



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 9, 2026 – 08:32 am BST

PDB ID : 8BCX / pdb_00008bcx
Title : Crystal structure of NrfA-1 from *Geobacter metallireducens*
Authors : Denkhaus, L.; Siffert, F.; Einsle, O.
Deposited on : 2022-10-17
Resolution : 1.94 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	:	1.8.4, 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

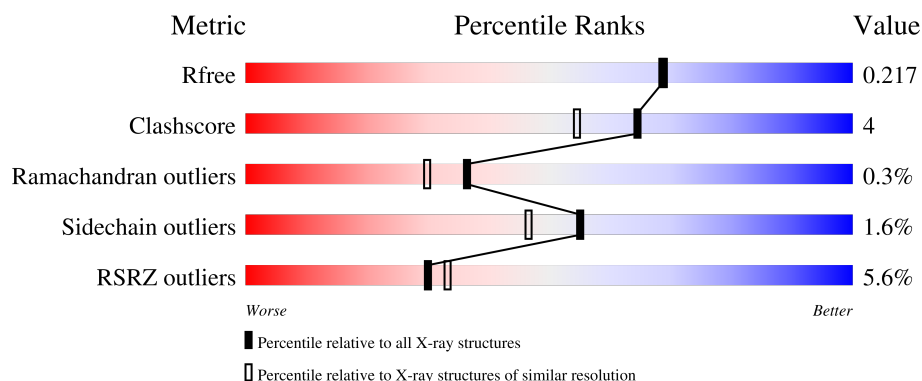
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	492	 3% 81% 8% • 11%
1	B	492	 6% 79% 9% 12%
1	C	492	 7% 80% 9% • 10%
1	D	492	 4% 80% 9% • 10%

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
2	HEC	A	501	X	-	-	-
2	HEC	A	502	X	-	-	-
2	HEC	A	503	X	-	-	-
2	HEC	A	504	X	-	-	-
2	HEC	A	505	X	-	-	-
2	HEC	B	501	X	-	-	-
2	HEC	B	502	X	-	-	-
2	HEC	B	503	X	-	-	-
2	HEC	B	504	X	-	-	-
2	HEC	B	505	X	-	-	-
2	HEC	C	501	X	-	-	-
2	HEC	C	502	X	-	-	-
2	HEC	C	503	X	-	-	-
2	HEC	C	504	X	-	-	-
2	HEC	C	505	X	-	-	-
2	HEC	D	501	X	-	-	-
2	HEC	D	502	X	-	-	-
2	HEC	D	503	X	-	-	-
2	HEC	D	504	X	-	-	-
2	HEC	D	505	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15471 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 Nitrite reductase (cytochrome; ammonia-forming).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3433	2185	594	631	23			
1	B	434	Total	C	N	O	S	0	0	0
			3398	2158	586	631	23			
1	C	443	Total	C	N	O	S	0	0	0
			3489	2217	608	641	23			
1	D	444	Total	C	N	O	S	0	0	0
			3493	2222	605	643	23			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP Q39YY5
A	-2	LYS	-	expression tag	UNP Q39YY5
A	-1	LYS	-	expression tag	UNP Q39YY5
A	0	THR	-	expression tag	UNP Q39YY5
A	1	ALA	-	expression tag	UNP Q39YY5
A	2	ILE	-	expression tag	UNP Q39YY5
A	3	ALA	-	expression tag	UNP Q39YY5
A	4	ILE	-	expression tag	UNP Q39YY5
A	5	ALA	-	expression tag	UNP Q39YY5
A	6	VAL	-	expression tag	UNP Q39YY5
A	7	ALA	-	expression tag	UNP Q39YY5
A	8	LEU	-	expression tag	UNP Q39YY5
A	9	ALA	-	expression tag	UNP Q39YY5
A	10	GLY	-	expression tag	UNP Q39YY5
A	11	PHE	-	expression tag	UNP Q39YY5
A	12	ALA	-	expression tag	UNP Q39YY5
A	13	THR	-	expression tag	UNP Q39YY5
A	14	VAL	-	expression tag	UNP Q39YY5
A	15	ALA	-	expression tag	UNP Q39YY5
A	16	GLN	-	expression tag	UNP Q39YY5
A	17	ALA	-	expression tag	UNP Q39YY5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ALA	-	expression tag	UNP Q39YY5
A	19	SER	-	expression tag	UNP Q39YY5
A	20	TRP	-	expression tag	UNP Q39YY5
A	21	SER	-	expression tag	UNP Q39YY5
A	22	HIS	-	expression tag	UNP Q39YY5
A	23	PRO	-	expression tag	UNP Q39YY5
A	24	GLN	-	expression tag	UNP Q39YY5
A	25	PHE	-	expression tag	UNP Q39YY5
A	26	GLU	-	expression tag	UNP Q39YY5
A	27	LYS	-	expression tag	UNP Q39YY5
A	28	GLY	-	expression tag	UNP Q39YY5
A	29	ALA	-	expression tag	UNP Q39YY5
B	-3	MET	-	initiating methionine	UNP Q39YY5
B	-2	LYS	-	expression tag	UNP Q39YY5
B	-1	LYS	-	expression tag	UNP Q39YY5
B	0	THR	-	expression tag	UNP Q39YY5
B	1	ALA	-	expression tag	UNP Q39YY5
B	2	ILE	-	expression tag	UNP Q39YY5
B	3	ALA	-	expression tag	UNP Q39YY5
B	4	ILE	-	expression tag	UNP Q39YY5
B	5	ALA	-	expression tag	UNP Q39YY5
B	6	VAL	-	expression tag	UNP Q39YY5
B	7	ALA	-	expression tag	UNP Q39YY5
B	8	LEU	-	expression tag	UNP Q39YY5
B	9	ALA	-	expression tag	UNP Q39YY5
B	10	GLY	-	expression tag	UNP Q39YY5
B	11	PHE	-	expression tag	UNP Q39YY5
B	12	ALA	-	expression tag	UNP Q39YY5
B	13	THR	-	expression tag	UNP Q39YY5
B	14	VAL	-	expression tag	UNP Q39YY5
B	15	ALA	-	expression tag	UNP Q39YY5
B	16	GLN	-	expression tag	UNP Q39YY5
B	17	ALA	-	expression tag	UNP Q39YY5
B	18	ALA	-	expression tag	UNP Q39YY5
B	19	SER	-	expression tag	UNP Q39YY5
B	20	TRP	-	expression tag	UNP Q39YY5
B	21	SER	-	expression tag	UNP Q39YY5
B	22	HIS	-	expression tag	UNP Q39YY5
B	23	PRO	-	expression tag	UNP Q39YY5
B	24	GLN	-	expression tag	UNP Q39YY5
B	25	PHE	-	expression tag	UNP Q39YY5
B	26	GLU	-	expression tag	UNP Q39YY5

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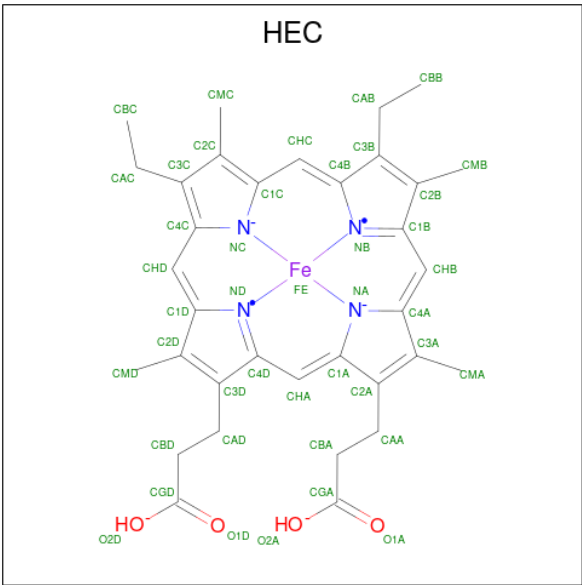
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	LYS	-	expression tag	UNP Q39YY5
B	28	GLY	-	expression tag	UNP Q39YY5
B	29	ALA	-	expression tag	UNP Q39YY5
C	-3	MET	-	initiating methionine	UNP Q39YY5
C	-2	LYS	-	expression tag	UNP Q39YY5
C	-1	LYS	-	expression tag	UNP Q39YY5
C	0	THR	-	expression tag	UNP Q39YY5
C	1	ALA	-	expression tag	UNP Q39YY5
C	2	ILE	-	expression tag	UNP Q39YY5
C	3	ALA	-	expression tag	UNP Q39YY5
C	4	ILE	-	expression tag	UNP Q39YY5
C	5	ALA	-	expression tag	UNP Q39YY5
C	6	VAL	-	expression tag	UNP Q39YY5
C	7	ALA	-	expression tag	UNP Q39YY5
C	8	LEU	-	expression tag	UNP Q39YY5
C	9	ALA	-	expression tag	UNP Q39YY5
C	10	GLY	-	expression tag	UNP Q39YY5
C	11	PHE	-	expression tag	UNP Q39YY5
C	12	ALA	-	expression tag	UNP Q39YY5
C	13	THR	-	expression tag	UNP Q39YY5
C	14	VAL	-	expression tag	UNP Q39YY5
C	15	ALA	-	expression tag	UNP Q39YY5
C	16	GLN	-	expression tag	UNP Q39YY5
C	17	ALA	-	expression tag	UNP Q39YY5
C	18	ALA	-	expression tag	UNP Q39YY5
C	19	SER	-	expression tag	UNP Q39YY5
C	20	TRP	-	expression tag	UNP Q39YY5
C	21	SER	-	expression tag	UNP Q39YY5
C	22	HIS	-	expression tag	UNP Q39YY5
C	23	PRO	-	expression tag	UNP Q39YY5
C	24	GLN	-	expression tag	UNP Q39YY5
C	25	PHE	-	expression tag	UNP Q39YY5
C	26	GLU	-	expression tag	UNP Q39YY5
C	27	LYS	-	expression tag	UNP Q39YY5
C	28	GLY	-	expression tag	UNP Q39YY5
C	29	ALA	-	expression tag	UNP Q39YY5
D	-3	MET	-	initiating methionine	UNP Q39YY5
D	-2	LYS	-	expression tag	UNP Q39YY5
D	-1	LYS	-	expression tag	UNP Q39YY5
D	0	THR	-	expression tag	UNP Q39YY5
D	1	ALA	-	expression tag	UNP Q39YY5
D	2	ILE	-	expression tag	UNP Q39YY5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	3	ALA	-	expression tag	UNP Q39YY5
D	4	ILE	-	expression tag	UNP Q39YY5
D	5	ALA	-	expression tag	UNP Q39YY5
D	6	VAL	-	expression tag	UNP Q39YY5
D	7	ALA	-	expression tag	UNP Q39YY5
D	8	LEU	-	expression tag	UNP Q39YY5
D	9	ALA	-	expression tag	UNP Q39YY5
D	10	GLY	-	expression tag	UNP Q39YY5
D	11	PHE	-	expression tag	UNP Q39YY5
D	12	ALA	-	expression tag	UNP Q39YY5
D	13	THR	-	expression tag	UNP Q39YY5
D	14	VAL	-	expression tag	UNP Q39YY5
D	15	ALA	-	expression tag	UNP Q39YY5
D	16	GLN	-	expression tag	UNP Q39YY5
D	17	ALA	-	expression tag	UNP Q39YY5
D	18	ALA	-	expression tag	UNP Q39YY5
D	19	SER	-	expression tag	UNP Q39YY5
D	20	TRP	-	expression tag	UNP Q39YY5
D	21	SER	-	expression tag	UNP Q39YY5
D	22	HIS	-	expression tag	UNP Q39YY5
D	23	PRO	-	expression tag	UNP Q39YY5
D	24	GLN	-	expression tag	UNP Q39YY5
D	25	PHE	-	expression tag	UNP Q39YY5
D	26	GLU	-	expression tag	UNP Q39YY5
D	27	LYS	-	expression tag	UNP Q39YY5
D	28	GLY	-	expression tag	UNP Q39YY5
D	29	ALA	-	expression tag	UNP Q39YY5

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



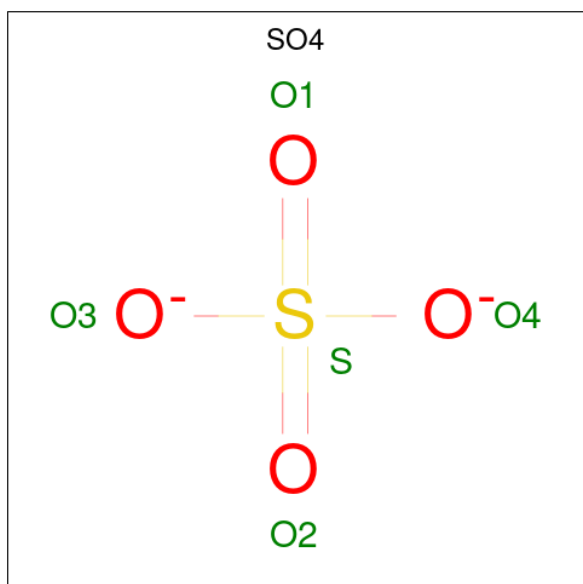
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S		
			5 4 1		0	0
3	A	1	Total	O S		
			5 4 1		0	0
3	A	1	Total	O S		
			5 4 1		0	0
3	B	1	Total	O S		
			5 4 1		0	0
3	B	1	Total	O S		
			5 4 1		0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

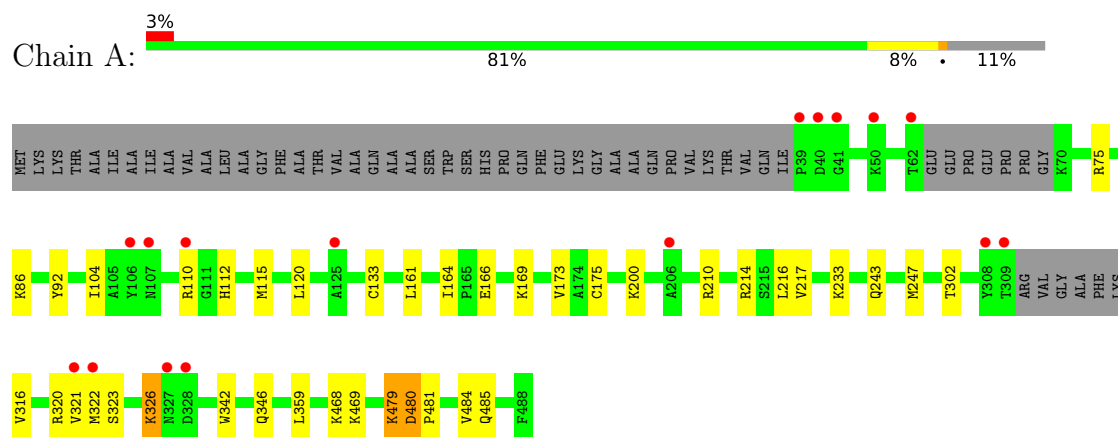
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total	O	0	1
			187	187		
4	B	154	Total	O	0	0
			154	154		
4	C	188	Total	O	0	1
			189	189		
4	D	197	Total	O	0	1
			198	198		

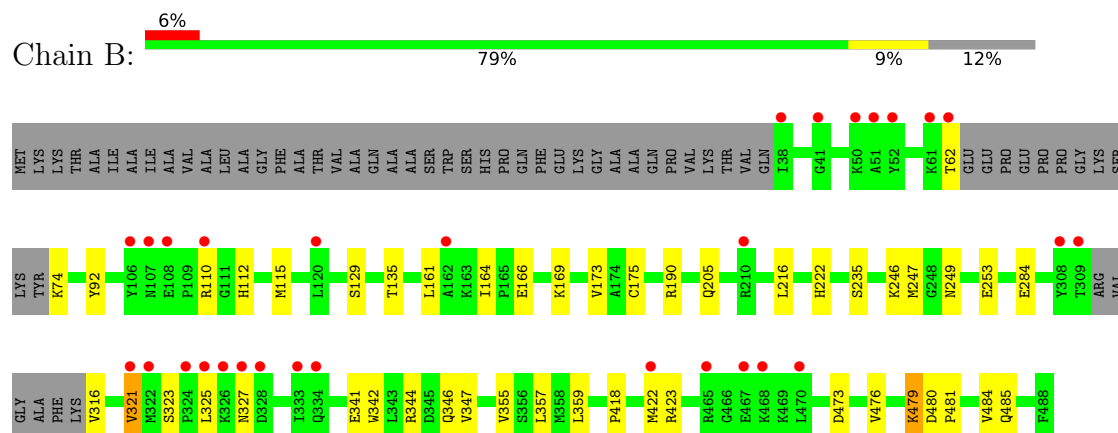
3 Residue-property plots [i](#)

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.

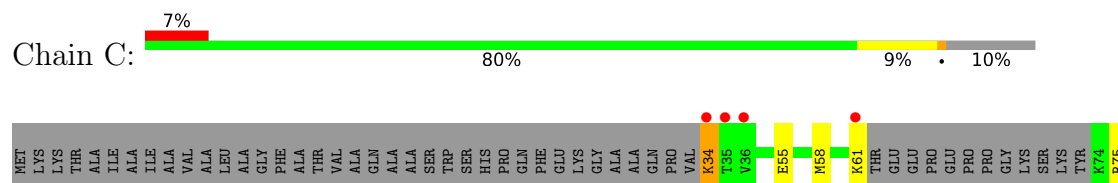
- Molecule 1: Nitrite reductase (cytochrome; ammonia-forming)

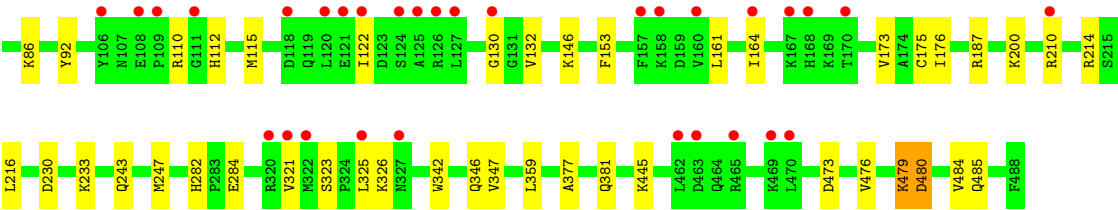


- Molecule 1: Nitrite reductase (cytochrome; ammonia-forming)

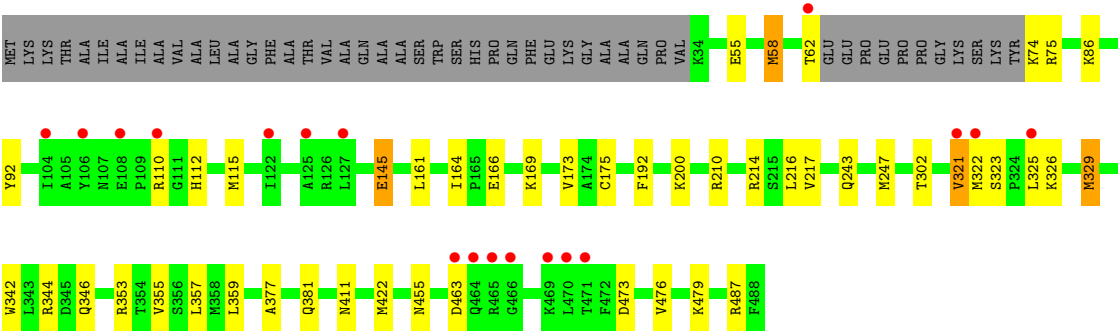
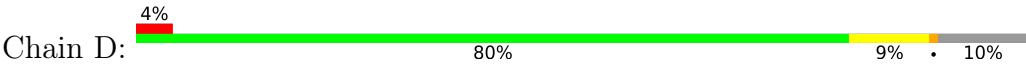


- Molecule 1: Nitrite reductase (cytochrome; ammonia-forming)





● Molecule 1: Nitrite reductase (cytochrome; ammonia-forming)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.08Å 91.97Å 123.94Å 90.00° 99.06° 90.00°	Depositor
Resolution (Å)	122.39 – 1.94 122.39 – 1.94	Depositor EDS
% Data completeness (in resolution range)	62.1 (122.39-1.94) 62.1 (122.39-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.94Å)	Xtriage
Refinement program	BUSTER 2.10.4 (8-JUN-2022)	Depositor
R, R_{free}	0.193 , 0.227 0.187 , 0.217	Depositor DCC
R_{free} test set	4540 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15471	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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 45.55 % 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 1.2998e-04. 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: SO4, HEC

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	0.72	0/3510	1.02	3/4733 (0.1%)
1	B	0.72	0/3473	1.02	2/4690 (0.0%)
1	C	0.73	0/3567	1.03	4/4814 (0.1%)
1	D	0.77	2/3572 (0.1%)	1.03	3/4823 (0.1%)
All	All	0.74	2/14122 (0.0%)	1.03	12/19060 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	329	MET	SD-CE	-7.71	1.60	1.79
1	D	58	MET	SD-CE	-6.48	1.63	1.79

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	480	ASP	CA-CB-CG	6.94	119.54	112.60
1	D	479	LYS	CA-C-N	6.33	130.29	120.60
1	D	479	LYS	C-N-CA	6.33	130.29	120.60
1	A	479	LYS	CA-C-N	5.84	129.55	120.68
1	A	479	LYS	C-N-CA	5.84	129.55	120.68

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	3433	0	3390	25	0
1	B	3398	0	3339	25	0
1	C	3489	0	3453	27	0
1	D	3493	0	3450	31	0
2	A	215	0	150	6	0
2	B	215	0	150	6	0
2	C	215	0	150	2	0
2	D	215	0	150	6	0
3	A	15	0	0	0	0
3	B	20	0	0	0	0
3	C	15	0	0	0	0
3	D	20	0	0	0	0
4	A	187	0	0	0	0
4	B	154	0	0	0	0
4	C	189	0	0	1	0
4	D	198	0	0	1	0
All	All	15471	0	14232	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 114 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)
2:B:503:HEC:HHA	2:B:503:HEC:HBD1	1.60	0.83
1:D:455:ASN:HB2	1:D:487:ARG:HE	1.42	0.81
1:A:210:ARG:HE	1:A:214:ARG:HH22	1.33	0.74
1:A:480:ASP:OD1	1:A:481:PRO:HD2	1.91	0.70
1:A:210:ARG:HE	1:A:214:ARG:NH2	1.88	0.69

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	431/492 (88%)	414 (96%)	16 (4%)	1 (0%)	43	37
1	B	428/492 (87%)	413 (96%)	14 (3%)	1 (0%)	43	37
1	C	439/492 (89%)	421 (96%)	16 (4%)	2 (0%)	24	15
1	D	440/492 (89%)	422 (96%)	17 (4%)	1 (0%)	43	37
All	All	1738/1968 (88%)	1670 (96%)	63 (4%)	5 (0%)	36	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	130	GLY
1	A	321	VAL
1	B	321	VAL
1	D	321	VAL
1	C	282	HIS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	360/407 (88%)	354 (98%)	6 (2%)	53	44
1	B	358/407 (88%)	353 (99%)	5 (1%)	59	52
1	C	368/407 (90%)	362 (98%)	6 (2%)	55	46
1	D	368/407 (90%)	362 (98%)	6 (2%)	55	46
All	All	1454/1628 (89%)	1431 (98%)	23 (2%)	55	46

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	146	LYS
1	D	145	GLU
1	C	284	GLU

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Mol	Chain	Res	Type
1	D	175	CYS
1	B	175	CYS

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

Mol	Chain	Res	Type
1	D	270	GLN
1	D	346	GLN
1	B	327	ASN
1	C	258	GLN
1	C	270	GLN

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](#)

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEC	B	501	1,4	50,50,50	1.57	8 (16%)	68,82,82	1.28	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	B	504	1	50,50,50	1.44	8 (16%)	68,82,82	1.20	2 (2%)
2	HEC	C	503	1,4	50,50,50	1.48	7 (14%)	68,82,82	1.21	2 (2%)
2	HEC	D	501	1	50,50,50	1.47	8 (16%)	68,82,82	1.18	3 (4%)
2	HEC	B	503	1	50,50,50	1.52	7 (14%)	68,82,82	1.35	4 (5%)
3	SO4	B	509	-	4,4,4	0.26	0	6,6,6	0.21	0
2	HEC	A	503	1	50,50,50	1.55	10 (20%)	68,82,82	1.44	5 (7%)
3	SO4	C	507	-	4,4,4	0.25	0	6,6,6	0.74	0
3	SO4	D	509	-	4,4,4	0.21	0	6,6,6	0.59	0
2	HEC	A	502	1,4	50,50,50	1.59	9 (18%)	68,82,82	1.16	2 (2%)
2	HEC	D	505	1,4	50,50,50	1.51	9 (18%)	68,82,82	1.22	2 (2%)
3	SO4	D	507	-	4,4,4	0.20	0	6,6,6	0.22	0
2	HEC	B	505	1	50,50,50	1.56	9 (18%)	68,82,82	1.21	2 (2%)
3	SO4	B	506	-	4,4,4	0.30	0	6,6,6	0.61	0
2	HEC	A	504	1	50,50,50	1.47	7 (14%)	68,82,82	1.18	2 (2%)
3	SO4	B	508	-	4,4,4	0.24	0	6,6,6	0.27	0
3	SO4	B	507	-	4,4,4	0.20	0	6,6,6	0.49	0
3	SO4	C	506	-	4,4,4	0.23	0	6,6,6	1.11	1 (16%)
3	SO4	D	506	-	4,4,4	0.26	0	6,6,6	0.77	0
3	SO4	D	508	-	4,4,4	0.26	0	6,6,6	0.32	0
2	HEC	A	501	1	50,50,50	1.45	8 (16%)	68,82,82	1.25	3 (4%)
2	HEC	C	505	1	50,50,50	1.52	8 (16%)	68,82,82	1.23	2 (2%)
2	HEC	C	502	1	50,50,50	1.52	10 (20%)	68,82,82	1.24	5 (7%)
2	HEC	B	502	1	50,50,50	1.58	9 (18%)	68,82,82	1.19	3 (4%)
3	SO4	A	506	-	4,4,4	0.24	0	6,6,6	0.26	0
3	SO4	C	508	-	4,4,4	0.22	0	6,6,6	0.35	0
2	HEC	D	503	1	50,50,50	1.54	11 (22%)	68,82,82	1.40	7 (10%)
3	SO4	A	507	-	4,4,4	0.20	0	6,6,6	0.23	0
3	SO4	A	508	-	4,4,4	0.19	0	6,6,6	0.18	0
2	HEC	A	505	1	50,50,50	1.53	9 (18%)	68,82,82	1.22	2 (2%)
2	HEC	C	501	1	50,50,50	1.52	9 (18%)	68,82,82	1.13	3 (4%)
2	HEC	D	502	1	50,50,50	1.53	8 (16%)	68,82,82	1.24	5 (7%)
2	HEC	C	504	1	50,50,50	1.47	10 (20%)	68,82,82	1.18	2 (2%)
2	HEC	D	504	1	50,50,50	1.47	10 (20%)	68,82,82	1.16	3 (4%)

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	B	501	1,4	1/1/3/7	11/14/54/54	-
2	HEC	B	504	1	1/1/3/7	7/14/54/54	-
2	HEC	C	503	1,4	1/1/3/7	2/14/54/54	-
2	HEC	D	501	1	1/1/3/7	8/14/54/54	-
2	HEC	B	503	1	1/1/3/7	5/14/54/54	-
2	HEC	A	503	1	1/1/3/7	9/14/54/54	-
2	HEC	A	502	1,4	1/1/3/7	8/14/54/54	-
2	HEC	D	505	1,4	1/1/3/7	5/14/54/54	-
2	HEC	B	505	1	1/1/3/7	8/14/54/54	-
2	HEC	A	504	1	1/1/3/7	7/14/54/54	-
2	HEC	A	501	1	1/1/3/7	6/14/54/54	-
2	HEC	C	505	1	1/1/3/7	8/14/54/54	-
2	HEC	C	502	1	1/1/3/7	6/14/54/54	-
2	HEC	B	502	1	1/1/3/7	5/14/54/54	-
2	HEC	D	503	1	1/1/3/7	9/14/54/54	-
2	HEC	A	505	1	1/1/3/7	10/14/54/54	-
2	HEC	C	501	1	1/1/3/7	6/14/54/54	-
2	HEC	D	502	1	1/1/3/7	9/14/54/54	-
2	HEC	C	504	1	1/1/3/7	5/14/54/54	-
2	HEC	D	504	1	1/1/3/7	6/14/54/54	-

The worst 5 of 174 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEC	CBB-CAB	-4.49	1.31	1.51
2	C	501	HEC	CBC-CAC	-4.46	1.31	1.51
2	A	502	HEC	CBB-CAB	-4.44	1.31	1.51
2	B	502	HEC	CBC-CAC	-4.42	1.31	1.51
2	D	501	HEC	CBB-CAB	-4.40	1.31	1.51

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	HEC	CBC-CAC-C3C	6.37	129.99	112.43
2	A	501	HEC	CBC-CAC-C3C	6.36	129.96	112.43
2	A	503	HEC	CBC-CAC-C3C	6.23	129.60	112.43
2	C	502	HEC	CBC-CAC-C3C	6.18	129.46	112.43
2	C	505	HEC	CBB-CAB-C3B	6.11	129.28	112.43

5 of 20 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	HEC	NA
2	A	502	HEC	NA
2	A	503	HEC	NA
2	A	504	HEC	NA
2	A	505	HEC	NA

5 of 140 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	HEC	C1A-C2A-CAA-CBA
2	B	501	HEC	C3A-C2A-CAA-CBA
2	B	503	HEC	C2D-C3D-CAD-CBD
2	D	502	HEC	C2A-CAA-CBA-CGA
2	C	505	HEC	C2B-C3B-CAB-CBB

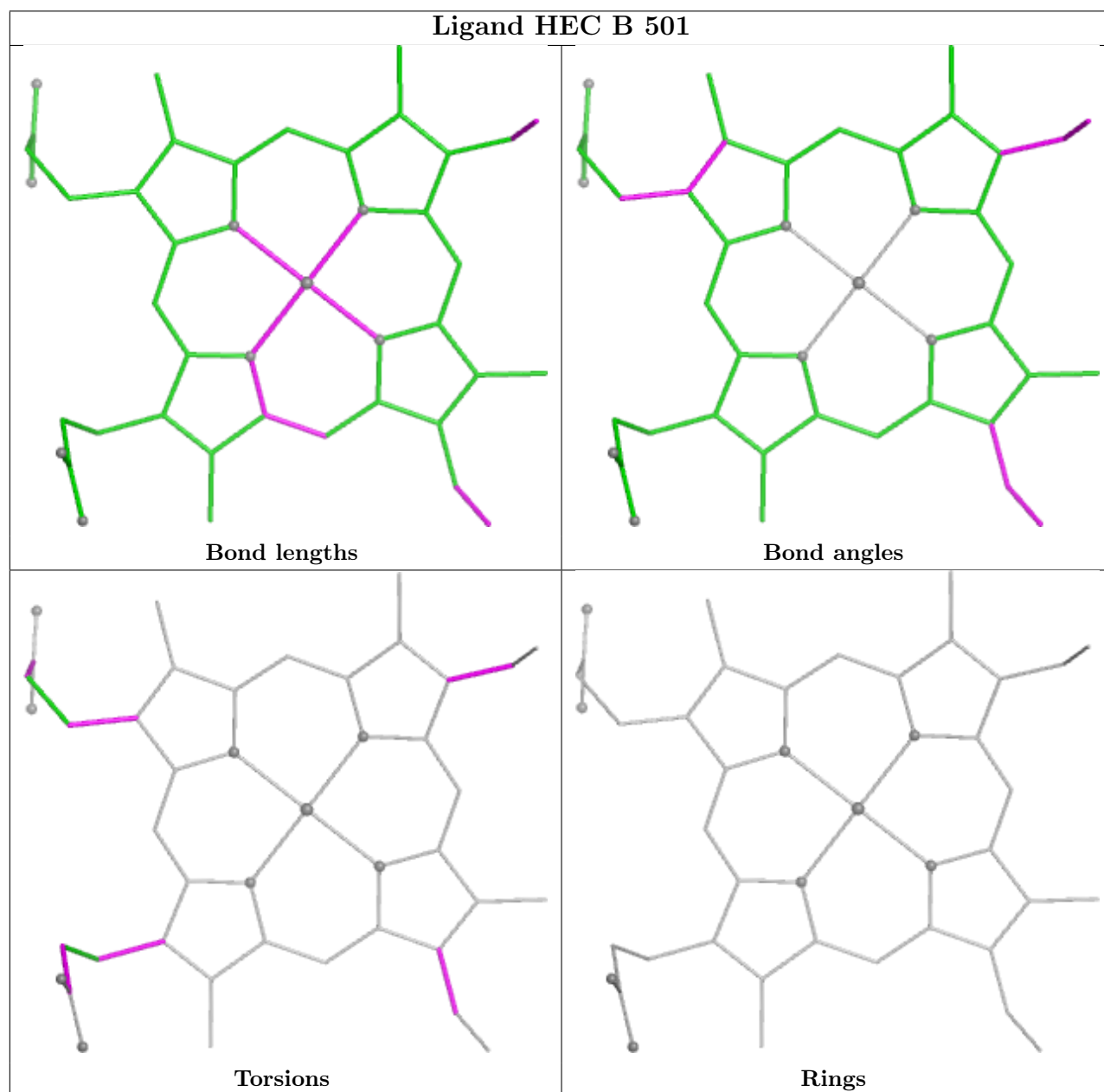
There are no ring outliers.

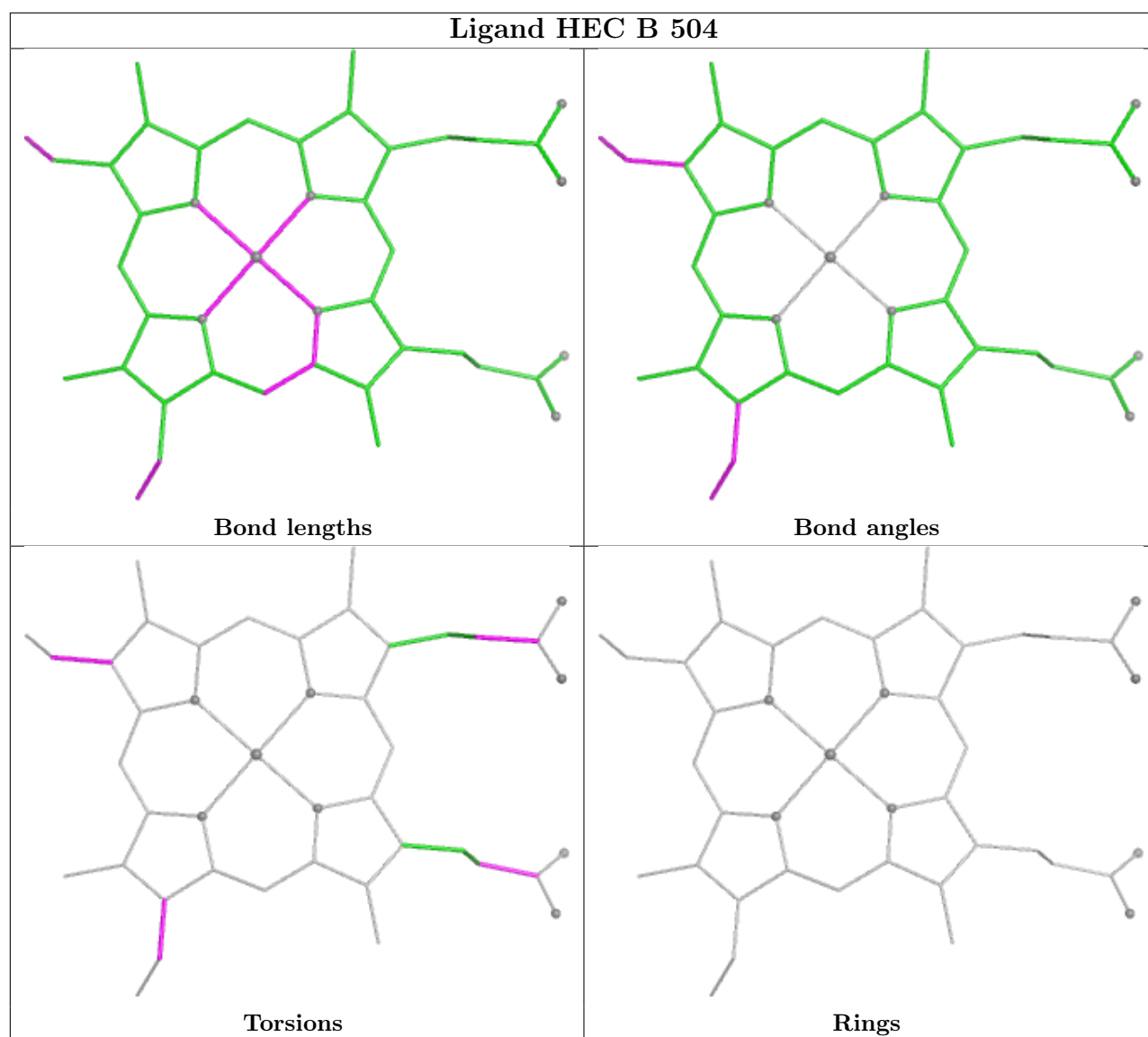
12 monomers are involved in 20 short contacts:

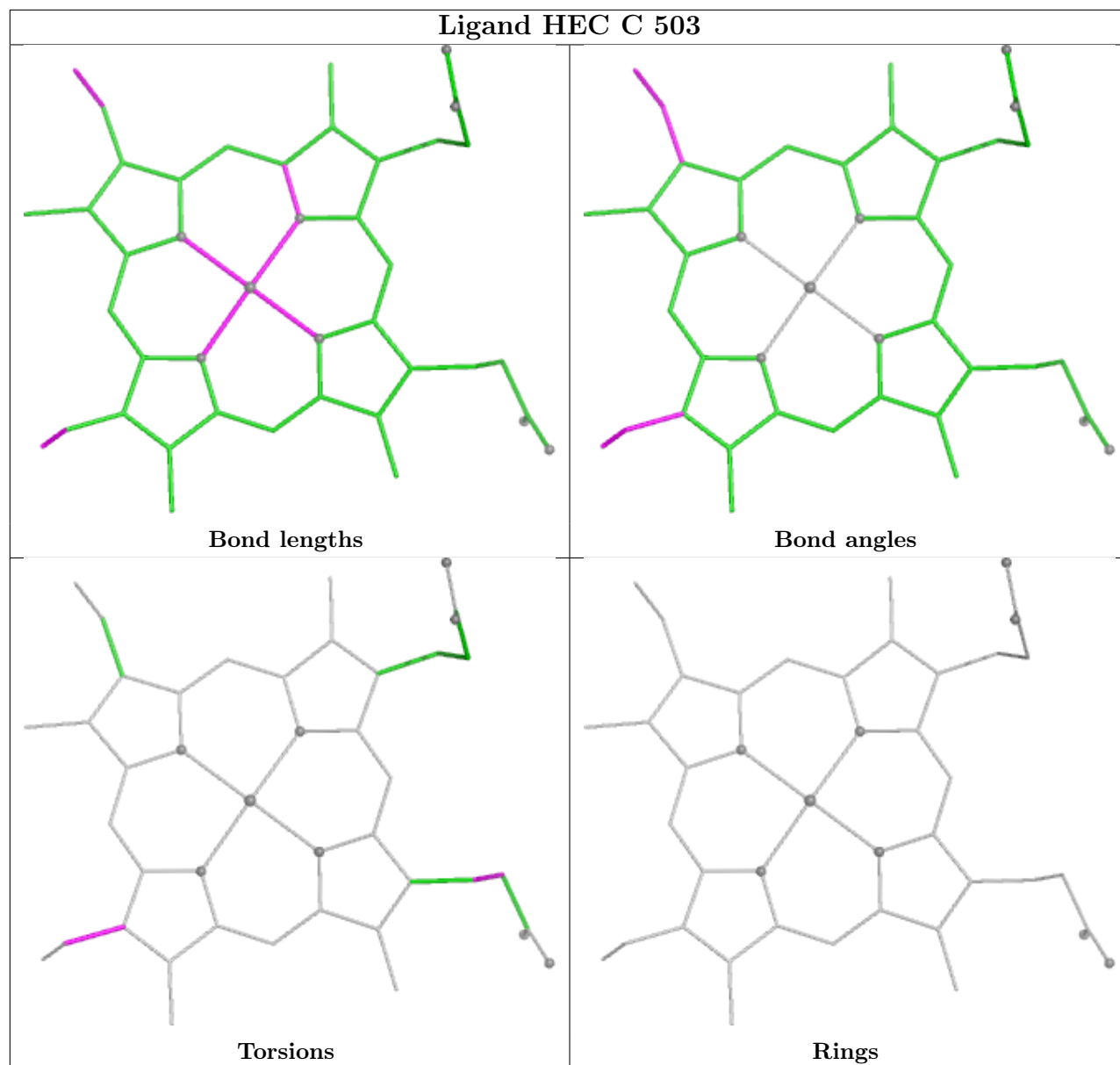
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEC	1	0
2	B	504	HEC	2	0
2	D	501	HEC	1	0
2	B	503	HEC	2	0
2	A	503	HEC	1	0
2	D	505	HEC	1	0
2	A	504	HEC	3	0
2	B	502	HEC	2	0
2	D	503	HEC	3	0
2	A	505	HEC	2	0
2	C	504	HEC	2	0
2	D	504	HEC	1	0

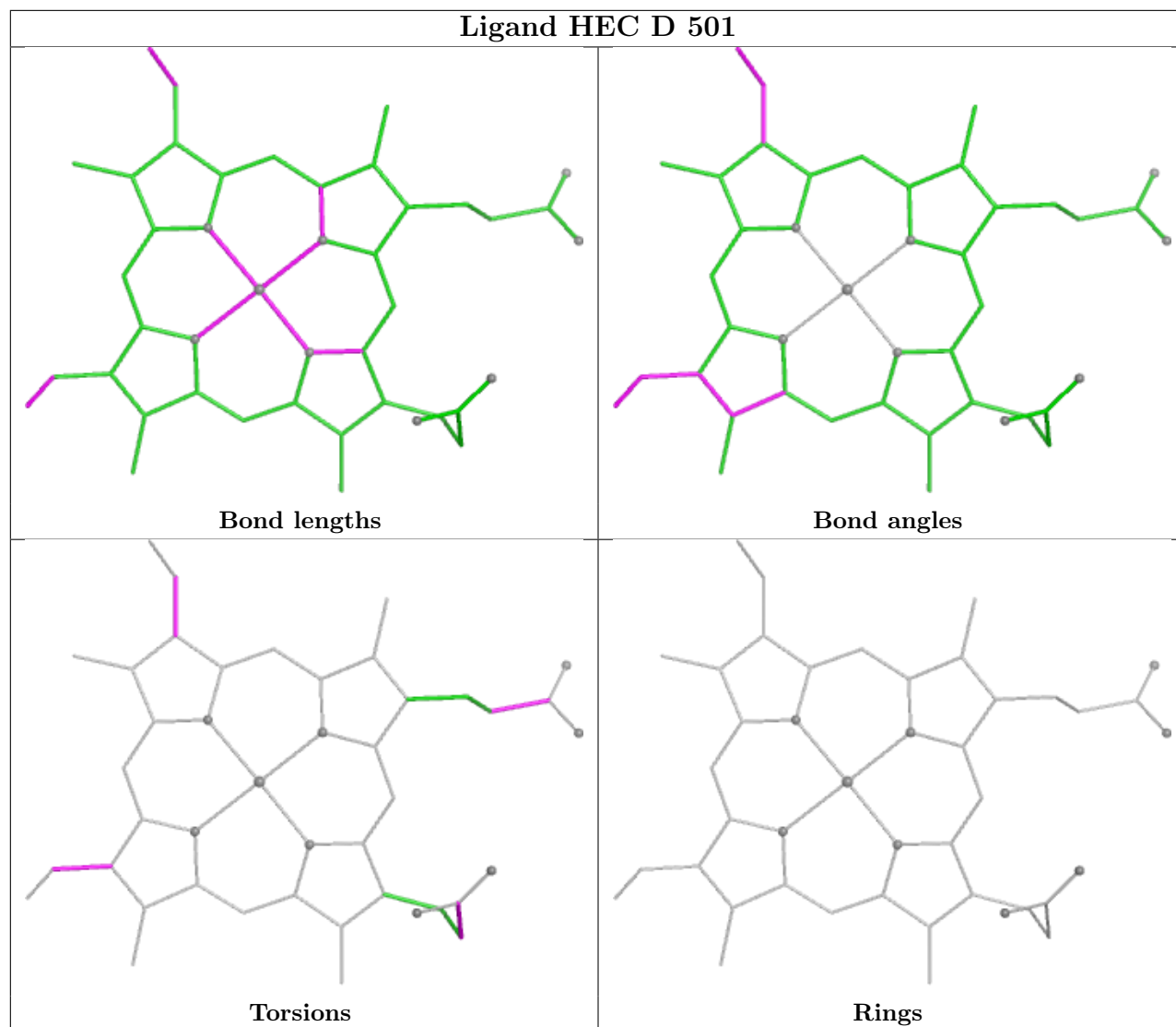
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

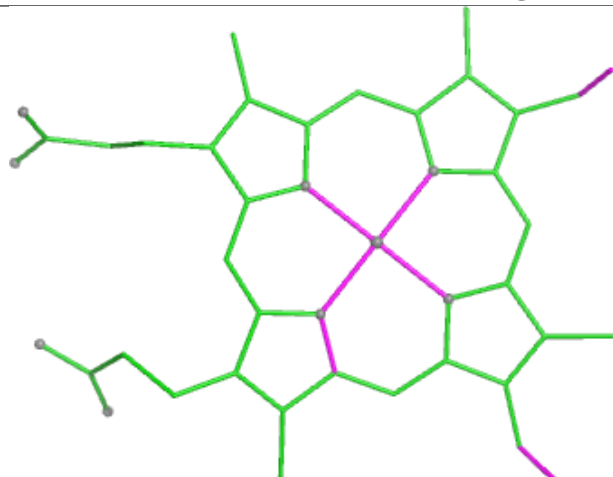




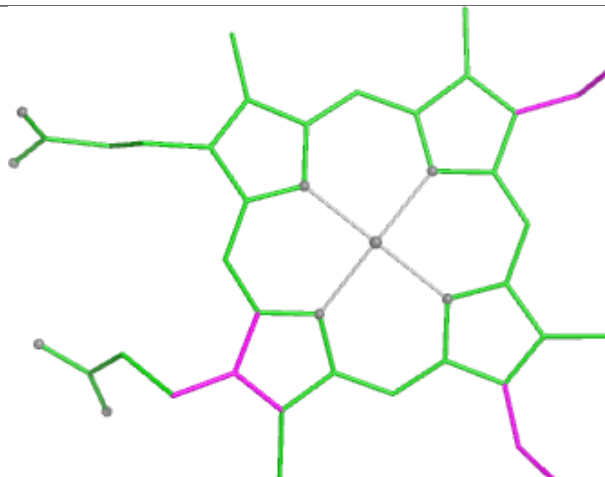




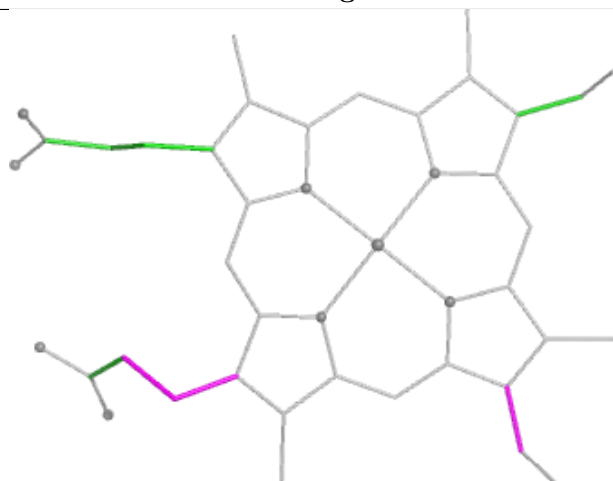
Ligand HEC B 503



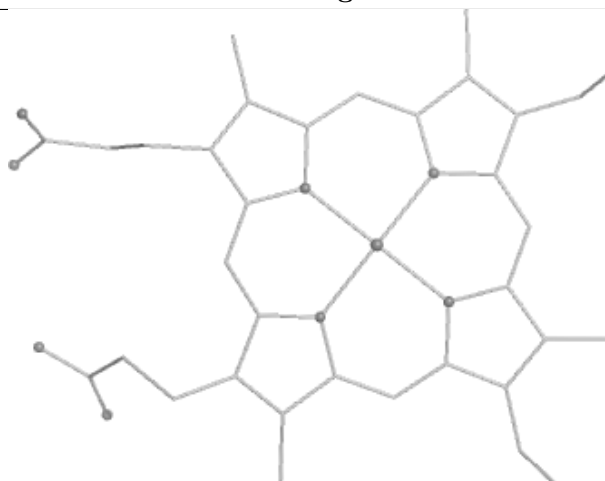
Bond lengths



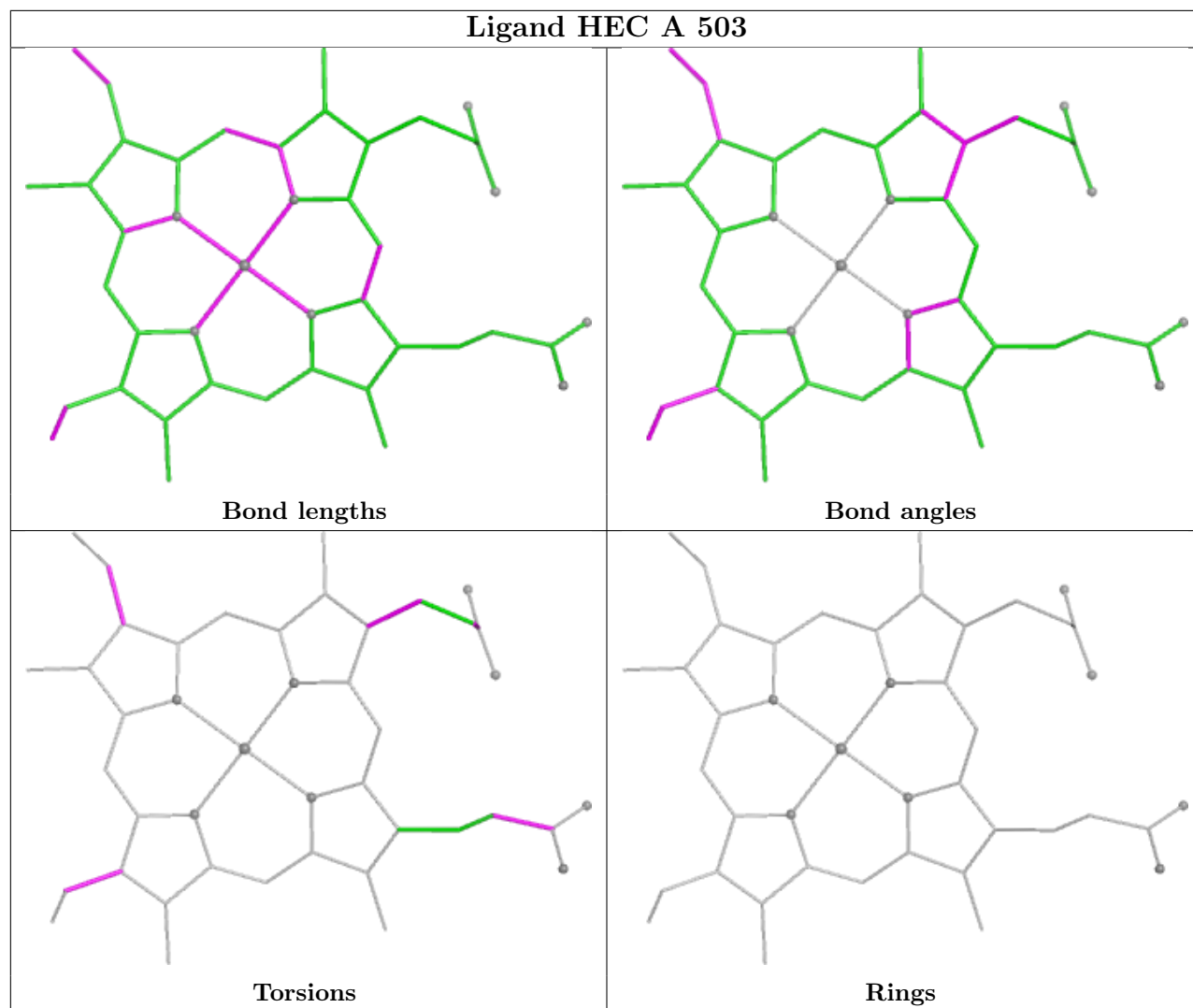
Bond angles

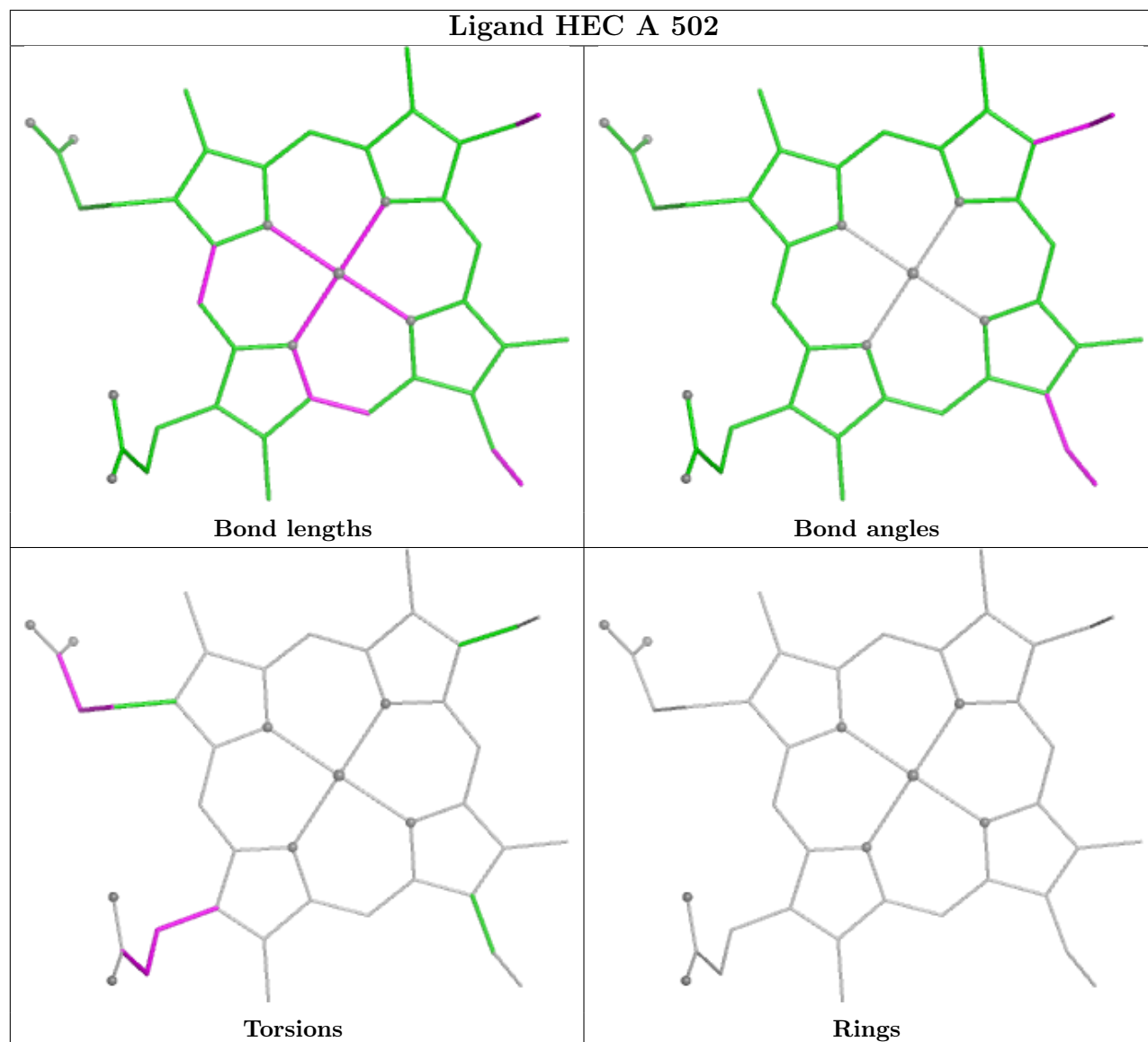


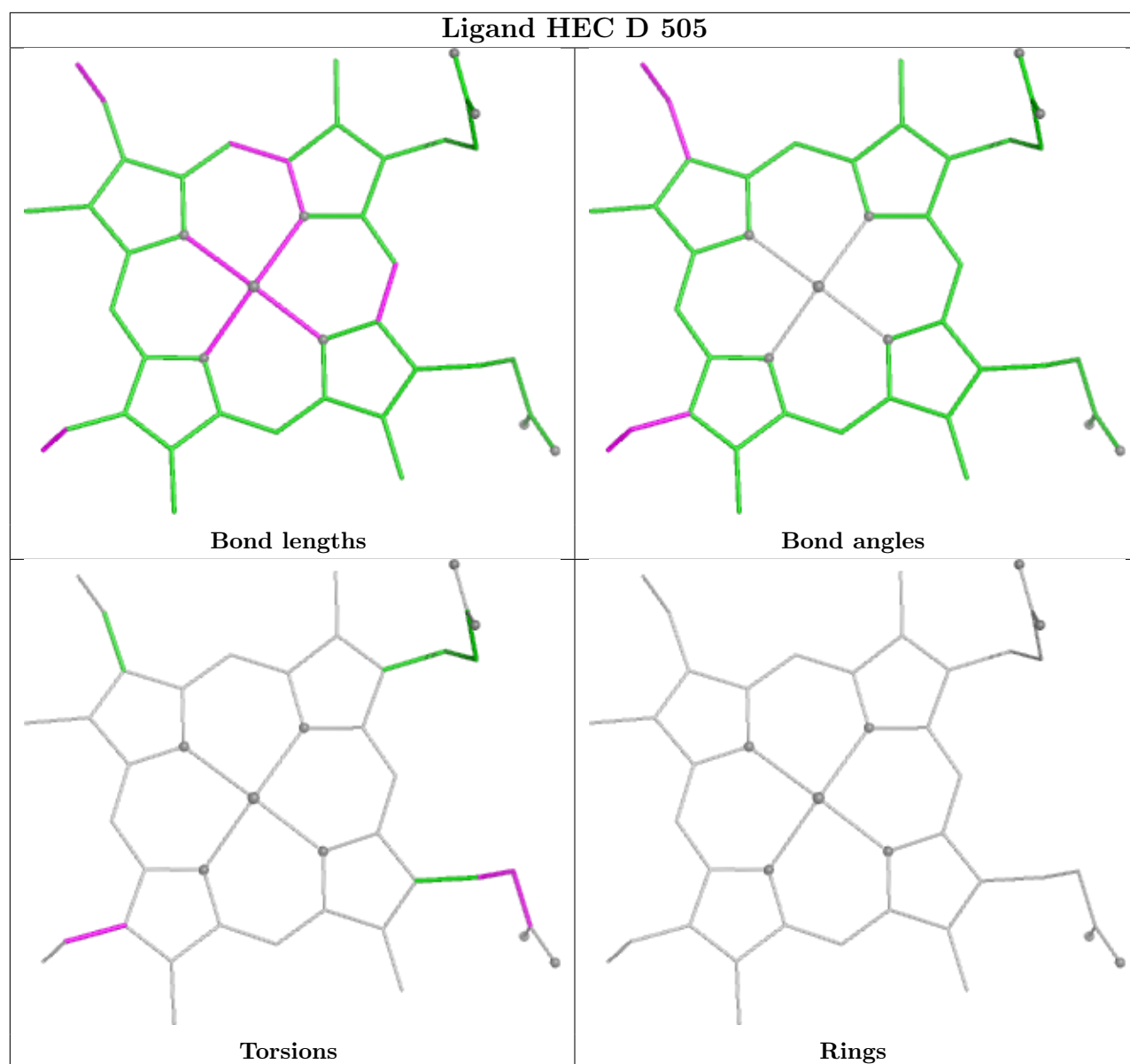
Torsions

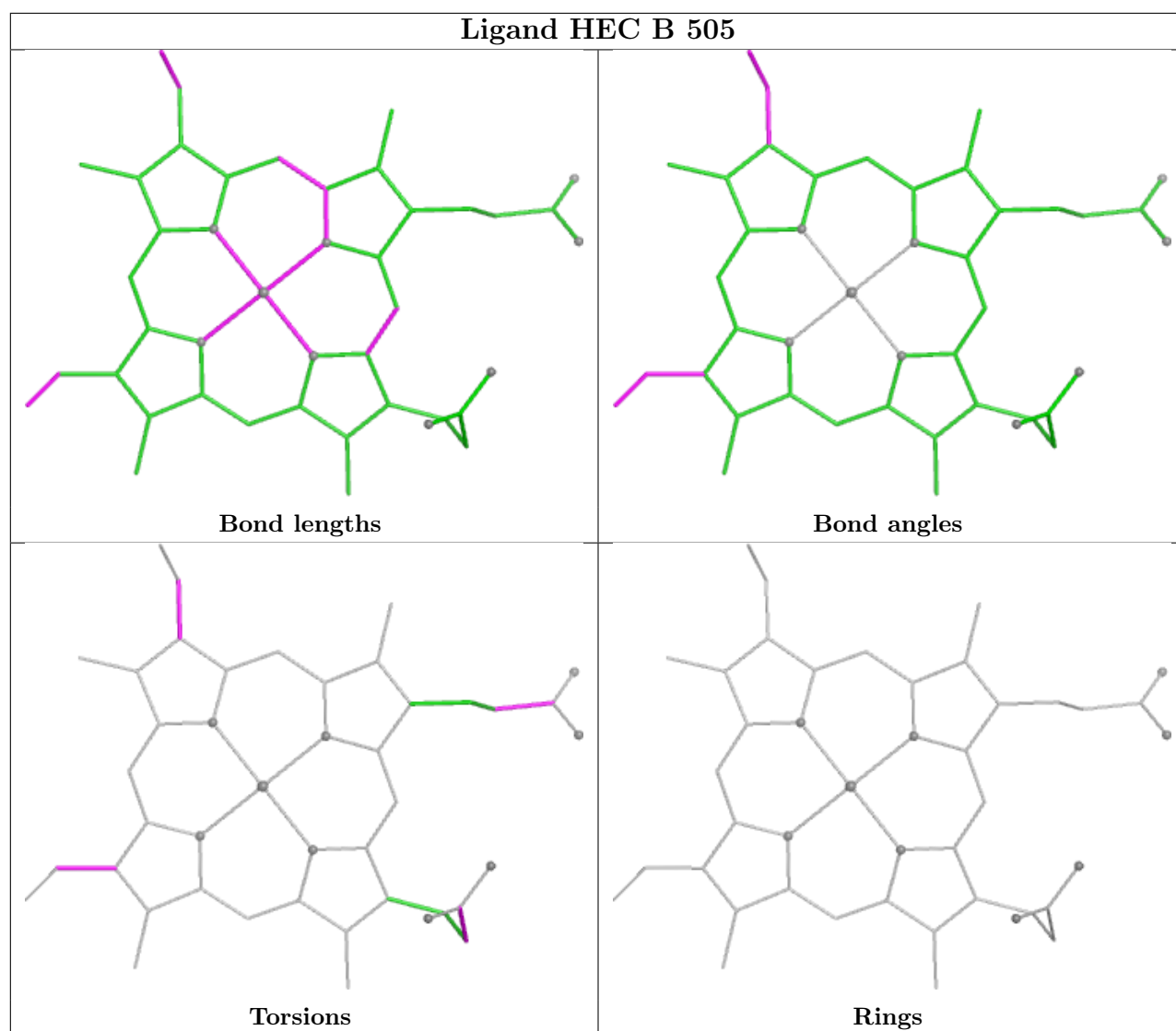


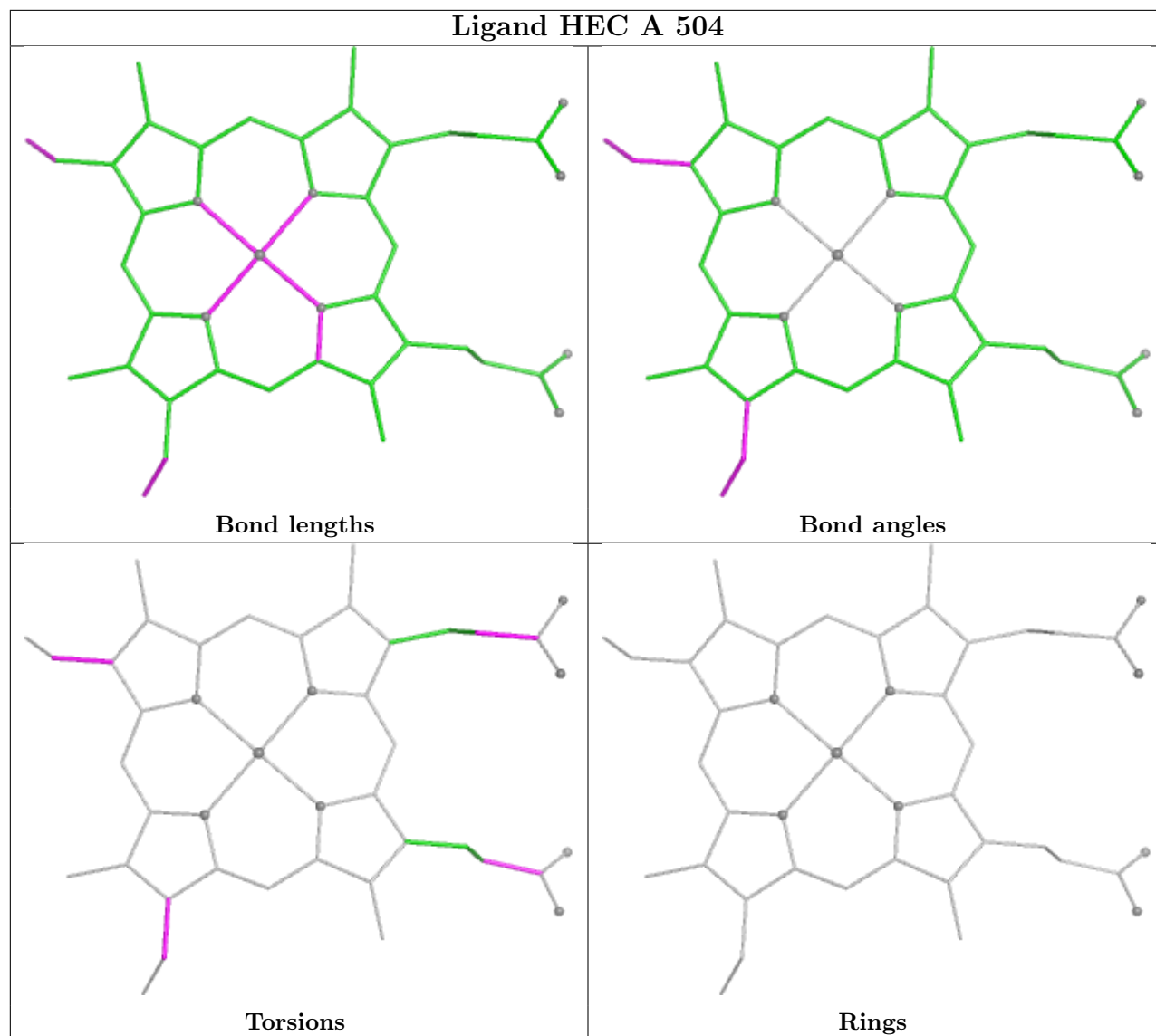
Rings

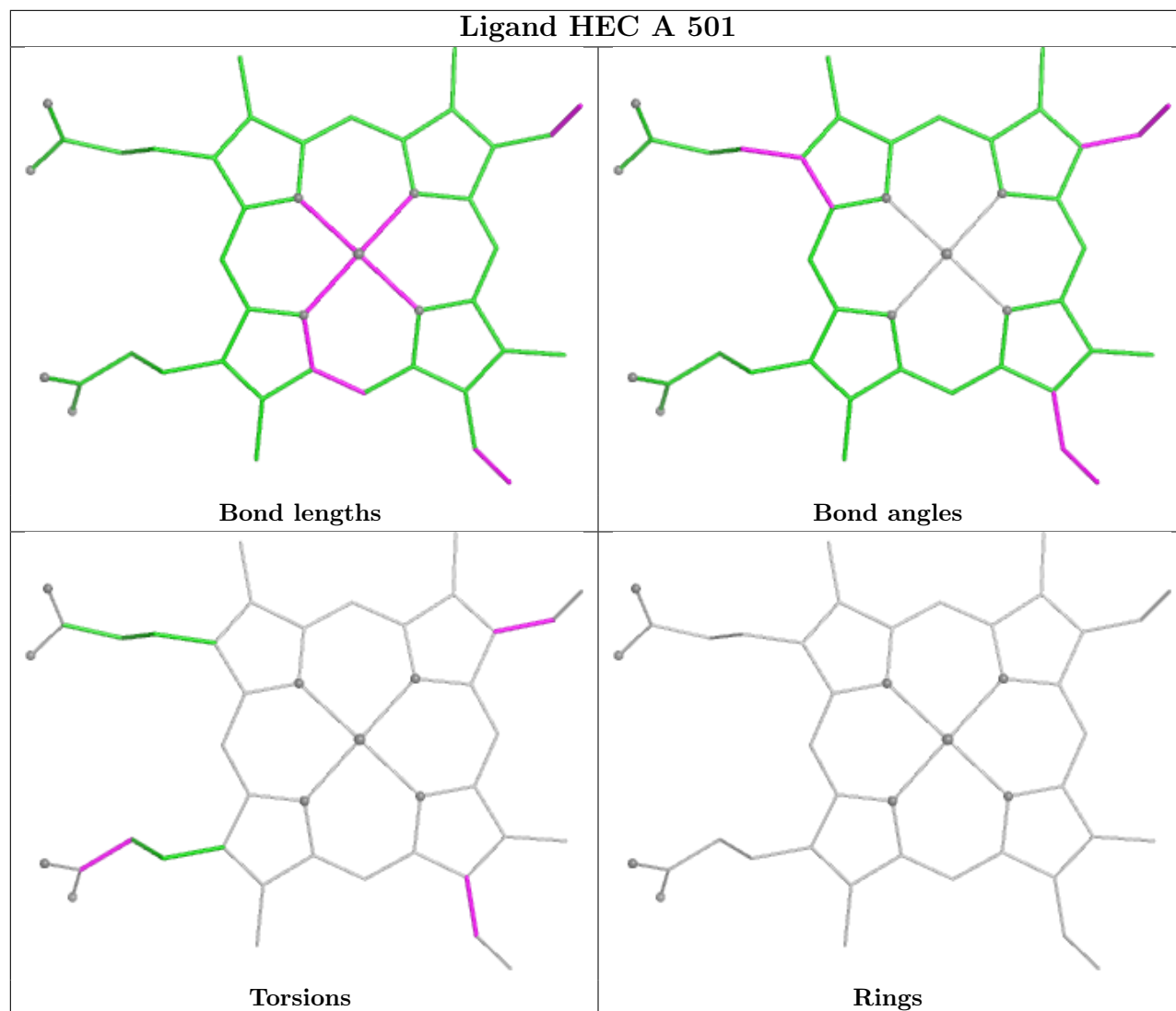




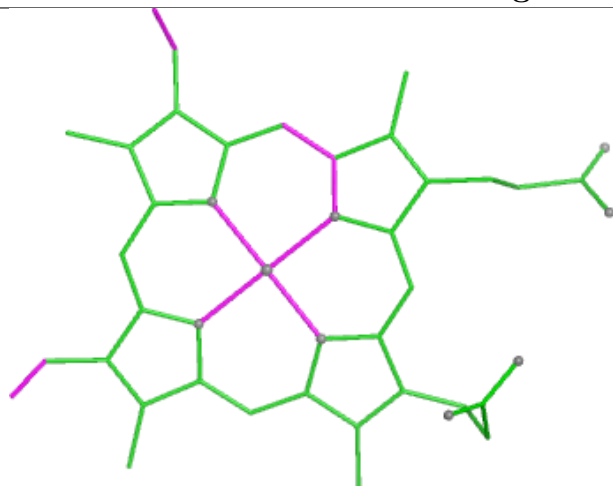




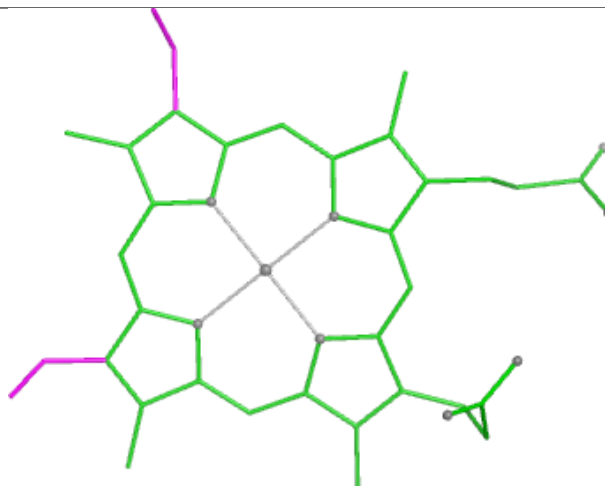




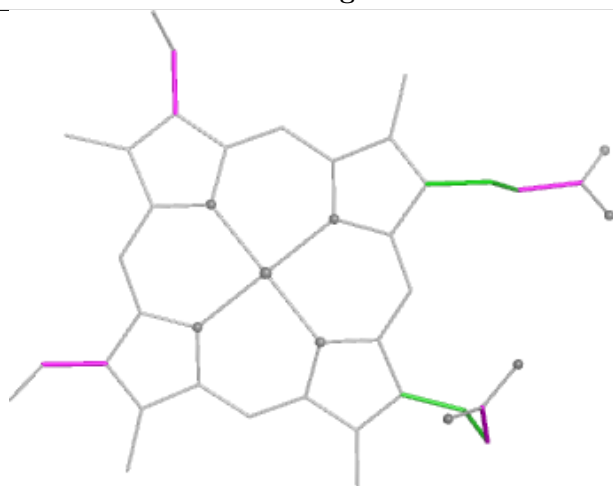
Ligand HEC C 505



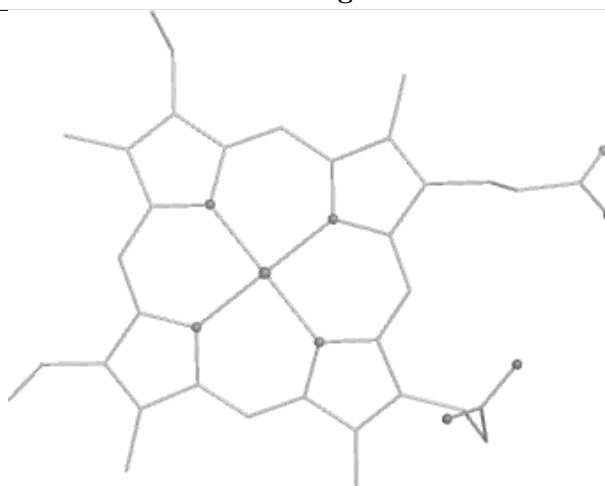
Bond lengths



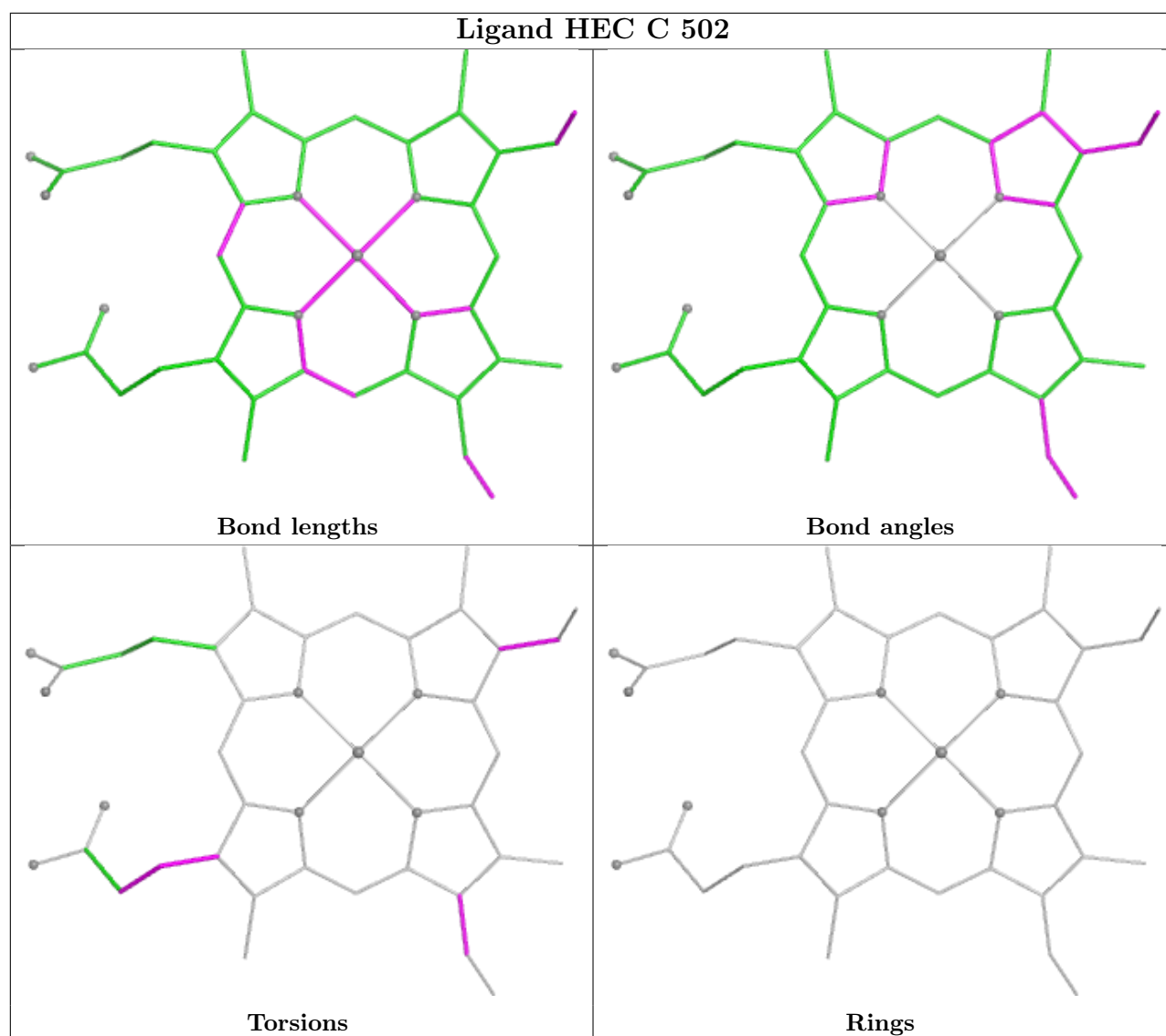
Bond angles

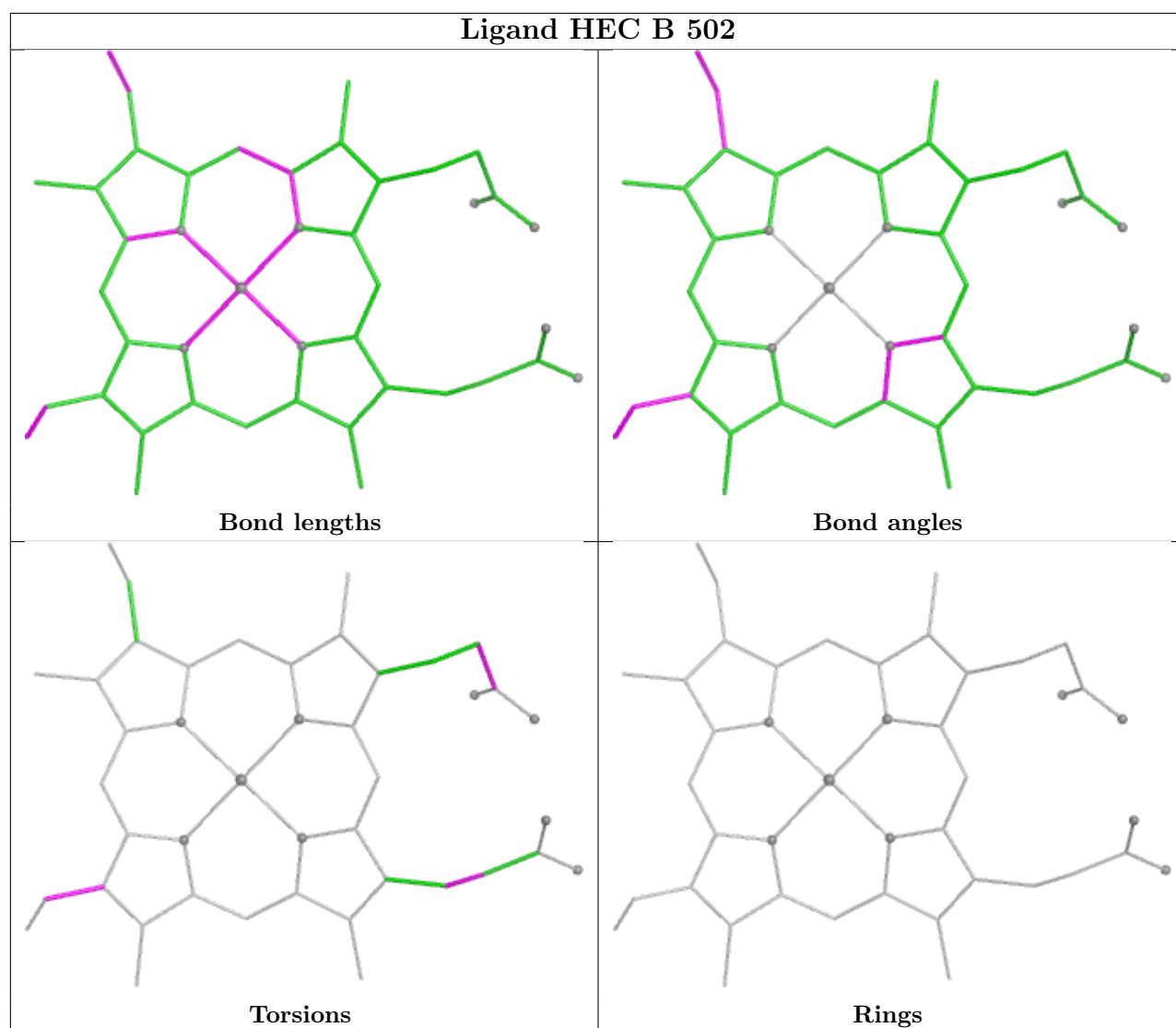


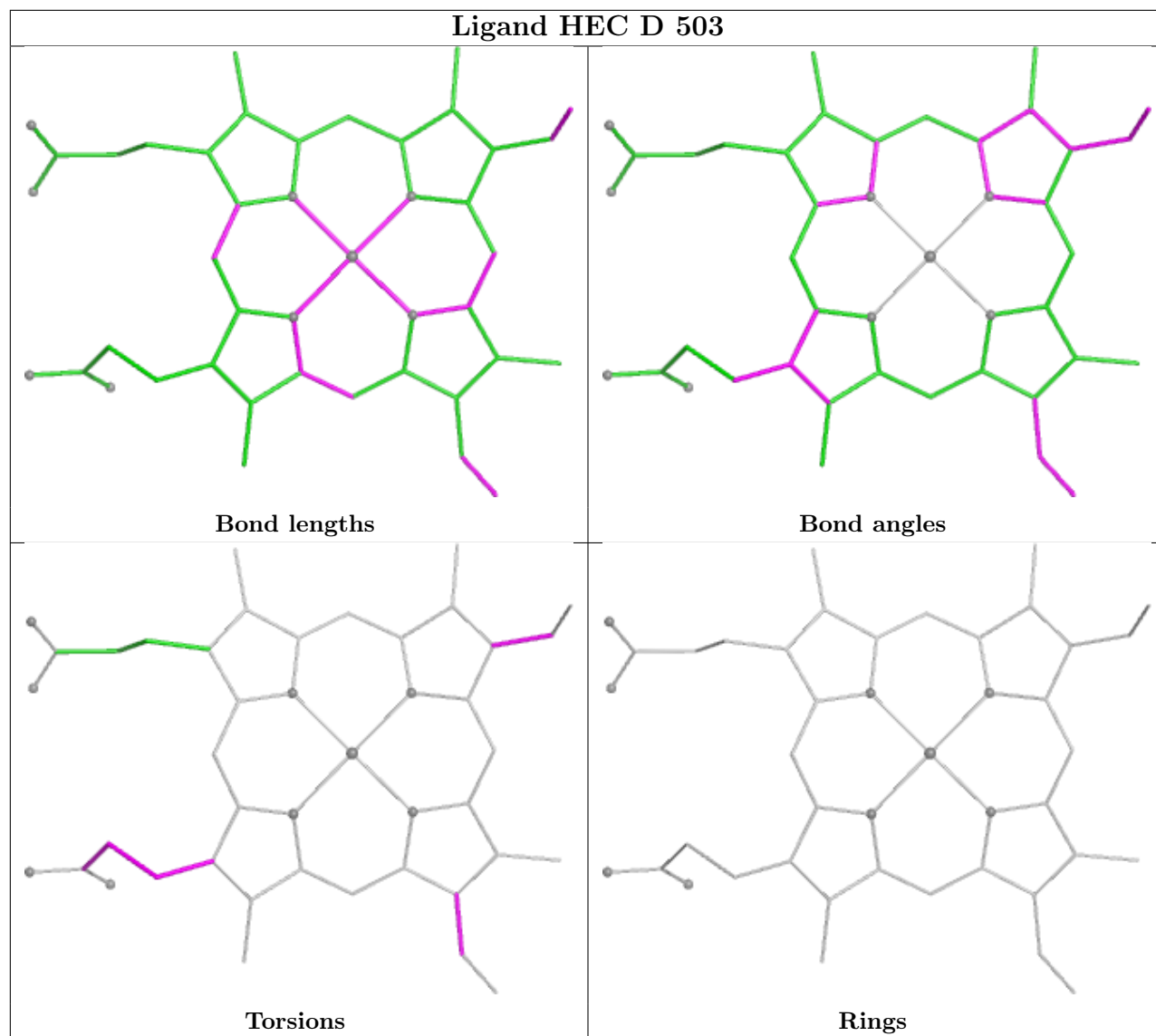
Torsions

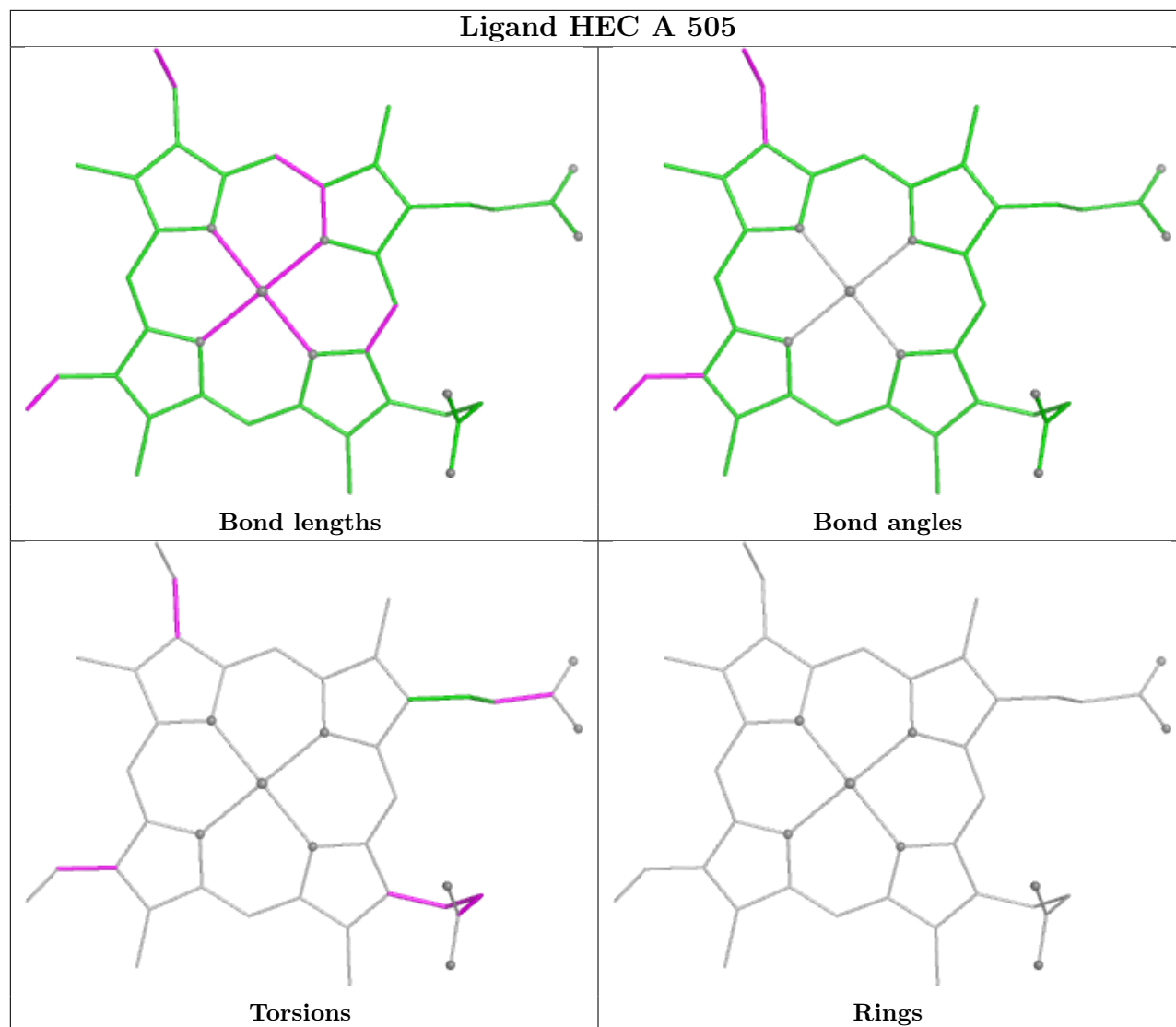


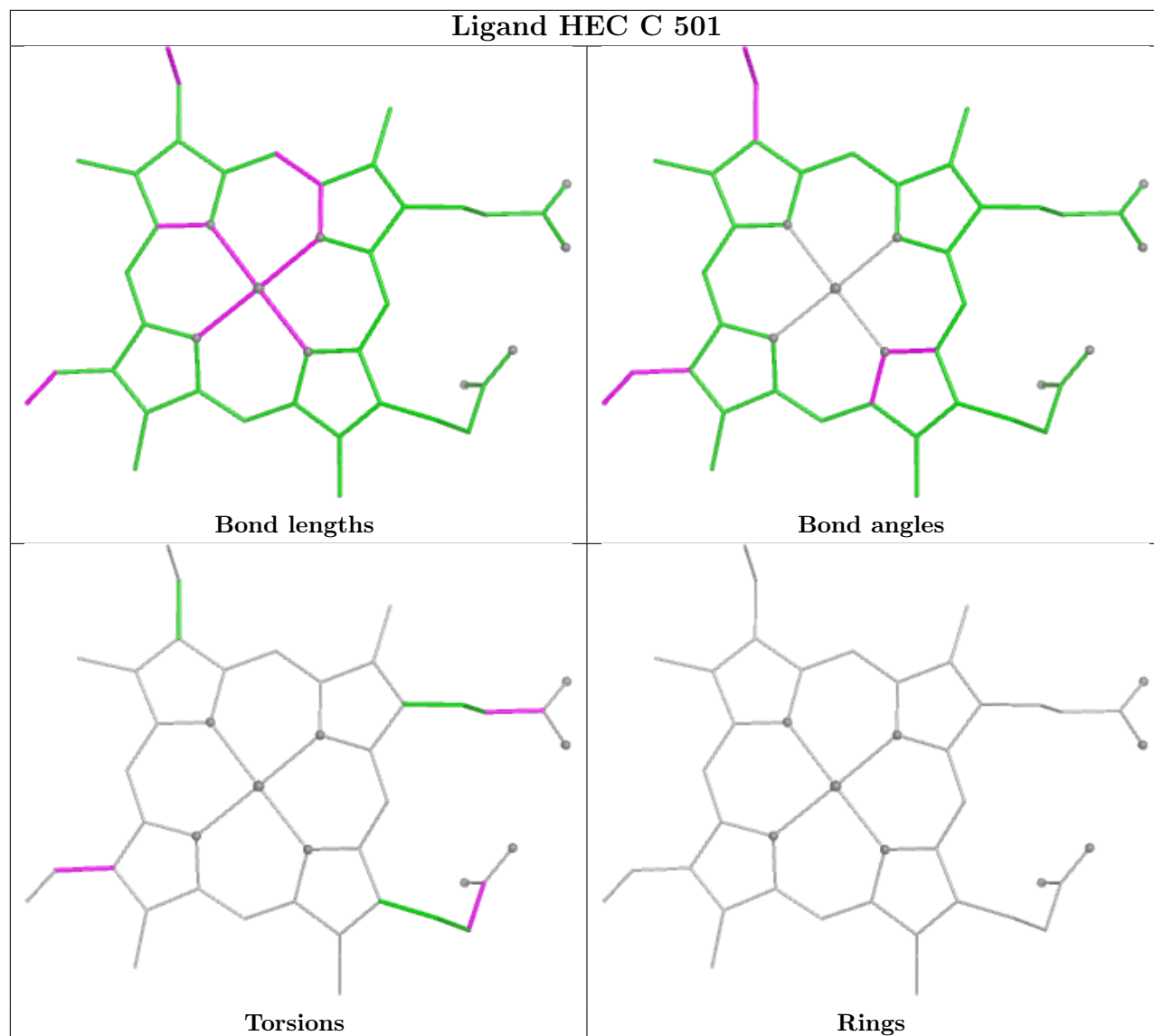
Rings

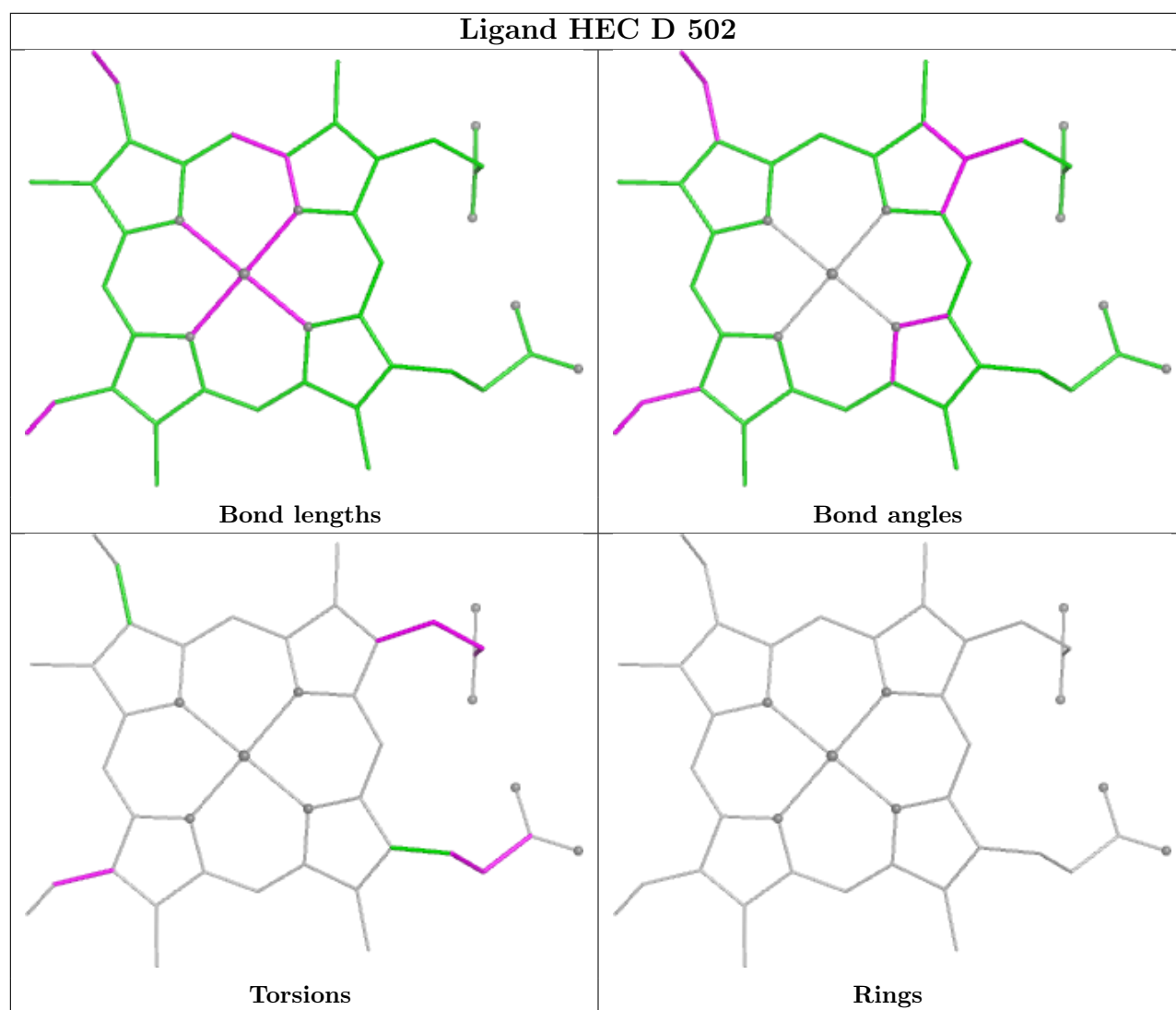


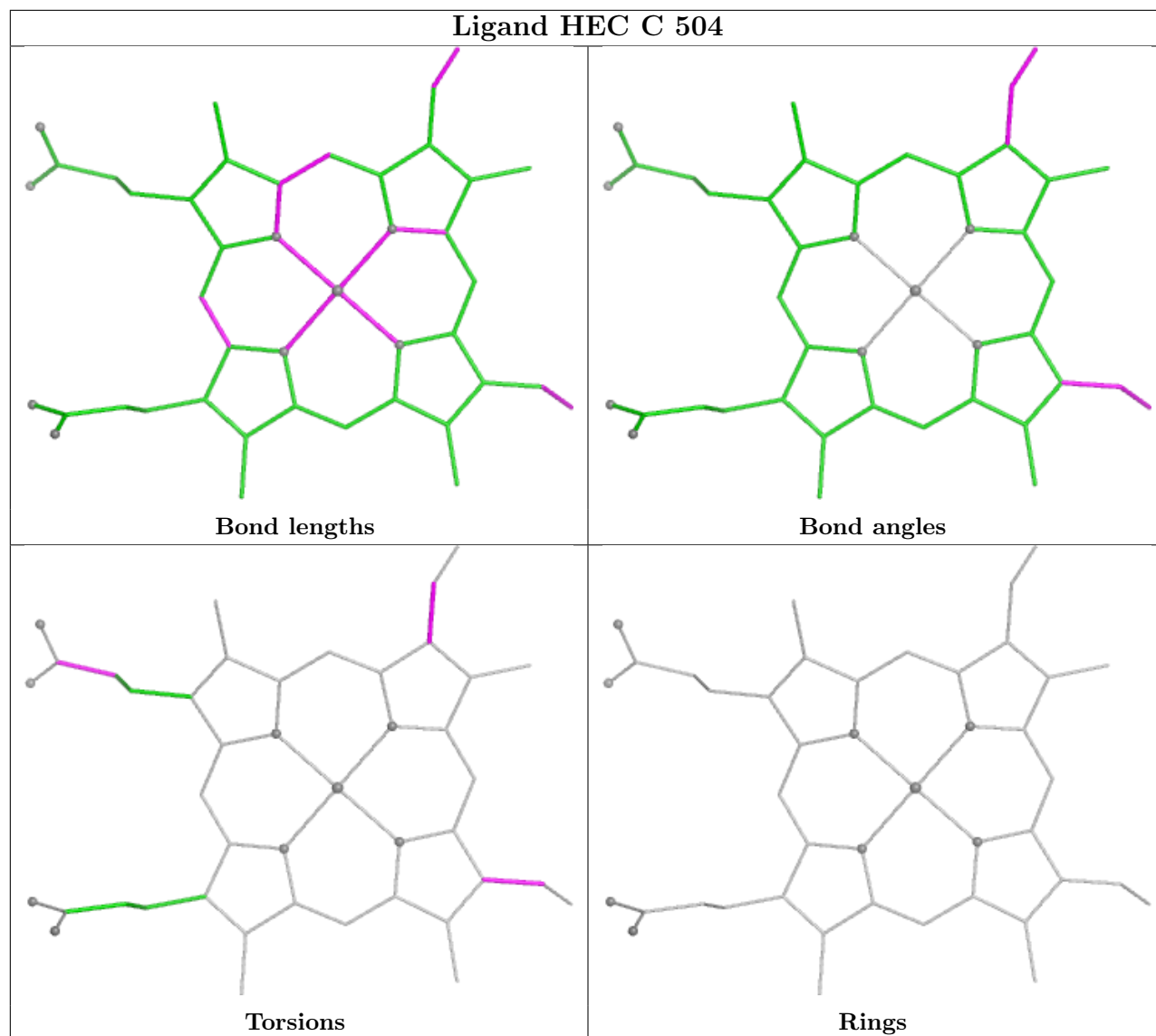


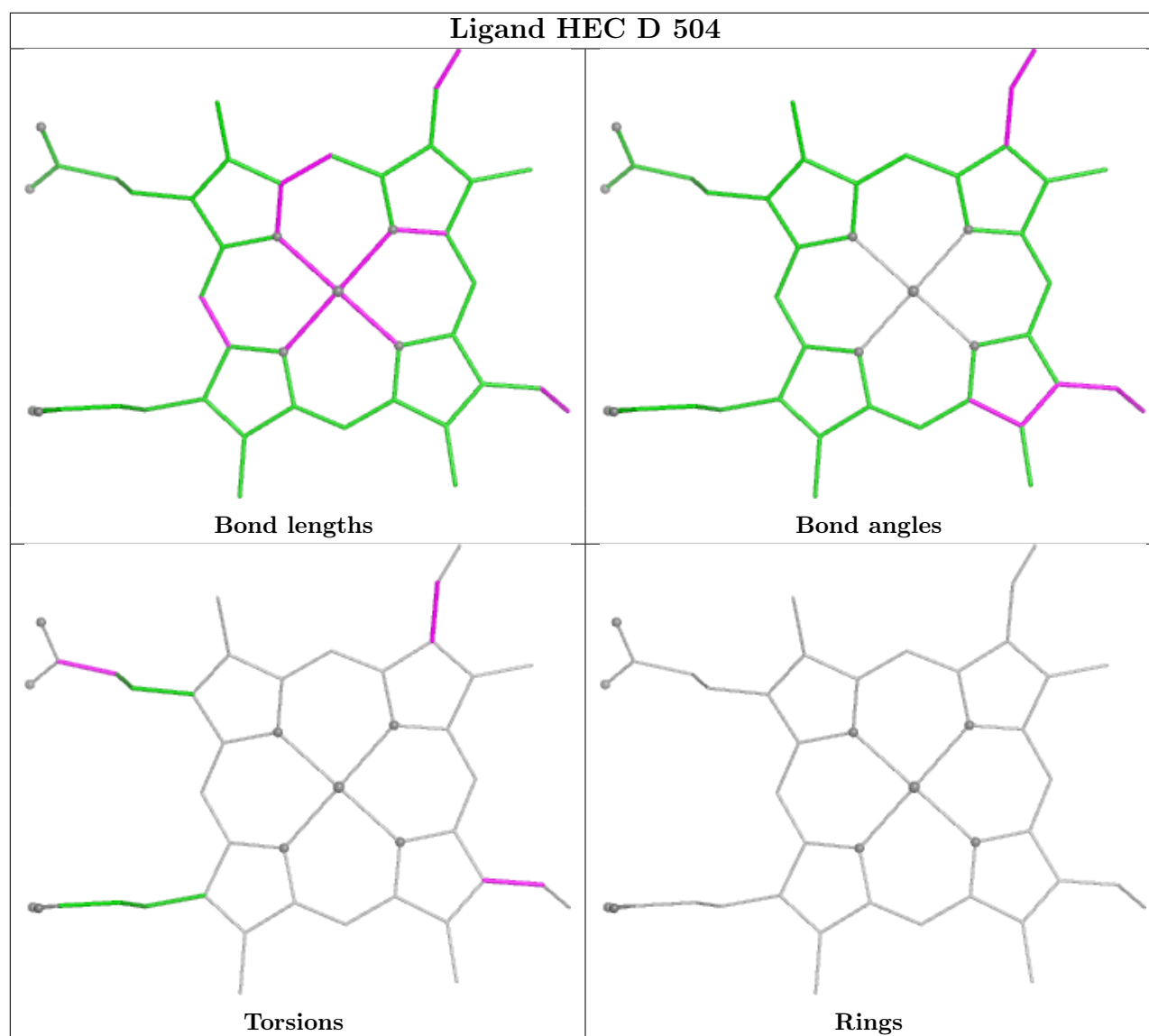












5.7 Other polymers [i](#)

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	437/492 (88%)	0.19	16 (3%) 45 51	15, 33, 59, 77	0
1	B	434/492 (88%)	0.28	30 (6%) 23 26	13, 34, 69, 87	0
1	C	443/492 (90%)	0.21	35 (7%) 18 21	13, 33, 75, 86	0
1	D	444/492 (90%)	0.00	18 (4%) 41 46	11, 29, 61, 82	0
All	All	1758/1968 (89%)	0.17	99 (5%) 30 33	11, 32, 67, 87	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	TYR	5.6
1	A	106	TYR	5.5
1	C	321	VAL	5.0
1	C	127	LEU	4.6
1	B	106	TYR	4.4

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 [i](#)

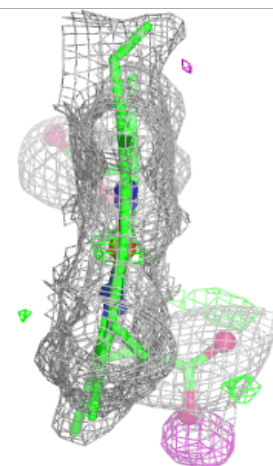
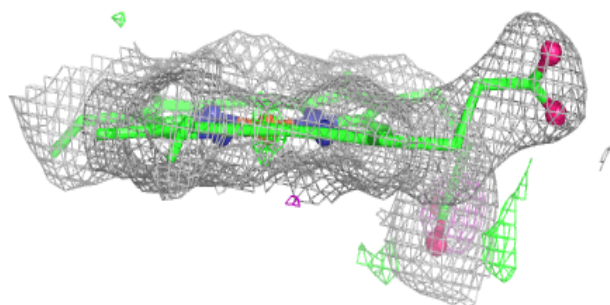
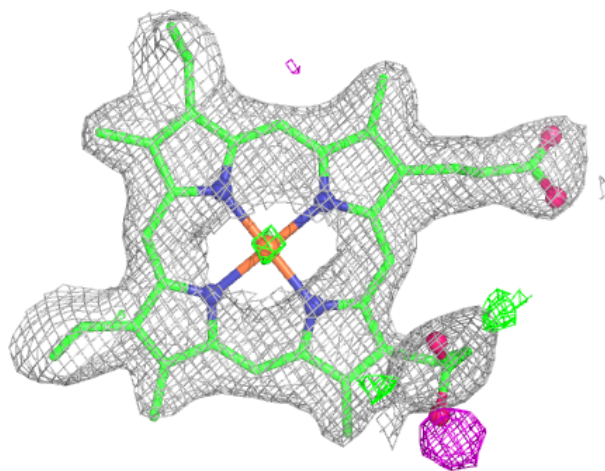
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	509	5/5	0.67	0.16	111,111,111,111	0
3	SO4	D	509	5/5	0.73	0.17	98,98,98,98	0
3	SO4	C	508	5/5	0.77	0.16	79,80,80,80	0
3	SO4	A	508	5/5	0.78	0.19	113,113,113,113	0
3	SO4	C	507	5/5	0.78	0.14	91,92,92,92	0
3	SO4	D	508	5/5	0.82	0.13	85,85,85,85	0
3	SO4	B	508	5/5	0.82	0.17	115,115,115,115	0
3	SO4	A	506	5/5	0.84	0.12	80,80,80,80	0
3	SO4	D	507	5/5	0.84	0.18	98,98,98,99	0
3	SO4	B	506	5/5	0.87	0.10	68,68,68,68	0
3	SO4	A	507	5/5	0.88	0.16	98,98,98,98	0
3	SO4	B	507	5/5	0.90	0.14	83,83,83,84	0
3	SO4	C	506	5/5	0.93	0.08	56,56,56,57	0
2	HEC	A	505	43/43	0.94	0.10	41,45,51,52	0
2	HEC	A	501	43/43	0.94	0.09	34,36,43,44	0
2	HEC	A	502	43/43	0.95	0.08	23,26,36,38	0
2	HEC	B	502	43/43	0.95	0.09	27,32,43,45	0
2	HEC	B	503	43/43	0.95	0.10	45,47,56,56	0
2	HEC	B	505	43/43	0.95	0.09	34,41,45,48	0
2	HEC	C	501	43/43	0.95	0.09	20,23,35,42	0
2	HEC	A	503	43/43	0.95	0.09	26,29,41,42	0
2	HEC	C	502	43/43	0.96	0.07	16,22,39,41	0
2	HEC	C	503	43/43	0.96	0.09	27,33,41,45	0
2	HEC	C	504	43/43	0.96	0.08	22,29,38,39	0
2	HEC	C	505	43/43	0.96	0.07	30,32,36,39	0
2	HEC	D	502	43/43	0.96	0.08	18,23,36,39	0
2	HEC	D	504	43/43	0.96	0.08	17,21,35,38	0
2	HEC	D	505	43/43	0.96	0.08	20,24,34,39	0
2	HEC	B	504	43/43	0.96	0.08	25,30,41,43	0
2	HEC	A	504	43/43	0.96	0.09	27,30,40,44	0
2	HEC	B	501	43/43	0.96	0.08	23,28,39,43	0
2	HEC	D	501	43/43	0.97	0.06	21,23,28,32	0
2	HEC	D	503	43/43	0.97	0.07	12,17,33,35	0
3	SO4	D	506	5/5	0.97	0.07	42,42,42,42	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.

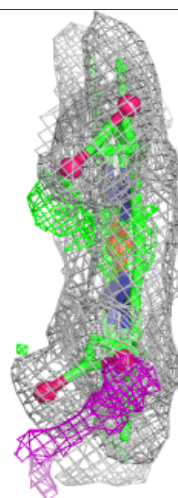
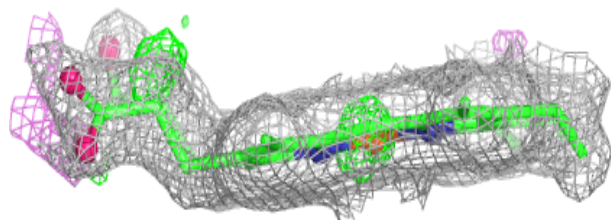
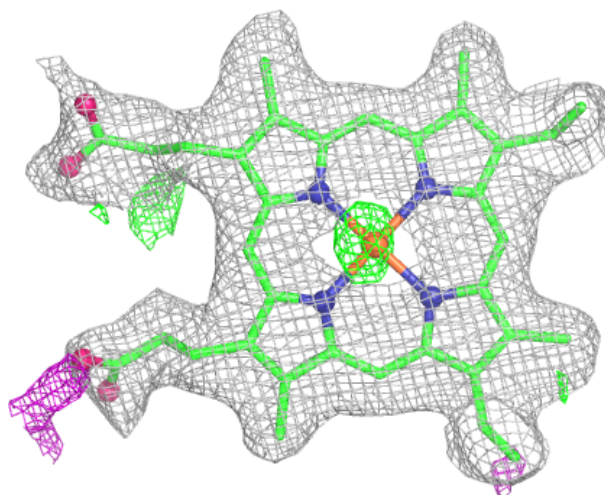
Electron density around HEC A 505:

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



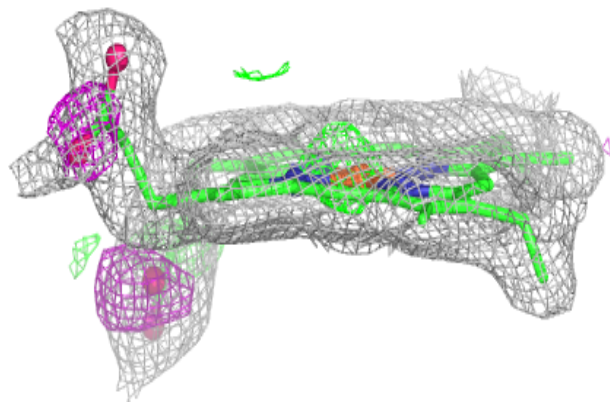
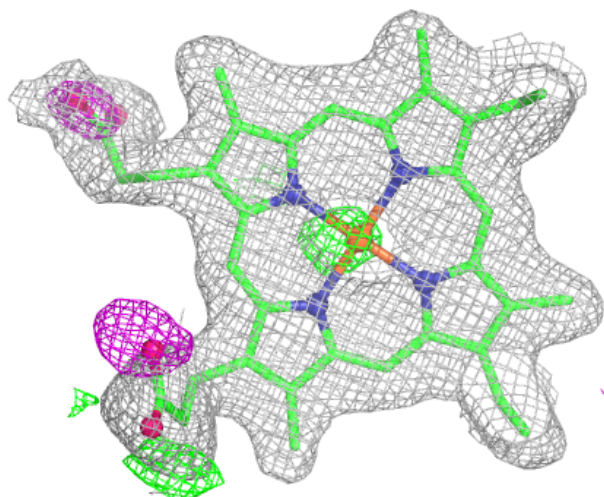
Electron density around HEC A 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



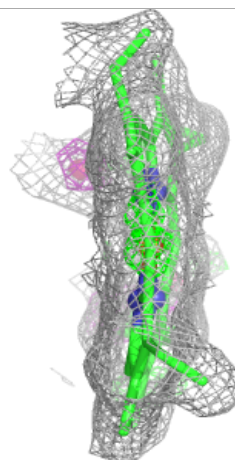
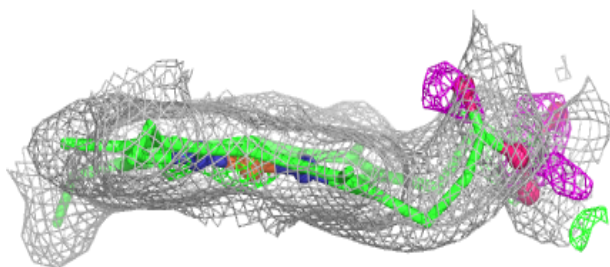
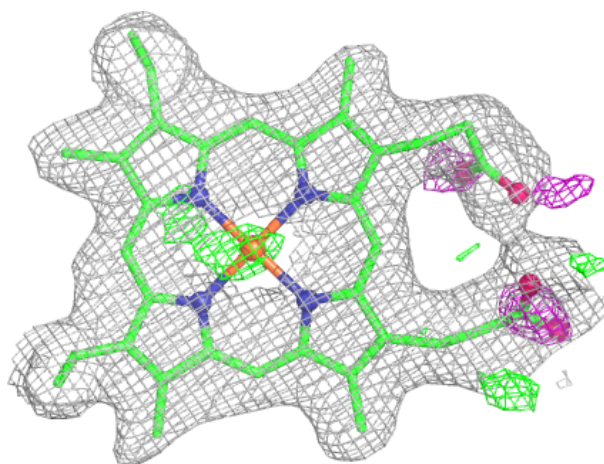
Electron density around HEC A 502:

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and green (positive)



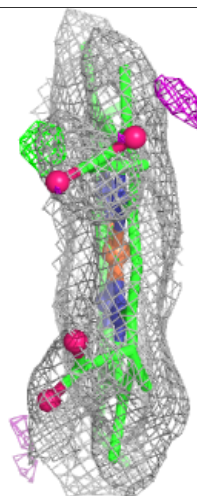
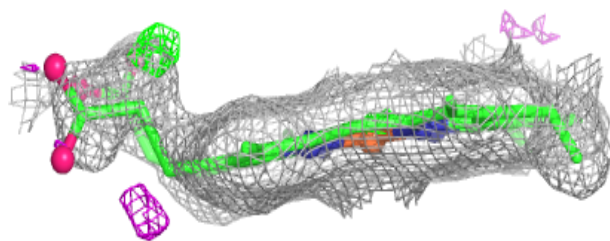
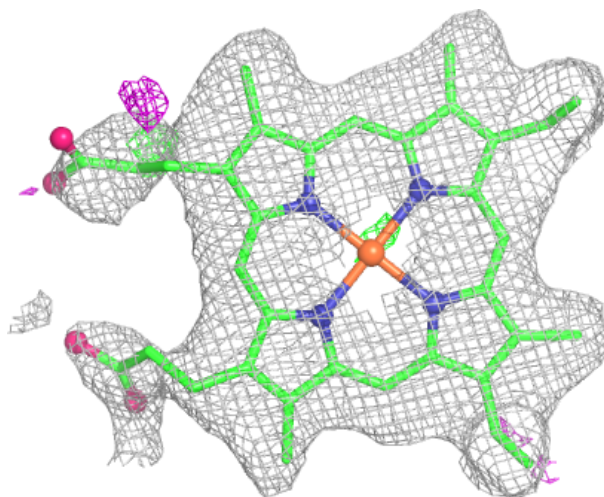
Electron density around HEC B 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



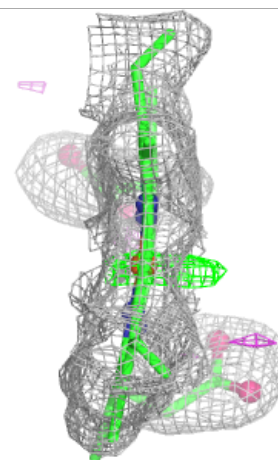
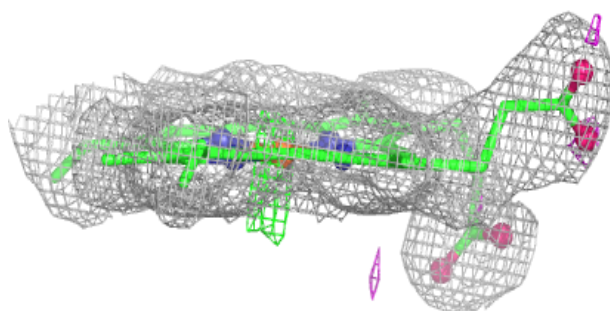
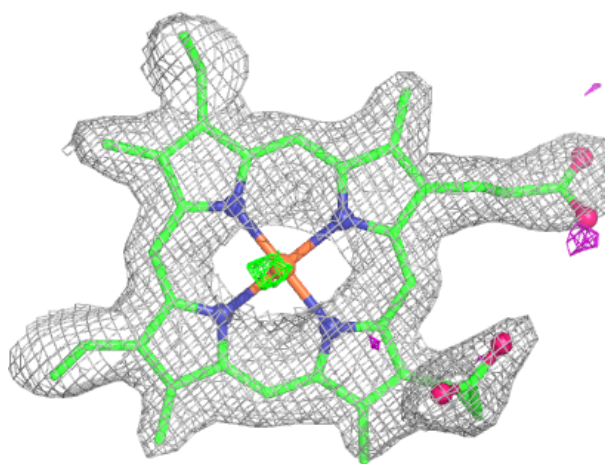
Electron density around HEC B 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



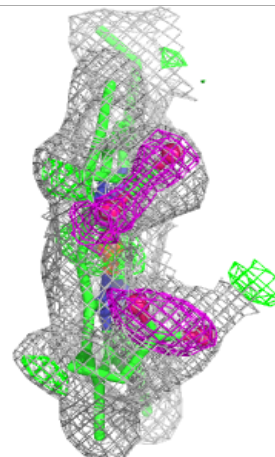
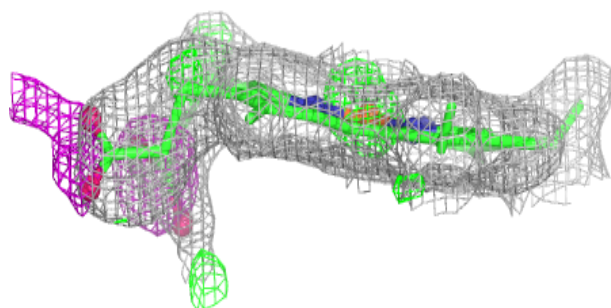
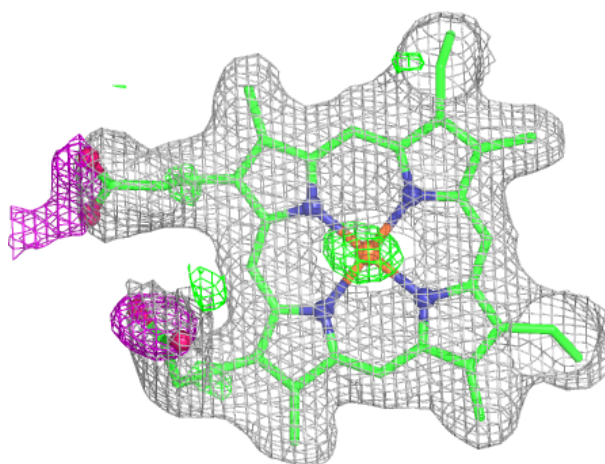
Electron density around HEC B 505:

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and green (positive)



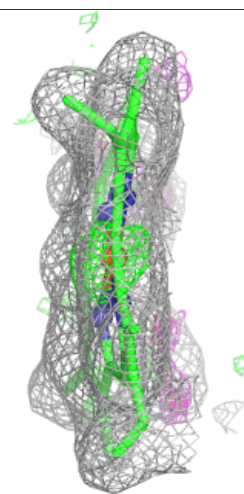
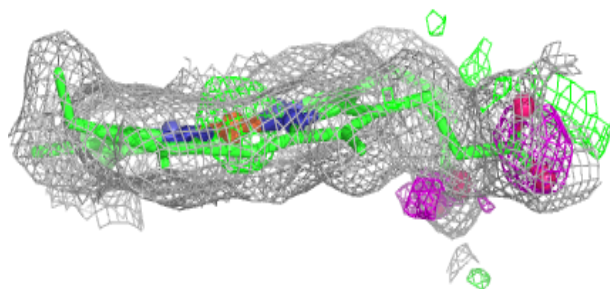
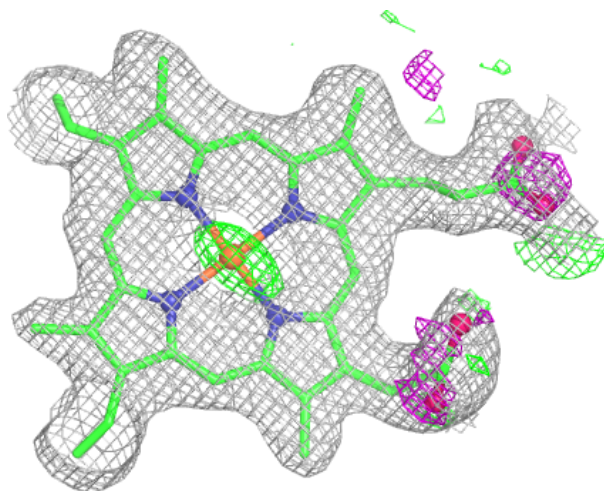
Electron density around HEC C 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



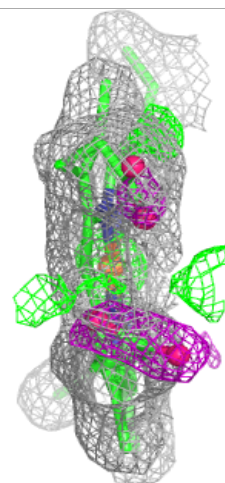
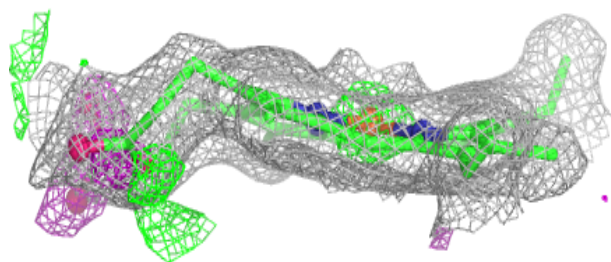
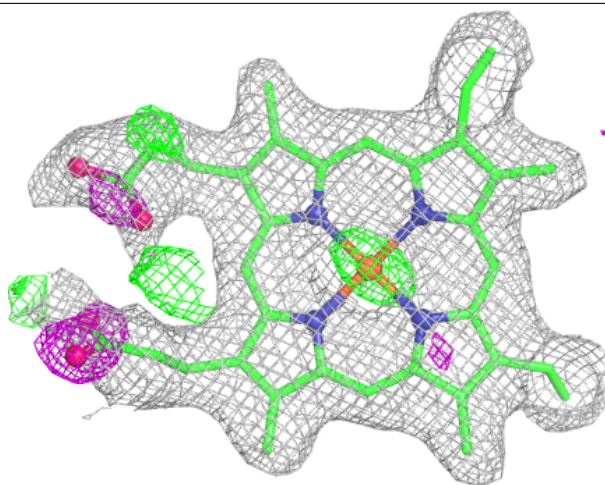
Electron density around HEC A 503:

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



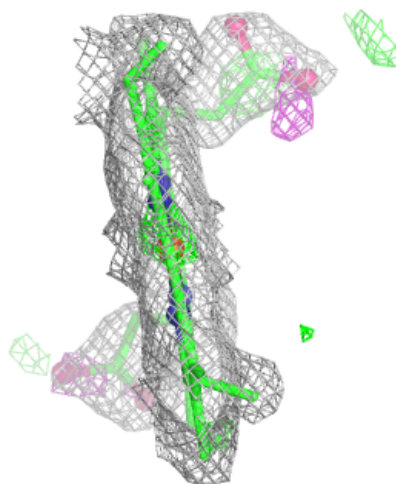
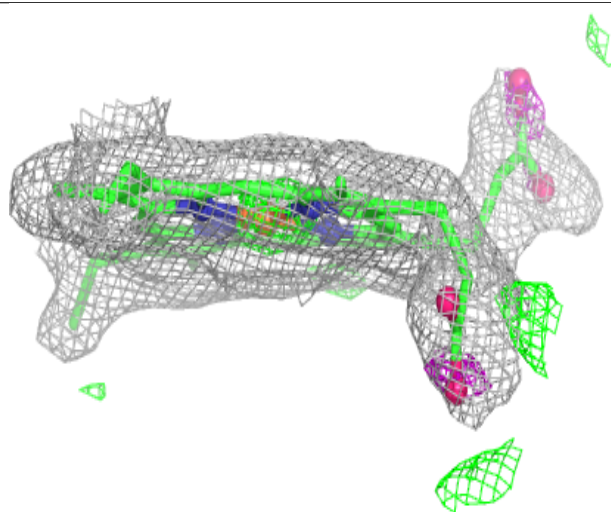
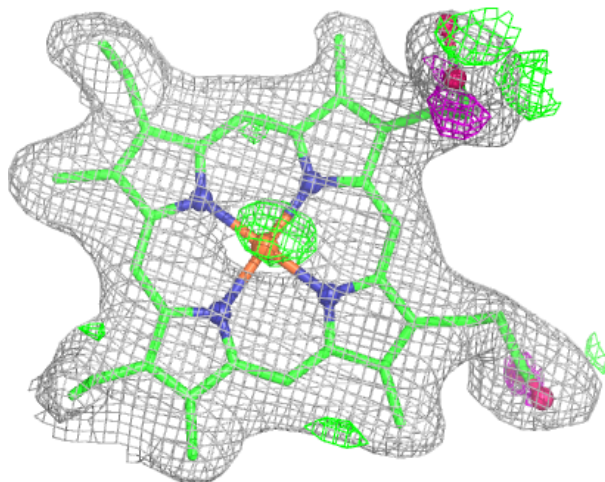
Electron density around HEC C 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



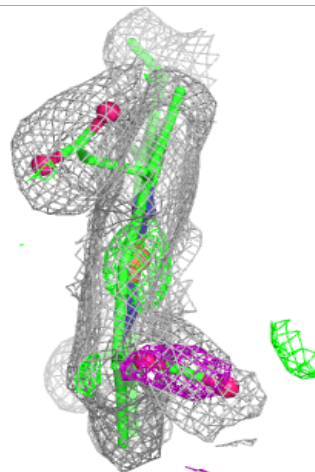
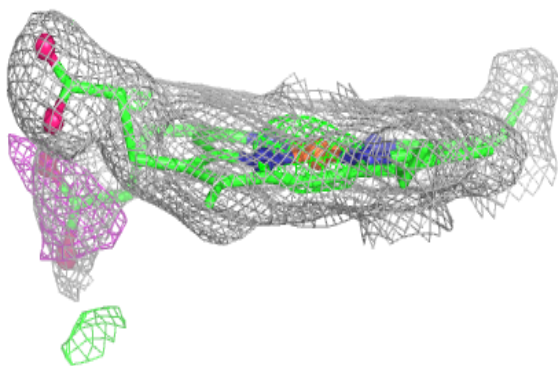
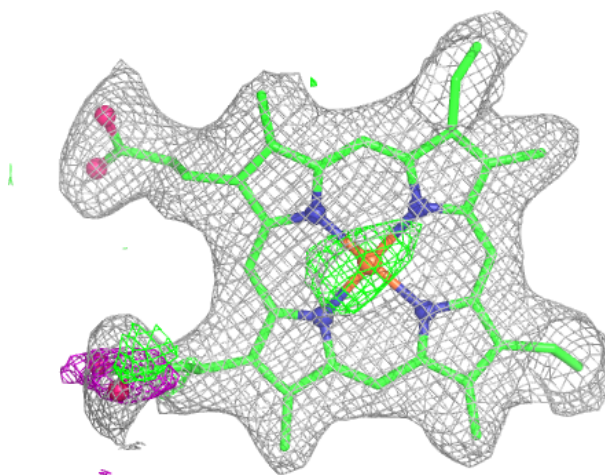
Electron density around HEC C 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



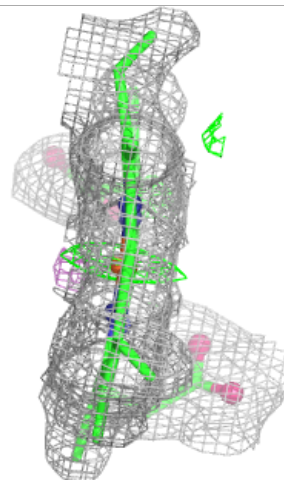
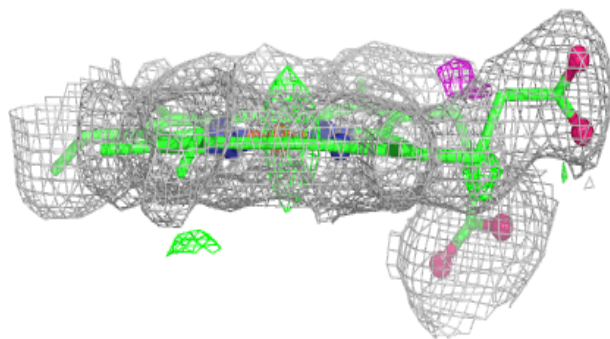
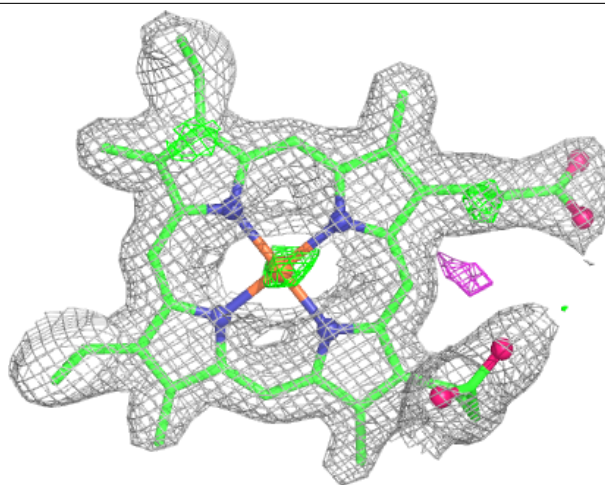
Electron density around HEC C 504:

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and green (positive)



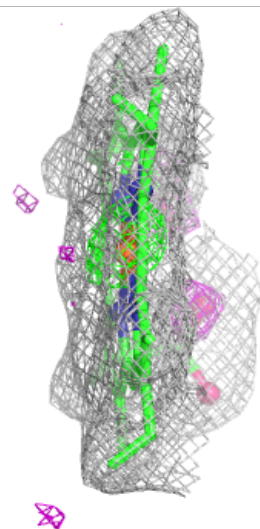
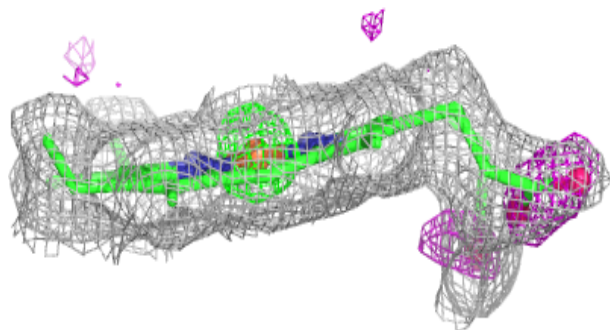
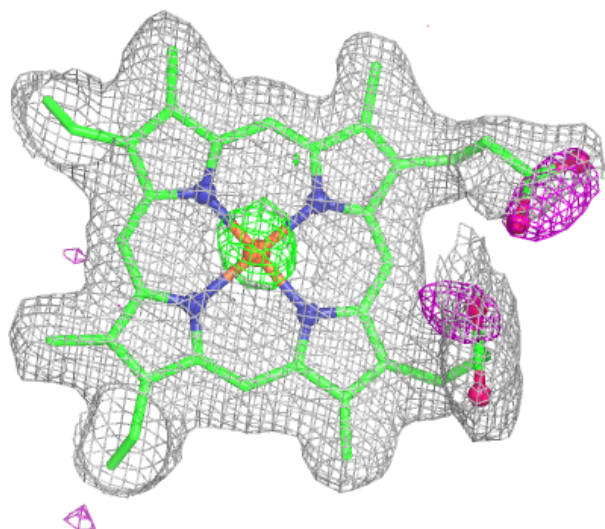
Electron density around HEC C 505:

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and green (positive)



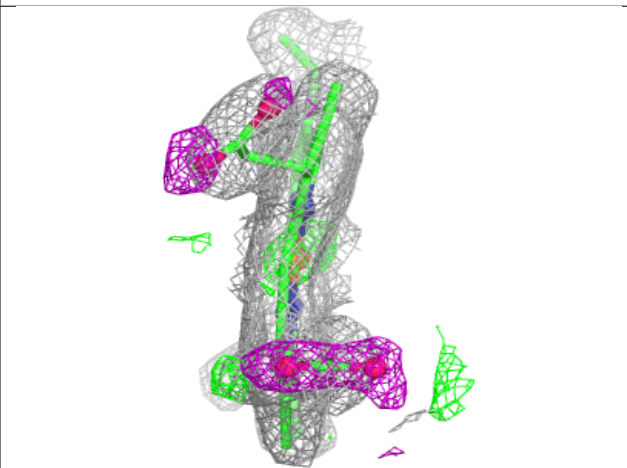
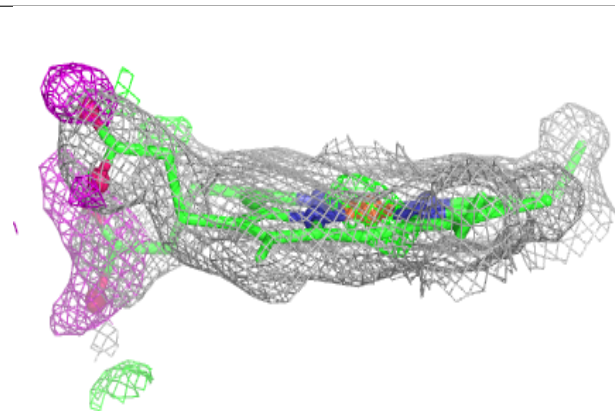
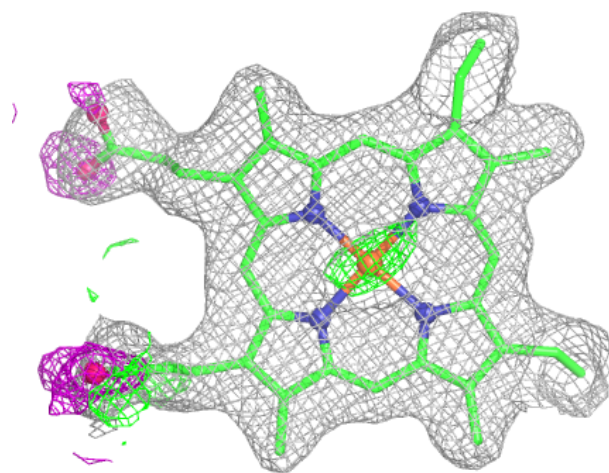
Electron density around HEC D 502:

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and green (positive)



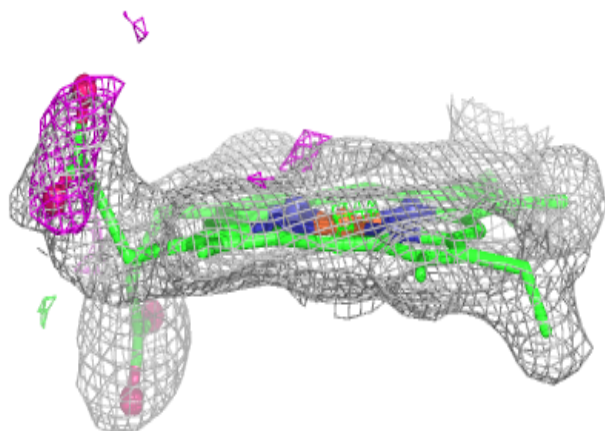
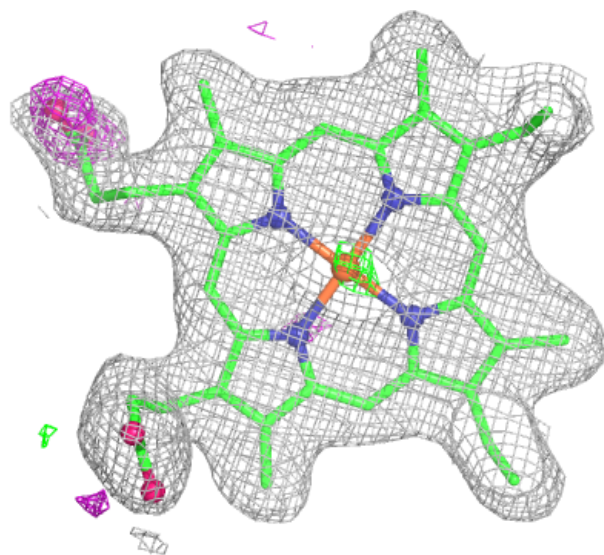
Electron density around HEC D 504:

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and green (positive)



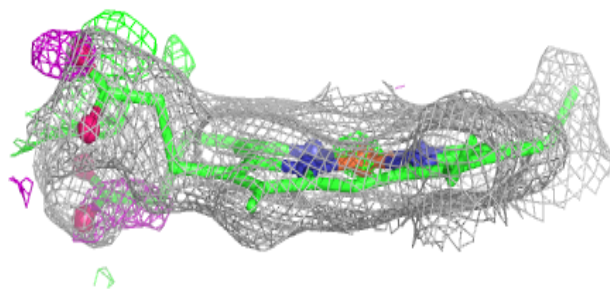
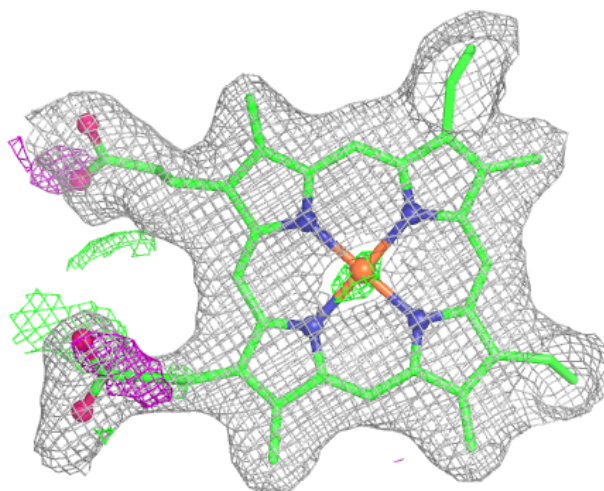
Electron density around HEC D 505:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



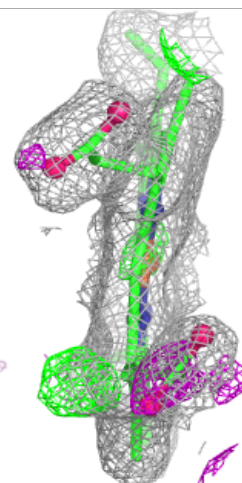
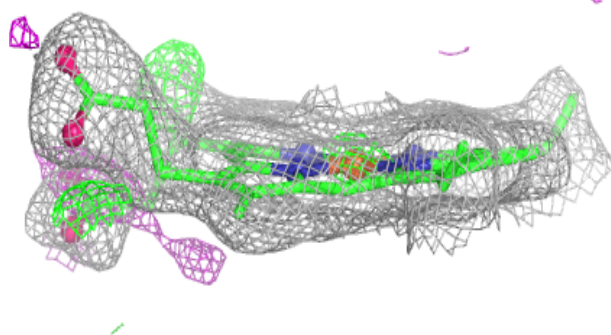
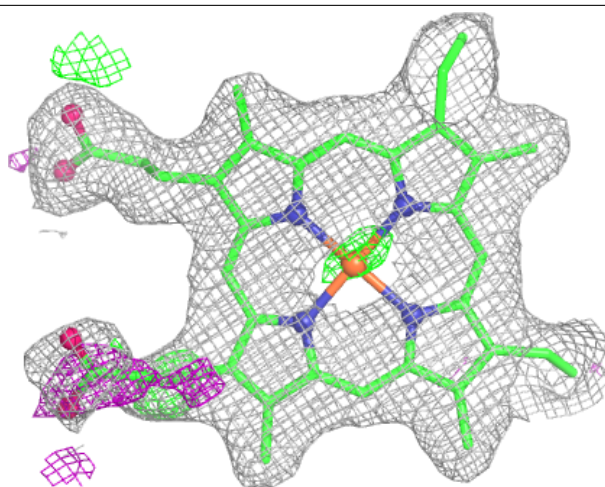
Electron density around HEC B 504:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



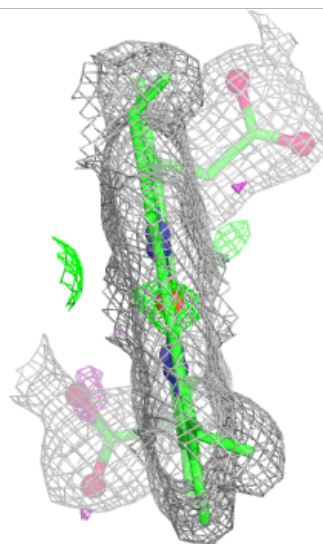
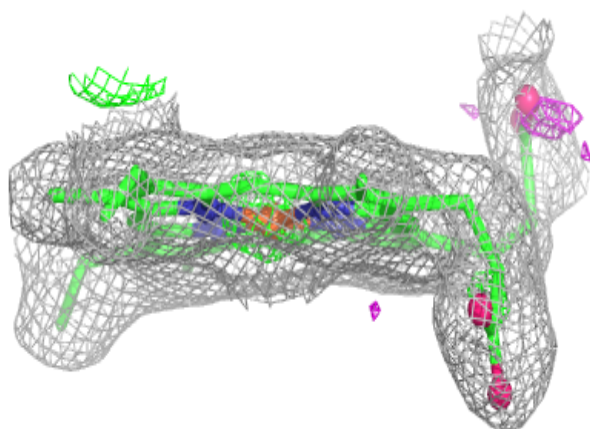
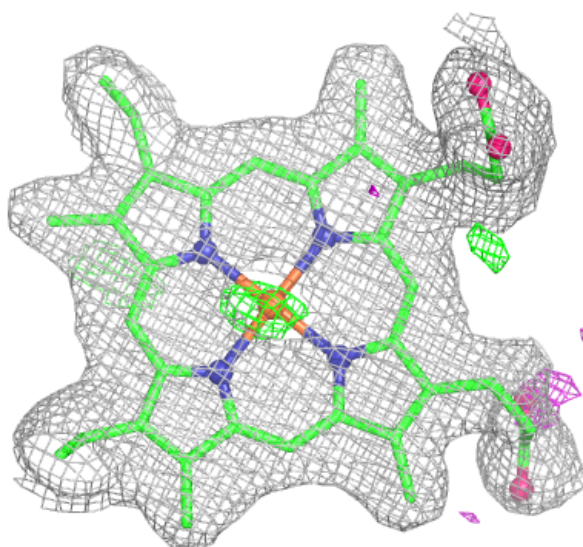
Electron density around HEC A 504:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



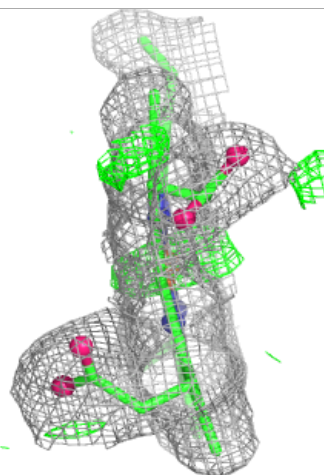
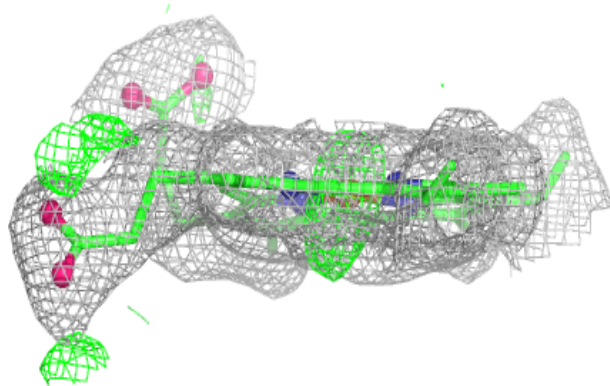
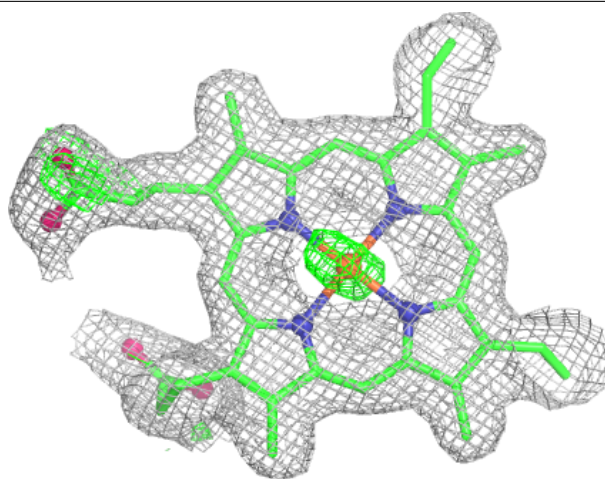
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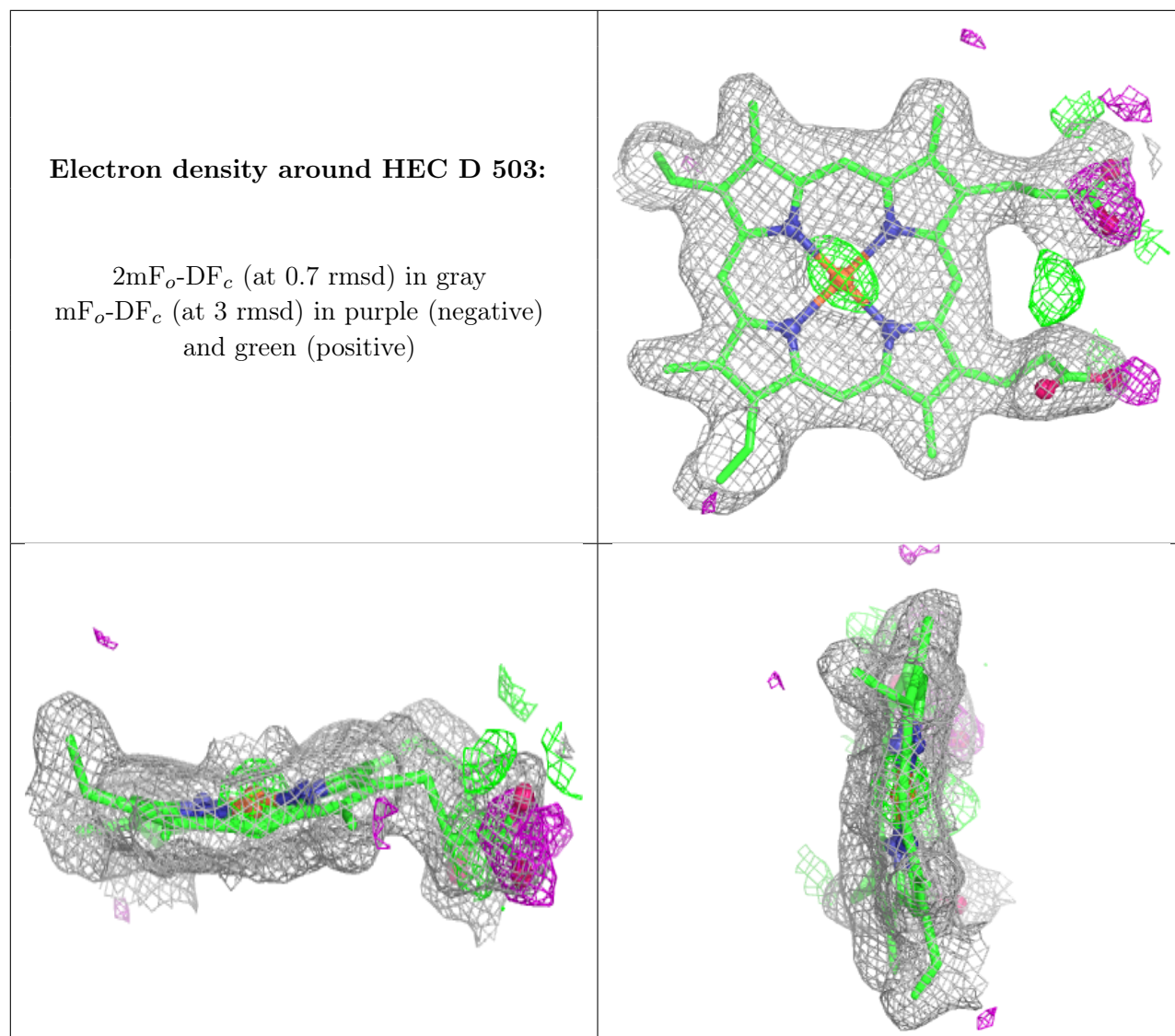
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC D 501:

$2mF_o-DF_c$ (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.