



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 09:53 am BST

PDB ID : 7O3E
EMDB ID : EMD-12705
Title : Murine supercomplex CIII2CIV in the intermediate locked conformation
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2021-04-01
Resolution : 3.60 Å(reported)
Based on initial models : 5Z62, 5IY5, 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

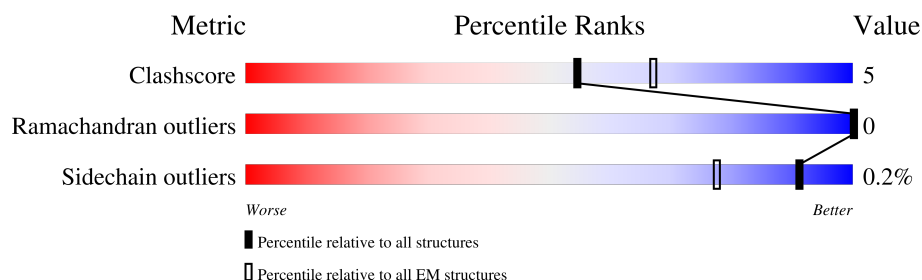
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.





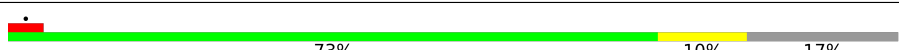
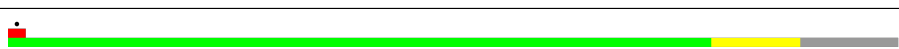

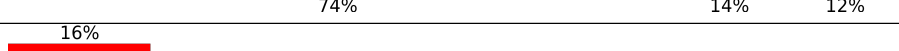
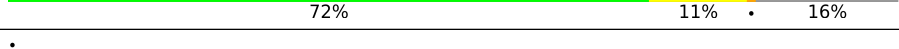
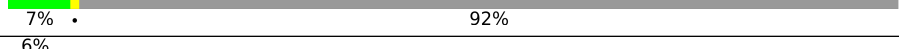
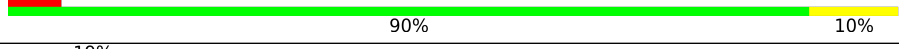

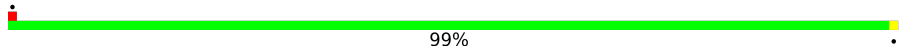
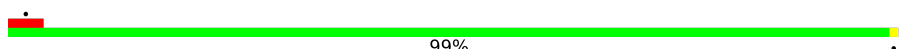
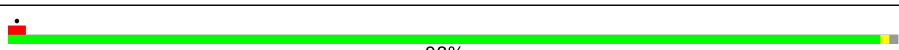

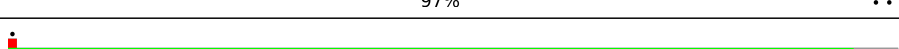
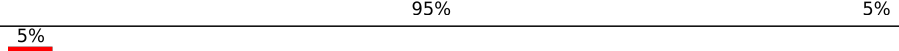
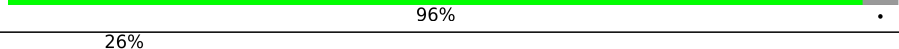

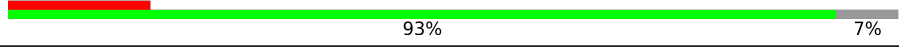
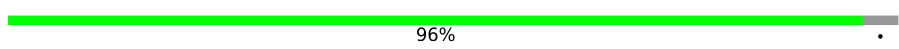

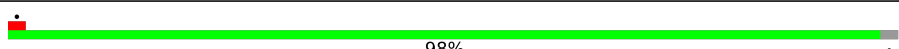
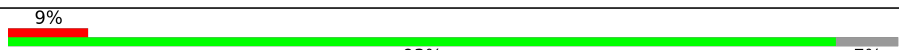
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	 87% 13%
1	L	446	 85% 15%
2	B	439	 80% 15% .
2	M	439	 84% 12% .
3	C	381	 91% 9%
3	N	381	 84% 15% .
4	D	241	 87% 13%
4	O	241	 88% 11% .

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Mol	Chain	Length	Quality of chain
5	F	110	
5	Q	110	
6	G	81	
6	R	81	
7	H	76	
7	S	76	
8	P	196	
9	T	78	
10	I	113	
11	a	514	
12	b	227	
13	c	261	
14	d	147	
15	e	109	
16	f	99	
17	g	85	
18	h	85	
19	i	75	
20	k	56	
21	l	47	
22	m	46	
23	J	63	
23	U	63	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 44039 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
			3045	2052	473	499	21		
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 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	101	Total	C	N	O	S	0	0
			894	572	159	160	3		
5	Q	101	Total	C	N	O	S	0	0
			894	572	159	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	67	Total	C	N	O		0	0
			565	364	107	94			
6	R	72	Total	C	N	O		0	0
			609	396	112	101			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	67	Total	C	N	O	S	0	0
			554	338	102	109	5		
7	S	64	Total	C	N	O	S	0	0
			530	322	99	104	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	15	Total	C	N	O	0	0
			128	79	24	25		

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

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

- Molecule 10 is a protein called Cox7a2l protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	111	Total	C	N	O	S	0	0
			834	543	138	148	5		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	514	Total	C	N	O	S	0	0
			4021	2691	623	675	32		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	227	Total	C	N	O	S	0	0
			1817	1180	282	336	19		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	259	Total	C	N	O	S	0	0
			2111	1414	338	349	10		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	144	Total	C	N	O	S	0	0
			1195	770	199	219	7		

- Molecule 15 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	104	Total	C	N	O	S	0	0
			842	538	141	161	2		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	95	Total	C	N	O	S	0	0
			727	452	127	140	8		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	75	Total	C	N	O	S	0	0
			605	392	114	96	3		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	79	Total	C	N	O	S	0	0
			654	416	116	117	5		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	72	Total	C	N	O	S	0	0
			572	372	103	94	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	k	49	Total	C	N	O	S	0	0
			383	248	65	68	2		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	l	46	Total	C	N	O	S	0	0
			380	253	64	61	2		

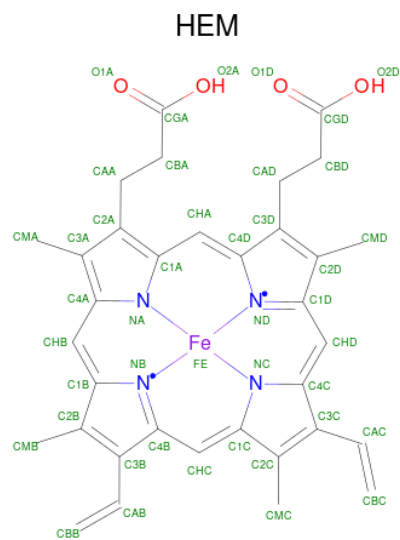
- Molecule 22 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	m	43	Total	C	N	O	S	0	0
			311	203	51	56	1		

- Molecule 23 is a protein called Cytochrome b-c1 complex subunit 9.

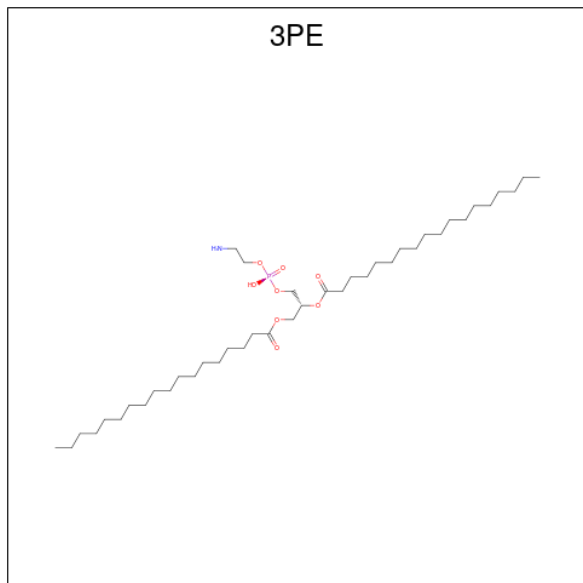
Mol	Chain	Residues	Atoms				AltConf	Trace
23	J	31	Total	C	N	O	0	0
			272	178	47	47		
23	U	31	Total	C	N	O	0	0
			272	178	47	47		

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



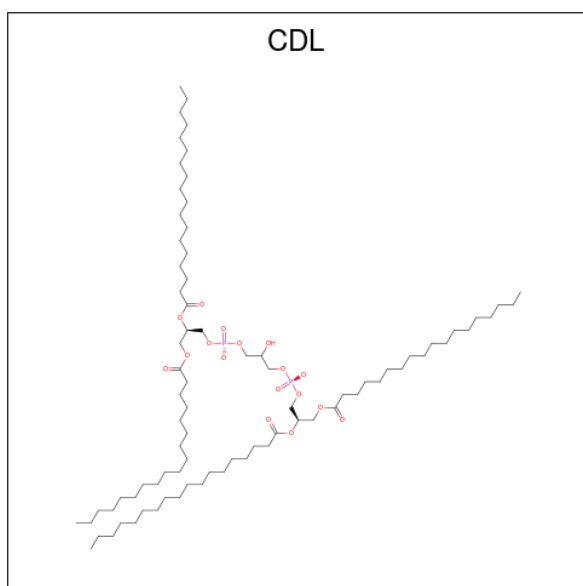
Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
24	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
24	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
24	N	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 25 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$).



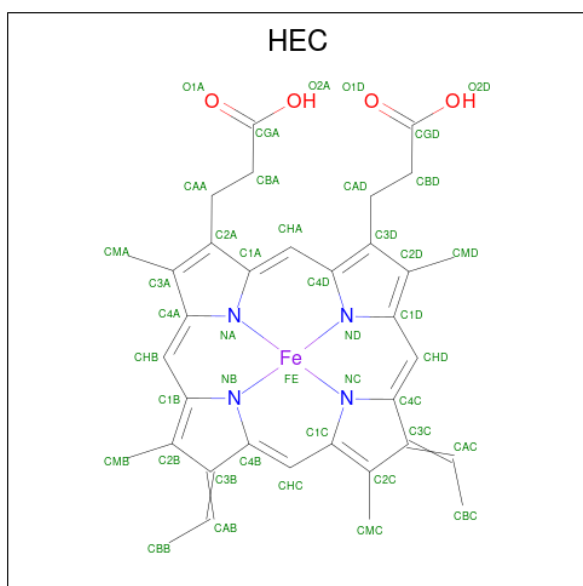
Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	F	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	F	1	Total	C	N	O	P	0
			34	24	1	8	1	
25	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
25	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	a	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	b	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	b	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	c	1	Total	C	N	O	P	0
			45	35	1	8	1	
25	d	1	Total	C	N	O	P	0
			34	24	1	8	1	
25	g	1	Total	C	N	O	P	0
			25	15	1	8	1	
25	k	1	Total	C	N	O	P	0
			27	17	1	8	1	

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



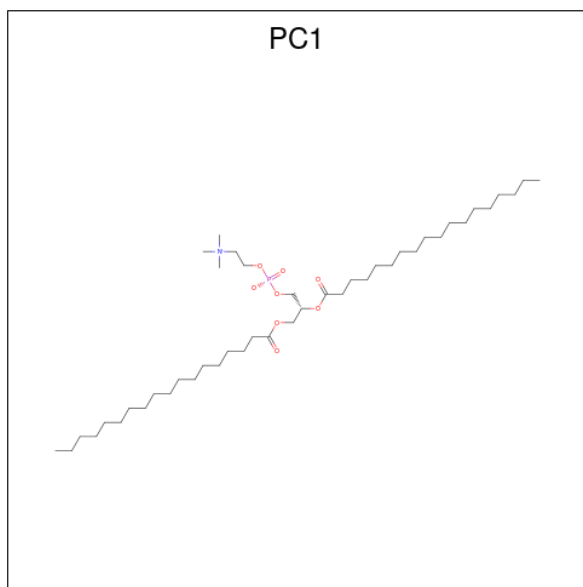
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	O	P	0
			42	23	17	2	
26	D	1	Total	C	O	P	0
			56	37	17	2	
26	L	1	Total	C	O	P	0
			46	27	17	2	
26	N	1	Total	C	O	P	0
			41	22	17	2	
26	O	1	Total	C	O	P	0
			57	38	17	2	

- Molecule 27 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 28 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
28	L	1	Total	C	N	O	P	0
			24	14	1	8	1	
28	a	1	Total	C	N	O	P	0
			43	33	1	8	1	

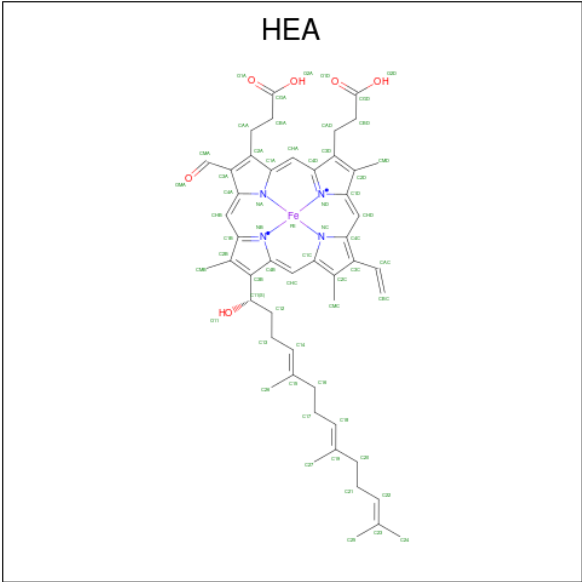
- Molecule 29 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
29	a	1	Total	Cu	0
			1	1	

- Molecule 30 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
30	a	1	Total	Na	0
			1	1	

- Molecule 31 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).

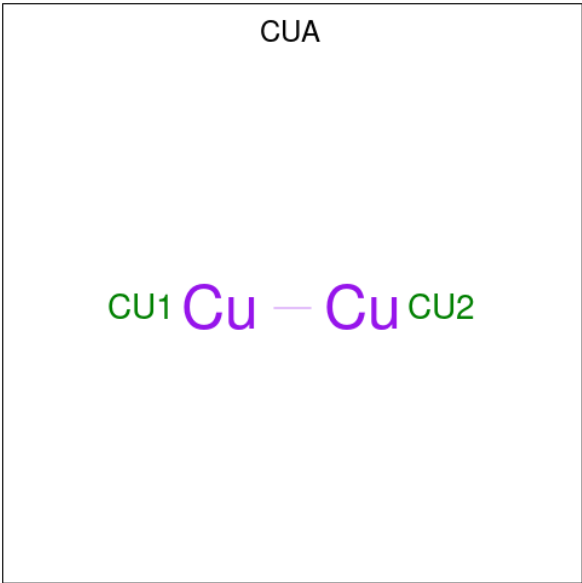


Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total 60	C 49	Fe 1	N 4	O 6	0
31	a	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	b	1	Total	Mg	0
			1	1	

- Molecule 33 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).

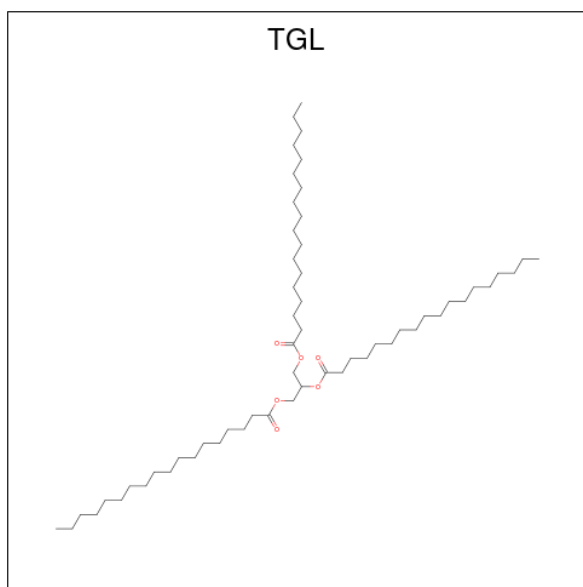


Mol	Chain	Residues	Atoms		AltConf
33	b	1	Total	Cu	0
			2	2	

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	f	1	Total	Zn	0
			1	1	

- Molecule 35 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).

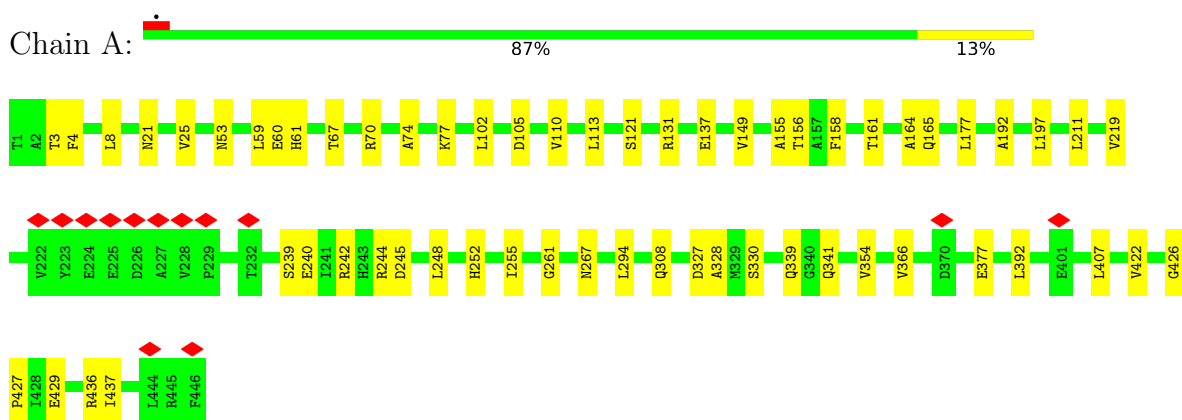


Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			44	38	6	

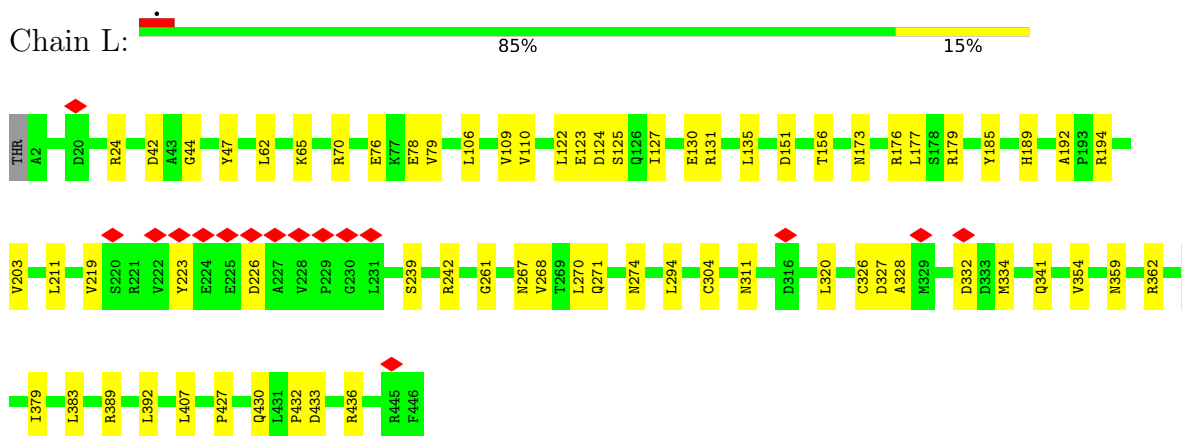
3 Residue-property plots

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

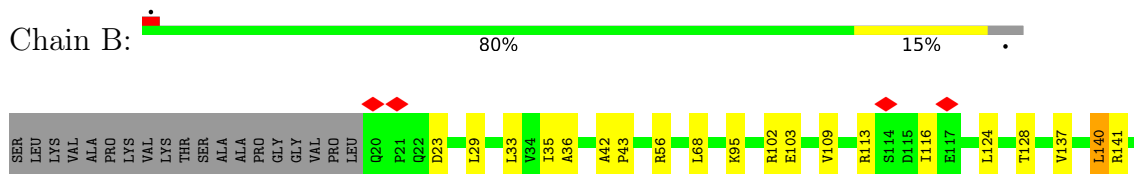
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

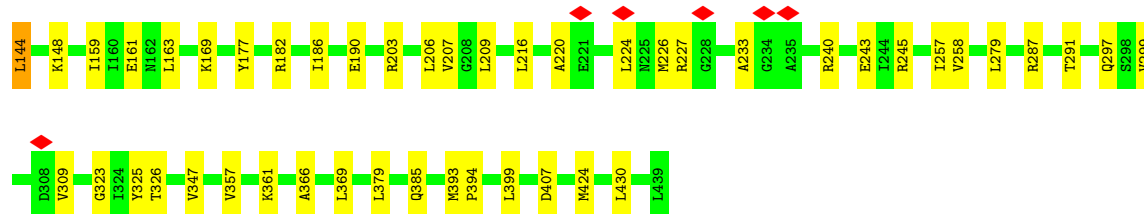


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



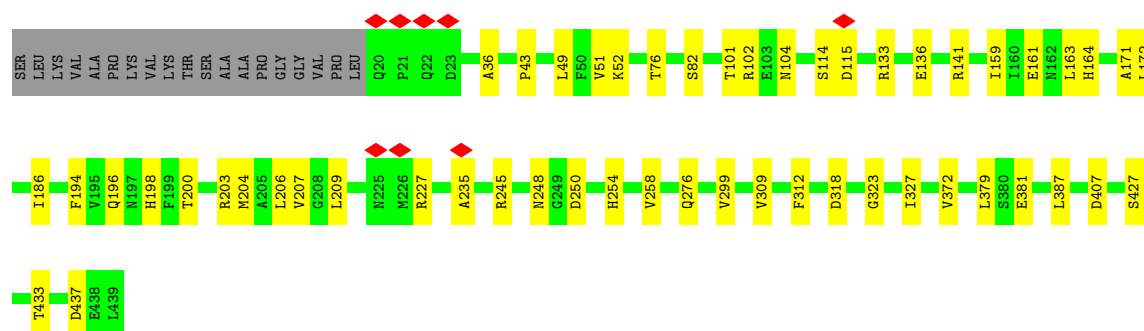
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





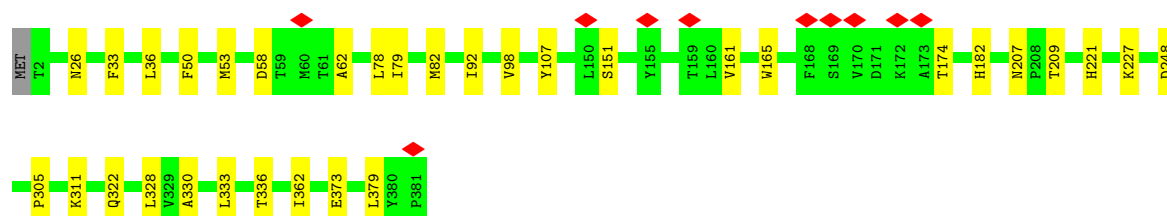
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 84% 12%



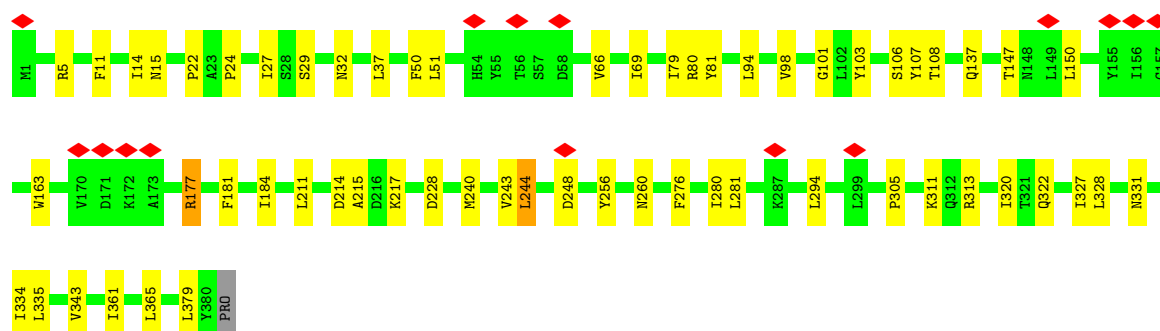
- Molecule 3: Cytochrome b

Chain C: 91% 9%



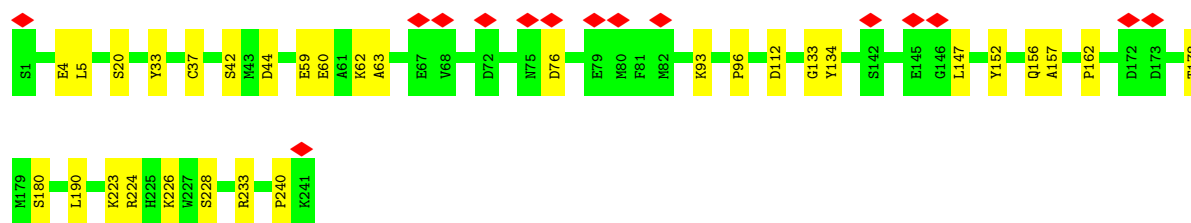
- Molecule 3: Cytochrome b

Chain N: 84% 15%

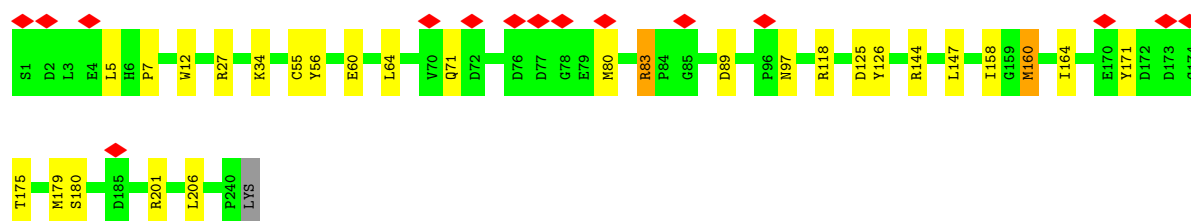
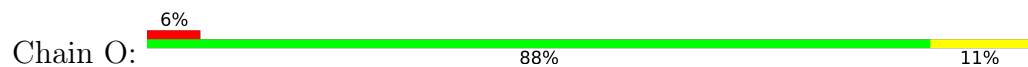


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

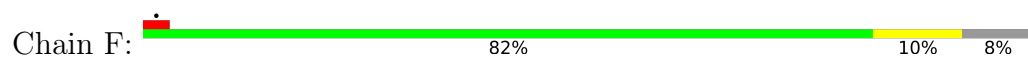
Chain D: 6% 87% 13%



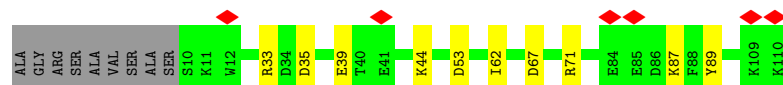
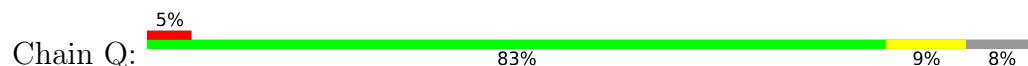
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 7



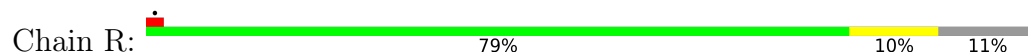
- Molecule 5: Cytochrome b-c1 complex subunit 7



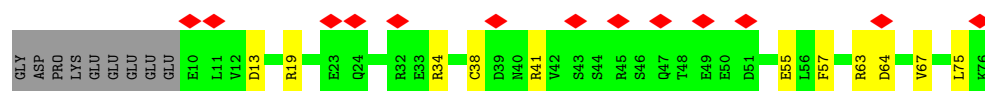
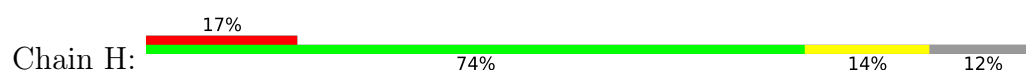
- Molecule 6: Cytochrome b-c1 complex subunit 8



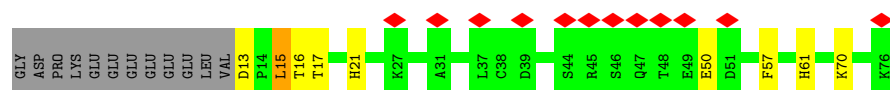
- Molecule 6: Cytochrome b-c1 complex subunit 8



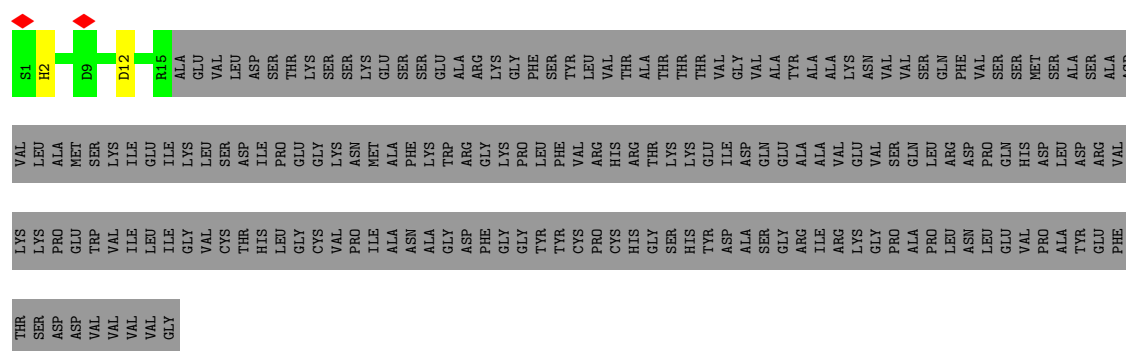
- Molecule 7: Cytochrome b-c1 complex subunit 6, mitochondrial



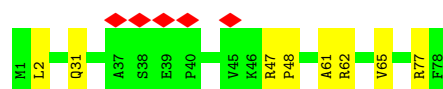
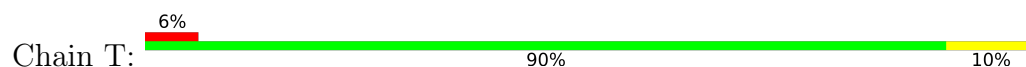
- Molecule 7: Cytochrome b-c1 complex subunit 6, mitochondrial



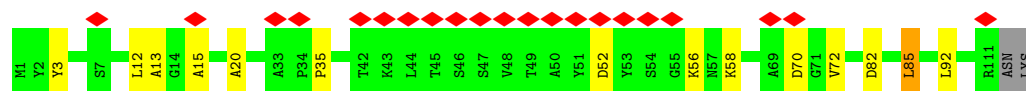
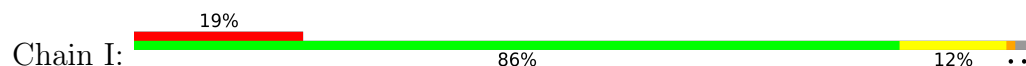
- Molecule 8: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 9: Cytochrome b-c1 complex subunit 9



- Molecule 10: Cox7a2l protein

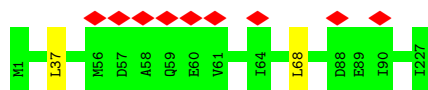


- Molecule 11: Cytochrome c oxidase subunit 1



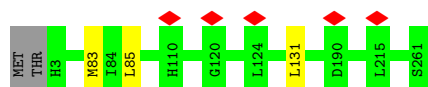
- Molecule 12: Cytochrome c oxidase subunit 2

Chain b:  99%



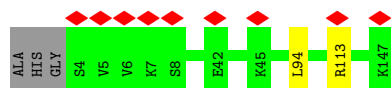
- Molecule 13: Cytochrome c oxidase subunit 3

Chain c:  98%



- Molecule 14: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain d:  97%



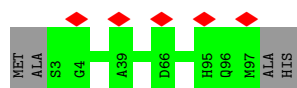
- Molecule 15: Cytochrome c oxidase subunit 5A, mitochondrial

Chain e:  95%




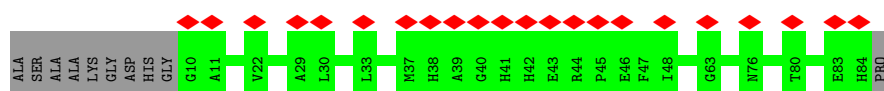
- Molecule 16: Cytochrome c oxidase subunit 5B, mitochondrial

Chain f:  96%



- Molecule 17: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain g:  88%



- Molecule 18: Cytochrome c oxidase subunit 6B1

Chain h:  93%



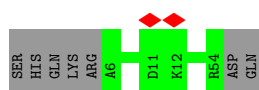
- Molecule 19: Cytochrome c oxidase subunit 6C

Chain i: 96%



- Molecule 20: Cytochrome c oxidase subunit 7B, mitochondrial

Chain k: 88% 12%



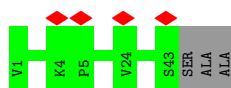
- Molecule 21: Cytochrome c oxidase subunit 7C, mitochondrial

Chain l: 98%



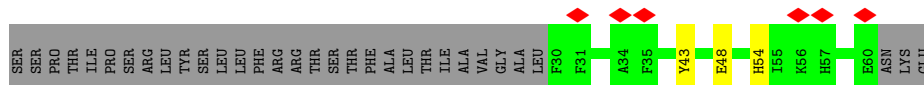
- Molecule 22: Cytochrome c oxidase subunit 8B, mitochondrial

Chain m: 9% 93% 7%



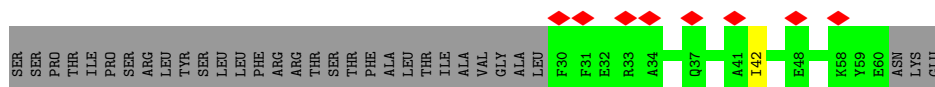
- Molecule 23: Cytochrome b-c1 complex subunit 9

Chain J: 10% 44% 5% 51%



- Molecule 23: Cytochrome b-c1 complex subunit 9

Chain U: 13% 48% 51%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8426	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	0.330	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	161.728, 214.92801, 180.88	wwPDB
Map dimensions	170, 202, 152	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, TGL, PC1, MG, HEC, CDL, CUA, HEA, CU, 3PE, NA, HEM

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	0/4803
1	L	0.28	0/3530	0.58	0/4793
2	B	0.29	0/3205	0.59	3/4332 (0.1%)
2	M	0.28	0/3205	0.54	0/4332
3	C	0.29	0/3147	0.58	0/4299
3	N	0.31	0/3147	0.62	2/4297 (0.0%)
4	D	0.29	0/1978	0.61	1/2685 (0.0%)
4	O	0.28	0/1968	0.58	0/2674
5	F	0.29	0/916	0.63	1/1226 (0.1%)
5	Q	0.29	0/916	0.59	1/1226 (0.1%)
6	G	0.32	0/578	0.62	0/777
6	R	0.34	0/627	0.70	0/848
7	H	0.32	0/561	0.64	0/751
7	S	0.35	0/537	0.77	1/718 (0.1%)
8	P	0.25	0/131	0.60	0/176
9	T	0.31	0/565	0.67	0/772
10	I	0.32	0/856	0.71	2/1164 (0.2%)
11	a	0.36	0/4162	0.59	3/5686 (0.1%)
12	b	0.34	0/1863	0.70	2/2542 (0.1%)
13	c	0.35	0/2195	0.63	3/3000 (0.1%)
14	d	0.33	0/1229	0.62	1/1659 (0.1%)
15	e	0.32	0/860	0.69	0/1167
16	f	0.32	0/744	0.66	0/1009
17	g	0.28	0/632	0.53	0/866
18	h	0.32	0/674	0.65	0/910
19	i	0.36	0/584	0.70	0/778
20	k	0.30	0/396	0.55	0/541
21	l	0.36	0/393	0.64	0/527
22	m	0.36	0/318	0.56	0/433
23	J	0.30	0/281	0.61	0/375
23	U	0.33	0/281	0.52	0/375
All	All	0.31	0/44015	0.61	20/59741 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	O	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
12	b	68	LEU	CA-CB-CG	8.15	134.06	115.30
10	I	85	LEU	CA-CB-CG	7.64	132.86	115.30
12	b	37	LEU	CA-CB-CG	7.32	132.14	115.30
5	Q	53	ASP	CB-CG-OD1	7.24	124.82	118.30
2	B	140	LEU	CA-CB-CG	7.16	131.76	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	SER	Peptide
4	O	160	MET	Peptide

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	37	0
1	L	3460	0	3367	41	0
2	B	3154	0	3158	39	0
2	M	3154	0	3158	34	0
3	C	3045	0	3107	23	0
3	N	3046	0	3112	39	0
4	D	1919	0	1867	22	0
4	O	1909	0	1854	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	894	0	882	8	0
5	Q	894	0	882	6	0
6	G	565	0	577	6	0
6	R	609	0	614	7	0
7	H	554	0	535	7	0
7	S	530	0	509	6	0
8	P	128	0	120	2	0
9	T	554	0	590	7	0
10	I	834	0	823	7	0
11	a	4021	0	3998	0	0
12	b	1817	0	1822	0	0
13	c	2111	0	2047	0	0
14	d	1195	0	1161	0	0
15	e	842	0	838	0	0
16	f	727	0	703	0	0
17	g	605	0	570	0	0
18	h	654	0	622	0	0
19	i	572	0	596	0	0
20	k	383	0	367	0	0
21	l	380	0	378	0	0
22	m	311	0	329	0	0
23	J	272	0	251	2	0
23	U	272	0	251	1	0
24	C	86	0	60	2	0
24	N	86	0	60	2	0
25	C	35	0	44	0	0
25	F	63	0	74	1	0
25	L	23	0	20	0	0
25	N	88	0	130	3	0
25	a	28	0	30	0	0
25	b	57	0	62	0	0
25	c	45	0	67	0	0
25	d	34	0	42	0	0
25	g	25	0	24	0	0
25	k	27	0	28	0	0
26	C	42	0	28	0	0
26	D	56	0	56	2	0
26	L	46	0	36	0	0
26	N	41	0	26	0	0
26	O	57	0	58	2	0
27	D	43	0	30	0	0
27	O	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	L	24	0	22	0	0
28	a	43	0	60	0	0
29	a	1	0	0	0	0
30	a	1	0	0	0	0
31	a	120	0	108	0	0
32	b	1	0	0	0	0
33	b	2	0	0	0	0
34	f	1	0	0	0	0
35	l	44	0	63	0	0
All	All	44039	0	43623	278	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 5.

The worst 5 of 278 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)
7:H:34:ARG:HG3	7:H:55:GLU:HG3	1.73	0.70
4:D:233:ARG:HA	6:G:16:TYR:O	1.91	0.69
2:B:226:MET:HG2	2:B:227:ARG:HG3	1.77	0.66
2:B:220:ALA:HA	2:B:224:LEU:HD23	1.80	0.63
4:O:71:GLN:HE21	4:O:80:MET:HG3	1.64	0.62

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%)	423 (95%)	21 (5%)	0	100	100
1	L	443/446 (99%)	426 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	418/439 (95%)	398 (95%)	20 (5%)	0	100	100
2	M	418/439 (95%)	400 (96%)	18 (4%)	0	100	100
3	C	378/381 (99%)	365 (97%)	13 (3%)	0	100	100
3	N	378/381 (99%)	359 (95%)	19 (5%)	0	100	100
4	D	239/241 (99%)	226 (95%)	13 (5%)	0	100	100
4	O	238/241 (99%)	227 (95%)	11 (5%)	0	100	100
5	F	99/110 (90%)	99 (100%)	0	0	100	100
5	Q	99/110 (90%)	99 (100%)	0	0	100	100
6	G	63/81 (78%)	60 (95%)	3 (5%)	0	100	100
6	R	70/81 (86%)	66 (94%)	4 (6%)	0	100	100
7	H	65/76 (86%)	62 (95%)	3 (5%)	0	100	100
7	S	62/76 (82%)	57 (92%)	5 (8%)	0	100	100
8	P	13/196 (7%)	12 (92%)	1 (8%)	0	100	100
9	T	76/78 (97%)	66 (87%)	10 (13%)	0	100	100
10	I	109/113 (96%)	96 (88%)	13 (12%)	0	100	100
11	a	512/514 (100%)	498 (97%)	14 (3%)	0	100	100
12	b	225/227 (99%)	210 (93%)	15 (7%)	0	100	100
13	c	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
14	d	142/147 (97%)	132 (93%)	10 (7%)	0	100	100
15	e	102/109 (94%)	97 (95%)	5 (5%)	0	100	100
16	f	93/99 (94%)	84 (90%)	9 (10%)	0	100	100
17	g	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
18	h	77/85 (91%)	75 (97%)	2 (3%)	0	100	100
19	i	70/75 (93%)	67 (96%)	3 (4%)	0	100	100
20	k	47/56 (84%)	47 (100%)	0	0	100	100
21	l	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
22	m	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
23	J	29/63 (46%)	28 (97%)	1 (3%)	0	100	100
23	U	29/63 (46%)	25 (86%)	4 (14%)	0	100	100
All	All	5353/5812 (92%)	5102 (95%)	251 (5%)	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%)	373 (100%)	0	100	100
1	L	372/373 (100%)	372 (100%)	0	100	100
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%)	330 (99%)	2 (1%)	84	92
4	D	206/206 (100%)	206 (100%)	0	100	100
4	O	205/206 (100%)	204 (100%)	1 (0%)	86	93
5	F	93/98 (95%)	93 (100%)	0	100	100
5	Q	93/98 (95%)	93 (100%)	0	100	100
6	G	61/73 (84%)	61 (100%)	0	100	100
6	R	66/73 (90%)	66 (100%)	0	100	100
7	H	64/72 (89%)	64 (100%)	0	100	100
7	S	61/72 (85%)	60 (98%)	1 (2%)	58	76
8	P	15/166 (9%)	15 (100%)	0	100	100
9	T	58/58 (100%)	58 (100%)	0	100	100
10	I	82/95 (86%)	81 (99%)	1 (1%)	67	82
11	a	425/425 (100%)	424 (100%)	1 (0%)	92	96
12	b	210/210 (100%)	210 (100%)	0	100	100
13	c	225/227 (99%)	225 (100%)	0	100	100
14	d	127/128 (99%)	126 (99%)	1 (1%)	79	88
15	e	91/95 (96%)	91 (100%)	0	100	100
16	f	81/83 (98%)	81 (100%)	0	100	100
17	g	62/67 (92%)	62 (100%)	0	100	100
18	h	70/75 (93%)	70 (100%)	0	100	100
19	i	54/56 (96%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	k	39/46 (85%)	39 (100%)	0	100	100
21	l	39/40 (98%)	39 (100%)	0	100	100
22	m	33/34 (97%)	33 (100%)	0	100	100
23	J	26/54 (48%)	26 (100%)	0	100	100
23	U	26/54 (48%)	26 (100%)	0	100	100
All	All	4581/4911 (93%)	4574 (100%)	7 (0%)	91	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	I	56	LYS
11	a	331	ASN
4	O	83	ARG
14	d	113	ARG
7	S	70	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
11	a	331	ASN
11	a	451	ASN
14	d	76	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	3PE	N	405	-	50,50,50	0.31	0	53,55,55	0.30	0
26	CDL	N	404	-	40,40,99	0.46	0	46,52,111	0.59	1 (2%)
25	3PE	b	302	-	28,28,50	0.39	0	31,33,55	0.35	0
24	HEM	C	401	3	41,50,50	1.24	5 (12%)	45,82,82	1.69	7 (15%)
31	HEA	a	603	11	57,67,67	1.43	8 (14%)	61,103,103	2.36	23 (37%)
27	HEC	D	302	4	32,50,50	2.18	3 (9%)	24,82,82	1.53	2 (8%)
26	CDL	D	301	-	55,55,99	0.38	0	61,67,111	0.32	0
28	PC1	L	501	-	23,23,53	0.45	0	29,31,61	0.67	1 (3%)
25	3PE	N	403	-	36,36,50	0.35	0	39,41,55	0.34	0
25	3PE	a	606	-	27,27,50	0.40	0	30,32,55	0.45	0
25	3PE	L	502	-	22,22,50	0.44	0	25,27,55	0.39	0
33	CUA	b	303	12	0,1,1	-	-	-	-	-
25	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.37	0
25	3PE	g	101	-	24,24,50	0.44	0	27,29,55	0.68	1 (3%)
24	HEM	N	402	3	41,50,50	1.26	3 (7%)	45,82,82	1.79	8 (17%)
25	3PE	b	304	-	27,27,50	0.40	0	30,32,55	0.39	0
25	3PE	c	301	-	44,44,50	0.32	0	47,49,55	0.37	0
27	HEC	O	302	4	32,50,50	2.19	4 (12%)	24,82,82	1.51	2 (8%)
28	PC1	a	605	-	42,42,53	0.33	0	48,50,61	0.33	0
25	3PE	F	202	-	33,33,50	0.37	0	36,38,55	0.32	0
26	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.32	0
26	CDL	L	503	-	45,45,99	0.44	0	51,57,111	0.55	1 (1%)
24	HEM	C	402	3	41,50,50	1.26	5 (12%)	45,82,82	1.68	8 (17%)
31	HEA	a	604	11	57,67,67	1.43	8 (14%)	61,103,103	2.28	22 (36%)
25	3PE	F	201	-	28,28,50	0.39	0	31,33,55	0.40	0
35	TGL	l	601	-	43,43,62	0.21	0	46,46,65	0.24	0
25	3PE	d	201	-	33,33,50	0.39	0	36,38,55	0.60	1 (2%)
24	HEM	N	401	3	41,50,50	1.22	4 (9%)	45,82,82	1.73	8 (17%)
25	3PE	k	101	-	26,26,50	0.41	0	29,31,55	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	C	404	-	41,41,99	0.44	0	47,53,111	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	N	405	-	-	13/54/54/54	-
26	CDL	N	404	-	-	12/51/51/110	-
25	3PE	b	302	-	-	8/32/32/54	-
24	HEM	C	401	3	-	4/12/54/54	-
31	HEA	a	603	11	-	10/32/76/76	-
27	HEC	D	302	4	-	0/10/54/54	-
26	CDL	D	301	-	-	18/66/66/110	-
28	PC1	L	501	-	-	8/27/27/57	-
25	3PE	N	403	-	-	6/40/40/54	-
25	3PE	a	606	-	-	12/31/31/54	-
25	3PE	L	502	-	-	9/26/26/54	-
25	3PE	C	403	-	-	10/38/38/54	-
25	3PE	g	101	-	-	10/28/28/54	-
24	HEM	N	402	3	-	8/12/54/54	-
25	3PE	b	304	-	-	7/31/31/54	-
25	3PE	c	301	-	-	7/48/48/54	-
27	HEC	O	302	4	-	0/10/54/54	-
28	PC1	a	605	-	-	8/46/46/57	-
25	3PE	F	202	-	-	9/37/37/54	-
26	CDL	O	301	-	-	20/67/67/110	-
26	CDL	L	503	-	-	16/56/56/110	-
24	HEM	C	402	3	-	6/12/54/54	-
31	HEA	a	604	11	-	5/32/76/76	-
25	3PE	F	201	-	-	6/32/32/54	-
35	TGL	l	601	-	-	4/46/46/65	-
25	3PE	d	201	-	-	9/37/37/54	-
24	HEM	N	401	3	-	5/12/54/54	-
25	3PE	k	101	-	-	6/30/30/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	C	404	-	-	12/52/52/110	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	302	HEC	C2B-C3B	-6.35	1.34	1.40
27	D	302	HEC	C3C-C2C	-6.25	1.34	1.40
27	O	302	HEC	C3C-C2C	-6.22	1.34	1.40
27	O	302	HEC	C2B-C3B	-6.21	1.34	1.40
27	O	302	HEC	C3D-C2D	5.44	1.53	1.37

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	604	HEA	CMC-C2C-C3C	7.05	137.88	124.68
31	a	603	HEA	CMC-C2C-C3C	6.99	137.75	124.68
31	a	604	HEA	CMC-C2C-C1C	-6.31	118.77	128.46
31	a	603	HEA	CMC-C2C-C1C	-6.15	119.02	128.46
24	N	401	HEM	CHC-C4B-NB	4.88	129.73	124.43

There are no chirality outliers.

5 of 248 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	C	401	HEM	C2B-C3B-CAB-CBB
24	C	401	HEM	C4B-C3B-CAB-CBB
24	C	402	HEM	C2B-C3B-CAB-CBB
24	C	402	HEM	C4B-C3B-CAB-CBB
24	N	401	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

8 monomers are involved in 12 short contacts:

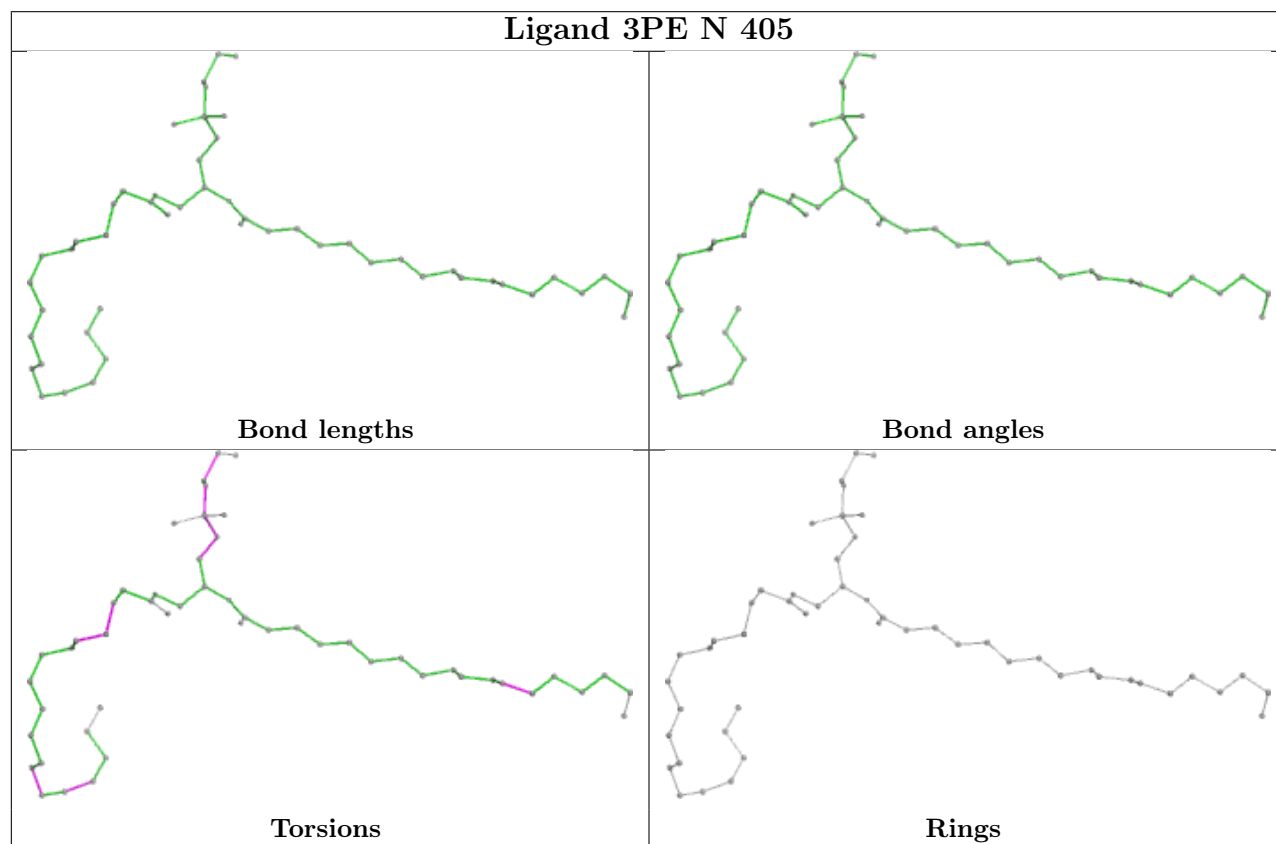
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	N	405	3PE	3	0
24	C	401	HEM	1	0
26	D	301	CDL	2	0
24	N	402	HEM	1	0
26	O	301	CDL	2	0
24	C	402	HEM	1	0
25	F	201	3PE	1	0

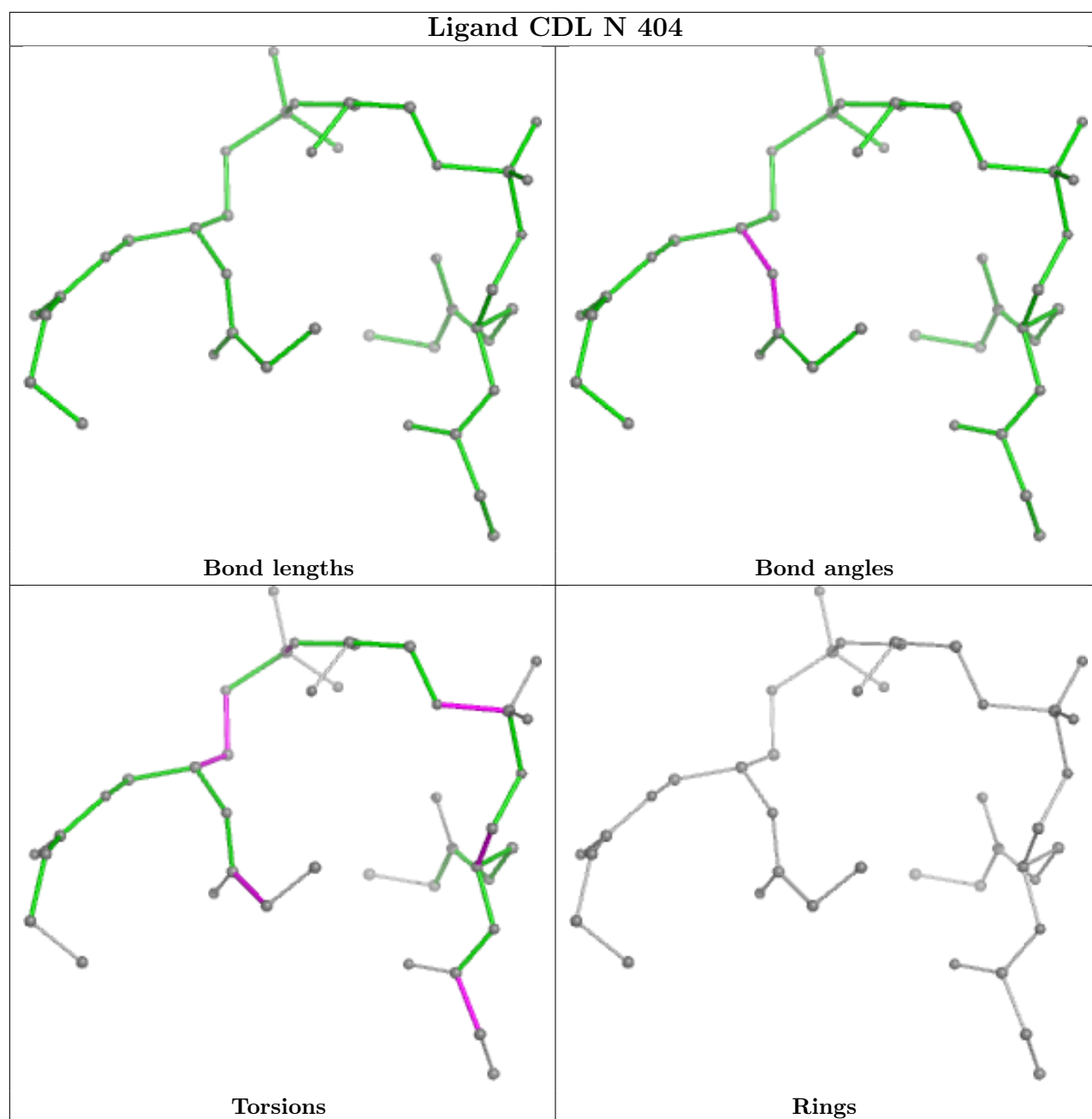
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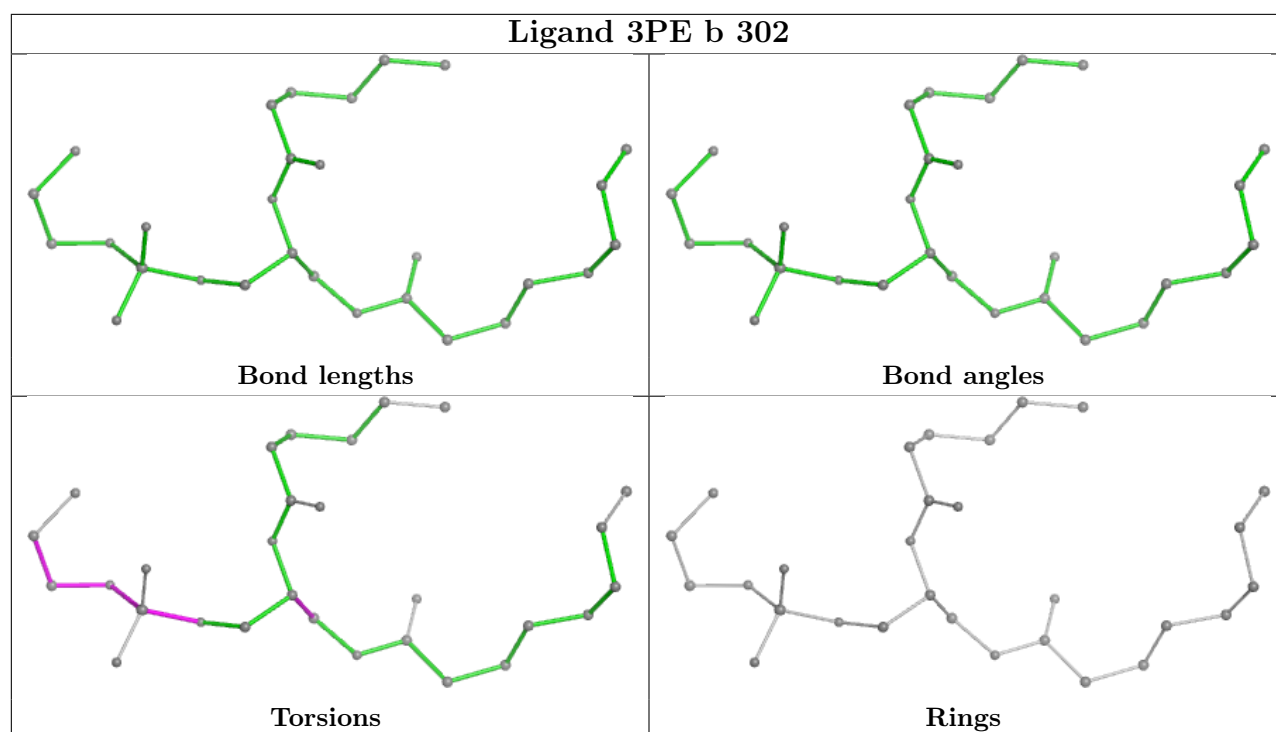
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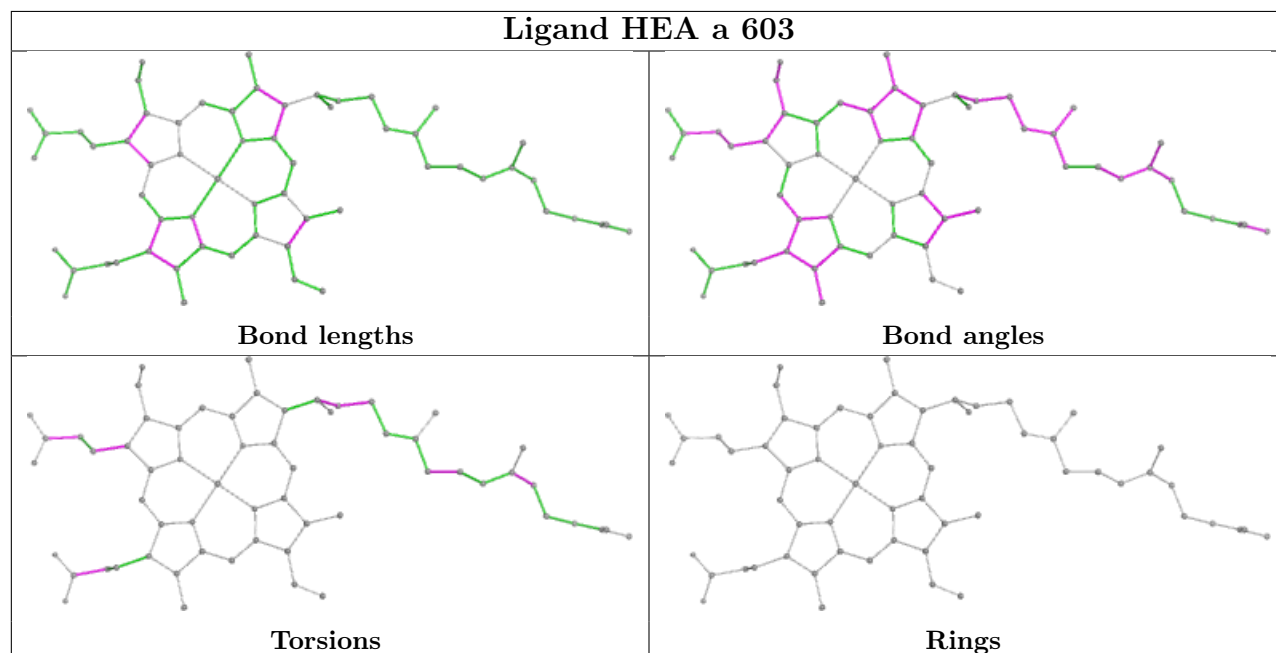
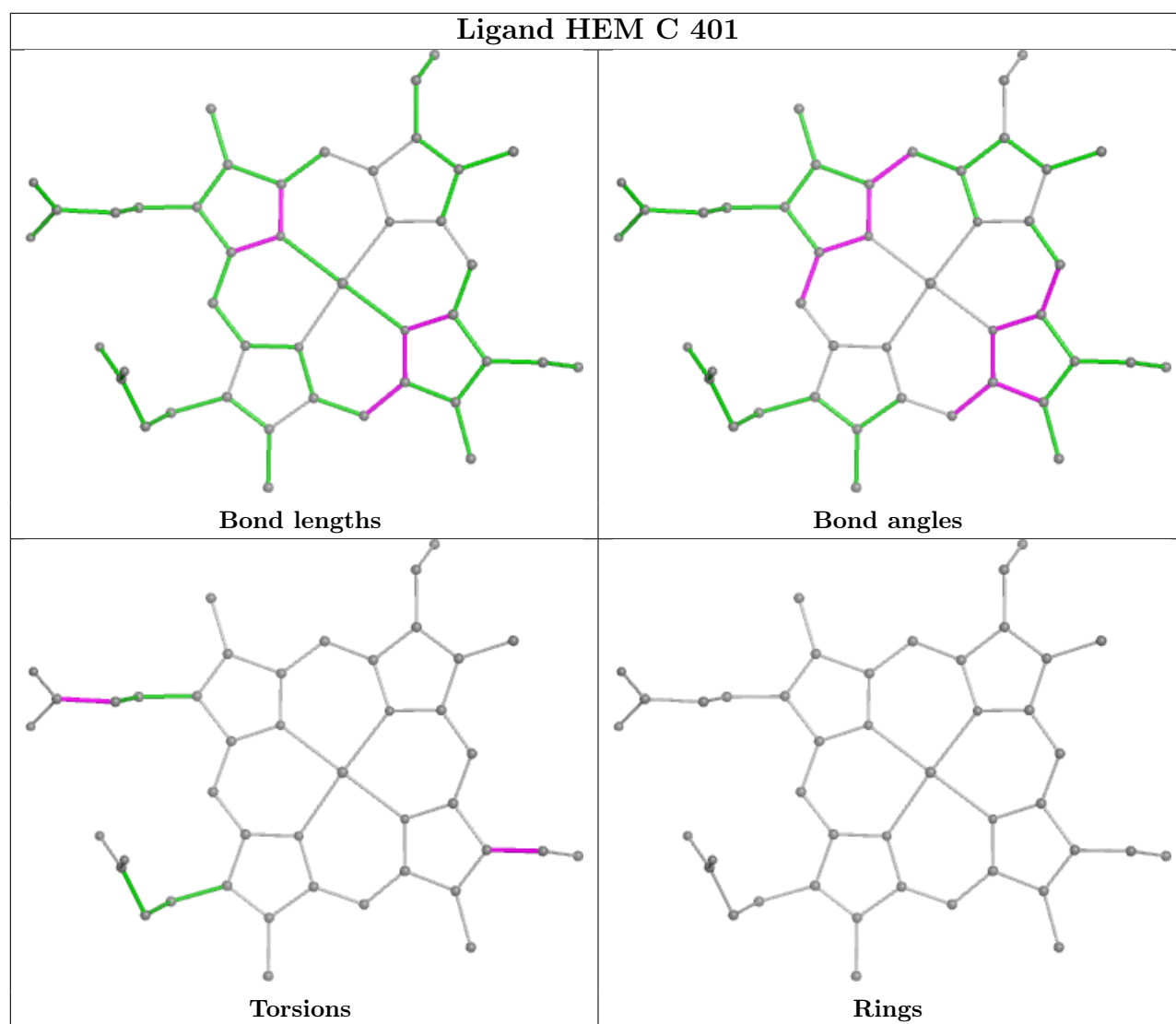
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	N	401	HEM	1	0

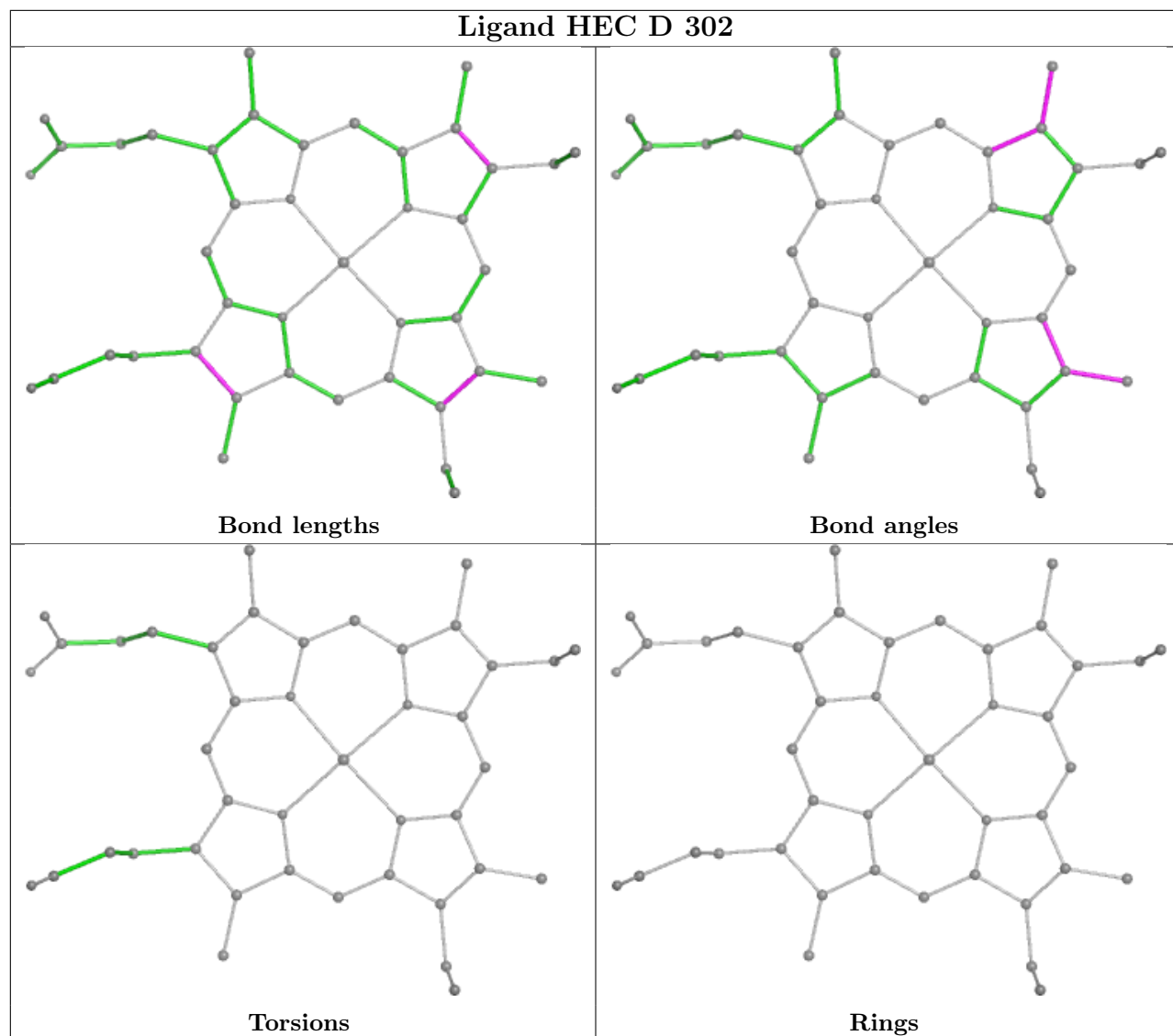
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

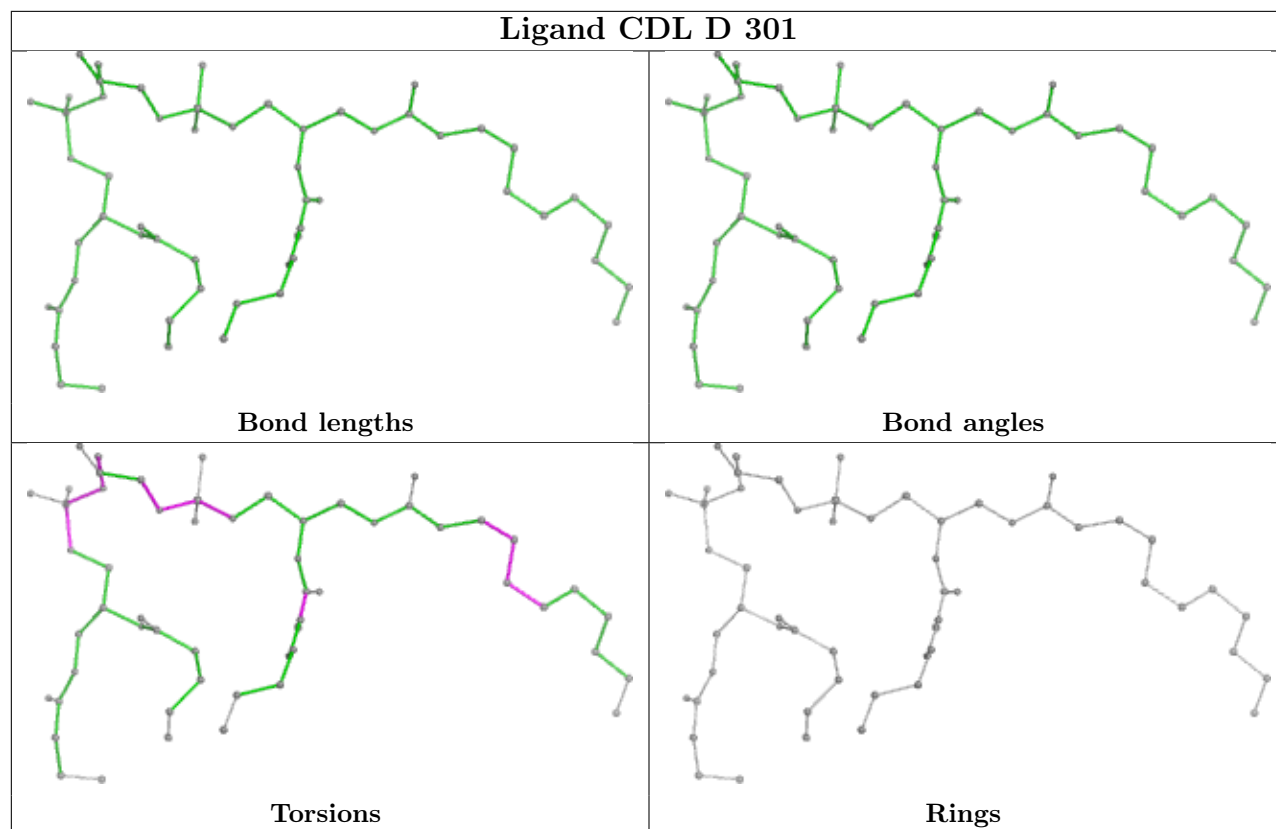




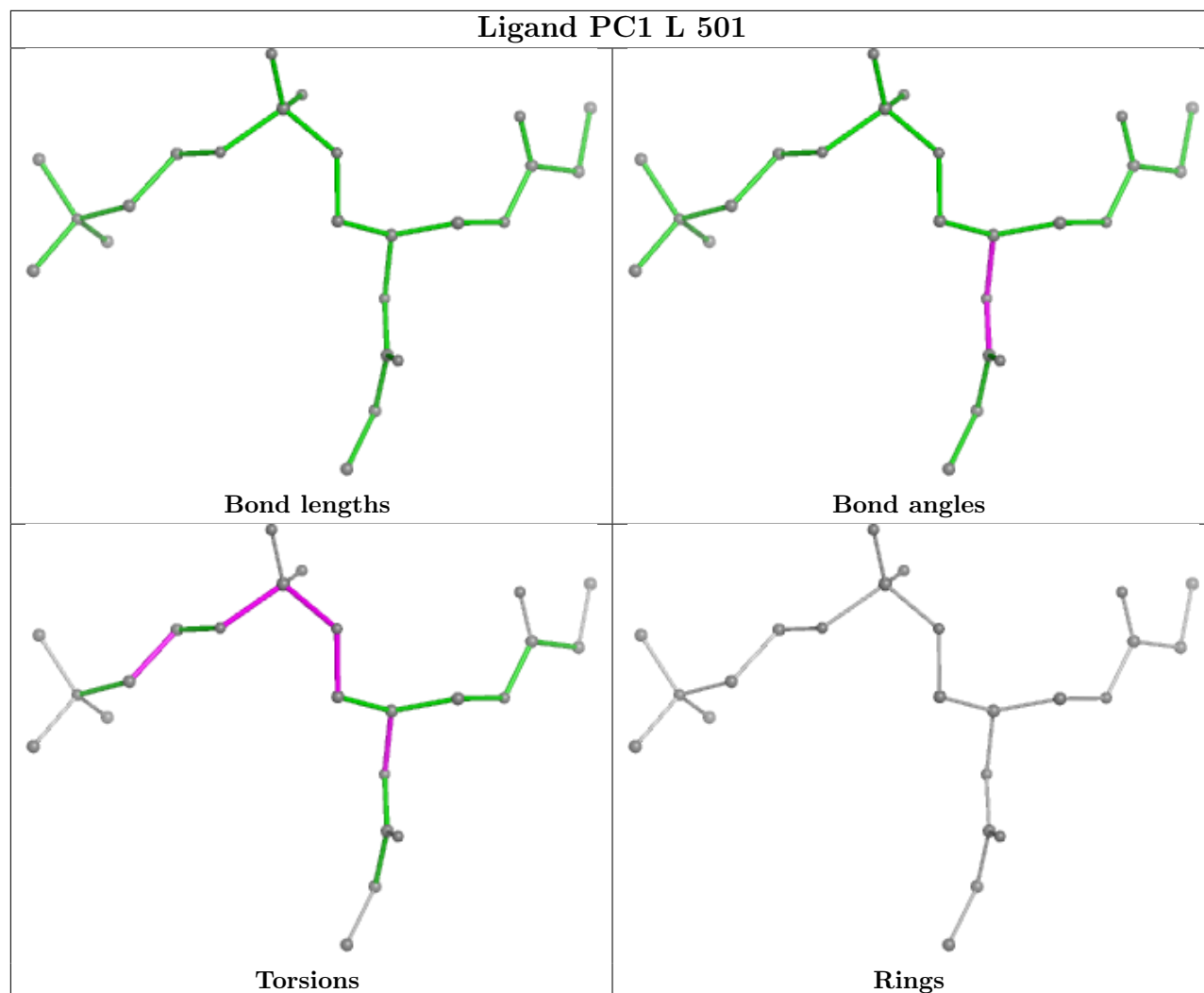




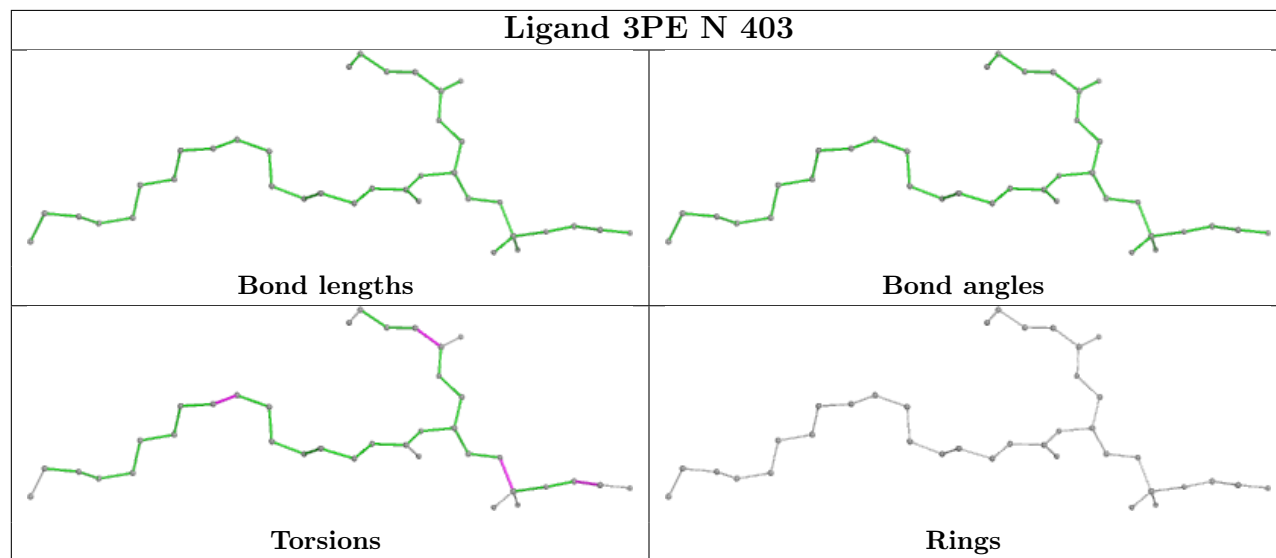


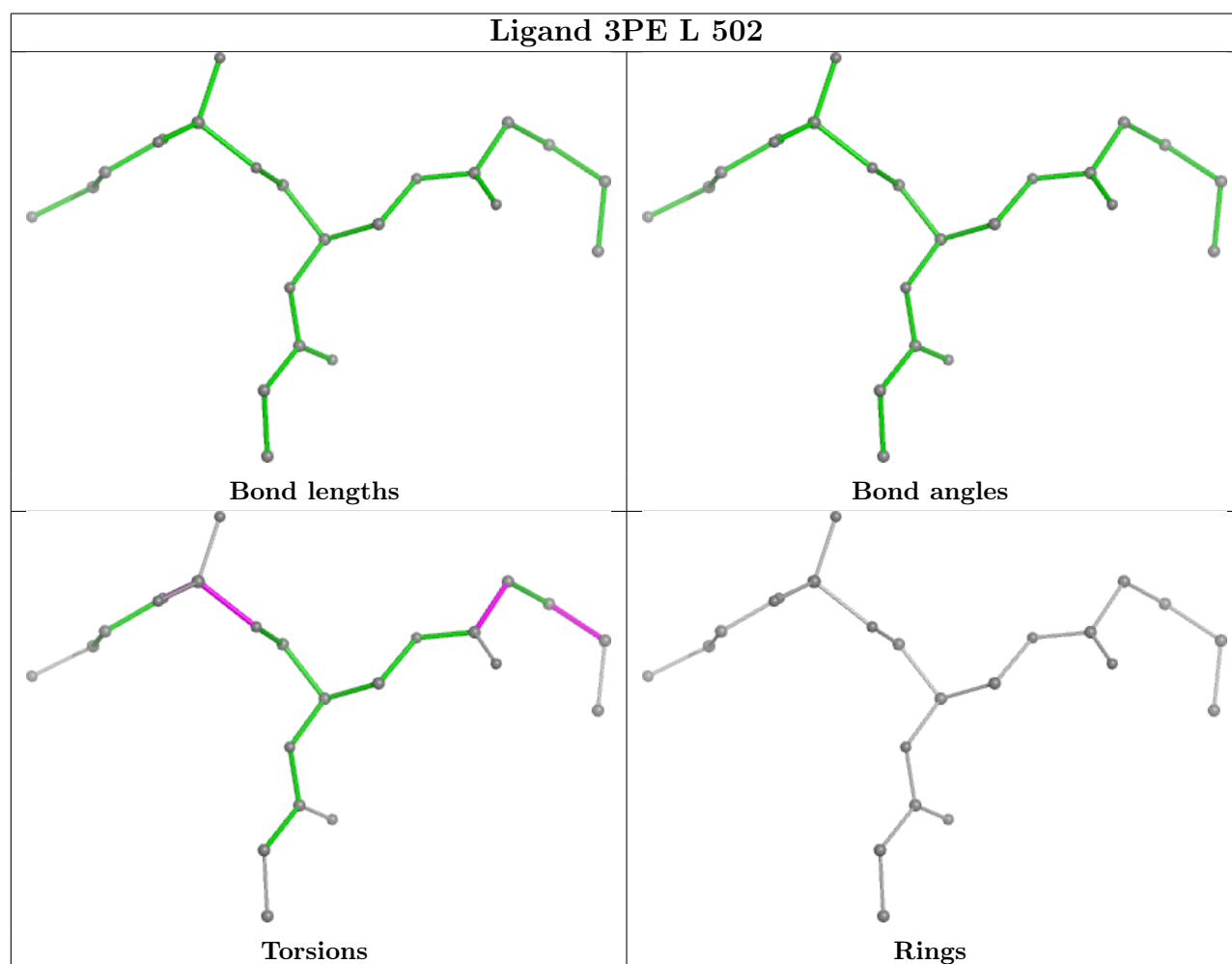
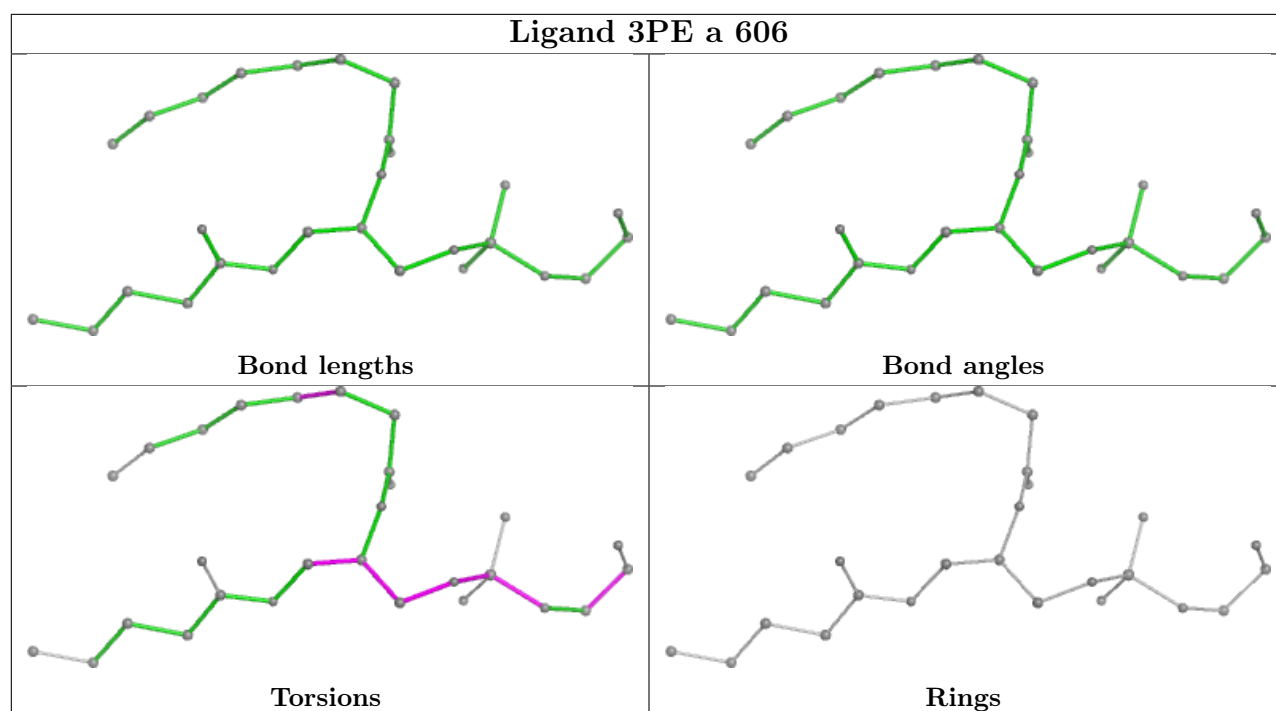


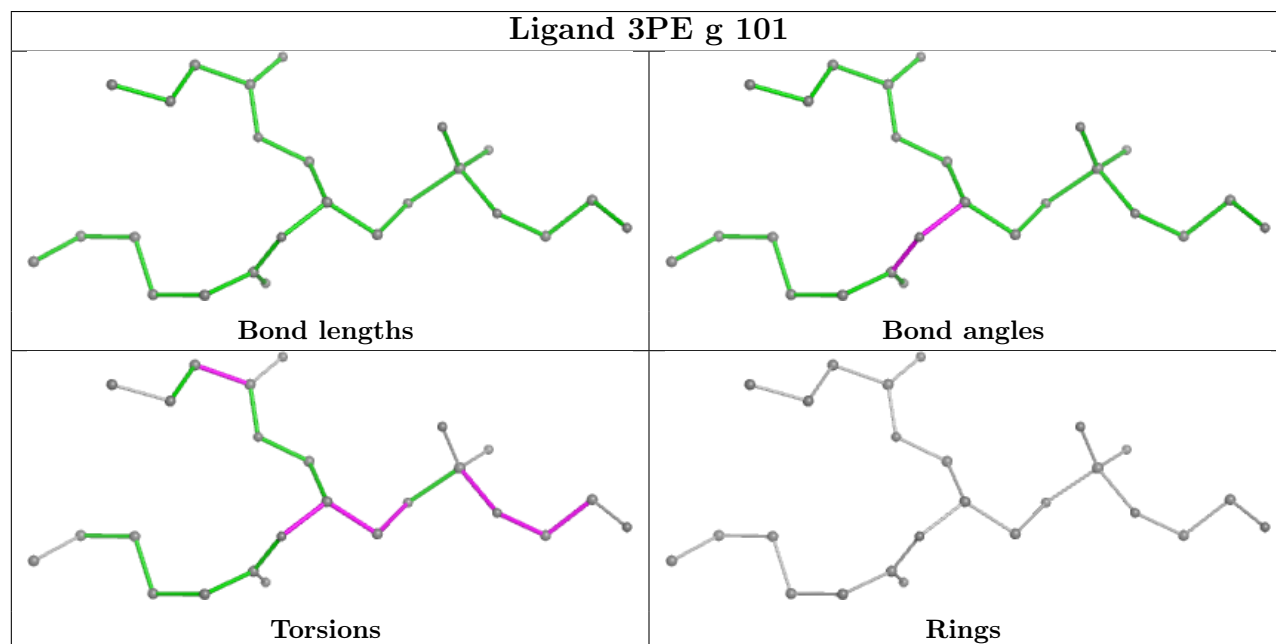
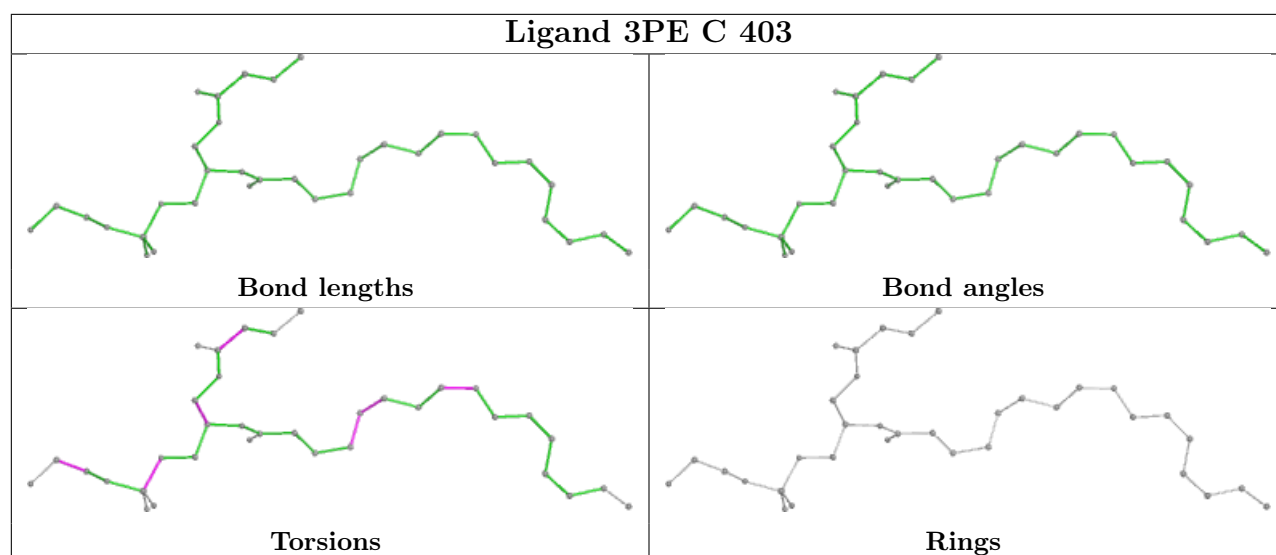
Ligand PC1 L 501

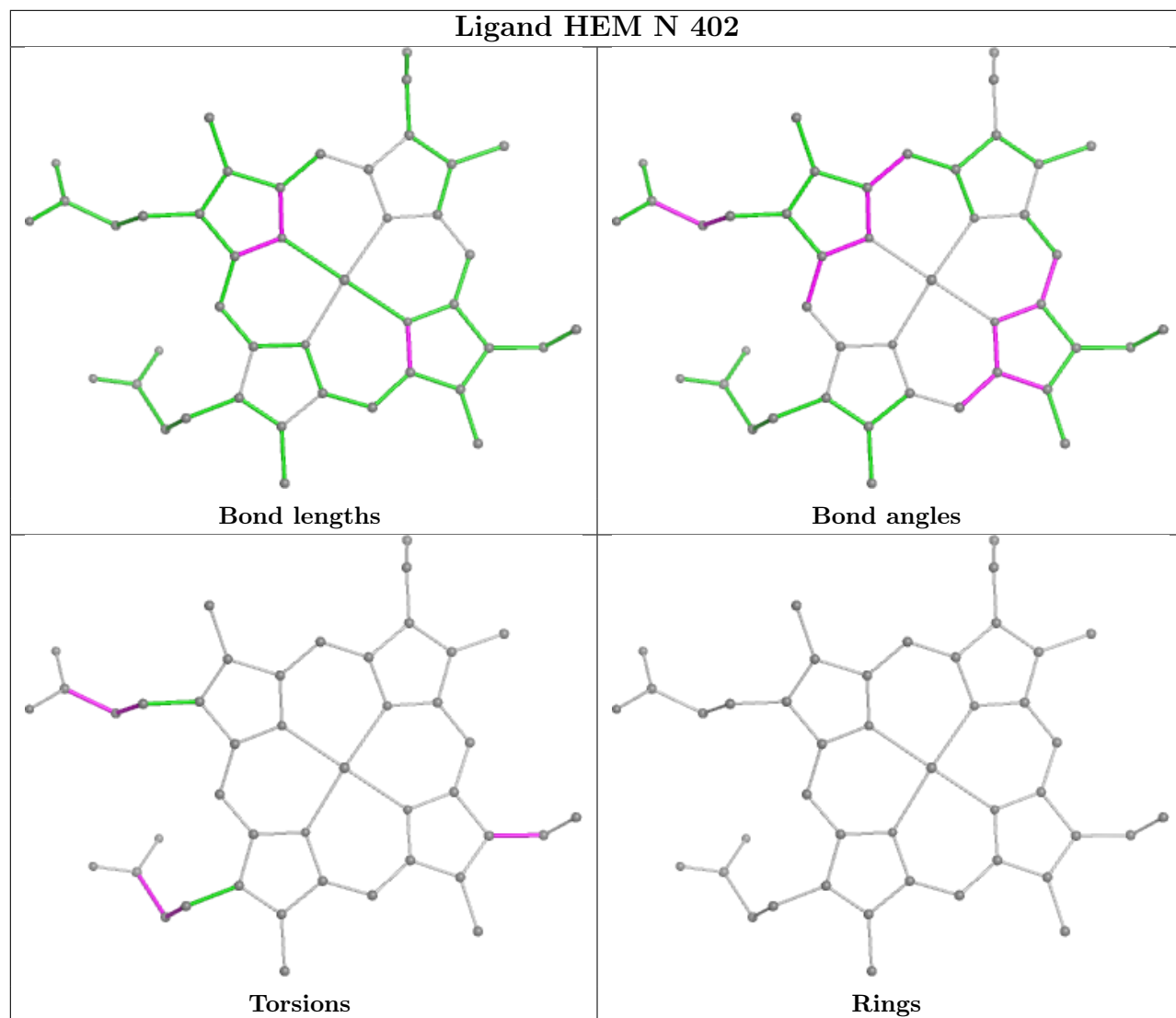


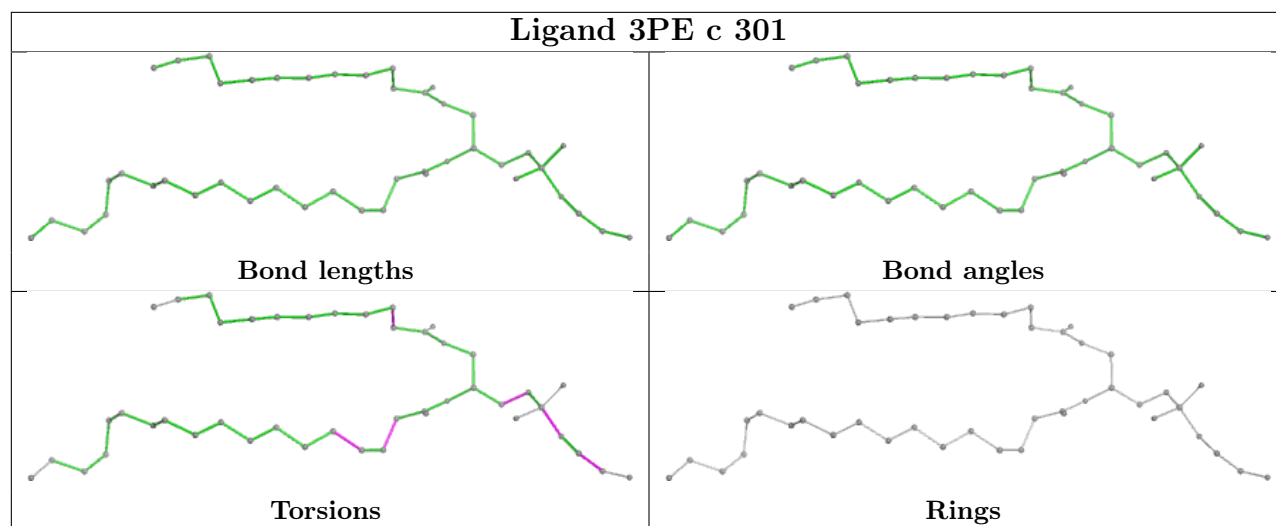
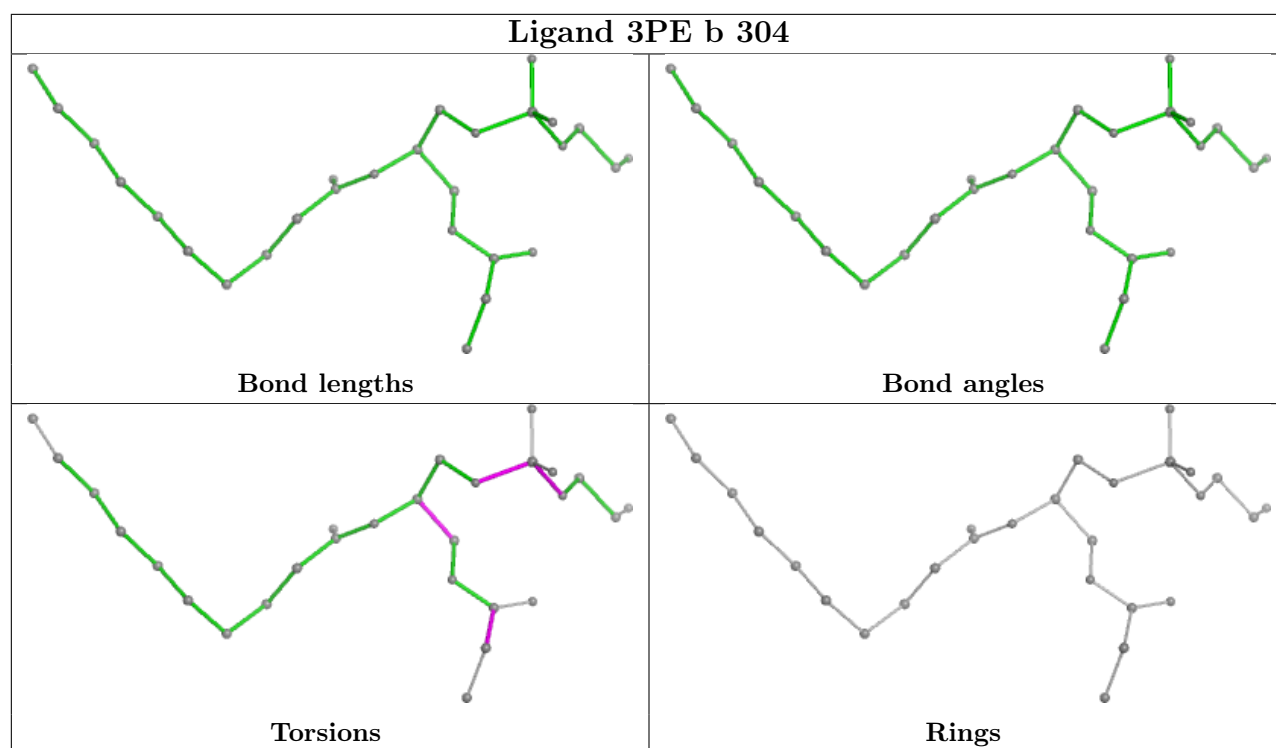
Ligand 3PE N 403

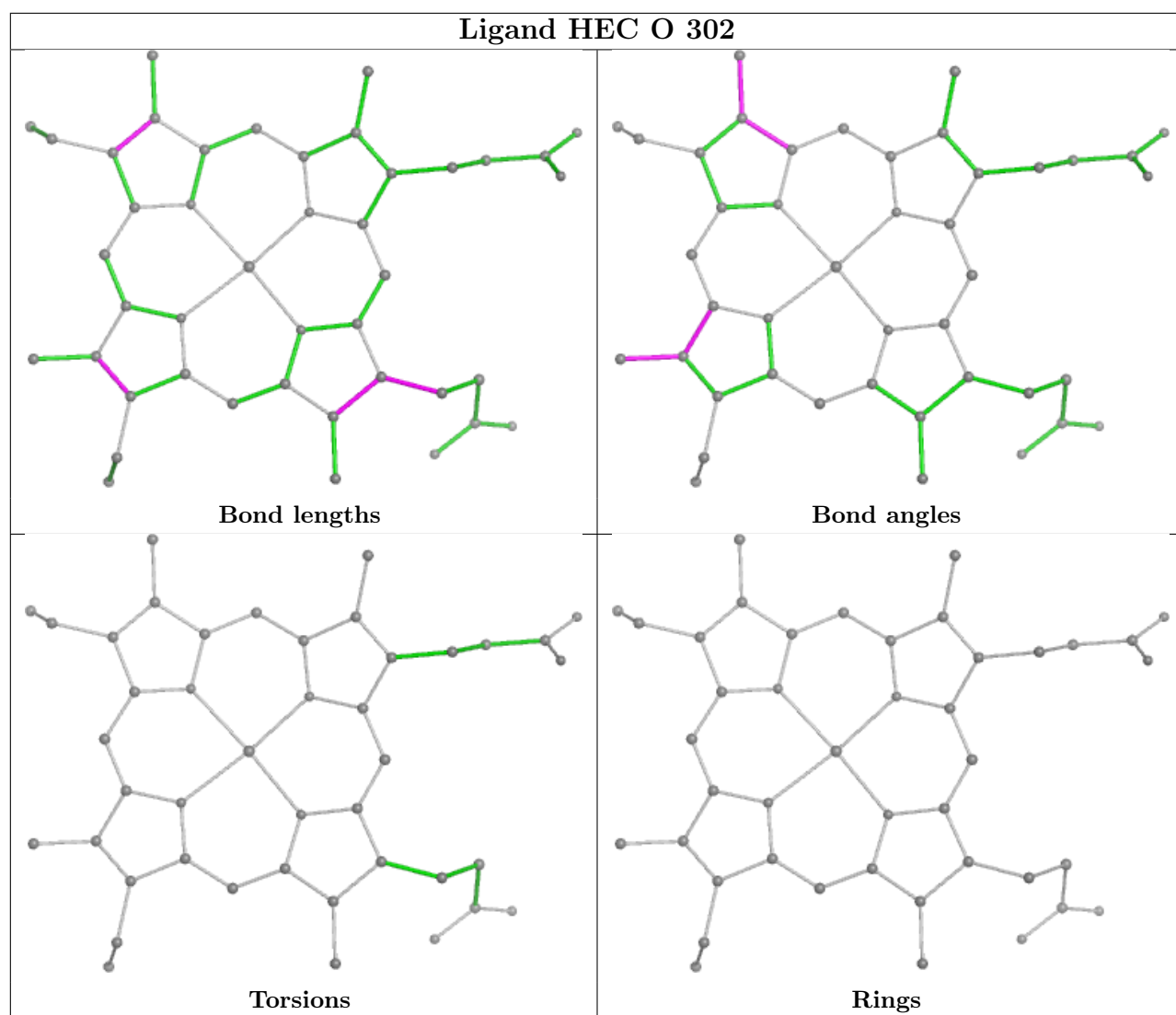


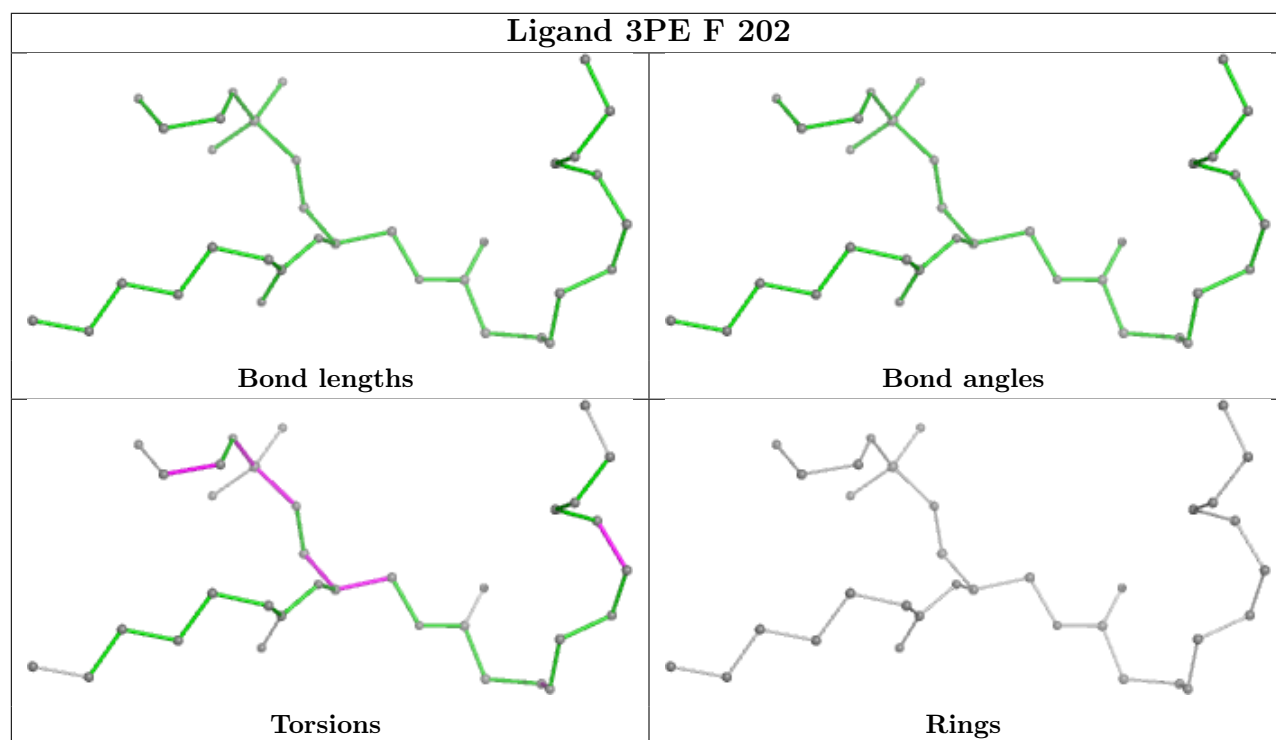
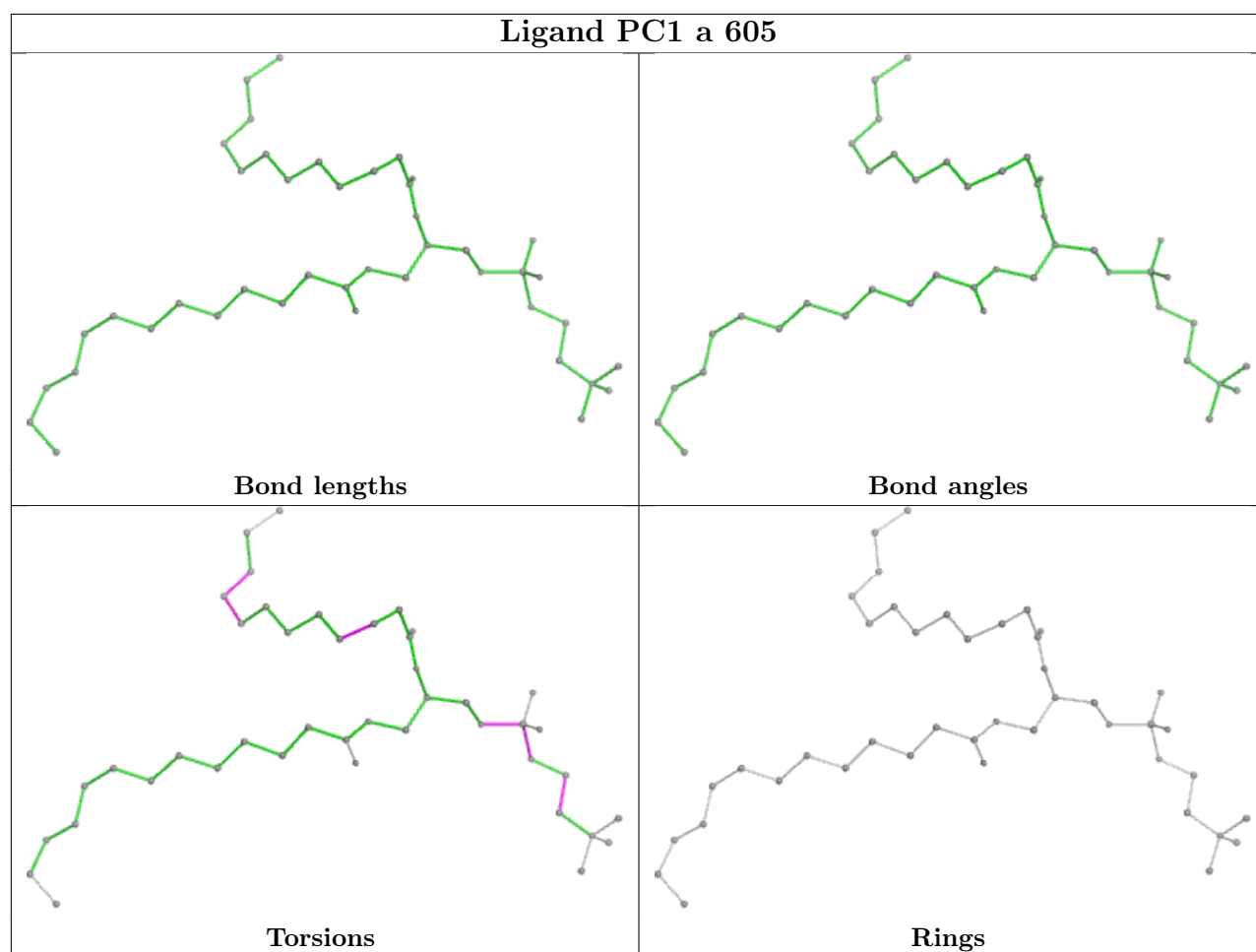


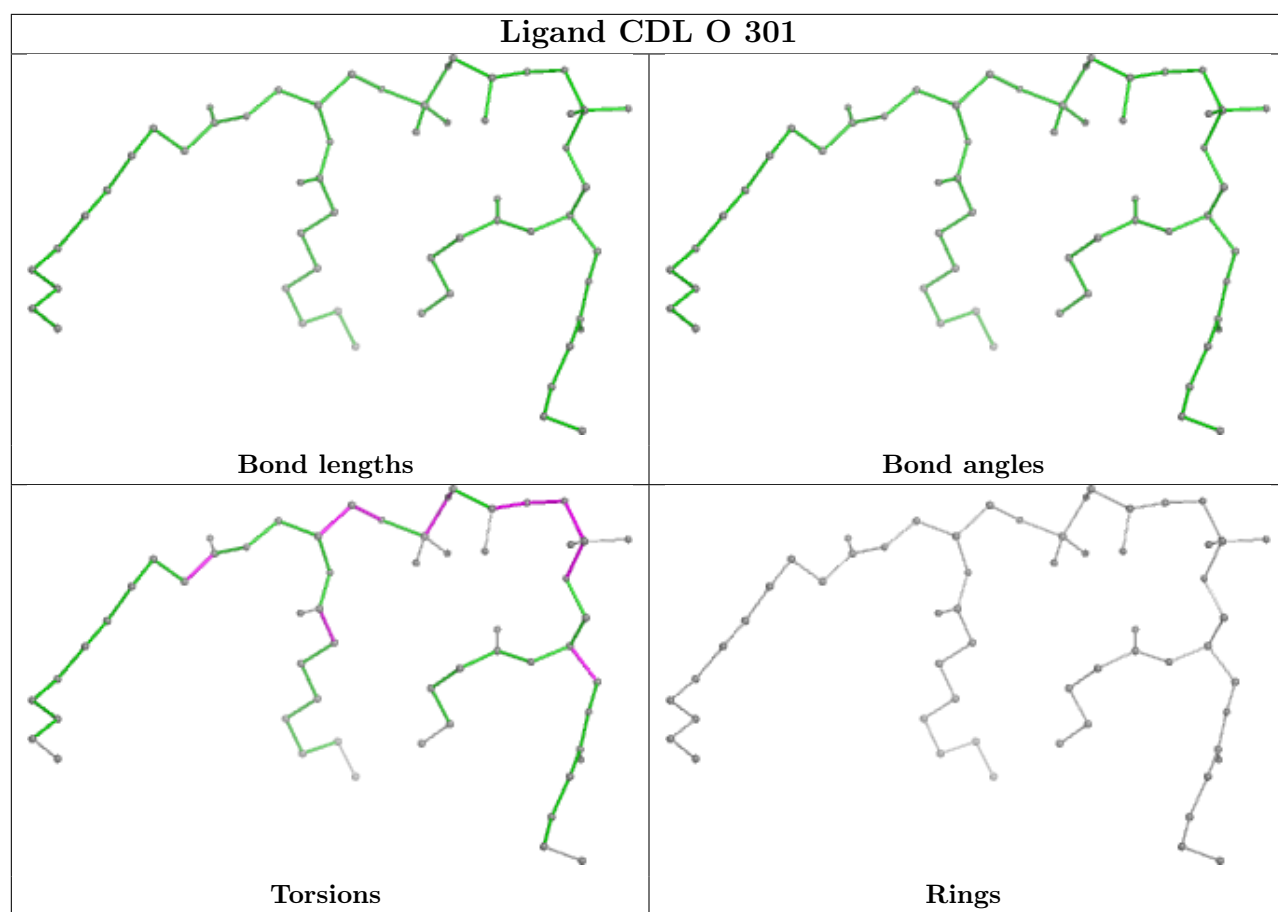




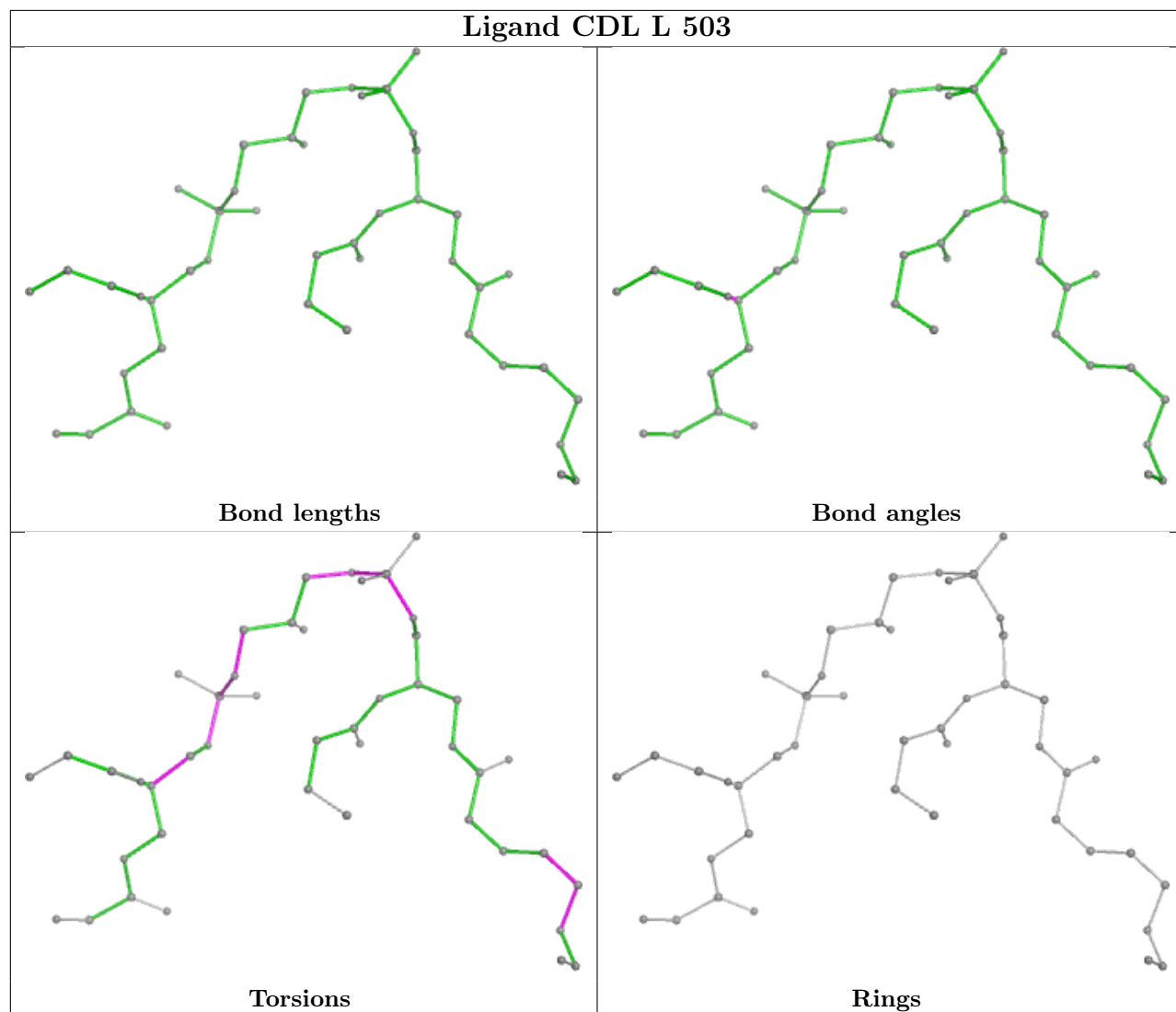


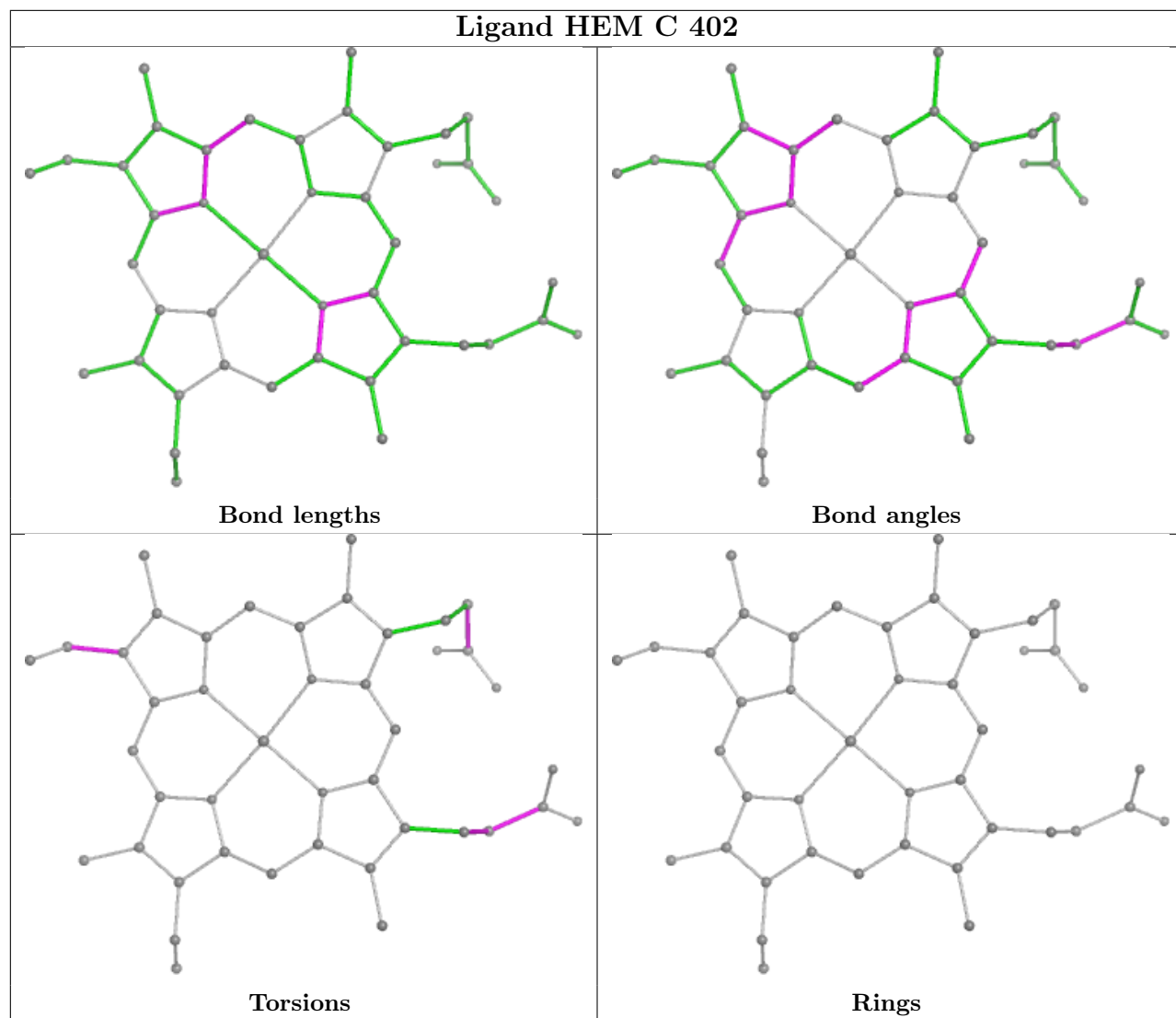




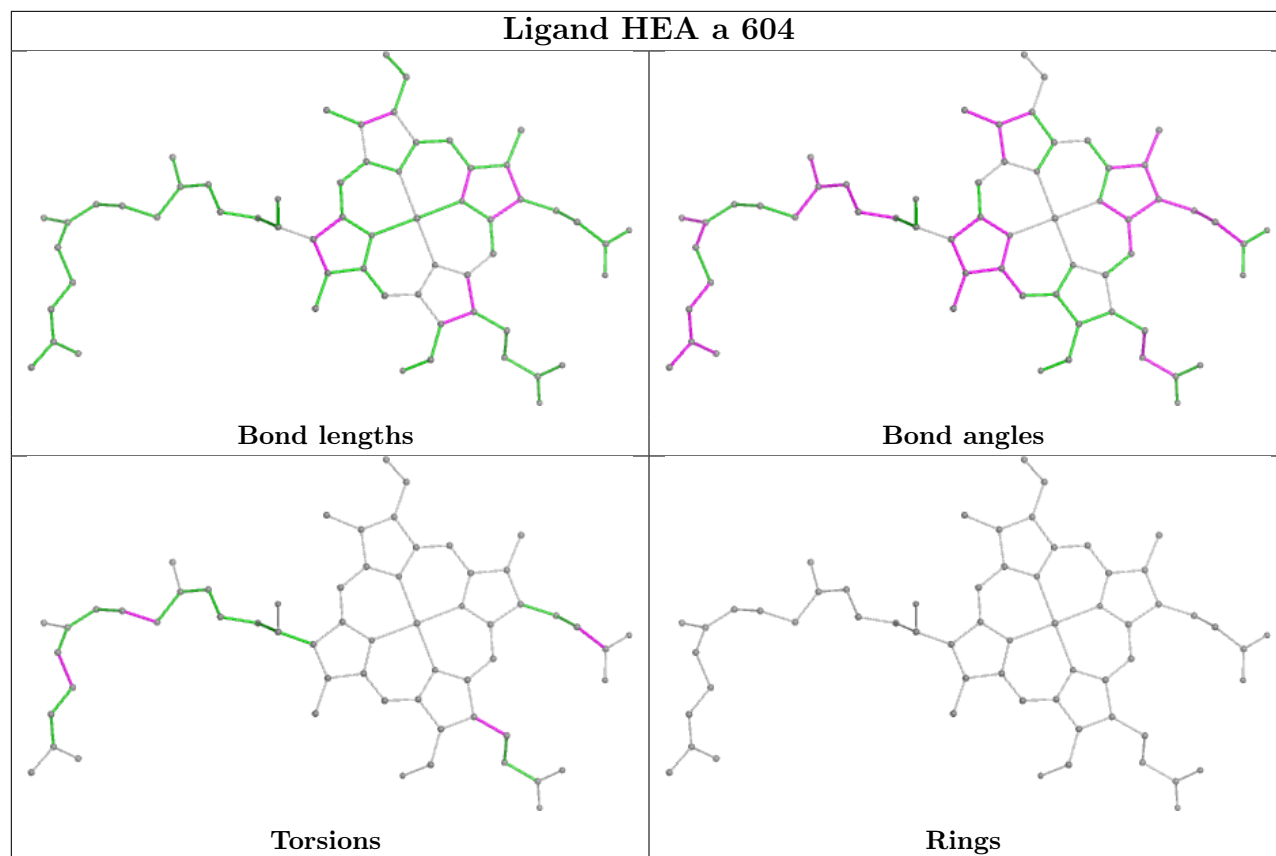


Ligand CDL L 503

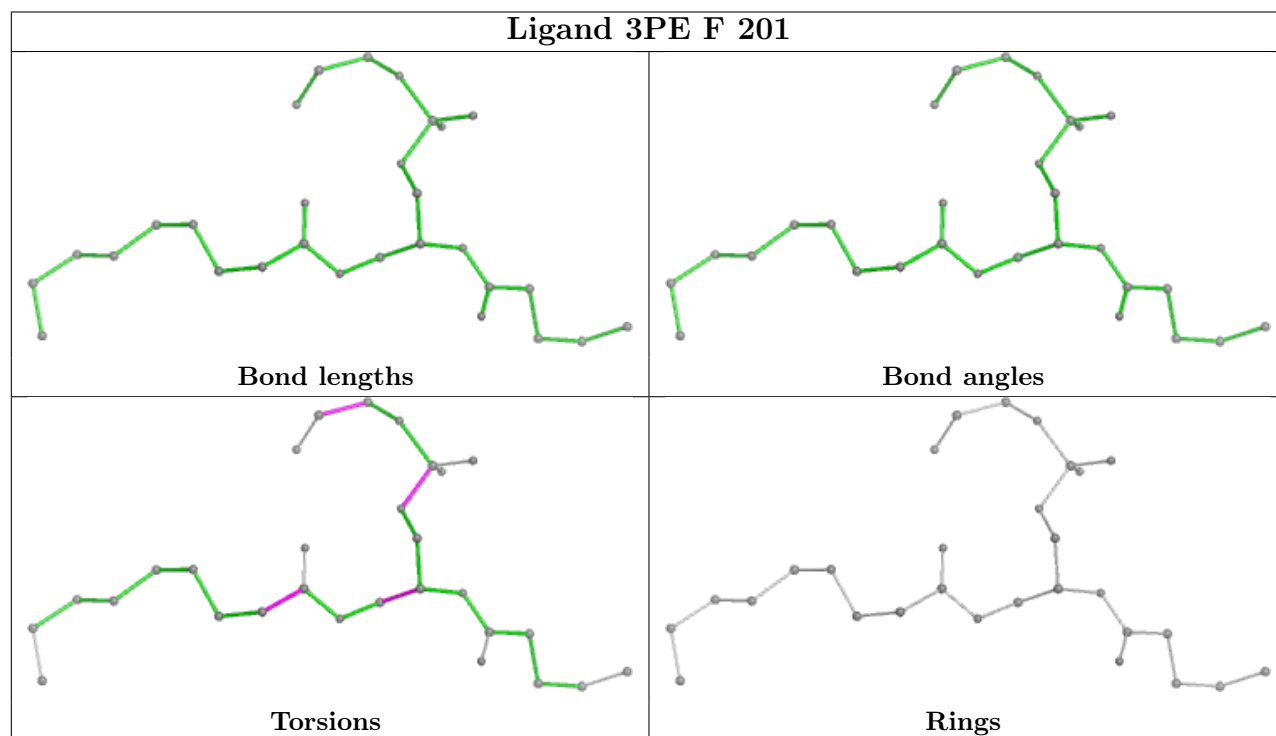


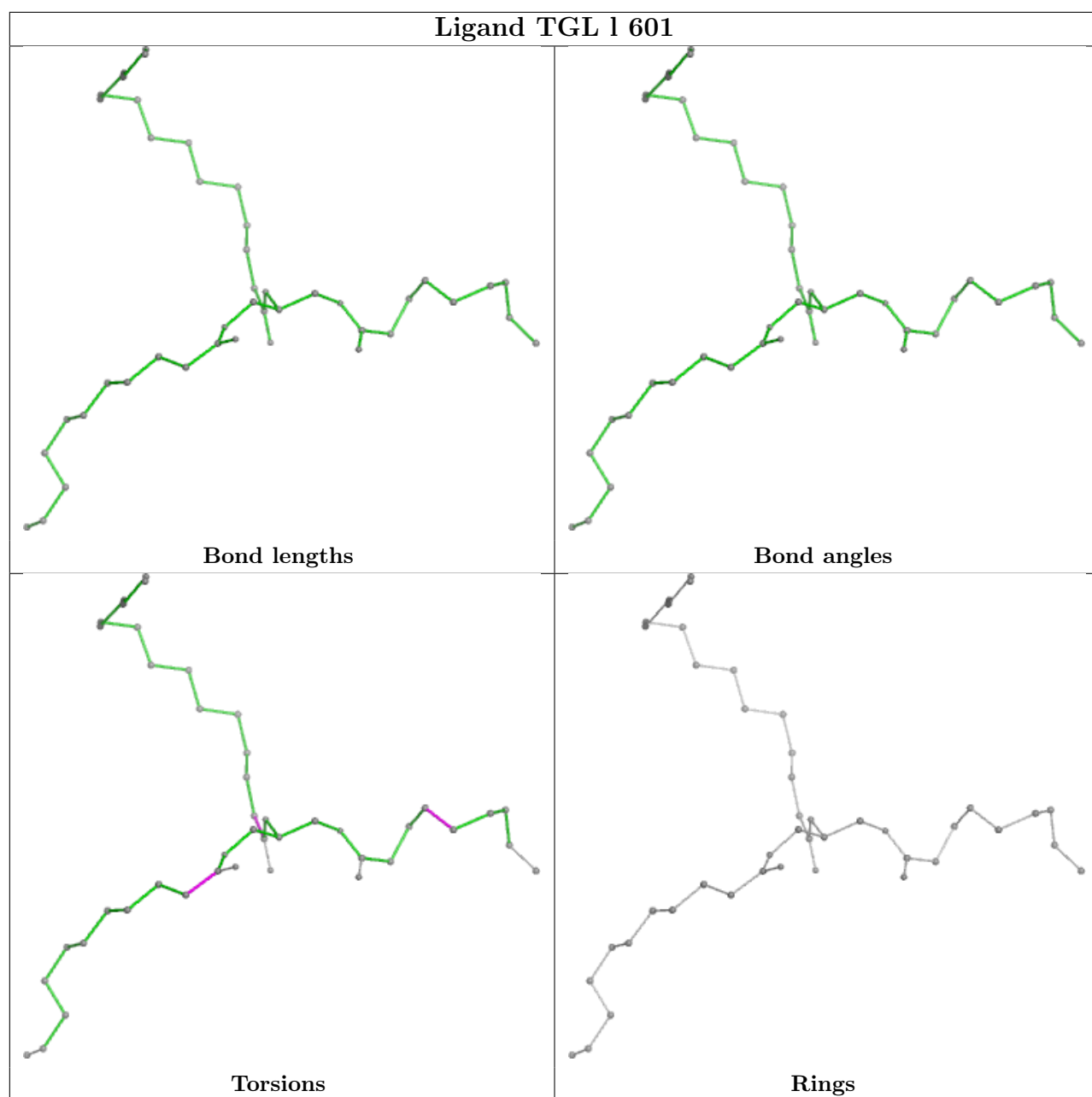


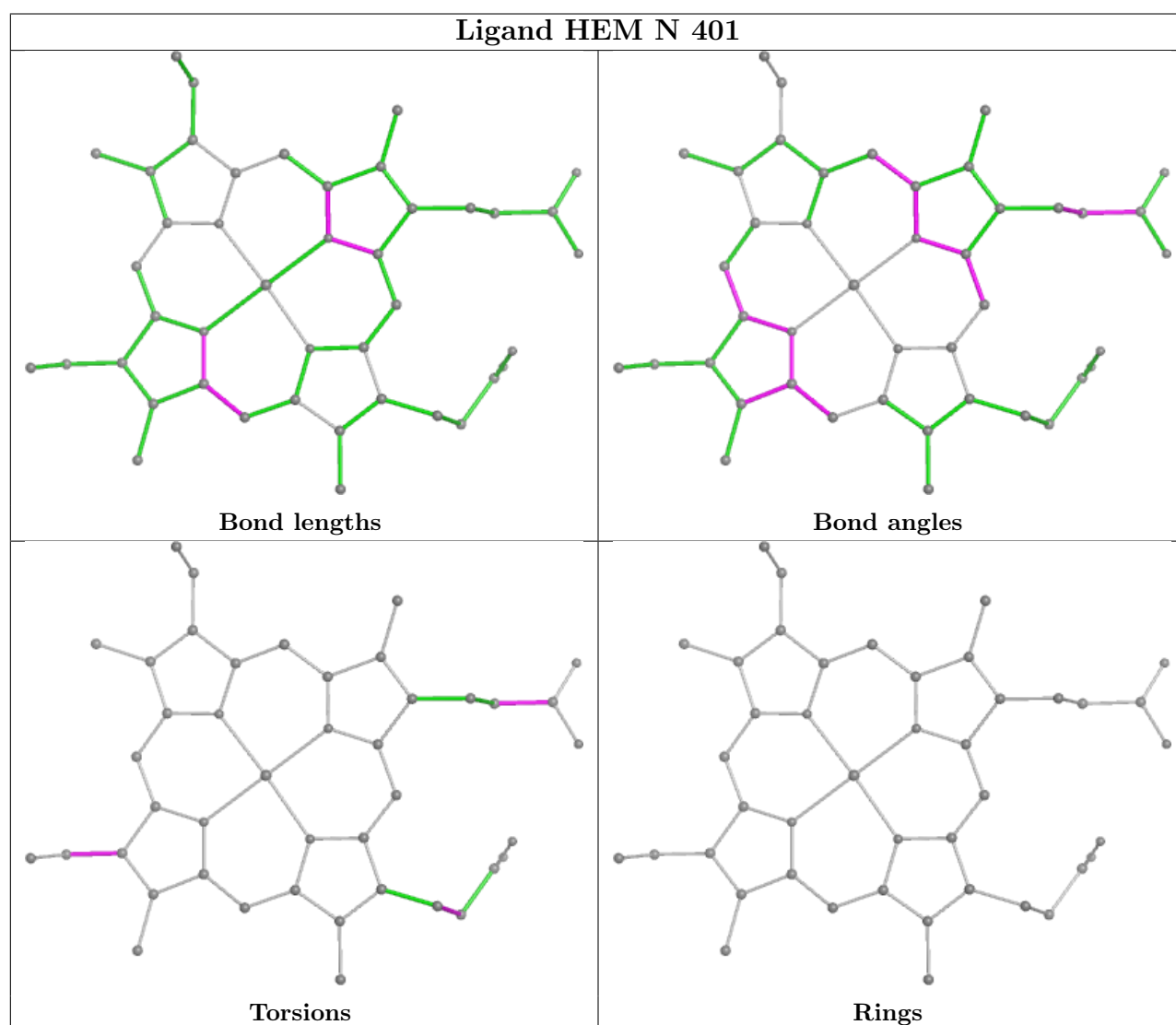
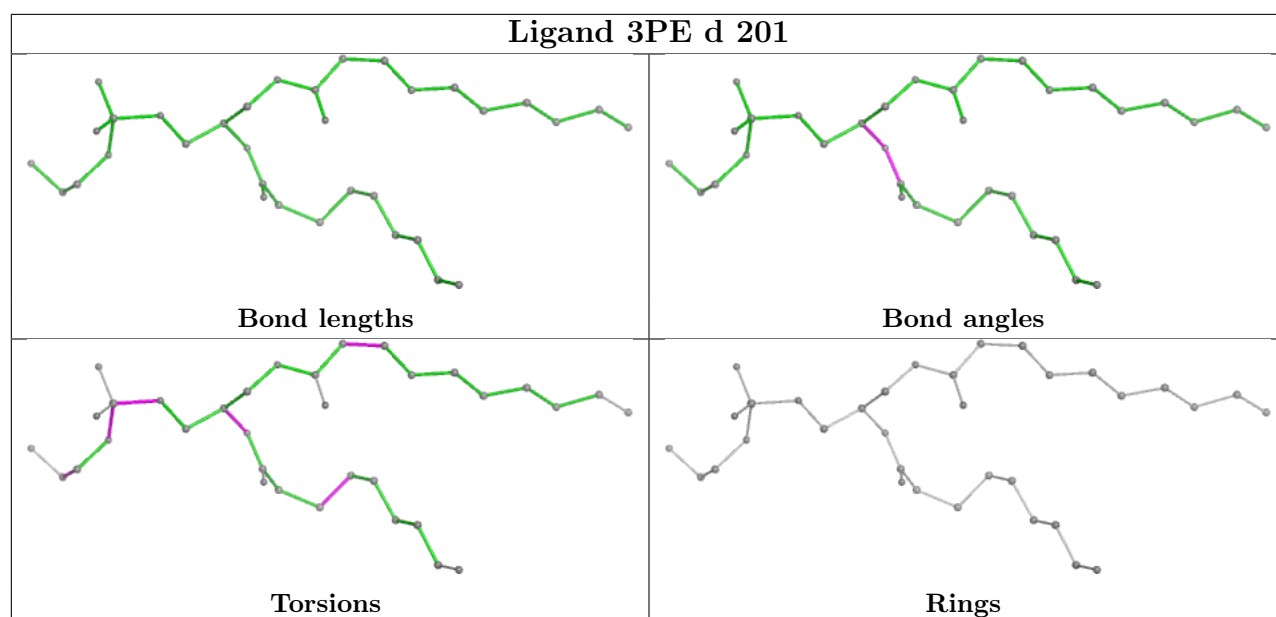
Ligand HEA a 604

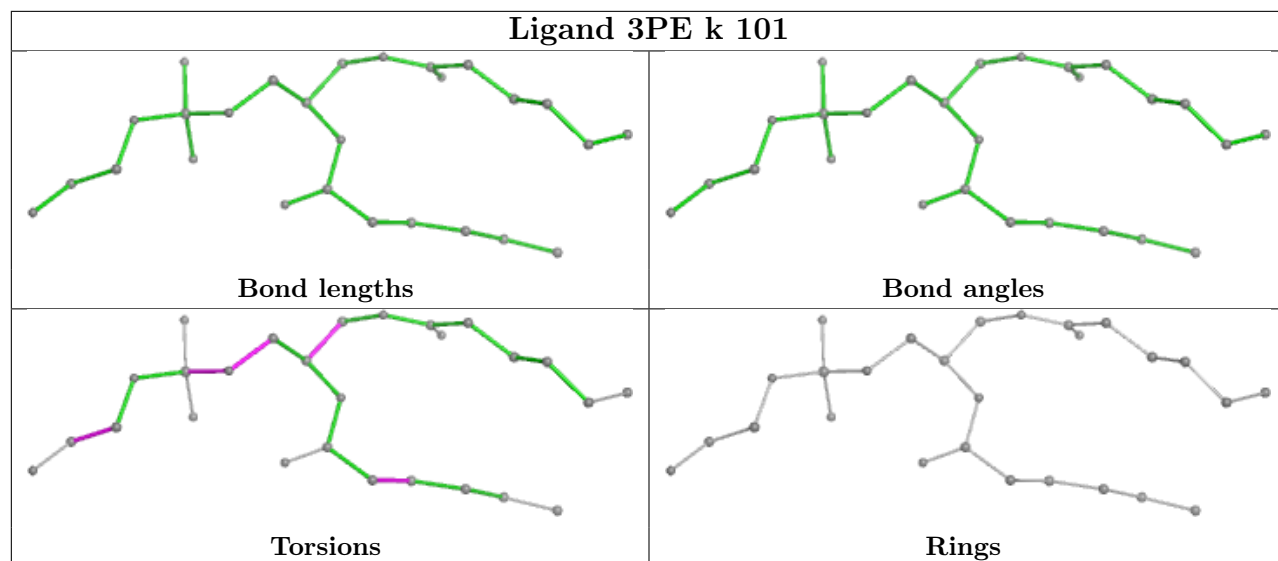


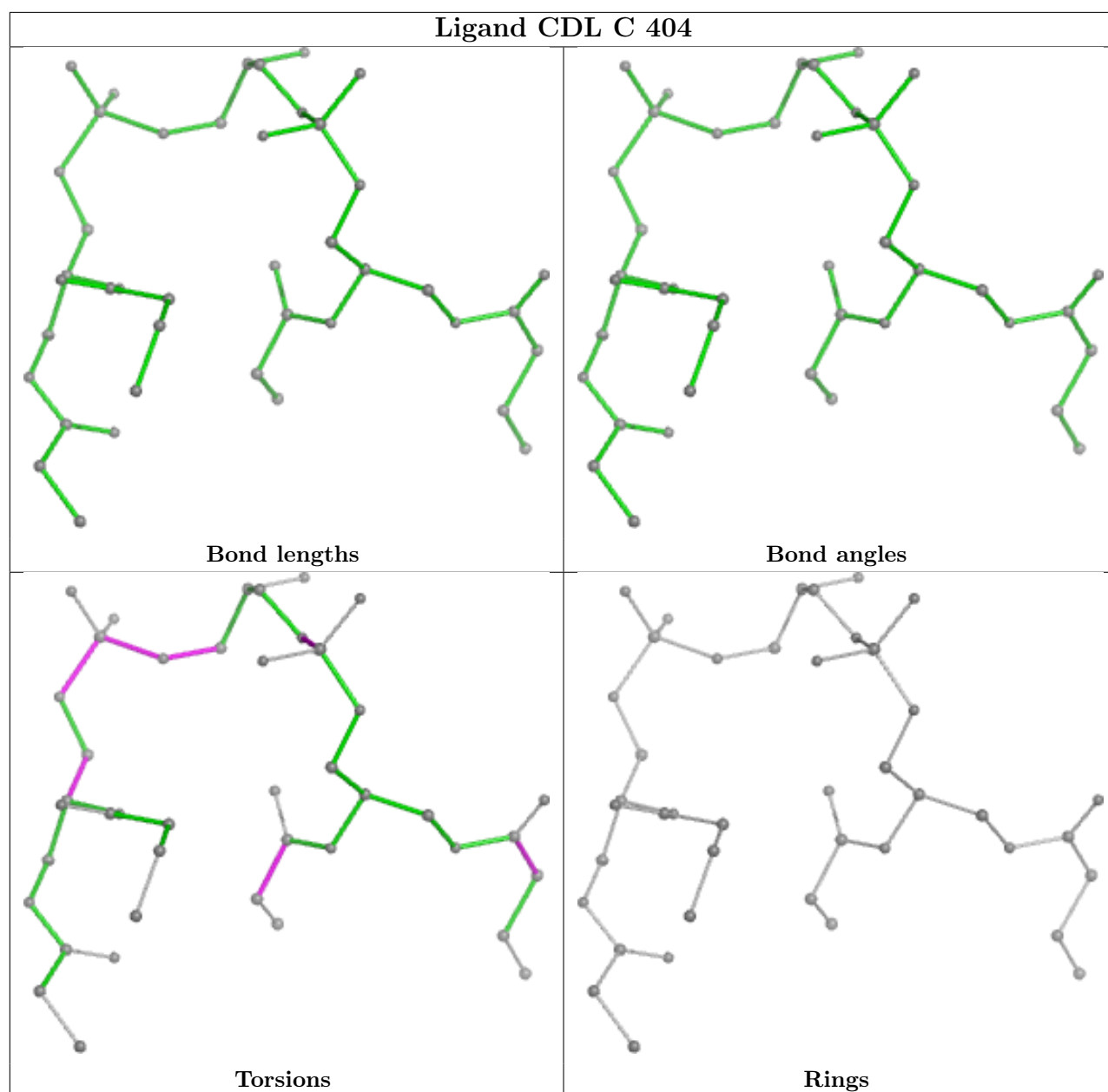
Ligand 3PE F 201











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.

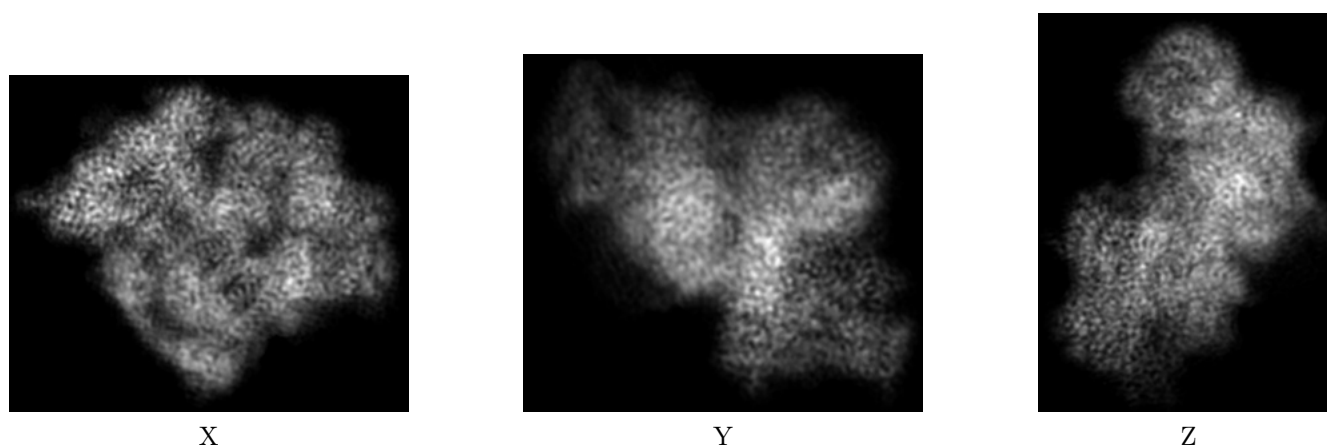
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12705. 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](#)

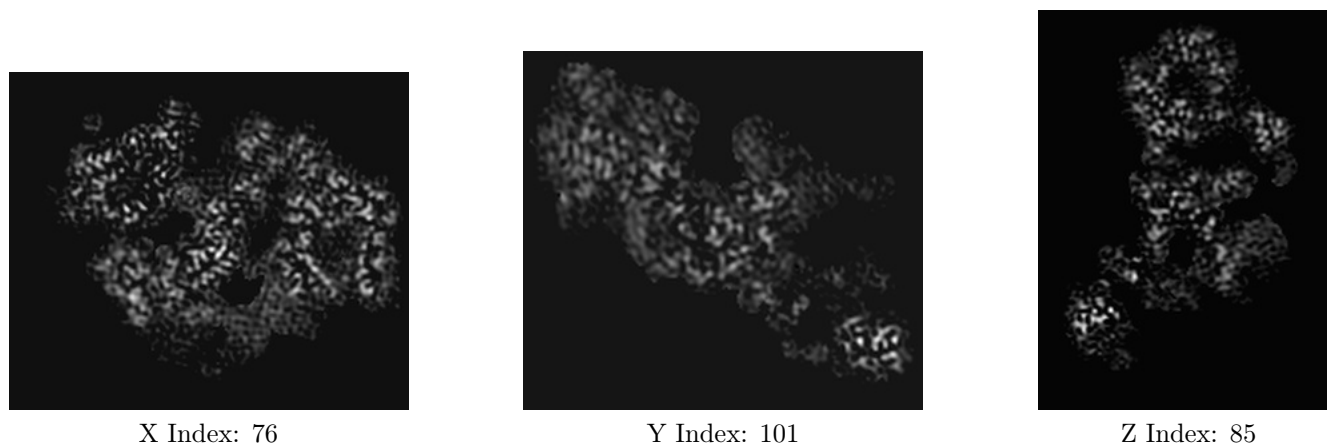
6.1.1 Primary map



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

6.2 Central slices [i](#)

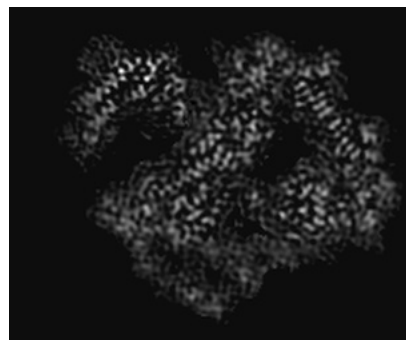
6.2.1 Primary map



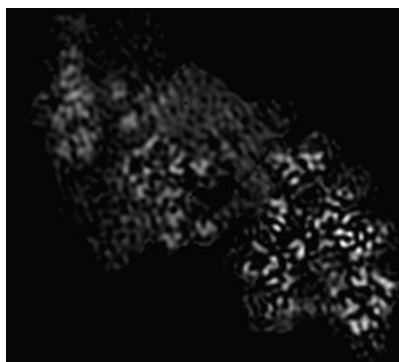
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

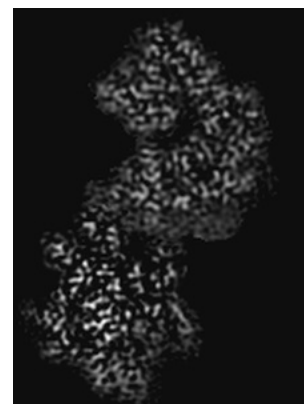
6.3.1 Primary map



X Index: 87



Y Index: 87

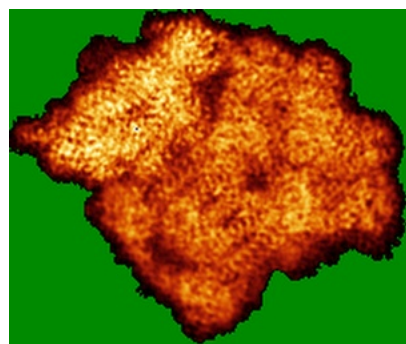


Z Index: 104

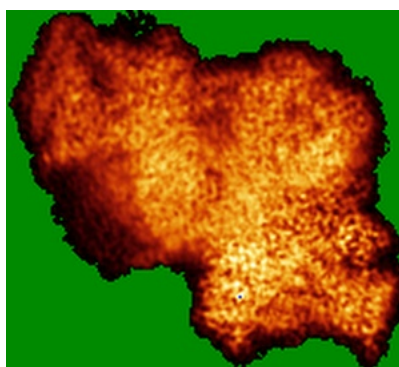
The images above show the largest variance slices of the map in three orthogonal directions.

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

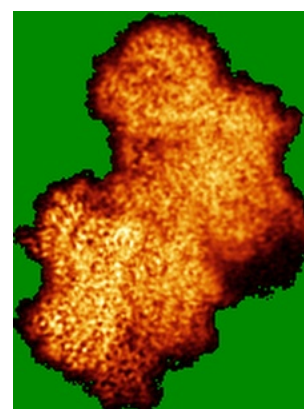
6.4.1 Primary map



X



Y

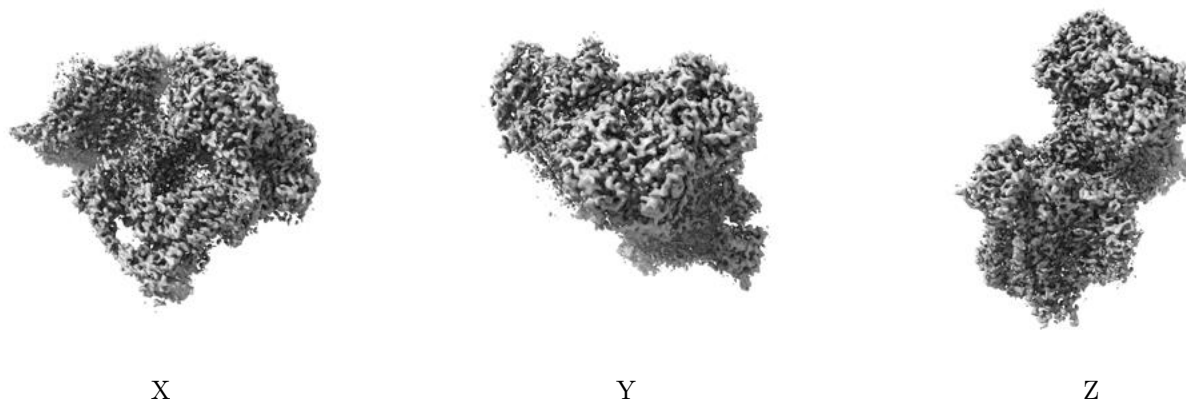


Z

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.

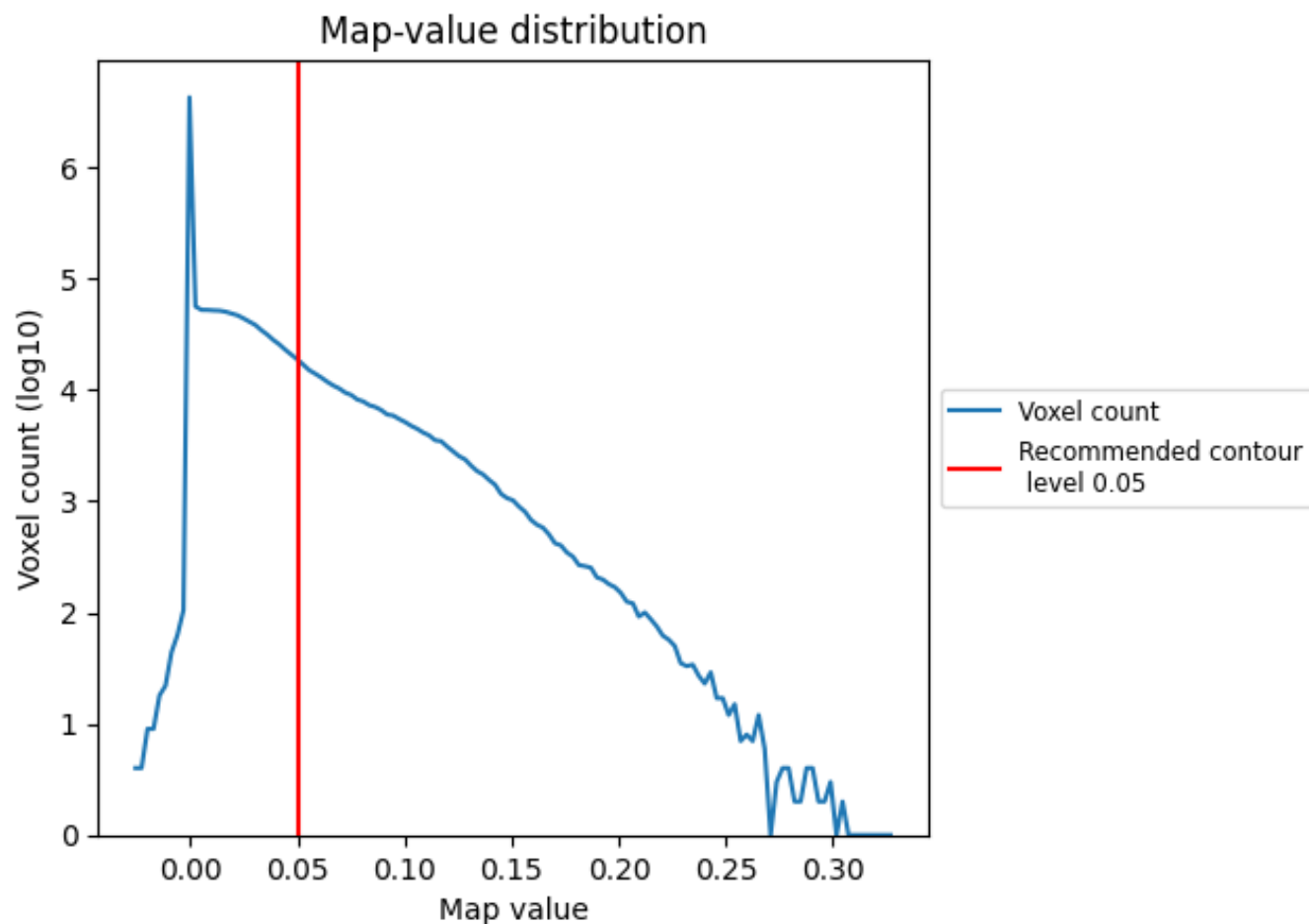
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

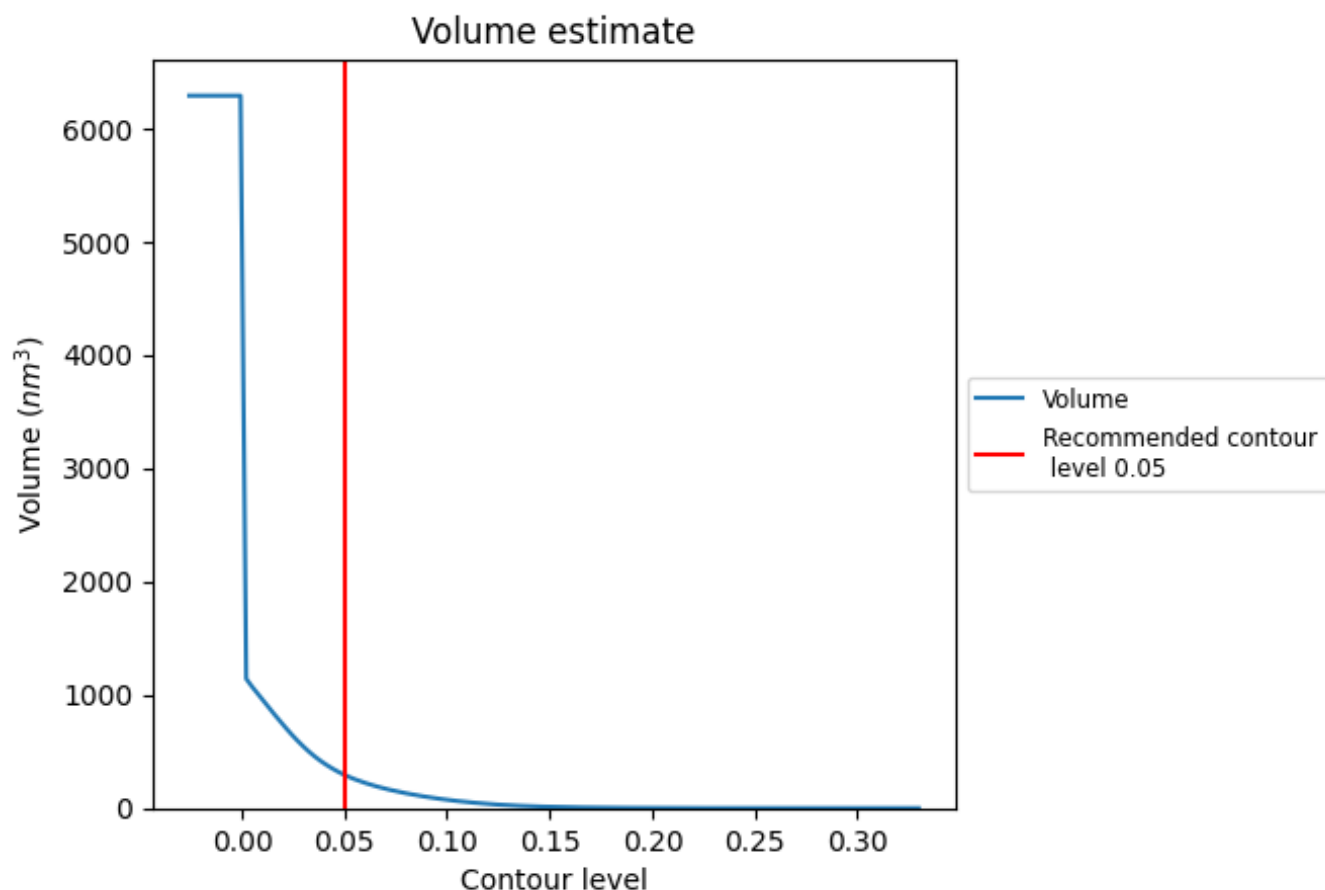
This section contains the results of statistical analysis of the map.

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 294 nm³; this corresponds to an approximate mass of 266 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.

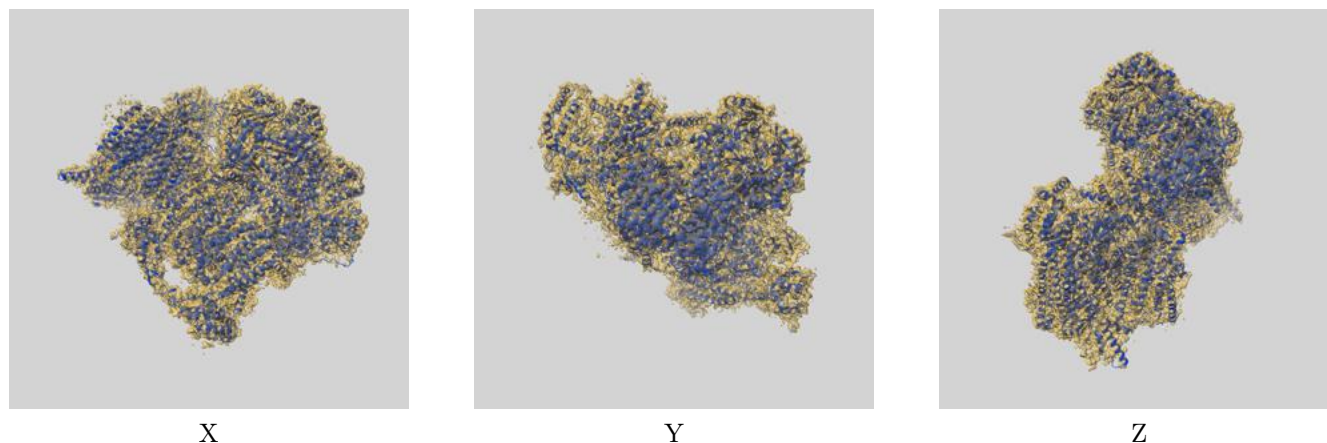
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

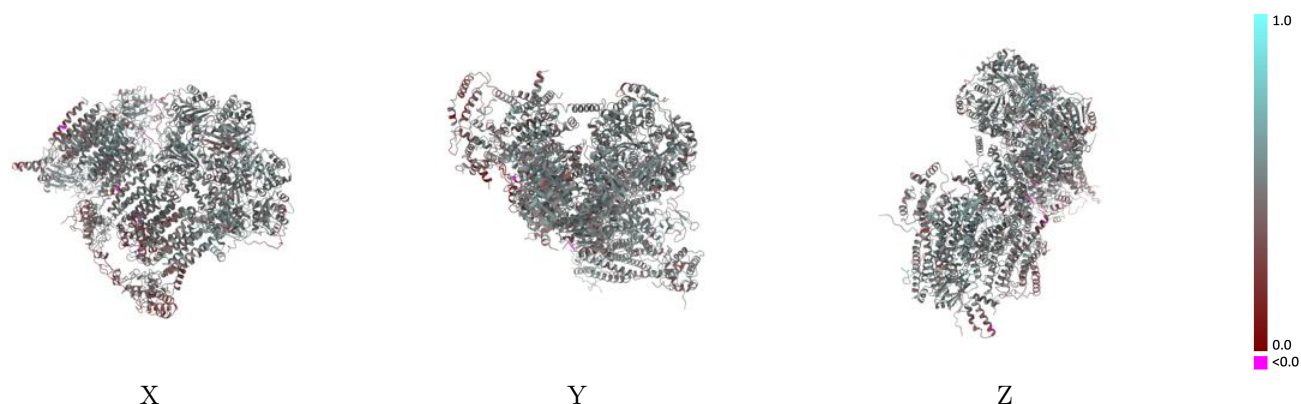
This section contains information regarding the fit between EMDB map EMD-12705 and PDB model 7O3E. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



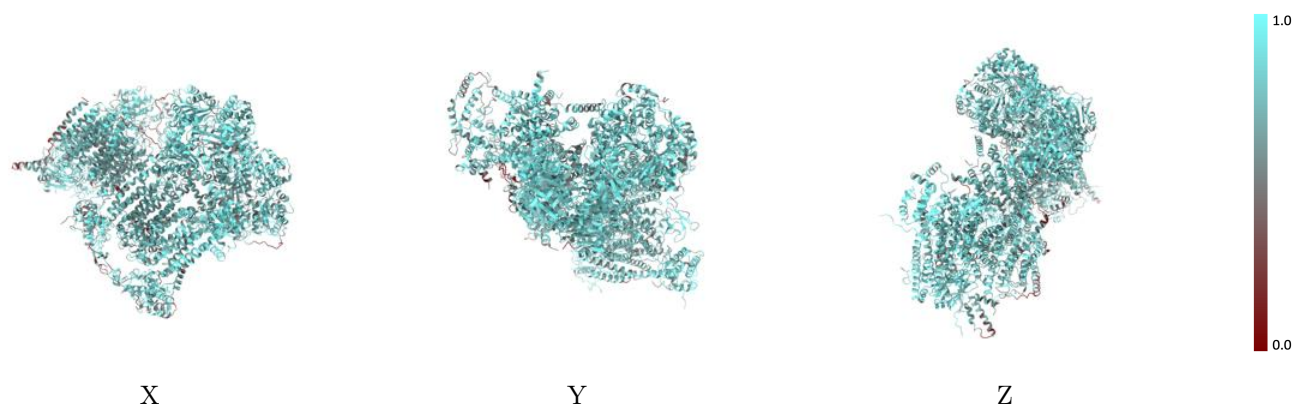
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



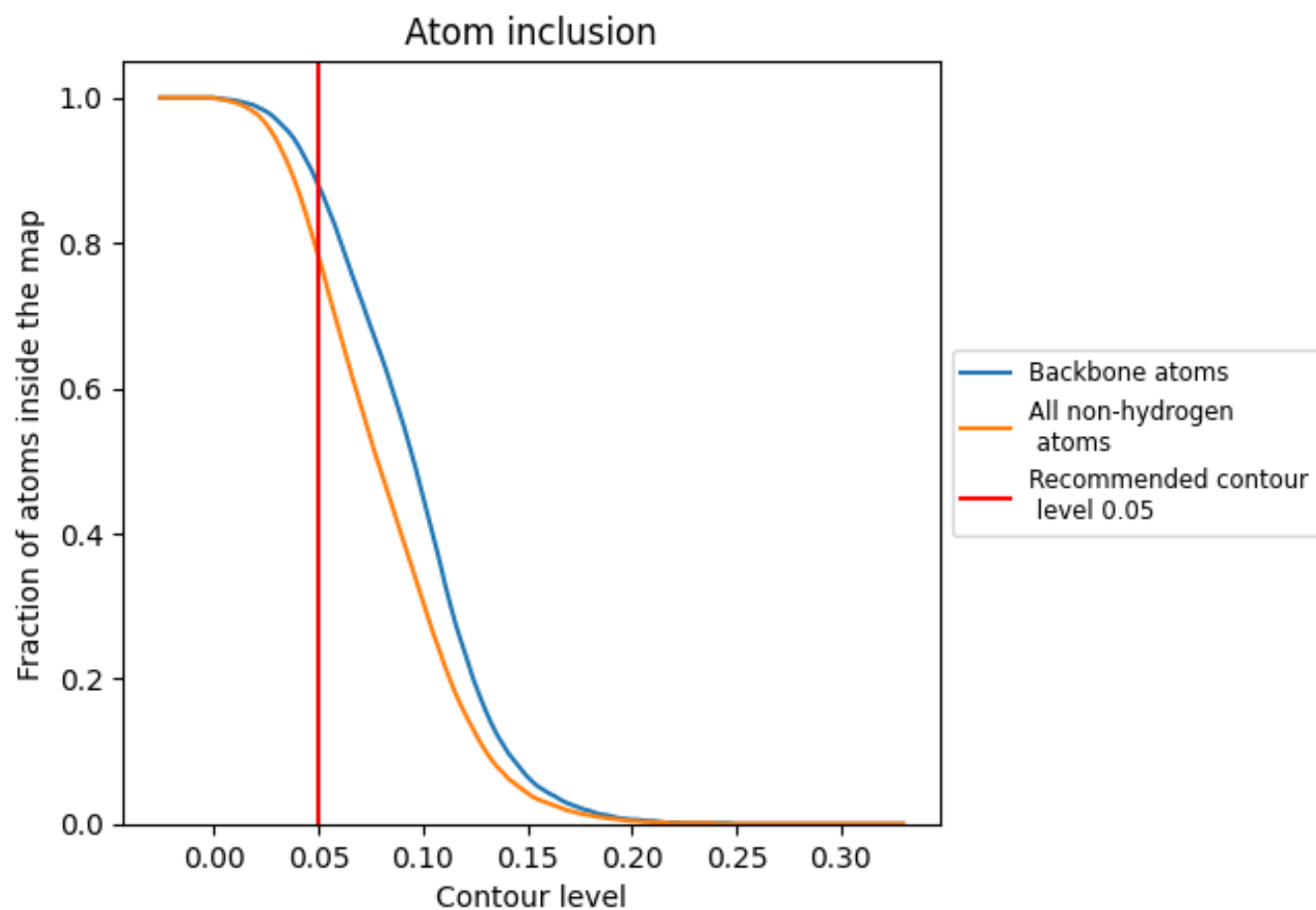
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 88% of all backbone atoms, 78% 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	 0.7820	 0.4800
A	 0.8050	 0.4950
B	 0.8170	 0.5000
C	 0.7750	 0.4670
D	 0.7710	 0.4430
F	 0.8000	 0.5140
G	 0.7880	 0.4790
H	 0.6530	 0.3540
I	 0.6590	 0.4410
J	 0.6440	 0.3610
L	 0.7820	 0.4840
M	 0.8110	 0.4950
N	 0.7580	 0.4620
O	 0.7760	 0.4420
P	 0.7970	 0.4970
Q	 0.8120	 0.4900
R	 0.8070	 0.4860
S	 0.6350	 0.3400
T	 0.7650	 0.4710
U	 0.6630	 0.3520
a	 0.8280	 0.5380
b	 0.8190	 0.5060
c	 0.7800	 0.4830
d	 0.7790	 0.4760
e	 0.8540	 0.4710
f	 0.7920	 0.5030
g	 0.5490	 0.4340
h	 0.6630	 0.4290
i	 0.8290	 0.4730
k	 0.7710	 0.4920
l	 0.7770	 0.5350
m	 0.7150	 0.4380

