



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:45 AM UTC

PDB ID : 5E58 / pdb_00005e58
Title : Crystal Structure Of Cytochrome P450 2B35 from Desert Woodrat Neotoma
Lepida in complex with 4-(4-chlorophenyl)imidazole
Authors : Shah, M.B.; Stout, C.D.; Halpert, J.R.
Deposited on : 2015-10-08
Resolution : 2.40 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:

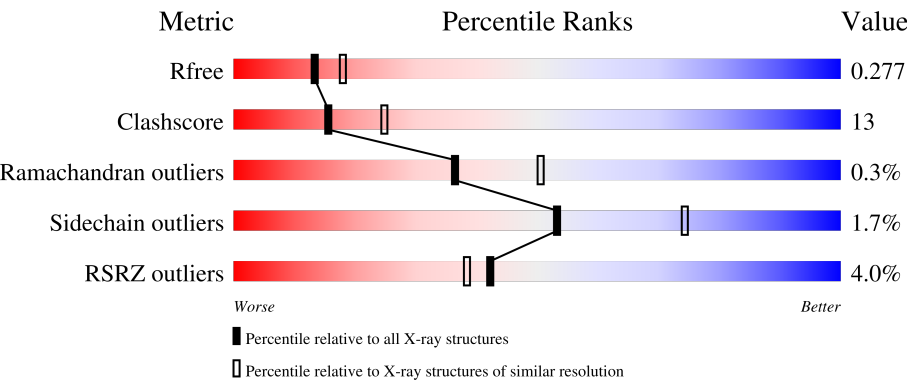
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	493	81%13%• 6%
1	B	493	70%22%• 7%
1	C	493	71%21%• 6%
1	D	493	76%17%• 6%
1	E	493	72%21%• 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	493	
2	G	2	

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	GLC	G	1	-	X	-	-
2	FRU	G	2	-	-	X	-
4	CPZ	A	502	-	-	X	-
4	CPZ	B	502	-	-	X	-
4	CPZ	B	503	-	-	X	-
4	CPZ	C	502	-	-	X	-
4	CPZ	D	502	-	-	X	-
4	CPZ	E	502	-	-	X	-
4	CPZ	F	502	-	-	X	-
4	CPZ	F	503	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23024 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.

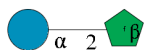
- Molecule 1 is a protein called Cytochrome P450 family 2 subfamily B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3727	2396	638	677	16			
1	B	458	Total	C	N	O	S	0	0	0
			3602	2321	607	659	15			
1	C	465	Total	C	N	O	S	0	0	0
			3685	2371	631	667	16			
1	D	463	Total	C	N	O	S	0	0	0
			3665	2360	623	666	16			
1	E	462	Total	C	N	O	S	0	0	0
			3661	2352	626	667	16			
1	F	458	Total	C	N	O	S	0	1	0
			3558	2284	608	651	15			

There are 12 discrepancies between the modelled and reference sequences:

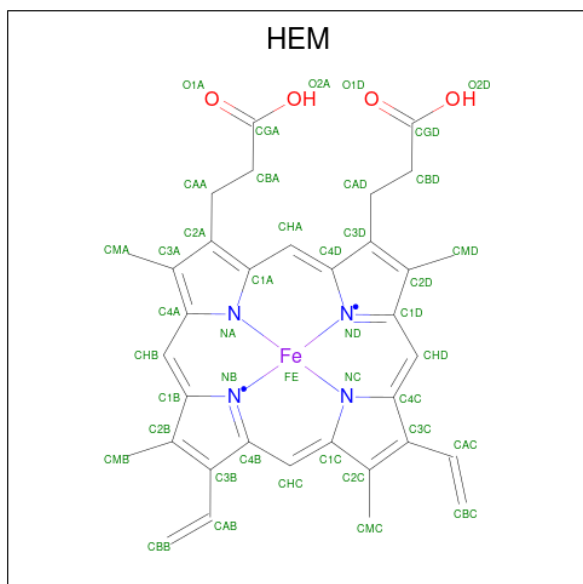
Chain	Residue	Modelled	Actual	Comment	Reference
A	492	HIS	-	expression tag	UNP J9JD66
A	493	HIS	-	expression tag	UNP J9JD66
B	492	HIS	-	expression tag	UNP J9JD66
B	493	HIS	-	expression tag	UNP J9JD66
C	492	HIS	-	expression tag	UNP J9JD66
C	493	HIS	-	expression tag	UNP J9JD66
D	492	HIS	-	expression tag	UNP J9JD66
D	493	HIS	-	expression tag	UNP J9JD66
E	492	HIS	-	expression tag	UNP J9JD66
E	493	HIS	-	expression tag	UNP J9JD66
F	492	HIS	-	expression tag	UNP J9JD66
F	493	HIS	-	expression tag	UNP J9JD66

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



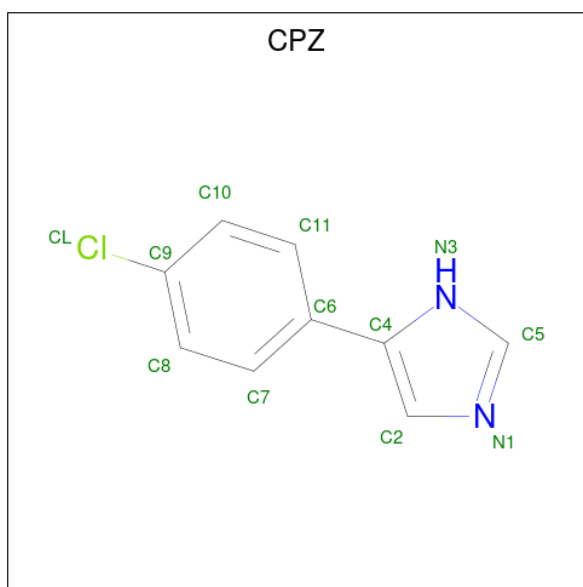
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



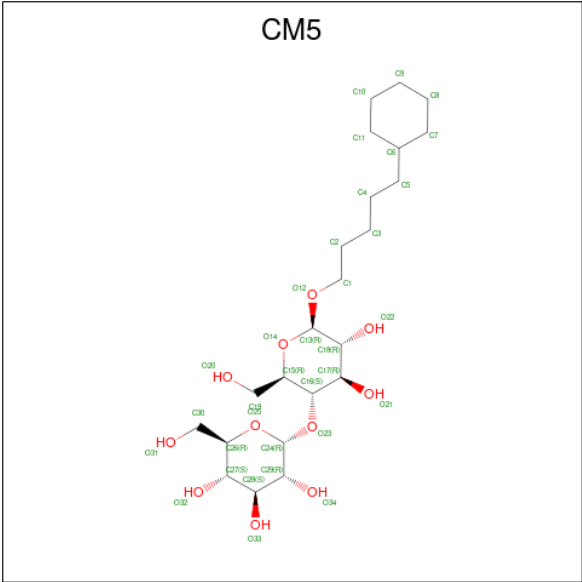
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is 4-(4-CHLOROPHENYL)IMIDAZOLE (CCD ID: CPZ) (formula: $C_9H_7ClN_2$).



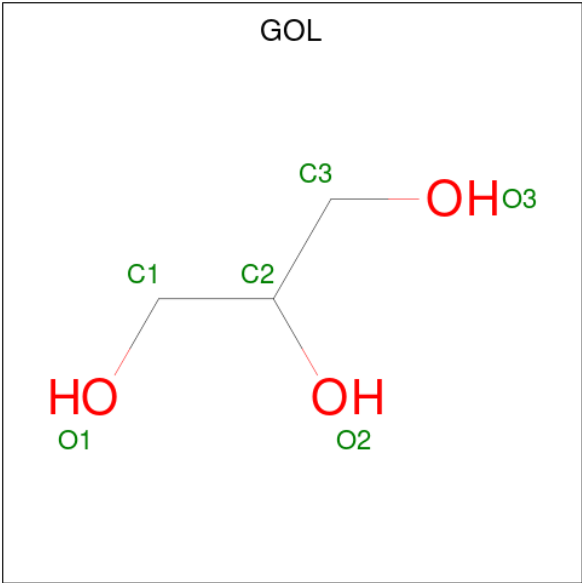
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	A	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	B	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	B	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	C	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	C	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	D	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	D	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	E	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	E	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	F	1	Total	C	Cl	N	0	0
			12	9	1	2		
4	F	1	Total	C	Cl	N	0	0
			12	9	1	2		

- Molecule 5 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (CCD ID: CM5) (formula: C₂₃H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C		0	0
			6	6			
5	E	1	Total	C	O	0	0
			12	11	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

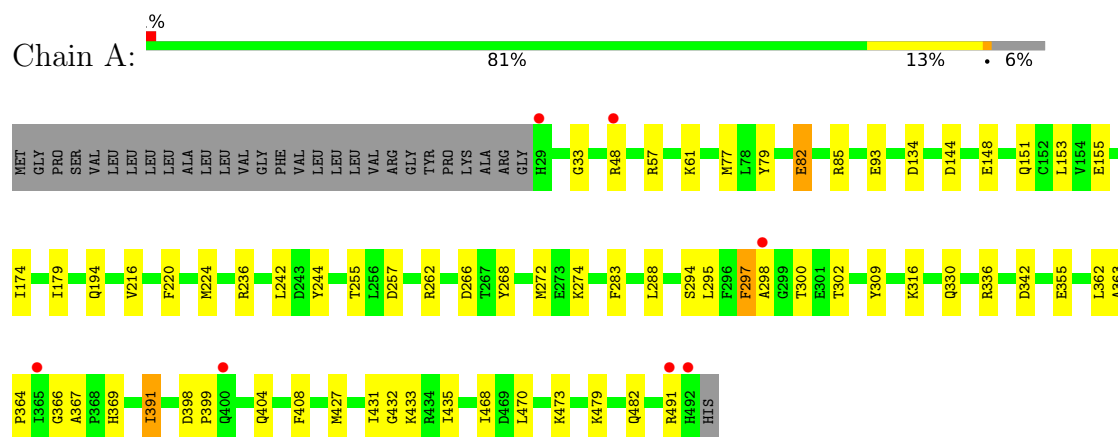
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	211	Total	O	0	0
			211	211		
7	B	59	Total	O	0	0
			59	59		
7	C	124	Total	O	0	0
			124	124		
7	D	106	Total	O	0	0
			106	106		
7	E	99	Total	O	0	0
			99	99		
7	F	60	Total	O	0	0
			60	60		

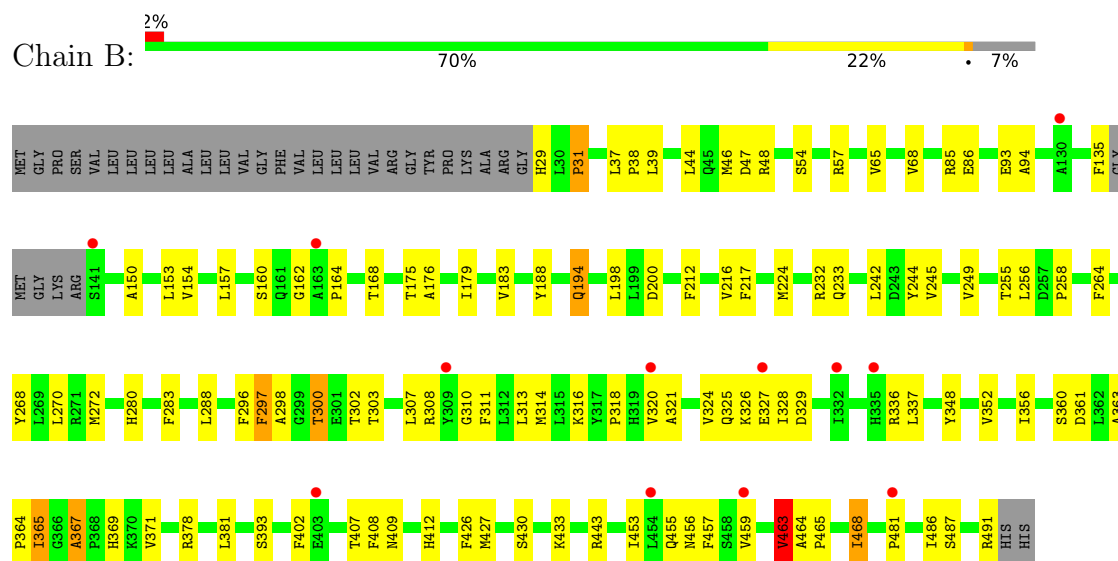
3 Residue-property plots [i](#)

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: Cytochrome P450 family 2 subfamily B

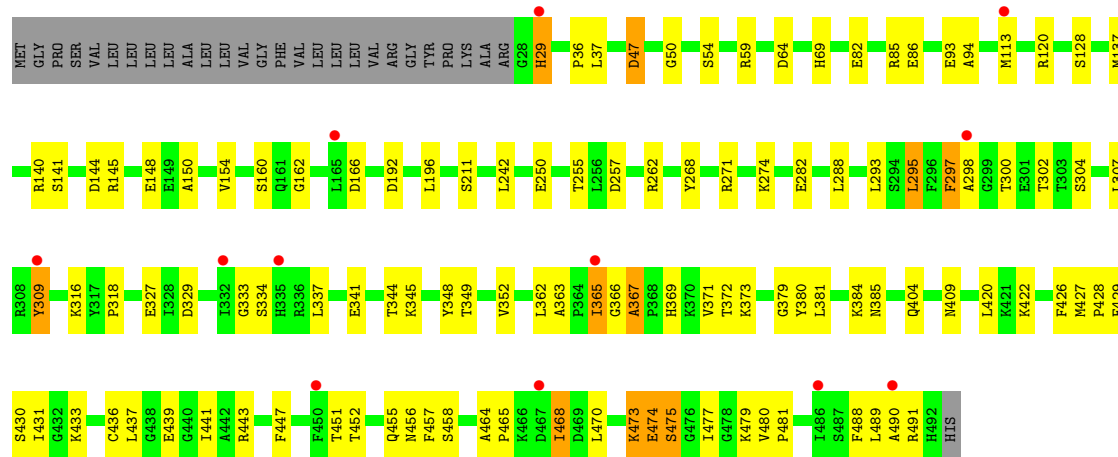


- Molecule 1: Cytochrome P450 family 2 subfamily B

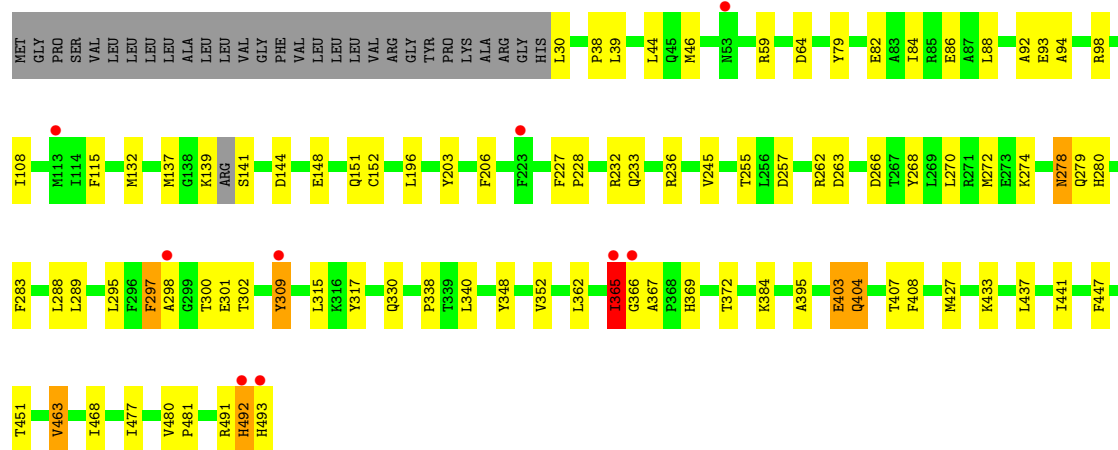
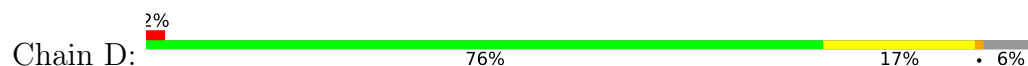


- Molecule 1: Cytochrome P450 family 2 subfamily B

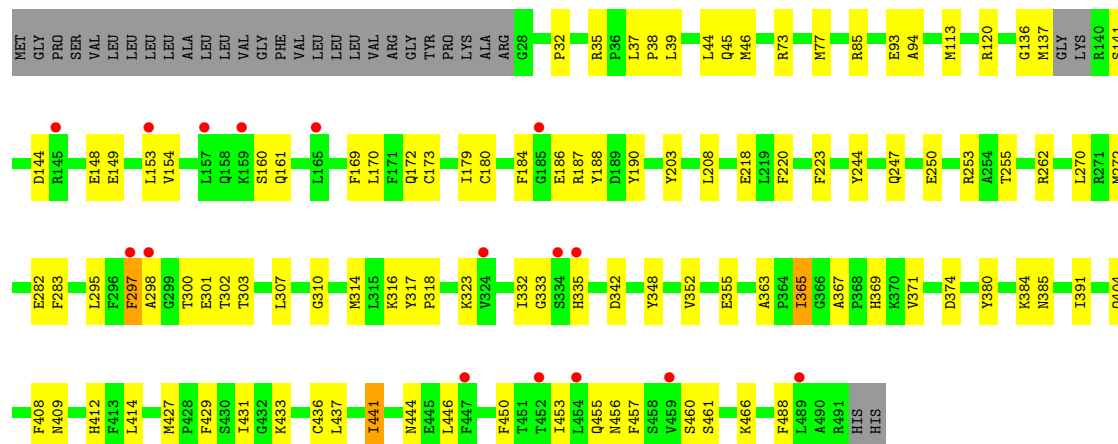




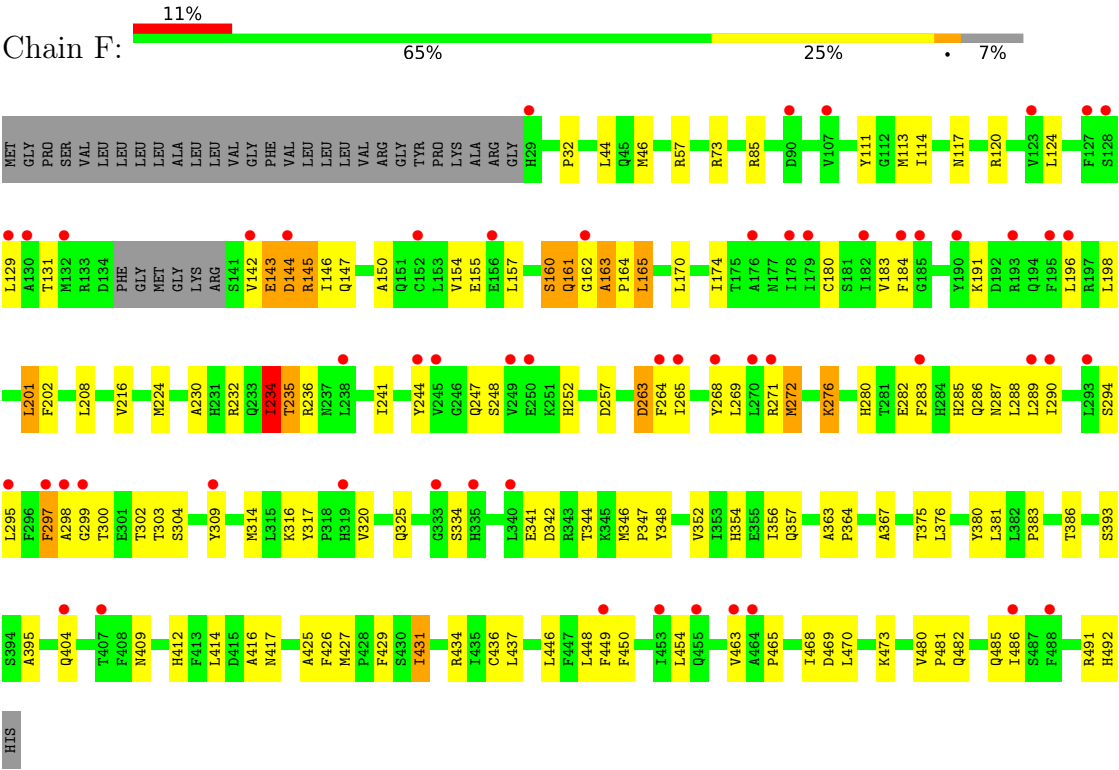
• Molecule 1: Cytochrome P450 family 2 subfamily B



• Molecule 1: Cytochrome P450 family 2 subfamily B



• Molecule 1: Cytochrome P450 family 2 subfamily B



● Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	98.08Å 106.07Å 106.20Å 64.61° 82.53° 69.93°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.00-2.40) 94.8 (40.00-2.40)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.216 , 0.283 0.229 , 0.277	Depositor DCC
R_{free} test set	6567 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23024	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FRU, CM5, GOL, CPZ, HEM, GLC

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	0.75	3/3819 (0.1%)	0.99	8/5163 (0.2%)
1	B	0.80	8/3692 (0.2%)	1.00	4/5008 (0.1%)
1	C	0.75	7/3778 (0.2%)	1.02	21/5114 (0.4%)
1	D	0.73	5/3757 (0.1%)	0.96	11/5090 (0.2%)
1	E	0.64	2/3752 (0.1%)	0.95	8/5080 (0.2%)
1	F	0.79	3/3637 (0.1%)	1.09	17/4936 (0.3%)
All	All	0.75	28/22435 (0.1%)	1.00	69/30391 (0.2%)

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	365	ILE	CA-CB	-8.80	1.44	1.54
1	C	295	LEU	C-N	8.57	1.45	1.33
1	F	299	GLY	C-O	-8.05	1.18	1.24
1	D	295	LEU	N-CA	-7.10	1.37	1.46
1	B	164	PRO	C-N	-6.69	1.25	1.33

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	365	ILE	N-CA-C	-8.08	101.24	110.05
1	F	131	THR	N-CA-C	7.54	119.28	111.14
1	A	257	ASP	CA-C-N	7.11	126.79	119.82
1	A	257	ASP	C-N-CA	7.11	126.79	119.82
1	E	136	GLY	N-CA-C	7.03	124.34	114.85

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	3727	0	3708	49	0
1	B	3602	0	3500	99	1
1	C	3685	0	3625	100	0
1	D	3665	0	3594	81	0
1	E	3661	0	3581	95	1
1	F	3558	0	3406	135	0
2	G	23	0	18	13	0
3	A	43	0	30	9	0
3	B	43	0	30	9	0
3	C	43	0	30	7	0
3	D	43	0	30	3	0
3	E	43	0	30	8	0
3	F	43	0	30	7	0
4	A	24	0	14	4	0
4	B	24	0	14	9	0
4	C	24	0	14	6	0
4	D	24	0	14	5	0
4	E	24	0	14	8	0
4	F	24	0	14	10	0
5	A	6	0	10	0	0
5	E	12	0	21	2	0
6	A	6	0	8	0	0
6	B	6	0	8	1	0
6	C	6	0	8	0	0
6	E	6	0	8	0	0
7	A	211	0	0	12	0
7	B	59	0	0	7	0
7	C	124	0	0	13	0
7	D	106	0	0	11	0
7	E	99	0	0	14	0
7	F	60	0	0	16	0
All	All	23024	0	21759	589	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 13.

The worst 5 of 589 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:E:455:GLN:NE2	7:E:601:HOH:O	1.79	1.15
2:G:1:GLC:O2	2:G:2:FRU:O3	1.70	1.06
1:A:297:PHE:O	1:A:298:ALA:HB3	1.60	1.02
1:B:297:PHE:O	1:B:298:ALA:HB3	1.60	1.01
1:F:157:LEU:O	1:F:160:SER:HB3	1.62	1.00

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)
1:B:280:HIS:O	1:E:335:HIS:NE2[1_554]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

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	462/493 (94%)	447 (97%)	15 (3%)	0	100	100
1	B	454/493 (92%)	432 (95%)	22 (5%)	0	100	100
1	C	463/493 (94%)	450 (97%)	12 (3%)	1 (0%)	43	58
1	D	459/493 (93%)	446 (97%)	12 (3%)	1 (0%)	43	58
1	E	458/493 (93%)	444 (97%)	14 (3%)	0	100	100
1	F	455/493 (92%)	424 (93%)	26 (6%)	5 (1%)	11	18
All	All	2751/2958 (93%)	2643 (96%)	101 (4%)	7 (0%)	36	50

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	475	SER
1	F	163	ALA
1	F	144	ASP
1	F	235	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	492	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	408/433 (94%)	400 (98%)	8 (2%)	48	70
1	B	384/433 (89%)	380 (99%)	4 (1%)	68	84
1	C	396/433 (92%)	390 (98%)	6 (2%)	57	77
1	D	395/433 (91%)	387 (98%)	8 (2%)	48	70
1	E	393/433 (91%)	391 (100%)	2 (0%)	81	91
1	F	370/433 (86%)	359 (97%)	11 (3%)	36	58
All	All	2346/2598 (90%)	2307 (98%)	39 (2%)	53	74

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	44	LEU
1	F	276	LYS
1	F	129	LEU
1	F	201	LEU
1	F	431	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	285	HIS
1	F	335	HIS
1	F	325	GLN
1	D	53	ASN
1	D	456	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 ⓘ

2 monosaccharides 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	GLC	G	1	2	11,11,12	3.20	8 (72%)	15,15,17	2.76	10 (66%)
2	FRU	G	2	2	11,12,12	0.56	0	10,18,18	0.55	0

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	GLC	G	1	2	-	2/2/19/22	0/1/1/1
2	FRU	G	2	2	-	3/5/24/24	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	GLC	O5-C1	-4.74	1.35	1.43
2	G	1	GLC	C4-C3	-3.98	1.42	1.52
2	G	1	GLC	O2-C2	-3.95	1.35	1.43
2	G	1	GLC	C2-C3	-3.92	1.46	1.52
2	G	1	GLC	O4-C4	-3.56	1.34	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	GLC	O5-C1-C2	-4.95	98.98	110.79
2	G	1	GLC	O4-C4-C3	-4.38	100.06	110.38
2	G	1	GLC	C1-C2-C3	3.25	114.38	109.64
2	G	1	GLC	C3-C4-C5	-3.24	104.36	110.23
2	G	1	GLC	O2-C2-C1	3.19	116.53	109.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

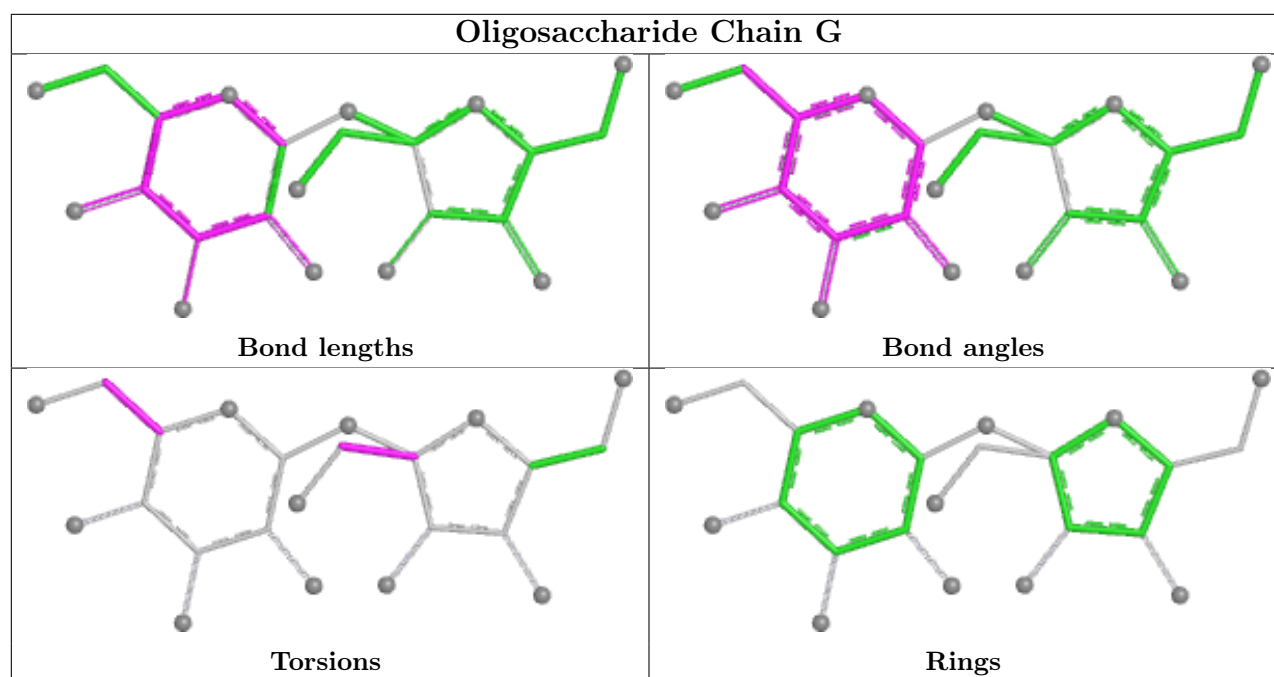
Mol	Chain	Res	Type	Atoms
2	G	2	FRU	O1-C1-C2-C3
2	G	2	FRU	O1-C1-C2-O2
2	G	1	GLC	C4-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	G	2	FRU	O1-C1-C2-O5

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	GLC	4	0
2	G	2	FRU	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
3	HEM	F	501	4	50,50,50	1.89	12 (24%)	67,82,82	1.54	10 (14%)
5	CM5	A	505	-	6,6,36	0.46	0	6,6,49	0.64	0
3	HEM	C	501	4,1	50,50,50	1.83	8 (16%)	67,82,82	1.20	7 (10%)
4	CPZ	E	503	-	12,13,13	1.00	1 (8%)	16,17,17	1.03	1 (6%)
4	CPZ	E	502	3	12,13,13	1.01	1 (8%)	16,17,17	1.02	1 (6%)
4	CPZ	C	502	3	12,13,13	1.02	1 (8%)	16,17,17	1.02	1 (6%)
6	GOL	A	506	-	5,5,5	0.60	0	5,5,5	0.99	0
4	CPZ	A	503	-	12,13,13	1.03	2 (16%)	16,17,17	1.02	1 (6%)
3	HEM	A	501	4,1	50,50,50	2.28	22 (44%)	67,82,82	1.24	9 (13%)
3	HEM	B	501	4,1	50,50,50	1.88	10 (20%)	67,82,82	1.23	8 (11%)
4	CPZ	F	503	-	12,13,13	1.03	2 (16%)	16,17,17	1.02	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CPZ	B	503	-	12,13,13	1.03	2 (16%)	16,17,17	1.45	3 (18%)
6	GOL	C	504	-	5,5,5	0.42	0	5,5,5	0.62	0
6	GOL	E	505	-	5,5,5	0.49	0	5,5,5	0.59	0
6	GOL	B	504	-	5,5,5	0.51	0	5,5,5	0.81	0
4	CPZ	C	503	-	12,13,13	1.02	1 (8%)	16,17,17	1.02	1 (6%)
3	HEM	E	501	4,1	50,50,50	1.98	11 (22%)	67,82,82	1.35	9 (13%)
4	CPZ	B	502	3	12,13,13	1.29	1 (8%)	16,17,17	1.47	3 (18%)
5	CM5	E	504	-	12,12,36	1.19	0	13,13,49	1.14	0
4	CPZ	F	502	3	12,13,13	1.02	2 (16%)	16,17,17	1.03	1 (6%)
3	HEM	D	501	4,1	50,50,50	1.71	7 (14%)	67,82,82	1.31	6 (8%)
4	CPZ	D	502	-	12,13,13	1.03	2 (16%)	16,17,17	1.02	1 (6%)
4	CPZ	D	503	3	12,13,13	0.99	2 (16%)	16,17,17	1.01	1 (6%)
4	CPZ	A	502	3	12,13,13	1.02	1 (8%)	16,17,17	1.03	1 (6%)

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
3	HEM	F	501	4	-	10/14/54/54	-
5	CM5	A	505	-	-	-	0/1/1/3
3	HEM	C	501	4,1	-	2/14/54/54	-
4	CPZ	E	503	-	-	4/4/4/4	0/2/2/2
4	CPZ	E	502	3	-	0/4/4/4	0/2/2/2
4	CPZ	C	502	3	-	0/4/4/4	0/2/2/2
6	GOL	A	506	-	-	2/4/4/4	-
4	CPZ	A	503	-	-	4/4/4/4	0/2/2/2
3	HEM	A	501	4,1	-	4/14/54/54	-
3	HEM	B	501	4,1	-	4/14/54/54	-
4	CPZ	F	503	-	-	4/4/4/4	0/2/2/2
4	CPZ	B	503	-	-	4/4/4/4	0/2/2/2
6	GOL	C	504	-	-	0/4/4/4	-
6	GOL	E	505	-	-	4/4/4/4	-
6	GOL	B	504	-	-	4/4/4/4	-
4	CPZ	C	503	-	-	0/4/4/4	0/2/2/2
3	HEM	E	501	4,1	-	6/14/54/54	-
4	CPZ	B	502	3	-	4/4/4/4	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CM5	E	504	-	-	2/6/14/65	0/1/1/3
4	CPZ	F	502	3	-	0/4/4/4	0/2/2/2
3	HEM	D	501	4,1	-	6/14/54/54	-
4	CPZ	D	502	-	-	0/4/4/4	0/2/2/2
4	CPZ	D	503	3	-	0/4/4/4	0/2/2/2
4	CPZ	A	502	3	-	0/4/4/4	0/2/2/2

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	501	HEM	C3D-C2D	8.14	1.54	1.36
3	C	501	HEM	C3D-C2D	7.86	1.53	1.36
3	B	501	HEM	C3D-C2D	7.65	1.53	1.36
3	F	501	HEM	C3D-C2D	7.38	1.52	1.36
3	D	501	HEM	C3D-C2D	6.89	1.51	1.36

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	HEM	C4D-ND-C1D	5.35	111.54	105.21
3	D	501	HEM	C4D-ND-C1D	4.87	110.98	105.21
3	F	501	HEM	C4D-ND-C1D	4.55	110.59	105.21
3	C	501	HEM	C4D-ND-C1D	3.82	109.73	105.21
3	F	501	HEM	CAD-CBD-CGD	-3.77	103.67	113.67

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	HEM	C2C-C3C-CAC-CBC
3	D	501	HEM	C4C-C3C-CAC-CBC
3	F	501	HEM	C1A-C2A-CAA-CBA
3	F	501	HEM	C2C-C3C-CAC-CBC
4	B	503	CPZ	C2-C4-C6-C11

There are no ring outliers.

20 monomers are involved in 79 short contacts:

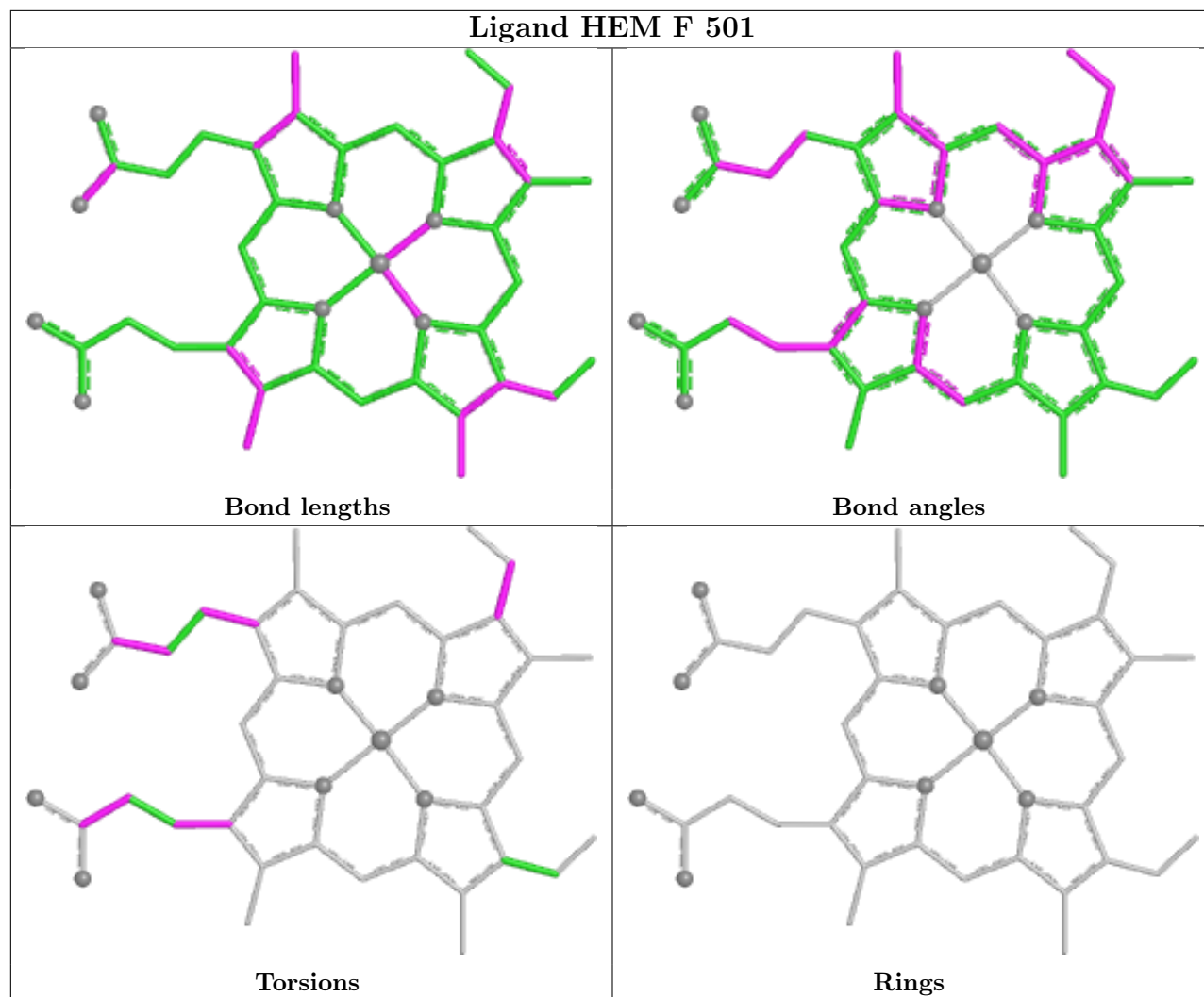
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	HEM	7	0

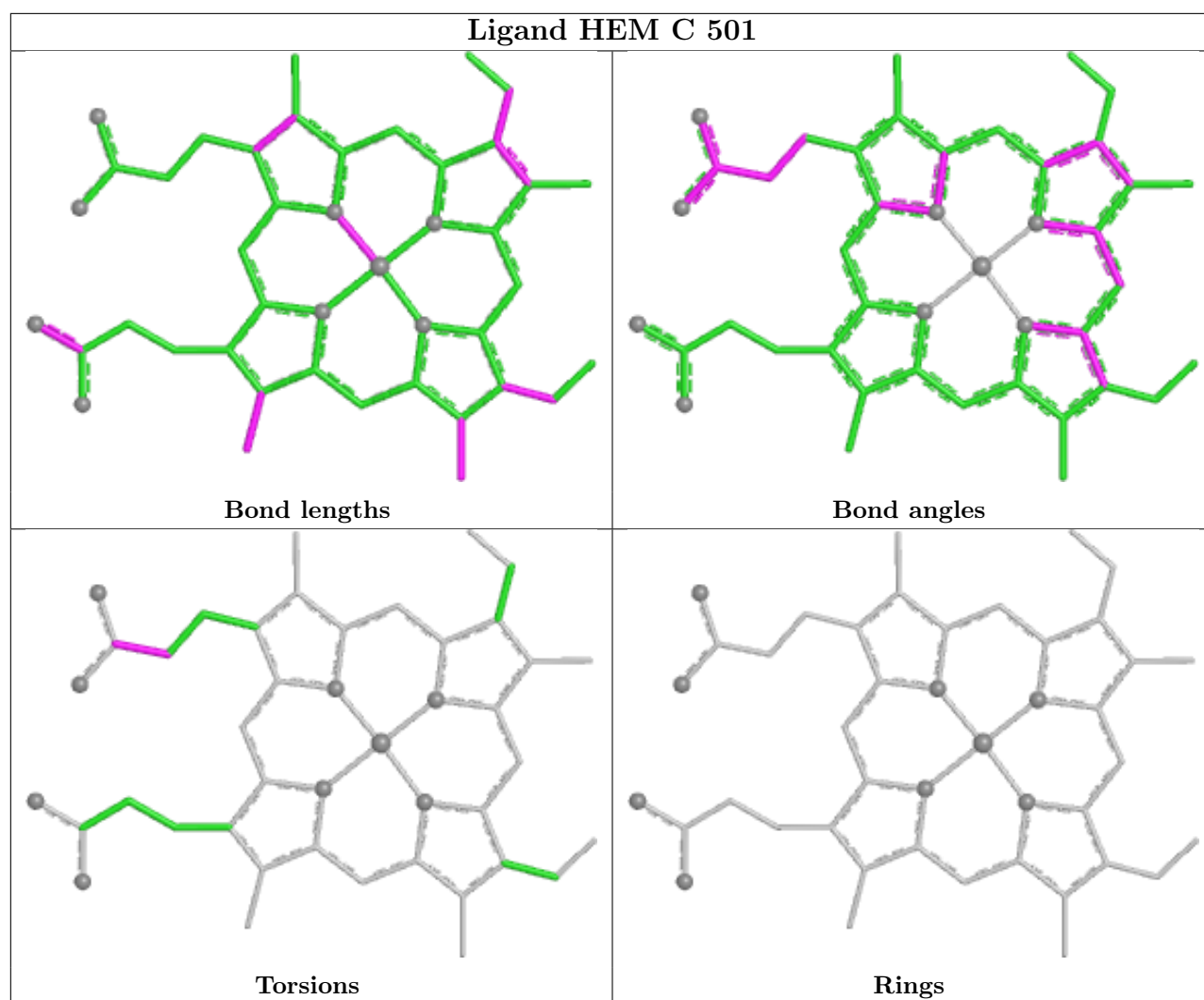
Continued on next page...

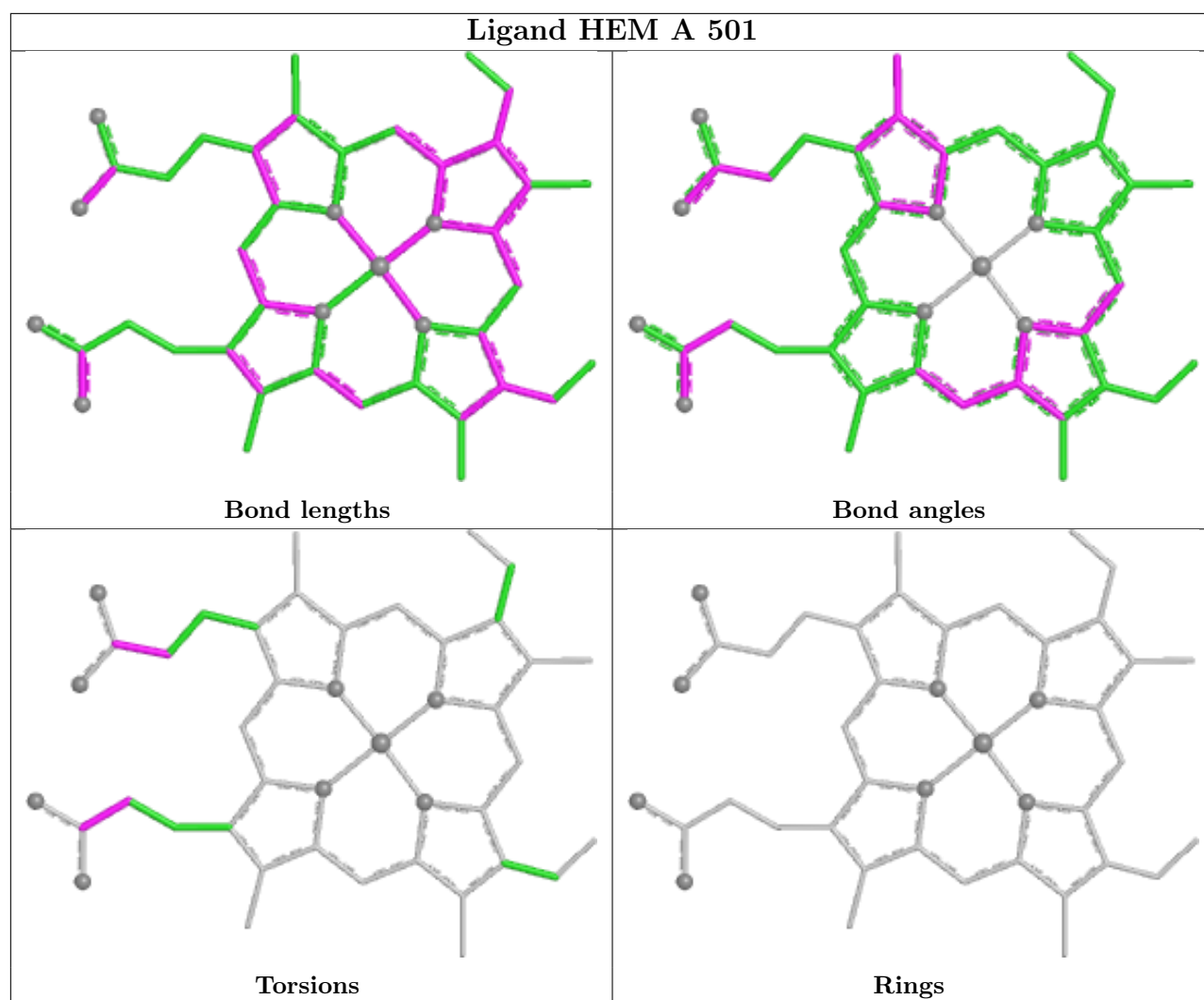
Continued from previous page...

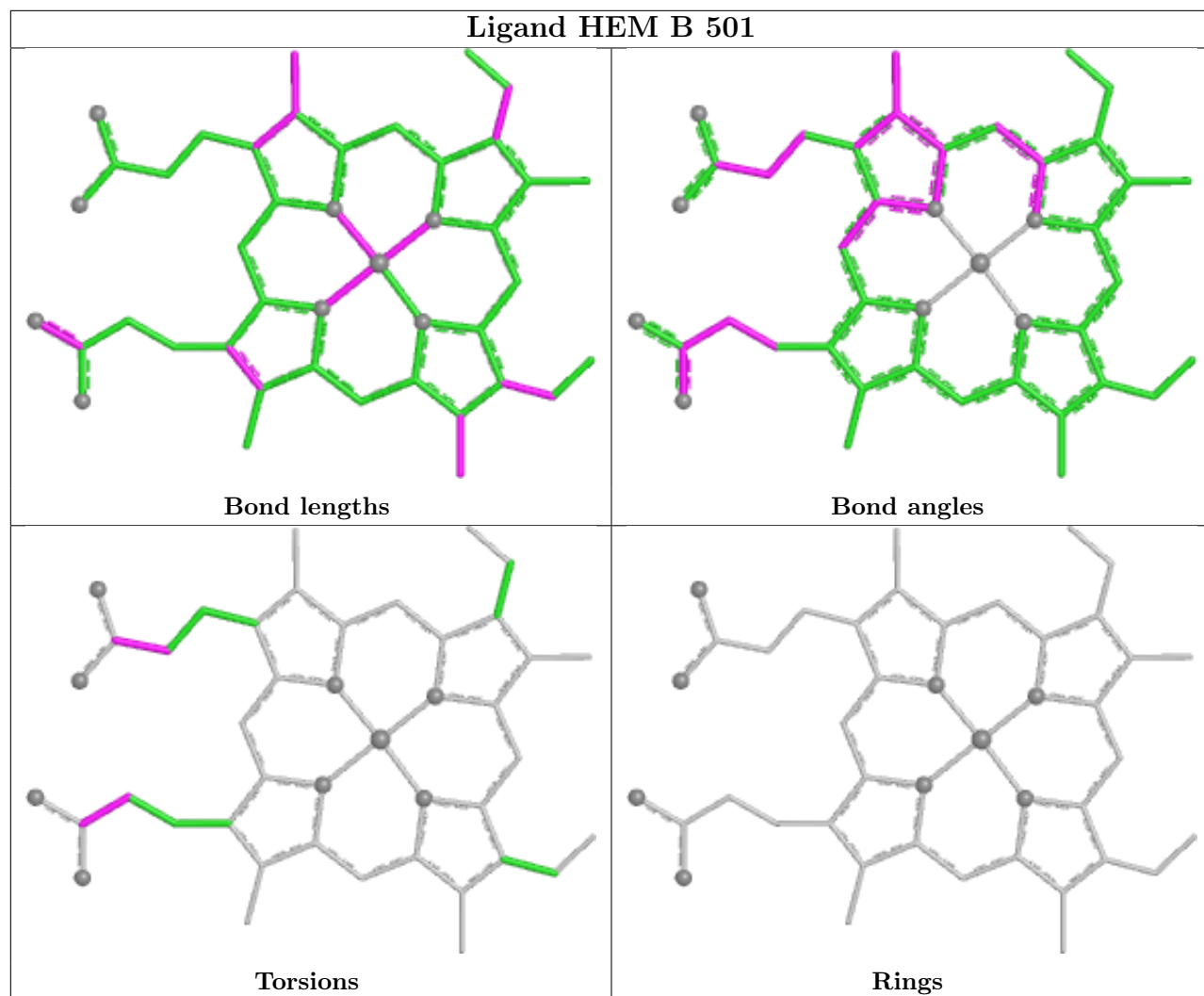
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	HEM	7	0
4	E	503	CPZ	3	0
4	E	502	CPZ	6	0
4	C	502	CPZ	4	0
4	A	503	CPZ	1	0
3	A	501	HEM	9	0
3	B	501	HEM	9	0
4	F	503	CPZ	6	0
4	B	503	CPZ	5	0
6	B	504	GOL	1	0
4	C	503	CPZ	3	0
3	E	501	HEM	8	0
4	B	502	CPZ	5	0
5	E	504	CM5	2	0
4	F	502	CPZ	5	0
3	D	501	HEM	3	0
4	D	502	CPZ	4	0
4	D	503	CPZ	2	0
4	A	502	CPZ	4	0

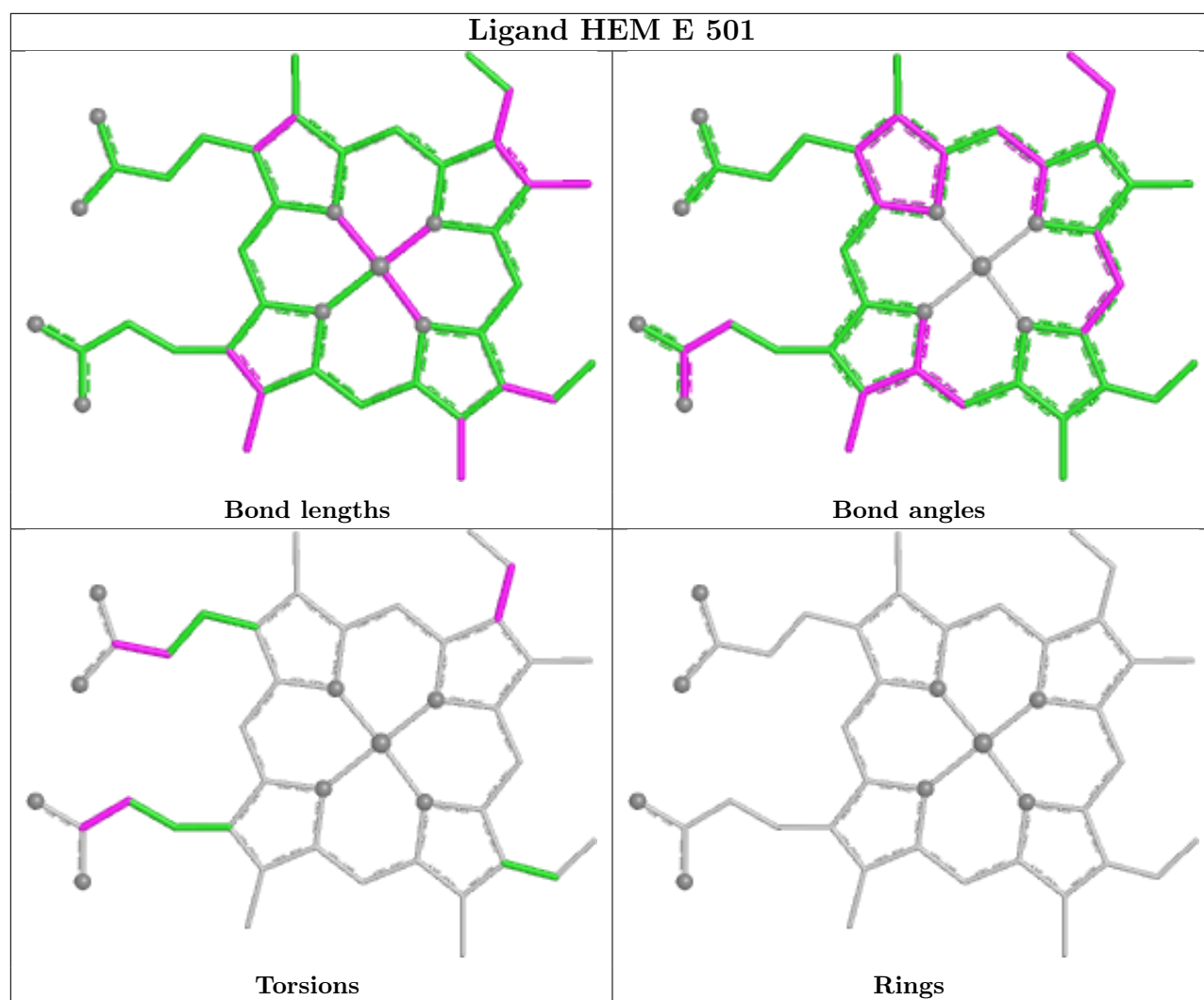
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

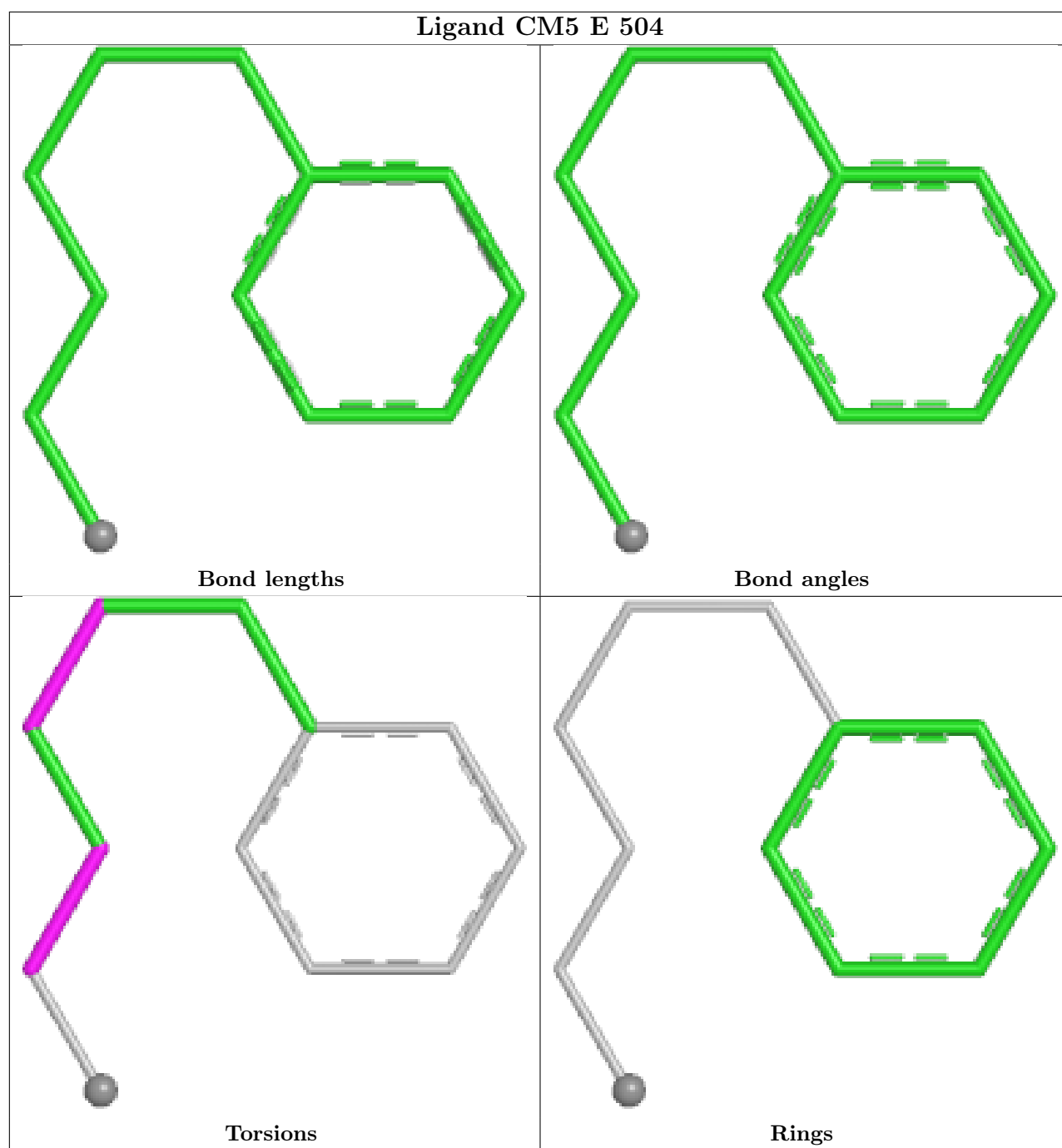


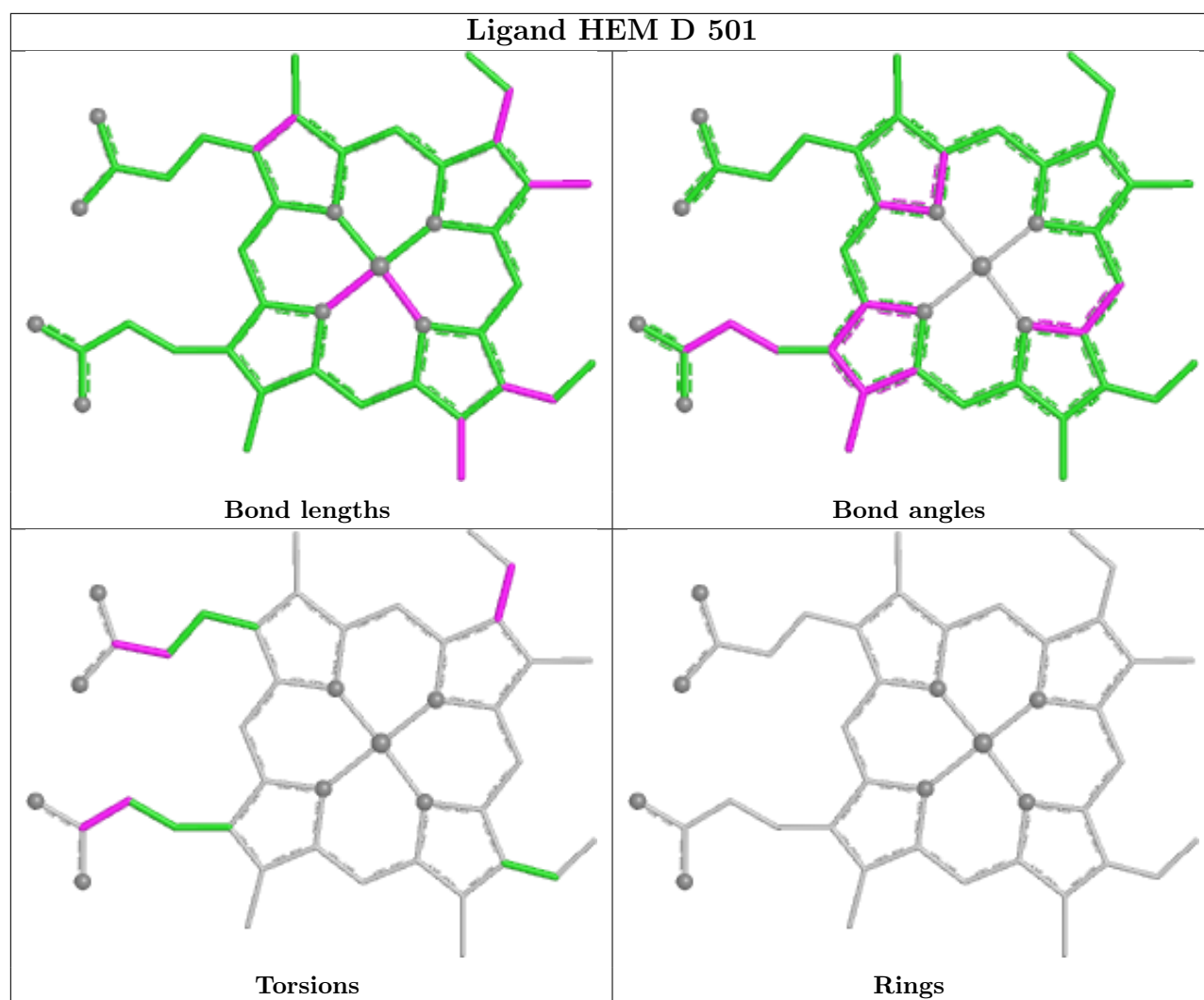












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	464/493 (94%)	-0.09	7 (1%) 72 68	19, 35, 60, 90	0
1	B	458/493 (92%)	0.43	12 (2%) 57 53	30, 50, 73, 86	0
1	C	465/493 (94%)	0.20	12 (2%) 57 53	22, 43, 71, 90	0
1	D	463/493 (93%)	0.24	9 (1%) 66 62	24, 45, 63, 84	0
1	E	462/493 (93%)	0.35	16 (3%) 47 43	27, 48, 71, 79	0
1	F	458/493 (92%)	0.87	56 (12%) 8 6	27, 57, 75, 95	1 (0%)
All	All	2770/2958 (93%)	0.33	112 (4%) 42 38	19, 47, 71, 95	1 (0%)

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	298	ALA	6.0
1	A	298	ALA	5.4
1	D	298	ALA	4.8
1	F	152	CYS	4.6
1	D	365	ILE	4.5

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

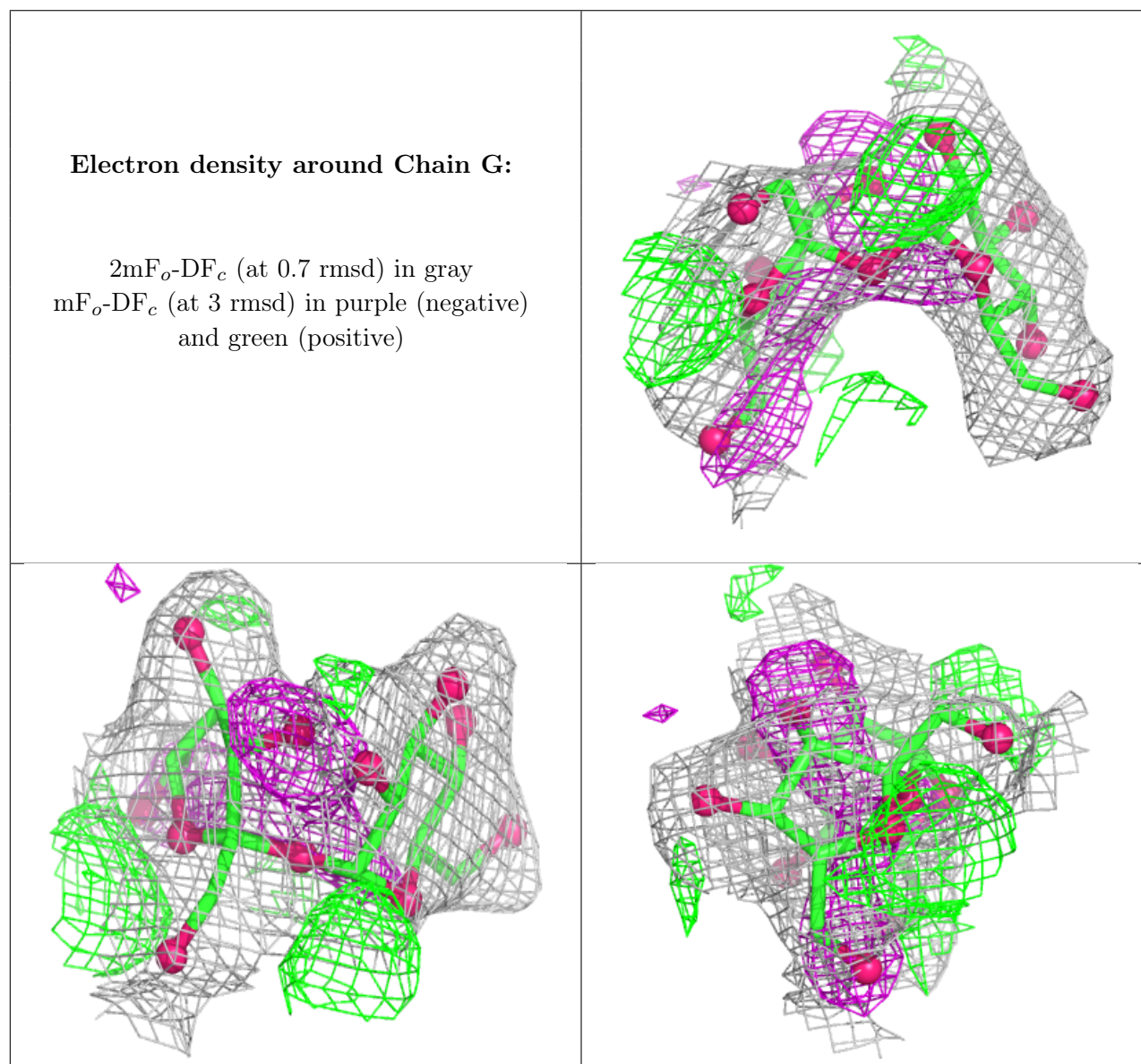
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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
2	GLC	G	1	11/12	0.66	0.14	59,60,62,63	0
2	FRU	G	2	12/12	0.66	0.17	35,45,54,55	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands ⓘ

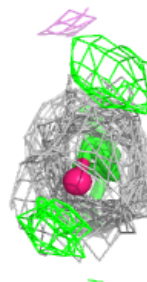
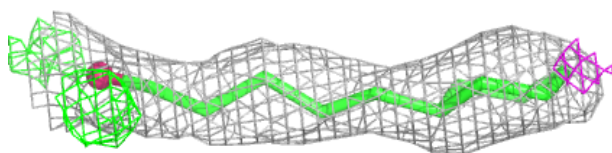
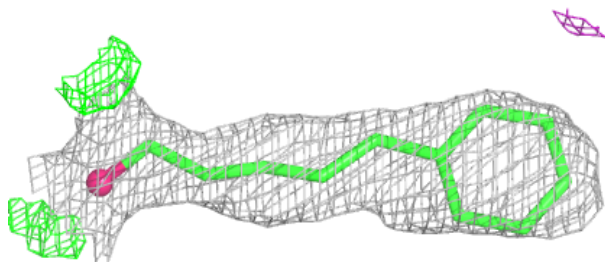
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	E	505	6/6	0.65	0.19	65,67,68,69	0
6	GOL	C	504	6/6	0.72	0.18	65,69,69,71	0
4	CPZ	D	502	12/12	0.80	0.17	57,58,61,65	0
6	GOL	A	506	6/6	0.82	0.14	47,52,53,54	0
6	GOL	B	504	6/6	0.82	0.10	54,59,60,61	0
4	CPZ	A	503	12/12	0.86	0.16	49,52,56,60	0
5	CM5	E	504	12/34	0.86	0.18	63,66,67,67	0
4	CPZ	F	503	12/12	0.87	0.15	68,69,71,71	0
4	CPZ	B	503	12/12	0.90	0.15	68,70,74,76	0
4	CPZ	E	503	12/12	0.90	0.15	69,71,72,76	0
4	CPZ	F	502	12/12	0.90	0.14	54,65,69,72	0
5	CM5	A	505	6/34	0.92	0.17	55,55,56,56	0
4	CPZ	C	503	12/12	0.94	0.11	49,51,53,60	0
4	CPZ	B	502	12/12	0.95	0.08	39,41,43,44	0
4	CPZ	C	502	12/12	0.95	0.08	40,42,44,45	0
4	CPZ	D	503	12/12	0.95	0.08	35,42,49,52	0
3	HEM	F	501	43/43	0.96	0.08	40,44,49,53	0
3	HEM	E	501	43/43	0.96	0.09	33,38,42,47	0
4	CPZ	E	502	12/12	0.96	0.09	42,46,46,47	0
4	CPZ	A	502	12/12	0.97	0.07	31,33,35,37	0
3	HEM	B	501	43/43	0.97	0.07	29,35,37,39	0
3	HEM	D	501	43/43	0.98	0.07	23,30,34,39	0
3	HEM	A	501	43/43	0.98	0.06	12,17,21,26	0
3	HEM	C	501	43/43	0.98	0.06	16,24,29,37	0

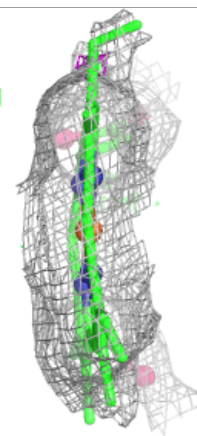
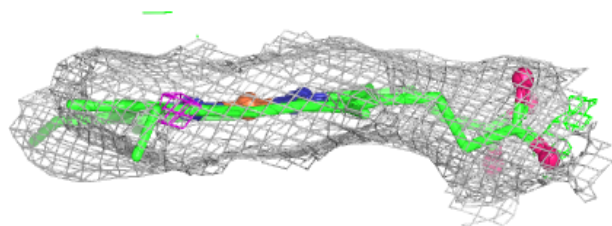
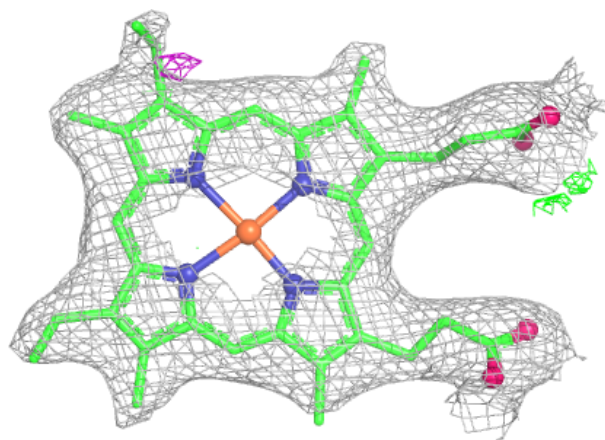
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CM5 E 504:

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

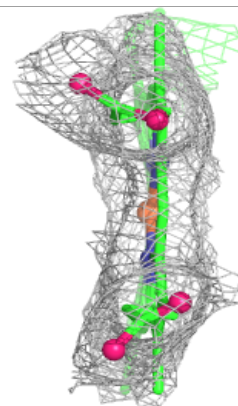
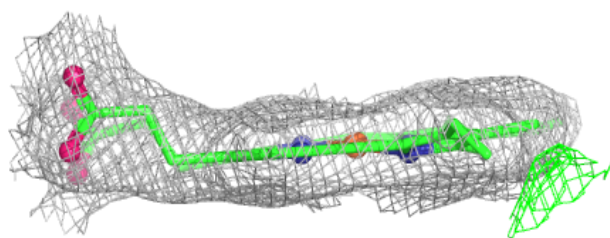
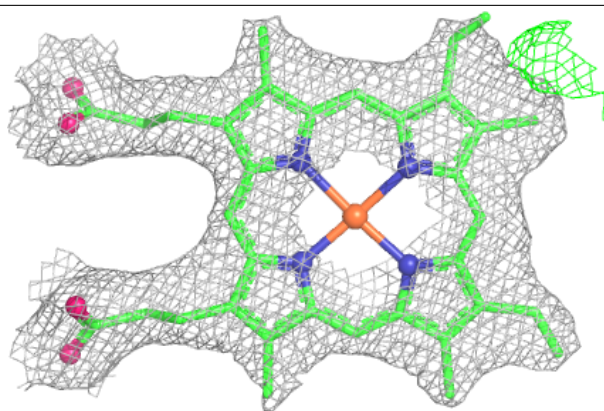
**Electron density around HEM F 501:**

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



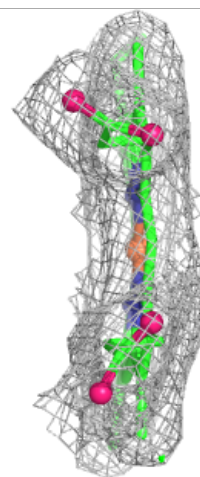
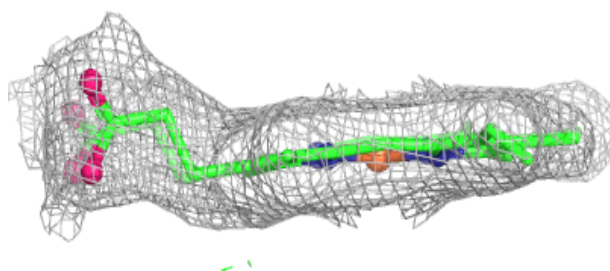
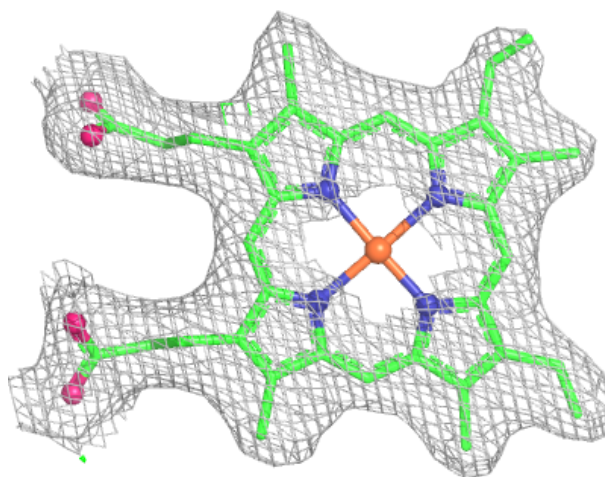
Electron density around HEM E 501:

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



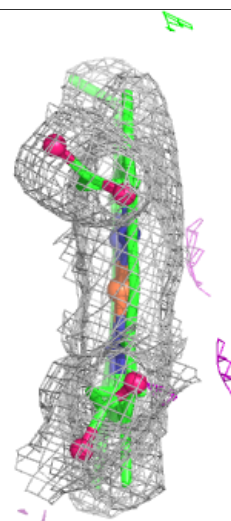
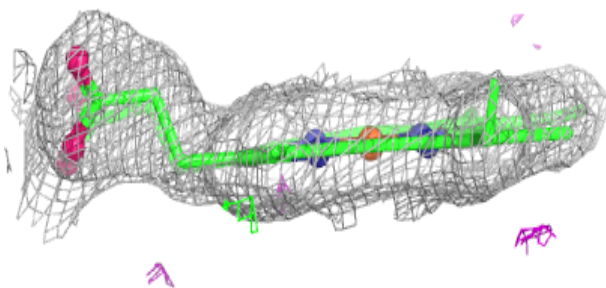
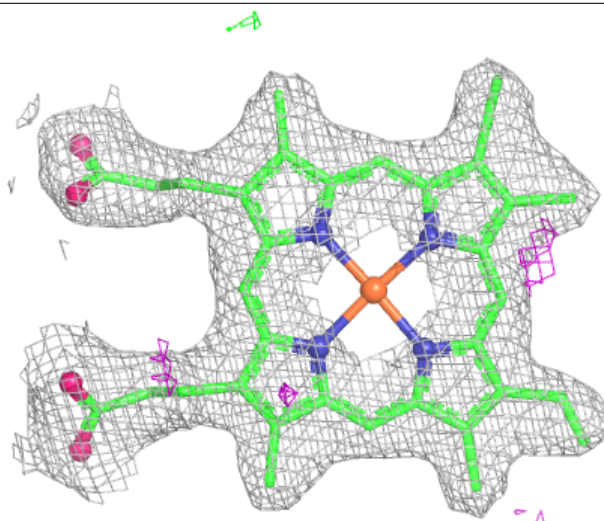
Electron density around HEM B 501:

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



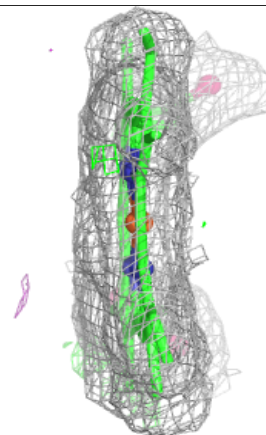
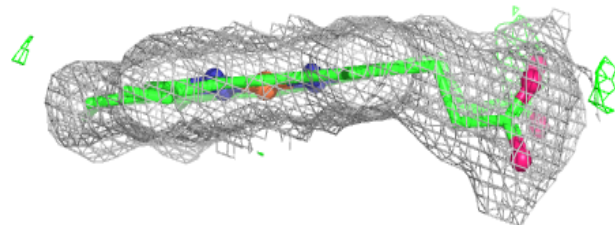
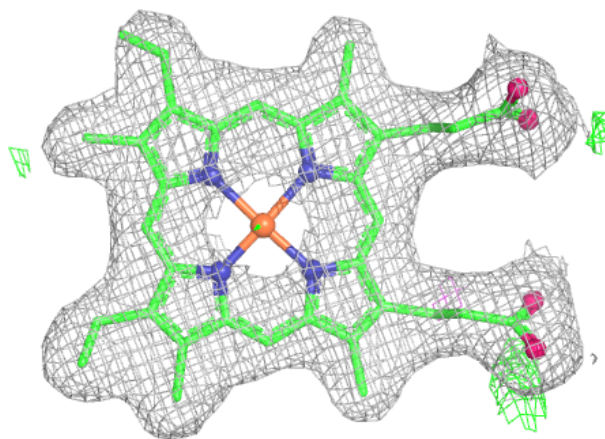
Electron density around HEM D 501:

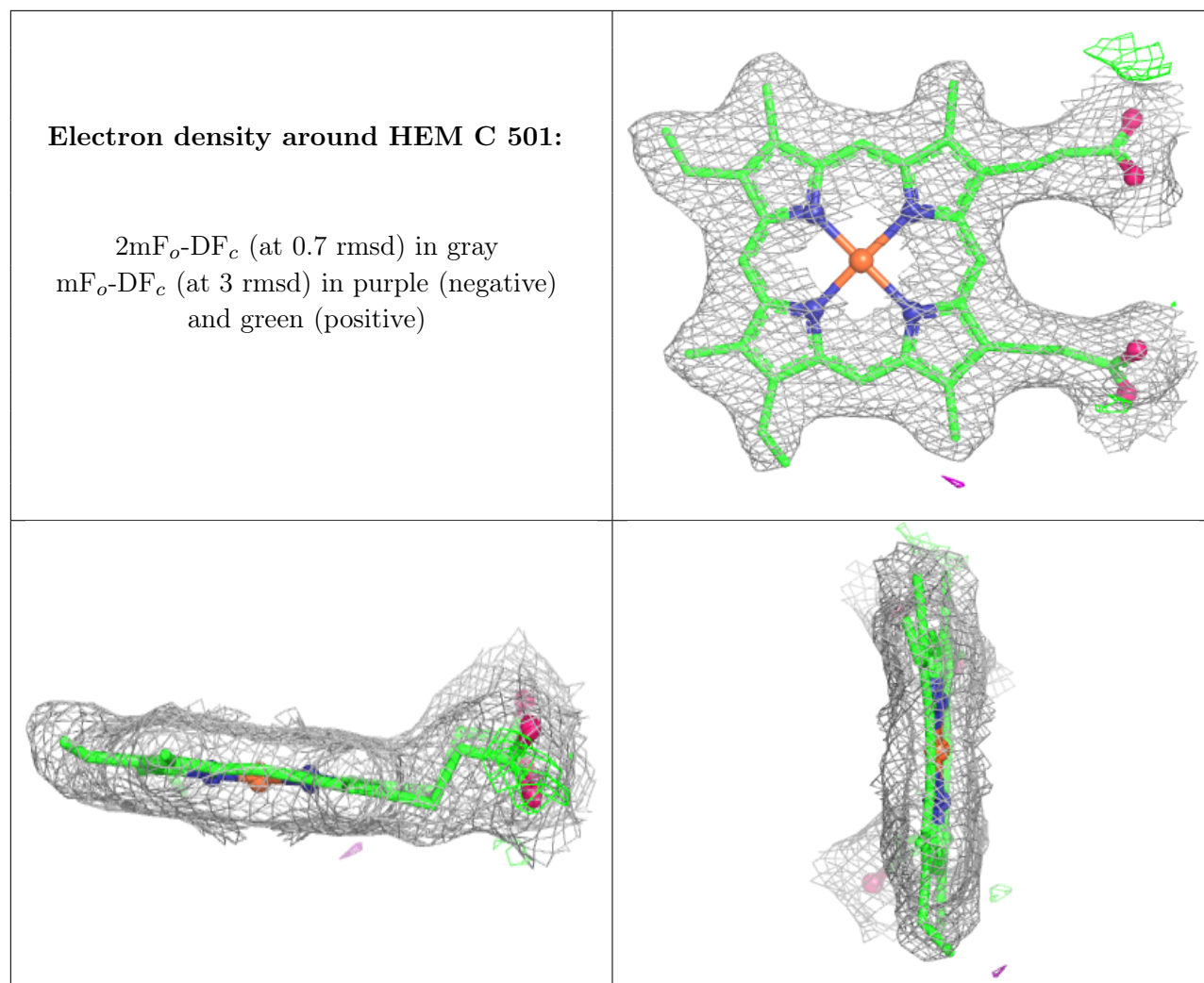
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 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.