



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:16 PM UTC

PDB ID : 3R1A / pdb_00003r1a
Title : Closed crystal structure of cytochrome P450 2B4 covalently bound to the mechanism-based inactivator tert-butylphenylacetylene
Authors : Gay, S.C.; Zhang, H.; Stout, C.D.; Hollenberg, P.F.; Halpert, J.R.
Deposited on : 2011-03-09
Resolution : 3.50 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 : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

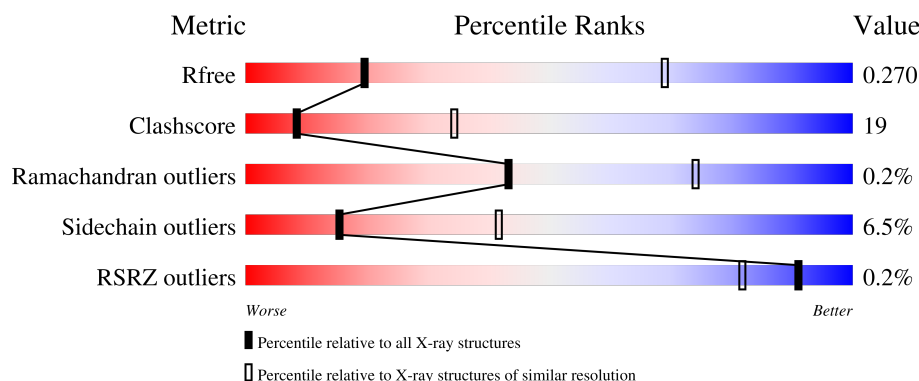
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	476	
1	B	476	
1	C	476	
1	D	476	
1	E	476	

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Mol	Chain	Length	Quality of chain
1	F	476	62% 33% . .
1	G	476	63% 30% . .
1	H	476	% 64% 32% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28813 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 Cytochrome P450 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3618	2332	613	663	10			
1	B	465	Total	C	N	O	S	0	0	0
			3582	2314	595	662	11			
1	C	465	Total	C	N	O	S	0	0	0
			3637	2346	618	662	11			
1	D	465	Total	C	N	O	S	0	0	0
			3608	2327	604	666	11			
1	E	465	Total	C	N	O	S	0	0	0
			3588	2319	592	666	11			
1	F	465	Total	C	N	O	S	0	0	0
			3540	2292	581	656	11			
1	G	465	Total	C	N	O	S	0	0	0
			3545	2293	583	659	10			
1	H	464	Total	C	N	O	S	0	0	0
			3239	2079	539	612	9			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	engineered mutation	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	SER	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	GLY	deletion	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	ARG	deletion	UNP P00178
A	22	LYS	GLY	engineered mutation	UNP P00178
A	23	LYS	HIS	engineered mutation	UNP P00178
A	24	THR	PRO	engineered mutation	UNP P00178
A	25	SER	LYS	engineered mutation	UNP P00178
A	26	SER	ALA	engineered mutation	UNP P00178
A	27	LYS	HIS	engineered mutation	UNP P00178
A	29	LYS	ARG	engineered mutation	UNP P00178
A	221	SER	PRO	conflict	UNP P00178
A	226	TYR	HIS	engineered mutation	UNP P00178
A	492	HIS	-	expression tag	UNP P00178
A	493	HIS	-	expression tag	UNP P00178
A	494	HIS	-	expression tag	UNP P00178
A	495	HIS	-	expression tag	UNP P00178
B	21	ALA	GLU	engineered mutation	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	SER	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	ALA	deletion	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	ALA	deletion	UNP P00178
B	?	-	GLY	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	LEU	deletion	UNP P00178
B	?	-	PHE	deletion	UNP P00178
B	?	-	ARG	deletion	UNP P00178
B	22	LYS	GLY	engineered mutation	UNP P00178
B	23	LYS	HIS	engineered mutation	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
B	24	THR	PRO	engineered mutation	UNP P00178
B	25	SER	LYS	engineered mutation	UNP P00178
B	26	SER	ALA	engineered mutation	UNP P00178
B	27	LYS	HIS	engineered mutation	UNP P00178
B	29	LYS	ARG	engineered mutation	UNP P00178
B	221	SER	PRO	conflict	UNP P00178
B	226	TYR	HIS	engineered mutation	UNP P00178
B	492	HIS	-	expression tag	UNP P00178
B	493	HIS	-	expression tag	UNP P00178
B	494	HIS	-	expression tag	UNP P00178
B	495	HIS	-	expression tag	UNP P00178
C	21	ALA	GLU	engineered mutation	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	SER	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	ALA	deletion	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	ALA	deletion	UNP P00178
C	?	-	GLY	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	LEU	deletion	UNP P00178
C	?	-	PHE	deletion	UNP P00178
C	?	-	ARG	deletion	UNP P00178
C	22	LYS	GLY	engineered mutation	UNP P00178
C	23	LYS	HIS	engineered mutation	UNP P00178
C	24	THR	PRO	engineered mutation	UNP P00178
C	25	SER	LYS	engineered mutation	UNP P00178
C	26	SER	ALA	engineered mutation	UNP P00178
C	27	LYS	HIS	engineered mutation	UNP P00178
C	29	LYS	ARG	engineered mutation	UNP P00178
C	221	SER	PRO	conflict	UNP P00178
C	226	TYR	HIS	engineered mutation	UNP P00178
C	492	HIS	-	expression tag	UNP P00178
C	493	HIS	-	expression tag	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
C	494	HIS	-	expression tag	UNP P00178
C	495	HIS	-	expression tag	UNP P00178
D	21	ALA	GLU	engineered mutation	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	SER	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	ALA	deletion	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	ALA	deletion	UNP P00178
D	?	-	GLY	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	LEU	deletion	UNP P00178
D	?	-	PHE	deletion	UNP P00178
D	?	-	ARG	deletion	UNP P00178
D	22	LYS	GLY	engineered mutation	UNP P00178
D	23	LYS	HIS	engineered mutation	UNP P00178
D	24	THR	PRO	engineered mutation	UNP P00178
D	25	SER	LYS	engineered mutation	UNP P00178
D	26	SER	ALA	engineered mutation	UNP P00178
D	27	LYS	HIS	engineered mutation	UNP P00178
D	29	LYS	ARG	engineered mutation	UNP P00178
D	221	SER	PRO	conflict	UNP P00178
D	226	TYR	HIS	engineered mutation	UNP P00178
D	492	HIS	-	expression tag	UNP P00178
D	493	HIS	-	expression tag	UNP P00178
D	494	HIS	-	expression tag	UNP P00178
D	495	HIS	-	expression tag	UNP P00178
E	21	ALA	GLU	engineered mutation	UNP P00178
E	?	-	PHE	deletion	UNP P00178
E	?	-	SER	deletion	UNP P00178
E	?	-	LEU	deletion	UNP P00178
E	?	-	LEU	deletion	UNP P00178
E	?	-	LEU	deletion	UNP P00178
E	?	-	LEU	deletion	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP P00178
E	?	-	ALA	deletion	UNP P00178
E	?	-	PHE	deletion	UNP P00178
E	?	-	LEU	deletion	UNP P00178
E	?	-	ALA	deletion	UNP P00178
E	?	-	GLY	deletion	UNP P00178
E	?	-	LEU	deletion	UNP P00178
E	?	-	LEU	deletion	UNP P00178
E	?	-	LEU	deletion	UNP P00178
E	?	-	LEU	deletion	UNP P00178
E	?	-	LEU	deletion	UNP P00178
E	?	-	PHE	deletion	UNP P00178
E	?	-	ARG	deletion	UNP P00178
E	22	LYS	GLY	engineered mutation	UNP P00178
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E	26	SER	ALA	engineered mutation	UNP P00178
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E	492	HIS	-	expression tag	UNP P00178
E	493	HIS	-	expression tag	UNP P00178
E	494	HIS	-	expression tag	UNP P00178
E	495	HIS	-	expression tag	UNP P00178
F	21	ALA	GLU	engineered mutation	UNP P00178
F	?	-	PHE	deletion	UNP P00178
F	?	-	SER	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	ALA	deletion	UNP P00178
F	?	-	PHE	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	ALA	deletion	UNP P00178
F	?	-	GLY	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	LEU	deletion	UNP P00178
F	?	-	LEU	deletion	UNP P00178
F	?	-	PHE	deletion	UNP P00178
F	?	-	ARG	deletion	UNP P00178
F	22	LYS	GLY	engineered mutation	UNP P00178
F	23	LYS	HIS	engineered mutation	UNP P00178
F	24	THR	PRO	engineered mutation	UNP P00178
F	25	SER	LYS	engineered mutation	UNP P00178
F	26	SER	ALA	engineered mutation	UNP P00178
F	27	LYS	HIS	engineered mutation	UNP P00178
F	29	LYS	ARG	engineered mutation	UNP P00178
F	221	SER	PRO	conflict	UNP P00178
F	226	TYR	HIS	engineered mutation	UNP P00178
F	492	HIS	-	expression tag	UNP P00178
F	493	HIS	-	expression tag	UNP P00178
F	494	HIS	-	expression tag	UNP P00178
F	495	HIS	-	expression tag	UNP P00178
G	21	ALA	GLU	engineered mutation	UNP P00178
G	?	-	PHE	deletion	UNP P00178
G	?	-	SER	deletion	UNP P00178
G	?	-	LEU	deletion	UNP P00178
G	?	-	LEU	deletion	UNP P00178
G	?	-	LEU	deletion	UNP P00178
G	?	-	LEU	deletion	UNP P00178
G	?	-	LEU	deletion	UNP P00178
G	?	-	ALA	deletion	UNP P00178
G	?	-	PHE	deletion	UNP P00178
G	?	-	LEU	deletion	UNP P00178
G	?	-	ALA	deletion	UNP P00178
G	?	-	GLY	deletion	UNP P00178
G	?	-	LEU	deletion	UNP P00178
G	?	-	LEU	deletion	UNP P00178
G	?	-	LEU	deletion	UNP P00178
G	?	-	LEU	deletion	UNP P00178
G	?	-	LEU	deletion	UNP P00178
G	?	-	PHE	deletion	UNP P00178
G	?	-	ARG	deletion	UNP P00178
G	22	LYS	GLY	engineered mutation	UNP P00178
G	23	LYS	HIS	engineered mutation	UNP P00178
G	24	THR	PRO	engineered mutation	UNP P00178
G	25	SER	LYS	engineered mutation	UNP P00178
G	26	SER	ALA	engineered mutation	UNP P00178

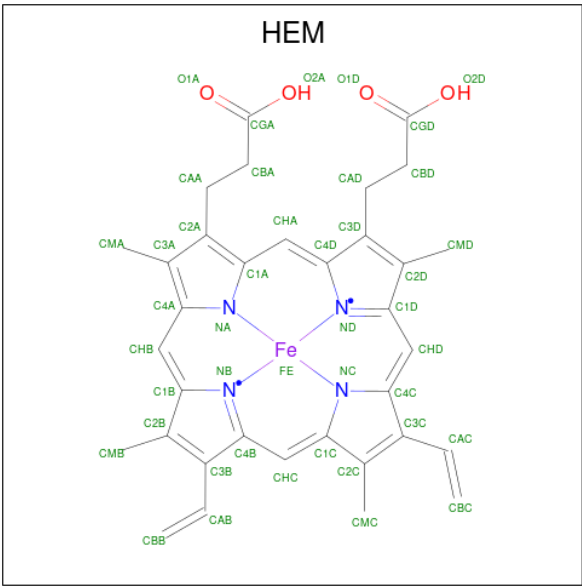
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Chain	Residue	Modelled	Actual	Comment	Reference
G	27	LYS	HIS	engineered mutation	UNP P00178
G	29	LYS	ARG	engineered mutation	UNP P00178
G	221	SER	PRO	conflict	UNP P00178
G	226	TYR	HIS	engineered mutation	UNP P00178
G	492	HIS	-	expression tag	UNP P00178
G	493	HIS	-	expression tag	UNP P00178
G	494	HIS	-	expression tag	UNP P00178
G	495	HIS	-	expression tag	UNP P00178
H	21	ALA	GLU	engineered mutation	UNP P00178
H	?	-	PHE	deletion	UNP P00178
H	?	-	SER	deletion	UNP P00178
H	?	-	LEU	deletion	UNP P00178
H	?	-	LEU	deletion	UNP P00178
H	?	-	LEU	deletion	UNP P00178
H	?	-	LEU	deletion	UNP P00178
H	?	-	LEU	deletion	UNP P00178
H	?	-	ALA	deletion	UNP P00178
H	?	-	PHE	deletion	UNP P00178
H	?	-	LEU	deletion	UNP P00178
H	?	-	ALA	deletion	UNP P00178
H	?	-	GLY	deletion	UNP P00178
H	?	-	LEU	deletion	UNP P00178
H	?	-	LEU	deletion	UNP P00178
H	?	-	LEU	deletion	UNP P00178
H	?	-	LEU	deletion	UNP P00178
H	?	-	LEU	deletion	UNP P00178
H	?	-	PHE	deletion	UNP P00178
H	?	-	ARG	deletion	UNP P00178
H	22	LYS	GLY	engineered mutation	UNP P00178
H	23	LYS	HIS	engineered mutation	UNP P00178
H	24	THR	PRO	engineered mutation	UNP P00178
H	25	SER	LYS	engineered mutation	UNP P00178
H	26	SER	ALA	engineered mutation	UNP P00178
H	27	LYS	HIS	engineered mutation	UNP P00178
H	29	LYS	ARG	engineered mutation	UNP P00178
H	221	SER	PRO	conflict	UNP P00178
H	226	TYR	HIS	engineered mutation	UNP P00178
H	492	HIS	-	expression tag	UNP P00178
H	493	HIS	-	expression tag	UNP P00178
H	494	HIS	-	expression tag	UNP P00178
H	495	HIS	-	expression tag	UNP P00178

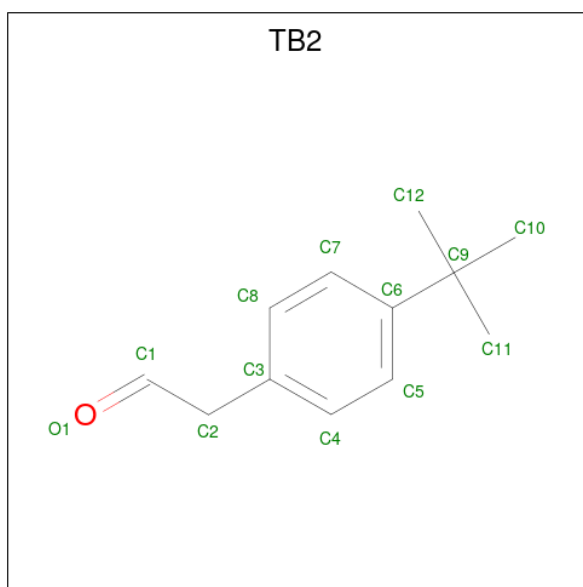
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is (4-tert-butylphenyl)acetaldehyde (CCD ID: TB2) (formula: C₁₂H₁₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	12	1		
3	B	1	Total	C	O	0	0
			13	12	1		
3	C	1	Total	C	O	0	0
			13	12	1		
3	D	1	Total	C	O	0	0
			13	12	1		
3	E	1	Total	C	O	0	0
			13	12	1		
3	F	1	Total	C	O	0	0
			13	12	1		
3	G	1	Total	C	O	0	0
			13	12	1		
3	H	1	Total	C	O	0	0
			13	12	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

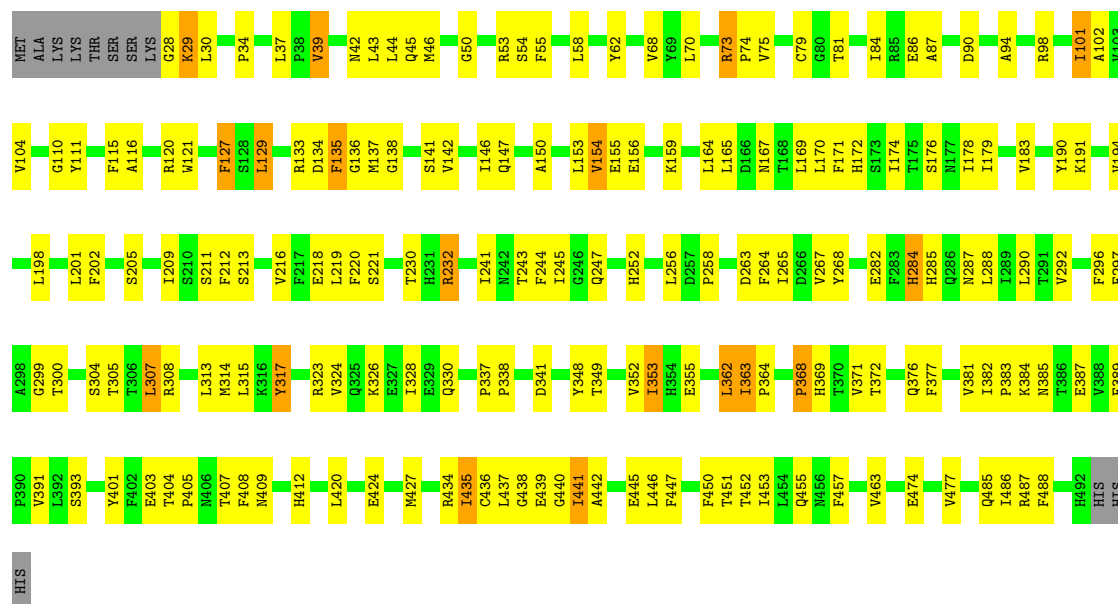
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	O 1	0	0
4	F	1	Total 1	O 1	0	0
4	G	1	Total 1	O 1	0	0
4	H	1	Total 1	O 1	0	0

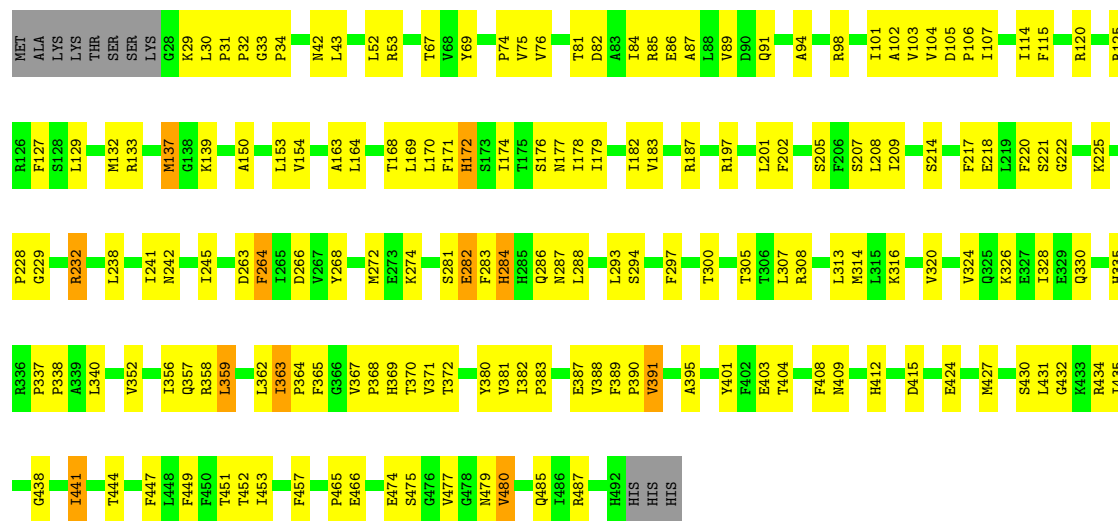
• Molecule 1: Cytochrome P450 2B4

Chain C:  59% 35%



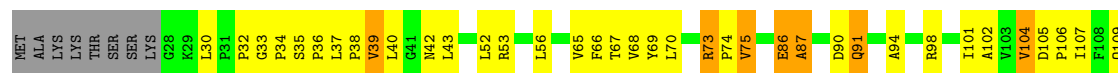
• Molecule 1: Cytochrome P450 2B4

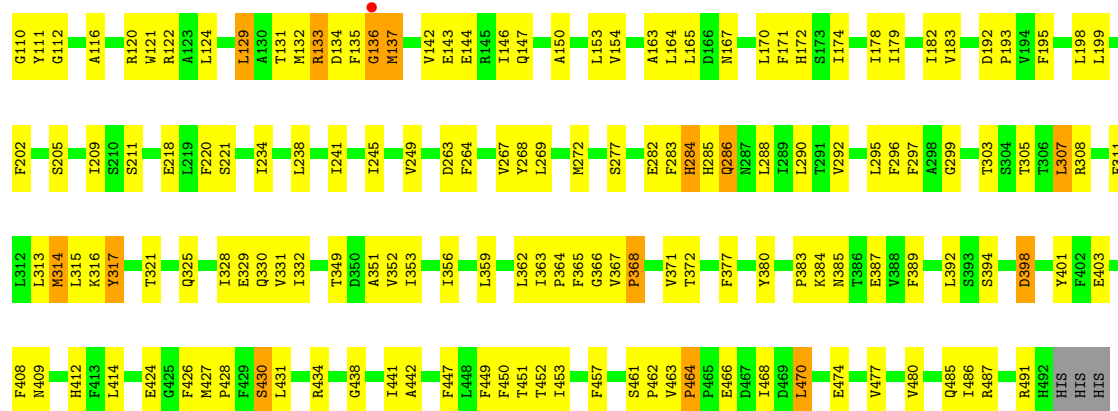
Chain D:  62% 33%



• Molecule 1: Cytochrome P450 2B4

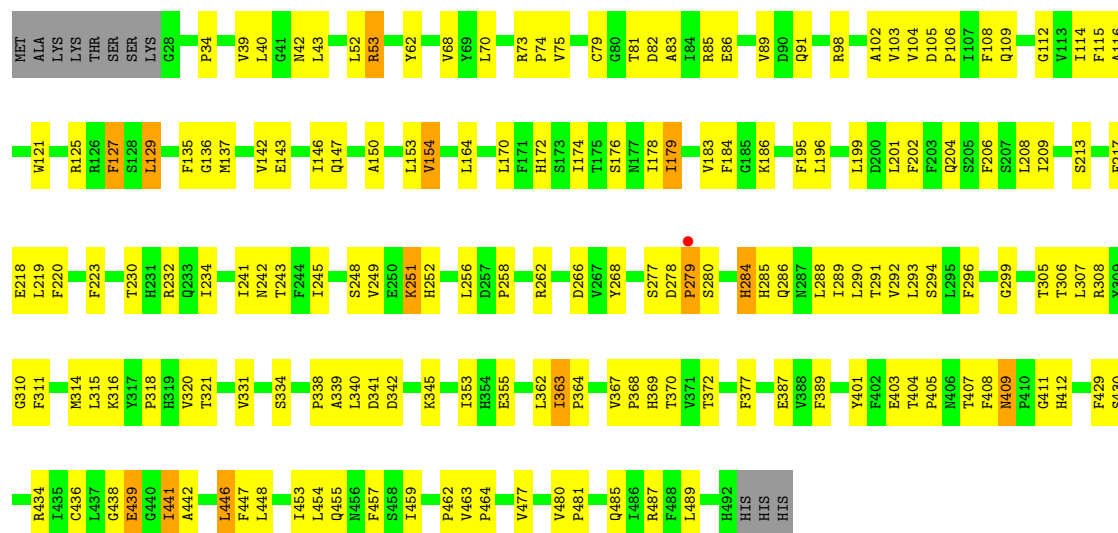
Chain E:  58% 35%





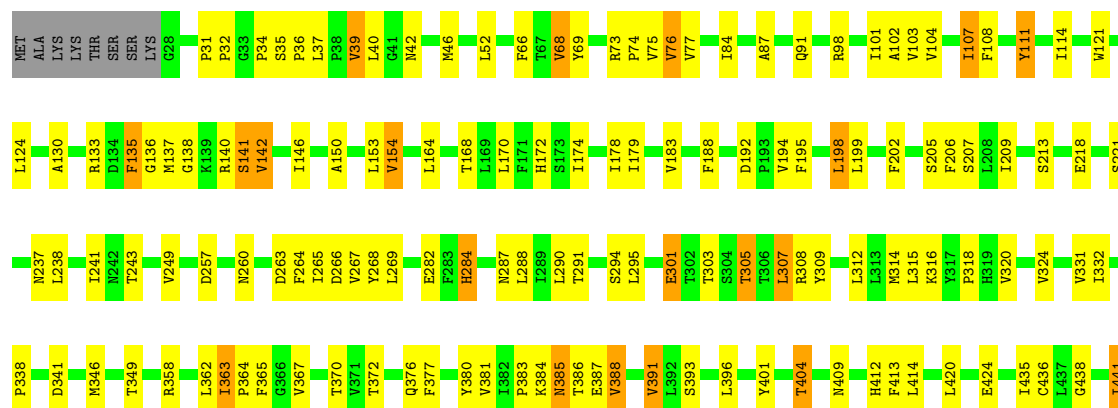
• Molecule 1: Cytochrome P450 2B4

Chain F: 62% 33%



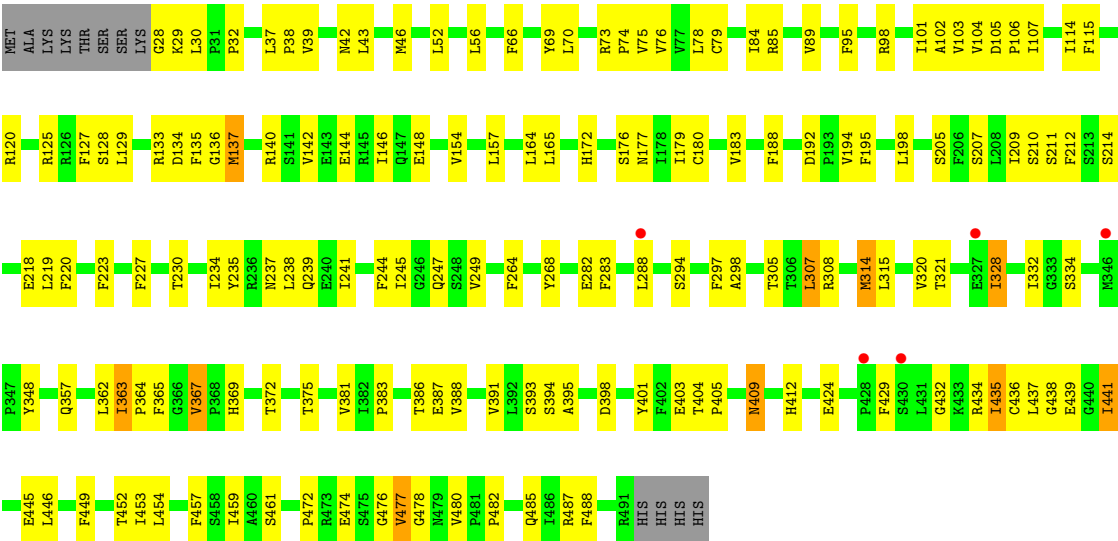
• Molecule 1: Cytochrome P450 2B4

Chain G: 63% 30%





● Molecule 1: Cytochrome P450 2B4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.38Å 144.55Å 229.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.93 – 3.50 115.93 – 3.50	Depositor EDS
% Data completeness (in resolution range)	85.5 (115.93-3.50) 89.8 (115.93-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.206 , 0.285 0.203 , 0.270	Depositor DCC
R_{free} test set	2603 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	80.2	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28813	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TB2, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.30	0/3711	0.86	11/5052 (0.2%)
1	B	0.29	0/3675	0.82	7/5010 (0.1%)
1	C	0.30	0/3730	0.83	10/5072 (0.2%)
1	D	0.29	0/3701	0.85	12/5041 (0.2%)
1	E	0.30	0/3681	0.87	16/5017 (0.3%)
1	F	0.30	0/3633	0.85	11/4960 (0.2%)
1	G	0.28	0/3638	0.86	16/4968 (0.3%)
1	H	0.42	3/3313 (0.1%)	0.93	11/4554 (0.2%)
All	All	0.31	3/29082 (0.0%)	0.86	94/39674 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	135	PHE	CA-C	-10.80	1.37	1.52
1	H	134	ASP	C-N	7.21	1.44	1.33
1	H	135	PHE	C-O	6.15	1.32	1.24

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	137	MET	N-CA-C	-14.23	95.75	113.97
1	A	301	GLU	N-CA-C	12.41	124.80	111.03
1	E	87	ALA	N-CA-C	11.86	125.87	111.40
1	B	301	GLU	N-CA-C	9.57	121.47	111.14
1	E	331	VAL	N-CA-C	9.05	120.26	111.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3618	0	3491	121	0
1	B	3582	0	3425	127	0
1	C	3637	0	3538	135	0
1	D	3608	0	3466	125	0
1	E	3588	0	3434	140	0
1	F	3540	0	3353	123	0
1	G	3545	0	3353	116	0
1	H	3239	0	2900	132	0
2	A	43	0	30	8	0
2	B	43	0	30	9	0
2	C	43	0	30	11	0
2	D	43	0	30	11	0
2	E	43	0	30	9	0
2	F	43	0	30	8	0
2	G	43	0	30	12	0
2	H	43	0	30	13	0
3	A	13	0	15	5	0
3	B	13	0	15	2	0
3	C	13	0	15	0	0
3	D	13	0	15	5	0
3	E	13	0	15	1	0
3	F	13	0	15	3	0
3	G	13	0	15	3	0
3	H	13	0	15	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	1	0
All	All	28813	0	27320	1069	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 19.

The worst 5 of 1069 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)
1:B:232:ARG:HH11	1:B:232:ARG:HG2	1.00	1.15
2:H:500:HEM:HBD2	2:H:500:HEM:HHA	1.30	1.09
1:H:136:GLY:O	1:H:142:VAL:HB	1.58	1.03
1:F:136:GLY:O	1:F:142:VAL:HB	1.63	0.97
1:G:138:GLY:O	1:G:142:VAL:HG11	1.66	0.94

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	463/476 (97%)	435 (94%)	28 (6%)	0	100	100
1	B	463/476 (97%)	433 (94%)	28 (6%)	2 (0%)	30	62
1	C	463/476 (97%)	435 (94%)	26 (6%)	2 (0%)	30	62
1	D	463/476 (97%)	433 (94%)	29 (6%)	1 (0%)	43	74
1	E	463/476 (97%)	432 (93%)	29 (6%)	2 (0%)	30	62
1	F	463/476 (97%)	429 (93%)	34 (7%)	0	100	100
1	G	463/476 (97%)	434 (94%)	29 (6%)	0	100	100
1	H	462/476 (97%)	432 (94%)	30 (6%)	0	100	100
All	All	3703/3808 (97%)	3463 (94%)	233 (6%)	7 (0%)	43	74

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	366	GLY
1	B	39	VAL
1	B	29	LYS
1	D	29	LYS

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Mol	Chain	Res	Type
1	C	29	LYS

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	385/421 (91%)	361 (94%)	24 (6%)	16	43
1	B	379/421 (90%)	357 (94%)	22 (6%)	18	44
1	C	389/421 (92%)	363 (93%)	26 (7%)	15	41
1	D	384/421 (91%)	361 (94%)	23 (6%)	17	44
1	E	381/421 (90%)	356 (93%)	25 (7%)	15	41
1	F	370/421 (88%)	345 (93%)	25 (7%)	14	40
1	G	371/421 (88%)	338 (91%)	33 (9%)	9	32
1	H	304/421 (72%)	290 (95%)	14 (5%)	24	50
All	All	2963/3368 (88%)	2771 (94%)	192 (6%)	15	42

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	430	SER
1	F	441	ILE
1	E	477	VAL
1	F	251	LYS
1	G	141	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	485	GLN
1	H	409	ASN
1	H	42	ASN
1	H	357	GLN

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Mol	Chain	Res	Type
1	D	177	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	HEM	H	500	-	50,50,50	1.93	10 (20%)	67,82,82	1.33	5 (7%)
3	TB2	F	501	1	12,13,13	0.58	0	18,18,18	1.14	1 (5%)
3	TB2	C	501	1	12,13,13	0.69	0	18,18,18	1.27	2 (11%)
2	HEM	D	500	1	50,50,50	1.84	9 (18%)	67,82,82	1.22	3 (4%)
2	HEM	A	500	1	50,50,50	1.90	10 (20%)	67,82,82	1.19	6 (8%)
3	TB2	A	501	1	12,13,13	0.64	0	18,18,18	1.56	2 (11%)
3	TB2	B	501	1	12,13,13	0.63	0	18,18,18	0.99	1 (5%)
3	TB2	E	501	1	12,13,13	0.60	0	18,18,18	0.98	0
2	HEM	B	500	1	50,50,50	1.94	8 (16%)	67,82,82	1.39	8 (11%)
2	HEM	F	500	1	50,50,50	1.90	10 (20%)	67,82,82	1.24	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	500	1	50,50,50	1.89	9 (18%)	67,82,82	1.23	4 (5%)
2	HEM	E	500	1,4	50,50,50	1.89	8 (16%)	67,82,82	1.34	8 (11%)
3	TB2	D	501	1	12,13,13	0.69	0	18,18,18	1.12	1 (5%)
3	TB2	H	501	1	12,13,13	0.68	0	18,18,18	0.96	0
2	HEM	G	500	1	50,50,50	1.93	11 (22%)	67,82,82	1.21	2 (2%)
3	TB2	G	501	1	12,13,13	0.61	0	18,18,18	1.01	1 (5%)

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	HEM	H	500	-	-	5/14/54/54	-
3	TB2	F	501	1	-	6/9/9/9	0/1/1/1
3	TB2	C	501	1	-	6/9/9/9	0/1/1/1
2	HEM	D	500	1	-	3/14/54/54	-
2	HEM	A	500	1	-	4/14/54/54	-
3	TB2	A	501	1	-	0/9/9/9	0/1/1/1
3	TB2	B	501	1	-	0/9/9/9	0/1/1/1
3	TB2	E	501	1	-	0/9/9/9	0/1/1/1
2	HEM	B	500	1	-	11/14/54/54	-
2	HEM	F	500	1	-	4/14/54/54	-
2	HEM	C	500	1	-	2/14/54/54	-
2	HEM	E	500	1,4	-	8/14/54/54	-
3	TB2	D	501	1	-	0/9/9/9	0/1/1/1
3	TB2	H	501	1	-	6/9/9/9	0/1/1/1
2	HEM	G	500	1	-	5/14/54/54	-
3	TB2	G	501	1	-	6/9/9/9	0/1/1/1

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	HEM	C3D-C2D	8.28	1.54	1.36
2	H	500	HEM	C3D-C2D	7.94	1.53	1.36
2	F	500	HEM	C3D-C2D	7.92	1.53	1.36
2	D	500	HEM	C3D-C2D	7.87	1.53	1.36
2	A	500	HEM	C3D-C2D	7.85	1.53	1.36

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	HEM	C4D-ND-C1D	5.82	112.10	105.21
2	B	500	HEM	C4D-ND-C1D	5.44	111.65	105.21
3	A	501	TB2	O1-C1-C2	-5.41	109.57	126.34
2	G	500	HEM	C4D-ND-C1D	5.35	111.54	105.21
2	F	500	HEM	C4D-ND-C1D	5.30	111.48	105.21

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500	HEM	C3A-C2A-CAA-CBA
2	G	500	HEM	C4D-C3D-CAD-CBD
2	H	500	HEM	C1A-C2A-CAA-CBA
2	H	500	HEM	C2D-C3D-CAD-CBD
2	H	500	HEM	C4D-C3D-CAD-CBD

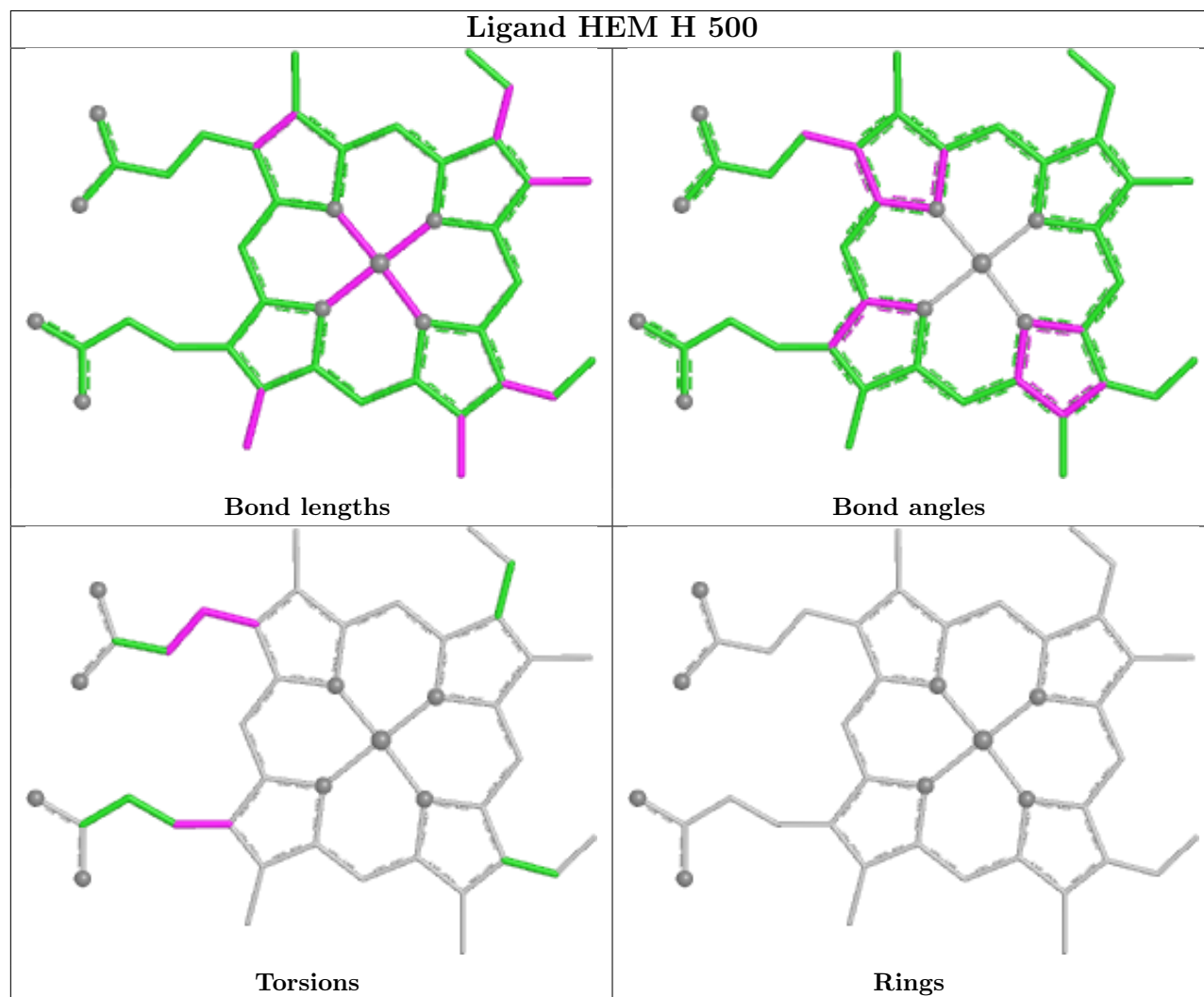
There are no ring outliers.

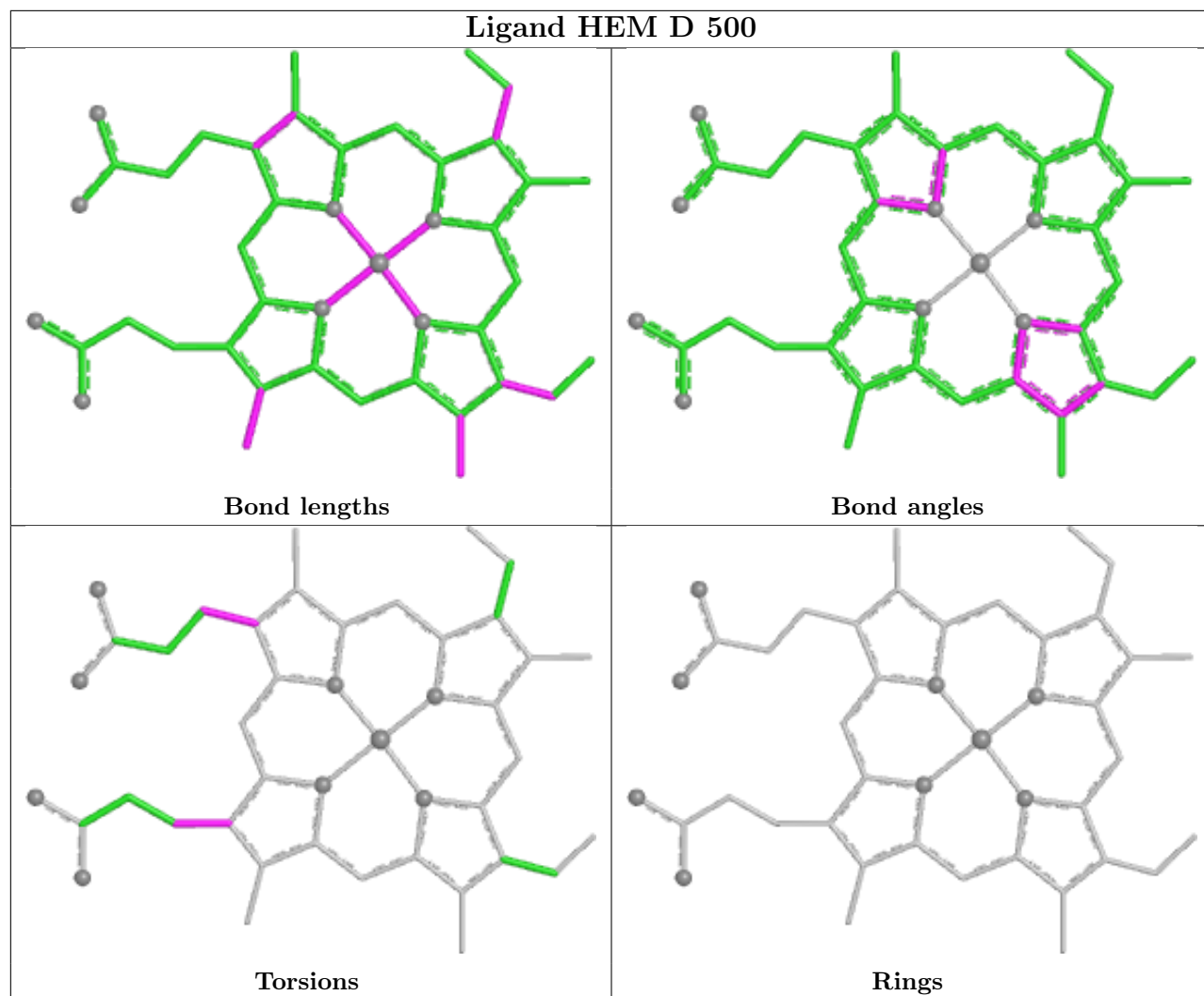
15 monomers are involved in 102 short contacts:

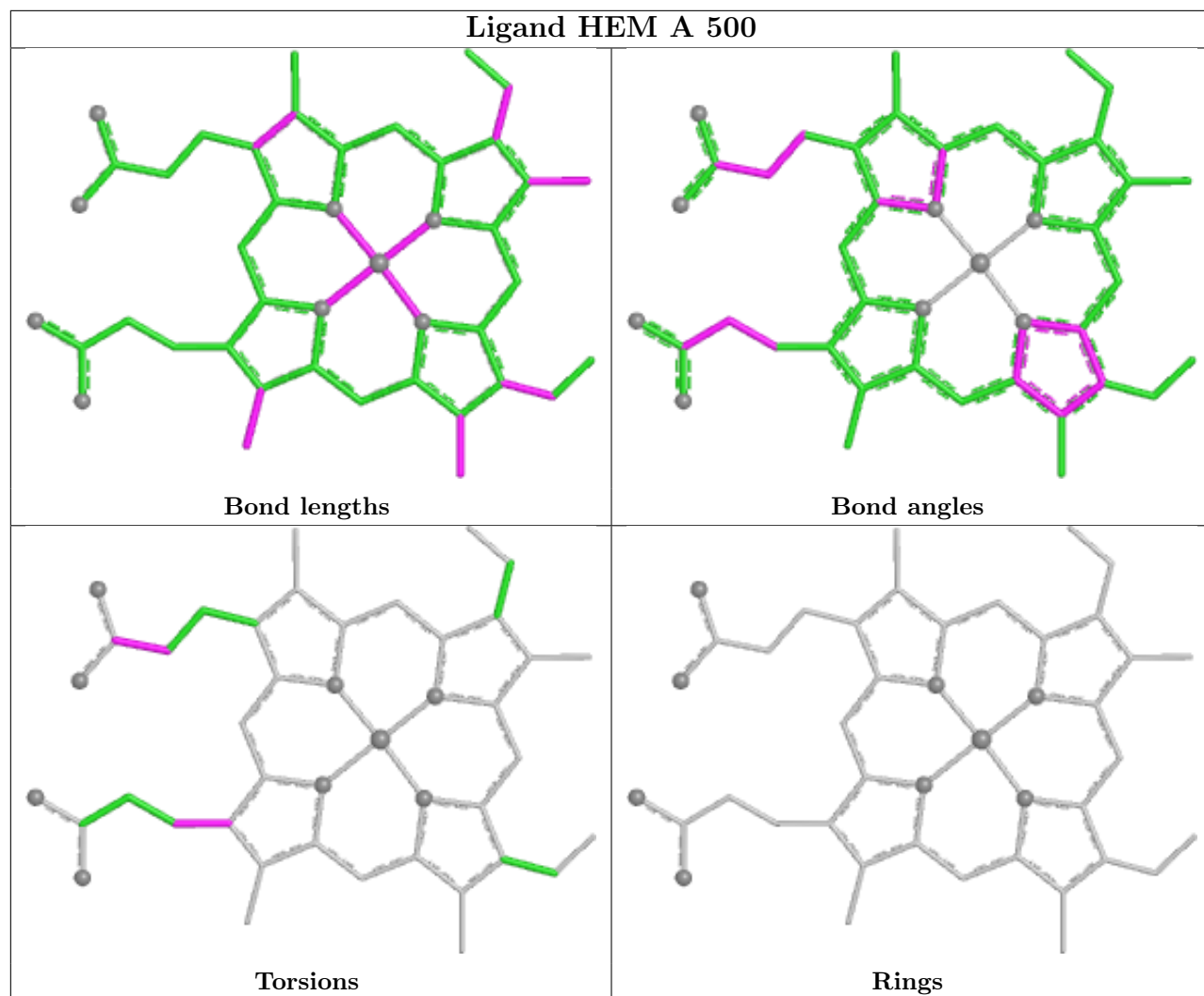
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	500	HEM	13	0
3	F	501	TB2	3	0
2	D	500	HEM	11	0
2	A	500	HEM	8	0
3	A	501	TB2	5	0
3	B	501	TB2	2	0
3	E	501	TB2	1	0
2	B	500	HEM	9	0
2	F	500	HEM	8	0
2	C	500	HEM	11	0
2	E	500	HEM	9	0
3	D	501	TB2	5	0
3	H	501	TB2	2	0
2	G	500	HEM	12	0
3	G	501	TB2	3	0

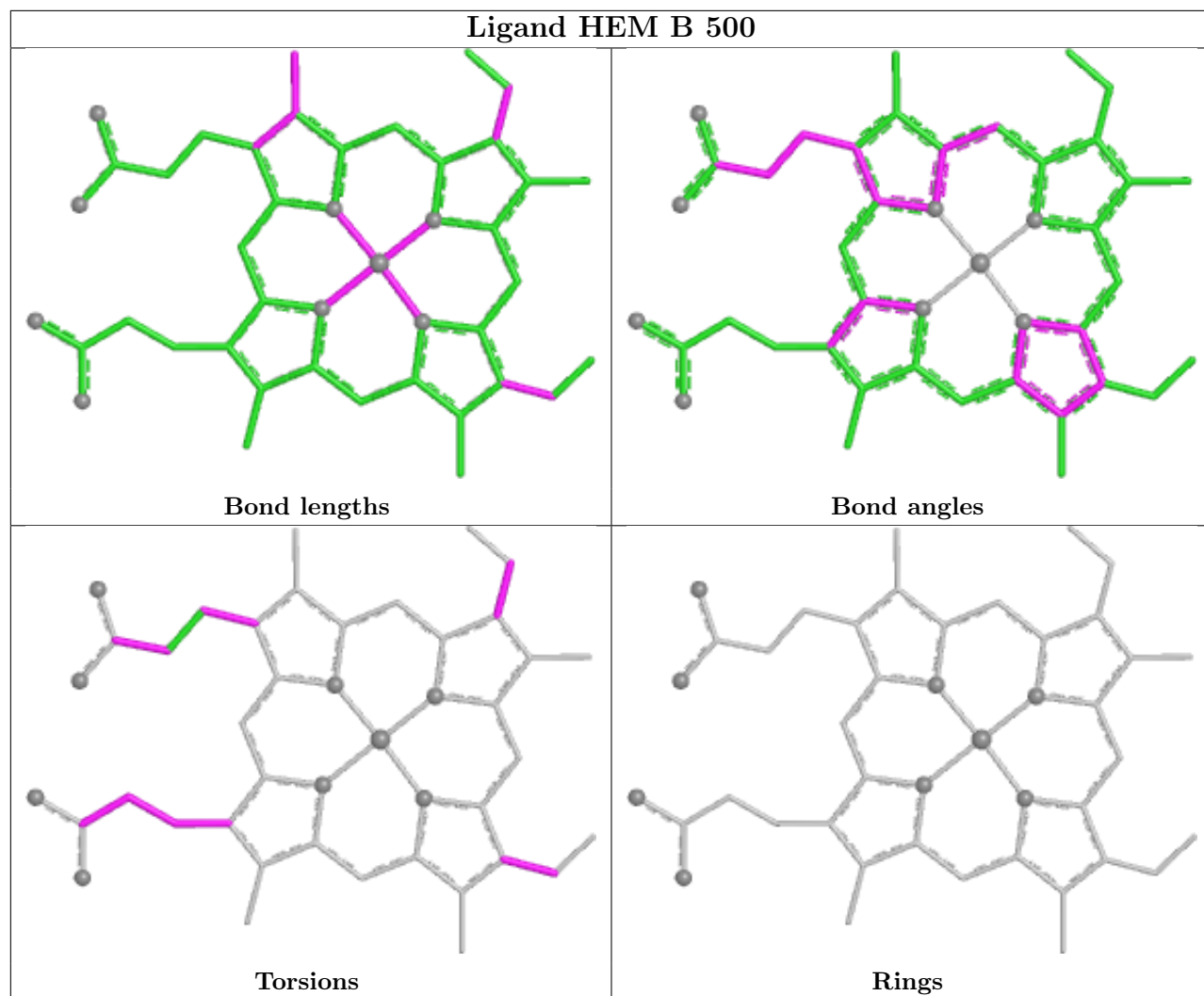
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

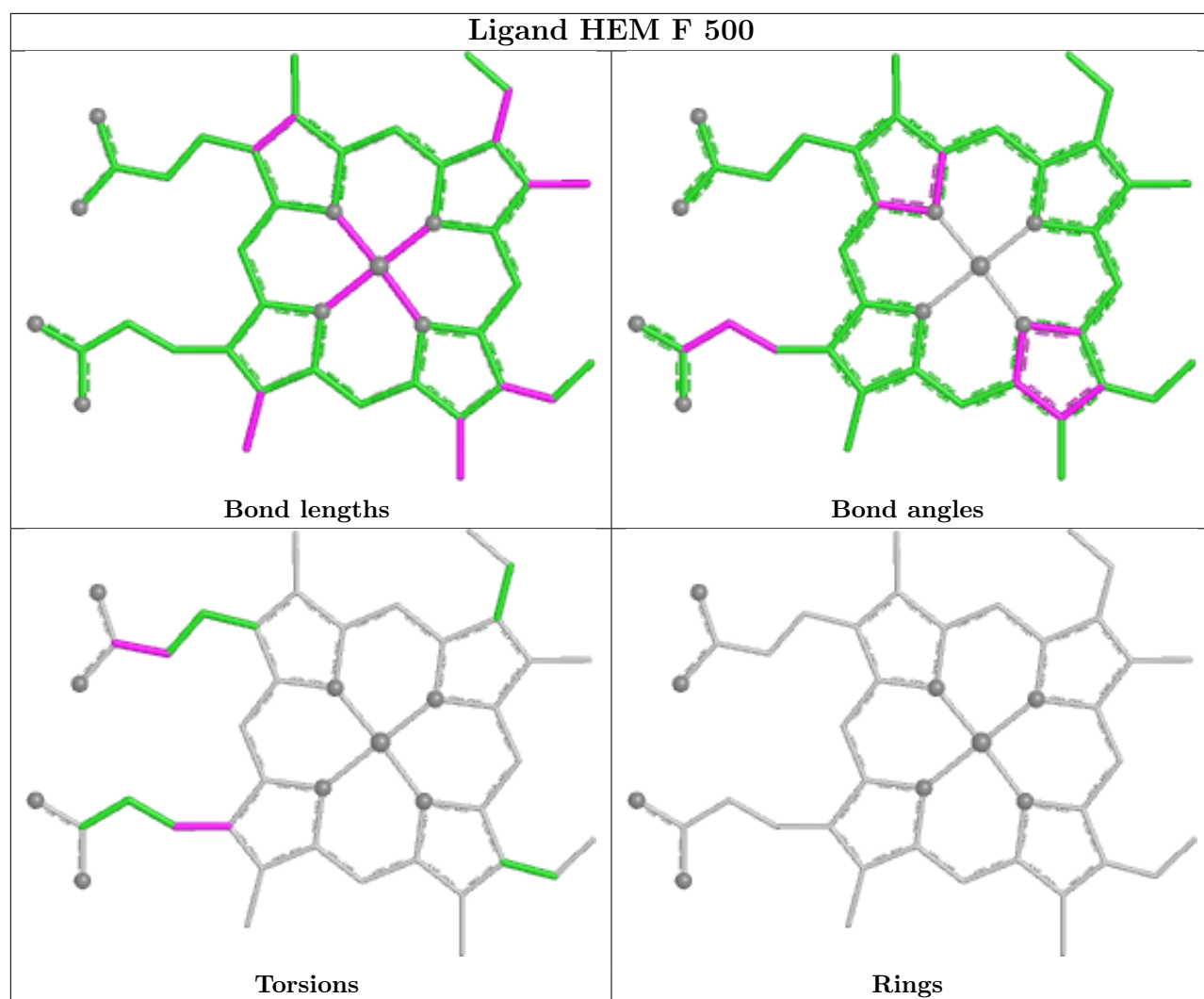
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

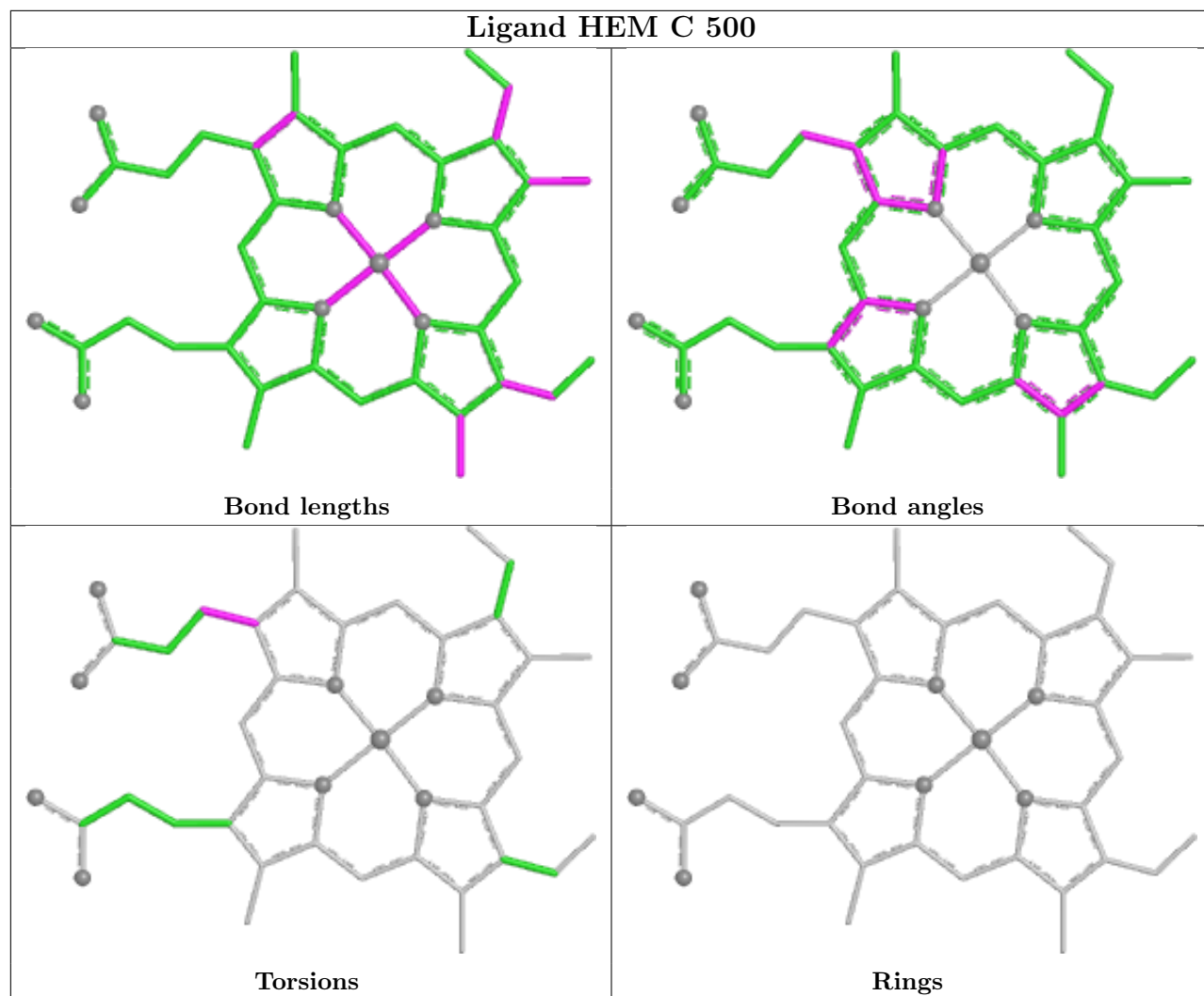


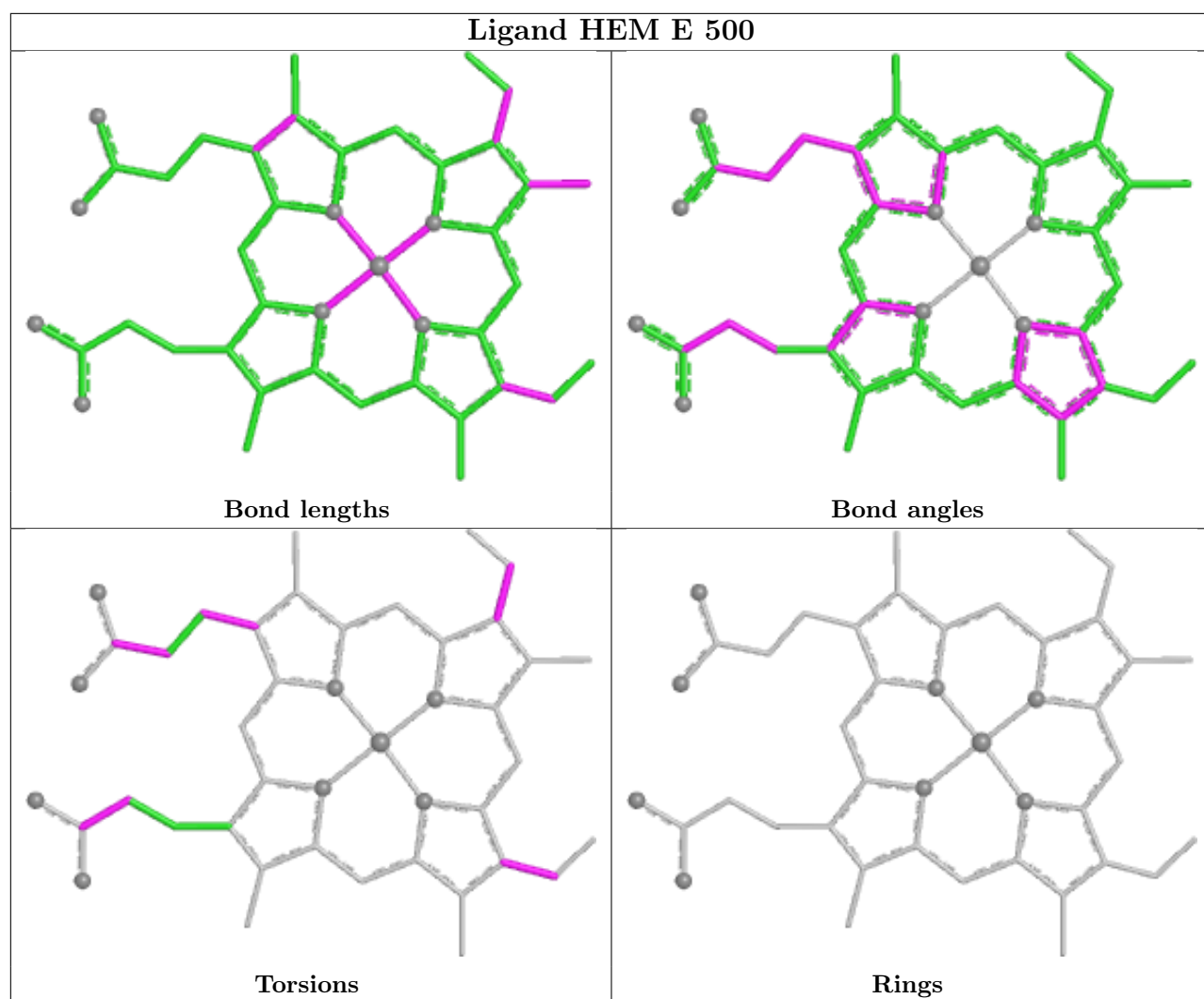


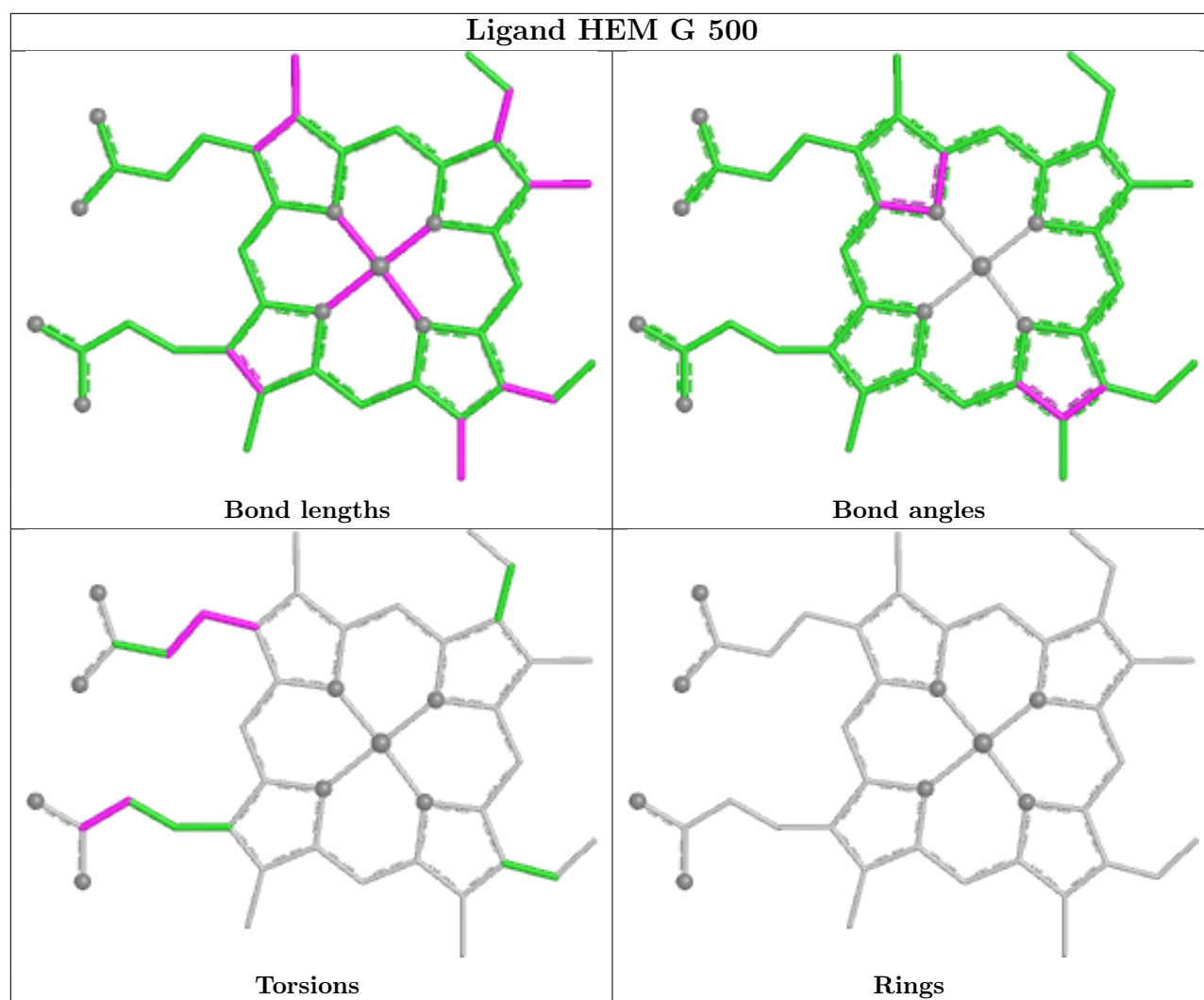












5.7 Other polymers [i](#)

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	465/476 (97%)	-0.47	2 (0%) 88 72	40, 59, 81, 119	0
1	B	465/476 (97%)	-0.41	0 100 100	41, 67, 94, 143	0
1	C	465/476 (97%)	-0.40	0 100 100	43, 67, 102, 147	0
1	D	465/476 (97%)	-0.48	0 100 100	41, 58, 82, 101	0
1	E	465/476 (97%)	-0.42	1 (0%) 91 82	49, 65, 87, 108	0
1	F	465/476 (97%)	-0.38	1 (0%) 91 82	40, 68, 96, 114	0
1	G	465/476 (97%)	-0.36	0 100 100	49, 75, 115, 133	0
1	H	464/476 (97%)	0.20	5 (1%) 78 54	93, 121, 143, 156	0
All	All	3719/3808 (97%)	-0.34	9 (0%) 91 82	40, 68, 126, 156	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	GLY	3.3
1	E	136	GLY	2.7
1	H	428	PRO	2.7
1	A	139	LYS	2.5
1	H	288	LEU	2.5

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

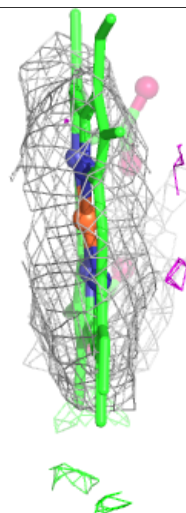
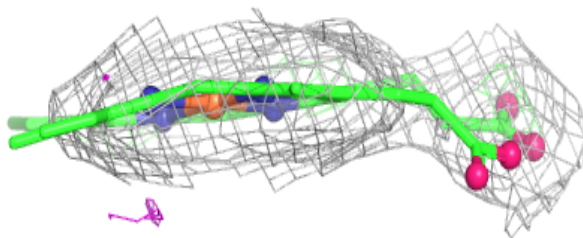
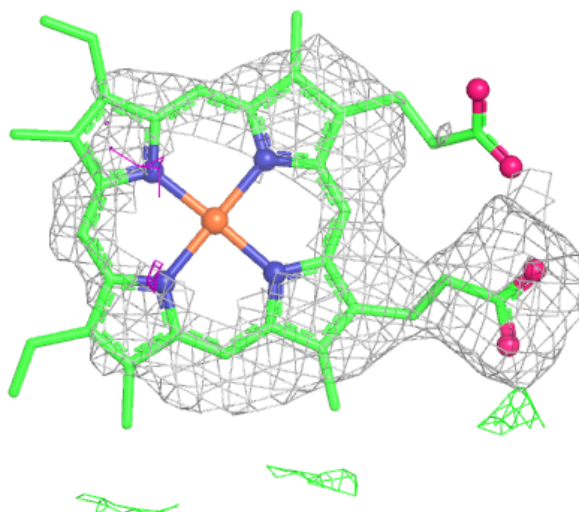
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	H	500	43/43	0.91	0.13	92,106,114,114	0
3	TB2	E	501	13/13	0.91	0.15	48,53,58,59	0
3	TB2	H	501	13/13	0.91	0.14	96,103,107,110	0
3	TB2	F	501	13/13	0.92	0.15	46,51,63,66	0
3	TB2	D	501	13/13	0.93	0.15	48,56,60,60	0
3	TB2	A	501	13/13	0.94	0.12	42,49,57,57	0
3	TB2	B	501	13/13	0.94	0.15	54,60,67,69	0
3	TB2	G	501	13/13	0.95	0.14	57,62,73,77	0
3	TB2	C	501	13/13	0.97	0.10	40,51,55,57	0
2	HEM	G	500	43/43	0.97	0.10	59,70,89,98	0
2	HEM	E	500	43/43	0.98	0.08	48,55,60,62	0
2	HEM	F	500	43/43	0.98	0.10	43,53,62,72	0
2	HEM	A	500	43/43	0.98	0.08	39,49,54,57	0
2	HEM	B	500	43/43	0.98	0.07	41,59,68,72	0
2	HEM	C	500	43/43	0.98	0.11	45,56,66,72	0
2	HEM	D	500	43/43	0.98	0.08	36,44,53,55	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.

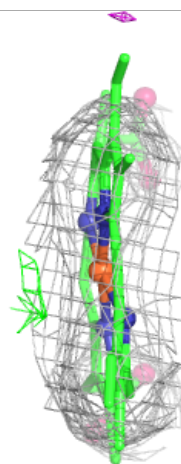
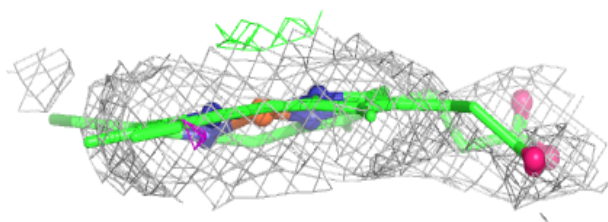
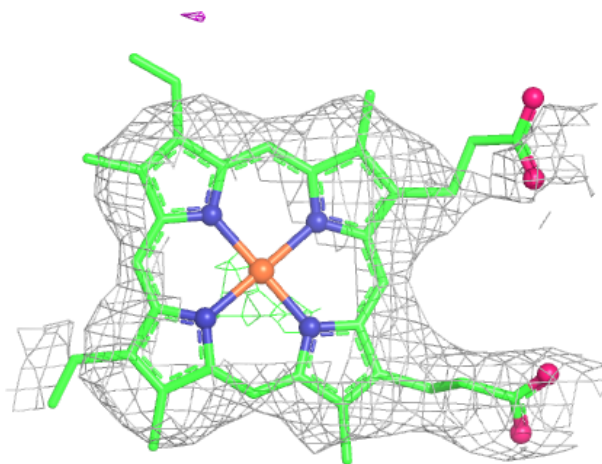
Electron density around HEM H 500:

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



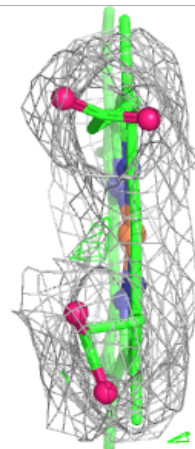
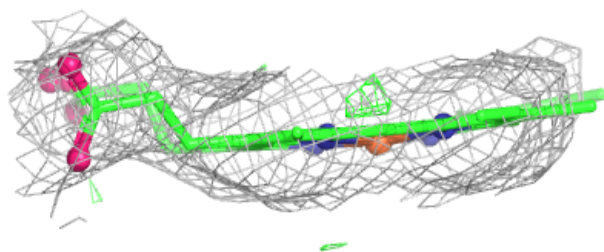
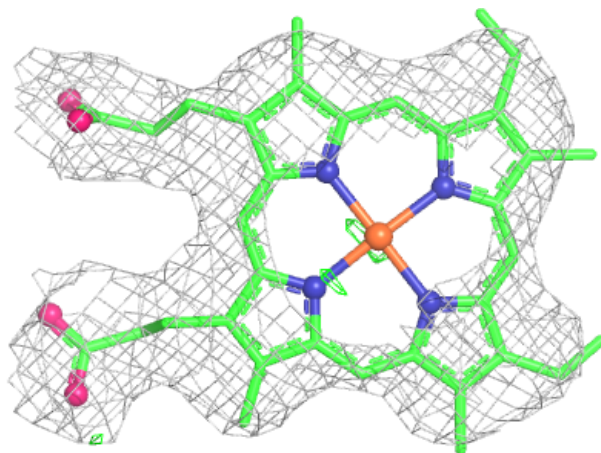
Electron density around HEM G 500:

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



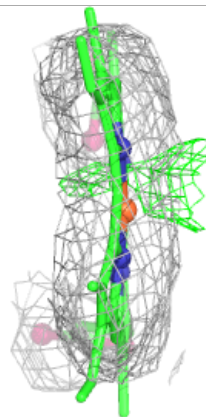
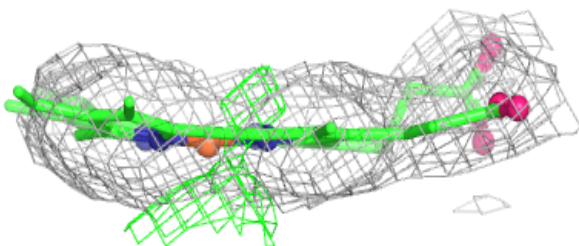
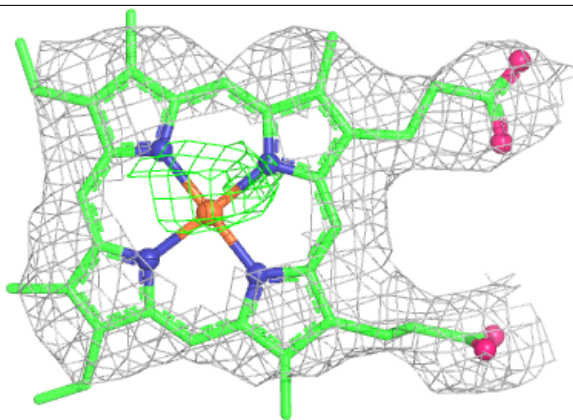
Electron density around HEM E 500:

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



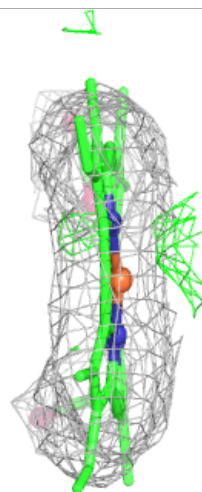
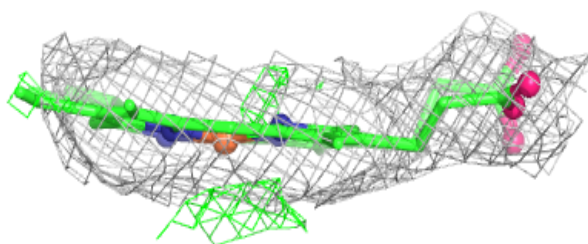
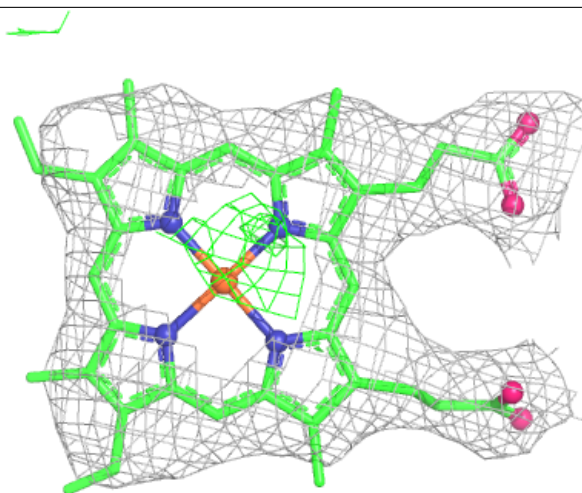
Electron density around HEM F 500:

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



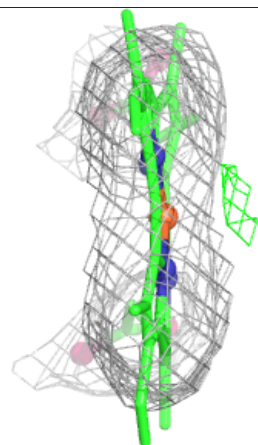
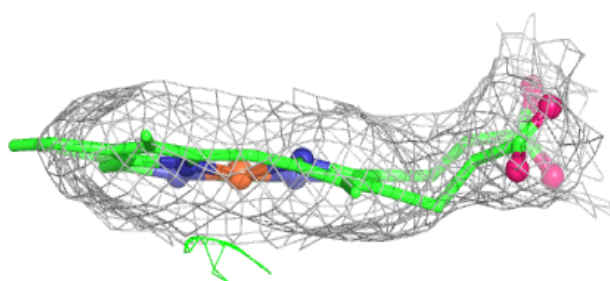
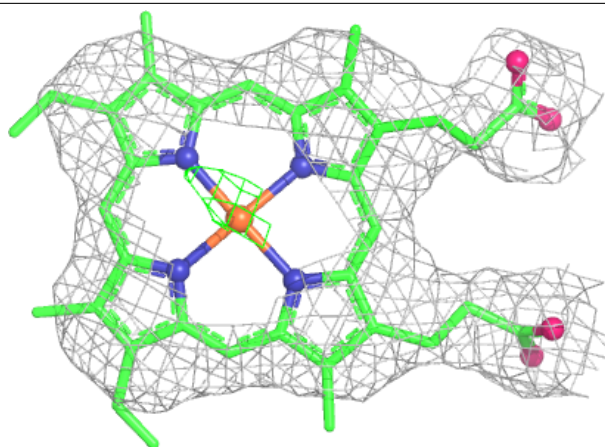
Electron density around HEM A 500:

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



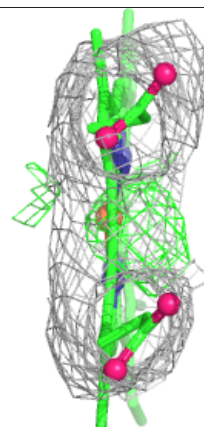
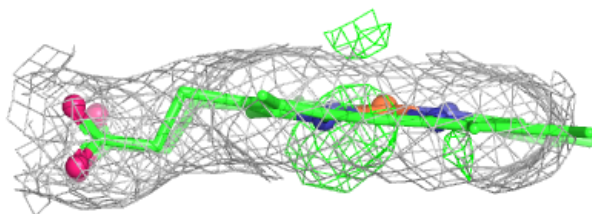
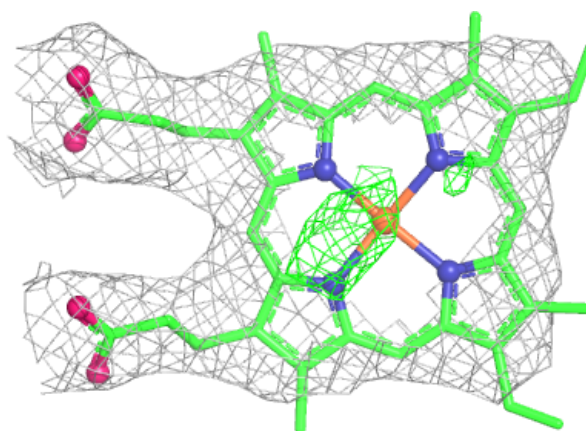
Electron density around HEM B 500:

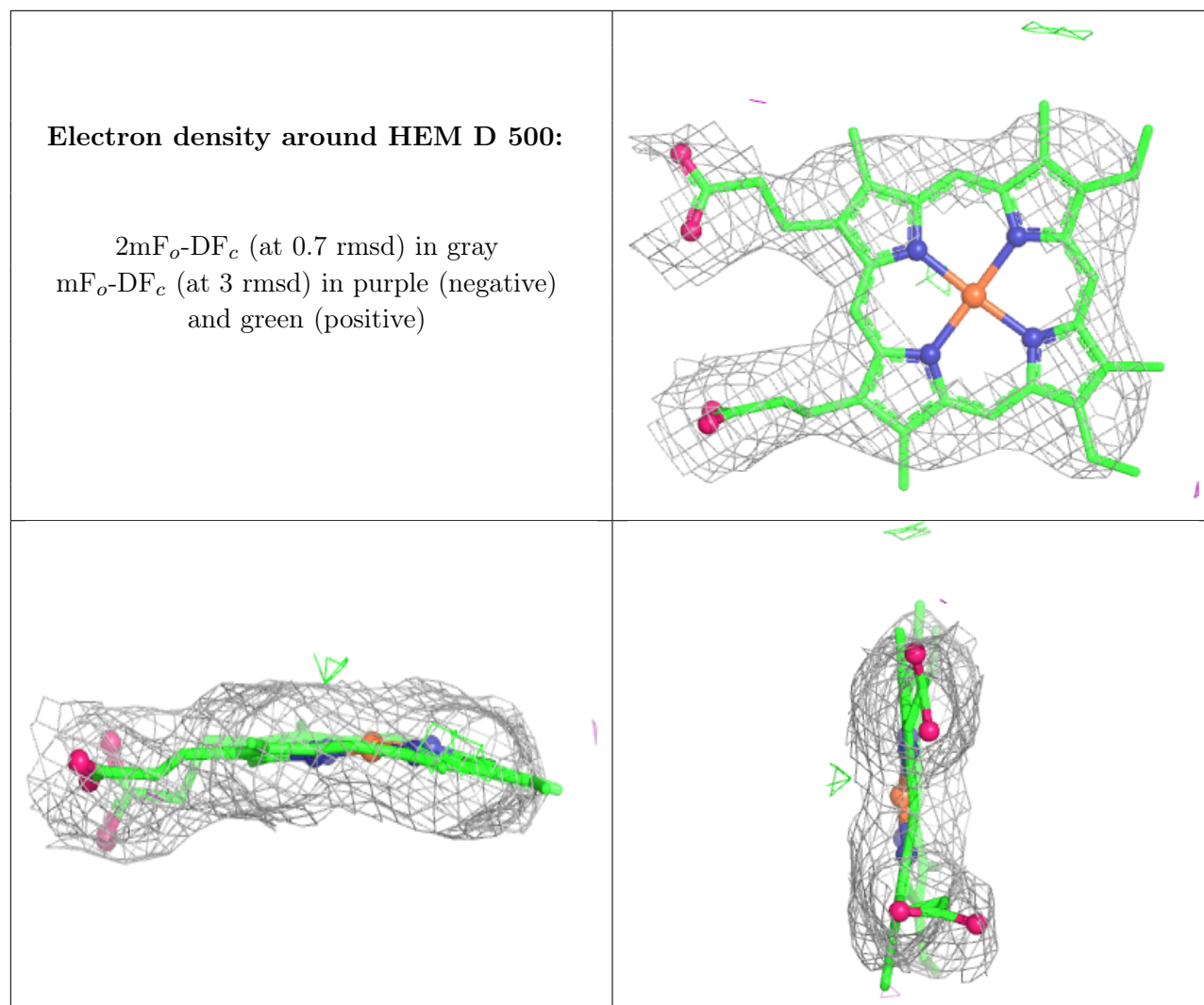
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 500:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.