



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 10:39 PM EDT

PDB ID : 6OVH / pdb_00006ovh
EMDB ID : EMD-20212
Title : Cryo-EM structure of Bimetallic dodecameric cage design 3 (BMC3) from cytochrome cb562
Authors : Golub, E.; Subramanian, R.H.; Yan, X.; Alberstein, R.G.; Tezcan, F.A.
Deposited on : 2019-05-07
Resolution : 2.60 Å(reported)
Based on initial model : 6OT7

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

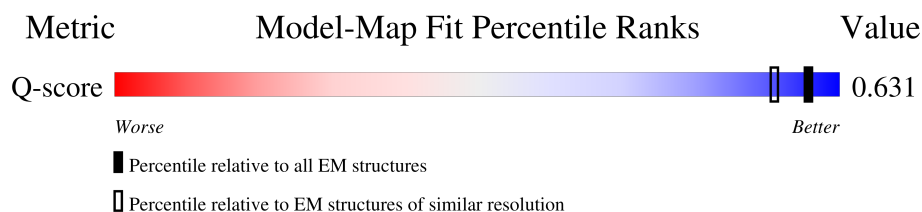
1 Overall quality at a glance

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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	8728 (2.10 - 3.10)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10895 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 Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	106	Total	C	N	O	S	1	0
			838	518	150	163	7		
1	B	106	Total	C	N	O	S	1	0
			838	518	150	163	7		
1	C	106	Total	C	N	O	S	1	0
			838	518	150	163	7		
1	D	106	Total	C	N	O	S	1	0
			838	518	150	163	7		
1	E	106	Total	C	N	O	S	1	0
			838	518	150	163	7		
1	F	106	Total	C	N	O	S	1	0
			838	518	150	163	7		
1	G	106	Total	C	N	O	S	1	0
			838	518	150	163	7		
1	H	106	Total	C	N	O	S	1	0
			838	518	150	163	7		
1	I	106	Total	C	N	O	S	1	0
			838	518	150	163	7		
1	J	106	Total	C	N	O	S	1	0
			838	518	150	163	7		
1	K	106	Total	C	N	O	S	1	0
			838	518	150	163	7		
1	L	106	Total	C	N	O	S	1	0
			838	518	150	163	7		

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	HIS	ASP	engineered mutation	UNP P0ABE7
A	8	HIS	GLU	engineered mutation	UNP P0ABE7
A	16	HIS	VAL	engineered mutation	UNP P0ABE7
A	24	THR	ALA	engineered mutation	UNP P0ABE7
A	25	THR	GLN	engineered mutation	UNP P0ABE7
A	34	GLN	ARG	engineered mutation	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLN	LEU	engineered mutation	UNP P0ABE7
A	41	TRP	GLN	engineered mutation	UNP P0ABE7
A	42	SER	LYS	engineered mutation	UNP P0ABE7
A	59	SER	LYS	engineered mutation	UNP P0ABE7
A	63	CYS	HIS	engineered mutation	UNP P0ABE7
A	66	TRP	ASP	engineered mutation	UNP P0ABE7
A	67	GLU	ILE	engineered mutation	UNP P0ABE7
A	69	ILE	VAL	engineered mutation	UNP P0ABE7
A	73	ASN	ASP	engineered mutation	UNP P0ABE7
A	74	ALA	ASP	engineered mutation	UNP P0ABE7
A	77	HIS	LYS	engineered mutation	UNP P0ABE7
A	80	LYS	ASN	engineered mutation	UNP P0ABE7
A	81	GLN	GLU	engineered mutation	UNP P0ABE7
A	82	CYS	GLY	engineered mutation	UNP P0ABE7
A	98	CYS	ARG	engineered mutation	UNP P0ABE7
A	101	CYS	TYR	engineered mutation	UNP P0ABE7
B	5	HIS	ASP	engineered mutation	UNP P0ABE7
B	8	HIS	GLU	engineered mutation	UNP P0ABE7
B	16	HIS	VAL	engineered mutation	UNP P0ABE7
B	24	THR	ALA	engineered mutation	UNP P0ABE7
B	25	THR	GLN	engineered mutation	UNP P0ABE7
B	34	GLN	ARG	engineered mutation	UNP P0ABE7
B	38	GLN	LEU	engineered mutation	UNP P0ABE7
B	41	TRP	GLN	engineered mutation	UNP P0ABE7
B	42	SER	LYS	engineered mutation	UNP P0ABE7
B	59	SER	LYS	engineered mutation	UNP P0ABE7
B	63	CYS	HIS	engineered mutation	UNP P0ABE7
B	66	TRP	ASP	engineered mutation	UNP P0ABE7
B	67	GLU	ILE	engineered mutation	UNP P0ABE7
B	69	ILE	VAL	engineered mutation	UNP P0ABE7
B	73	ASN	ASP	engineered mutation	UNP P0ABE7
B	74	ALA	ASP	engineered mutation	UNP P0ABE7
B	77	HIS	LYS	engineered mutation	UNP P0ABE7
B	80	LYS	ASN	engineered mutation	UNP P0ABE7
B	81	GLN	GLU	engineered mutation	UNP P0ABE7
B	82	CYS	GLY	engineered mutation	UNP P0ABE7
B	98	CYS	ARG	engineered mutation	UNP P0ABE7
B	101	CYS	TYR	engineered mutation	UNP P0ABE7
C	5	HIS	ASP	engineered mutation	UNP P0ABE7
C	8	HIS	GLU	engineered mutation	UNP P0ABE7
C	16	HIS	VAL	engineered mutation	UNP P0ABE7
C	24	THR	ALA	engineered mutation	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	25	THR	GLN	engineered mutation	UNP P0ABE7
C	34	GLN	ARG	engineered mutation	UNP P0ABE7
C	38	GLN	LEU	engineered mutation	UNP P0ABE7
C	41	TRP	GLN	engineered mutation	UNP P0ABE7
C	42	SER	LYS	engineered mutation	UNP P0ABE7
C	59	SER	LYS	engineered mutation	UNP P0ABE7
C	63	CYS	HIS	engineered mutation	UNP P0ABE7
C	66	TRP	ASP	engineered mutation	UNP P0ABE7
C	67	GLU	ILE	engineered mutation	UNP P0ABE7
C	69	ILE	VAL	engineered mutation	UNP P0ABE7
C	73	ASN	ASP	engineered mutation	UNP P0ABE7
C	74	ALA	ASP	engineered mutation	UNP P0ABE7
C	77	HIS	LYS	engineered mutation	UNP P0ABE7
C	80	LYS	ASN	engineered mutation	UNP P0ABE7
C	81	GLN	GLU	engineered mutation	UNP P0ABE7
C	82	CYS	GLY	engineered mutation	UNP P0ABE7
C	98	CYS	ARG	engineered mutation	UNP P0ABE7
C	101	CYS	TYR	engineered mutation	UNP P0ABE7
D	5	HIS	ASP	engineered mutation	UNP P0ABE7
D	8	HIS	GLU	engineered mutation	UNP P0ABE7
D	16	HIS	VAL	engineered mutation	UNP P0ABE7
D	24	THR	ALA	engineered mutation	UNP P0ABE7
D	25	THR	GLN	engineered mutation	UNP P0ABE7
D	34	GLN	ARG	engineered mutation	UNP P0ABE7
D	38	GLN	LEU	engineered mutation	UNP P0ABE7
D	41	TRP	GLN	engineered mutation	UNP P0ABE7
D	42	SER	LYS	engineered mutation	UNP P0ABE7
D	59	SER	LYS	engineered mutation	UNP P0ABE7
D	63	CYS	HIS	engineered mutation	UNP P0ABE7
D	66	TRP	ASP	engineered mutation	UNP P0ABE7
D	67	GLU	ILE	engineered mutation	UNP P0ABE7
D	69	ILE	VAL	engineered mutation	UNP P0ABE7
D	73	ASN	ASP	engineered mutation	UNP P0ABE7
D	74	ALA	ASP	engineered mutation	UNP P0ABE7
D	77	HIS	LYS	engineered mutation	UNP P0ABE7
D	80	LYS	ASN	engineered mutation	UNP P0ABE7
D	81	GLN	GLU	engineered mutation	UNP P0ABE7
D	82	CYS	GLY	engineered mutation	UNP P0ABE7
D	98	CYS	ARG	engineered mutation	UNP P0ABE7
D	101	CYS	TYR	engineered mutation	UNP P0ABE7
E	5	HIS	ASP	engineered mutation	UNP P0ABE7
E	8	HIS	GLU	engineered mutation	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	16	HIS	VAL	engineered mutation	UNP P0ABE7
E	24	THR	ALA	engineered mutation	UNP P0ABE7
E	25	THR	GLN	engineered mutation	UNP P0ABE7
E	34	GLN	ARG	engineered mutation	UNP P0ABE7
E	38	GLN	LEU	engineered mutation	UNP P0ABE7
E	41	TRP	GLN	engineered mutation	UNP P0ABE7
E	42	SER	LYS	engineered mutation	UNP P0ABE7
E	59	SER	LYS	engineered mutation	UNP P0ABE7
E	63	CYS	HIS	engineered mutation	UNP P0ABE7
E	66	TRP	ASP	engineered mutation	UNP P0ABE7
E	67	GLU	ILE	engineered mutation	UNP P0ABE7
E	69	ILE	VAL	engineered mutation	UNP P0ABE7
E	73	ASN	ASP	engineered mutation	UNP P0ABE7
E	74	ALA	ASP	engineered mutation	UNP P0ABE7
E	77	HIS	LYS	engineered mutation	UNP P0ABE7
E	80	LYS	ASN	engineered mutation	UNP P0ABE7
E	81	GLN	GLU	engineered mutation	UNP P0ABE7
E	82	CYS	GLY	engineered mutation	UNP P0ABE7
E	98	CYS	ARG	engineered mutation	UNP P0ABE7
E	101	CYS	TYR	engineered mutation	UNP P0ABE7
F	5	HIS	ASP	engineered mutation	UNP P0ABE7
F	8	HIS	GLU	engineered mutation	UNP P0ABE7
F	16	HIS	VAL	engineered mutation	UNP P0ABE7
F	24	THR	ALA	engineered mutation	UNP P0ABE7
F	25	THR	GLN	engineered mutation	UNP P0ABE7
F	34	GLN	ARG	engineered mutation	UNP P0ABE7
F	38	GLN	LEU	engineered mutation	UNP P0ABE7
F	41	TRP	GLN	engineered mutation	UNP P0ABE7
F	42	SER	LYS	engineered mutation	UNP P0ABE7
F	59	SER	LYS	engineered mutation	UNP P0ABE7
F	63	CYS	HIS	engineered mutation	UNP P0ABE7
F	66	TRP	ASP	engineered mutation	UNP P0ABE7
F	67	GLU	ILE	engineered mutation	UNP P0ABE7
F	69	ILE	VAL	engineered mutation	UNP P0ABE7
F	73	ASN	ASP	engineered mutation	UNP P0ABE7
F	74	ALA	ASP	engineered mutation	UNP P0ABE7
F	77	HIS	LYS	engineered mutation	UNP P0ABE7
F	80	LYS	ASN	engineered mutation	UNP P0ABE7
F	81	GLN	GLU	engineered mutation	UNP P0ABE7
F	82	CYS	GLY	engineered mutation	UNP P0ABE7
F	98	CYS	ARG	engineered mutation	UNP P0ABE7
F	101	CYS	TYR	engineered mutation	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	5	HIS	ASP	engineered mutation	UNP P0ABE7
G	8	HIS	GLU	engineered mutation	UNP P0ABE7
G	16	HIS	VAL	engineered mutation	UNP P0ABE7
G	24	THR	ALA	engineered mutation	UNP P0ABE7
G	25	THR	GLN	engineered mutation	UNP P0ABE7
G	34	GLN	ARG	engineered mutation	UNP P0ABE7
G	38	GLN	LEU	engineered mutation	UNP P0ABE7
G	41	TRP	GLN	engineered mutation	UNP P0ABE7
G	42	SER	LYS	engineered mutation	UNP P0ABE7
G	59	SER	LYS	engineered mutation	UNP P0ABE7
G	63	CYS	HIS	engineered mutation	UNP P0ABE7
G	66	TRP	ASP	engineered mutation	UNP P0ABE7
G	67	GLU	ILE	engineered mutation	UNP P0ABE7
G	69	ILE	VAL	engineered mutation	UNP P0ABE7
G	73	ASN	ASP	engineered mutation	UNP P0ABE7
G	74	ALA	ASP	engineered mutation	UNP P0ABE7
G	77	HIS	LYS	engineered mutation	UNP P0ABE7
G	80	LYS	ASN	engineered mutation	UNP P0ABE7
G	81	GLN	GLU	engineered mutation	UNP P0ABE7
G	82	CYS	GLY	engineered mutation	UNP P0ABE7
G	98	CYS	ARG	engineered mutation	UNP P0ABE7
G	101	CYS	TYR	engineered mutation	UNP P0ABE7
H	5	HIS	ASP	engineered mutation	UNP P0ABE7
H	8	HIS	GLU	engineered mutation	UNP P0ABE7
H	16	HIS	VAL	engineered mutation	UNP P0ABE7
H	24	THR	ALA	engineered mutation	UNP P0ABE7
H	25	THR	GLN	engineered mutation	UNP P0ABE7
H	34	GLN	ARG	engineered mutation	UNP P0ABE7
H	38	GLN	LEU	engineered mutation	UNP P0ABE7
H	41	TRP	GLN	engineered mutation	UNP P0ABE7
H	42	SER	LYS	engineered mutation	UNP P0ABE7
H	59	SER	LYS	engineered mutation	UNP P0ABE7
H	63	CYS	HIS	engineered mutation	UNP P0ABE7
H	66	TRP	ASP	engineered mutation	UNP P0ABE7
H	67	GLU	ILE	engineered mutation	UNP P0ABE7
H	69	ILE	VAL	engineered mutation	UNP P0ABE7
H	73	ASN	ASP	engineered mutation	UNP P0ABE7
H	74	ALA	ASP	engineered mutation	UNP P0ABE7
H	77	HIS	LYS	engineered mutation	UNP P0ABE7
H	80	LYS	ASN	engineered mutation	UNP P0ABE7
H	81	GLN	GLU	engineered mutation	UNP P0ABE7
H	82	CYS	GLY	engineered mutation	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	98	CYS	ARG	engineered mutation	UNP P0ABE7
H	101	CYS	TYR	engineered mutation	UNP P0ABE7
I	5	HIS	ASP	engineered mutation	UNP P0ABE7
I	8	HIS	GLU	engineered mutation	UNP P0ABE7
I	16	HIS	VAL	engineered mutation	UNP P0ABE7
I	24	THR	ALA	engineered mutation	UNP P0ABE7
I	25	THR	GLN	engineered mutation	UNP P0ABE7
I	34	GLN	ARG	engineered mutation	UNP P0ABE7
I	38	GLN	LEU	engineered mutation	UNP P0ABE7
I	41	TRP	GLN	engineered mutation	UNP P0ABE7
I	42	SER	LYS	engineered mutation	UNP P0ABE7
I	59	SER	LYS	engineered mutation	UNP P0ABE7
I	63	CYS	HIS	engineered mutation	UNP P0ABE7
I	66	TRP	ASP	engineered mutation	UNP P0ABE7
I	67	GLU	ILE	engineered mutation	UNP P0ABE7
I	69	ILE	VAL	engineered mutation	UNP P0ABE7
I	73	ASN	ASP	engineered mutation	UNP P0ABE7
I	74	ALA	ASP	engineered mutation	UNP P0ABE7
I	77	HIS	LYS	engineered mutation	UNP P0ABE7
I	80	LYS	ASN	engineered mutation	UNP P0ABE7
I	81	GLN	GLU	engineered mutation	UNP P0ABE7
I	82	CYS	GLY	engineered mutation	UNP P0ABE7
I	98	CYS	ARG	engineered mutation	UNP P0ABE7
I	101	CYS	TYR	engineered mutation	UNP P0ABE7
J	5	HIS	ASP	engineered mutation	UNP P0ABE7
J	8	HIS	GLU	engineered mutation	UNP P0ABE7
J	16	HIS	VAL	engineered mutation	UNP P0ABE7
J	24	THR	ALA	engineered mutation	UNP P0ABE7
J	25	THR	GLN	engineered mutation	UNP P0ABE7
J	34	GLN	ARG	engineered mutation	UNP P0ABE7
J	38	GLN	LEU	engineered mutation	UNP P0ABE7
J	41	TRP	GLN	engineered mutation	UNP P0ABE7
J	42	SER	LYS	engineered mutation	UNP P0ABE7
J	59	SER	LYS	engineered mutation	UNP P0ABE7
J	63	CYS	HIS	engineered mutation	UNP P0ABE7
J	66	TRP	ASP	engineered mutation	UNP P0ABE7
J	67	GLU	ILE	engineered mutation	UNP P0ABE7
J	69	ILE	VAL	engineered mutation	UNP P0ABE7
J	73	ASN	ASP	engineered mutation	UNP P0ABE7
J	74	ALA	ASP	engineered mutation	UNP P0ABE7
J	77	HIS	LYS	engineered mutation	UNP P0ABE7
J	80	LYS	ASN	engineered mutation	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	81	GLN	GLU	engineered mutation	UNP P0ABE7
J	82	CYS	GLY	engineered mutation	UNP P0ABE7
J	98	CYS	ARG	engineered mutation	UNP P0ABE7
J	101	CYS	TYR	engineered mutation	UNP P0ABE7
K	5	HIS	ASP	engineered mutation	UNP P0ABE7
K	8	HIS	GLU	engineered mutation	UNP P0ABE7
K	16	HIS	VAL	engineered mutation	UNP P0ABE7
K	24	THR	ALA	engineered mutation	UNP P0ABE7
K	25	THR	GLN	engineered mutation	UNP P0ABE7
K	34	GLN	ARG	engineered mutation	UNP P0ABE7
K	38	GLN	LEU	engineered mutation	UNP P0ABE7
K	41	TRP	GLN	engineered mutation	UNP P0ABE7
K	42	SER	LYS	engineered mutation	UNP P0ABE7
K	59	SER	LYS	engineered mutation	UNP P0ABE7
K	63	CYS	HIS	engineered mutation	UNP P0ABE7
K	66	TRP	ASP	engineered mutation	UNP P0ABE7
K	67	GLU	ILE	engineered mutation	UNP P0ABE7
K	69	ILE	VAL	engineered mutation	UNP P0ABE7
K	73	ASN	ASP	engineered mutation	UNP P0ABE7
K	74	ALA	ASP	engineered mutation	UNP P0ABE7
K	77	HIS	LYS	engineered mutation	UNP P0ABE7
K	80	LYS	ASN	engineered mutation	UNP P0ABE7
K	81	GLN	GLU	engineered mutation	UNP P0ABE7
K	82	CYS	GLY	engineered mutation	UNP P0ABE7
K	98	CYS	ARG	engineered mutation	UNP P0ABE7
K	101	CYS	TYR	engineered mutation	UNP P0ABE7
L	5	HIS	ASP	engineered mutation	UNP P0ABE7
L	8	HIS	GLU	engineered mutation	UNP P0ABE7
L	16	HIS	VAL	engineered mutation	UNP P0ABE7
L	24	THR	ALA	engineered mutation	UNP P0ABE7
L	25	THR	GLN	engineered mutation	UNP P0ABE7
L	34	GLN	ARG	engineered mutation	UNP P0ABE7
L	38	GLN	LEU	engineered mutation	UNP P0ABE7
L	41	TRP	GLN	engineered mutation	UNP P0ABE7
L	42	SER	LYS	engineered mutation	UNP P0ABE7
L	59	SER	LYS	engineered mutation	UNP P0ABE7
L	63	CYS	HIS	engineered mutation	UNP P0ABE7
L	66	TRP	ASP	engineered mutation	UNP P0ABE7
L	67	GLU	ILE	engineered mutation	UNP P0ABE7
L	69	ILE	VAL	engineered mutation	UNP P0ABE7
L	73	ASN	ASP	engineered mutation	UNP P0ABE7
L	74	ALA	ASP	engineered mutation	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
L	77	HIS	LYS	engineered mutation	UNP P0ABE7
L	80	LYS	ASN	engineered mutation	UNP P0ABE7
L	81	GLN	GLU	engineered mutation	UNP P0ABE7
L	82	CYS	GLY	engineered mutation	UNP P0ABE7
L	98	CYS	ARG	engineered mutation	UNP P0ABE7
L	101	CYS	TYR	engineered mutation	UNP P0ABE7

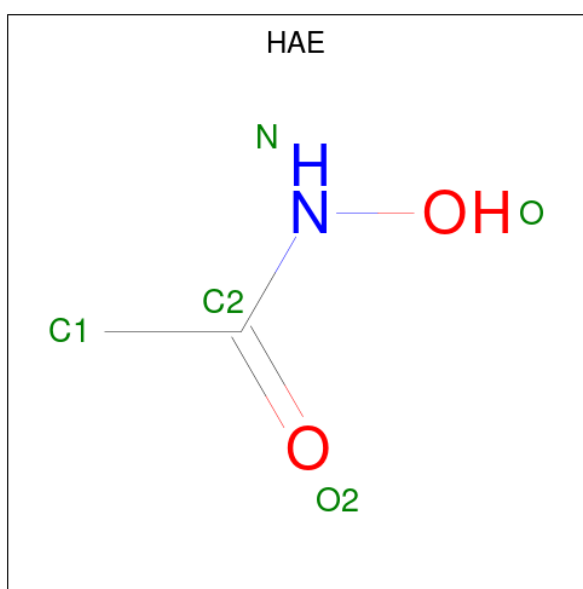
- # HEC
-
- Chemical structure of HEC (Hexaethylcyclen) complexed with an iron(II) ion. The structure shows a central iron atom (Fe) coordinated by six nitrogen atoms (N) in a hexagonal arrangement. The nitrogen atoms are part of a 1,4,7-triazacyclononane ring. The rings are substituted with ethyl groups (C2C, C3C, C4C, C5C, C6C, C7C) and methyl groups (C8C, C9C, C10C, C11C, C12C, C13C). The iron atom is also coordinated by two water molecules (H2O) in the axial positions, represented by O1D and O2A. The overall structure is highly symmetrical.

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Mol	Chain	Residues	Atoms					AltConf
2	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 3 is ACETOHYDROXAMIC ACID (CCD ID: HAE) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			5	2	1	2	
3	A	1	Total	C	N	O	0
			5	2	1	2	
3	B	1	Total	C	N	O	0
			5	2	1	2	
3	B	1	Total	C	N	O	0
			5	2	1	2	
3	C	1	Total	C	N	O	0
			5	2	1	2	
3	C	1	Total	C	N	O	0
			5	2	1	2	
3	D	1	Total	C	N	O	0
			5	2	1	2	

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Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	N	O	0
			5	2	1	2	
3	E	1	Total	C	N	O	0
			5	2	1	2	
3	E	1	Total	C	N	O	0
			5	2	1	2	
3	F	1	Total	C	N	O	0
			5	2	1	2	
3	F	1	Total	C	N	O	0
			5	2	1	2	
3	G	1	Total	C	N	O	0
			5	2	1	2	
3	G	1	Total	C	N	O	0
			5	2	1	2	
3	H	1	Total	C	N	O	0
			5	2	1	2	
3	H	1	Total	C	N	O	0
			5	2	1	2	
3	I	1	Total	C	N	O	0
			5	2	1	2	
3	I	1	Total	C	N	O	0
			5	2	1	2	
3	J	1	Total	C	N	O	0
			5	2	1	2	
3	J	1	Total	C	N	O	0
			5	2	1	2	
3	K	1	Total	C	N	O	0
			5	2	1	2	
3	K	1	Total	C	N	O	0
			5	2	1	2	
3	L	1	Total	C	N	O	0
			5	2	1	2	
3	L	1	Total	C	N	O	0
			5	2	1	2	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	Zn	0
			3	3	
4	B	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	C	2	Total 2	Zn 2	0
4	D	3	Total 3	Zn 3	0
4	E	3	Total 3	Zn 3	0
4	F	1	Total 1	Zn 1	0
4	G	1	Total 1	Zn 1	0
4	H	2	Total 2	Zn 2	0
4	I	2	Total 2	Zn 2	0
4	J	2	Total 2	Zn 2	0
4	K	2	Total 2	Zn 2	0
4	L	2	Total 2	Zn 2	0

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Fe 1	0
5	B	2	Total 2	Fe 2	0
5	C	1	Total 1	Fe 1	0
5	D	1	Total 1	Fe 1	0
5	E	1	Total 1	Fe 1	0
5	H	1	Total 1	Fe 1	0
5	I	1	Total 1	Fe 1	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	16	Total 16	O 16	0
6	B	15	Total 15	O 15	0
6	C	14	Total 14	O 14	0
6	D	12	Total 12	O 12	0
6	E	14	Total 14	O 14	0
6	F	14	Total 14	O 14	0
6	G	15	Total 15	O 15	0
6	H	12	Total 12	O 12	0
6	I	14	Total 14	O 14	0
6	J	17	Total 17	O 17	0
6	K	15	Total 15	O 15	0
6	L	13	Total 13	O 13	0

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	25391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.026	Depositor
Map size ($\text{\AA}$)	216.3712, 216.3712, 216.3712	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8452, 0.8452, 0.8452	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 32 are monoatomic - leaving 36 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
2	HEC	G	201	1	50,50,50	1.59	8 (16%)	68,82,82	1.52	10 (14%)
3	HAE	C	204	1,5	4,4,4	4.75	1 (25%)	2,4,4	1.85	1 (50%)
3	HAE	I	202	1,5	4,4,4	4.59	1 (25%)	2,4,4	1.92	1 (50%)
3	HAE	A	202	1,5	4,4,4	4.57	1 (25%)	2,4,4	1.93	1 (50%)
3	HAE	A	203	1,5	4,4,4	4.73	1 (25%)	2,4,4	1.87	1 (50%)
2	HEC	H	202	1	50,50,50	1.59	8 (16%)	68,82,82	1.53	10 (14%)
2	HEC	K	202	1	50,50,50	1.59	9 (18%)	68,82,82	1.53	10 (14%)
2	HEC	J	202	1	50,50,50	1.59	9 (18%)	68,82,82	1.53	10 (14%)
2	HEC	C	202	1	50,50,50	1.59	9 (18%)	68,82,82	1.52	10 (14%)
2	HEC	D	201	1	50,50,50	1.59	8 (16%)	68,82,82	1.53	10 (14%)
3	HAE	F	203	1,5	4,4,4	4.77	1 (25%)	2,4,4	1.85	1 (50%)
3	HAE	H	204	1,5	4,4,4	4.73	1 (25%)	2,4,4	1.83	1 (50%)
3	HAE	E	202	1,5	4,4,4	4.60	1 (25%)	2,4,4	1.90	1 (50%)
3	HAE	K	204	1,5	4,4,4	4.78	1 (25%)	2,4,4	1.82	1 (50%)
3	HAE	L	203	1,5	4,4,4	4.57	1 (25%)	2,4,4	1.93	1 (50%)
3	HAE	J	204	1,5	4,4,4	4.75	1 (25%)	2,4,4	1.84	1 (50%)
2	HEC	E	201	1	50,50,50	1.59	8 (16%)	68,82,82	1.53	10 (14%)
3	HAE	G	202	1,5	4,4,4	4.59	1 (25%)	2,4,4	1.90	1 (50%)
2	HEC	L	202	1	50,50,50	1.59	8 (16%)	68,82,82	1.53	10 (14%)
3	HAE	D	203	1,5	4,4,4	4.77	1 (25%)	2,4,4	1.84	1 (50%)
2	HEC	F	201	1	50,50,50	1.59	8 (16%)	68,82,82	1.53	10 (14%)
3	HAE	I	203	1,5	4,4,4	4.74	1 (25%)	2,4,4	1.84	1 (50%)
2	HEC	I	201	1	50,50,50	1.59	9 (18%)	68,82,82	1.53	10 (14%)
3	HAE	D	202	1,5	4,4,4	4.58	1 (25%)	2,4,4	1.92	1 (50%)
3	HAE	L	204	1,5	4,4,4	4.76	1 (25%)	2,4,4	1.85	1 (50%)
3	HAE	F	202	1,5	4,4,4	4.59	1 (25%)	2,4,4	1.92	1 (50%)
2	HEC	A	201	1	50,50,50	1.59	8 (16%)	68,82,82	1.53	10 (14%)
3	HAE	K	203	1,5	4,4,4	4.58	1 (25%)	2,4,4	1.92	1 (50%)
2	HEC	B	201	1	50,50,50	1.59	8 (16%)	68,82,82	1.52	10 (14%)
3	HAE	H	203	1,5	4,4,4	4.60	1 (25%)	2,4,4	1.90	1 (50%)
3	HAE	E	203	1,5	4,4,4	4.73	1 (25%)	2,4,4	1.84	1 (50%)
3	HAE	G	203	1,5	4,4,4	4.75	1 (25%)	2,4,4	1.84	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HAE	B	202	1,5	4,4,4	4.56	1 (25%)	2,4,4	1.92	1 (50%)
3	HAE	J	203	1,5	4,4,4	4.59	1 (25%)	2,4,4	1.92	1 (50%)
3	HAE	B	203	1,5	4,4,4	4.72	1 (25%)	2,4,4	1.87	1 (50%)
3	HAE	C	203	1,5	4,4,4	4.57	1 (25%)	2,4,4	1.94	1 (50%)

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
2	HEC	G	201	1	1/1/3/7	6/14/54/54	-
3	HAE	C	204	1,5	-	0/1/2/2	-
3	HAE	I	202	1,5	-	0/1/2/2	-
3	HAE	A	202	1,5	-	0/1/2/2	-
3	HAE	A	203	1,5	-	0/1/2/2	-
2	HEC	H	202	1	1/1/3/7	6/14/54/54	-
2	HEC	K	202	1	1/1/3/7	6/14/54/54	-
2	HEC	J	202	1	1/1/3/7	6/14/54/54	-
2	HEC	C	202	1	1/1/3/7	6/14/54/54	-
2	HEC	D	201	1	1/1/3/7	6/14/54/54	-
3	HAE	F	203	1,5	-	0/1/2/2	-
3	HAE	H	204	1,5	-	0/1/2/2	-
3	HAE	E	202	1,5	-	0/1/2/2	-
3	HAE	K	204	1,5	-	0/1/2/2	-
3	HAE	L	203	1,5	-	0/1/2/2	-
3	HAE	J	204	1,5	-	0/1/2/2	-
2	HEC	E	201	1	1/1/3/7	6/14/54/54	-
3	HAE	G	202	1,5	-	0/1/2/2	-
2	HEC	L	202	1	1/1/3/7	6/14/54/54	-
3	HAE	D	203	1,5	-	0/1/2/2	-
2	HEC	F	201	1	1/1/3/7	6/14/54/54	-
3	HAE	I	203	1,5	-	0/1/2/2	-
2	HEC	I	201	1	1/1/3/7	6/14/54/54	-
3	HAE	D	202	1,5	-	0/1/2/2	-
3	HAE	L	204	1,5	-	0/1/2/2	-
3	HAE	F	202	1,5	-	0/1/2/2	-
2	HEC	A	201	1	1/1/3/7	6/14/54/54	-
3	HAE	K	203	1,5	-	0/1/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	B	201	1	1/1/3/7	6/14/54/54	-
3	HAE	H	203	1,5	-	0/1/2/2	-
3	HAE	E	203	1,5	-	0/1/2/2	-
3	HAE	G	203	1,5	-	0/1/2/2	-
3	HAE	B	202	1,5	-	0/1/2/2	-
3	HAE	J	203	1,5	-	0/1/2/2	-
3	HAE	B	203	1,5	-	0/1/2/2	-
3	HAE	C	203	1,5	-	0/1/2/2	-

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	204	HAE	C2-N	9.25	1.45	1.33
3	D	203	HAE	C2-N	9.24	1.45	1.33
3	F	203	HAE	C2-N	9.24	1.45	1.33
3	L	204	HAE	C2-N	9.22	1.45	1.33
3	C	204	HAE	C2-N	9.21	1.45	1.33
3	G	203	HAE	C2-N	9.19	1.45	1.33
3	J	204	HAE	C2-N	9.19	1.45	1.33
3	I	203	HAE	C2-N	9.18	1.45	1.33
3	A	203	HAE	C2-N	9.16	1.45	1.33
3	E	203	HAE	C2-N	9.16	1.45	1.33
3	H	204	HAE	C2-N	9.16	1.45	1.33
3	B	203	HAE	C2-N	9.15	1.45	1.33
3	H	203	HAE	C2-N	8.90	1.45	1.33
3	E	202	HAE	C2-N	8.88	1.45	1.33
3	J	203	HAE	C2-N	8.87	1.45	1.33
3	I	202	HAE	C2-N	8.87	1.45	1.33
3	F	202	HAE	C2-N	8.87	1.45	1.33
3	D	202	HAE	C2-N	8.86	1.45	1.33
3	G	202	HAE	C2-N	8.86	1.45	1.33
3	K	203	HAE	C2-N	8.84	1.45	1.33
3	C	203	HAE	C2-N	8.84	1.45	1.33
3	A	202	HAE	C2-N	8.84	1.45	1.33
3	L	203	HAE	C2-N	8.83	1.45	1.33
3	B	202	HAE	C2-N	8.82	1.45	1.33
2	G	201	HEC	CBB-CAB	-4.08	1.34	1.51
2	K	202	HEC	CBB-CAB	-4.08	1.34	1.51
2	L	202	HEC	CBB-CAB	-4.08	1.34	1.51
2	B	201	HEC	CBB-CAB	-4.07	1.34	1.51
2	F	201	HEC	CBB-CAB	-4.07	1.34	1.51
2	E	201	HEC	CBB-CAB	-4.07	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	HEC	CBB-CAB	-4.07	1.34	1.51
2	I	201	HEC	CBB-CAB	-4.06	1.34	1.51
2	J	202	HEC	CBB-CAB	-4.06	1.34	1.51
2	C	202	HEC	CBB-CAB	-4.06	1.34	1.51
2	A	201	HEC	CBB-CAB	-4.06	1.34	1.51
2	H	202	HEC	CBB-CAB	-4.05	1.34	1.51
2	H	202	HEC	CBC-CAC	-4.04	1.34	1.51
2	A	201	HEC	CBC-CAC	-4.03	1.34	1.51
2	J	202	HEC	CBC-CAC	-4.03	1.34	1.51
2	D	201	HEC	CBC-CAC	-4.03	1.34	1.51
2	C	202	HEC	CBC-CAC	-4.03	1.34	1.51
2	L	202	HEC	CBC-CAC	-4.03	1.34	1.51
2	K	202	HEC	CBC-CAC	-4.03	1.34	1.51
2	B	201	HEC	CBC-CAC	-4.03	1.34	1.51
2	G	201	HEC	CBC-CAC	-4.02	1.34	1.51
2	F	201	HEC	CBC-CAC	-4.02	1.34	1.51
2	I	201	HEC	CBC-CAC	-4.02	1.34	1.51
2	E	201	HEC	CBC-CAC	-4.01	1.34	1.51
2	D	201	HEC	FE-NB	3.84	2.06	1.94
2	I	201	HEC	FE-NB	3.84	2.06	1.94
2	E	201	HEC	FE-NB	3.83	2.06	1.94
2	H	202	HEC	FE-NB	3.83	2.06	1.94
2	J	202	HEC	FE-NB	3.83	2.06	1.94
2	A	201	HEC	FE-NB	3.82	2.06	1.94
2	C	202	HEC	FE-NB	3.82	2.06	1.94
2	F	201	HEC	FE-NB	3.82	2.06	1.94
2	G	201	HEC	FE-NB	3.81	2.06	1.94
2	L	202	HEC	FE-NB	3.81	2.06	1.94
2	B	201	HEC	FE-NB	3.81	2.06	1.94
2	K	202	HEC	FE-NB	3.80	2.06	1.94
2	K	202	HEC	FE-ND	3.46	2.05	1.94
2	G	201	HEC	FE-ND	3.45	2.05	1.94
2	I	201	HEC	FE-ND	3.45	2.05	1.94
2	J	202	HEC	FE-ND	3.45	2.05	1.94
2	B	201	HEC	FE-ND	3.44	2.05	1.94
2	F	201	HEC	FE-ND	3.44	2.05	1.94
2	L	202	HEC	FE-ND	3.44	2.05	1.94
2	A	201	HEC	FE-ND	3.43	2.05	1.94
2	H	202	HEC	FE-ND	3.42	2.05	1.94
2	C	202	HEC	FE-ND	3.42	2.05	1.94
2	D	201	HEC	FE-ND	3.42	2.05	1.94
2	E	201	HEC	FE-ND	3.42	2.05	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	202	HEC	FE-NC	3.39	2.06	1.95
2	A	201	HEC	FE-NC	3.38	2.06	1.95
2	C	202	HEC	FE-NC	3.38	2.06	1.95
2	E	201	HEC	FE-NC	3.38	2.06	1.95
2	B	201	HEC	FE-NC	3.37	2.06	1.95
2	D	201	HEC	FE-NC	3.37	2.06	1.95
2	H	202	HEC	FE-NC	3.37	2.06	1.95
2	F	201	HEC	FE-NC	3.36	2.06	1.95
2	L	202	HEC	FE-NC	3.36	2.06	1.95
2	G	201	HEC	FE-NC	3.36	2.06	1.95
2	I	201	HEC	FE-NC	3.36	2.06	1.95
2	K	202	HEC	FE-NC	3.36	2.06	1.95
2	I	201	HEC	FE-NA	2.72	2.04	1.95
2	H	202	HEC	FE-NA	2.71	2.04	1.95
2	G	201	HEC	FE-NA	2.71	2.04	1.95
2	L	202	HEC	FE-NA	2.71	2.04	1.95
2	F	201	HEC	FE-NA	2.71	2.04	1.95
2	K	202	HEC	FE-NA	2.71	2.04	1.95
2	A	201	HEC	FE-NA	2.70	2.04	1.95
2	C	202	HEC	FE-NA	2.70	2.04	1.95
2	E	201	HEC	FE-NA	2.70	2.04	1.95
2	D	201	HEC	FE-NA	2.69	2.04	1.95
2	B	201	HEC	FE-NA	2.68	2.04	1.95
2	J	202	HEC	FE-NA	2.68	2.04	1.95
2	H	202	HEC	CMC-C2C	2.13	1.55	1.50
2	F	201	HEC	CMC-C2C	2.13	1.55	1.50
2	D	201	HEC	CMC-C2C	2.13	1.55	1.50
2	J	202	HEC	CMC-C2C	2.13	1.55	1.50
2	B	201	HEC	CMC-C2C	2.12	1.55	1.50
2	L	202	HEC	CMC-C2C	2.12	1.55	1.50
2	E	201	HEC	CMC-C2C	2.11	1.55	1.50
2	A	201	HEC	CMC-C2C	2.11	1.55	1.50
2	G	201	HEC	CMC-C2C	2.10	1.55	1.50
2	K	202	HEC	CMC-C2C	2.10	1.55	1.50
2	C	202	HEC	CMC-C2C	2.09	1.55	1.50
2	I	201	HEC	CMC-C2C	2.08	1.55	1.50
2	A	201	HEC	CAC-C3C	2.07	1.56	1.51
2	J	202	HEC	CAC-C3C	2.07	1.56	1.51
2	I	201	HEC	CAC-C3C	2.06	1.56	1.51
2	B	201	HEC	CAC-C3C	2.06	1.56	1.51
2	G	201	HEC	CAC-C3C	2.06	1.56	1.51
2	F	201	HEC	CAC-C3C	2.06	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	202	HEC	CAC-C3C	2.05	1.56	1.51
2	L	202	HEC	CAC-C3C	2.04	1.56	1.51
2	K	202	HEC	CAC-C3C	2.04	1.56	1.51
2	D	201	HEC	CAC-C3C	2.04	1.56	1.51
2	E	201	HEC	CAC-C3C	2.04	1.56	1.51
2	C	202	HEC	CAC-C3C	2.03	1.56	1.51
2	K	202	HEC	CMD-C2D	2.02	1.54	1.50
2	I	201	HEC	CMD-C2D	2.02	1.54	1.50
2	J	202	HEC	CMD-C2D	2.02	1.54	1.50
2	C	202	HEC	CMD-C2D	2.01	1.54	1.50

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	HEC	CBC-CAC-C3C	5.76	128.03	112.42
2	B	201	HEC	CBC-CAC-C3C	5.75	128.00	112.42
2	E	201	HEC	CBC-CAC-C3C	5.74	127.99	112.42
2	J	202	HEC	CBC-CAC-C3C	5.74	127.98	112.42
2	H	202	HEC	CBC-CAC-C3C	5.74	127.97	112.42
2	D	201	HEC	CBC-CAC-C3C	5.73	127.97	112.42
2	F	201	HEC	CBC-CAC-C3C	5.73	127.96	112.42
2	C	202	HEC	CBC-CAC-C3C	5.73	127.96	112.42
2	K	202	HEC	CBC-CAC-C3C	5.73	127.96	112.42
2	G	201	HEC	CBC-CAC-C3C	5.73	127.96	112.42
2	L	202	HEC	CBC-CAC-C3C	5.73	127.95	112.42
2	I	201	HEC	CBC-CAC-C3C	5.72	127.94	112.42
2	L	202	HEC	CAC-C3C-C2C	3.80	132.91	126.89
2	D	201	HEC	CAC-C3C-C2C	3.79	132.89	126.89
2	K	202	HEC	CAC-C3C-C2C	3.79	132.89	126.89
2	H	202	HEC	CAC-C3C-C2C	3.79	132.88	126.89
2	C	202	HEC	CAC-C3C-C2C	3.78	132.88	126.89
2	G	201	HEC	CAC-C3C-C2C	3.78	132.87	126.89
2	F	201	HEC	CAC-C3C-C2C	3.78	132.87	126.89
2	E	201	HEC	CAC-C3C-C2C	3.77	132.86	126.89
2	I	201	HEC	CAC-C3C-C2C	3.77	132.86	126.89
2	J	202	HEC	CAC-C3C-C2C	3.77	132.86	126.89
2	B	201	HEC	CAC-C3C-C2C	3.76	132.84	126.89
2	A	201	HEC	CAC-C3C-C2C	3.74	132.81	126.89
2	I	201	HEC	CAC-C3C-C4C	-3.48	120.12	124.91
2	F	201	HEC	CAC-C3C-C4C	-3.47	120.14	124.91
2	K	202	HEC	CAC-C3C-C4C	-3.46	120.15	124.91
2	H	202	HEC	CAC-C3C-C4C	-3.46	120.15	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	202	HEC	CAC-C3C-C4C	-3.46	120.16	124.91
2	C	202	HEC	CAC-C3C-C4C	-3.45	120.16	124.91
2	G	201	HEC	CAC-C3C-C4C	-3.45	120.17	124.91
2	J	202	HEC	CAC-C3C-C4C	-3.44	120.17	124.91
2	D	201	HEC	CAC-C3C-C4C	-3.44	120.17	124.91
2	E	201	HEC	CAC-C3C-C4C	-3.44	120.18	124.91
2	B	201	HEC	CAC-C3C-C4C	-3.44	120.18	124.91
2	A	201	HEC	CAC-C3C-C4C	-3.41	120.22	124.91
2	K	202	HEC	C2A-C1A-NA	-3.04	107.39	110.32
2	A	201	HEC	C2A-C1A-NA	-3.03	107.40	110.32
2	C	202	HEC	C2A-C1A-NA	-3.03	107.40	110.32
2	H	202	HEC	C2A-C1A-NA	-3.02	107.41	110.32
2	G	201	HEC	C2A-C1A-NA	-3.02	107.41	110.32
2	F	201	HEC	C2A-C1A-NA	-3.02	107.41	110.32
2	D	201	HEC	C2A-C1A-NA	-3.01	107.42	110.32
2	I	201	HEC	C2A-C1A-NA	-3.00	107.43	110.32
2	L	202	HEC	C2A-C1A-NA	-2.99	107.44	110.32
2	E	201	HEC	C2A-C1A-NA	-2.99	107.44	110.32
2	B	201	HEC	C2A-C1A-NA	-2.98	107.45	110.32
2	J	202	HEC	C2A-C1A-NA	-2.95	107.47	110.32
3	C	203	HAE	C1-C2-N	2.71	120.60	116.10
3	L	203	HAE	C1-C2-N	2.69	120.57	116.10
3	D	202	HAE	C1-C2-N	2.69	120.57	116.10
3	A	202	HAE	C1-C2-N	2.69	120.57	116.10
3	B	202	HAE	C1-C2-N	2.68	120.56	116.10
3	J	203	HAE	C1-C2-N	2.68	120.56	116.10
3	K	203	HAE	C1-C2-N	2.68	120.56	116.10
3	F	202	HAE	C1-C2-N	2.68	120.55	116.10
3	I	202	HAE	C1-C2-N	2.68	120.55	116.10
3	E	202	HAE	C1-C2-N	2.66	120.53	116.10
3	H	203	HAE	C1-C2-N	2.66	120.52	116.10
3	G	202	HAE	C1-C2-N	2.65	120.51	116.10
2	C	202	HEC	C3D-C4D-ND	-2.54	107.90	110.35
2	E	201	HEC	C3D-C4D-ND	-2.54	107.90	110.35
2	G	201	HEC	C3D-C4D-ND	-2.53	107.91	110.35
2	A	201	HEC	C3D-C4D-ND	-2.53	107.91	110.35
2	J	202	HEC	C3D-C4D-ND	-2.52	107.91	110.35
2	H	202	HEC	C3D-C4D-ND	-2.51	107.92	110.35
2	K	202	HEC	C3D-C4D-ND	-2.51	107.93	110.35
2	D	201	HEC	C3D-C4D-ND	-2.50	107.94	110.35
2	I	201	HEC	C3D-C4D-ND	-2.49	107.94	110.35
2	L	202	HEC	C3D-C4D-ND	-2.48	107.95	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	HEC	C4B-NB-C1B	2.48	108.14	105.21
2	B	201	HEC	C3D-C4D-ND	-2.47	107.96	110.35
2	I	201	HEC	C4B-NB-C1B	2.47	108.14	105.21
2	L	202	HEC	C4B-NB-C1B	2.47	108.13	105.21
2	D	201	HEC	C4B-NB-C1B	2.47	108.13	105.21
2	F	201	HEC	C3D-C4D-ND	-2.47	107.97	110.35
2	A	201	HEC	CBB-CAB-C3B	2.46	119.09	112.42
2	F	201	HEC	CBB-CAB-C3B	2.46	119.08	112.42
2	J	202	HEC	C4B-NB-C1B	2.46	108.12	105.21
2	G	201	HEC	CBB-CAB-C3B	2.46	119.08	112.42
2	K	202	HEC	CBB-CAB-C3B	2.46	119.08	112.42
2	K	202	HEC	C4B-NB-C1B	2.45	108.11	105.21
2	D	201	HEC	CBB-CAB-C3B	2.45	119.07	112.42
2	H	202	HEC	C4B-NB-C1B	2.45	108.11	105.21
2	A	201	HEC	C4B-NB-C1B	2.45	108.11	105.21
2	B	201	HEC	CBB-CAB-C3B	2.45	119.06	112.42
2	E	201	HEC	CBB-CAB-C3B	2.44	119.05	112.42
2	J	202	HEC	CMC-C2C-C1C	-2.44	121.70	125.42
2	J	202	HEC	CBB-CAB-C3B	2.44	119.04	112.42
2	B	201	HEC	C4B-NB-C1B	2.44	108.10	105.21
2	F	201	HEC	C4B-NB-C1B	2.44	108.10	105.21
2	L	202	HEC	CBB-CAB-C3B	2.44	119.03	112.42
2	C	202	HEC	CBB-CAB-C3B	2.44	119.03	112.42
2	I	201	HEC	CBB-CAB-C3B	2.44	119.03	112.42
2	F	201	HEC	CMC-C2C-C1C	-2.44	121.71	125.42
2	H	202	HEC	CBB-CAB-C3B	2.43	119.00	112.42
2	C	202	HEC	C4B-NB-C1B	2.43	108.08	105.21
2	G	201	HEC	CMC-C2C-C1C	-2.42	121.73	125.42
2	G	201	HEC	C4B-NB-C1B	2.42	108.08	105.21
2	D	201	HEC	CMC-C2C-C1C	-2.42	121.73	125.42
2	A	201	HEC	CMC-C2C-C1C	-2.42	121.74	125.42
2	L	202	HEC	CMC-C2C-C1C	-2.41	121.75	125.42
2	H	202	HEC	CMC-C2C-C1C	-2.41	121.75	125.42
2	K	202	HEC	CMC-C2C-C1C	-2.41	121.75	125.42
2	B	201	HEC	CMC-C2C-C1C	-2.40	121.76	125.42
2	C	202	HEC	CMC-C2C-C1C	-2.40	121.77	125.42
2	E	201	HEC	CMC-C2C-C1C	-2.40	121.77	125.42
3	B	203	HAE	C1-C2-N	2.39	120.08	116.10
3	A	203	HAE	C1-C2-N	2.39	120.08	116.10
2	I	201	HEC	CMC-C2C-C1C	-2.38	121.79	125.42
3	J	204	HAE	C1-C2-N	2.38	120.05	116.10
3	D	203	HAE	C1-C2-N	2.37	120.05	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	203	HAE	C1-C2-N	2.37	120.04	116.10
3	E	203	HAE	C1-C2-N	2.37	120.04	116.10
3	C	204	HAE	C1-C2-N	2.37	120.04	116.10
3	L	204	HAE	C1-C2-N	2.37	120.04	116.10
2	A	201	HEC	CMC-C2C-C3C	2.36	130.63	125.62
2	F	201	HEC	CMC-C2C-C3C	2.36	130.63	125.62
3	H	204	HAE	C1-C2-N	2.36	120.03	116.10
3	G	203	HAE	C1-C2-N	2.36	120.03	116.10
3	I	203	HAE	C1-C2-N	2.36	120.03	116.10
2	J	202	HEC	CMC-C2C-C3C	2.35	130.61	125.62
2	I	201	HEC	CMC-C2C-C3C	2.35	130.61	125.62
2	G	201	HEC	CMC-C2C-C3C	2.35	130.61	125.62
2	B	201	HEC	CMC-C2C-C3C	2.35	130.61	125.62
2	K	202	HEC	CMC-C2C-C3C	2.35	130.61	125.62
2	C	202	HEC	CMC-C2C-C3C	2.35	130.60	125.62
2	D	201	HEC	CMC-C2C-C3C	2.34	130.59	125.62
2	E	201	HEC	CMC-C2C-C3C	2.34	130.59	125.62
3	K	204	HAE	C1-C2-N	2.34	120.00	116.10
2	K	202	HEC	C1D-ND-C4D	2.34	107.97	105.21
2	L	202	HEC	CMC-C2C-C3C	2.33	130.58	125.62
2	H	202	HEC	CMC-C2C-C3C	2.33	130.57	125.62
2	J	202	HEC	C1D-ND-C4D	2.32	107.95	105.21
2	A	201	HEC	C1D-ND-C4D	2.29	107.92	105.21
2	G	201	HEC	C1D-ND-C4D	2.29	107.92	105.21
2	H	202	HEC	C1D-ND-C4D	2.29	107.92	105.21
2	E	201	HEC	C1D-ND-C4D	2.28	107.91	105.21
2	C	202	HEC	C1D-ND-C4D	2.28	107.91	105.21
2	I	201	HEC	C1D-ND-C4D	2.28	107.91	105.21
2	F	201	HEC	C1D-ND-C4D	2.27	107.89	105.21
2	D	201	HEC	C1D-ND-C4D	2.26	107.89	105.21
2	B	201	HEC	C1D-ND-C4D	2.25	107.88	105.21
2	L	202	HEC	C1D-ND-C4D	2.24	107.86	105.21

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	201	HEC	NA
2	B	201	HEC	NA
2	C	202	HEC	NA
2	D	201	HEC	NA
2	E	201	HEC	NA
2	F	201	HEC	NA

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Mol	Chain	Res	Type	Atom
2	G	201	HEC	NA
2	H	202	HEC	NA
2	I	201	HEC	NA
2	J	202	HEC	NA
2	K	202	HEC	NA
2	L	202	HEC	NA

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	HEC	C4C-C3C-CAC-CBC
2	B	201	HEC	C4C-C3C-CAC-CBC
2	C	202	HEC	C4C-C3C-CAC-CBC
2	D	201	HEC	C4C-C3C-CAC-CBC
2	E	201	HEC	C4C-C3C-CAC-CBC
2	F	201	HEC	C4C-C3C-CAC-CBC
2	G	201	HEC	C4C-C3C-CAC-CBC
2	H	202	HEC	C4C-C3C-CAC-CBC
2	I	201	HEC	C4C-C3C-CAC-CBC
2	J	202	HEC	C4C-C3C-CAC-CBC
2	K	202	HEC	C4C-C3C-CAC-CBC
2	L	202	HEC	C4C-C3C-CAC-CBC
2	A	201	HEC	C2C-C3C-CAC-CBC
2	B	201	HEC	C2C-C3C-CAC-CBC
2	C	202	HEC	C2C-C3C-CAC-CBC
2	D	201	HEC	C2C-C3C-CAC-CBC
2	E	201	HEC	C2C-C3C-CAC-CBC
2	F	201	HEC	C2C-C3C-CAC-CBC
2	G	201	HEC	C2C-C3C-CAC-CBC
2	H	202	HEC	C2C-C3C-CAC-CBC
2	I	201	HEC	C2C-C3C-CAC-CBC
2	J	202	HEC	C2C-C3C-CAC-CBC
2	K	202	HEC	C2C-C3C-CAC-CBC
2	L	202	HEC	C2C-C3C-CAC-CBC
2	A	201	HEC	C3D-CAD-CBD-CGD
2	B	201	HEC	C3D-CAD-CBD-CGD
2	C	202	HEC	C3D-CAD-CBD-CGD
2	D	201	HEC	C3D-CAD-CBD-CGD
2	E	201	HEC	C3D-CAD-CBD-CGD
2	F	201	HEC	C3D-CAD-CBD-CGD
2	G	201	HEC	C3D-CAD-CBD-CGD
2	H	202	HEC	C3D-CAD-CBD-CGD

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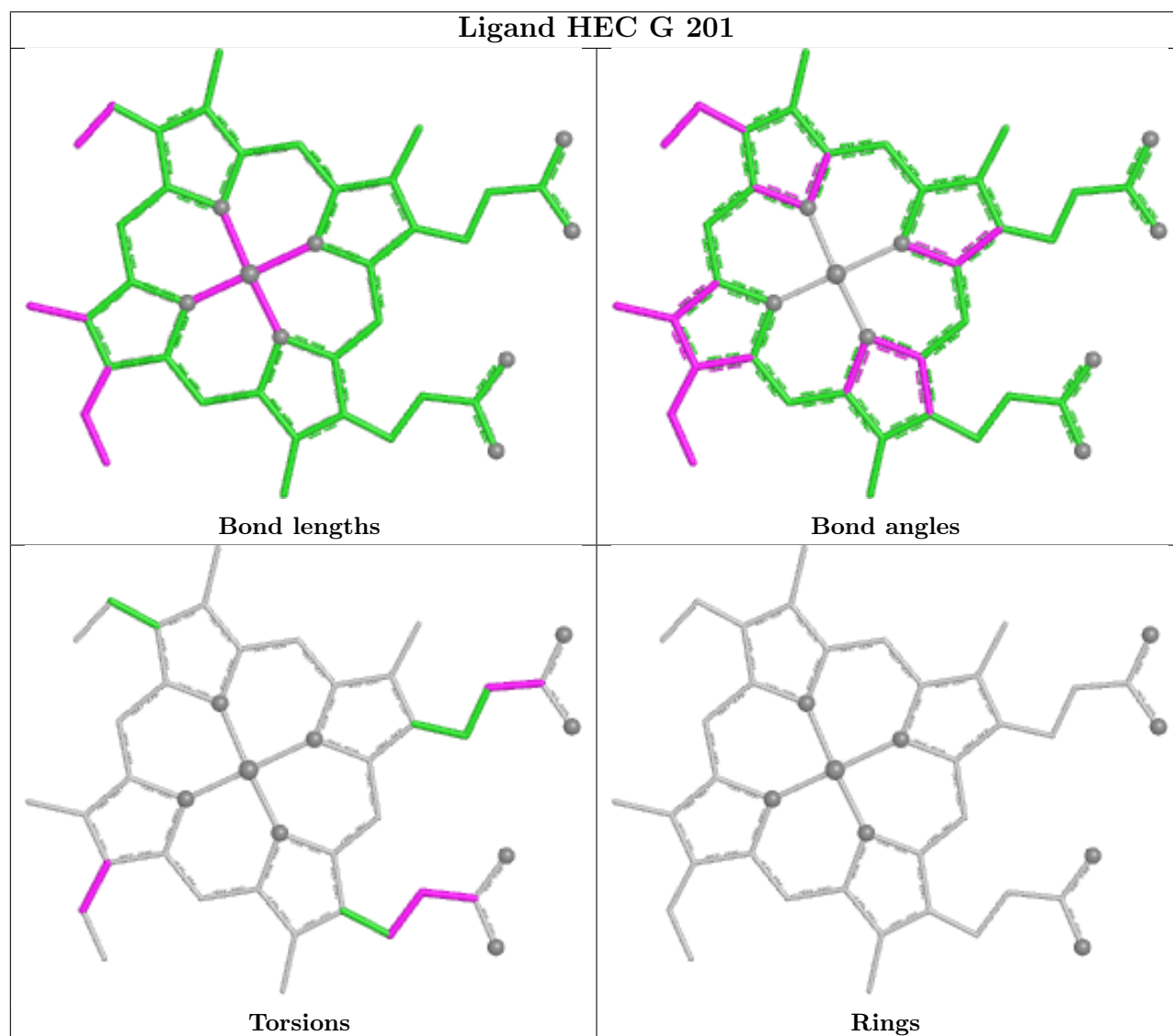
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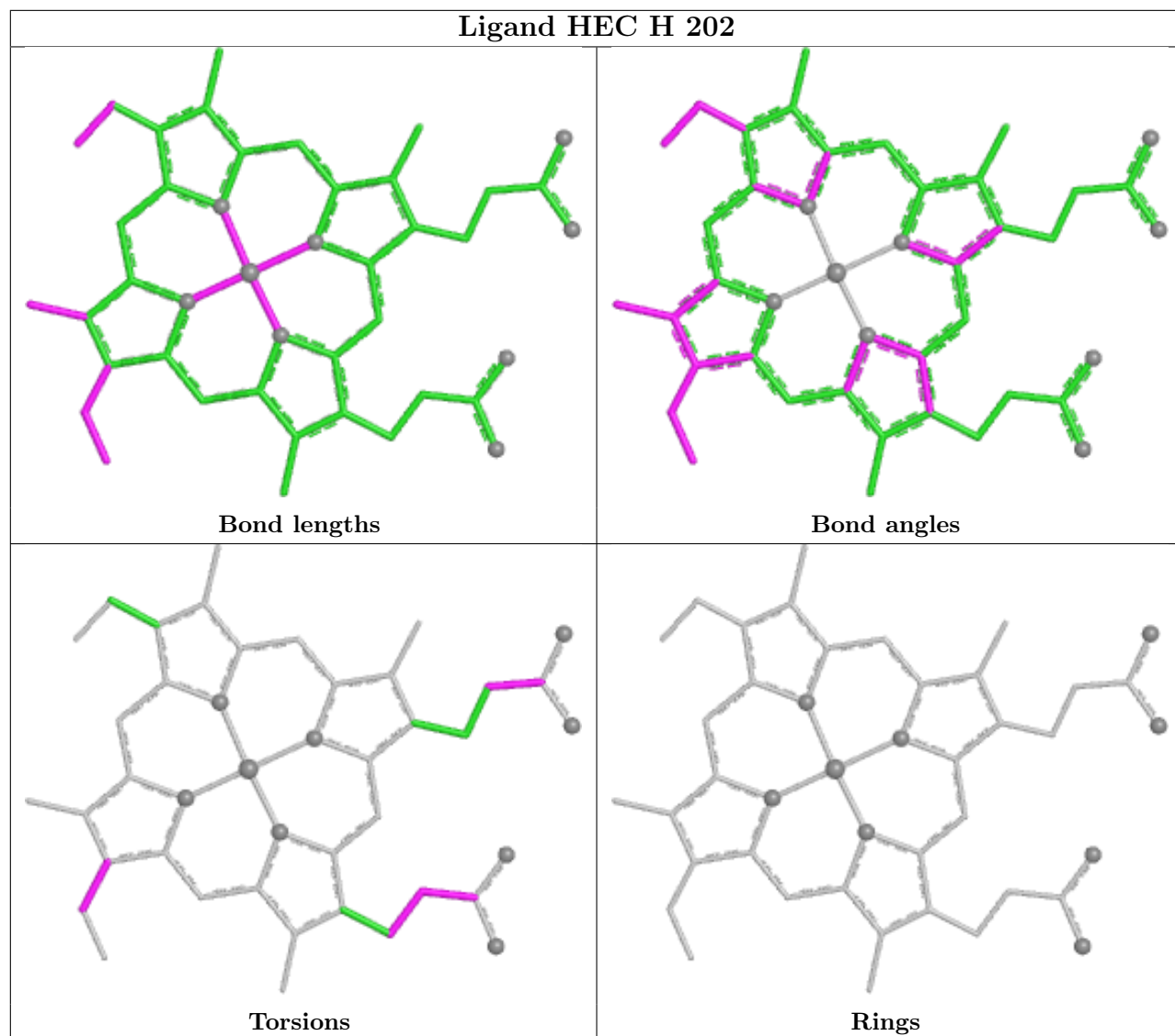
Mol	Chain	Res	Type	Atoms
2	I	201	HEC	C3D-CAD-CBD-CGD
2	J	202	HEC	C3D-CAD-CBD-CGD
2	K	202	HEC	C3D-CAD-CBD-CGD
2	L	202	HEC	C3D-CAD-CBD-CGD
2	C	202	HEC	CAD-CBD-CGD-O2D
2	B	201	HEC	CAD-CBD-CGD-O2D
2	D	201	HEC	CAD-CBD-CGD-O2D
2	G	201	HEC	CAD-CBD-CGD-O2D
2	J	202	HEC	CAD-CBD-CGD-O2D
2	K	202	HEC	CAD-CBD-CGD-O2D
2	L	202	HEC	CAD-CBD-CGD-O2D
2	A	201	HEC	CAD-CBD-CGD-O2D
2	E	201	HEC	CAD-CBD-CGD-O2D
2	F	201	HEC	CAD-CBD-CGD-O2D
2	H	202	HEC	CAD-CBD-CGD-O2D
2	I	201	HEC	CAD-CBD-CGD-O2D
2	A	201	HEC	CAD-CBD-CGD-O1D
2	C	202	HEC	CAD-CBD-CGD-O1D
2	F	201	HEC	CAD-CBD-CGD-O1D
2	G	201	HEC	CAD-CBD-CGD-O1D
2	H	202	HEC	CAD-CBD-CGD-O1D
2	I	201	HEC	CAD-CBD-CGD-O1D
2	J	202	HEC	CAD-CBD-CGD-O1D
2	K	202	HEC	CAD-CBD-CGD-O1D
2	L	202	HEC	CAD-CBD-CGD-O1D
2	B	201	HEC	CAD-CBD-CGD-O1D
2	D	201	HEC	CAD-CBD-CGD-O1D
2	E	201	HEC	CAD-CBD-CGD-O1D
2	A	201	HEC	CAA-CBA-CGA-O2A
2	B	201	HEC	CAA-CBA-CGA-O2A
2	C	202	HEC	CAA-CBA-CGA-O2A
2	D	201	HEC	CAA-CBA-CGA-O2A
2	E	201	HEC	CAA-CBA-CGA-O2A
2	F	201	HEC	CAA-CBA-CGA-O2A
2	G	201	HEC	CAA-CBA-CGA-O2A
2	H	202	HEC	CAA-CBA-CGA-O2A
2	I	201	HEC	CAA-CBA-CGA-O2A
2	J	202	HEC	CAA-CBA-CGA-O2A
2	K	202	HEC	CAA-CBA-CGA-O2A
2	L	202	HEC	CAA-CBA-CGA-O2A

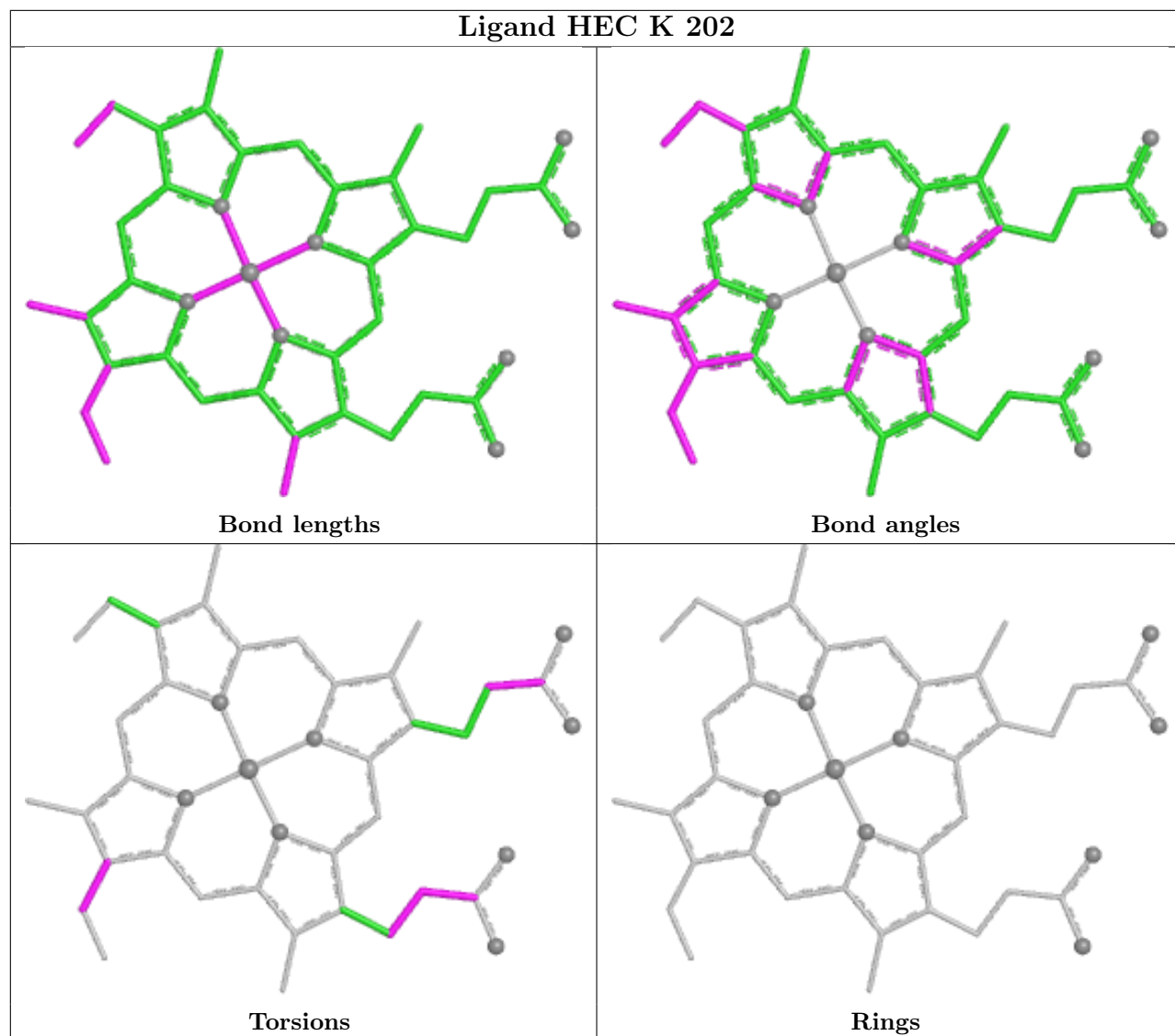
There are no ring outliers.

No monomer is involved in short contacts.

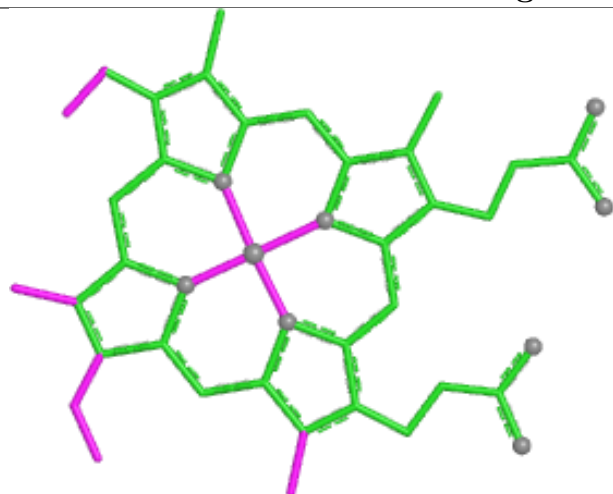
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



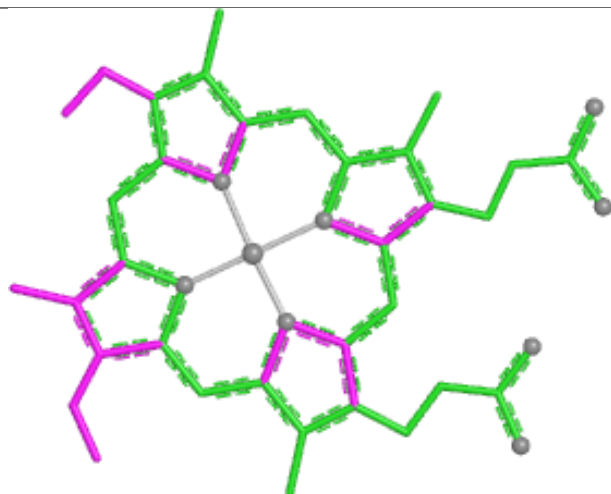




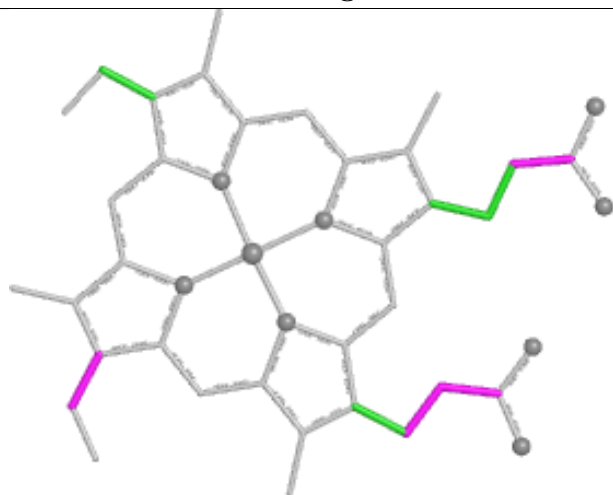
Ligand HEC J 202



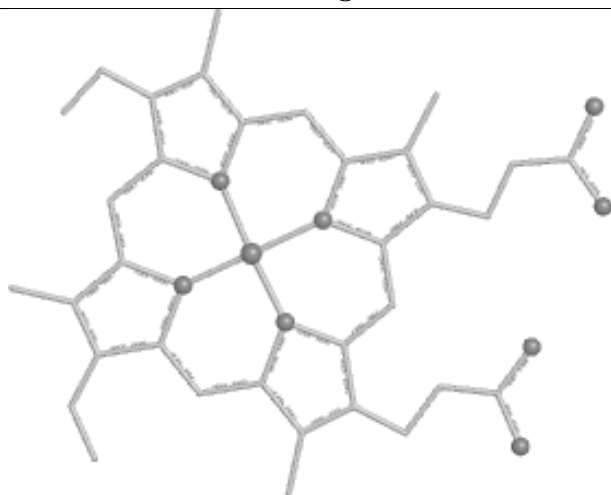
Bond lengths



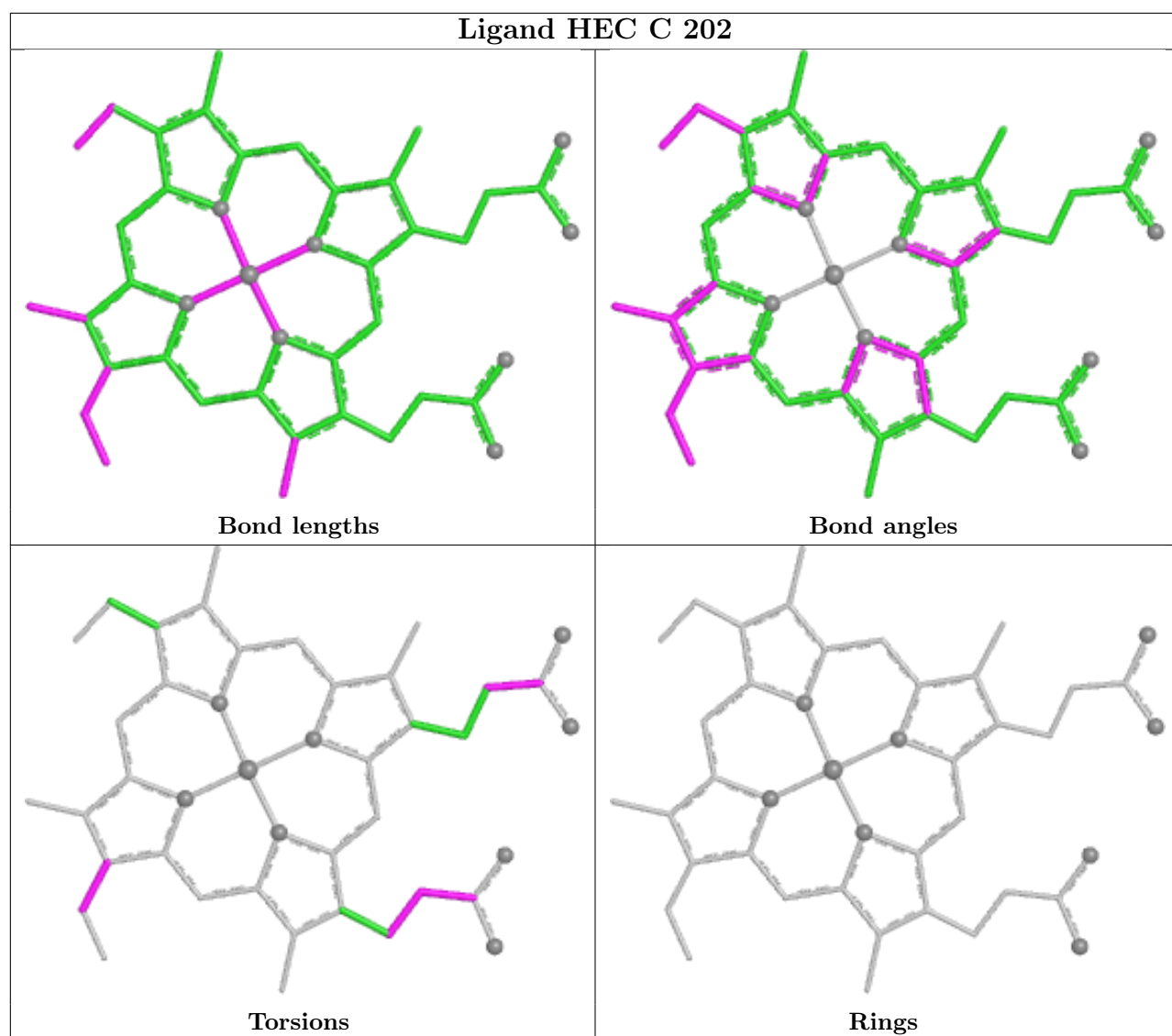
Bond angles

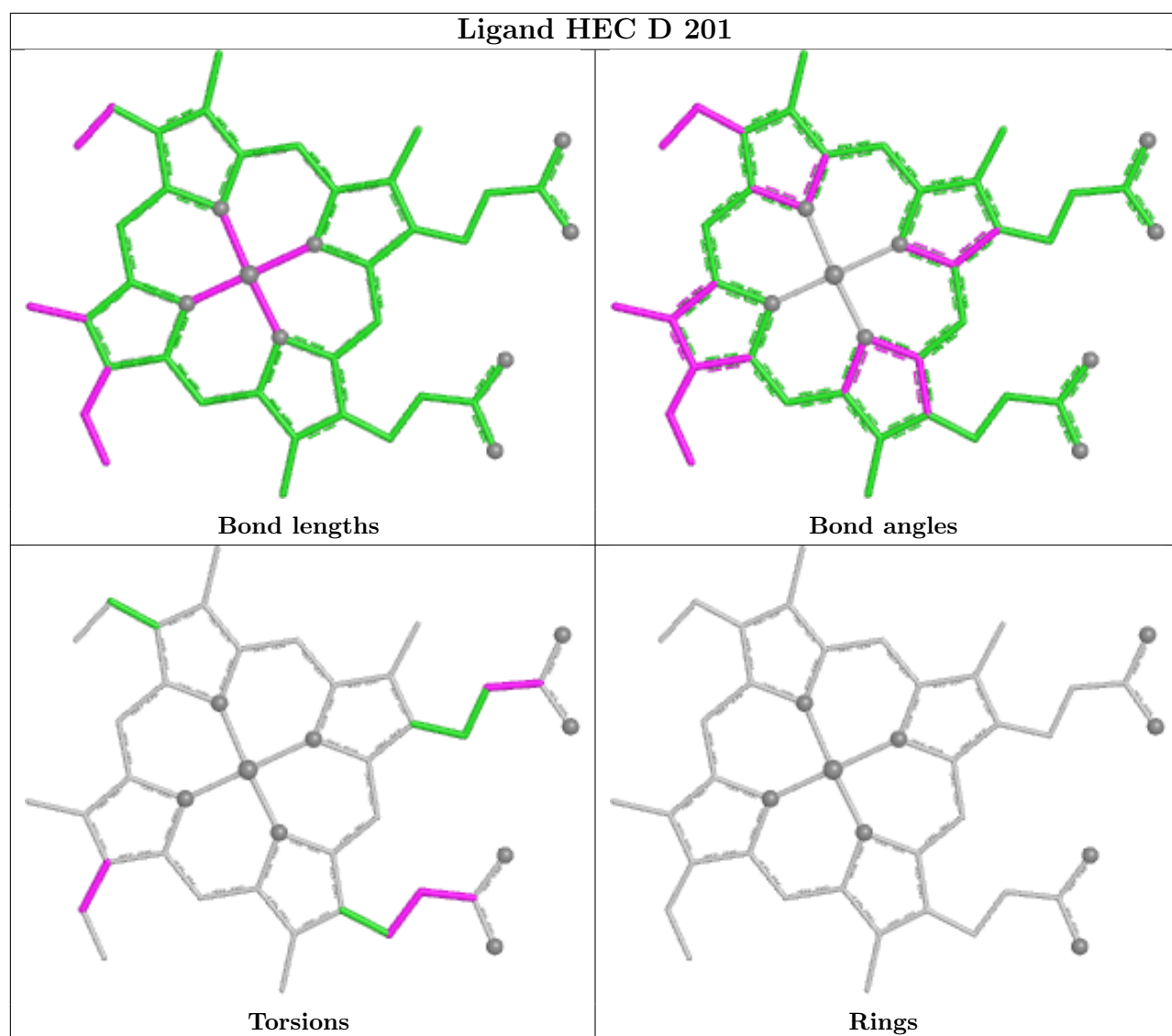


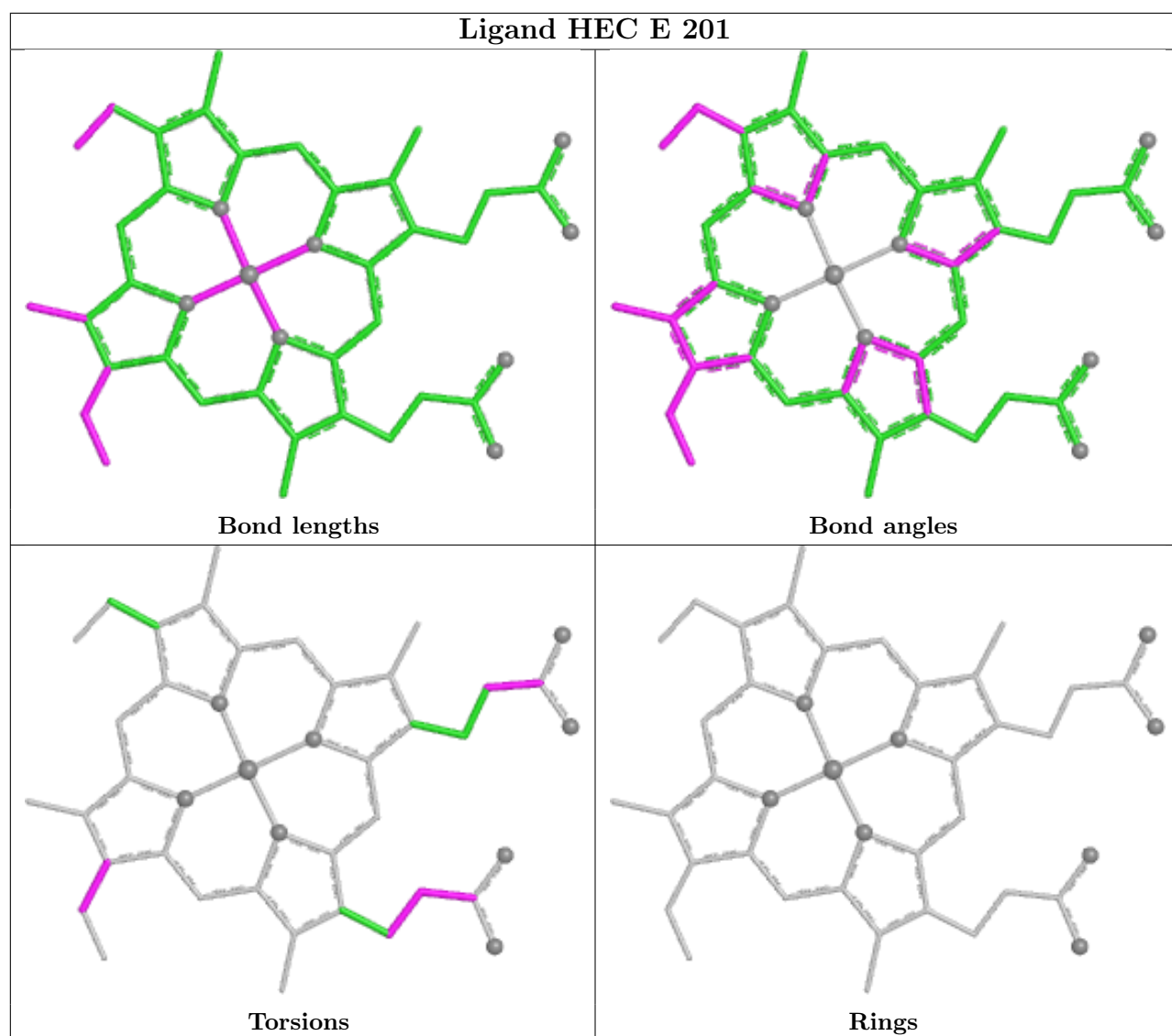
Torsions



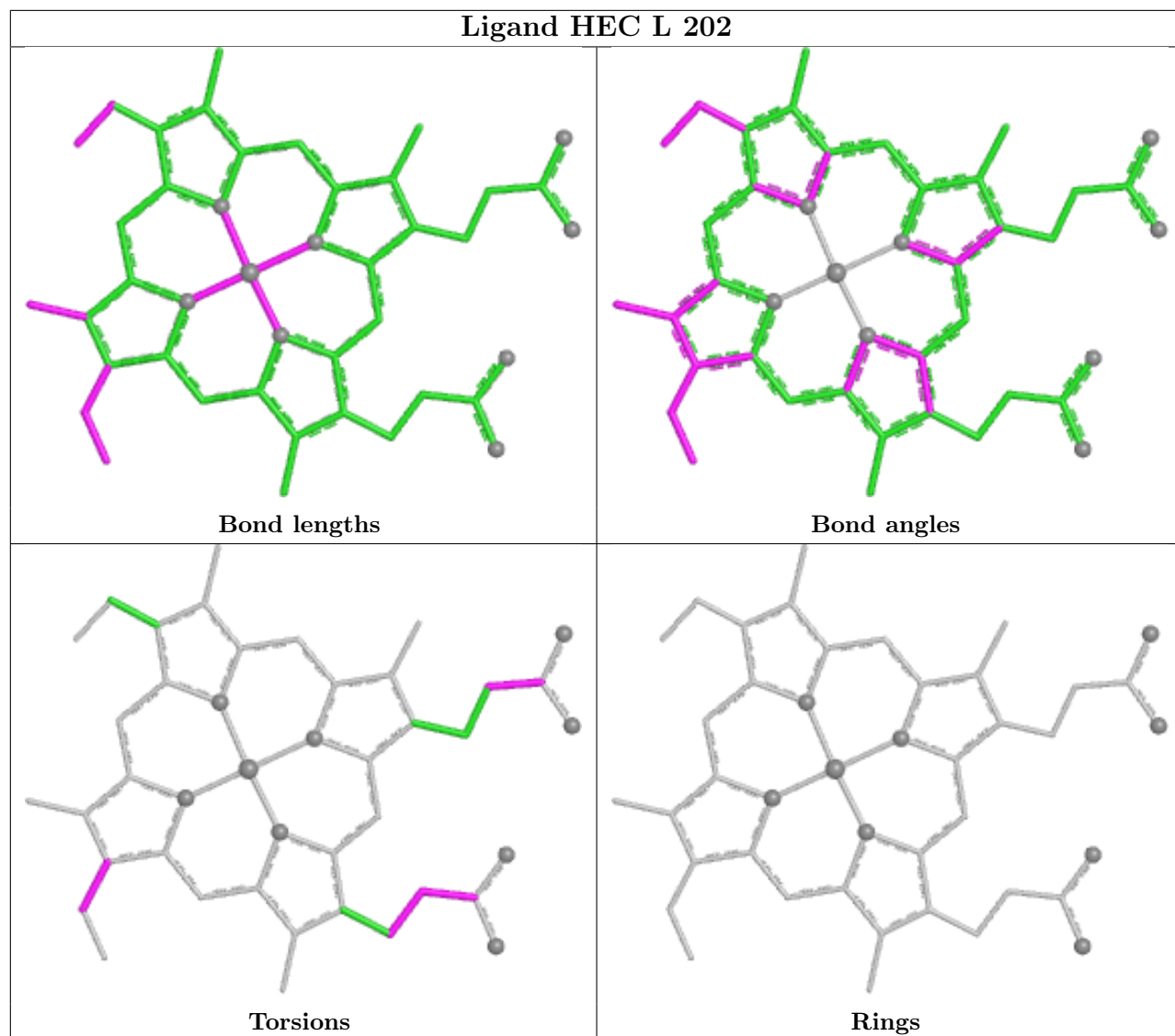
Rings



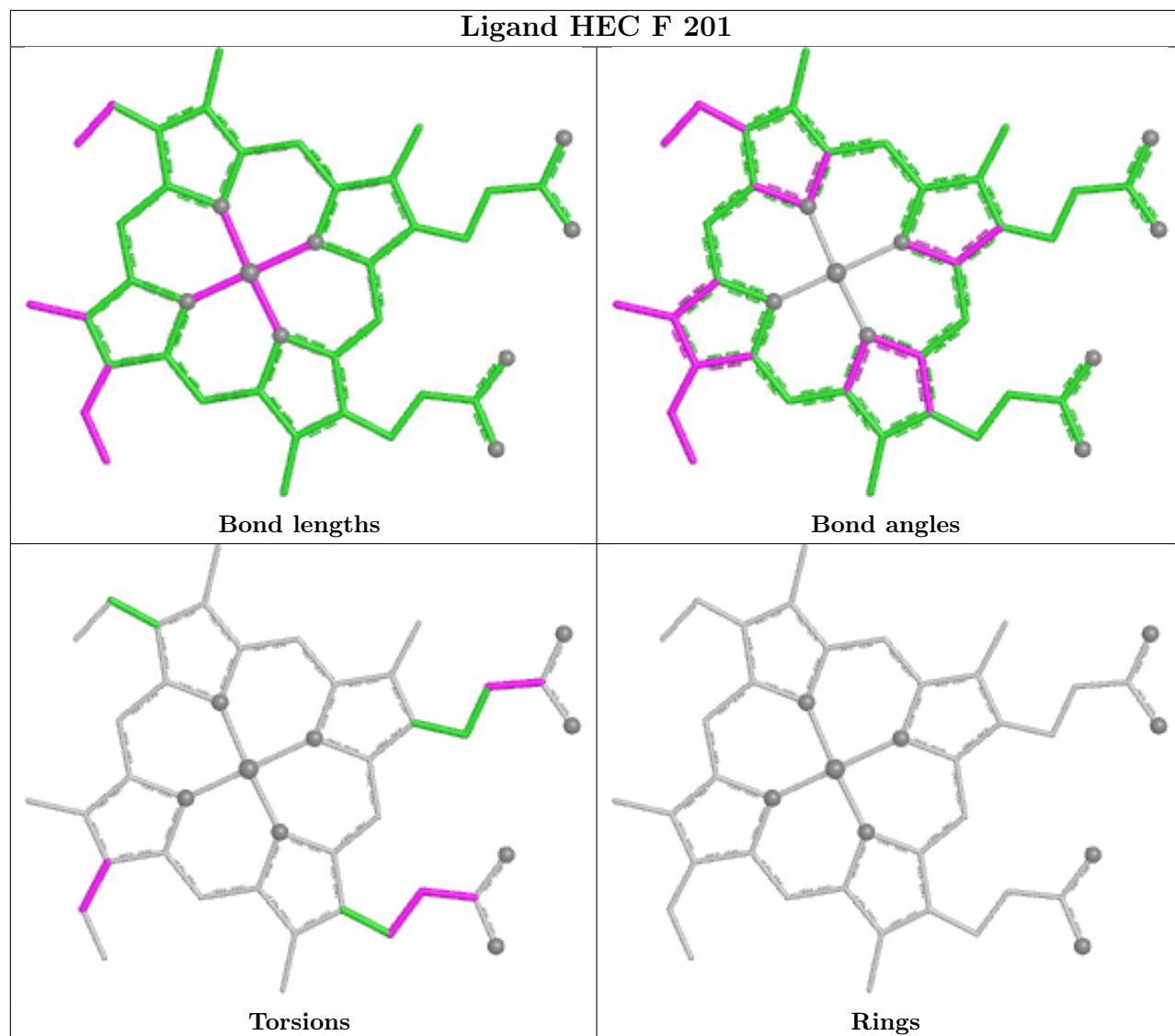




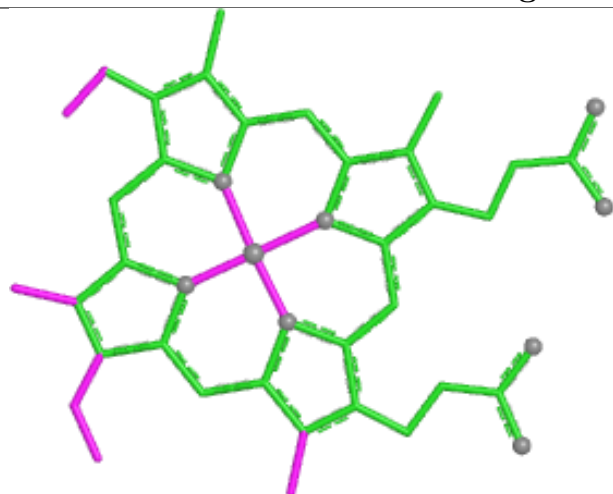
Ligand HEC L 202



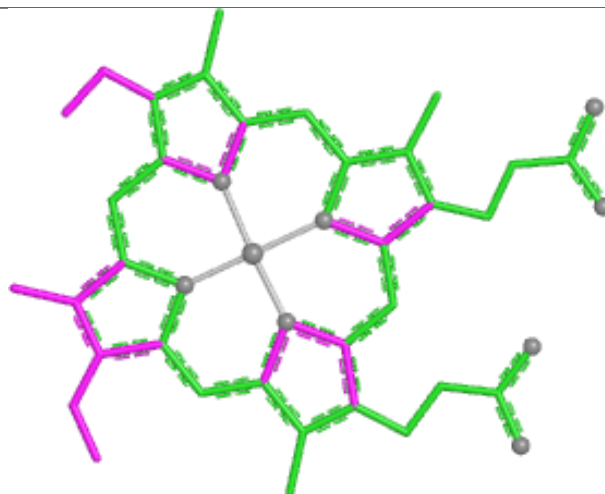
Ligand HEC F 201



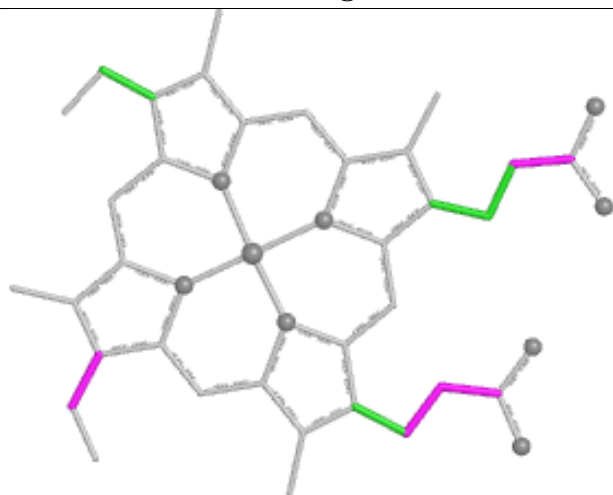
Ligand HEC I 201



Bond lengths



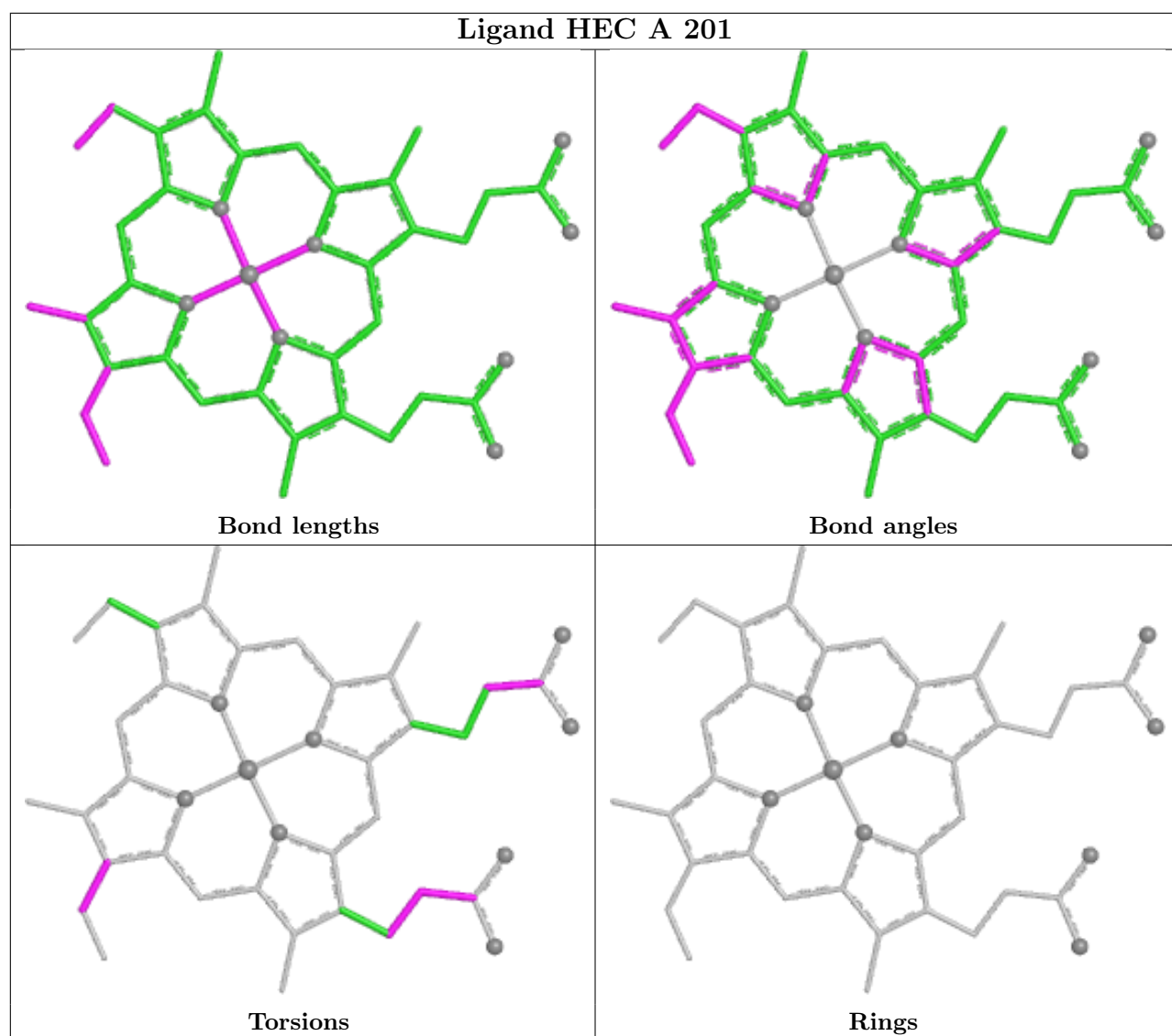
Bond angles

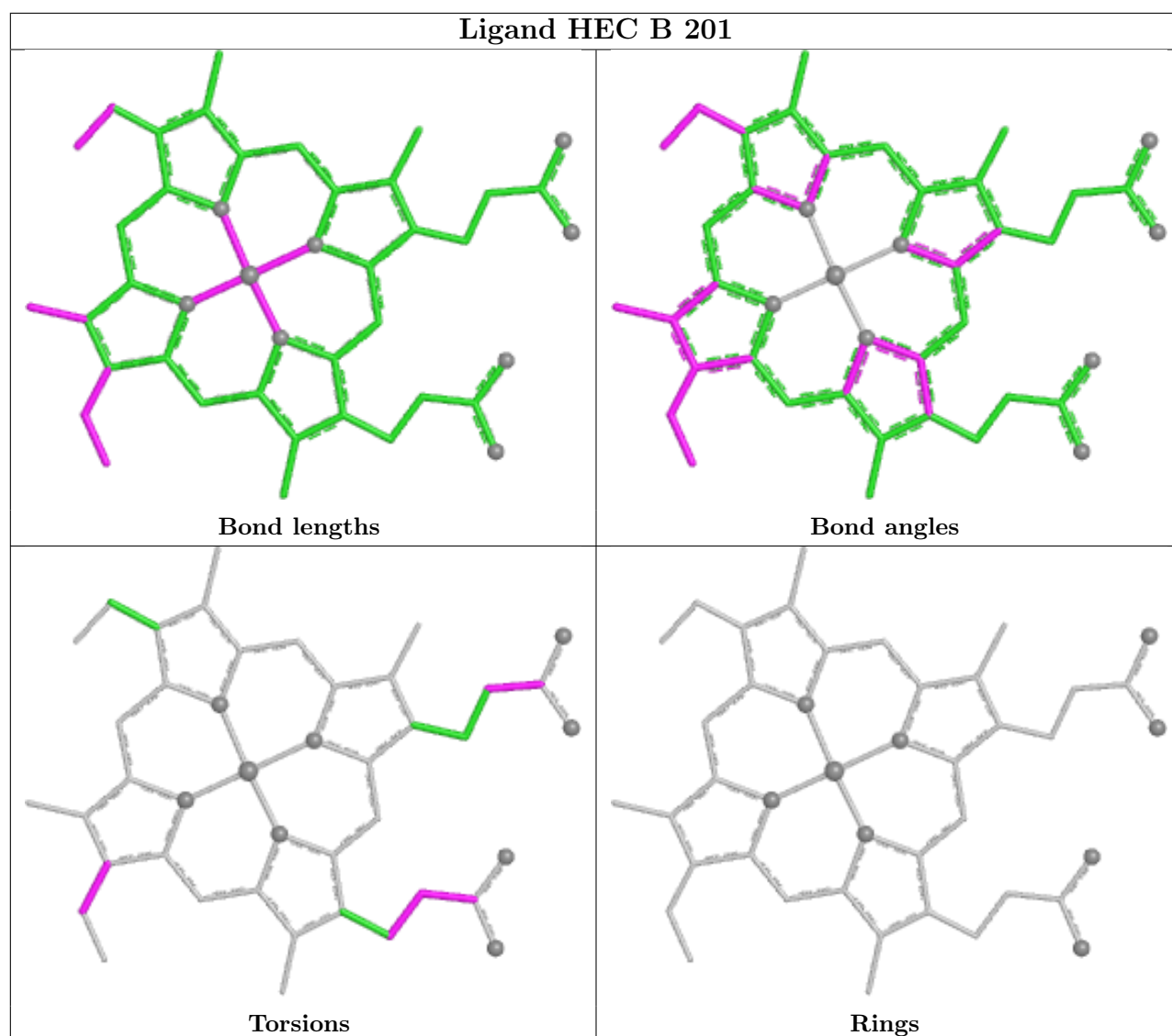


Torsions



Rings





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

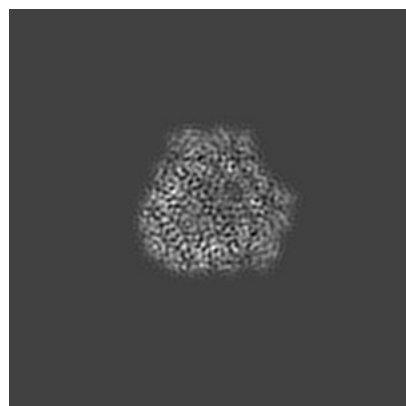
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20212. These allow visual inspection of the internal detail of the map and identification of artifacts.

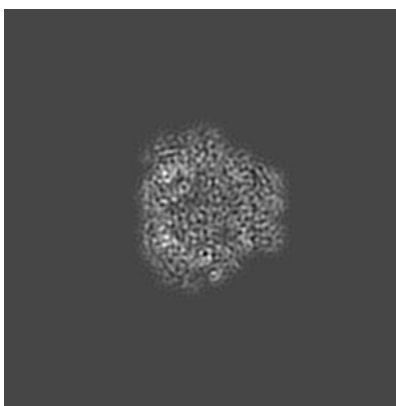
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

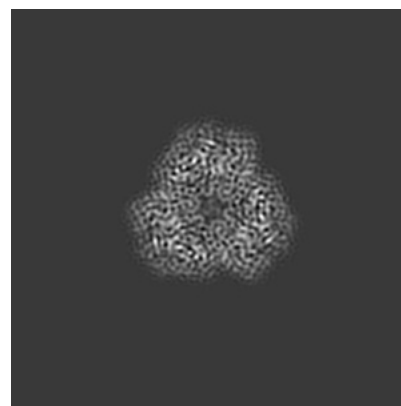
5.1.1 Primary map



X

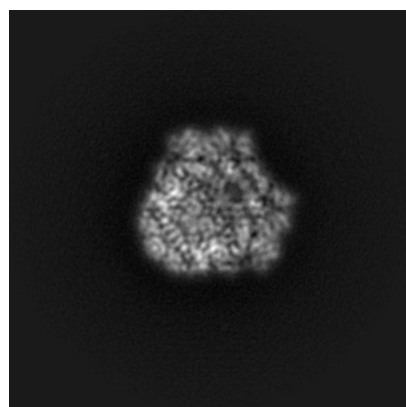


Y

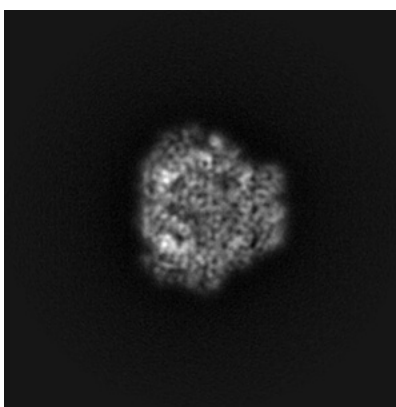


Z

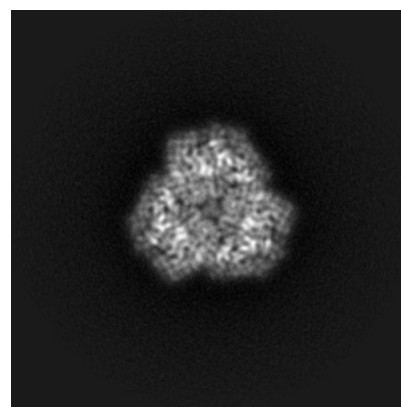
5.1.2 Raw map



X



Y

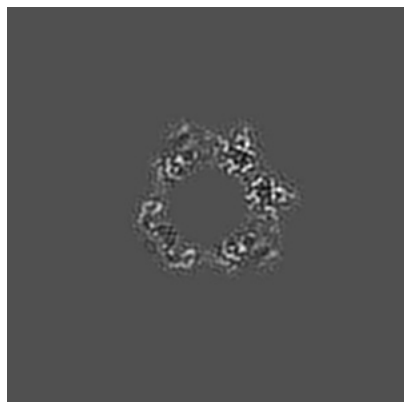


Z

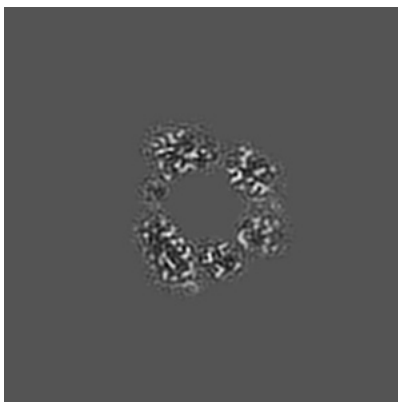
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

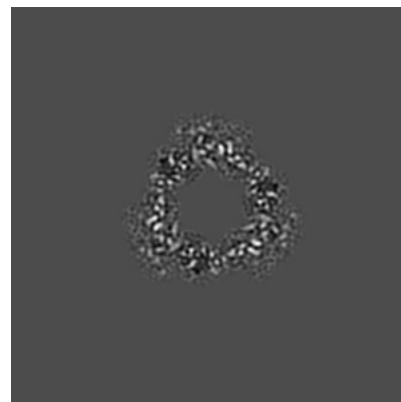
5.2.1 Primary map



X Index: 128

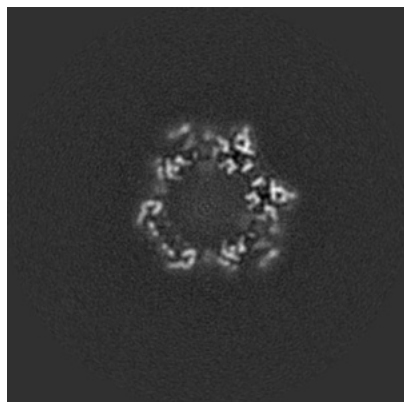


Y Index: 128

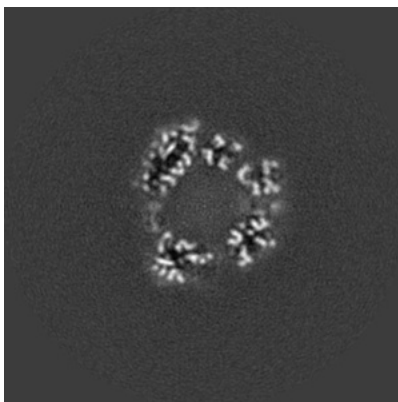


Z Index: 128

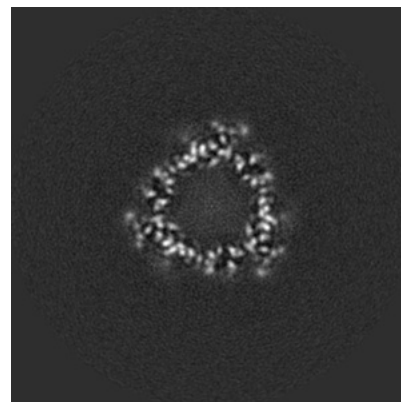
5.2.2 Raw map



X Index: 128



Y Index: 128

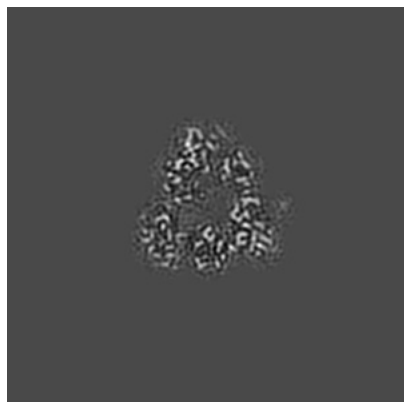


Z Index: 128

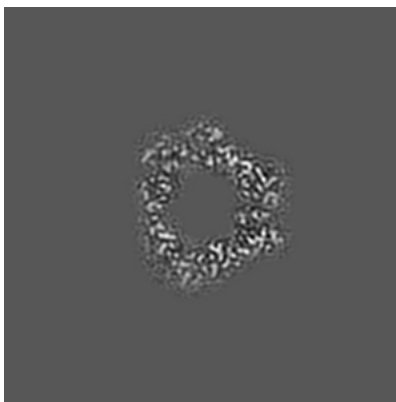
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

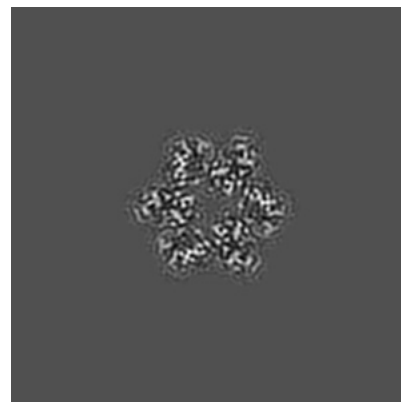
5.3.1 Primary map



X Index: 106

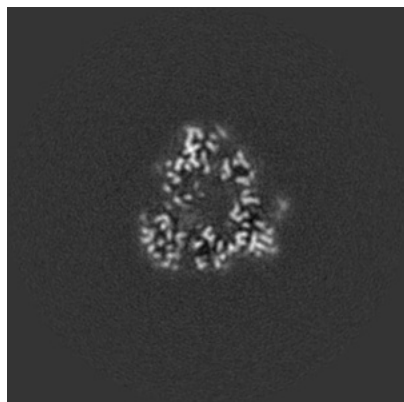


Y Index: 118

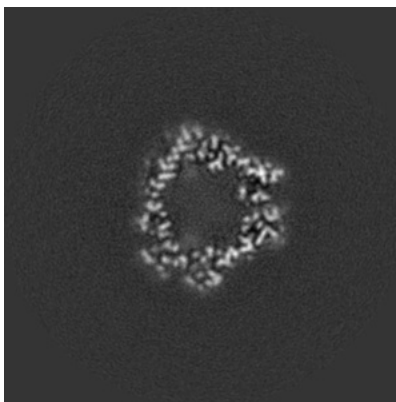


Z Index: 104

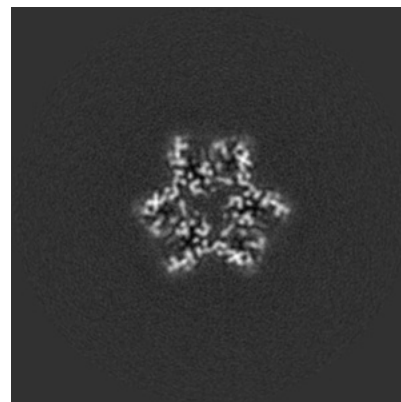
5.3.2 Raw map



X Index: 150



Y Index: 118

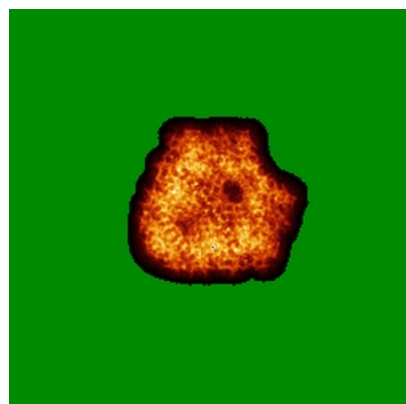


Z Index: 103

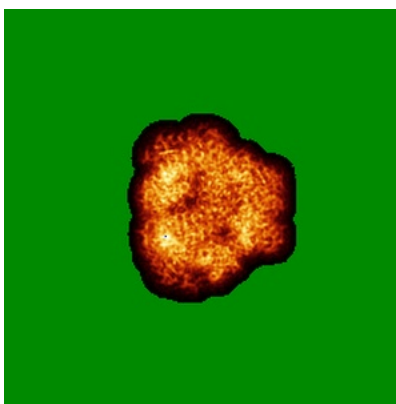
The images above show the largest variance slices of the map in three orthogonal directions.

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

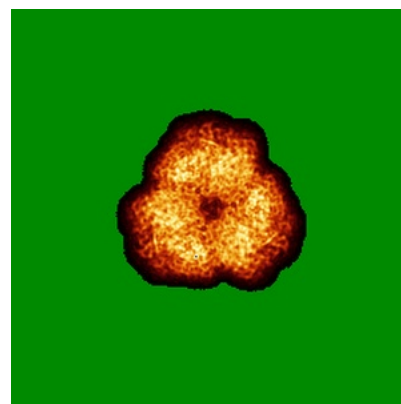
5.4.1 Primary map



X

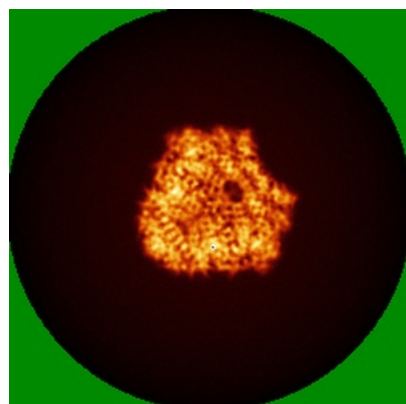


Y

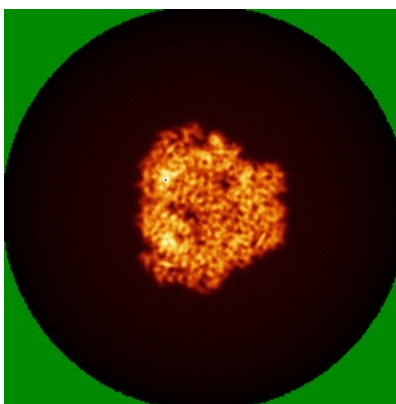


Z

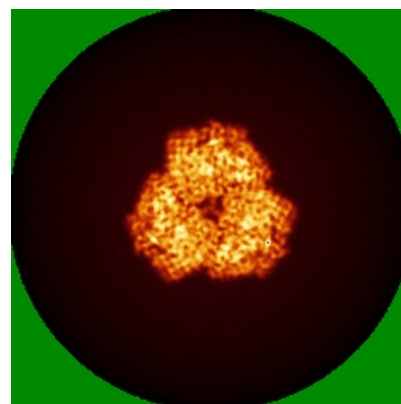
5.4.2 Raw map



X



Y

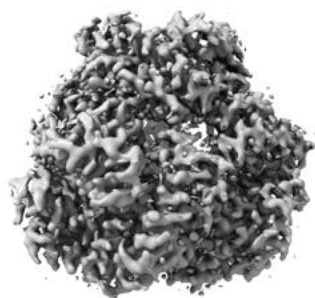


Z

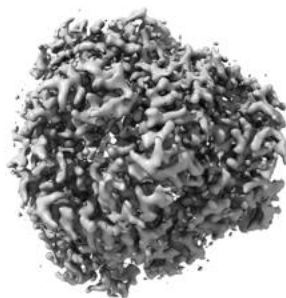
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

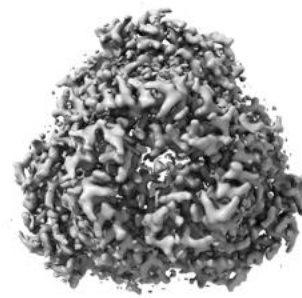
5.5.1 Primary map



X



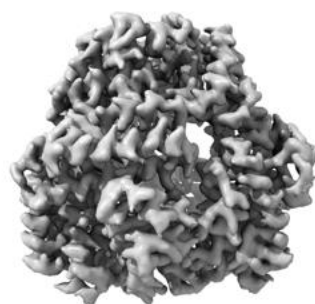
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

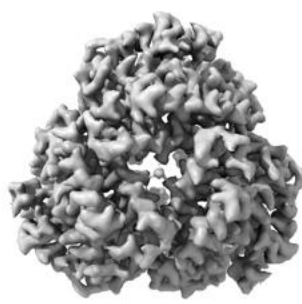
5.5.2 Raw map



X



Y



Z

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

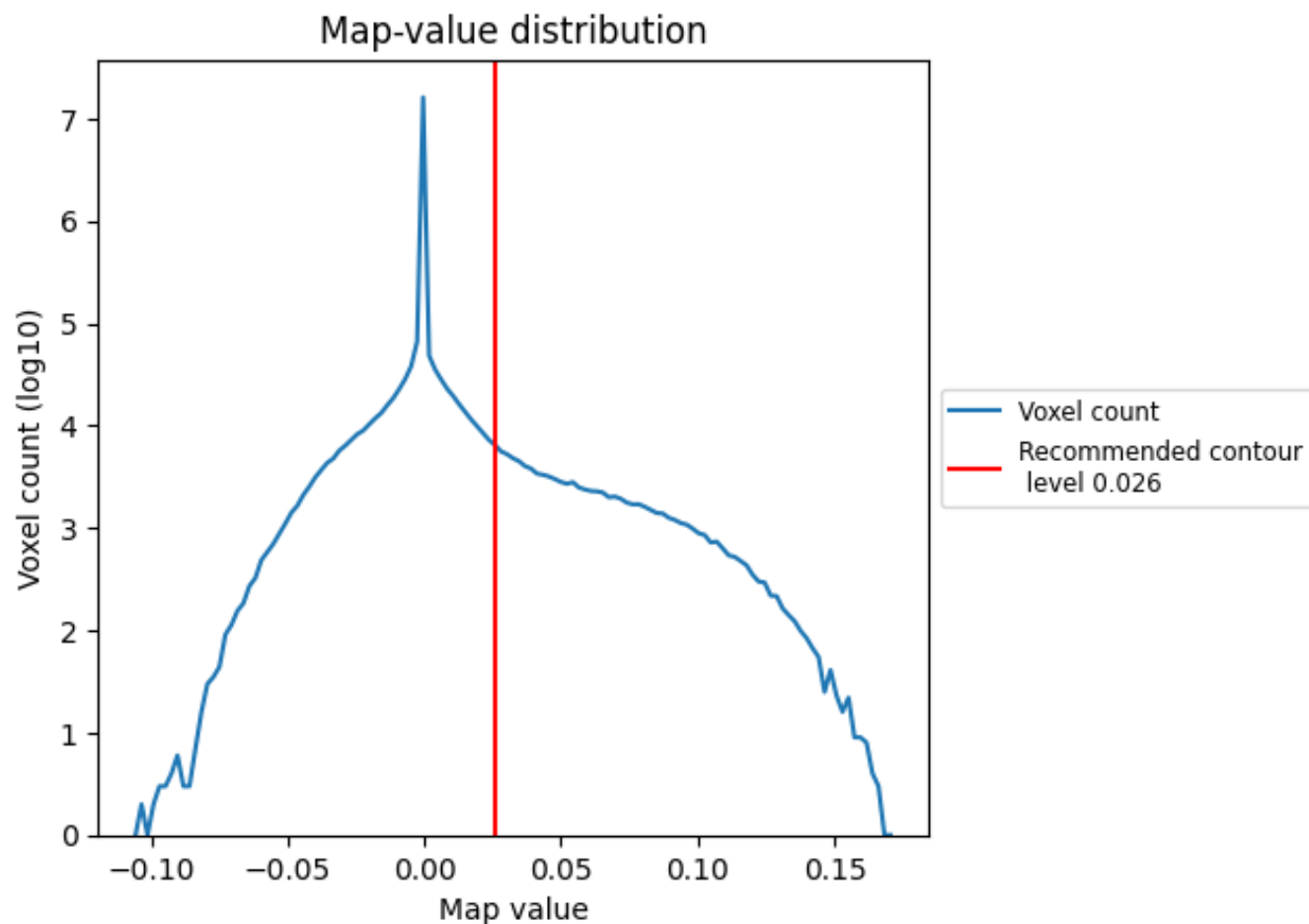
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

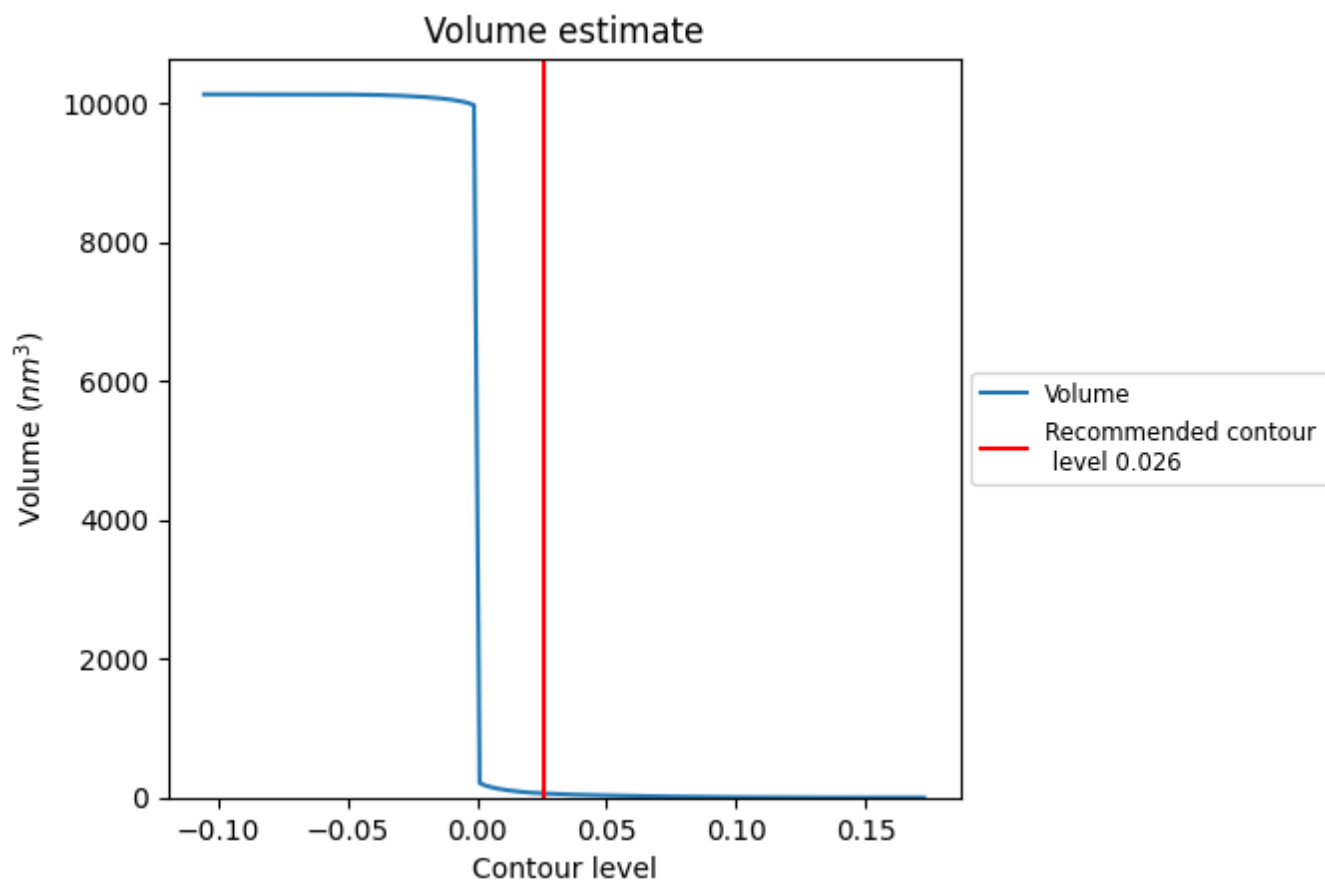
This section contains the results of statistical analysis of the map.

6.1 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.

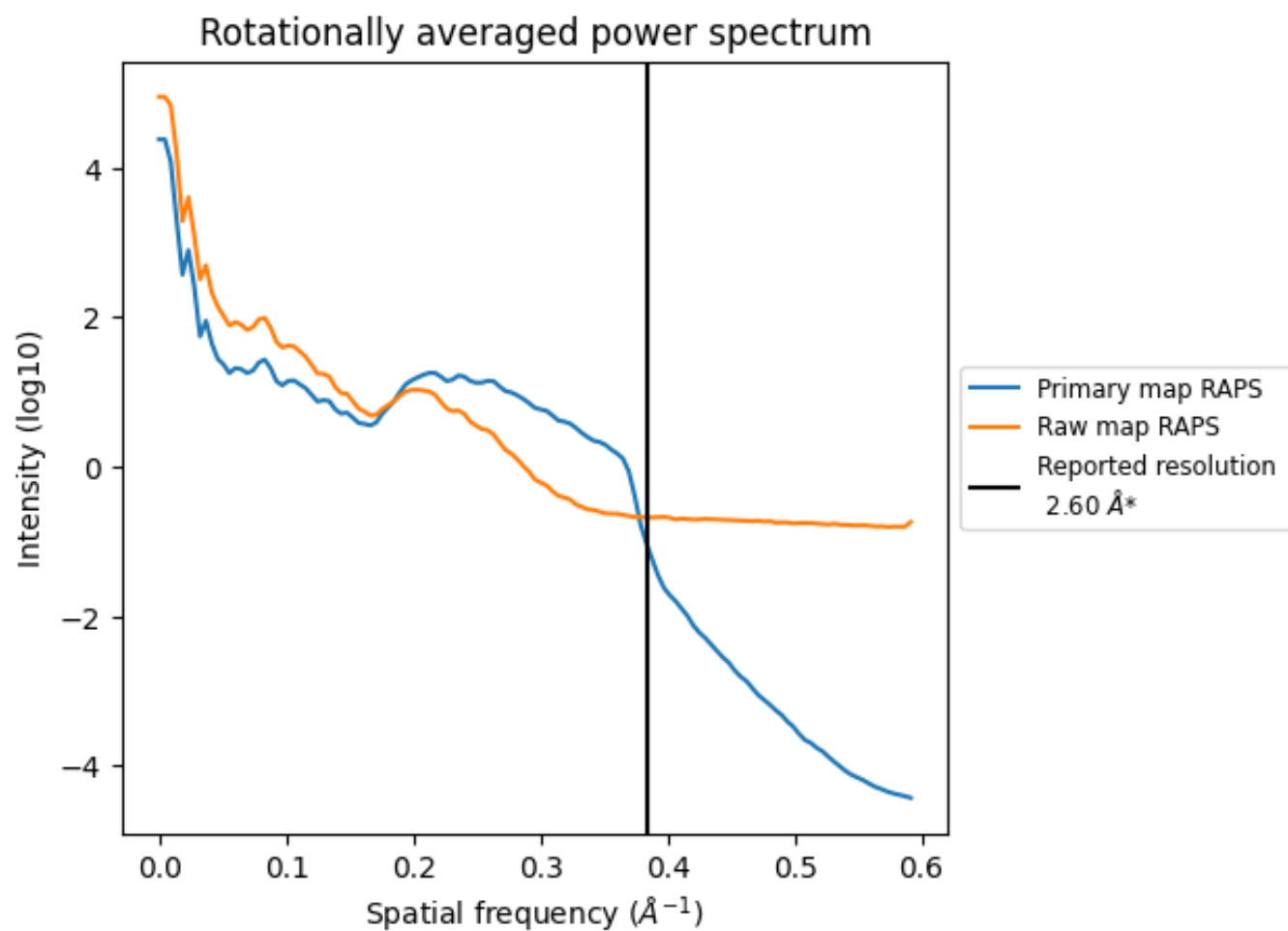
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 59 nm³; this corresponds to an approximate mass of 53 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.

6.3 Rotationally averaged power spectrum ⓘ

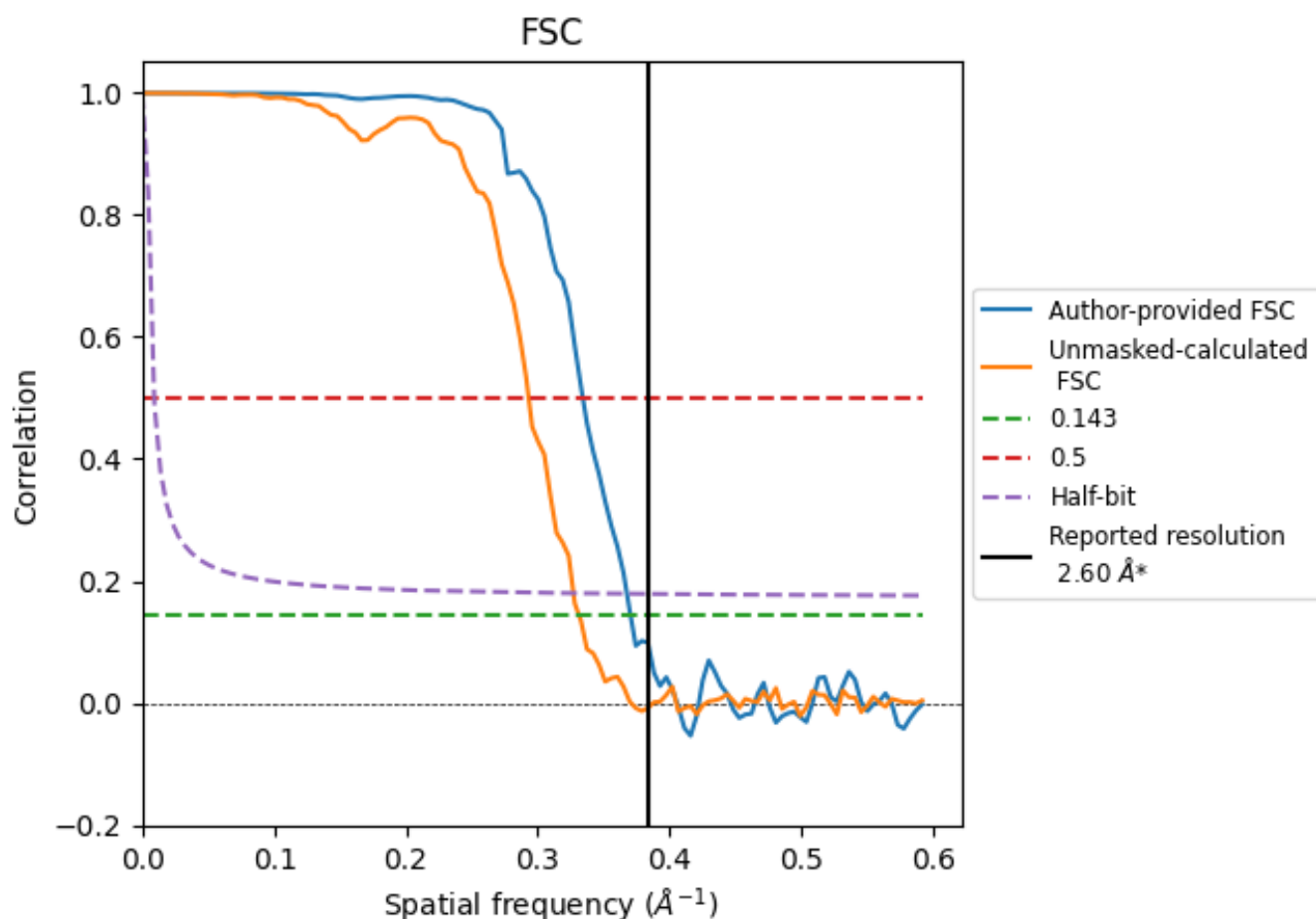


*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

7 Fourier-Shell correlation [i](#)

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

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

7.2 Resolution estimates [i](#)

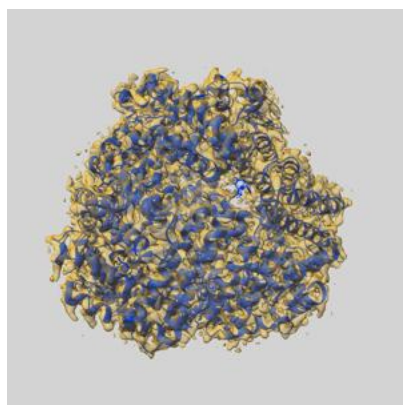
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.70	2.99	2.72
Unmasked-calculated*	3.02	3.41	3.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 2.6 by more than 10 %

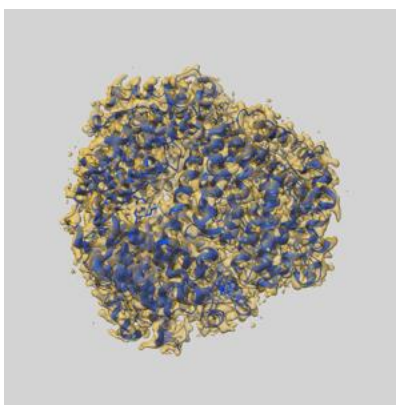
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20212 and PDB model 6OVH. Per-residue inclusion information can be found in section ?? on page ??.

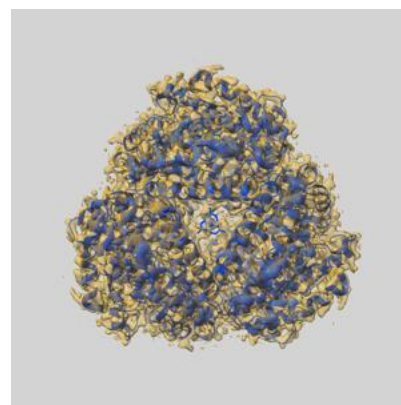
8.1 Map-model overlay [i](#)



X



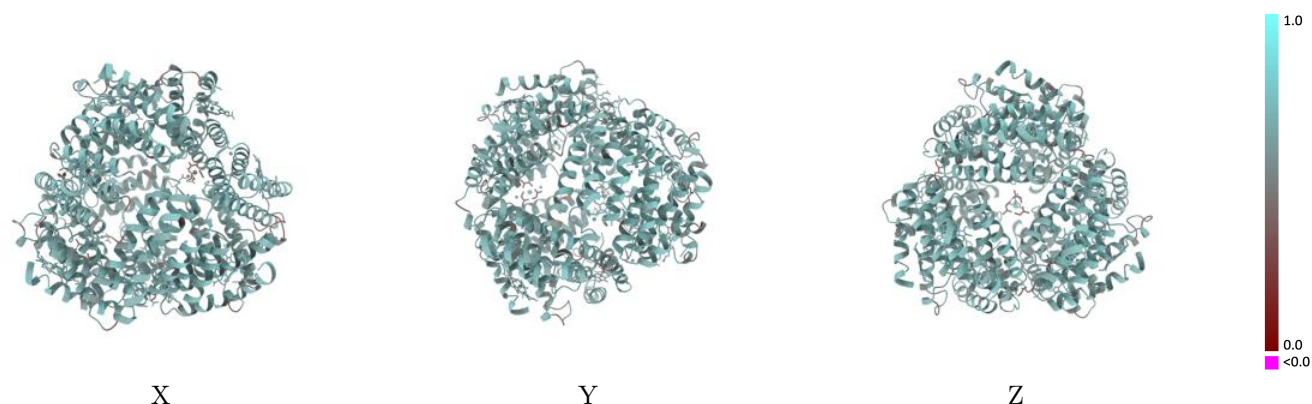
Y



Z

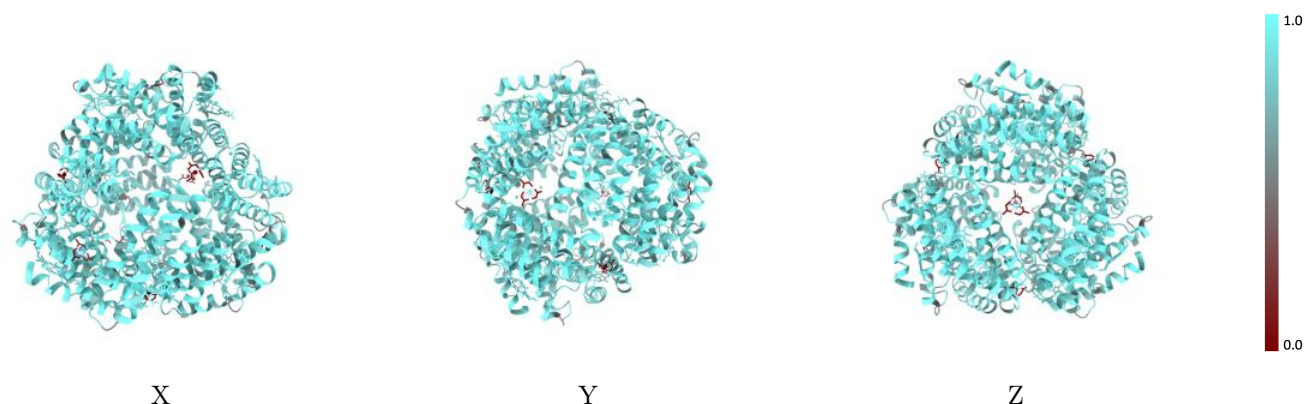
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



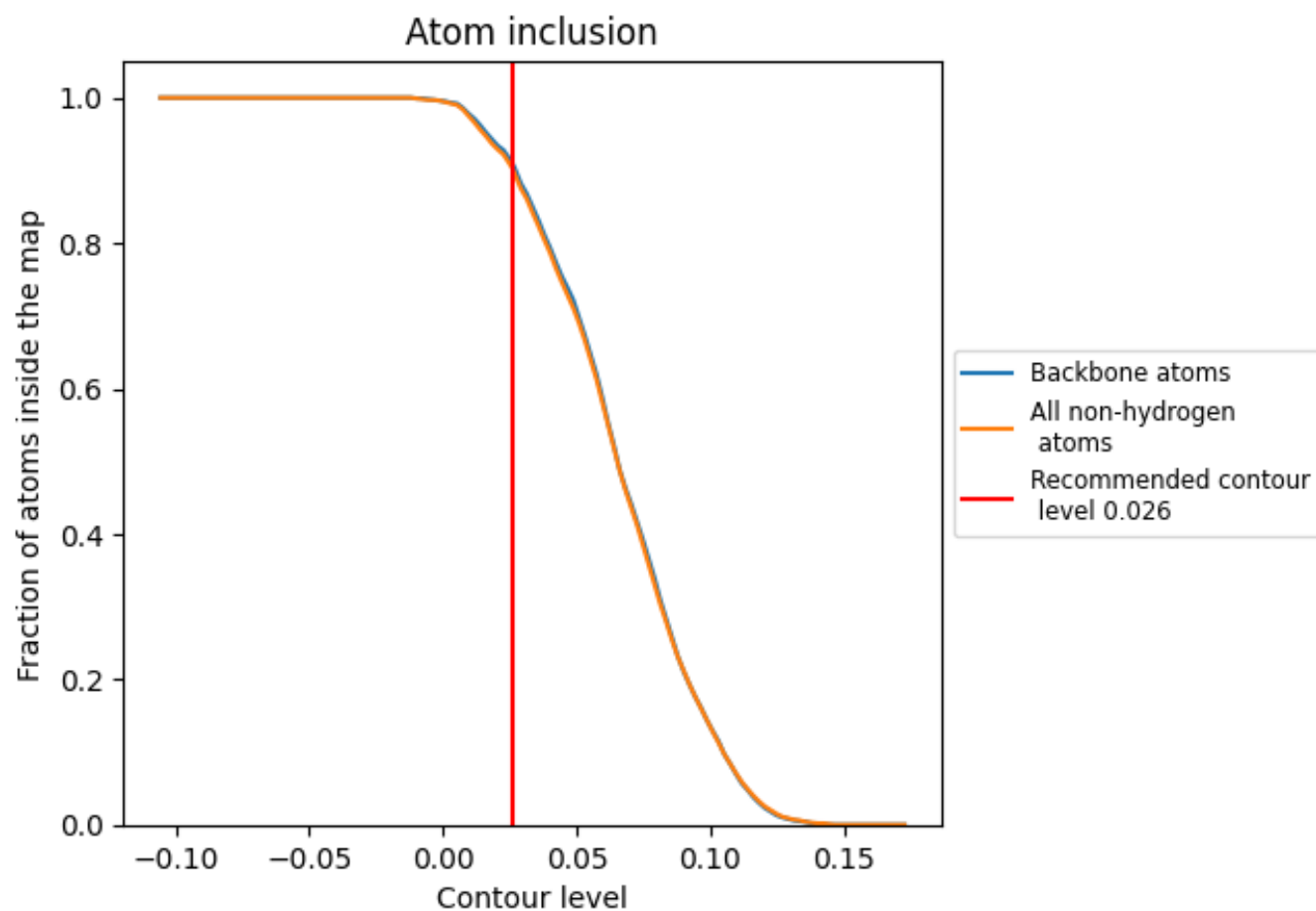
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.026).

8.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9030	0.6310
A	0.9020	0.6320
B	0.9000	0.6280
C	0.9080	0.6320
D	0.9050	0.6330
E	0.8950	0.6250
F	0.9030	0.6280
G	0.9050	0.6330
H	0.8990	0.6300
I	0.9030	0.6310
J	0.9050	0.6340
K	0.9030	0.6310
L	0.9040	0.6320

1.0

0.0

<0.0