



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 05:49 AM JST

PDB ID : 5GUW / pdb_00005guw
Title : Complex of Cytochrome cd1 Nitrite Reductase and Nitric Oxide Reductase in Denitrification of *Pseudomonas aeruginosa*
Authors : Terasaka, E.; Sugimoto, H.; Shiro, Y.; Tosha, T.
Deposited on : 2016-08-31
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

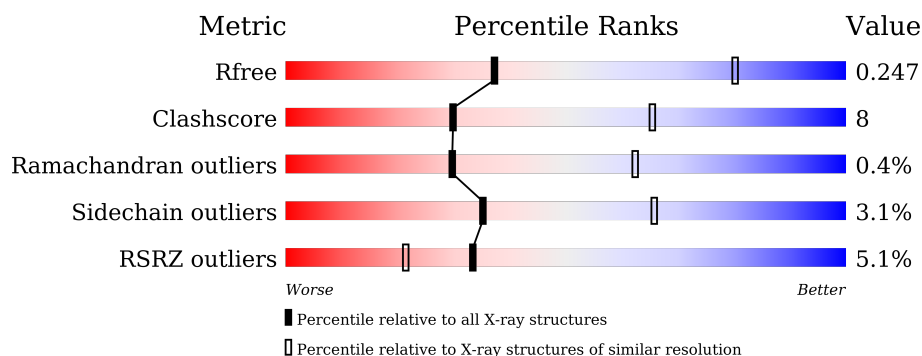
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	146	7% 83% 13% • •
1	C	146	3% 85% 12% •
2	B	465	9% 75% 20% • •
2	D	465	4% 76% 18% • •
3	M	568	3% 75% 19% • 5%
3	N	568	5% 75% 19% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HEC	A	201	X	-	-	-
4	HEC	C	201	X	-	-	-
4	HEC	M	601	X	-	-	-
4	HEC	N	601	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18387 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Nitric oxide reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			
1	C	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	LYS	ASN	conflict	UNP Q59646
C	100	LYS	ASN	conflict	UNP Q59646

- Molecule 2 is a protein called Nitric oxide reductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	449	Total	C	N	O	S	0	0	0
			3576	2416	563	572	25			
2	D	449	Total	C	N	O	S	0	0	0
			3576	2416	563	572	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	deletion	UNP Q59647
D	?	-	ARG	deletion	UNP Q59647

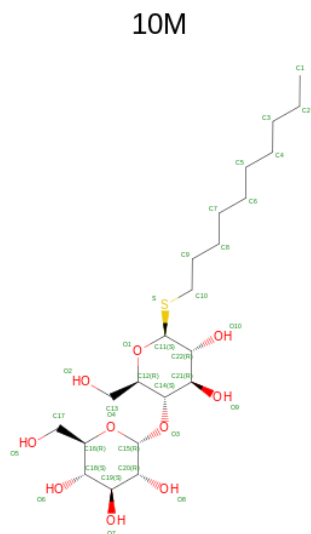
- Molecule 3 is a protein called Nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	538	Total	C	N	O	S	0	0	0
			4203	2665	733	793	12			
3	N	538	Total	C	N	O	S	0	0	0
			4203	2665	733	793	12			

- # HEC
-
- The diagram illustrates the chemical structure of HEC (Hexaethylcyclotriphosphazene). The central core consists of a square planar arrangement of four nitrogen (N) atoms, each with a positive charge (N⁺), coordinated by a central iron (Fe) atom. The Fe atom is also coordinated by four nitrogen (N) atoms, each with a negative charge (N⁻), forming a square planar geometry. The substituents are labeled as follows: C1A, C1B, C1C, C1D, C2A, C2B, C2C, C2D, C3A, C3B, C3C, C3D, C4A, C4B, C4C, C4D, C5A, C5B, C5C, C5D, C6A, C6B, C6C, C6D, C7A, C7B, C7C, C7D, C8A, C8B, C8C, C8D, C9A, C9B, C9C, C9D, C10A, C10B, C10C, C10D, C11A, C11B, C11C, C11D, C12A, C12B, C12C, C12D, C13A, C13B, C13C, C13D, C14A, C14B, C14C, C14D, C15A, C15B, C15C, C15D, C16A, C16B, C16C, C16D, C17A, C17B, C17C, C17D, C18A, C18B, C18C, C18D, C19A, C19B, C19C, C19D, C20A, C20B, C20C, C20D, C21A, C21B, C21C, C21D, C22A, C22B, C22C, C22D, C23A, C23B, C23C, C23D, C24A, C24B, C24C, C24D, C25A, C25B, C25C, C25D, C26A, C26B, C26C, C26D, C27A, C27B, C27C, C27D, C28A, C28B, C28C, C28D, C29A, C29B, C29C, C29D, C30A, C30B, C30C, C30D, C31A, C31B, C31C, C31D, C32A, C32B, C32C, C32D, C33A, C33B, C33C, C33D, C34A, C34B, C34C, C34D, C35A, C35B, C35C, C35D, C36A, C36B, C36C, C36D, C37A, C37B, C37C, C37D, C38A, C38B, C38C, C38D, C39A, C39B, C39C, C39D, C40A, C40B, C40C, C40D, C41A, C41B, C41C, C41D, C42A, C42B, C42C, C42D, C43A, C43B, C43C, C43D, C44A, C44B, C44C, C44D, C45A, C45B, C45C, C45D, C46A, C46B, C46C, C46D, C47A, C47B, C47C, C47D, C48A, C48B, C48C, C48D, C49A, C49B, C49C, C49D, C50A, C50B, C50C, C50D, C51A, C51B, C51C, C51D, C52A, C52B, C52C, C52D, C53A, C53B, C53C, C53D, C54A, C54B, C54C, C54D, C55A, C55B, C55C, C55D, C56A, C56B, C56C, C56D, C57A, C57B, C57C, C57D, C58A, C58B, C58C, C58D, C59A, C59B, C59C, C59D, C60A, C60B, C60C, C60D, C61A, C61B, C61C, C61D, C62A, C62B, C62C, C62D, C63A, C63B, C63C, C63D, C64A, C64B, C64C, C64D, C65A, C65B, C65C, C65D, C66A, C66B, C66C, C66D, C67A, C67B, C67C, C67D, C68A, C68B, C68C, C68D, C69A, C69B, C69C, C69D, C70A, C70B, C70C, C70D, C71A, C71B, C71C, C71D, C72A, C72B, C72C, C72D, C73A, C73B, C73C, C73D, C74A, C74B, C74C, C74D, C75A, C75B, C75C, C75D, C76A, C76B, C76C, C76D, C77A, C77B, C77C, C77D, C78A, C78B, C78C, C78D, C79A, C79B, C79C, C79D, C80A, C80B, C80C, C80D, C81A, C81B, C81C, C81D, C82A, C82B, C82C, C82D, C83A, C83B, C83C, C83D, C84A, C84B, C84C, C84D, C85A, C85B, C85C, C85D, C86A, C86B, C86C, C86D, C87A, C87B, C87C, C87D, C88A, C88B, C88C, C88D, C89A, C89B, C89C, C89D, C90A, C90B, C90C, C90D, C91A, C91B, C91C, C91D, C92A, C92B, C92C, C92D, C93A, C93B, C93C, C93D, C94A, C94B, C94C, C94D, C95A, C95B, C95C, C95D, C96A, C96B, C96C, C96D, C97A, C97B, C97C, C97D, C98A, C98B, C98C, C98D, C99A, C99B, C99C, C99D, C100A, C100B, C100C, C100D, C101A, C101B, C101C, C101D, C102A, C102B, C102C, C102D, C103A, C103B, C103C, C103D, C104A, C104B, C104C, C104D, C105A, C105B, C105C, C105D, C106A, C106B, C106C, C106D, C107A, C107B, C107C, C107D, C108A, C108B, C108C, C108D, C109A, C109B, C109C, C109D, C110A, C110B, C110C, C110D, C111A, C111B, C111C, C111D, C112A, C112B, C112C, C112D, C113A, C113B, C113C, C113D, C114A, C114B, C114C, C114D, C115A, C115B, C115C, C115D, C116A, C116B, C116C, C116D, C117A, C117B, C117C, C117D, C118A, C118B, C118C, C118D, C119A, C119B, C119C, C119D, C120A, C120B, C120C, C120D, C121A, C121B, C121C, C121D, C122A, C122B, C122C, C122D, C123A, C123B, C123C, C123D, C124A, C124B, C124C, C124D, C125A, C125B, C125C, C125D, C126A, C126B, C126C, C126D, C127A, C127B, C127C, C127D, C128A, C128B, C128C, C128D, C129A, C129B, C129C, C129D, C130A, C130B, C130C, C130D, C131A, C131B, C131C, C131D, C132A, C132B, C132C, C132D, C133A, C133B, C133C, C133D, C134A, C134B, C134C, C134D, C135A, C135B, C135C, C135D, C136A, C136B, C136C, C136D, C137A, C137B, C137C, C137D, C138A, C138B, C138C, C138D, C139A, C139B, C139C, C139D, C140A, C140B, C140C, C140D, C141A, C141B, C141C, C141D, C142A, C142B, C142C, C142D, C143A, C143B, C143C, C143D, C144A, C144B, C144C, C144D, C145A, C145B, C145C, C145D, C146A, C146B, C146C, C146D, C147A, C147B, C147C, C147D, C148A, C148B, C148C, C148D, C149A, C149B, C149C, C149D, C150A, C150B, C150C, C150D, C151A, C151B, C151C, C151D, C152A, C152B, C152C, C152D, C153A, C153B, C153C, C153D, C154A, C154B, C154C, C154D, C155A, C155B, C155C, C155D, C156A, C156B, C156C, C156D, C157A, C157B, C157C, C157D, C158A, C158B, C158C, C158D, C159A, C159B, C159C, C159D, C160A, C160B, C160C, C160D, C161A, C161B, C161C, C161D, C162A, C162B, C162C, C162D, C163A, C163B, C163C, C163D, C164A, C164B, C164C, C164D, C165A, C165B, C165C, C165D, C166A, C166B, C166C, C166D, C167A, C167B, C167C, C167D, C168A, C168B, C168C, C168D, C169A, C169B, C169C, C169D, C170A, C170B, C170C, C170D, C171A, C171B, C171C, C171D, C172A, C172B, C172C, C172D, C173A, C173B, C173C, C173D, C174A, C174B, C174C, C174D, C175A, C175B, C175C, C175D, C176A, C176B, C176C, C176D, C177A, C177B, C177C, C177D, C178A, C178B, C178C, C178D, C179A, C179B, C179C, C179D, C180A, C180B, C180C, C180D, C181A, C181B, C181C, C181D, C182A, C182B, C1

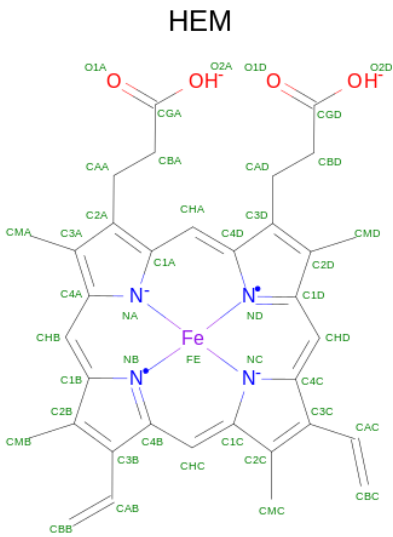
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

- Molecule 6 is decyl 4-O-alpha-D-glucopyranosyl-1-thio-beta-D-glucopyranoside (CCD ID: 10M) (formula: C₂₂H₄₂O₁₀S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 33	C 22	O 10	S 1	0	0
6	C	1	Total 33	C 22	O 10	S 1	0	0
6	D	1	Total 33	C 22	O 10	S 1	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

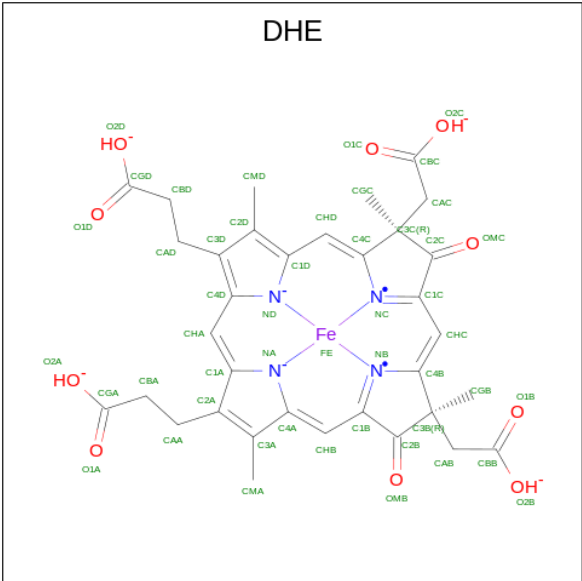
- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Fe		
			1	1	0	0
8	D	1	Total	Fe		
			1	1	0	0

- Molecule 9 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	O		
			1	1	0	0
9	D	1	Total	O		
			1	1	0	0

- Molecule 10 is HEME D (CCD ID: DHE) (formula: C₃₄H₃₂FeN₄O₁₀).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	M	1	Total 49	C 34	Fe 1	N 4	O 10	0	0
10	N	1	Total 49	C 34	Fe 1	N 4	O 10	0	0

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total 1	Cl 1	0	0
11	N	1	Total 1	Cl 1	0	0

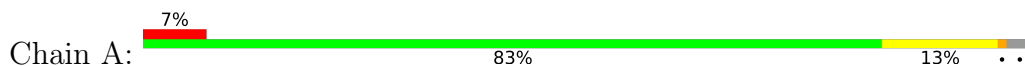
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	3	Total 3	O 3	0	0
12	B	11	Total 11	O 11	0	0
12	C	6	Total 6	O 6	0	0
12	D	6	Total 6	O 6	0	0
12	M	5	Total 5	O 5	0	0
12	N	3	Total 3	O 3	0	0

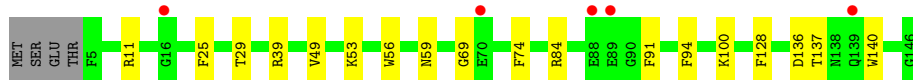
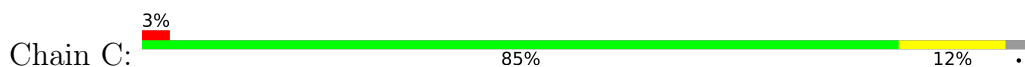
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

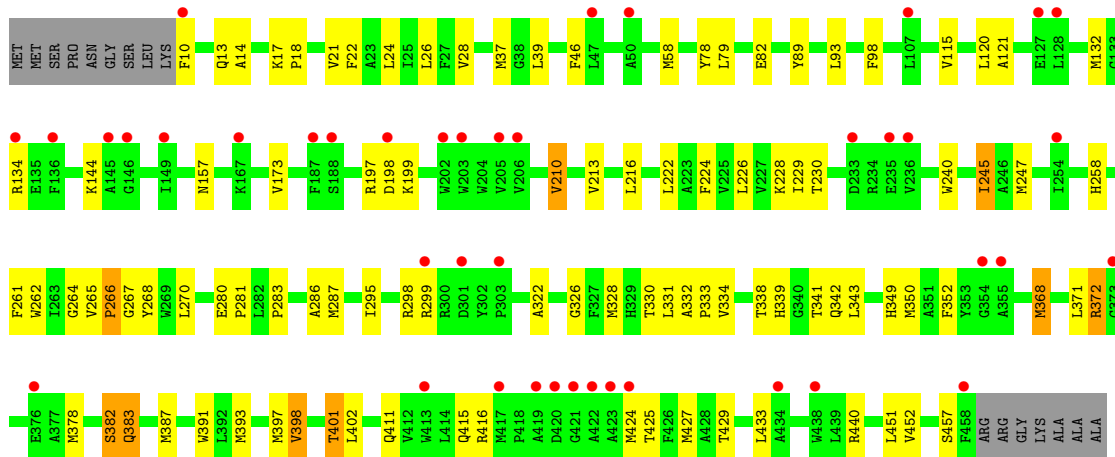
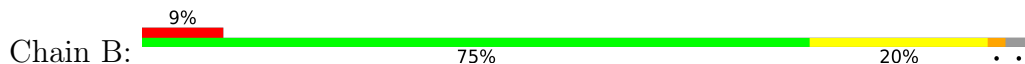
• Molecule 1: Nitric oxide reductase subunit C



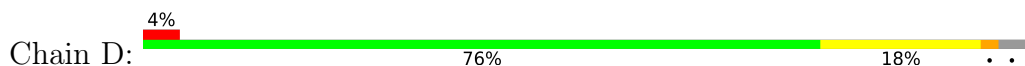
• Molecule 1: Nitric oxide reductase subunit C

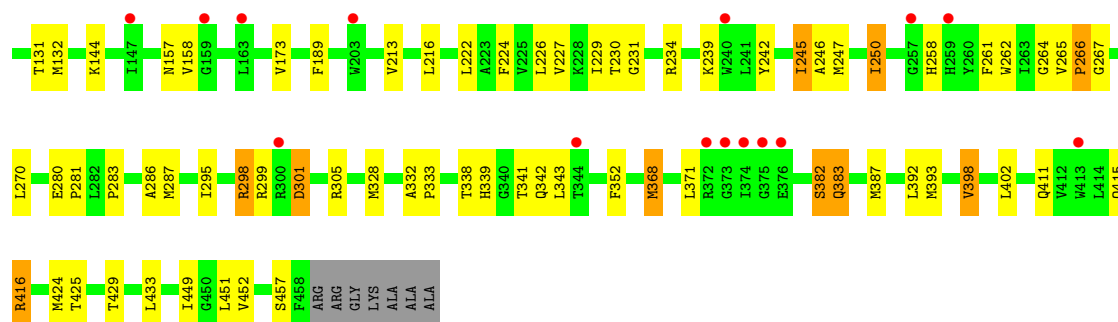


• Molecule 2: Nitric oxide reductase subunit B

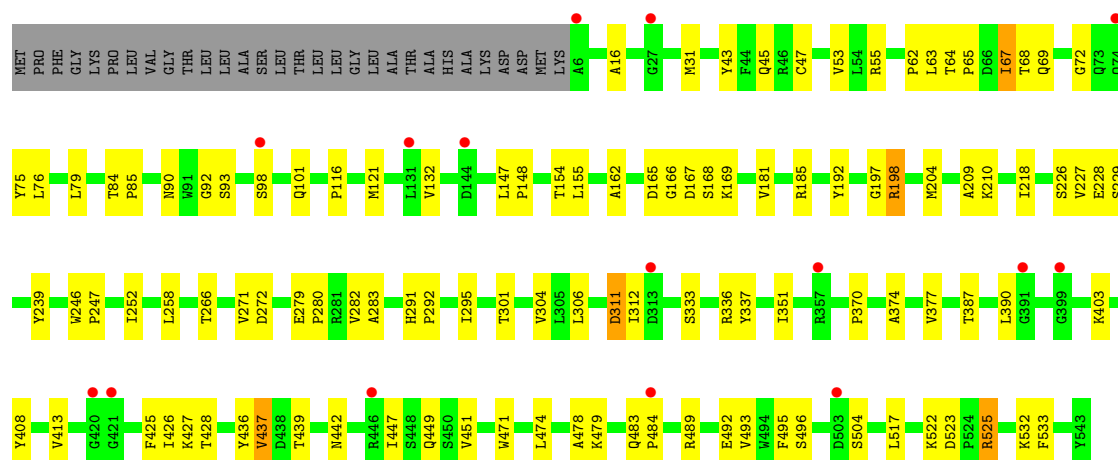
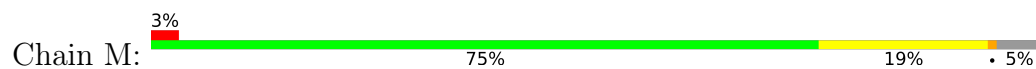


• Molecule 2: Nitric oxide reductase subunit B

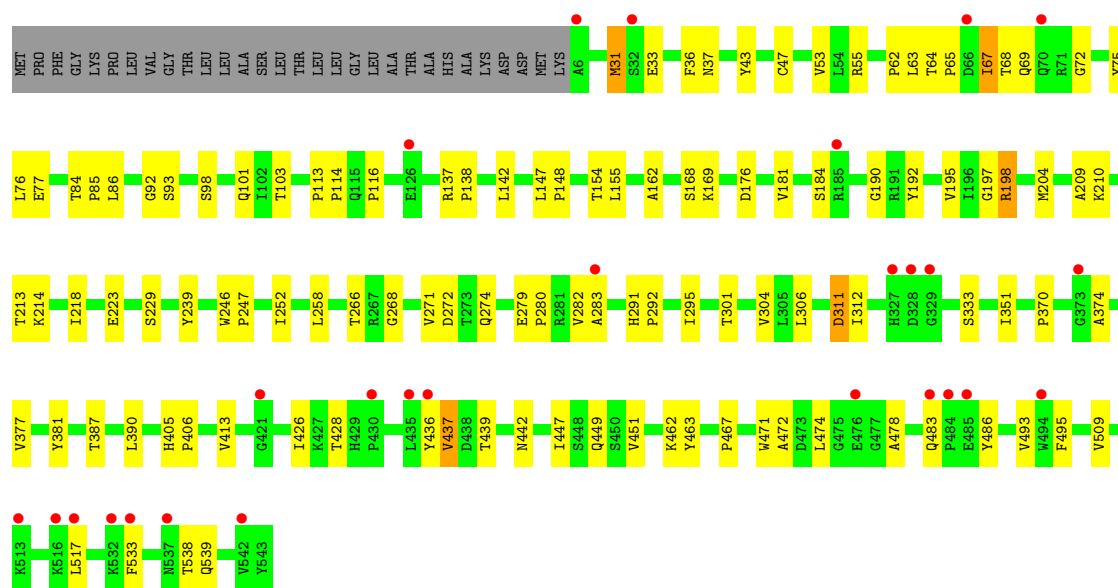
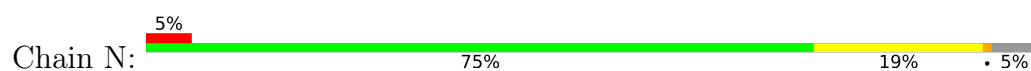




• Molecule 3: Nitrite reductase



• Molecule 3: Nitrite reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.87Å 128.61Å 127.81Å 90.00° 106.83° 90.00°	Depositor
Resolution (Å)	49.48 – 3.20 49.48 – 3.20	Depositor EDS
% Data completeness (in resolution range)	87.7 (49.48-3.20) 87.7 (49.48-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.210 , 0.254 0.208 , 0.247	Depositor DCC
R_{free} test set	2551 reflections (3.67%)	wwPDB-VP
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18387	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6858e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 10M, CA, O, DHE, HEM, HEC, CL, FE

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	0.56	0/1153	0.85	0/1559
1	C	0.61	0/1153	0.88	0/1559
2	B	0.56	0/3693	0.90	1/5039 (0.0%)
2	D	0.60	0/3693	0.91	1/5039 (0.0%)
3	M	0.60	0/4308	0.84	2/5854 (0.0%)
3	N	0.56	0/4308	0.84	3/5854 (0.1%)
All	All	0.58	0/18308	0.87	7/24904 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	245	ILE	CB-CA-C	-5.82	104.52	111.97
3	N	64	THR	CA-C-N	5.63	126.87	119.84
3	N	64	THR	C-N-CA	5.63	126.87	119.84
2	B	245	ILE	CB-CA-C	-5.39	105.07	111.97
3	M	64	THR	CA-C-N	5.25	126.40	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1123	0	1091	20	0
1	C	1123	0	1091	14	0
2	B	3576	0	3619	80	1
2	D	3576	0	3619	70	1
3	M	4203	0	4158	68	0
3	N	4203	0	4158	70	0
4	A	43	0	31	4	0
4	C	43	0	32	2	0
4	M	43	0	31	1	0
4	N	43	0	32	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	33	0	42	0	0
6	C	33	0	42	0	0
6	D	33	0	42	0	0
7	B	86	0	60	8	0
7	D	86	0	60	6	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	M	49	0	28	7	0
10	N	49	0	28	3	0
11	M	1	0	0	0	0
11	N	1	0	0	0	0
12	A	3	0	0	0	0
12	B	11	0	0	1	0
12	C	6	0	0	0	0
12	D	6	0	0	0	0
12	M	5	0	0	0	0
12	N	3	0	0	0	0
All	All	18387	0	18164	310	1

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 8.

The worst 5 of 310 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:M:16:ALA:HB3	3:N:223:GLU:HG3	1.56	0.87
3:M:169:LYS:NZ	3:M:492:GLU:OE2	2.10	0.82
3:M:165:ASP:HB3	3:M:168:SER:HB3	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:NH1	4:A:201:HEC:O2A	2.16	0.78
3:N:471:TRP:CE3	3:N:517:LEU:HB3	2.19	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:ARG:O	2:D:298:ARG:NH2[1_654]	2.12	0.08

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 X-ray entries followed by that with respect to entries of similar resolution.

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	140/146 (96%)	131 (94%)	9 (6%)	0	100	100
1	C	140/146 (96%)	131 (94%)	9 (6%)	0	100	100
2	B	447/465 (96%)	409 (92%)	36 (8%)	2 (0%)	30	62
2	D	447/465 (96%)	415 (93%)	30 (7%)	2 (0%)	30	62
3	M	536/568 (94%)	493 (92%)	40 (8%)	3 (1%)	21	56
3	N	536/568 (94%)	493 (92%)	41 (8%)	2 (0%)	30	62
All	All	2246/2358 (95%)	2072 (92%)	165 (7%)	9 (0%)	30	62

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	283	ALA
3	N	283	ALA
2	B	328	MET
2	D	328	MET
2	B	266	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	116/120 (97%)	114 (98%)	2 (2%)	53	75
1	C	116/120 (97%)	115 (99%)	1 (1%)	70	81
2	B	360/371 (97%)	346 (96%)	14 (4%)	28	62
2	D	360/371 (97%)	347 (96%)	13 (4%)	31	63
3	M	453/476 (95%)	439 (97%)	14 (3%)	35	66
3	N	453/476 (95%)	439 (97%)	14 (3%)	35	66
All	All	1858/1934 (96%)	1800 (97%)	58 (3%)	35	66

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	416	ARG
3	N	390	LEU
3	M	229	SER
3	N	377	VAL
3	N	198	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	45	GLN
3	N	375	ASN
3	M	90	ASN
3	M	291	HIS
3	M	375	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	$\# Z > 2$
6	10M	D	805	-	34,34,34	0.83	0	44,45,45	1.28	5 (11%)
7	HEM	D	801	5,2	50,50,50	1.76	10 (20%)	66,82,82	2.48	24 (36%)
4	HEC	C	201	1	50,50,50	1.64	9 (18%)	68,82,82	1.61	14 (20%)
6	10M	A	203	-	34,34,34	0.54	0	44,45,45	0.82	0
7	HEM	D	802	5,2,9	50,50,50	1.73	6 (12%)	66,82,82	1.81	13 (19%)
4	HEC	M	601	3	50,50,50	1.70	7 (14%)	68,82,82	1.68	15 (22%)
7	HEM	B	802	5,2,9	50,50,50	1.76	7 (14%)	66,82,82	1.83	12 (18%)
10	DHE	M	602	3	52,56,56	2.56	23 (44%)	53,94,94	2.26	21 (39%)
4	HEC	N	601	3	50,50,50	1.81	7 (14%)	68,82,82	1.69	14 (20%)
6	10M	C	203	-	34,34,34	0.59	0	44,45,45	0.83	1 (2%)
4	HEC	A	201	1	50,50,50	1.84	9 (18%)	68,82,82	2.04	19 (27%)
7	HEM	B	801	5,2	50,50,50	1.94	11 (22%)	66,82,82	2.44	21 (31%)
10	DHE	N	602	3	52,56,56	2.60	23 (44%)	53,94,94	1.84	17 (32%)

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
6	10M	D	805	-	-	10/19/59/59	0/2/2/2
7	HEM	D	801	5,2	-	5/14/54/54	-
4	HEC	C	201	1	1/1/3/7	9/14/54/54	-
6	10M	A	203	-	-	4/19/59/59	0/2/2/2
7	HEM	D	802	5,2,9	-	5/14/54/54	-
4	HEC	M	601	3	1/1/3/7	8/14/54/54	-
7	HEM	B	802	5,2,9	-	4/14/54/54	-
10	DHE	M	602	3	-	9/20/108/108	-
4	HEC	N	601	3	1/1/3/7	6/14/54/54	-
6	10M	C	203	-	-	4/19/59/59	0/2/2/2
4	HEC	A	201	1	1/1/3/7	6/14/54/54	-
7	HEM	B	801	5,2	-	3/14/54/54	-
10	DHE	N	602	3	-	10/20/108/108	-

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	801	HEM	C3D-C2D	7.66	1.53	1.36
4	N	601	HEC	C3D-C2D	7.64	1.53	1.36
7	D	802	HEM	C3D-C2D	7.60	1.52	1.36
7	B	801	HEM	C3D-C2D	7.58	1.52	1.36
7	B	802	HEM	C3D-C2D	7.52	1.52	1.36

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	802	HEM	C4D-ND-C1D	7.90	113.23	105.07
4	A	201	HEC	CAB-C3B-C4B	7.28	134.26	124.81
7	B	801	HEM	C4D-ND-C1D	6.62	111.91	105.07
7	B	802	HEM	CAD-CBD-CGD	-6.58	99.45	113.60
7	D	801	HEM	C4D-ND-C1D	6.38	111.66	105.07

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	201	HEC	NA
4	C	201	HEC	NA
4	M	601	HEC	NA
4	N	601	HEC	NA

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	HEC	C2B-C3B-CAB-CBB
4	A	201	HEC	C4B-C3B-CAB-CBB
10	M	602	DHE	C2B-C3B-CAB-CBB
10	M	602	DHE	CGB-C3B-CAB-CBB
10	M	602	DHE	C4B-C3B-CAB-CBB

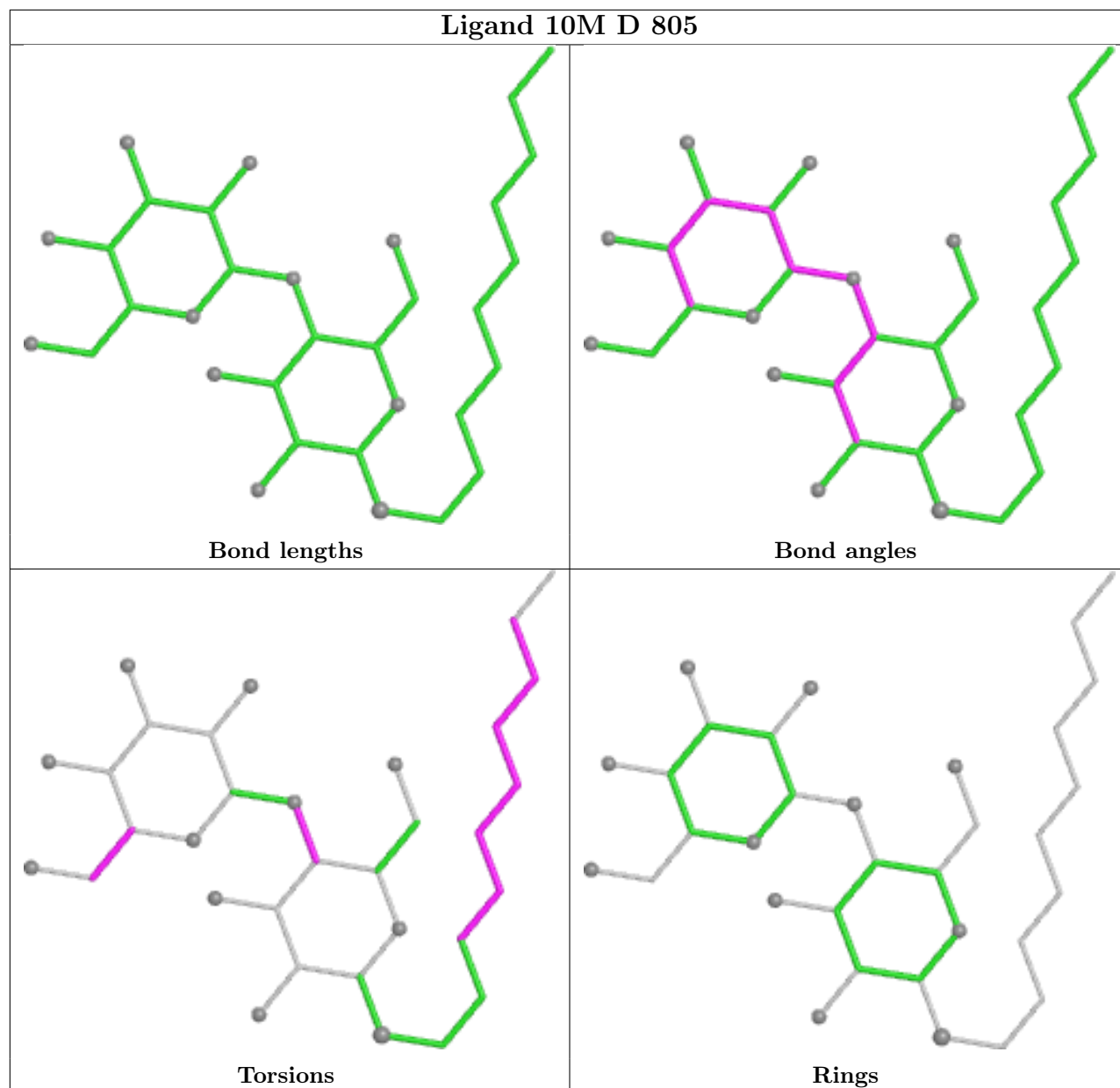
There are no ring outliers.

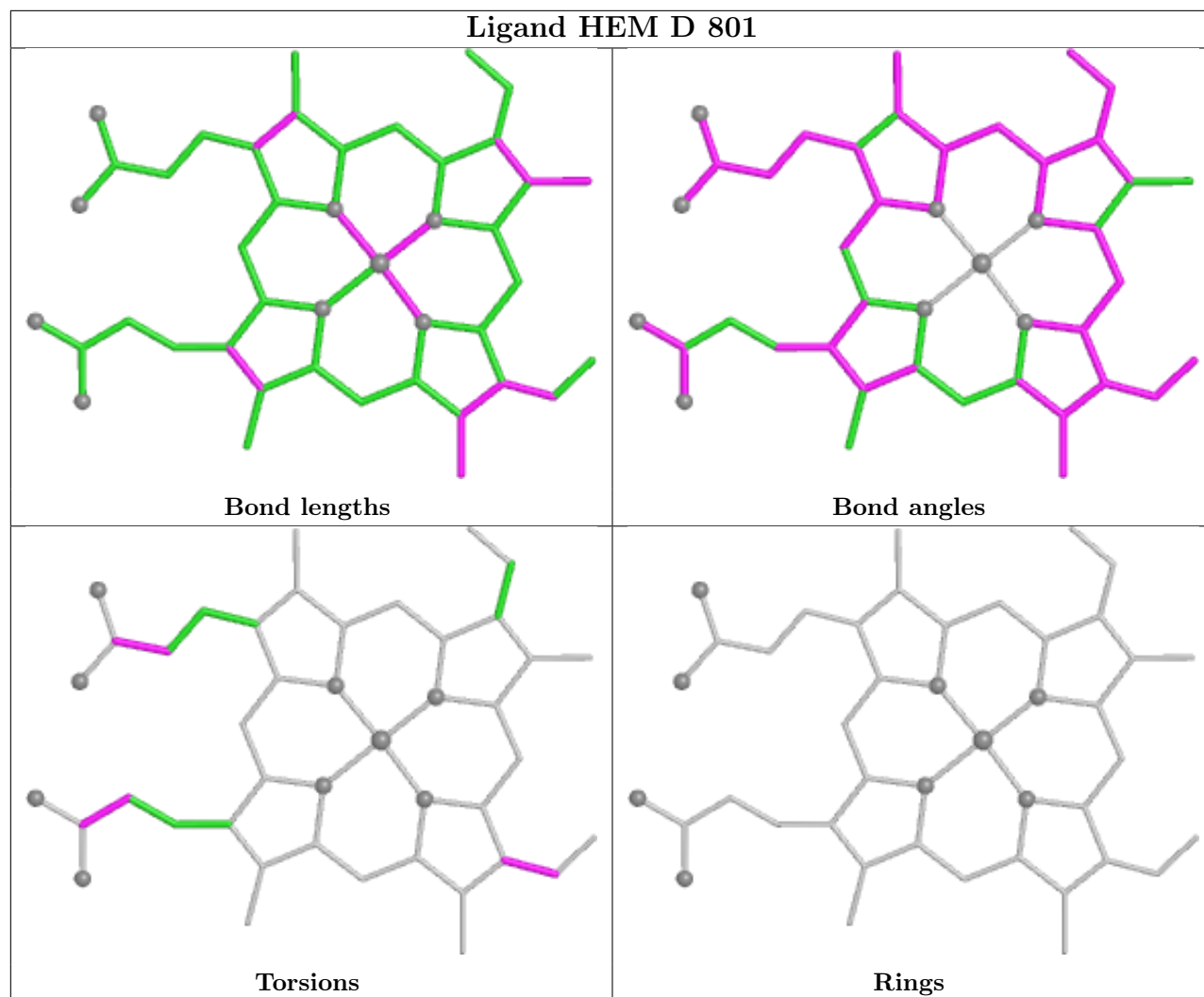
10 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	801	HEM	4	0
4	C	201	HEC	2	0
7	D	802	HEM	2	0
4	M	601	HEC	1	0
7	B	802	HEM	3	0
10	M	602	DHE	7	0
4	N	601	HEC	2	0
4	A	201	HEC	4	0
7	B	801	HEM	5	0
10	N	602	DHE	3	0

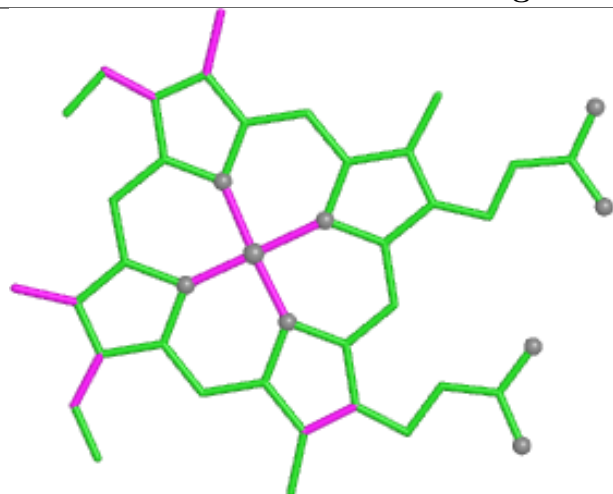
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 10M D 805

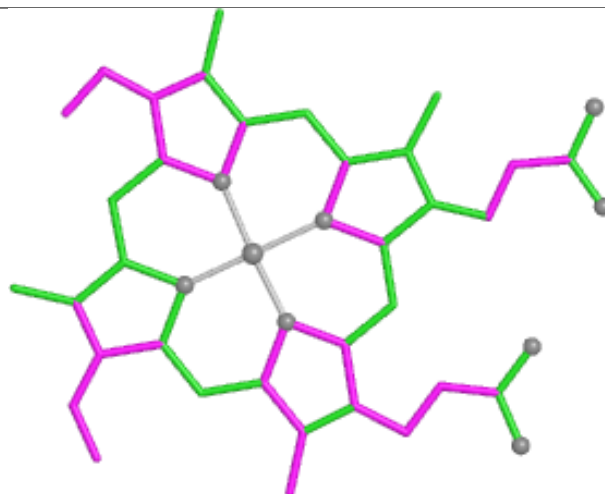




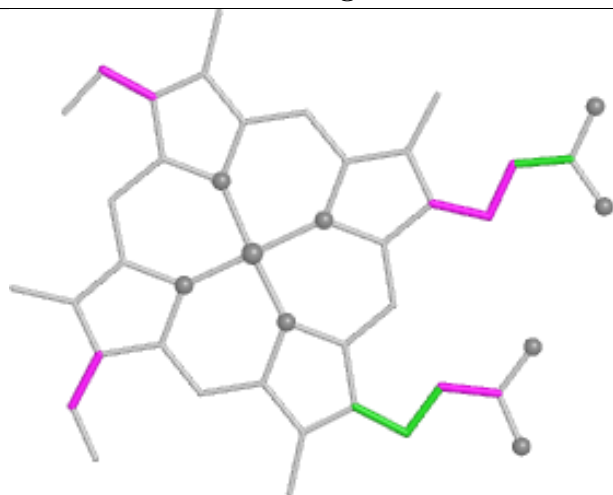
Ligand HEC C 201



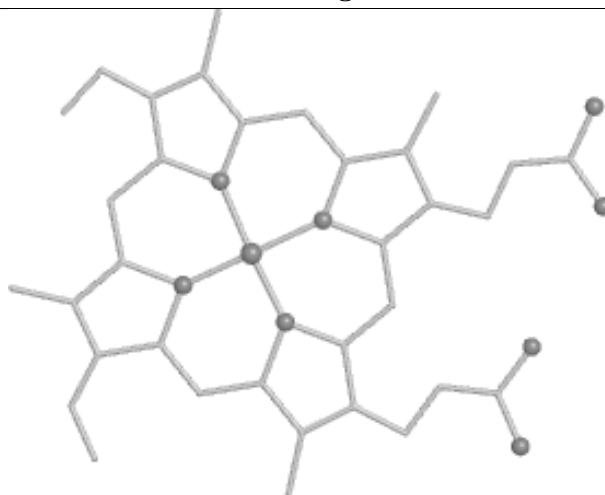
Bond lengths



Bond angles

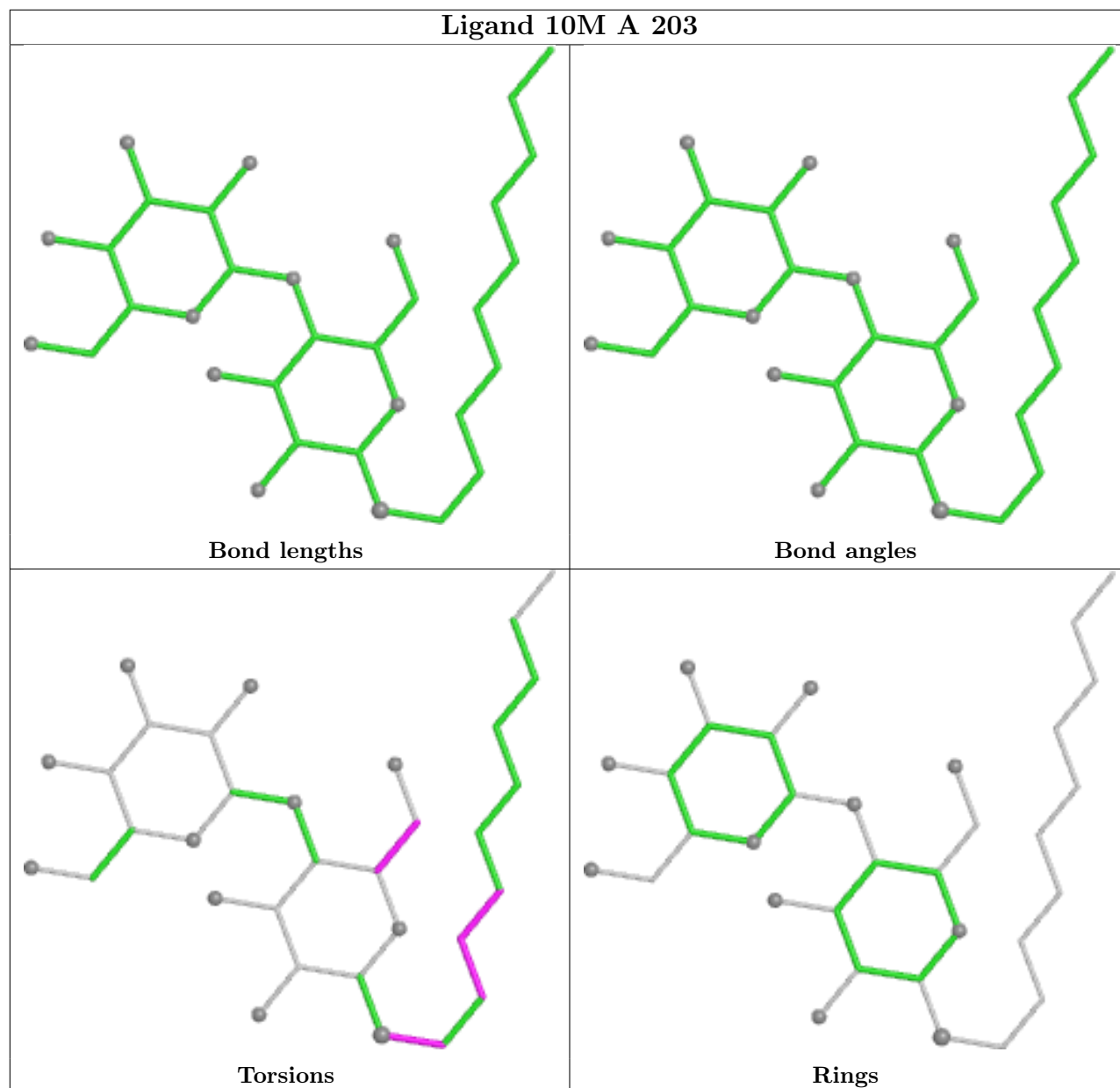


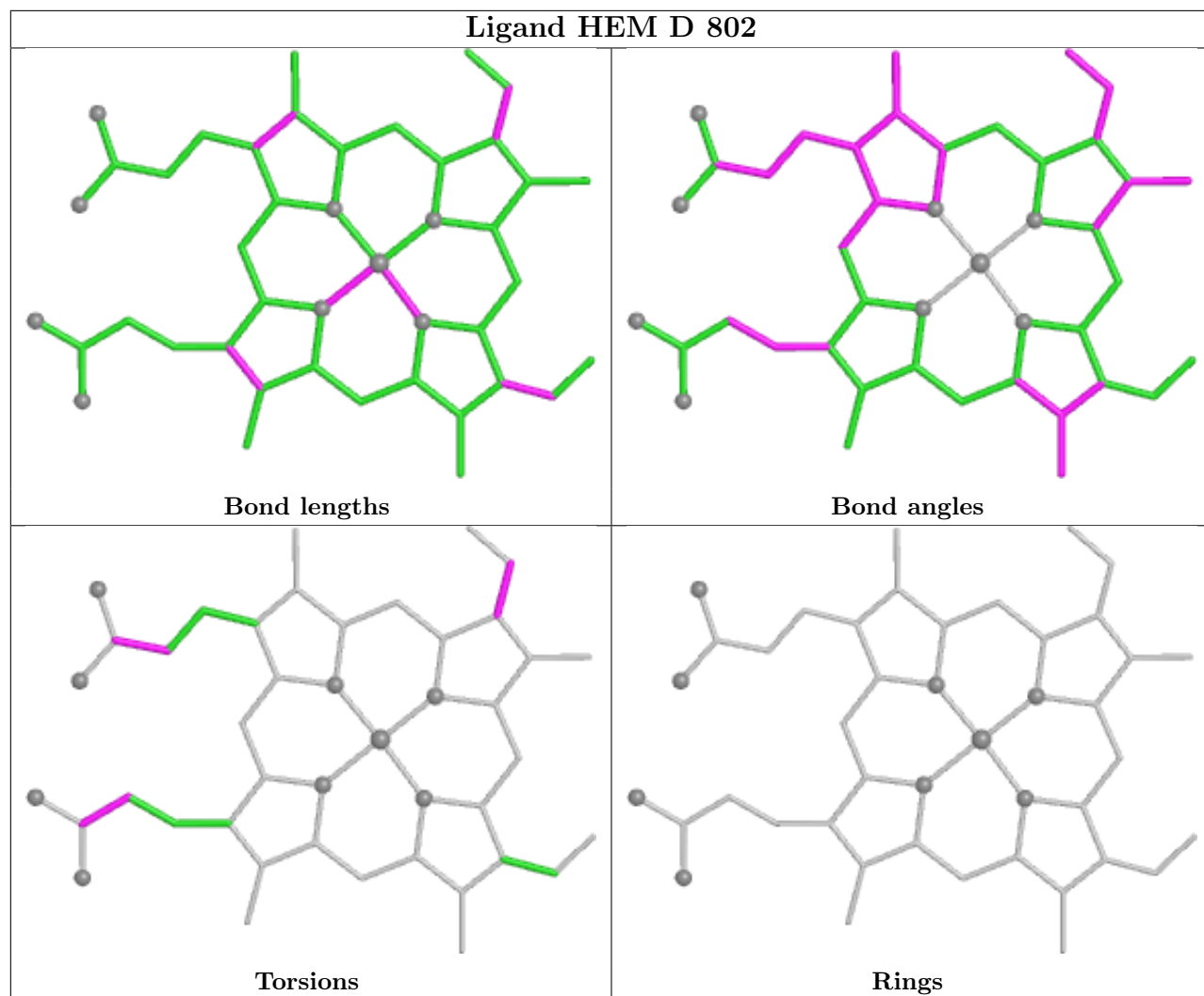
Torsions

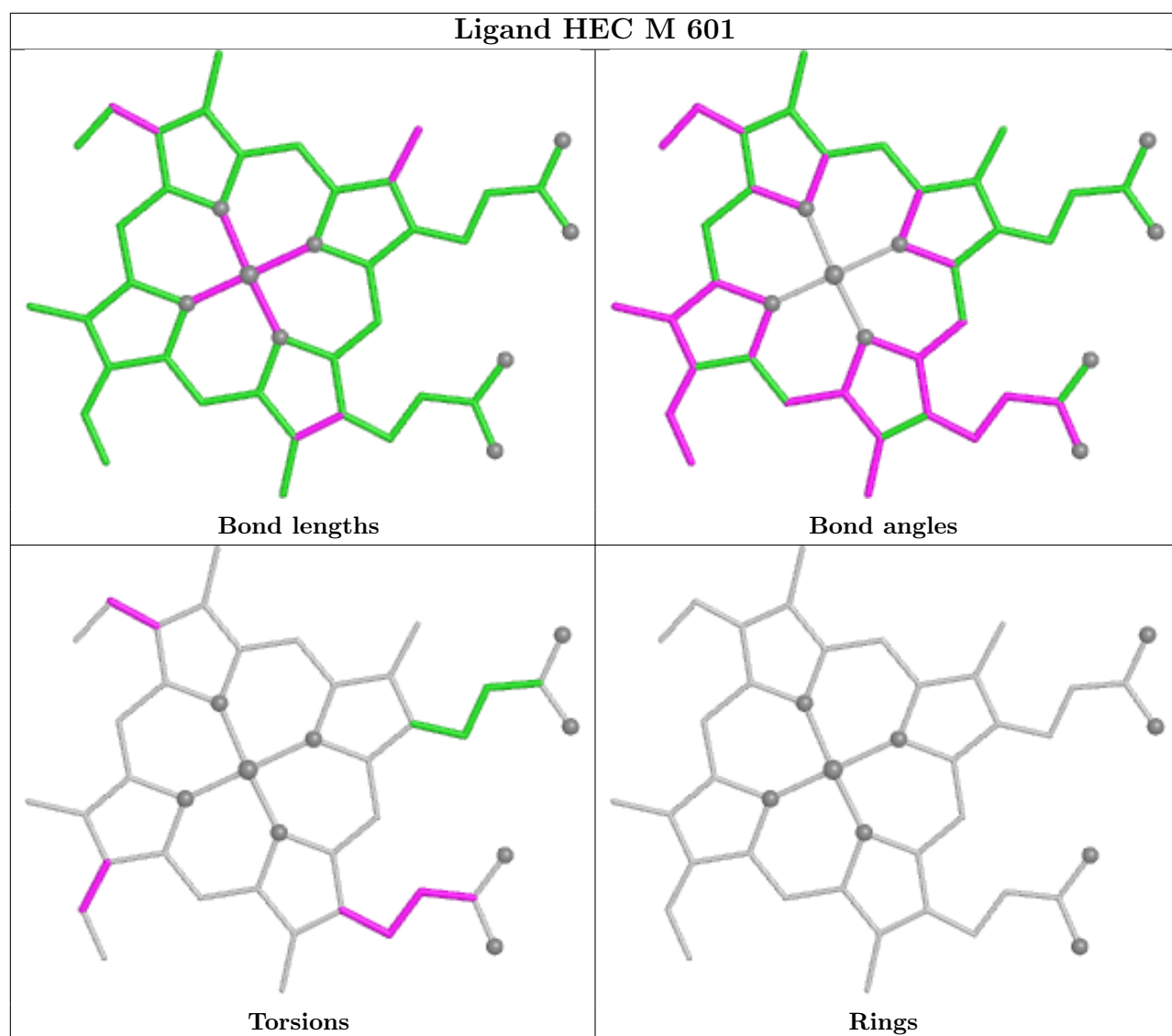


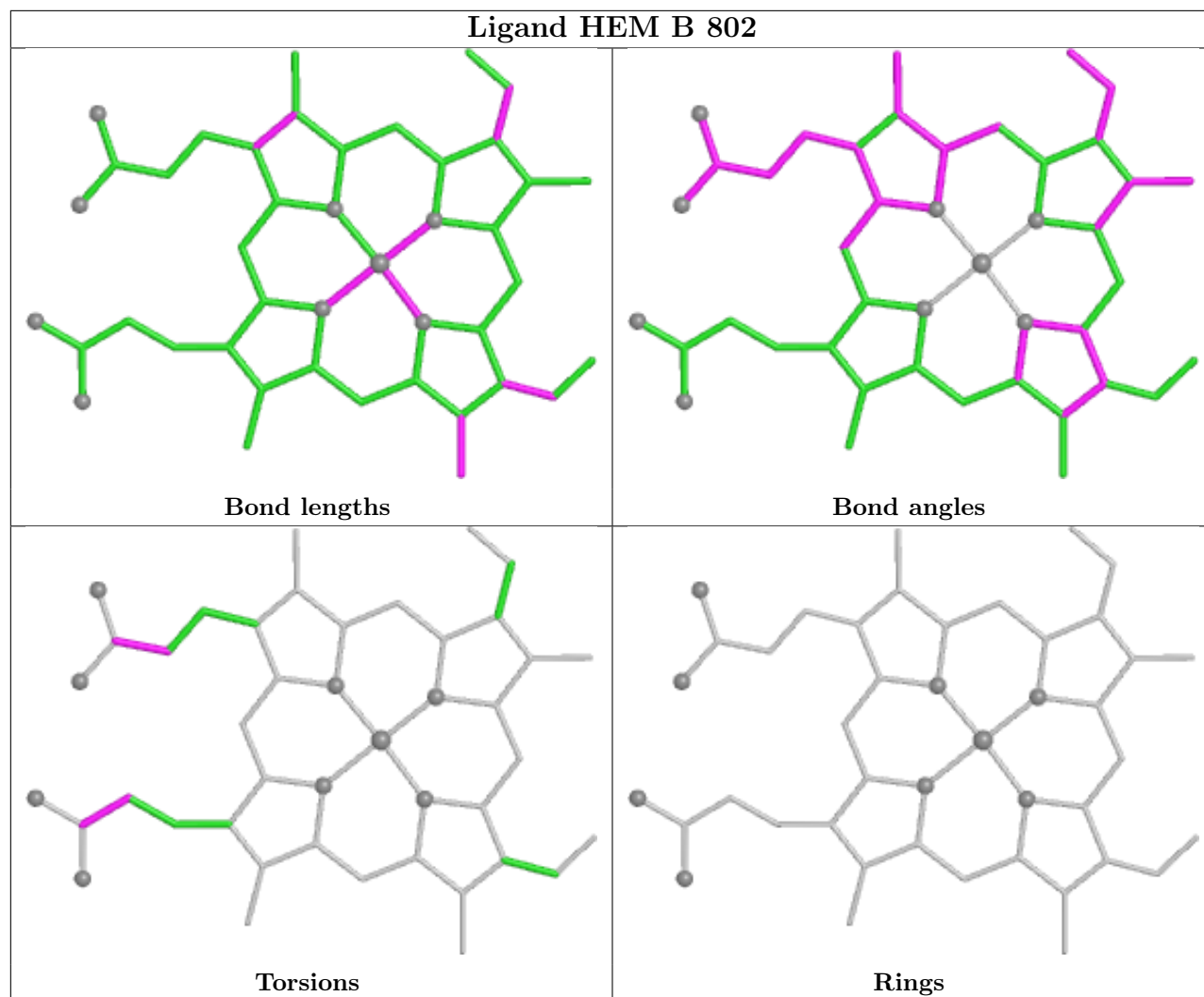
Rings

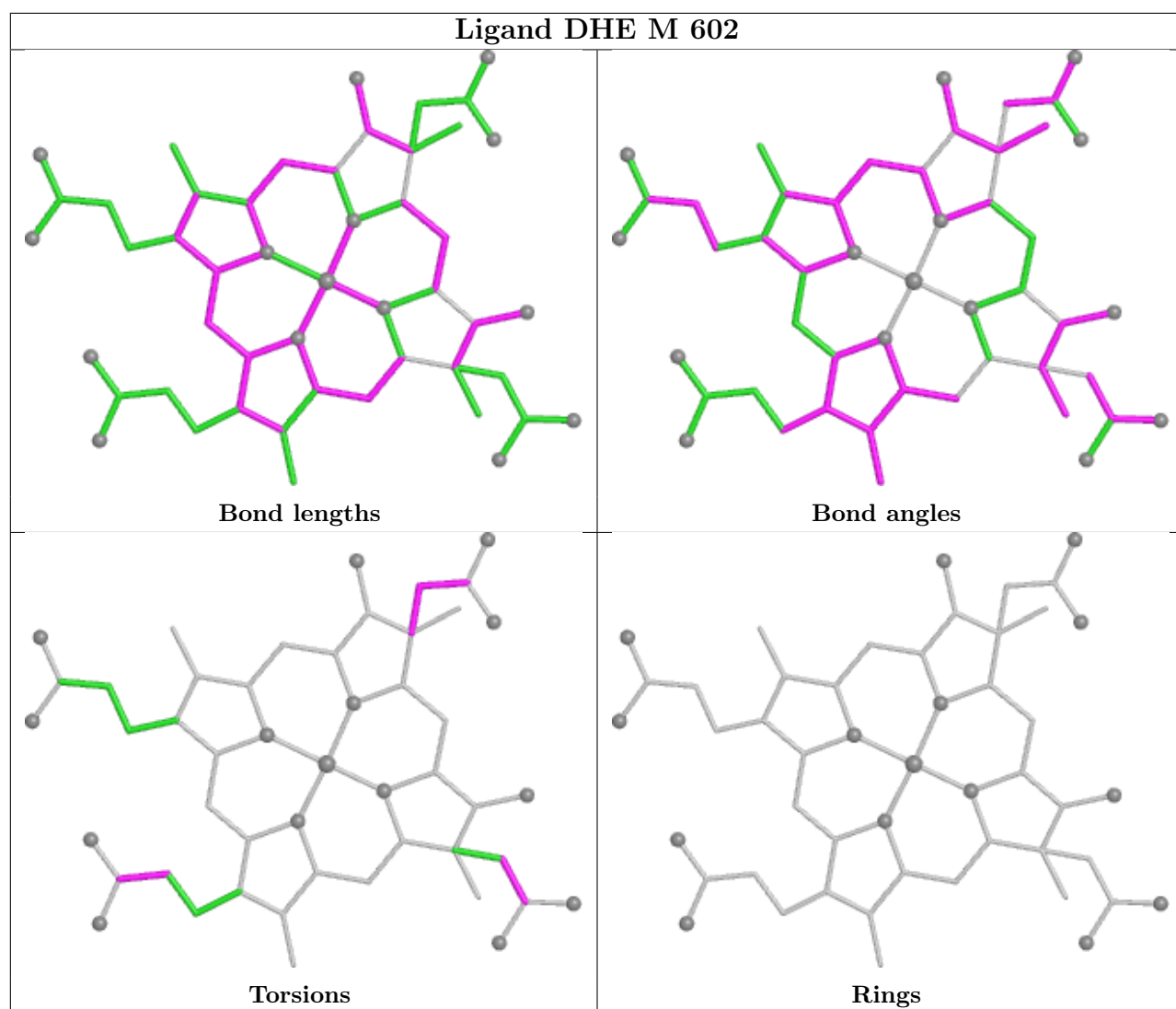
Ligand 10M A 203

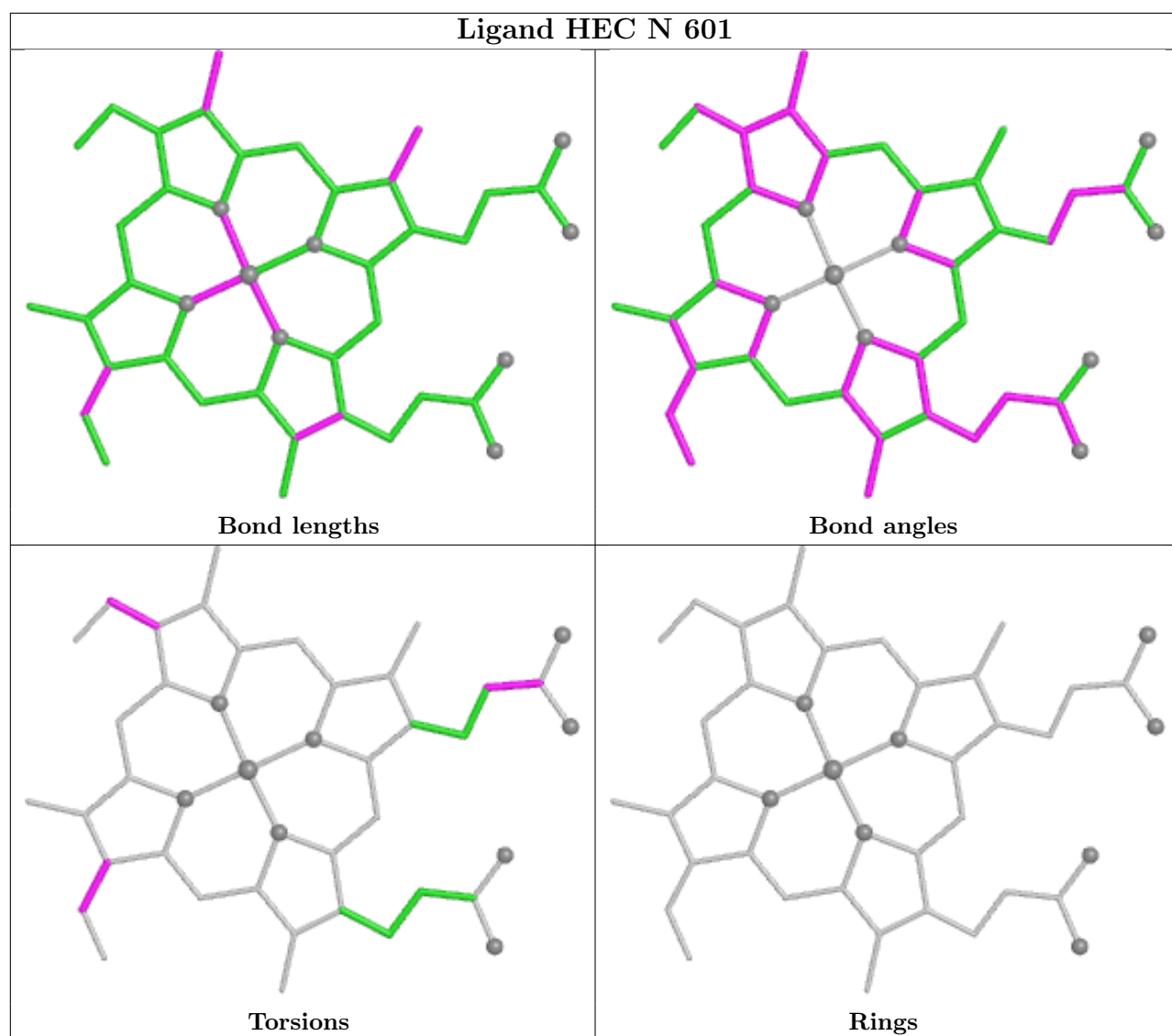




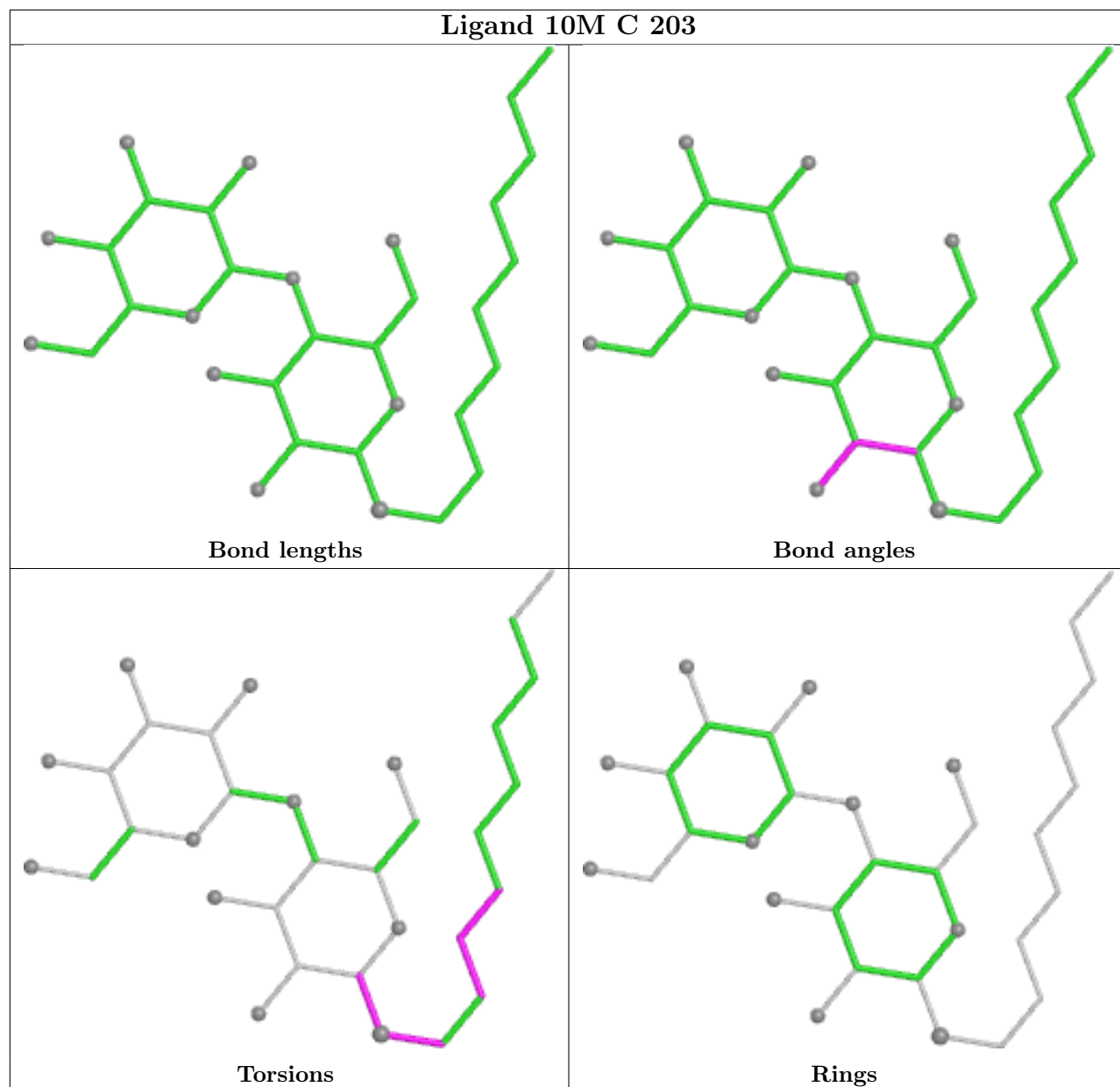


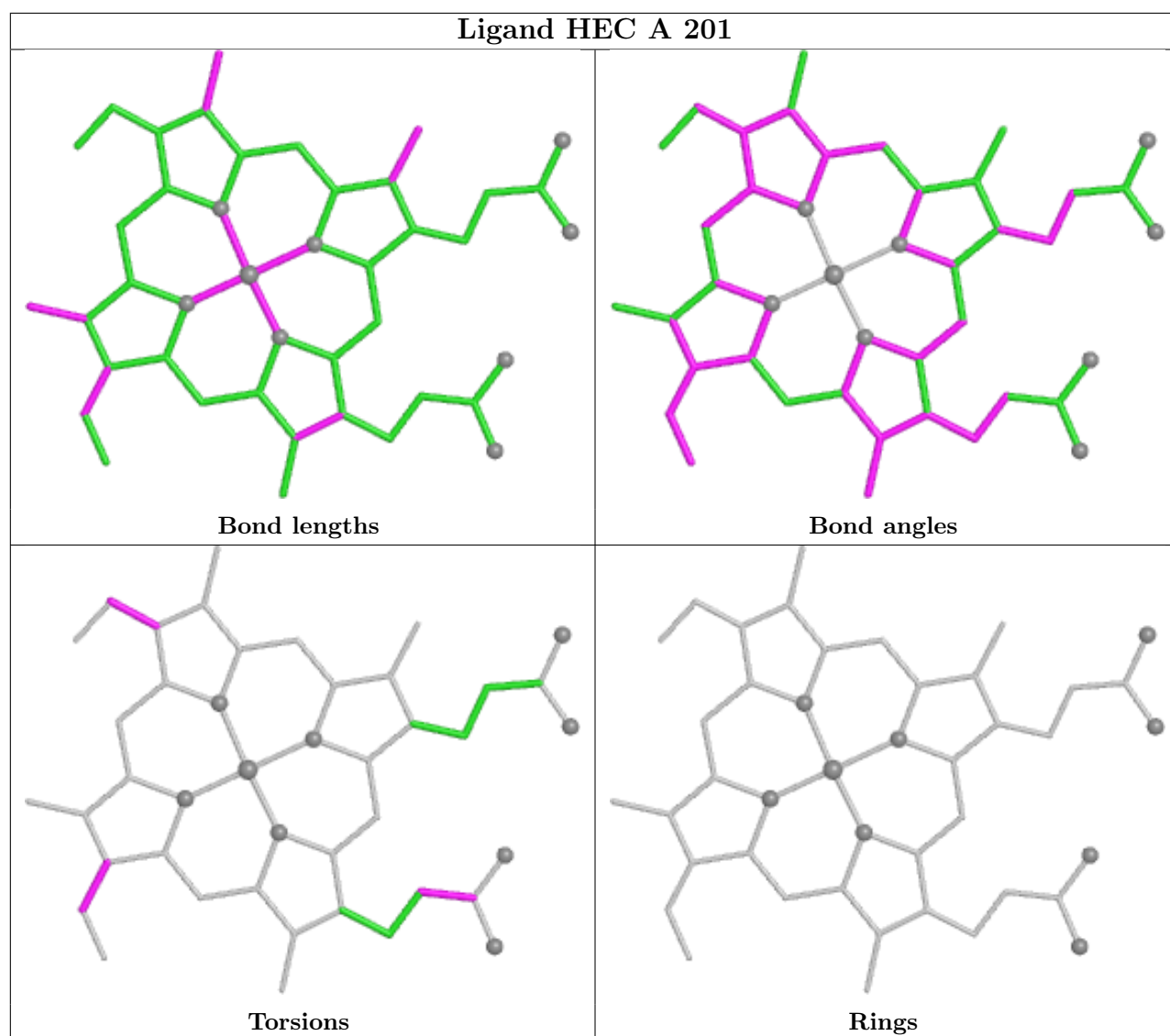


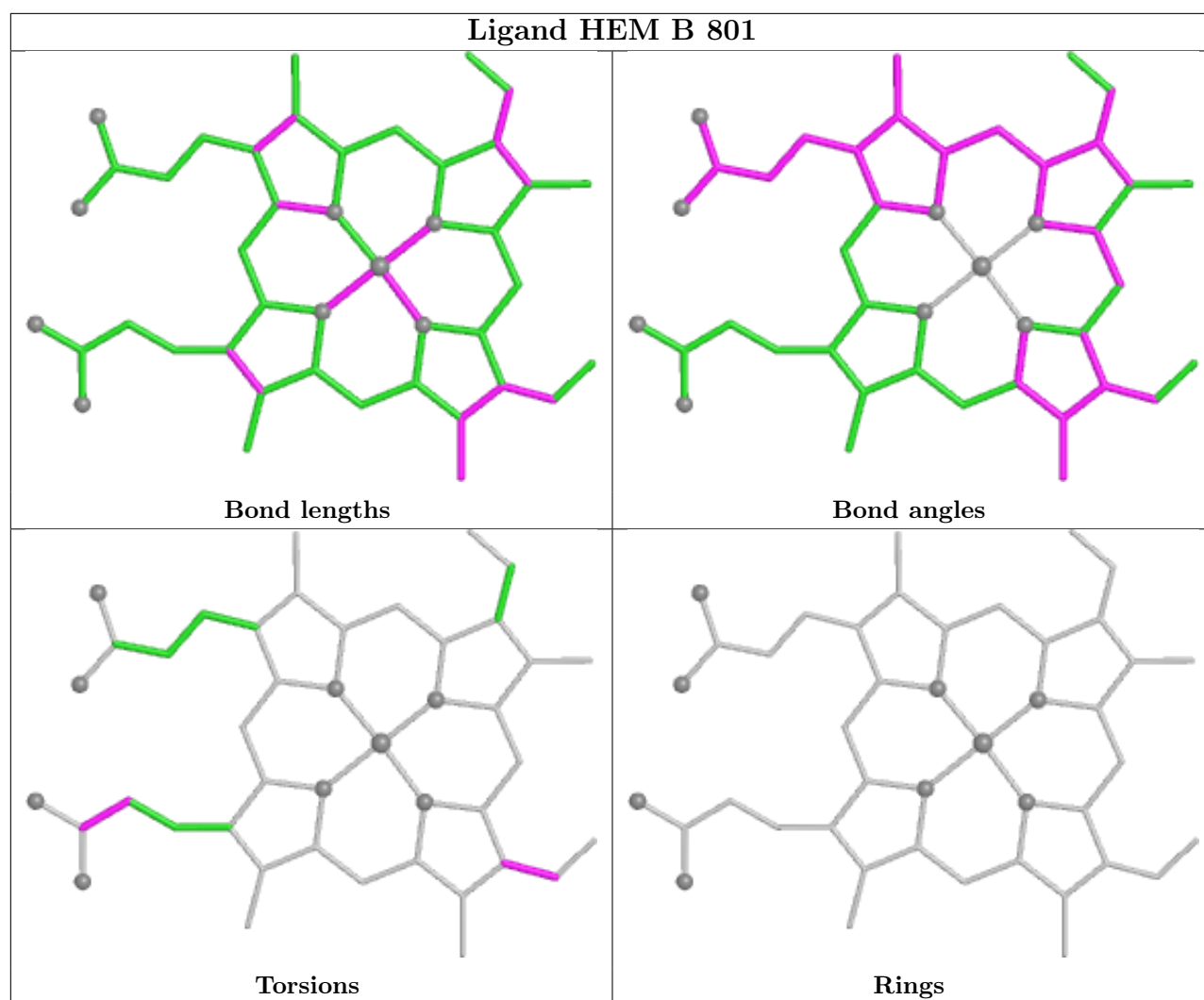


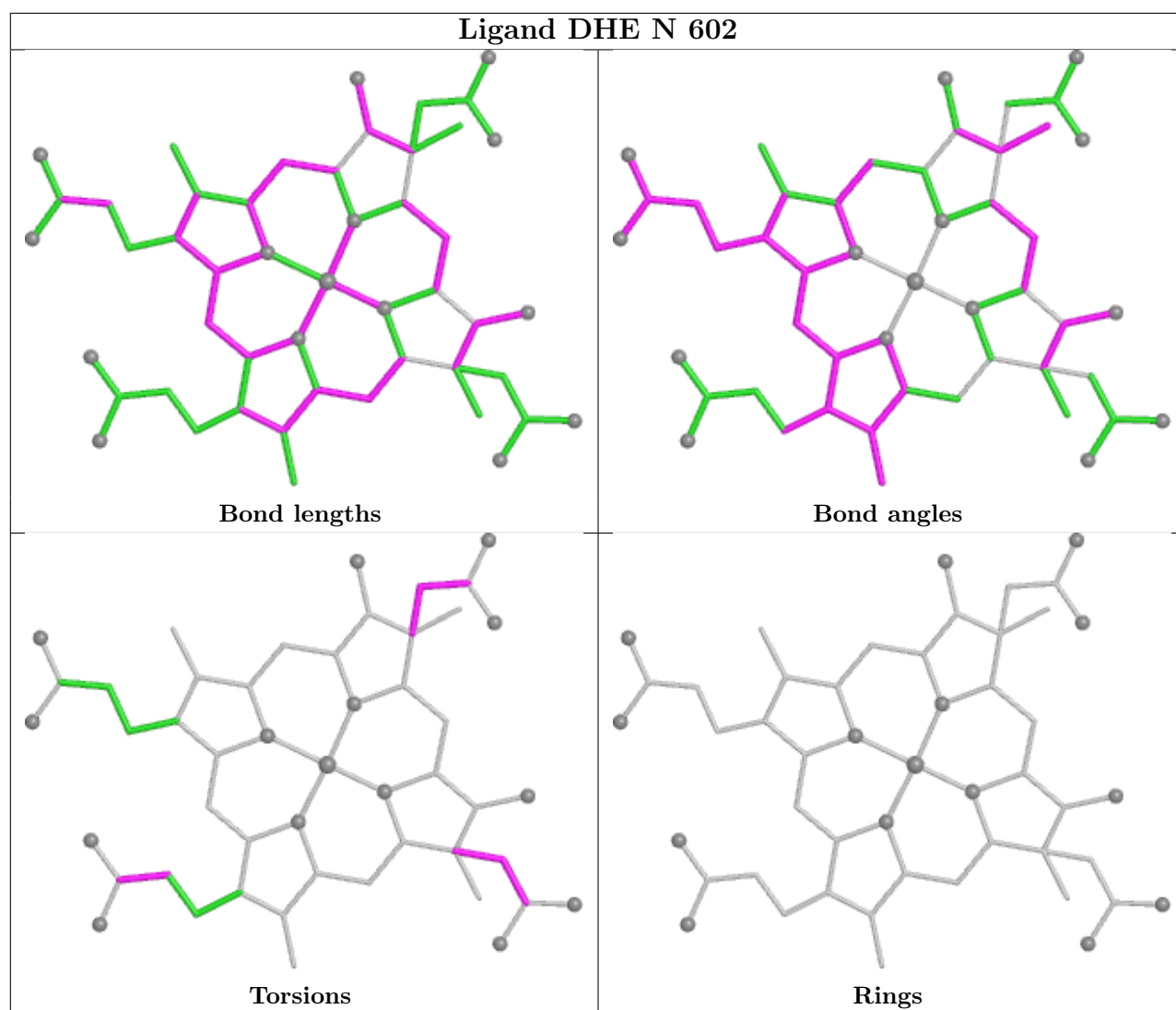


Ligand 10M C 203









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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	142/146 (97%)	0.45	10 (7%) 22 14	49, 74, 127, 147	0
1	C	142/146 (97%)	0.16	5 (3%) 47 29	34, 57, 97, 116	0
2	B	449/465 (96%)	0.53	41 (9%) 15 9	43, 72, 104, 134	0
2	D	449/465 (96%)	0.21	18 (4%) 42 26	32, 56, 89, 123	0
3	M	538/568 (94%)	0.05	15 (2%) 55 35	31, 56, 88, 108	0
3	N	538/568 (94%)	0.30	27 (5%) 34 22	38, 76, 113, 133	0
All	All	2258/2358 (95%)	0.27	116 (5%) 33 21	31, 65, 105, 147	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	485	GLU	7.0
2	B	206	VAL	5.9
2	D	373	GLY	5.8
3	N	542	VAL	5.4
2	B	233	ASP	4.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

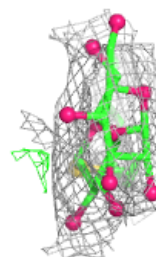
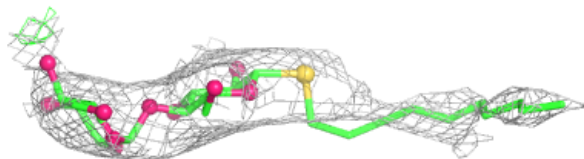
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	10M	A	203	33/33	0.79	0.13	71,107,122,128	0
6	10M	D	805	33/33	0.82	0.17	93,114,125,130	0
6	10M	C	203	33/33	0.88	0.14	71,82,98,110	0
11	CL	M	603	1/1	0.93	0.09	44,44,44,44	0
10	DHE	N	602	49/49	0.95	0.12	44,53,67,70	0
11	CL	N	603	1/1	0.95	0.12	44,44,44,44	0
5	CA	A	202	1/1	0.96	0.22	32,32,32,32	0
7	HEM	D	802	43/43	0.96	0.12	41,44,48,51	0
9	O	B	804	1/1	0.96	0.09	33,33,33,33	0
7	HEM	B	801	43/43	0.97	0.10	43,45,53,63	0
10	DHE	M	602	49/49	0.97	0.09	25,28,34,36	0
7	HEM	B	802	43/43	0.97	0.12	51,57,70,78	0
7	HEM	D	801	43/43	0.97	0.11	37,39,44,46	0
4	HEC	A	201	43/43	0.97	0.09	43,46,57,63	0
9	O	D	804	1/1	0.98	0.07	11,11,11,11	0
4	HEC	M	601	43/43	0.98	0.07	31,35,40,42	0
4	HEC	N	601	43/43	0.98	0.07	37,42,53,58	0
4	HEC	C	201	43/43	0.98	0.07	22,25,32,37	0
5	CA	C	202	1/1	0.98	0.27	8,8,8,8	0
8	FE	B	803	1/1	0.99	0.04	47,47,47,47	0
8	FE	D	803	1/1	1.00	0.09	19,19,19,19	0

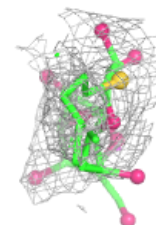
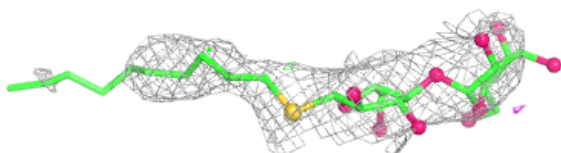
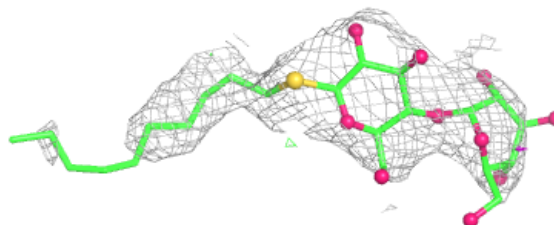
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 10M A 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

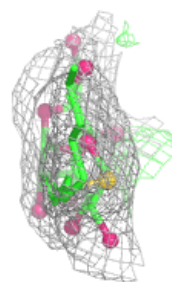
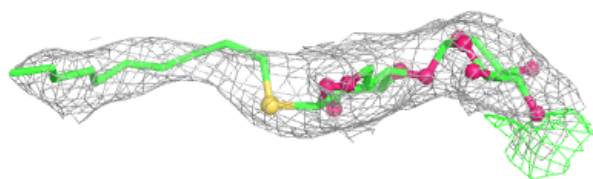
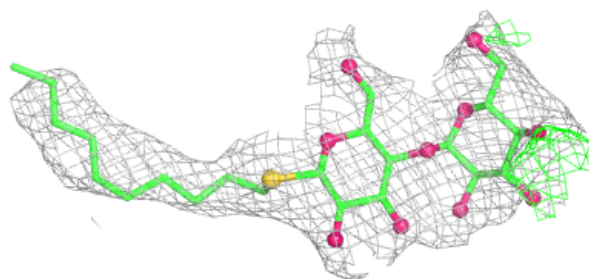
**Electron density around 10M D 805:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



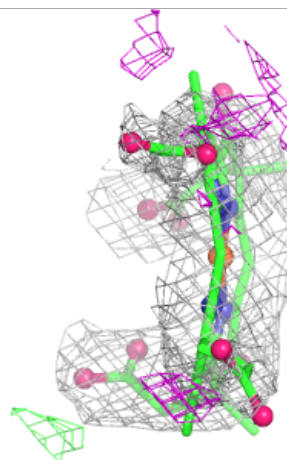
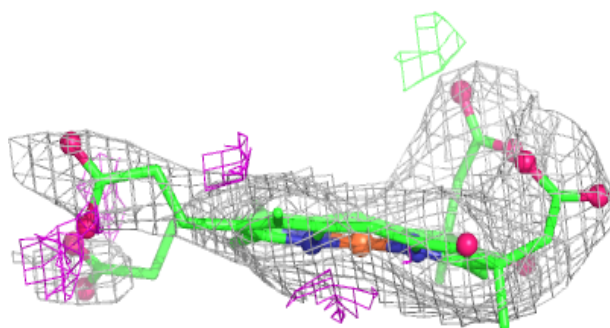
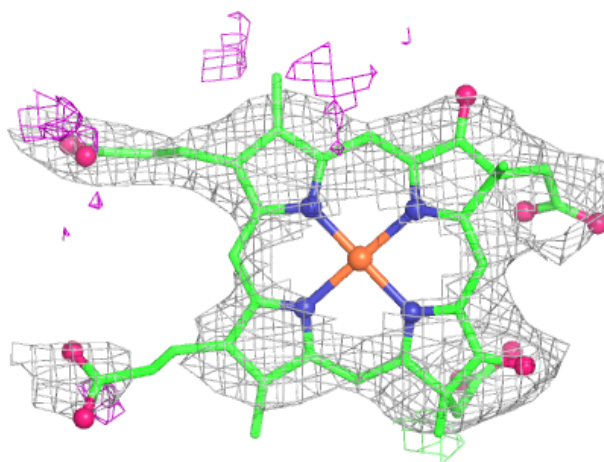
Electron density around 10M C 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



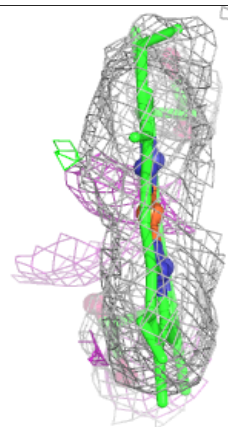
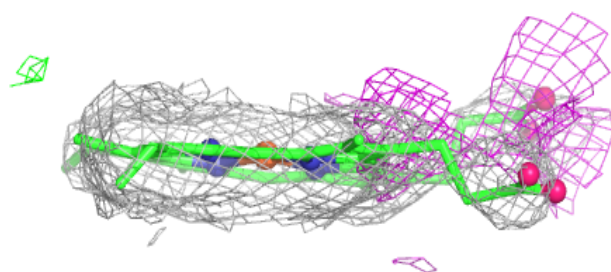
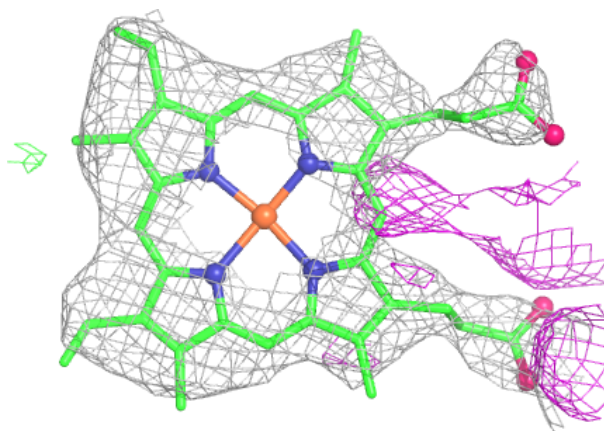
Electron density around DHE N 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



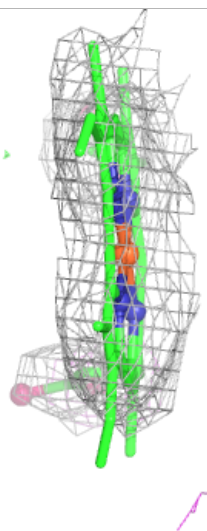
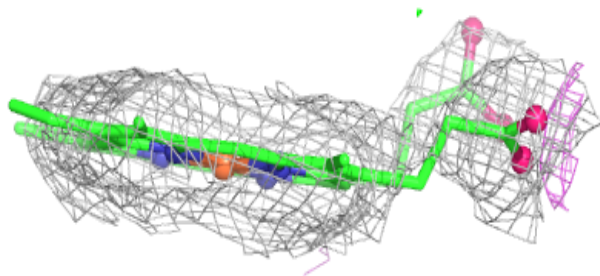
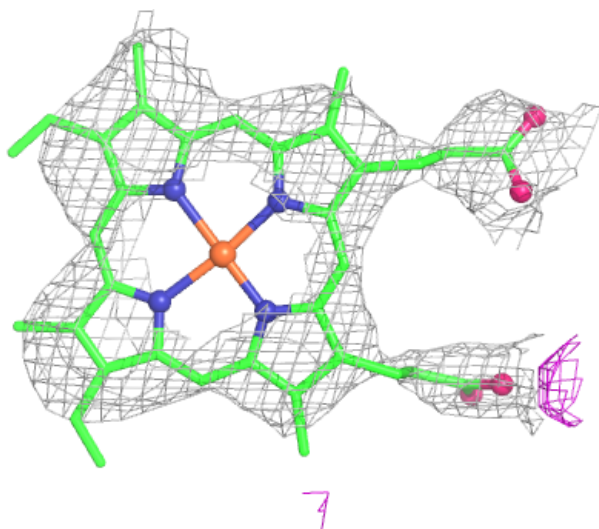
Electron density around HEM D 802:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



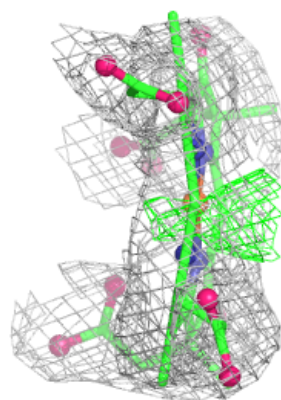
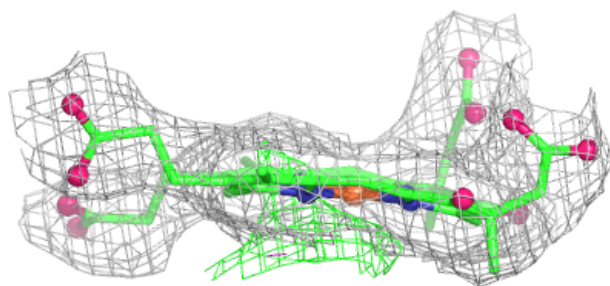
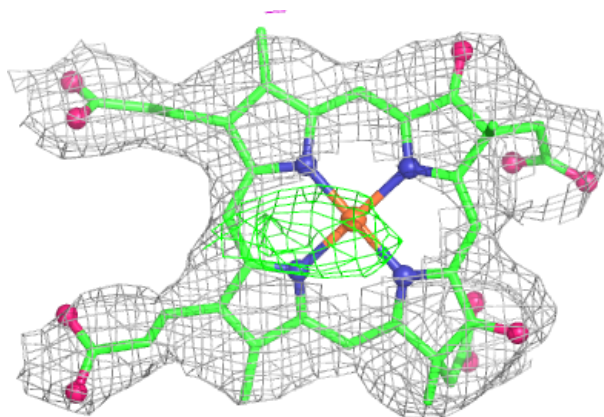
Electron density around HEM B 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



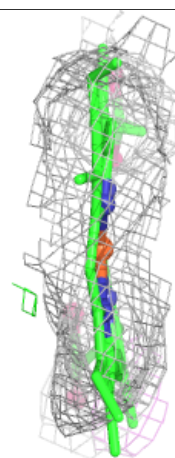
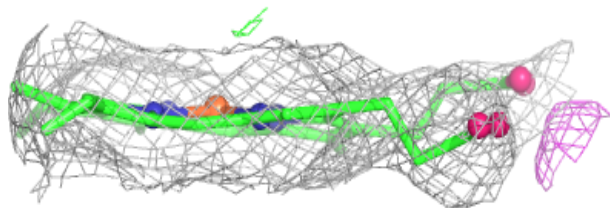
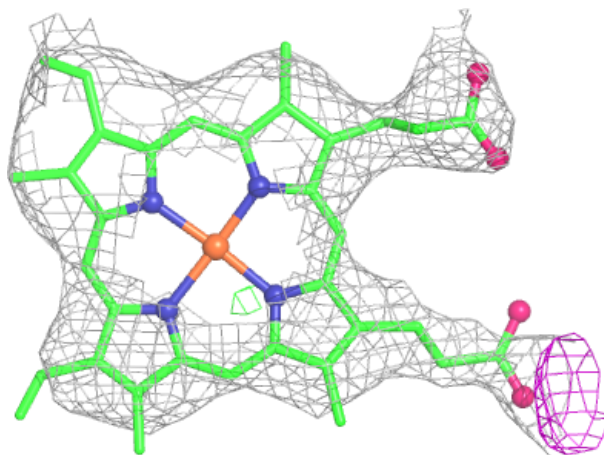
Electron density around DHE M 602:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



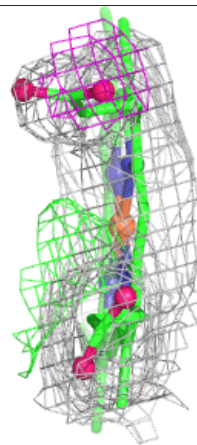
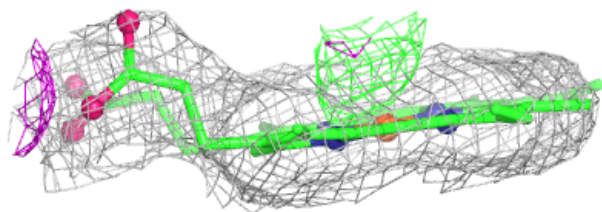
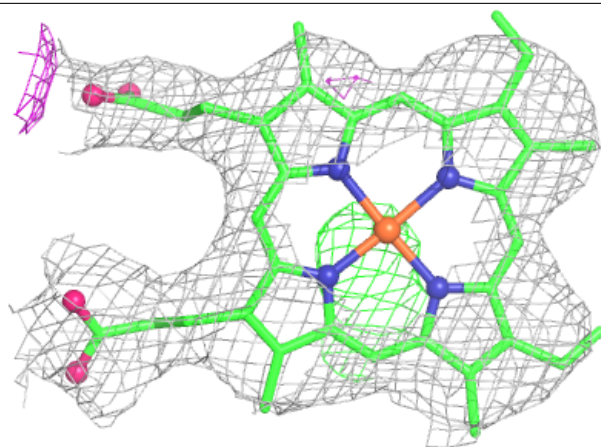
Electron density around HEM B 802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



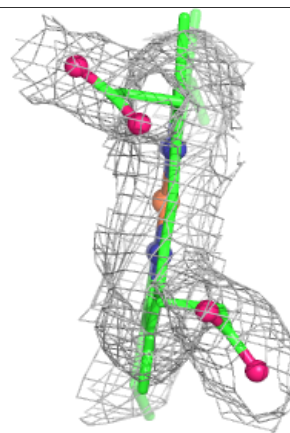
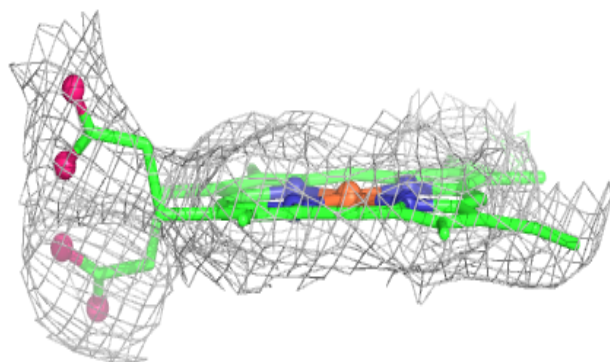
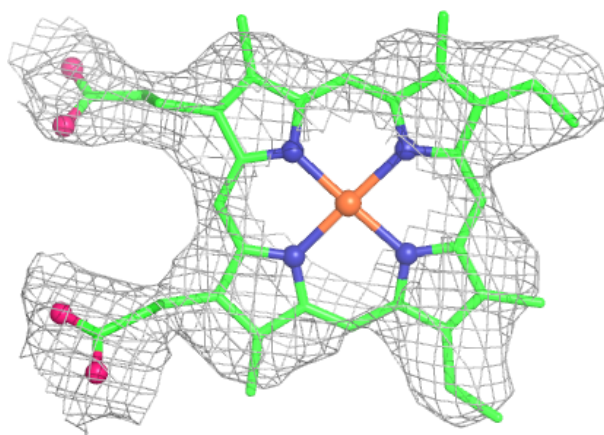
Electron density around HEM D 801:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



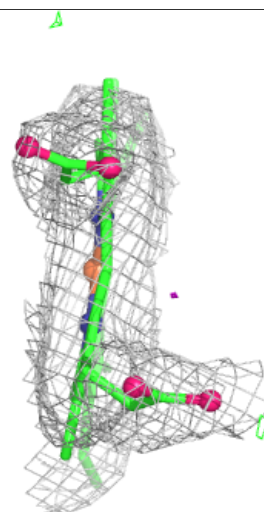
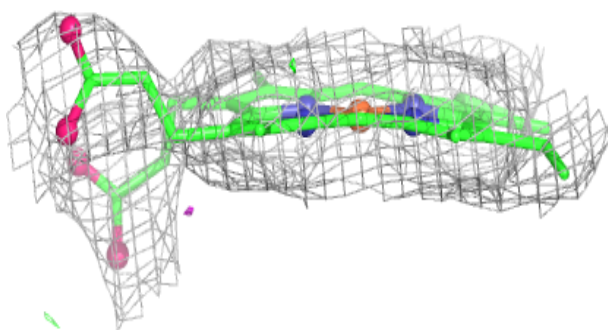
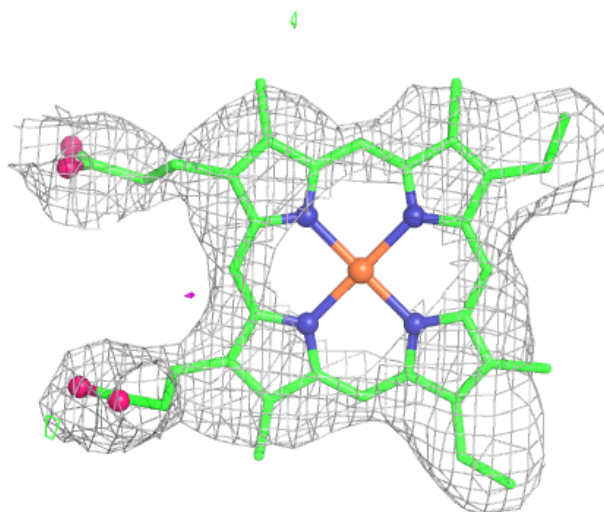
Electron density around HEC A 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



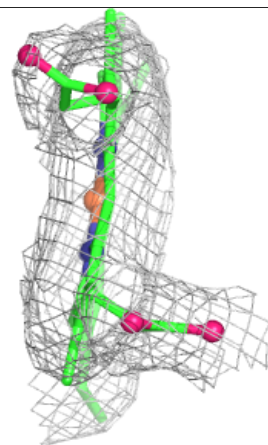
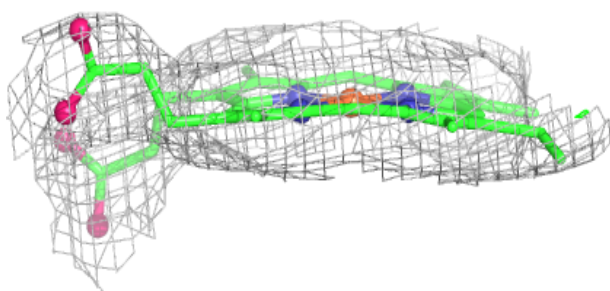
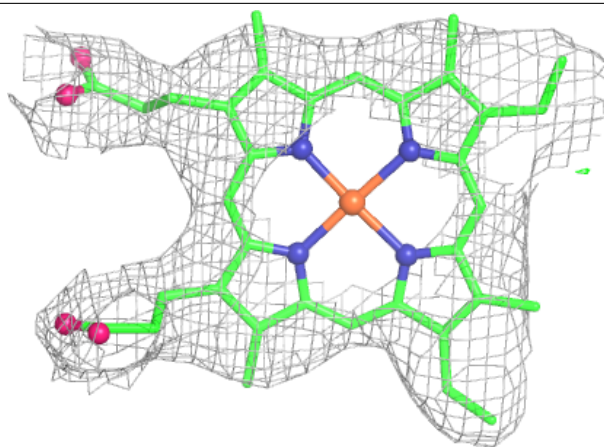
Electron density around HEC M 601:

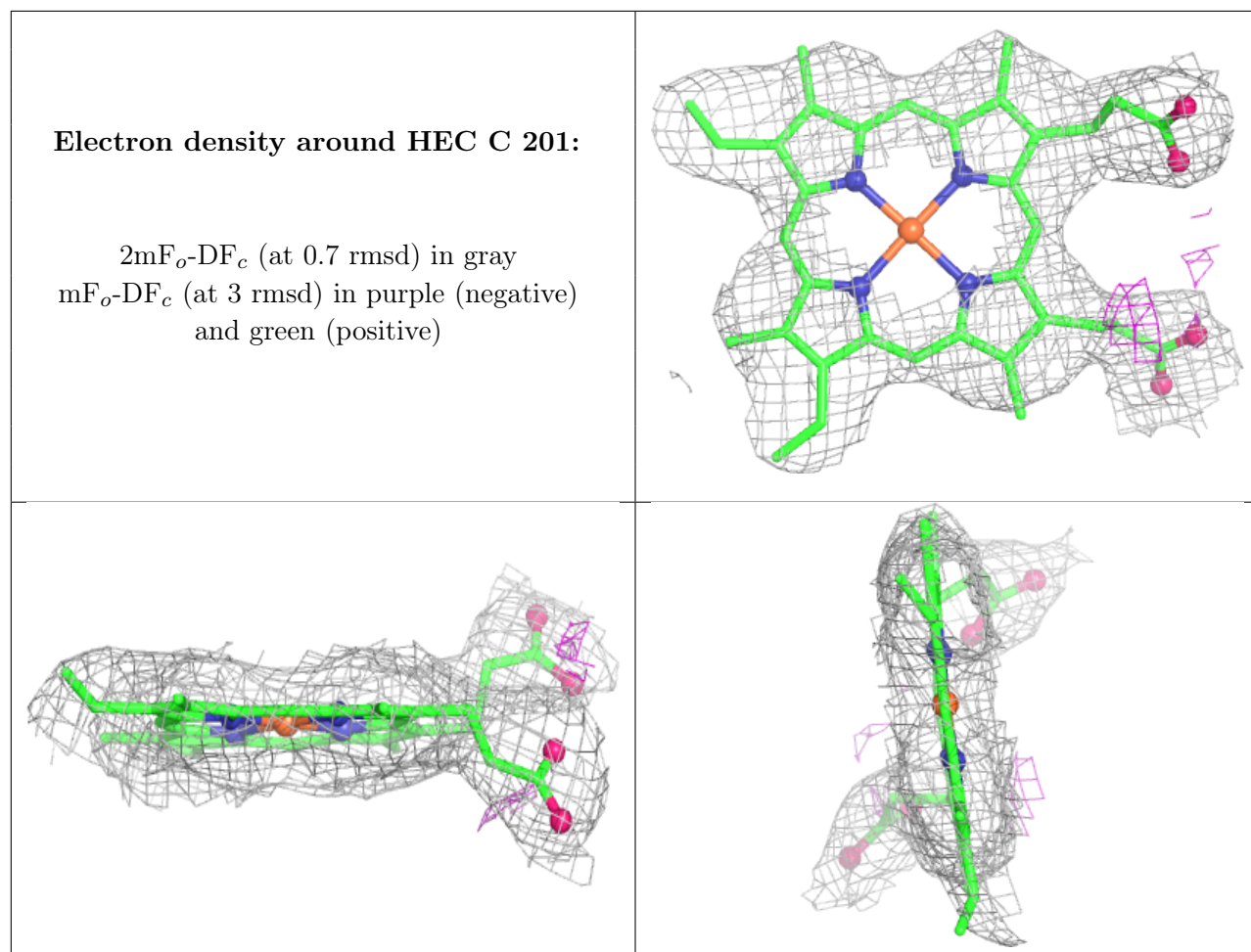
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC N 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.