



## wwPDB EM Validation Summary Report ⓘ

Apr 2, 2025 – 12:17 AM JST

PDB ID : 8HCR / pdb\_00008hcr  
EMDB ID : EMD-34664  
Title : Cryo-EM structure of the Mycobacterium tuberculosis cytochrome bcc:aa3 supercomplex and a novel inhibitor targeting subunit cytochrome cI  
Authors : Mathiyazakan, V.; Gruber, G.  
Deposited on : 2022-11-02  
Resolution : 4.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), 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) : 2.42

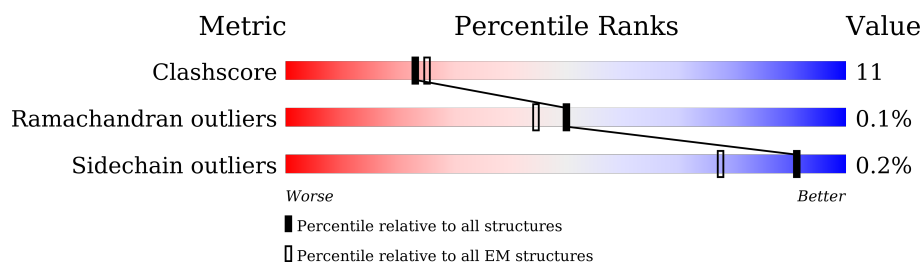
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	429	72% 16% 12%
1	M	429	68% 19% 13%
2	B	573	70% 22% 9%
2	N	573	70% 21% 9%
3	C	280	59% 19% 22%
3	O	280	59% 17% 24%
4	E	363	55% 21% 24%
4	Q	363	55% 23% 22%
5	F	573	66% 30% .

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Mol	Chain	Length	Quality of chain
5	R	573	
6	G	203	
6	S	203	
7	H	139	
7	T	139	
8	I	79	
8	U	79	
9	J	155	
9	V	155	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 38845 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 bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	378	Total	C	N	O	S	0	0
			2912	1884	499	518	11		
1	M	372	Total	C	N	O	S	0	0
			2882	1869	494	508	11		

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	524	Total	C	N	O	S	0	0
			4130	2729	703	681	17		
2	N	524	Total	C	N	O	S	0	0
			4118	2723	701	677	17		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	550	GLY	-	expression tag	UNP A0A0K2HYC0
B	551	GLY	-	expression tag	UNP A0A0K2HYC0
B	552	GLY	-	expression tag	UNP A0A0K2HYC0
B	553	GLY	-	expression tag	UNP A0A0K2HYC0
B	554	GLU	-	expression tag	UNP A0A0K2HYC0
B	555	ASN	-	expression tag	UNP A0A0K2HYC0
B	556	LEU	-	expression tag	UNP A0A0K2HYC0
B	557	TYR	-	expression tag	UNP A0A0K2HYC0
B	558	PHE	-	expression tag	UNP A0A0K2HYC0
B	559	GLN	-	expression tag	UNP A0A0K2HYC0
B	560	ASP	-	expression tag	UNP A0A0K2HYC0
B	561	TYR	-	expression tag	UNP A0A0K2HYC0
B	562	LYS	-	expression tag	UNP A0A0K2HYC0
B	563	ASP	-	expression tag	UNP A0A0K2HYC0
B	564	ASP	-	expression tag	UNP A0A0K2HYC0
B	565	ASP	-	expression tag	UNP A0A0K2HYC0
B	566	ASP	-	expression tag	UNP A0A0K2HYC0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	567	LYS	-	expression tag	UNP A0A0K2HYC0
B	568	HIS	-	expression tag	UNP A0A0K2HYC0
B	569	HIS	-	expression tag	UNP A0A0K2HYC0
B	570	HIS	-	expression tag	UNP A0A0K2HYC0
B	571	HIS	-	expression tag	UNP A0A0K2HYC0
B	572	HIS	-	expression tag	UNP A0A0K2HYC0
B	573	HIS	-	expression tag	UNP A0A0K2HYC0
N	550	GLY	-	expression tag	UNP A0A0K2HYC0
N	551	GLY	-	expression tag	UNP A0A0K2HYC0
N	552	GLY	-	expression tag	UNP A0A0K2HYC0
N	553	GLY	-	expression tag	UNP A0A0K2HYC0
N	554	GLU	-	expression tag	UNP A0A0K2HYC0
N	555	ASN	-	expression tag	UNP A0A0K2HYC0
N	556	LEU	-	expression tag	UNP A0A0K2HYC0
N	557	TYR	-	expression tag	UNP A0A0K2HYC0
N	558	PHE	-	expression tag	UNP A0A0K2HYC0
N	559	GLN	-	expression tag	UNP A0A0K2HYC0
N	560	ASP	-	expression tag	UNP A0A0K2HYC0
N	561	TYR	-	expression tag	UNP A0A0K2HYC0
N	562	LYS	-	expression tag	UNP A0A0K2HYC0
N	563	ASP	-	expression tag	UNP A0A0K2HYC0
N	564	ASP	-	expression tag	UNP A0A0K2HYC0
N	565	ASP	-	expression tag	UNP A0A0K2HYC0
N	566	ASP	-	expression tag	UNP A0A0K2HYC0
N	567	LYS	-	expression tag	UNP A0A0K2HYC0
N	568	HIS	-	expression tag	UNP A0A0K2HYC0
N	569	HIS	-	expression tag	UNP A0A0K2HYC0
N	570	HIS	-	expression tag	UNP A0A0K2HYC0
N	571	HIS	-	expression tag	UNP A0A0K2HYC0
N	572	HIS	-	expression tag	UNP A0A0K2HYC0
N	573	HIS	-	expression tag	UNP A0A0K2HYC0

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	218	Total	C	N	O	S	0	0
			1487	930	274	274	9		
3	O	213	Total	C	N	O	S	0	0
			1458	921	261	268	8		

- Molecule 4 is a protein called CYTOCHROME AA3 SUBUNIT CtaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	276	Total	C	N	O	S	0	0
			2204	1440	365	390	9		
4	Q	283	Total	C	N	O	S	0	0
			2247	1465	375	398	9		

- Molecule 5 is a protein called Probable cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	552	Total	C	N	O	S	0	0
			4358	2926	692	715	25		
5	R	552	Total	C	N	O	S	0	0
			4358	2926	692	715	25		

- Molecule 6 is a protein called Probable cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	186	Total	C	N	O	S	0	0
			1473	987	234	245	7		
6	S	185	Total	C	N	O	S	0	0
			1467	984	233	243	7		

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	139	Total	C	N	O	S	0	0
			1048	699	163	182	4		
7	T	139	Total	C	N	O	S	0	0
			1045	698	163	180	4		

- Molecule 8 is a protein called CYTOCHROME AA3 SUBUNIT CtaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	67	Total	C	N	O	S	0	0
			511	344	82	84	1		
8	U	67	Total	C	N	O	S	0	0
			510	344	82	83	1		

- Molecule 9 is a protein called DUF5130 domain-containing protein.

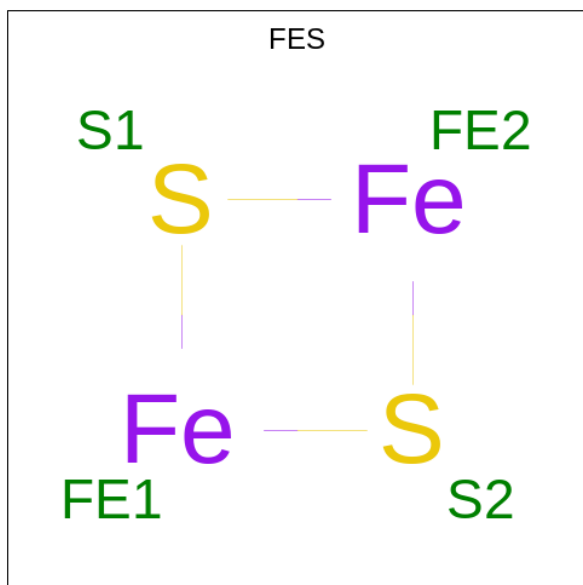
Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	143	Total	C	N	O	S	0	0
			1019	645	177	195	2		

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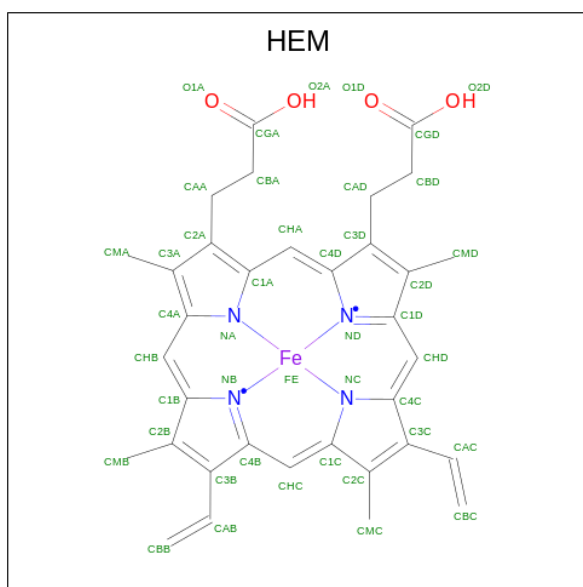
Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	143	Total	C	N	O	S	0	0
			1028	649	180	197	2		

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).



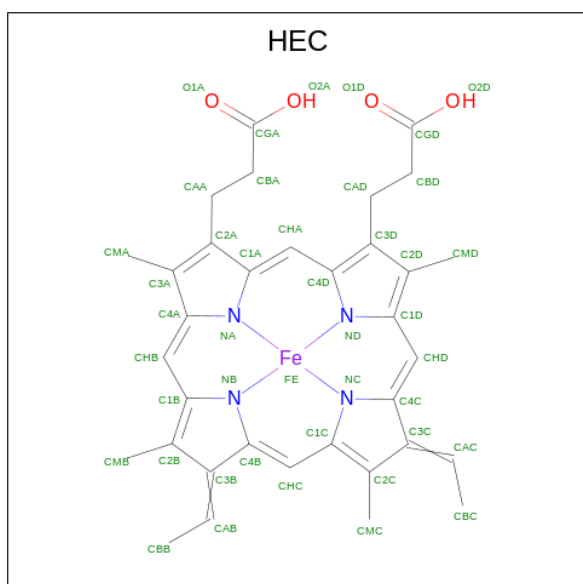
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	Fe	S	0
			4	2	2	
10	M	1	Total	Fe	S	0
			4	2	2	

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
11	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	N	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
11	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

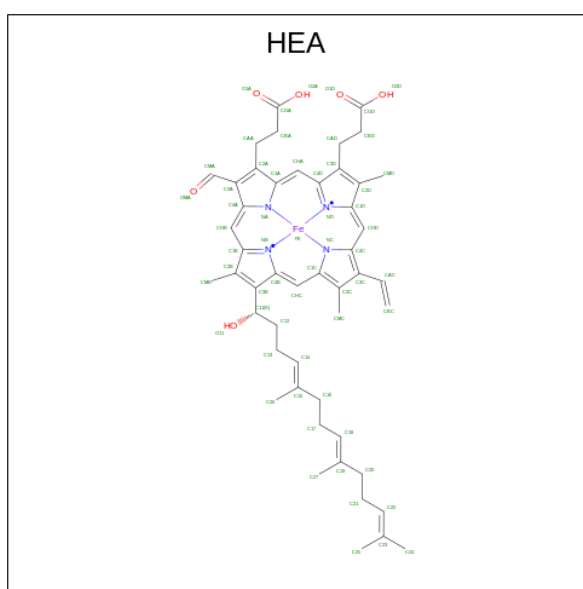
- Molecule 12 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 13 is HEME-A (CCD ID: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).

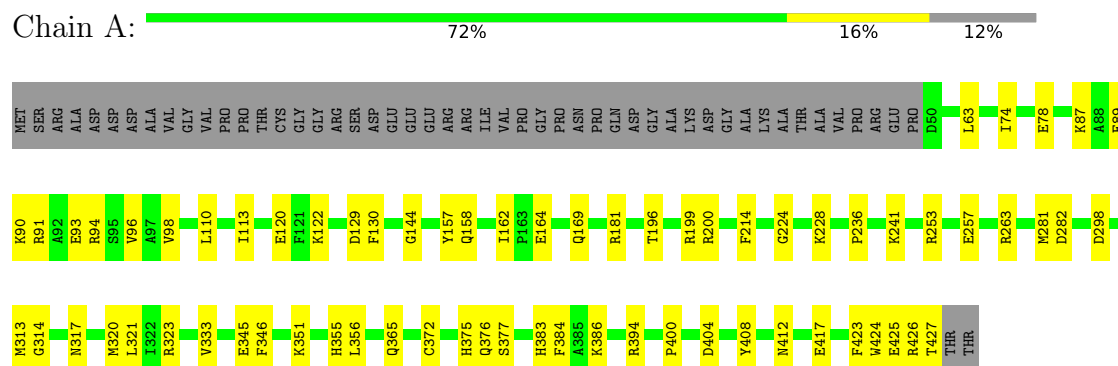


Mol	Chain	Residues	Atoms					AltConf
13	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
13	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
13	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
13	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

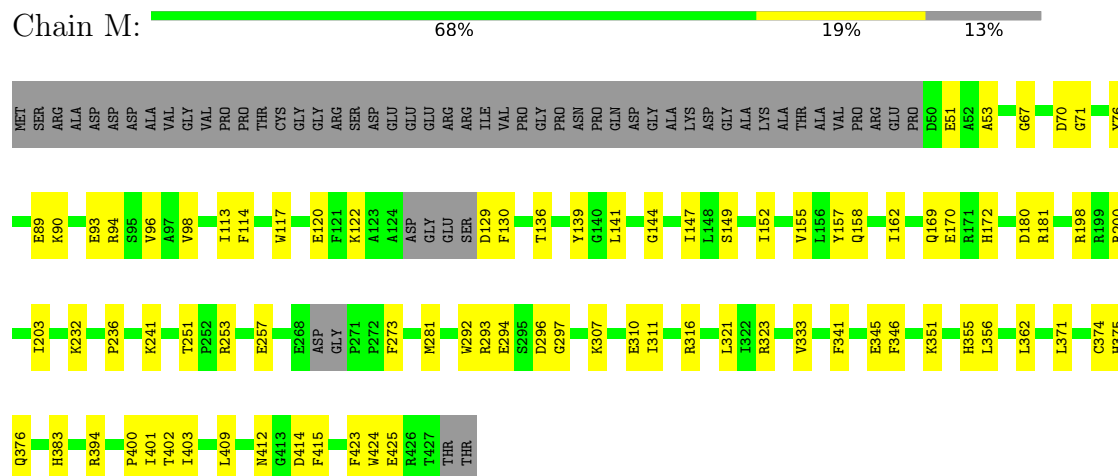
### 3 Residue-property plots

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. 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. 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.

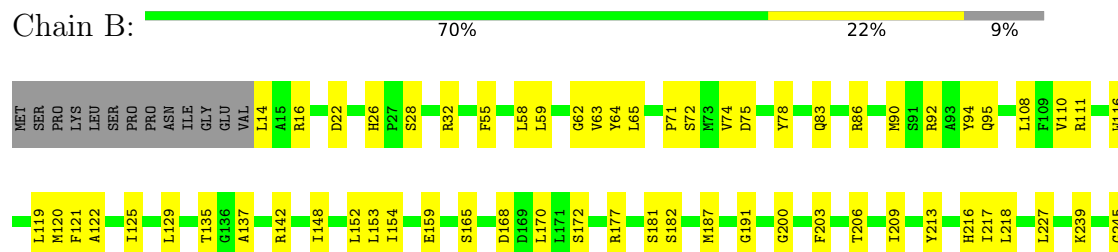
- Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit



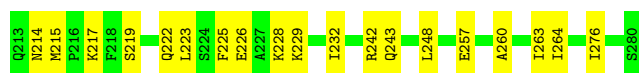
- Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit



- Molecule 2: Cytochrome bc1 complex cytochrome b subunit

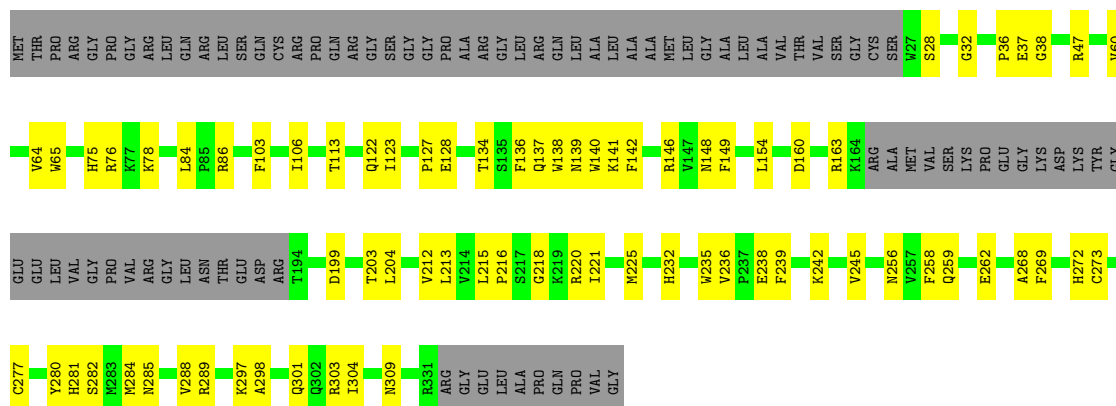






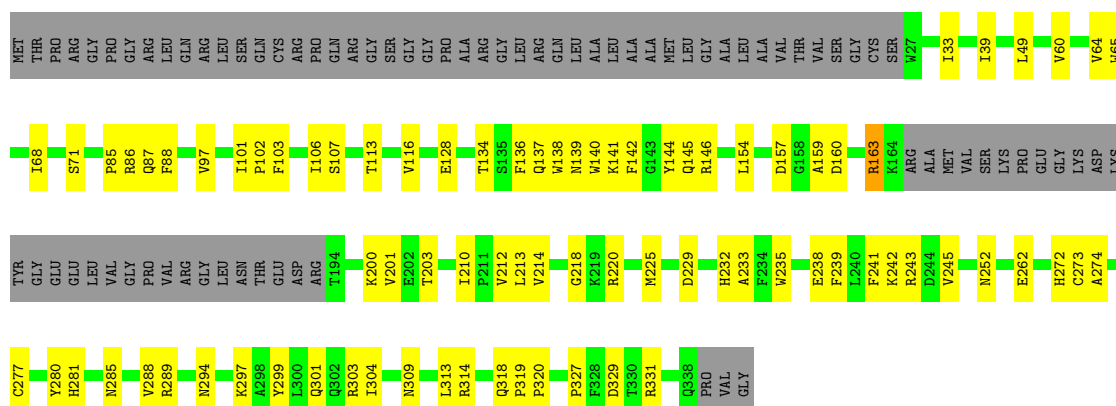
• Molecule 4: CYTOCHROME AA3 SUBUNIT CtaC

Chain E: 55% 21% 24%



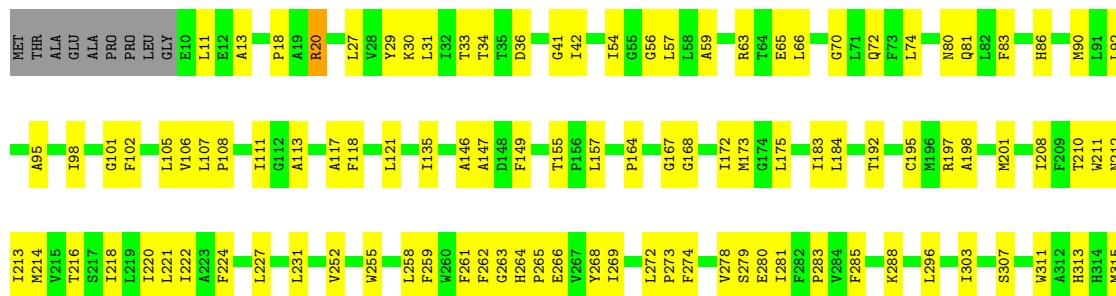
• Molecule 4: CYTOCHROME AA3 SUBUNIT CtaC

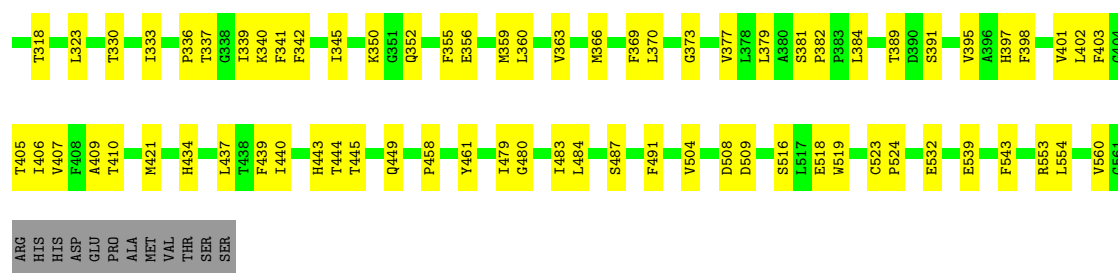
Chain Q: 55% 23% 22%



• Molecule 5: Probable cytochrome c oxidase subunit 1

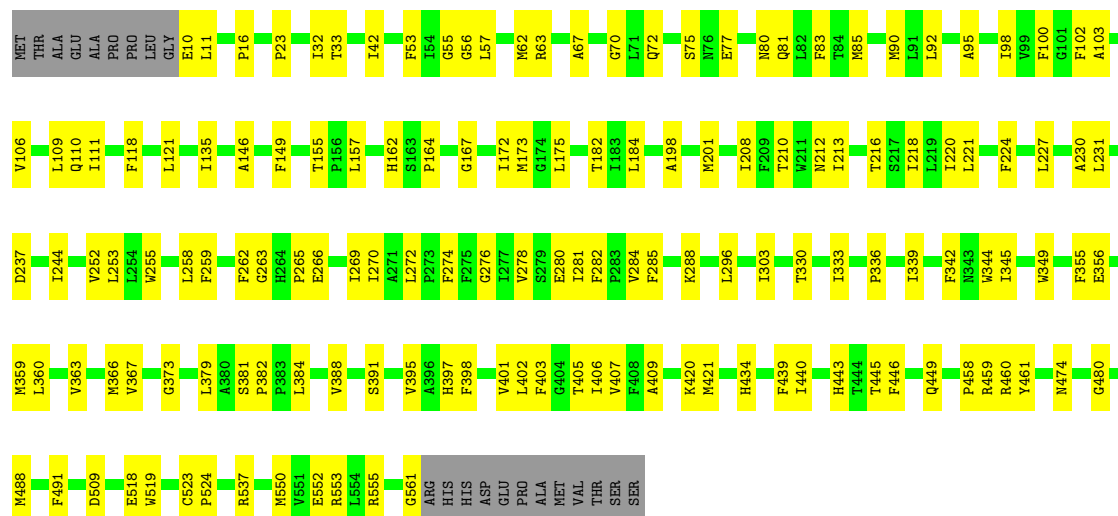
Chain F: 66% 30% 4%





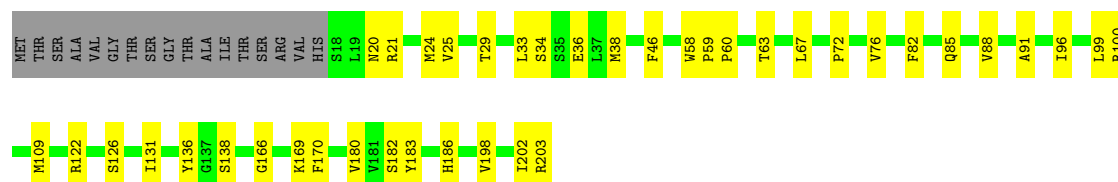
- Molecule 5: Probable cytochrome c oxidase subunit 1

Chain R: 71% 26% .



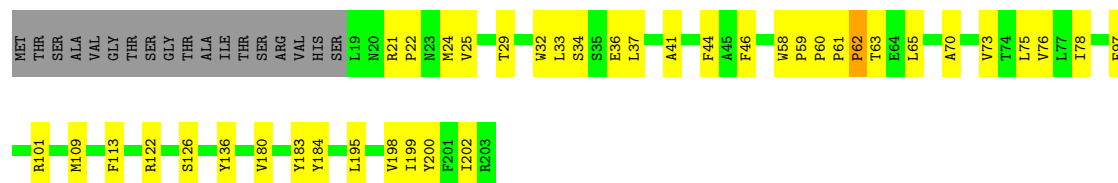
- Molecule 6: Probable cytochrome c oxidase subunit 3

Chain G: 72% 20% 8%




- Molecule 6: Probable cytochrome c oxidase subunit 3

Chain S: 71% 19% 9%




- Molecule 7: Cytochrome c oxidase polypeptide 4

Chain H:  84% 16%



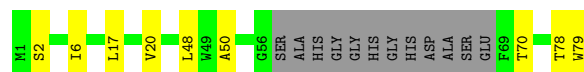
- Molecule 7: Cytochrome c oxidase polypeptide 4

Chain T:  83% 17%



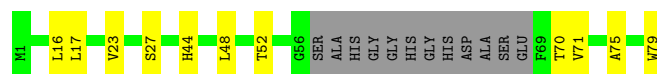
- Molecule 8: CYTOCHROME AA3 SUBUNIT CtaJ

Chain I:  73% 11% 15%



- Molecule 8: CYTOCHROME AA3 SUBUNIT CtaJ

Chain U:  71% 14% 15%



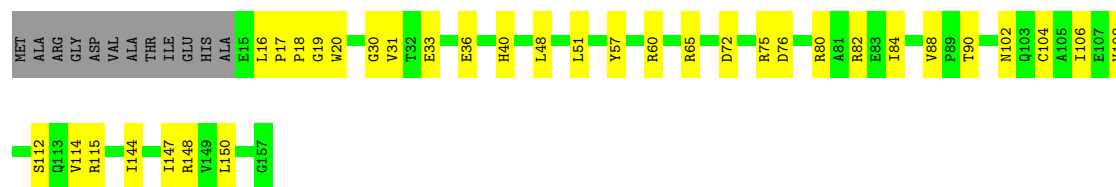
- Molecule 9: DUF5130 domain-containing protein

Chain J:  77% 14% 8%



- Molecule 9: DUF5130 domain-containing protein

Chain V:  70% 22% 8%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	
Number of tilted images used	100	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum voxel value	1.927	Depositor
Minimum voxel value	-0.639	Depositor
Average voxel value	0.002	Depositor
Voxel value standard deviation	0.034	Depositor
Recommended contour level	Not applicable	
Tomogram size (Å)	530.0, 530.0, 530.0	wwPDB
Tomogram dimensions	500, 500, 500	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, HEC, FES, 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	0.25	0/2989	0.51	0/4056
1	M	0.25	0/2957	0.50	0/4008
2	B	0.25	0/4266	0.49	1/5821 (0.0%)
2	N	0.25	0/4253	0.49	0/5804
3	C	0.25	0/1516	0.51	0/2061
3	O	0.26	0/1487	0.51	0/2022
4	E	0.24	0/2266	0.47	0/3090
4	Q	0.25	0/2310	0.47	0/3151
5	F	0.27	0/4517	0.49	0/6171
5	R	0.27	0/4517	0.49	0/6171
6	G	0.27	0/1523	0.47	0/2078
6	S	0.28	0/1517	0.50	0/2070
7	H	0.25	0/1081	0.45	0/1477
7	T	0.25	0/1078	0.44	0/1473
8	I	0.24	0/530	0.50	0/729
8	U	0.23	0/529	0.49	0/728
9	J	0.25	0/1038	0.51	0/1421
9	V	0.26	0/1047	0.54	0/1432
All	All	0.26	0/39421	0.49	1/53763 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	MET	CA-CB-CG	5.04	121.86	113.30

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	2912	0	2891	54	0
1	M	2882	0	2877	67	0
2	B	4130	0	4148	94	0
2	N	4118	0	4137	97	0
3	C	1487	0	1398	46	0
3	O	1458	0	1367	51	0
4	E	2204	0	2173	55	0
4	Q	2247	0	2204	56	0
5	F	4358	0	4320	133	0
5	R	4358	0	4321	113	0
6	G	1473	0	1458	29	0
6	S	1467	0	1453	35	0
7	H	1048	0	1027	16	0
7	T	1045	0	1025	22	0
8	I	511	0	516	10	0
8	U	510	0	513	10	0
9	J	1019	0	1019	19	0
9	V	1028	0	1032	26	0
10	A	4	0	0	0	0
10	M	4	0	0	0	0
11	B	85	0	57	8	0
11	N	85	0	57	7	0
12	C	86	0	63	7	0
12	O	86	0	64	20	0
13	F	120	0	107	26	0
13	R	120	0	108	18	0
All	All	38845	0	38335	843	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 11.

The worst 5 of 843 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:O:194:PRO:HD3	12:O:302:HEC:HAD2	1.35	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:36:PRO:O	4:E:47:ARG:NH2	2.09	0.86
3:O:194:PRO:HG2	12:O:302:HEC:HBA1	1.57	0.85
3:O:174:CYS:SG	12:O:302:HEC:HBB3	2.17	0.84
3:O:194:PRO:CD	12:O:302:HEC:HAD2	2.06	0.84

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	376/429 (88%)	345 (92%)	31 (8%)	0	100	100
1	M	366/429 (85%)	338 (92%)	28 (8%)	0	100	100
2	B	522/573 (91%)	477 (91%)	45 (9%)	0	100	100
2	N	522/573 (91%)	482 (92%)	40 (8%)	0	100	100
3	C	214/280 (76%)	198 (92%)	16 (8%)	0	100	100
3	O	207/280 (74%)	192 (93%)	15 (7%)	0	100	100
4	E	272/363 (75%)	256 (94%)	16 (6%)	0	100	100
4	Q	279/363 (77%)	260 (93%)	18 (6%)	1 (0%)	30	68
5	F	550/573 (96%)	528 (96%)	22 (4%)	0	100	100
5	R	550/573 (96%)	528 (96%)	22 (4%)	0	100	100
6	G	184/203 (91%)	179 (97%)	5 (3%)	0	100	100
6	S	183/203 (90%)	177 (97%)	5 (3%)	1 (0%)	25	64
7	H	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
7	T	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
8	I	63/79 (80%)	58 (92%)	5 (8%)	0	100	100
8	U	63/79 (80%)	62 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	141/155 (91%)	135 (96%)	5 (4%)	1 (1%)	19	56
9	V	141/155 (91%)	137 (97%)	4 (3%)	0	100	100
All	All	4907/5588 (88%)	4617 (94%)	287 (6%)	3 (0%)	50	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	18	PRO
4	Q	33	ILE
6	S	62	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/343 (86%)	296 (100%)	0	100	100
1	M	294/343 (86%)	293 (100%)	1 (0%)	91	91
2	B	422/466 (91%)	422 (100%)	0	100	100
2	N	419/466 (90%)	419 (100%)	0	100	100
3	C	131/207 (63%)	131 (100%)	0	100	100
3	O	128/207 (62%)	128 (100%)	0	100	100
4	E	236/306 (77%)	235 (100%)	1 (0%)	89	90
4	Q	238/306 (78%)	236 (99%)	2 (1%)	79	84
5	F	449/466 (96%)	448 (100%)	1 (0%)	92	93
5	R	449/466 (96%)	448 (100%)	1 (0%)	92	93
6	G	153/166 (92%)	153 (100%)	0	100	100
6	S	152/166 (92%)	152 (100%)	0	100	100
7	H	100/101 (99%)	100 (100%)	0	100	100
7	T	99/101 (98%)	99 (100%)	0	100	100
8	I	54/62 (87%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	53/62 (86%)	53 (100%)	0	100	100
9	J	103/115 (90%)	102 (99%)	1 (1%)	73	81
9	V	105/115 (91%)	104 (99%)	1 (1%)	73	81
All	All	3881/4464 (87%)	3873 (100%)	8 (0%)	91	93

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	V	16	LEU
5	R	555	ARG
4	Q	163	ARG
1	M	316	ARG
4	Q	314	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	O	179	ASN
5	R	434	HIS
6	S	186	HIS
3	C	213	GLN
3	C	179	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

14 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
11	HEM	N	601	2	41,49,50	1.28	3 (7%)	46,81,82	1.21	3 (6%)
11	HEM	B	602	2	41,50,50	1.33	5 (12%)	45,82,82	1.76	8 (17%)
12	HEC	O	302	3	32,50,50	2.38	12 (37%)	24,82,82	2.11	6 (25%)
13	HEA	F	601	5	57,67,67	1.99	14 (24%)	61,103,103	2.43	26 (42%)
11	HEM	B	601	2	41,49,50	1.27	3 (7%)	46,81,82	1.21	3 (6%)
13	HEA	F	602	-	57,67,67	2.03	14 (24%)	61,103,103	2.33	24 (39%)
12	HEC	C	301	-	32,50,50	2.25	4 (12%)	24,82,82	1.27	2 (8%)
13	HEA	R	602	5	57,67,67	1.98	14 (24%)	61,103,103	2.38	23 (37%)
11	HEM	N	602	2	41,50,50	1.47	3 (7%)	45,82,82	1.43	7 (15%)
12	HEC	C	302	3	32,50,50	2.24	3 (9%)	24,82,82	1.37	2 (8%)
13	HEA	R	601	5	57,67,67	1.99	14 (24%)	61,103,103	2.43	24 (39%)
10	FES	A	501	1	0,4,4	-	-	-	-	-
10	FES	M	501	1	0,4,4	-	-	-	-	-
12	HEC	O	301	3	32,50,50	2.22	3 (9%)	24,82,82	1.33	2 (8%)

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
11	HEM	N	601	2	-	0/12/52/54	-
11	HEM	B	602	2	-	4/12/54/54	-
12	HEC	O	302	3	-	1/10/54/54	-
13	HEA	F	601	5	-	15/32/76/76	-
11	HEM	B	601	2	-	0/12/52/54	-
13	HEA	F	602	-	-	19/32/76/76	-
12	HEC	C	301	-	-	3/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEA	R	602	5	-	17/32/76/76	-
11	HEM	N	602	2	-	2/12/54/54	-
12	HEC	C	302	3	-	0/10/54/54	-
13	HEA	R	601	5	-	11/32/76/76	-
10	FES	A	501	1	-	-	0/1/1/1
10	FES	M	501	1	-	-	0/1/1/1
12	HEC	O	301	3	-	3/10/54/54	-

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	302	HEC	C2B-C3B	7.01	1.48	1.40
12	C	301	HEC	C3C-C2C	-6.61	1.33	1.40
12	C	302	HEC	C3C-C2C	-6.57	1.33	1.40
12	C	301	HEC	C2B-C3B	-6.56	1.33	1.40
12	O	301	HEC	C2B-C3B	-6.56	1.33	1.40

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R	601	HEA	C3D-C4D-ND	6.46	116.61	110.36
13	F	601	HEA	C3D-C4D-ND	6.46	116.61	110.36
12	O	302	HEC	C1D-C2D-C3D	-6.43	102.52	107.00
13	F	602	HEA	C3D-C4D-ND	6.05	116.22	110.36
13	R	602	HEA	C3D-C4D-ND	6.03	116.20	110.36

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

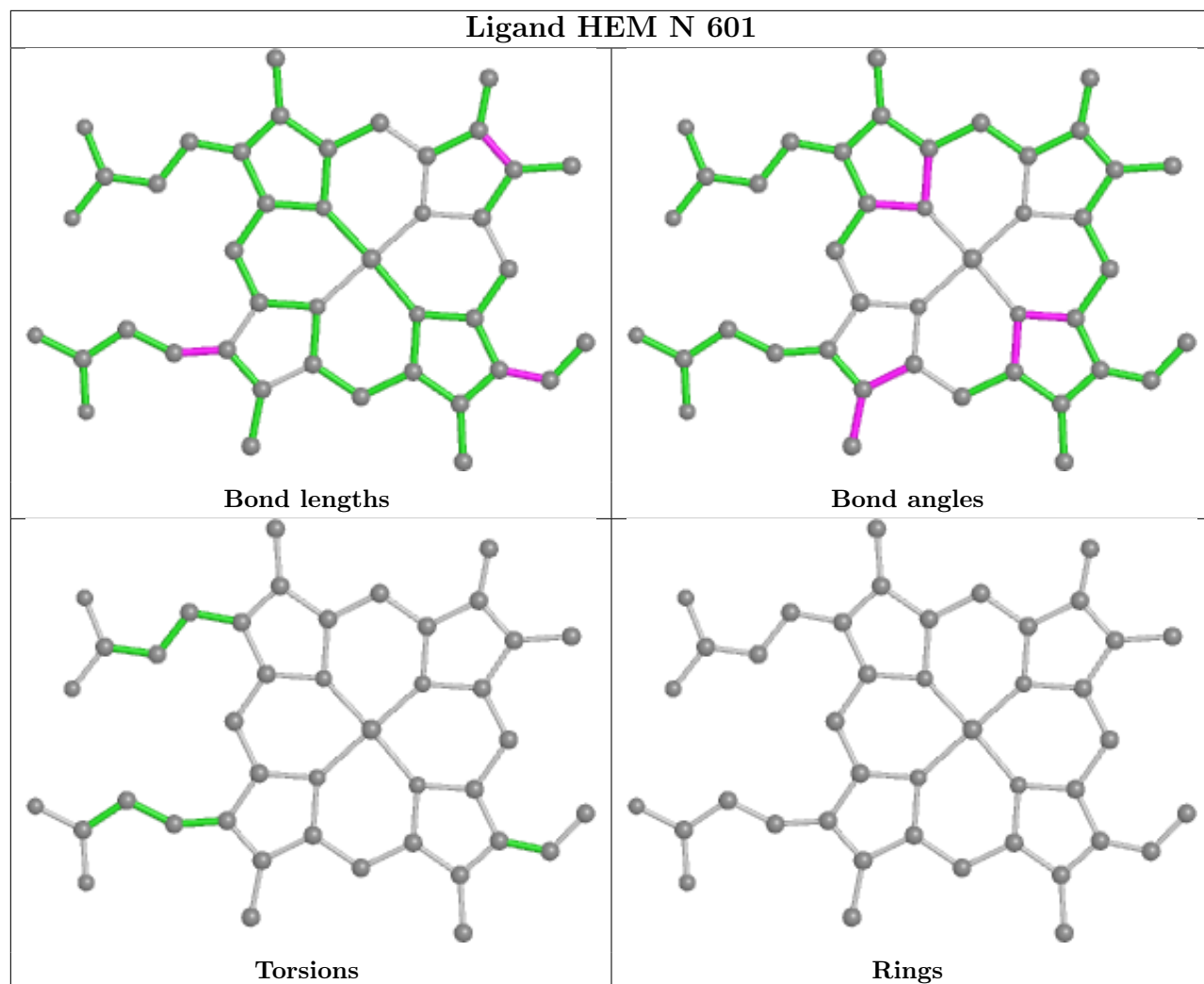
Mol	Chain	Res	Type	Atoms
12	O	301	HEC	C2A-CAA-CBA-CGA
13	F	601	HEA	C4D-C3D-CAD-CBD
13	F	601	HEA	C13-C14-C15-C16
13	F	601	HEA	C13-C14-C15-C26
13	F	601	HEA	C14-C15-C16-C17

There are no ring outliers.

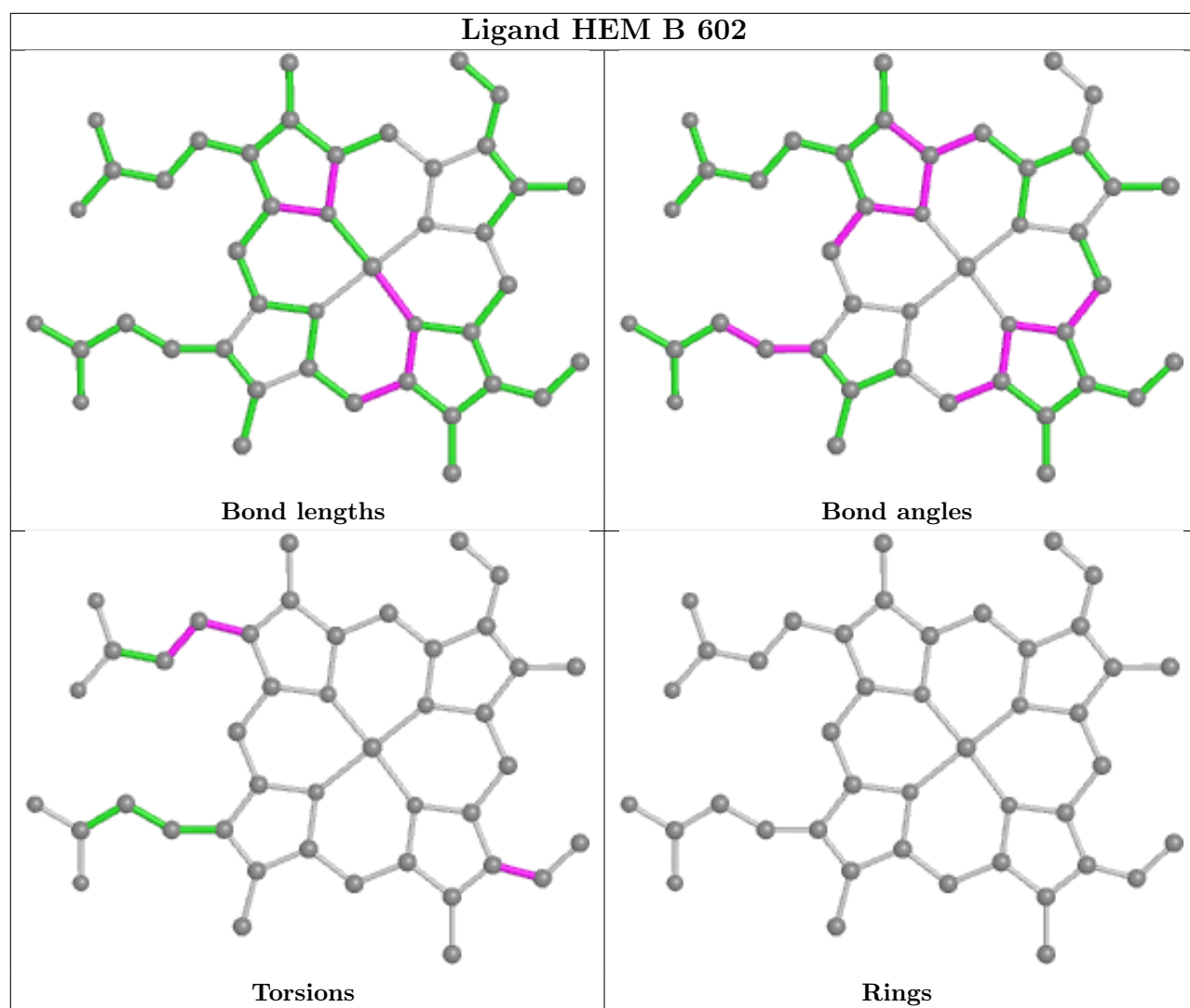
12 monomers are involved in 86 short contacts:

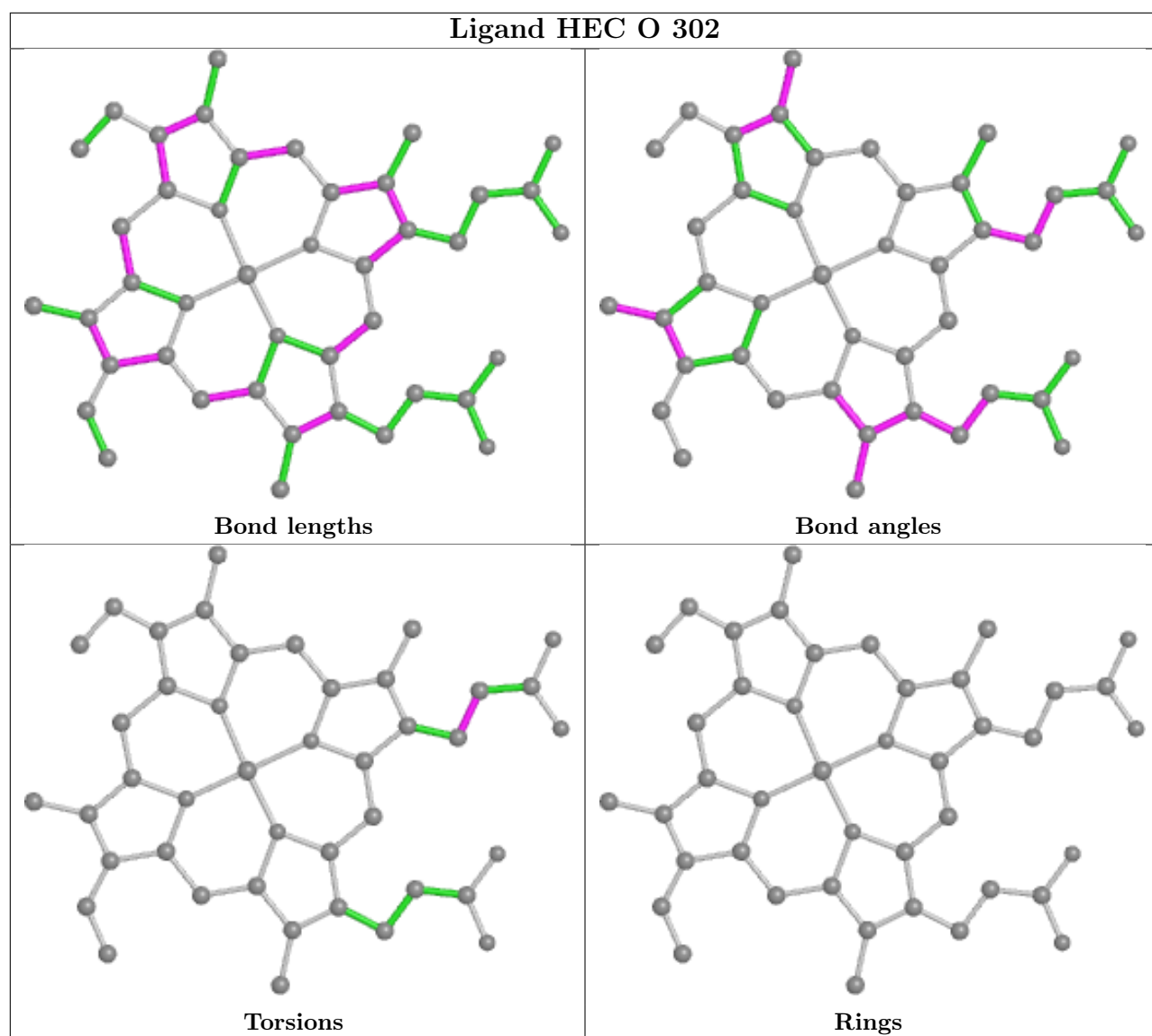
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	N	601	HEM	2	0
11	B	602	HEM	6	0
12	O	302	HEC	16	0
13	F	601	HEA	13	0
11	B	601	HEM	2	0
13	F	602	HEA	13	0
12	C	301	HEC	4	0
13	R	602	HEA	10	0
11	N	602	HEM	5	0
12	C	302	HEC	3	0
13	R	601	HEA	8	0
12	O	301	HEC	4	0

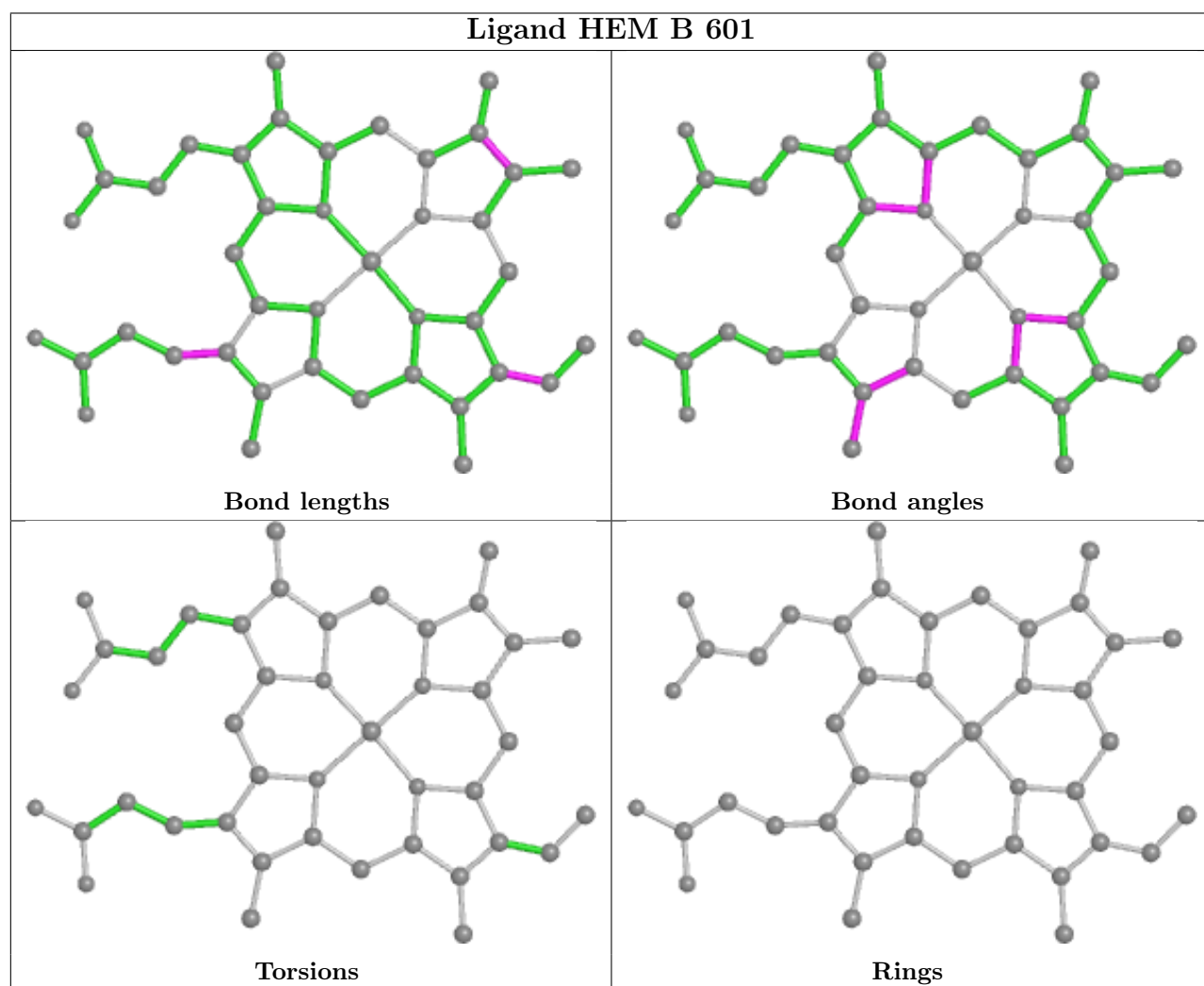
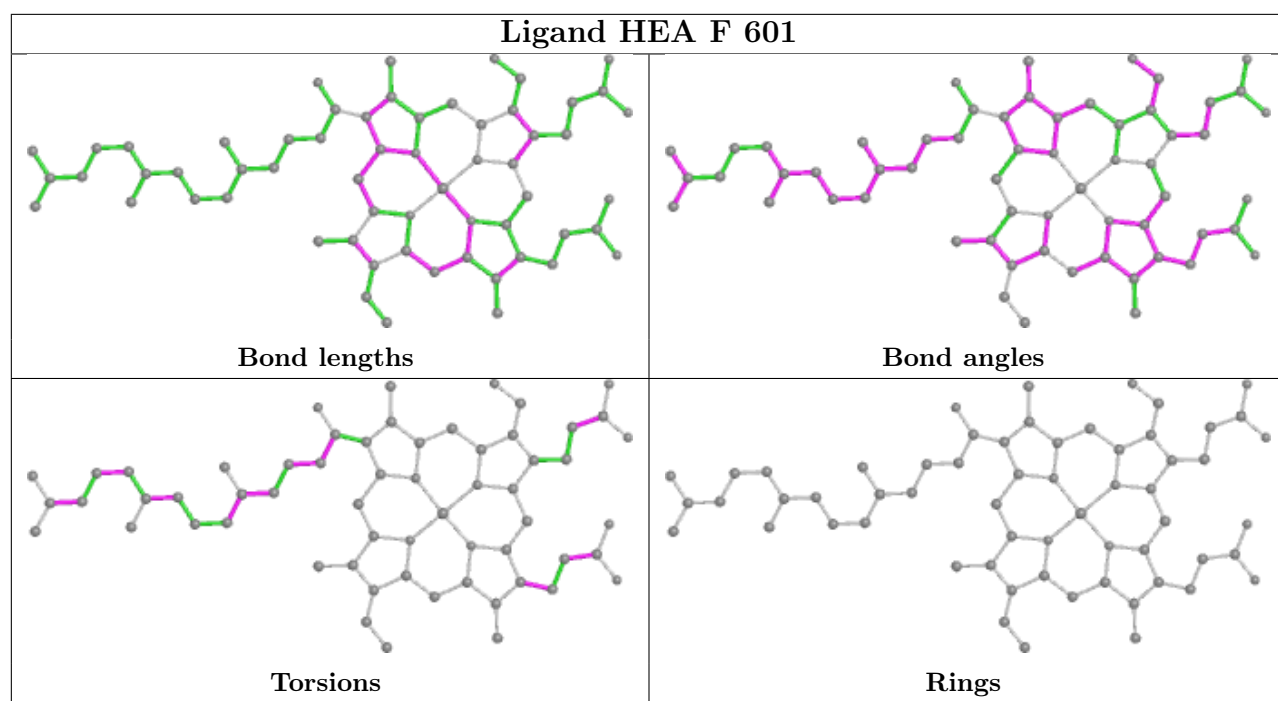
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

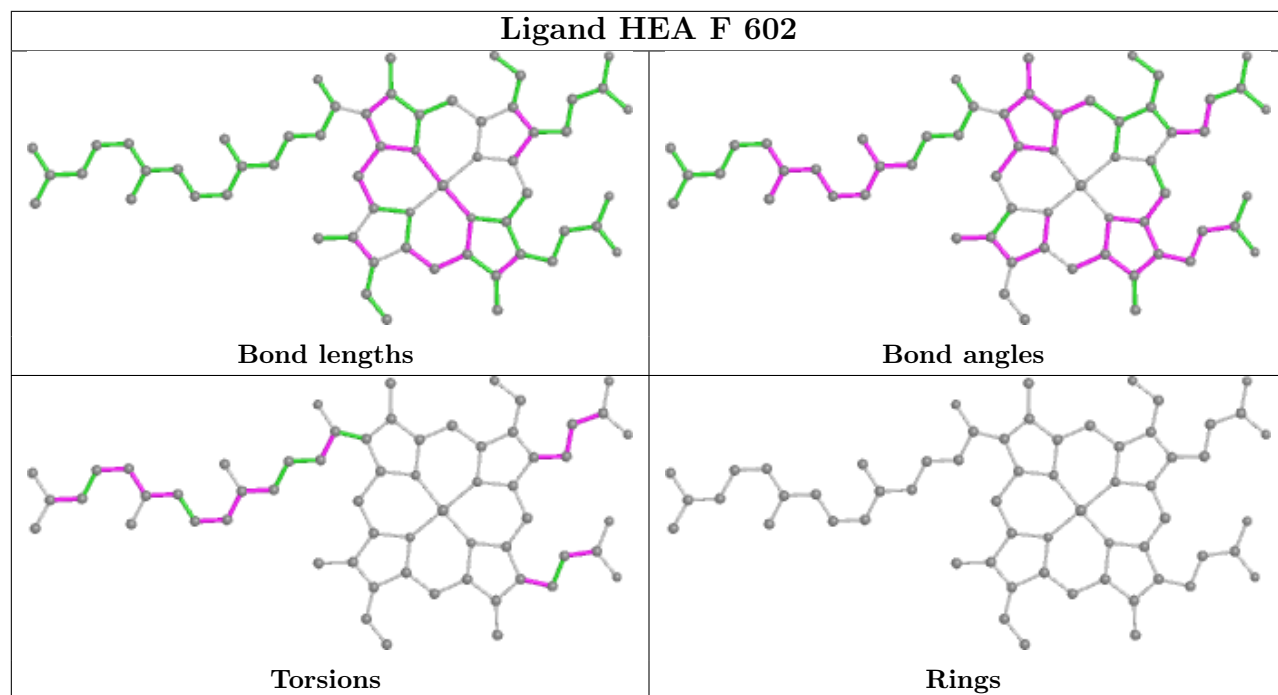


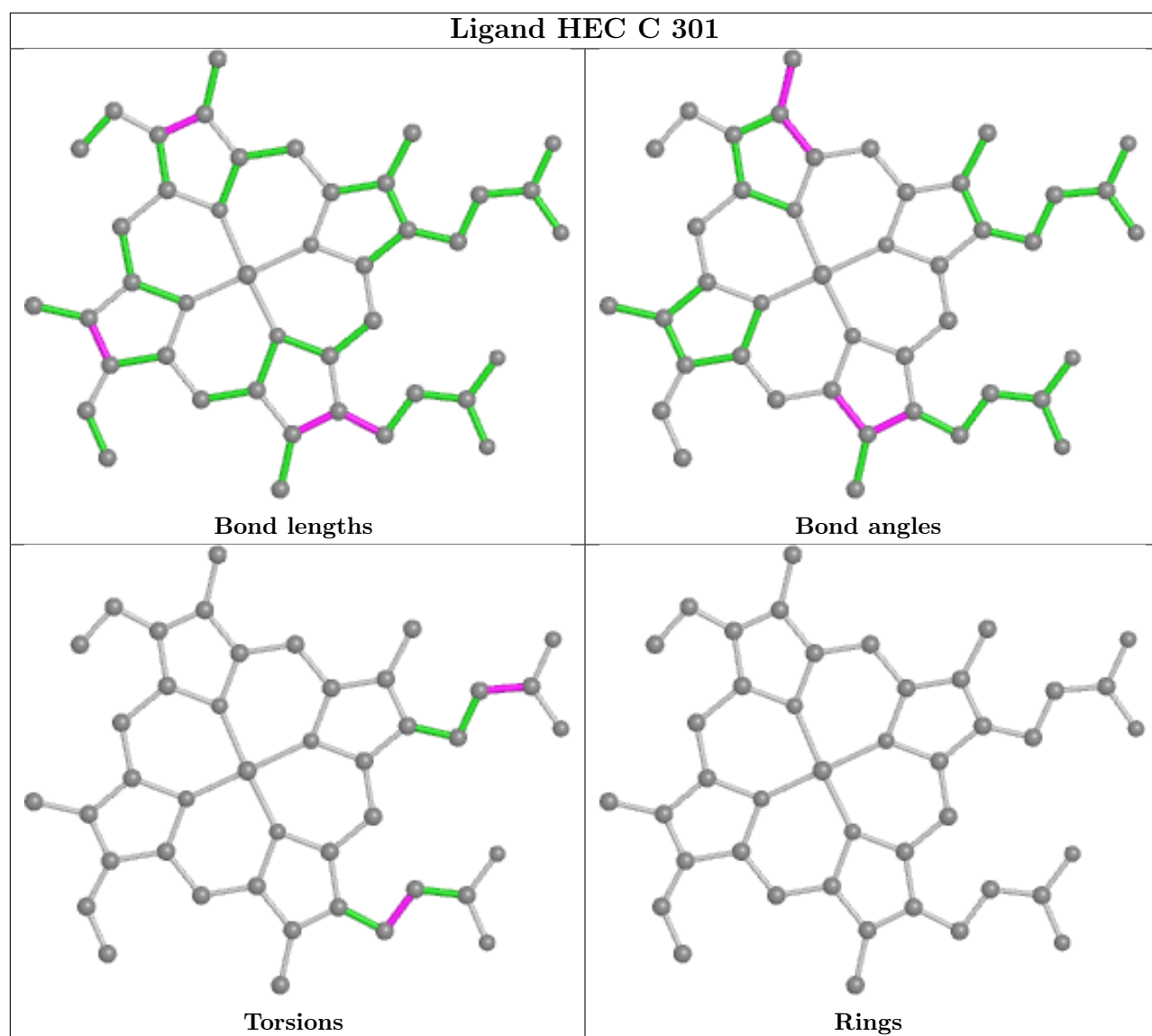


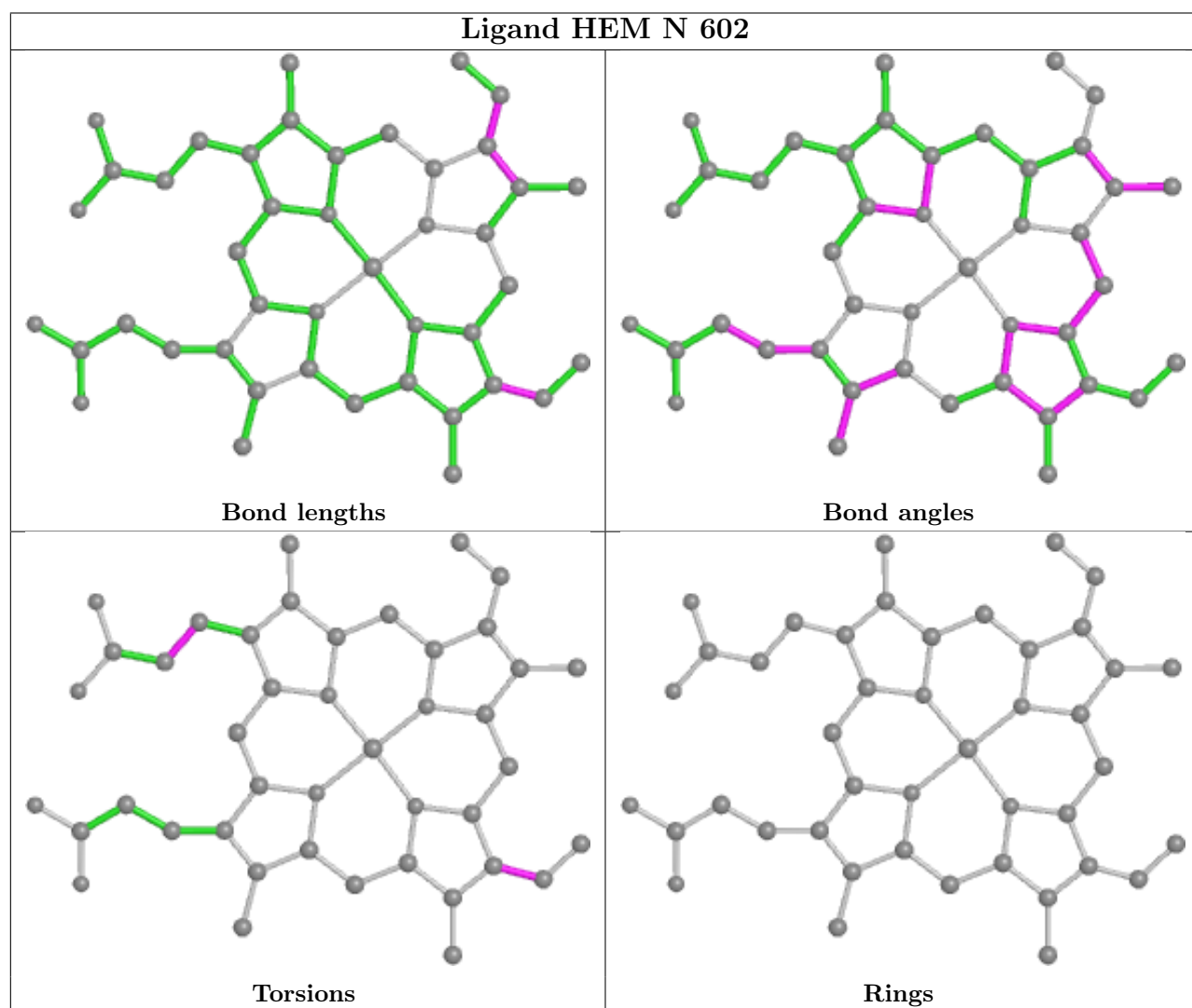
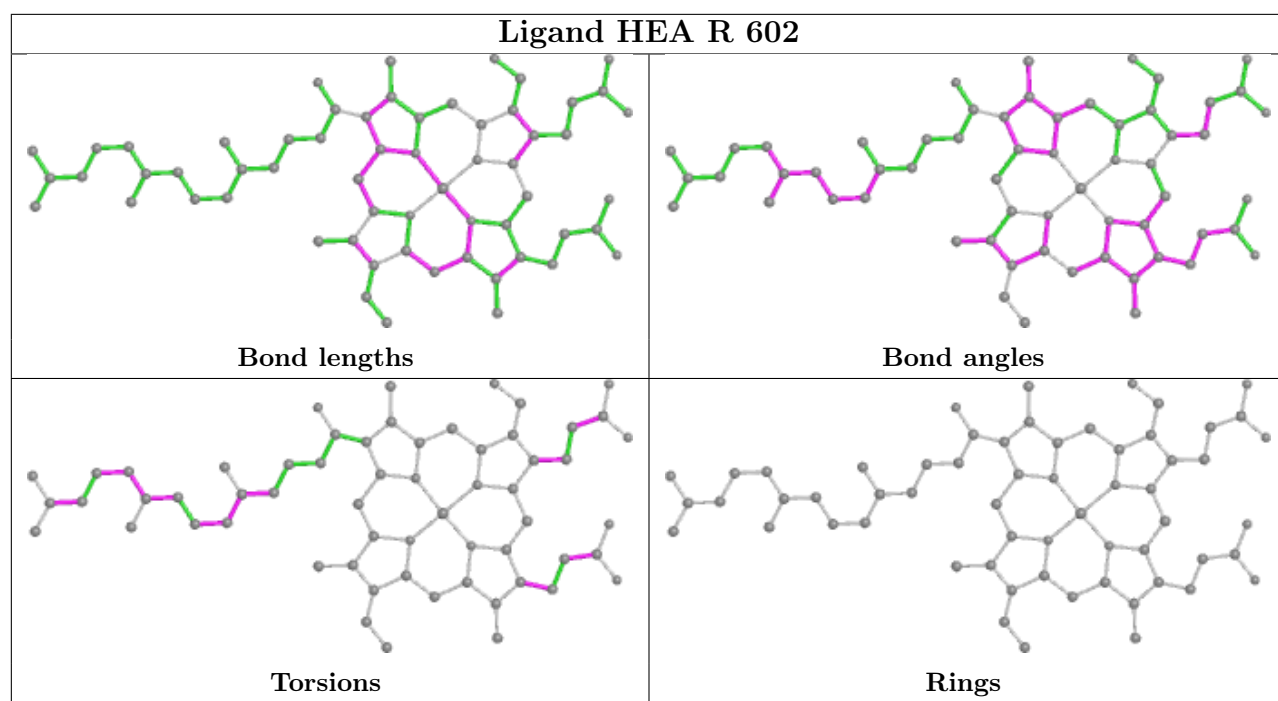


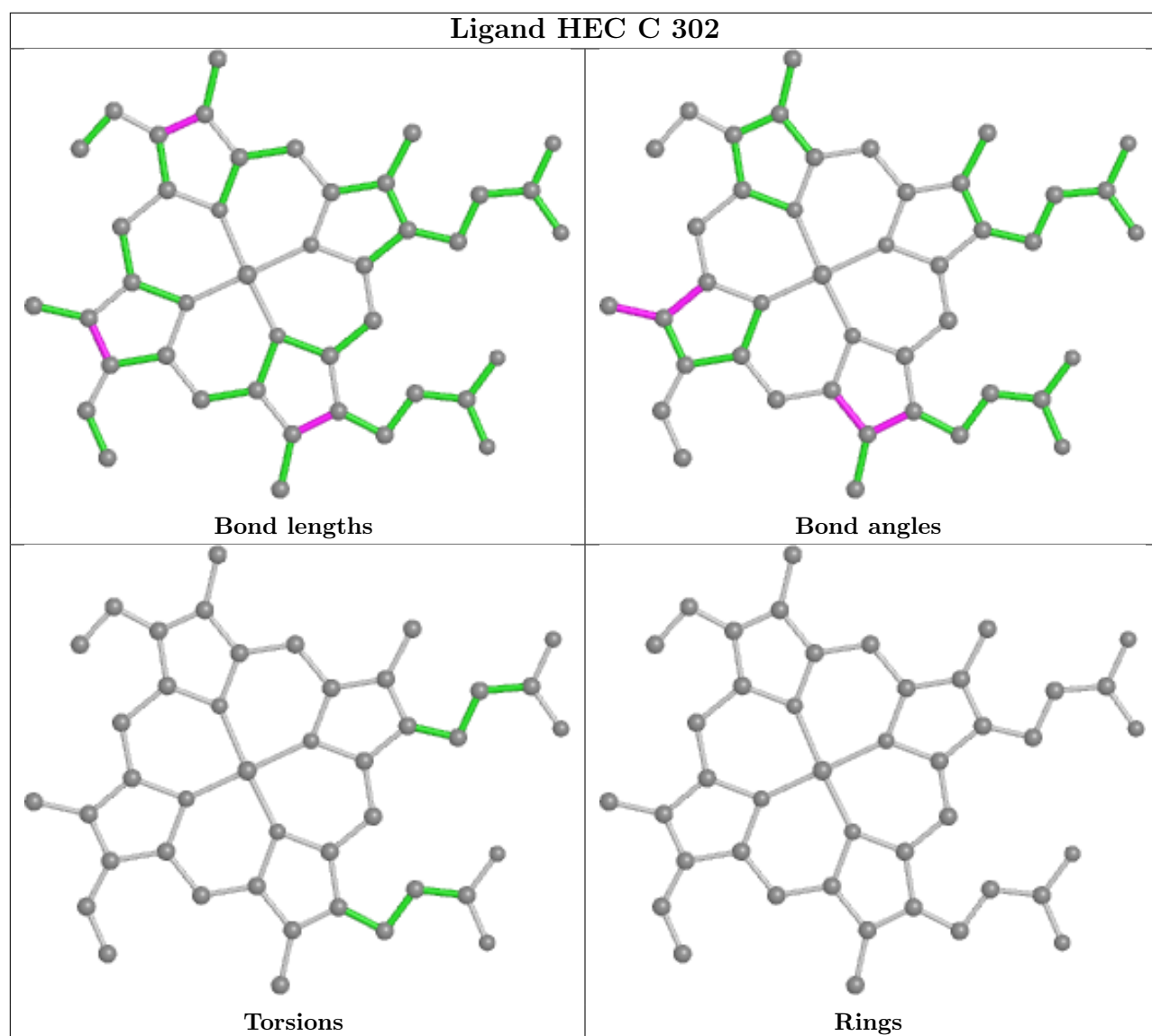


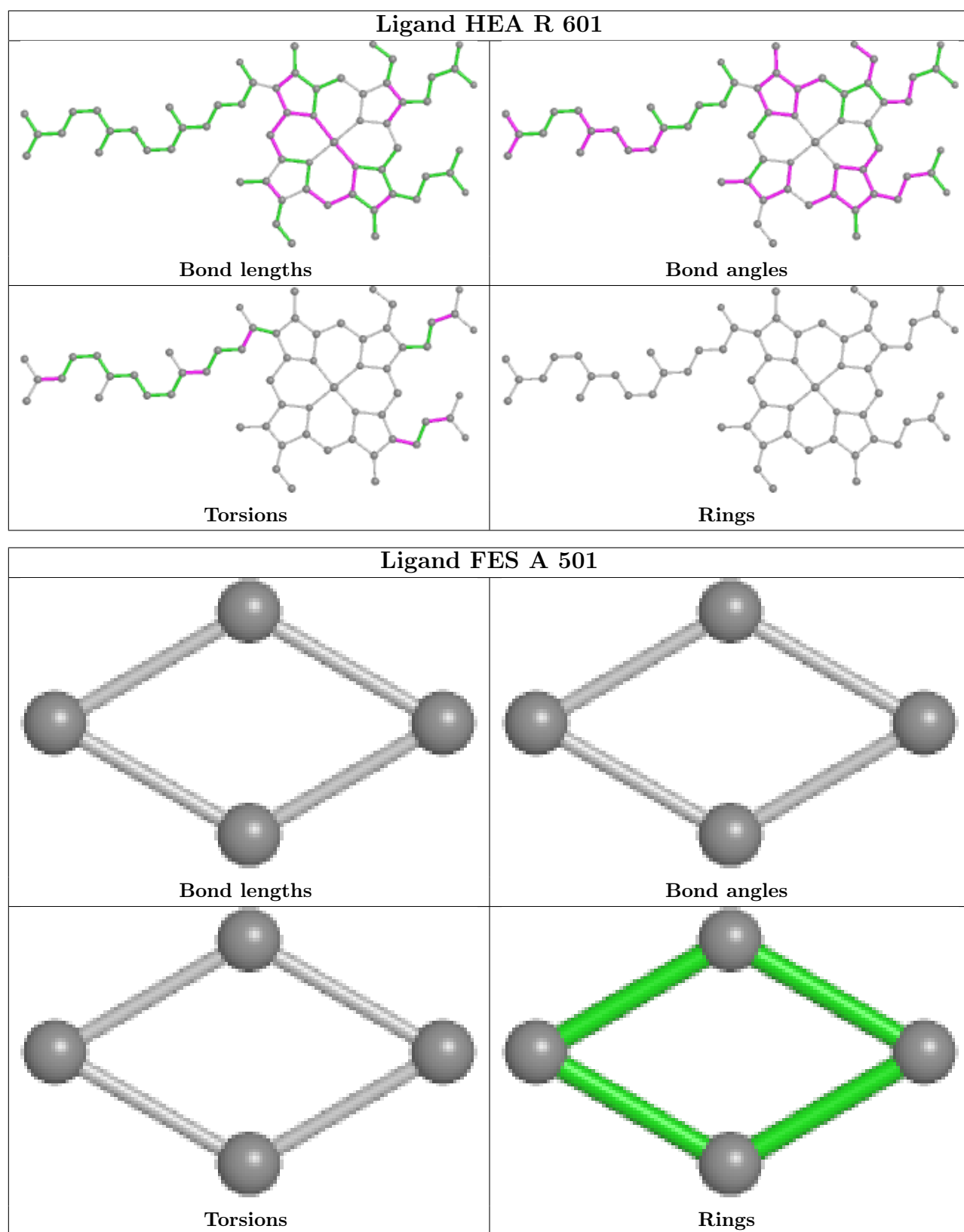




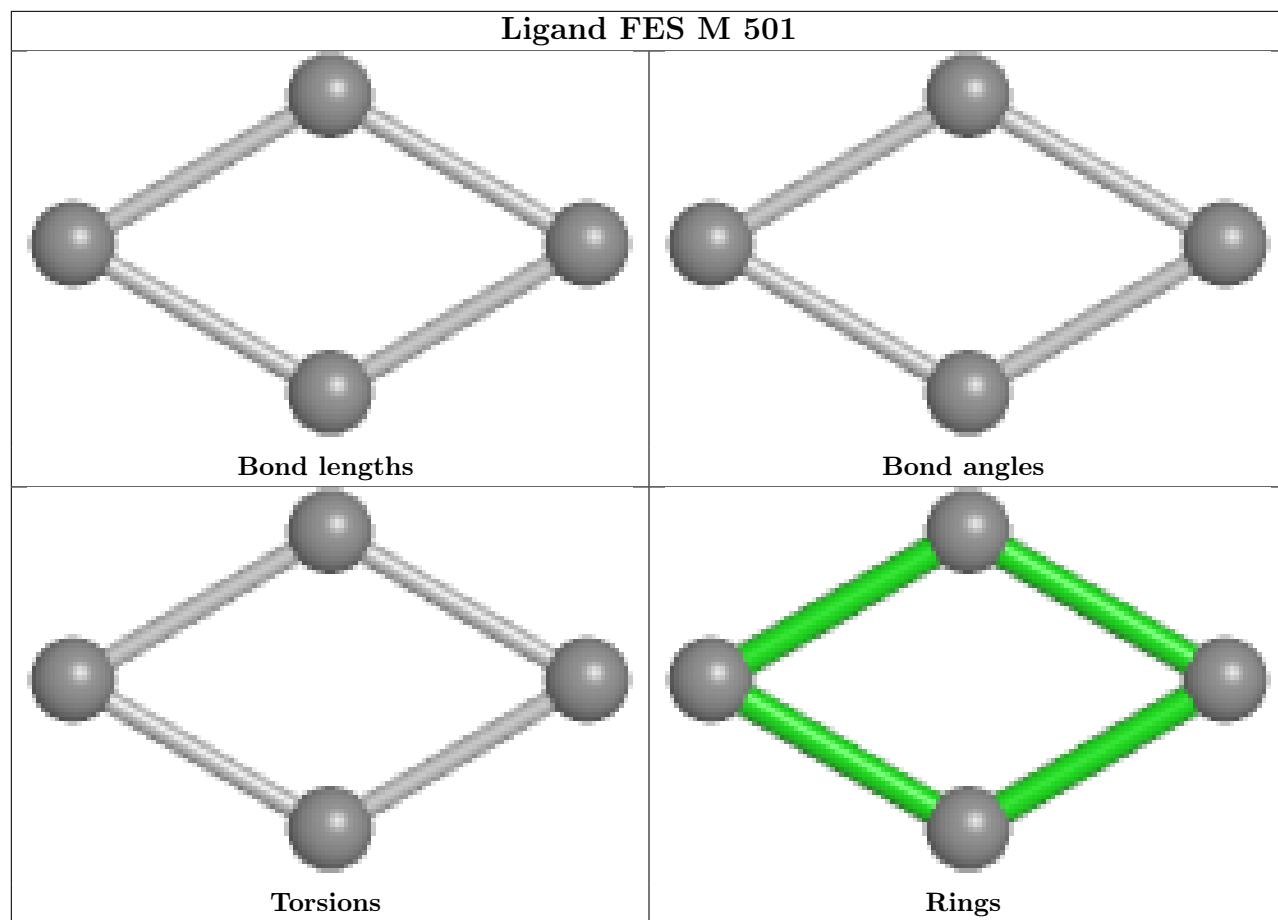


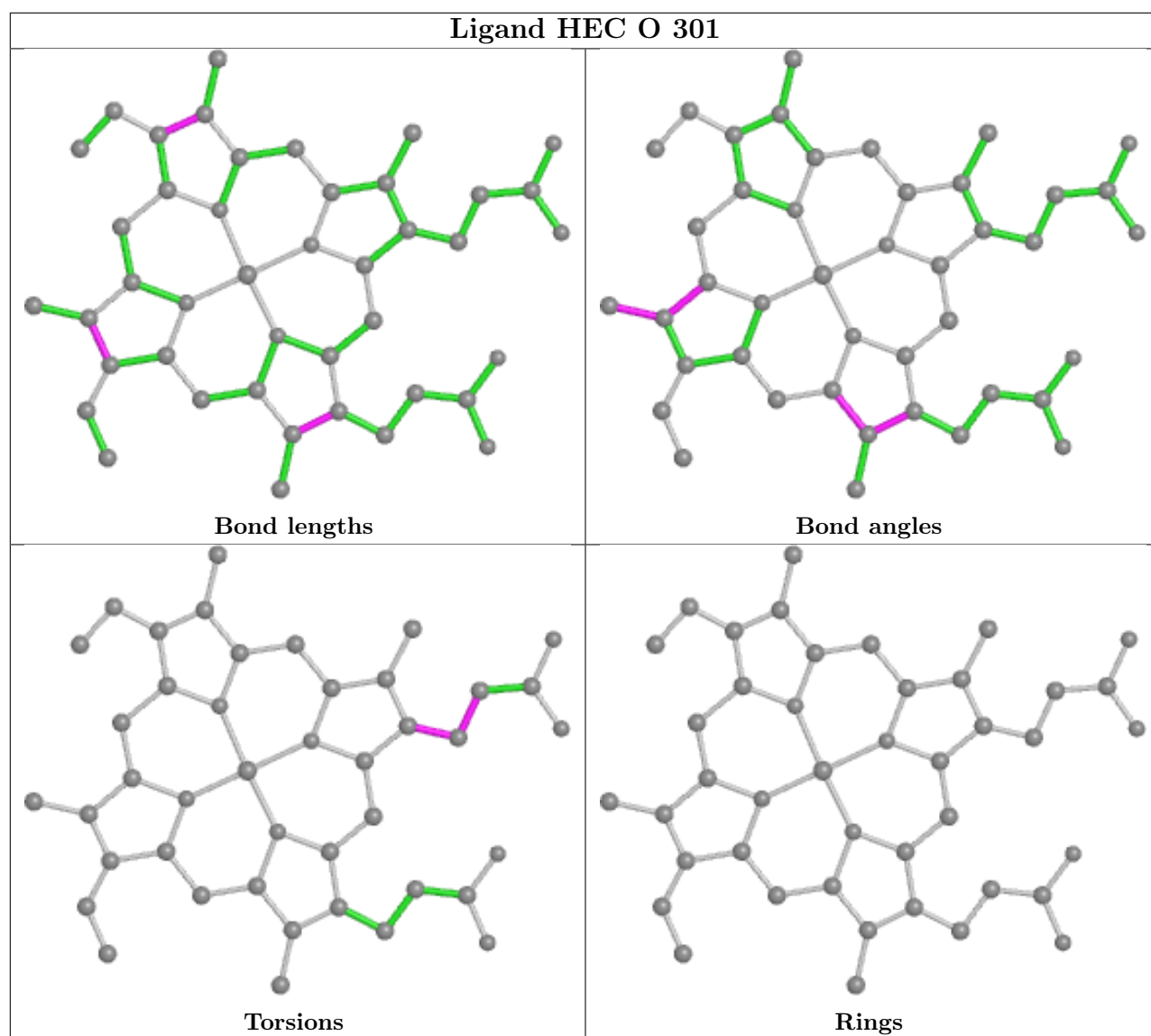












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

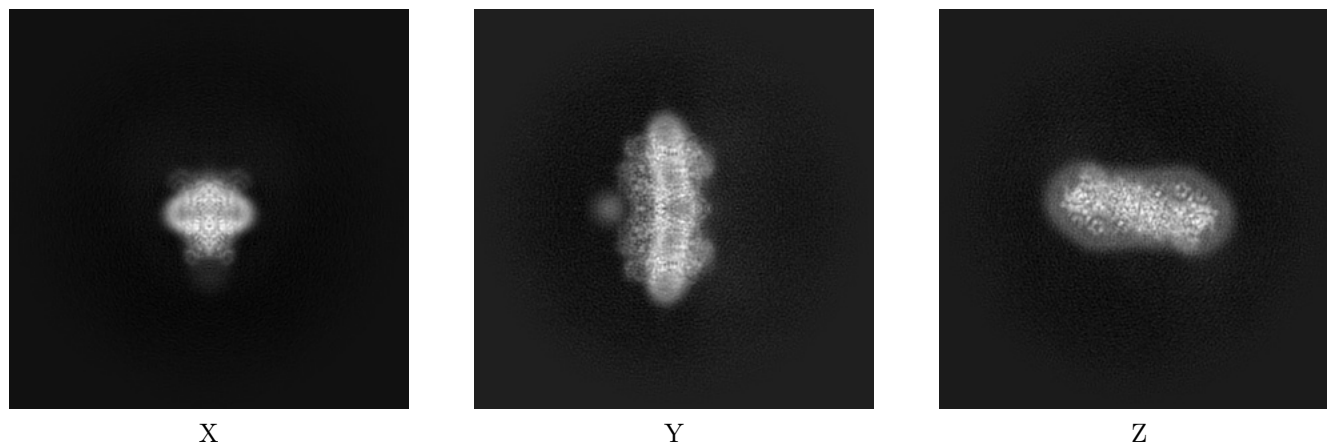
## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Tomogram visualisation [i](#)

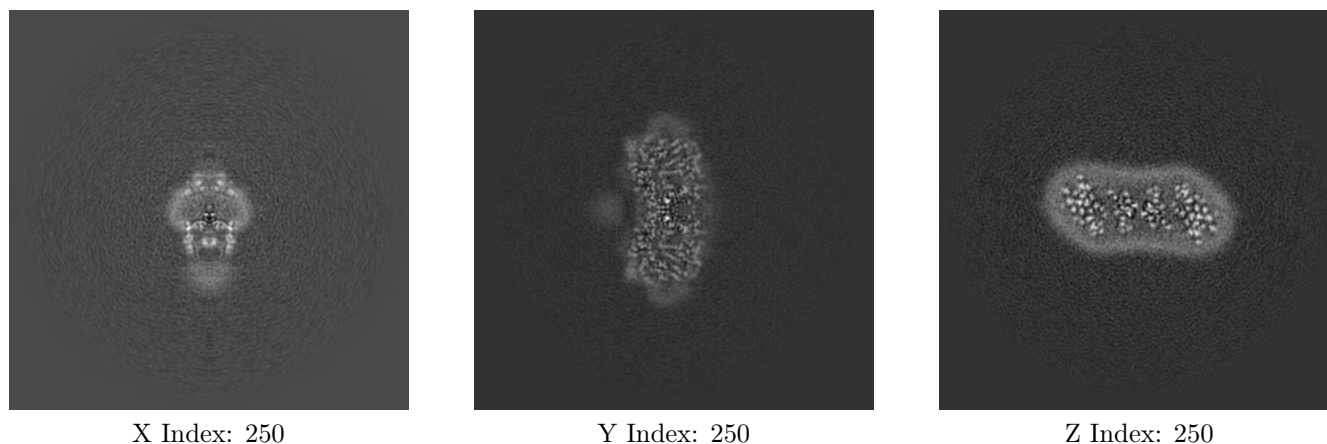
This section contains visualisations of the EMDB entry EMD-34664. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

### 6.1 Orthogonal projections [i](#)



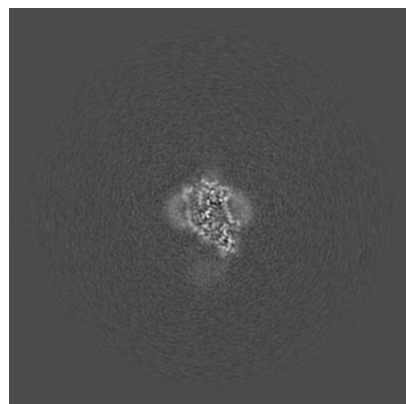
The images above show the tomogram projected in three orthogonal directions.

### 6.2 Central slices [i](#)

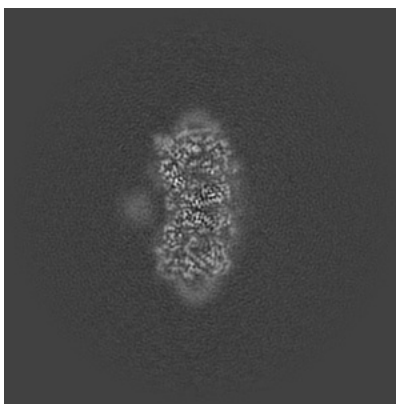


The images above show central slices of the tomogram in three orthogonal directions.

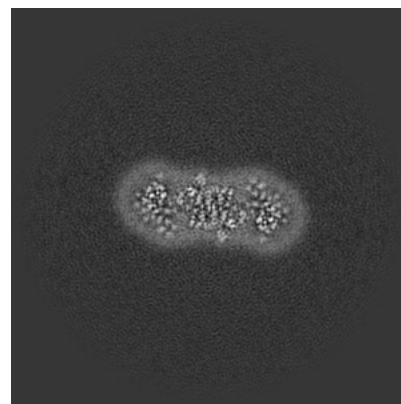
### 6.3 Largest variance slices [i](#)



X Index: 232



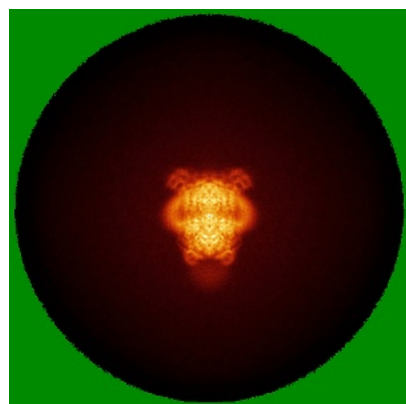
Y Index: 247



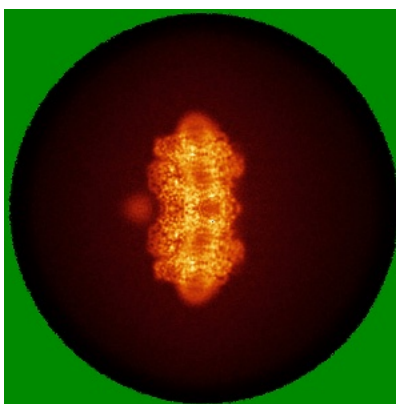
Z Index: 230

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

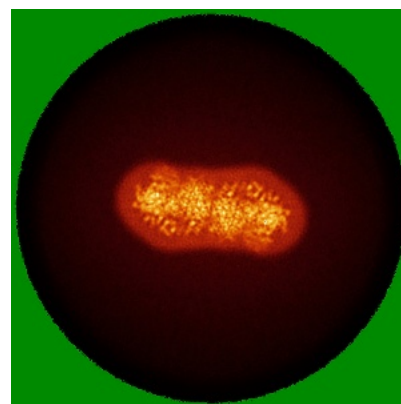
### 6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

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

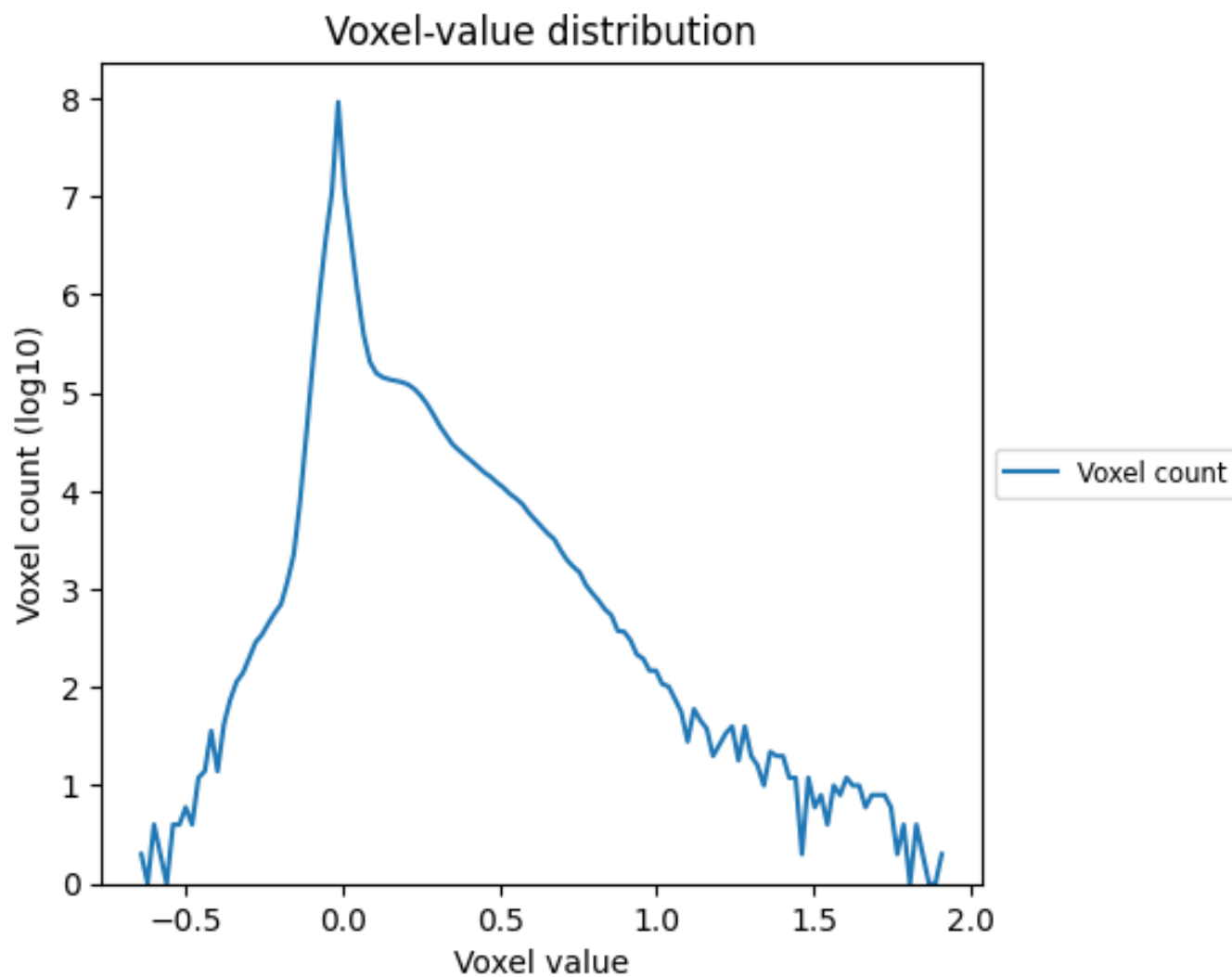
### 6.5 Mask visualisation [i](#)

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

## 7 Tomogram analysis [i](#)

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

### 7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

## 8 Map-model fit

This section was not generated.