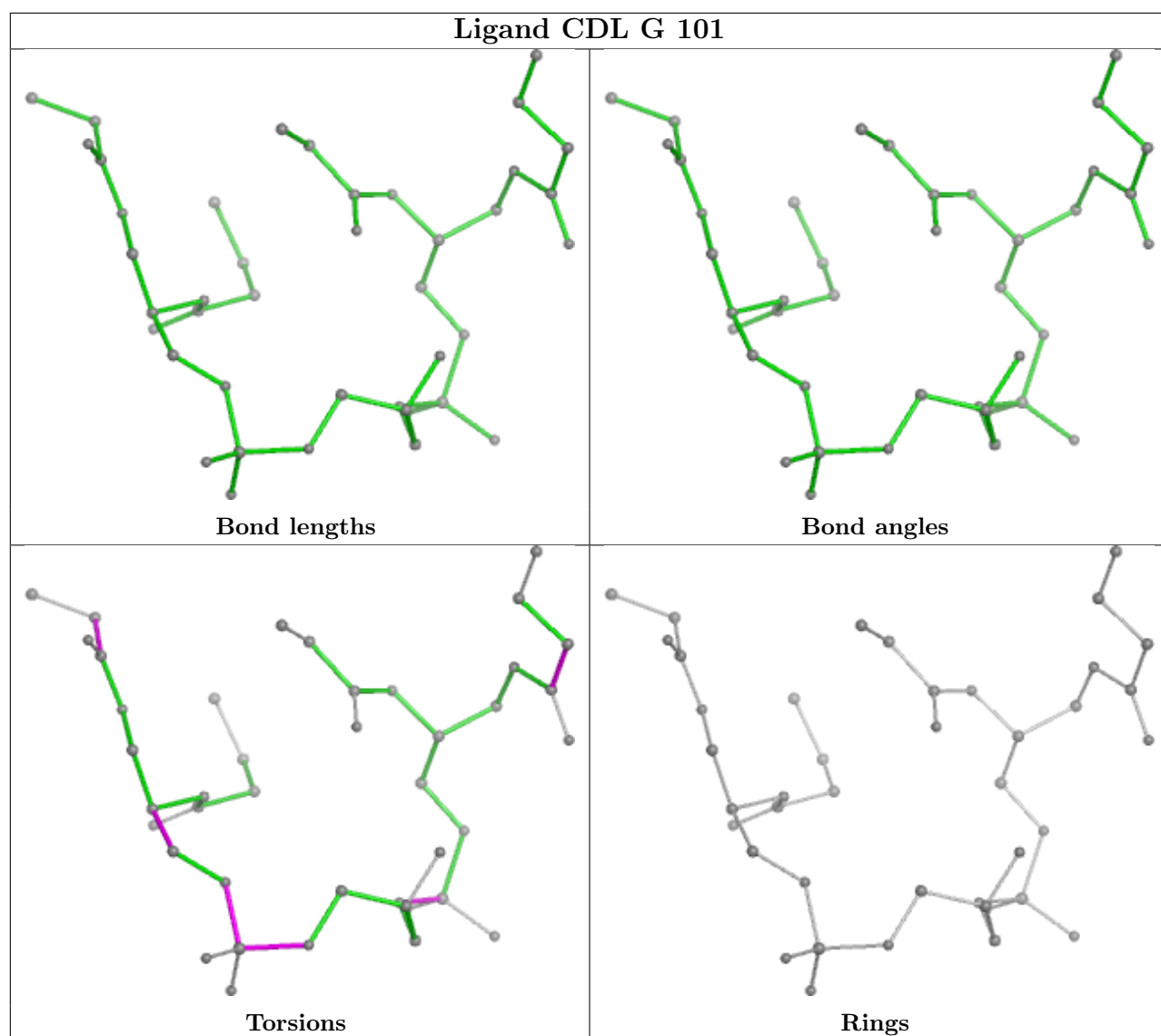
Ligand 3PE L 501

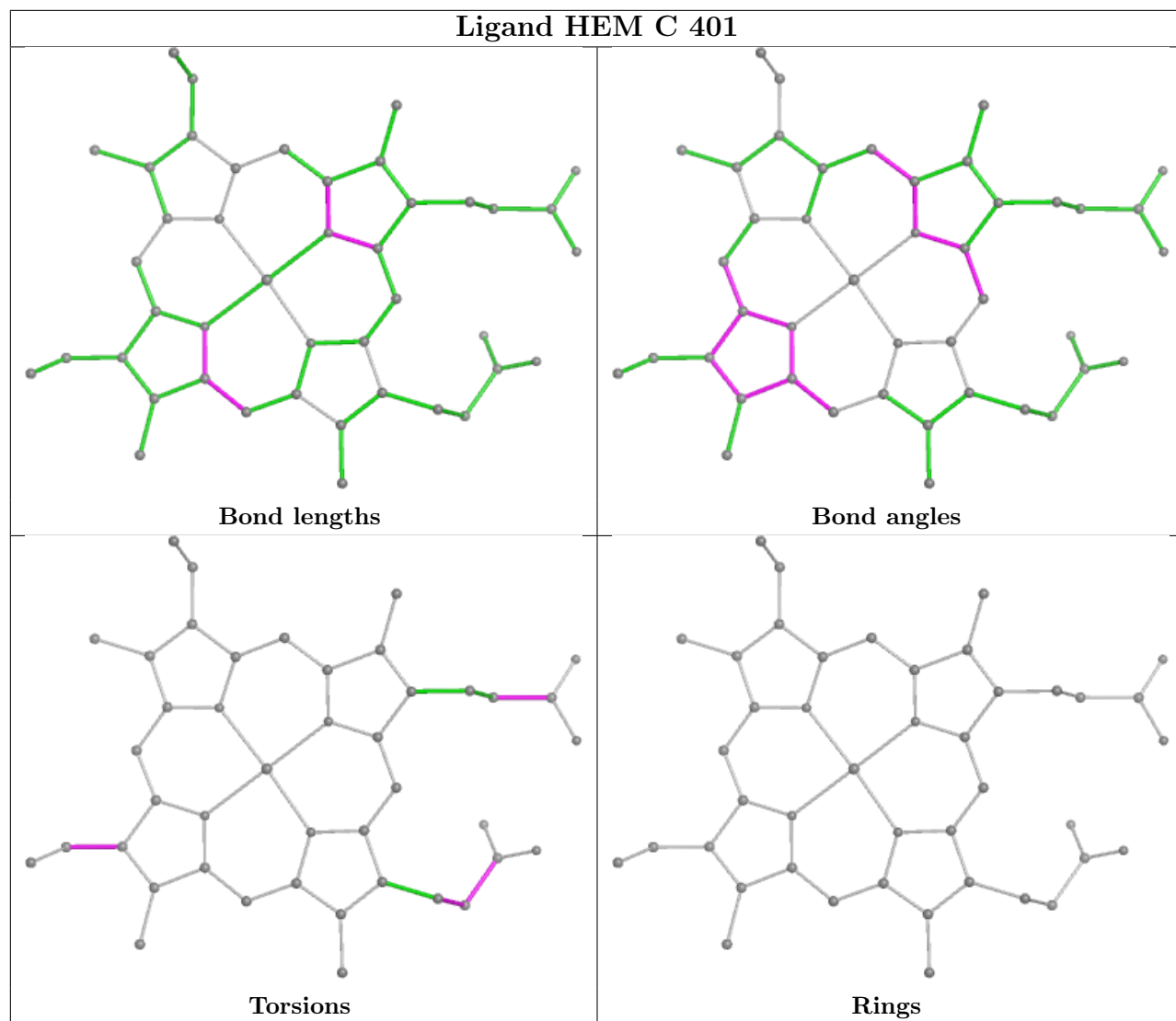


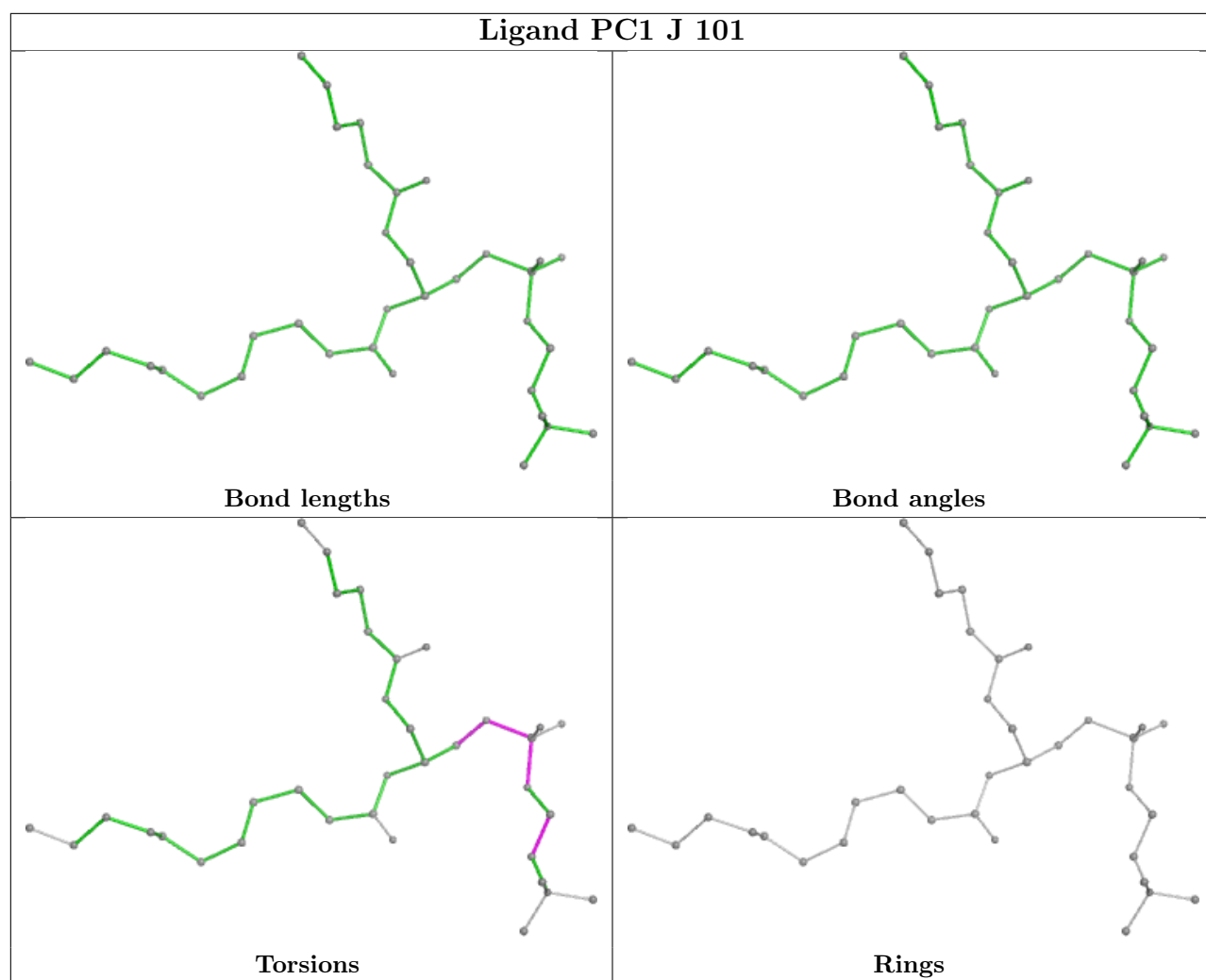
Ligand 3PE A 501

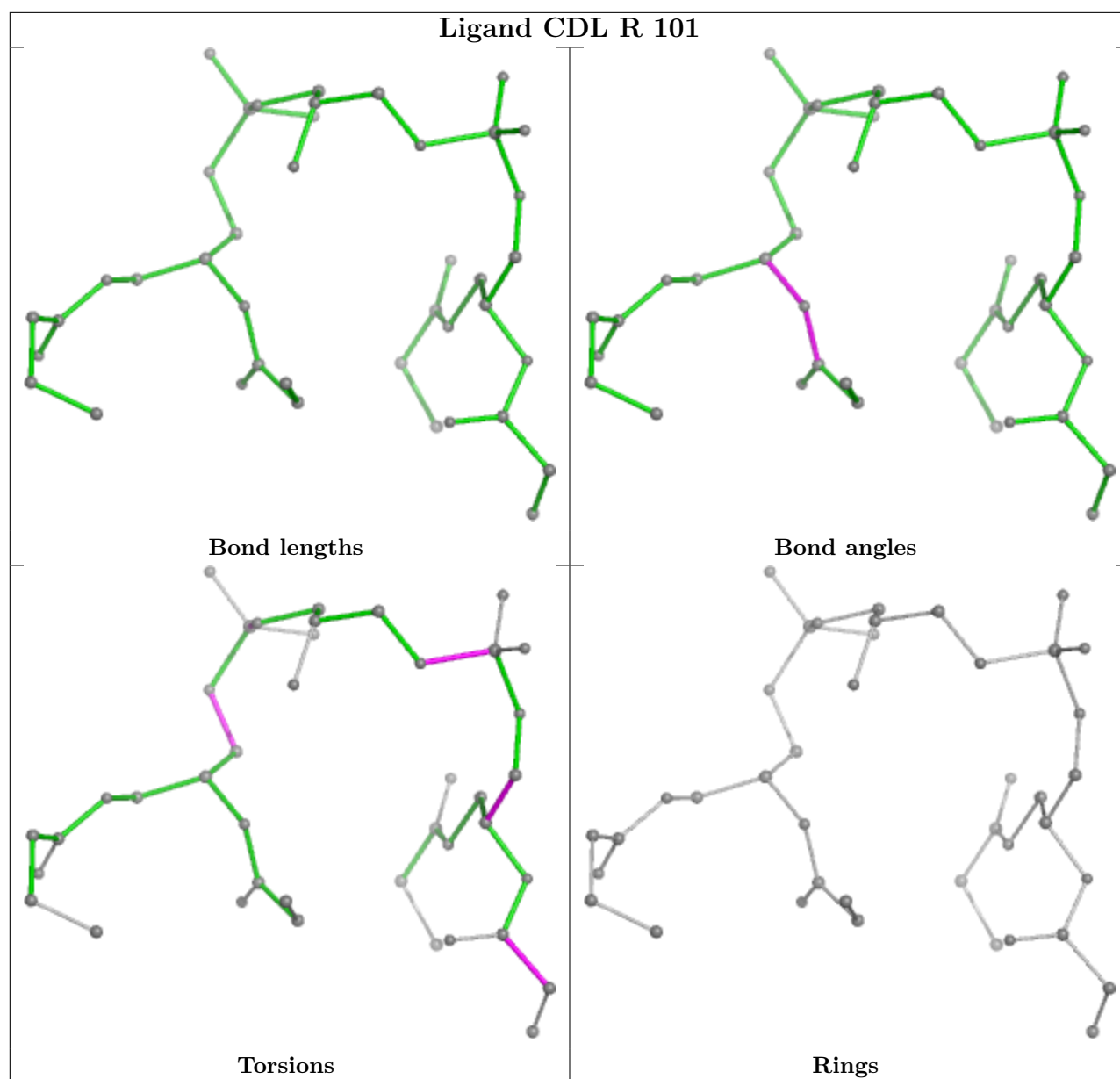












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

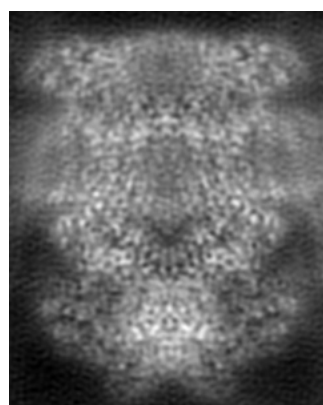
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12706. These allow visual inspection of the internal detail of the map and identification of artifacts.

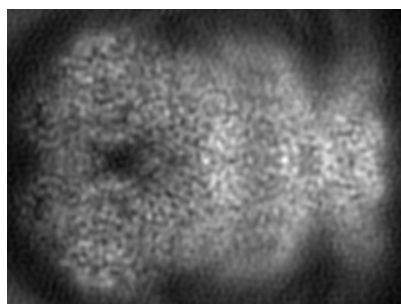
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

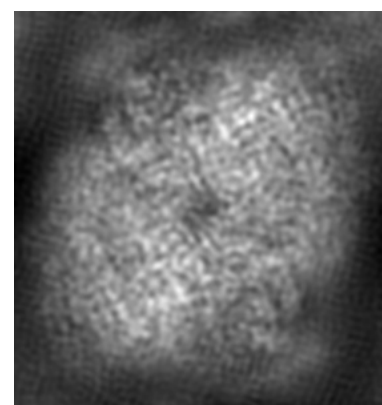
6.1.1 Primary map



X



Y

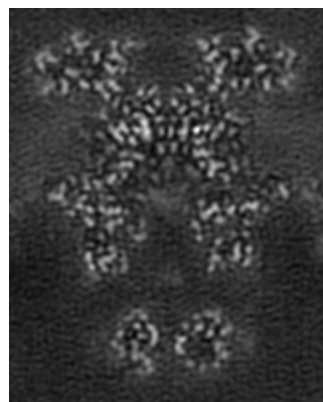


Z

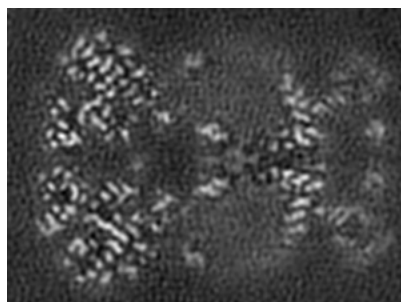
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

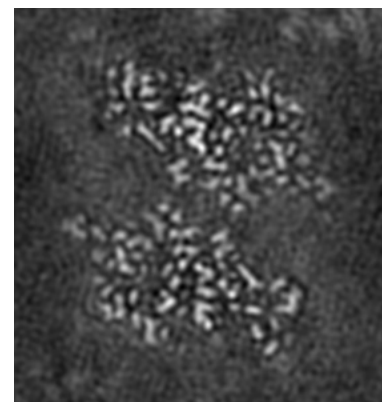
6.2.1 Primary map



X Index: 121



Y Index: 128

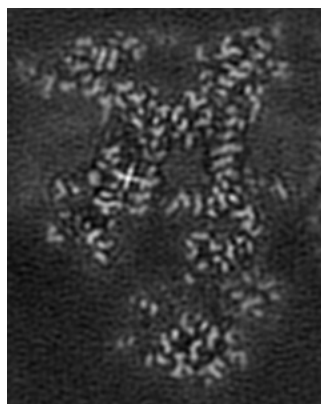


Z Index: 162

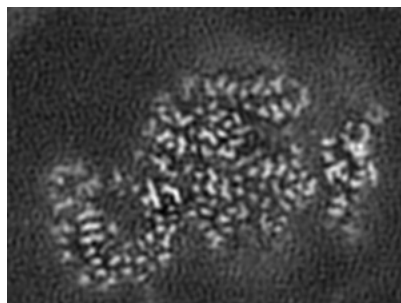
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

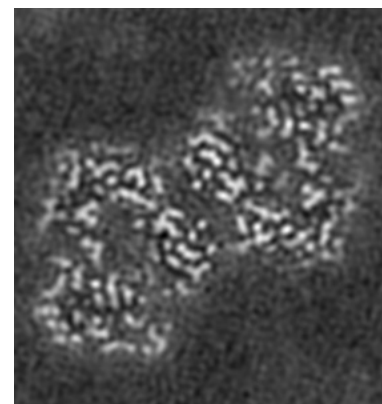
6.3.1 Primary map



X Index: 134



Y Index: 72

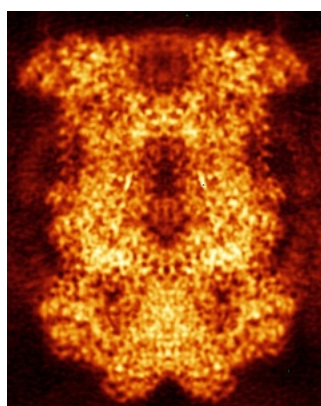


Z Index: 61

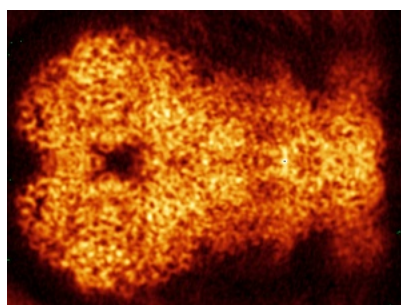
The images above show the largest variance slices of the map in three orthogonal directions.

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

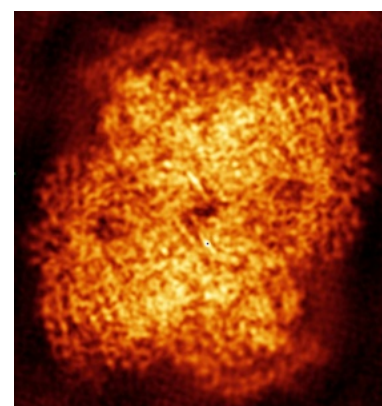
6.4.1 Primary map



X



Y



Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

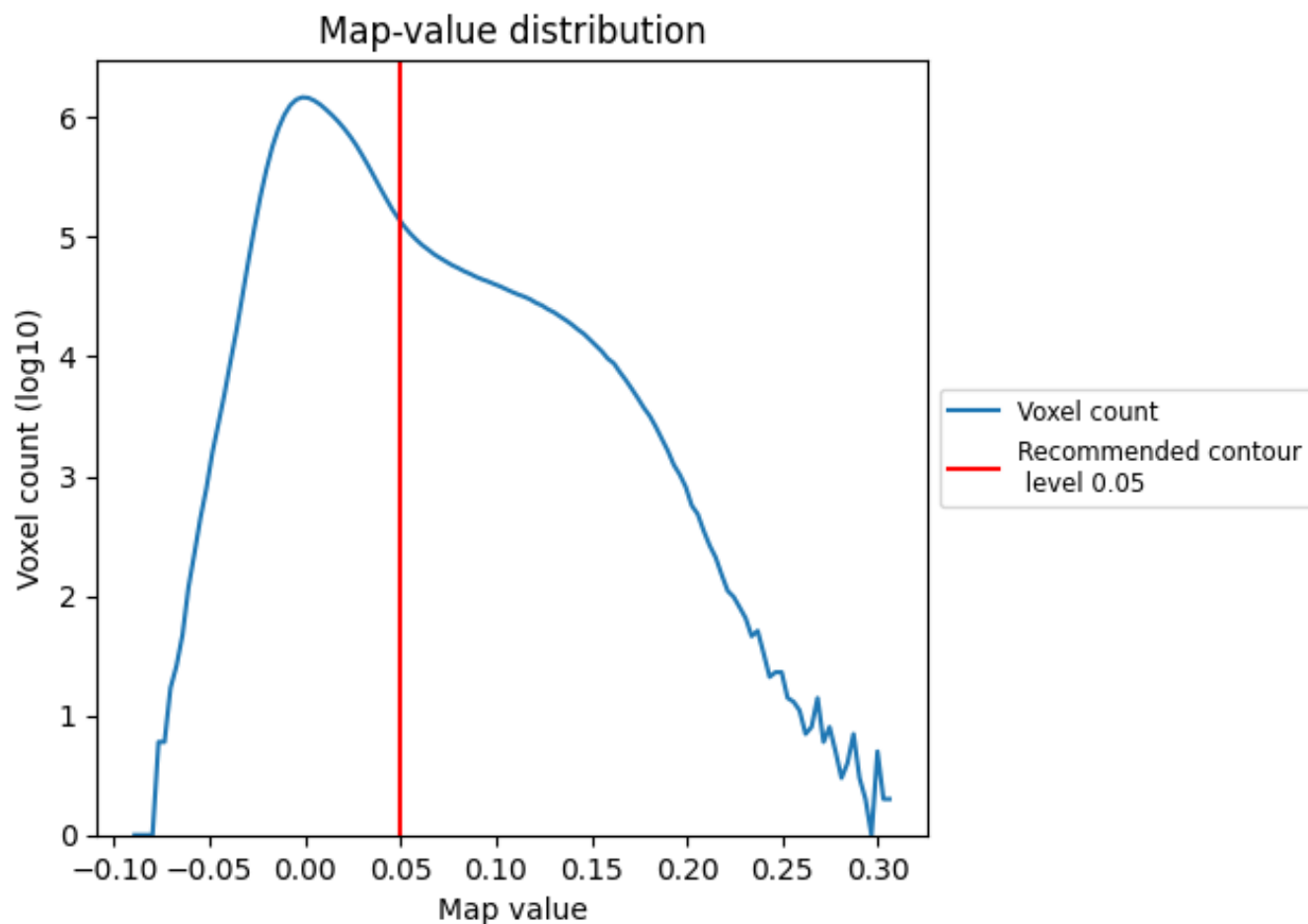
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

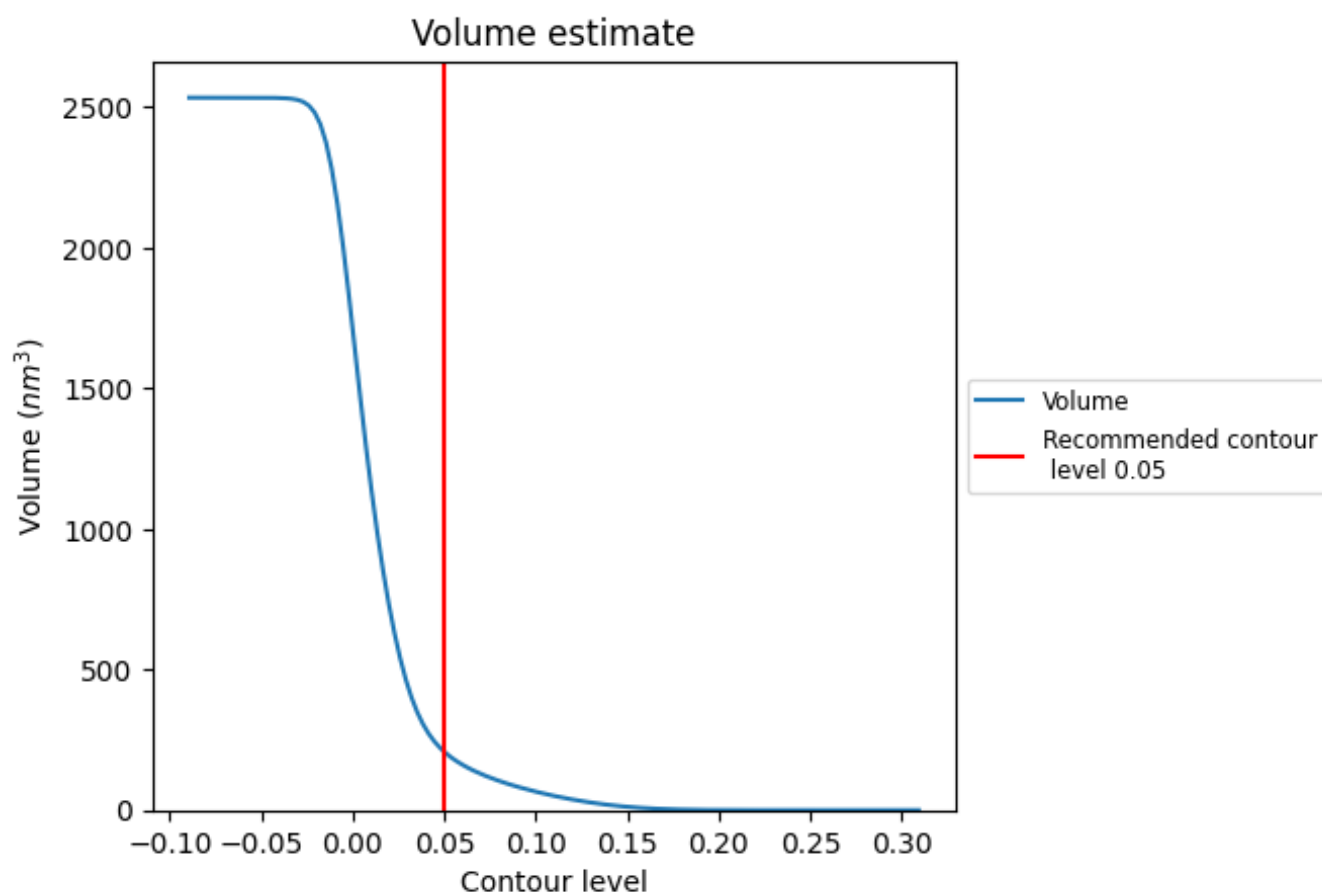
This section contains the results of statistical analysis of the map.

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 208 nm^3 ; this corresponds to an approximate mass of 188 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

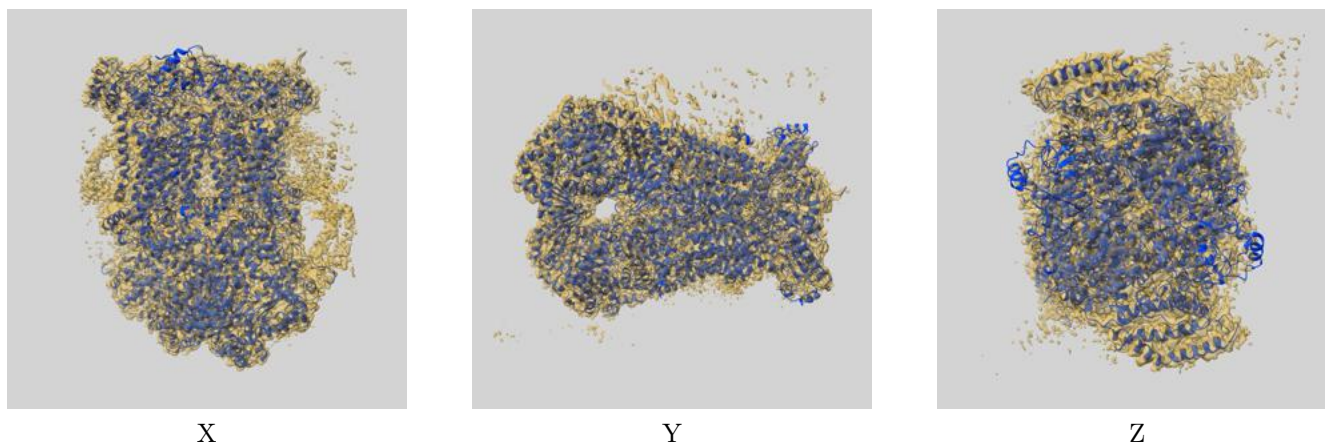
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

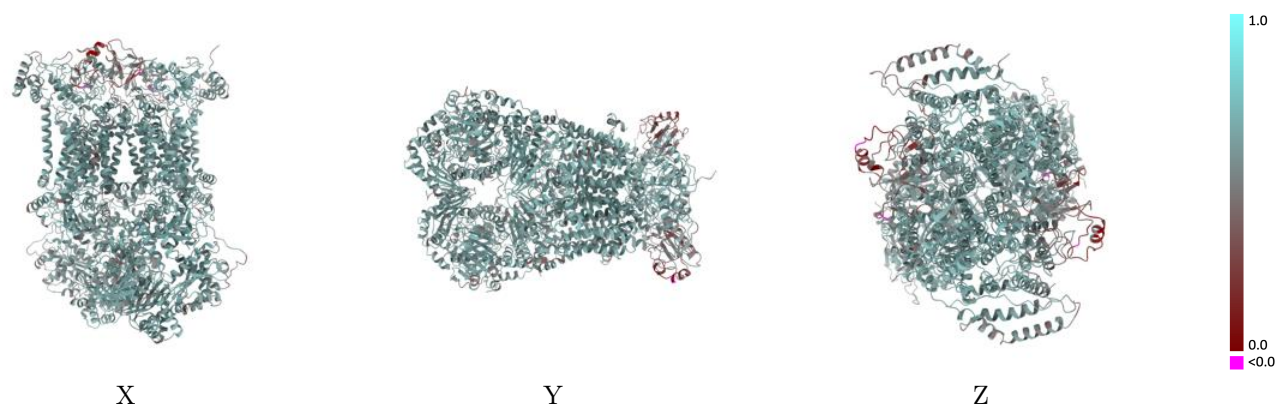
This section contains information regarding the fit between EMDB map EMD-12706 and PDB model 7O3H. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



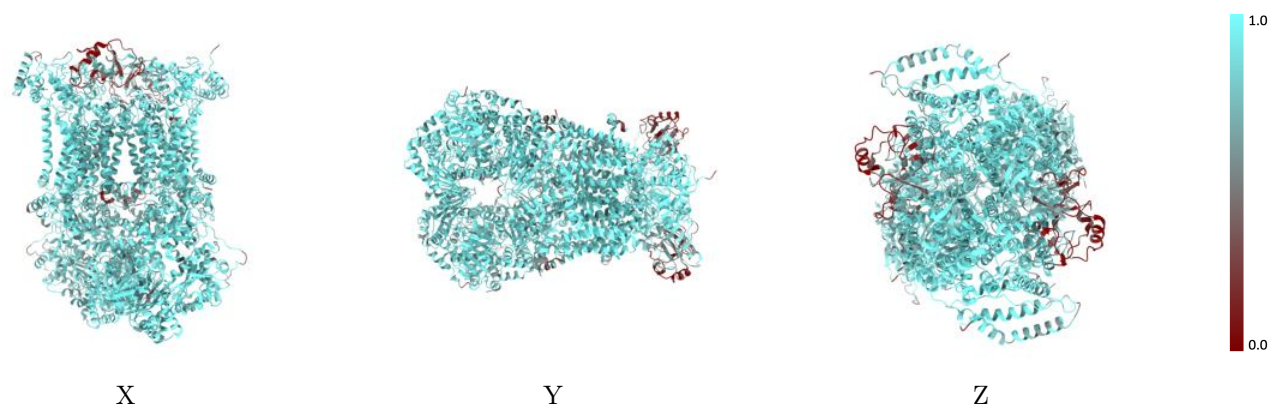
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



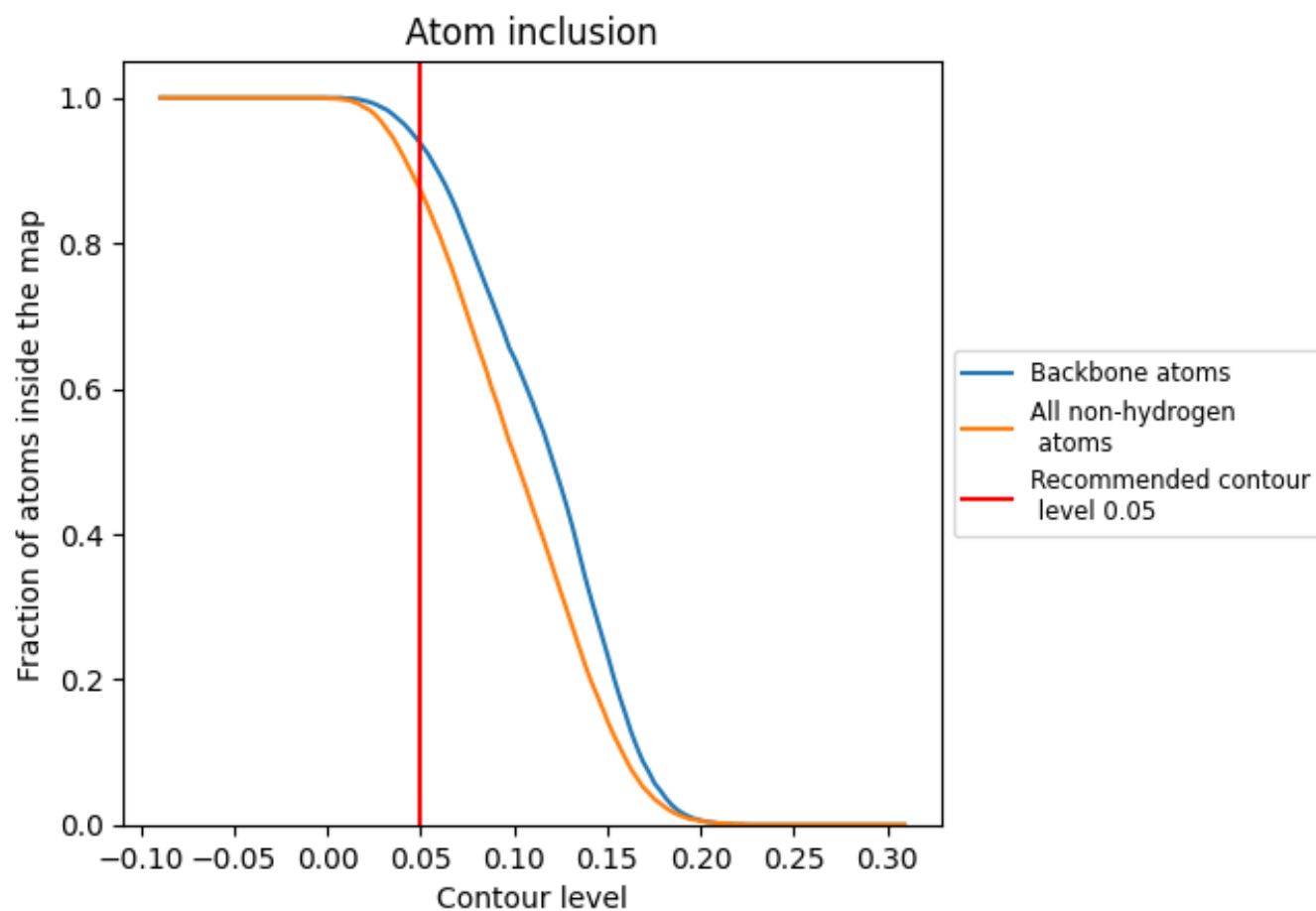
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8720	 0.5930
A	 0.9130	 0.6120
B	 0.9120	 0.6070
C	 0.9440	 0.6300
D	 0.9350	 0.6140
E	 0.5390	 0.4550
F	 0.8630	 0.6030
G	 0.8750	 0.5940
H	 0.8260	 0.5260
J	 0.8650	 0.5910
K	 0.7030	 0.5660
L	 0.9080	 0.6130
M	 0.9020	 0.6080
N	 0.9330	 0.6220
O	 0.9420	 0.6130
P	 0.5690	 0.4550
Q	 0.8780	 0.6040
R	 0.9190	 0.5950
S	 0.8220	 0.5480
T	 0.8540	 0.5790
U	 0.8780	 0.5950
V	 0.6770	 0.5450

