



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:05 PM UTC

PDB ID : 8U2M / pdb_00008u2m
Title : Structure of P450Blt from Micromonospora sp. MW-13 in Complex with Biarylthide
Authors : Hansen, M.H.; Cryle, M.J.
Deposited on : 2023-09-06
Resolution : 1.79 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

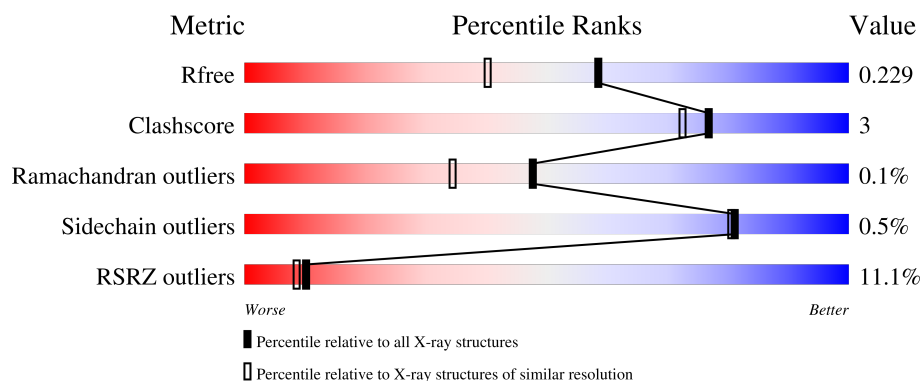
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	420	9% 86% 10%
1	B	420	3% 85% 6% 9%
1	C	420	18% 87% 9%
2	D	5	60% 60% 20% 20%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18649 atoms, of which 8994 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-SU1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	380	Total	C	H	N	O	S	0	6	0
			5844	1832	2925	554	529	4			
1	B	382	Total	C	H	N	O	S	0	1	0
			5840	1832	2925	551	528	4			
1	C	382	Total	C	H	N	O	S	0	3	0
			5864	1838	2938	555	529	4			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A3E2YLT4
A	-19	GLY	-	expression tag	UNP A0A3E2YLT4
A	-18	SER	-	expression tag	UNP A0A3E2YLT4
A	-17	SER	-	expression tag	UNP A0A3E2YLT4
A	-16	HIS	-	expression tag	UNP A0A3E2YLT4
A	-15	HIS	-	expression tag	UNP A0A3E2YLT4
A	-14	HIS	-	expression tag	UNP A0A3E2YLT4
A	-13	HIS	-	expression tag	UNP A0A3E2YLT4
A	-12	HIS	-	expression tag	UNP A0A3E2YLT4
A	-11	HIS	-	expression tag	UNP A0A3E2YLT4
A	-10	SER	-	expression tag	UNP A0A3E2YLT4
A	-9	SER	-	expression tag	UNP A0A3E2YLT4
A	-8	GLY	-	expression tag	UNP A0A3E2YLT4
A	-7	LEU	-	expression tag	UNP A0A3E2YLT4
A	-6	VAL	-	expression tag	UNP A0A3E2YLT4
A	-5	PRO	-	expression tag	UNP A0A3E2YLT4
A	-4	ARG	-	expression tag	UNP A0A3E2YLT4
A	-3	GLY	-	expression tag	UNP A0A3E2YLT4
A	-2	SER	-	expression tag	UNP A0A3E2YLT4
A	-1	HIS	-	expression tag	UNP A0A3E2YLT4
A	0	MET	-	expression tag	UNP A0A3E2YLT4
B	-20	MET	-	initiating methionine	UNP A0A3E2YLT4
B	-19	GLY	-	expression tag	UNP A0A3E2YLT4

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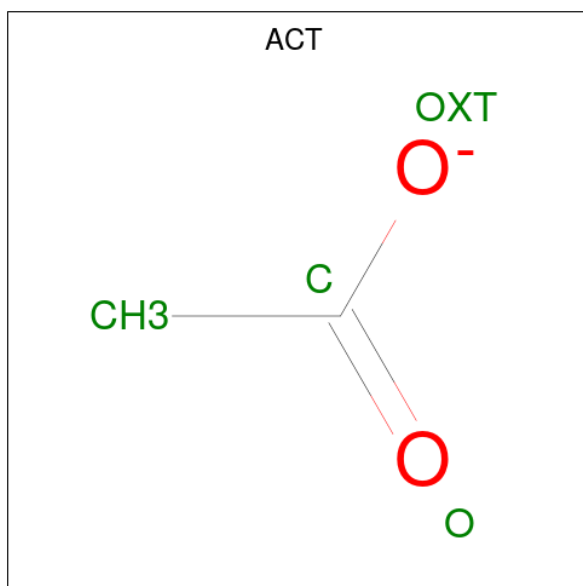
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	expression tag	UNP A0A3E2YLT4
B	-17	SER	-	expression tag	UNP A0A3E2YLT4
B	-16	HIS	-	expression tag	UNP A0A3E2YLT4
B	-15	HIS	-	expression tag	UNP A0A3E2YLT4
B	-14	HIS	-	expression tag	UNP A0A3E2YLT4
B	-13	HIS	-	expression tag	UNP A0A3E2YLT4
B	-12	HIS	-	expression tag	UNP A0A3E2YLT4
B	-11	HIS	-	expression tag	UNP A0A3E2YLT4
B	-10	SER	-	expression tag	UNP A0A3E2YLT4
B	-9	SER	-	expression tag	UNP A0A3E2YLT4
B	-8	GLY	-	expression tag	UNP A0A3E2YLT4
B	-7	LEU	-	expression tag	UNP A0A3E2YLT4
B	-6	VAL	-	expression tag	UNP A0A3E2YLT4
B	-5	PRO	-	expression tag	UNP A0A3E2YLT4
B	-4	ARG	-	expression tag	UNP A0A3E2YLT4
B	-3	GLY	-	expression tag	UNP A0A3E2YLT4
B	-2	SER	-	expression tag	UNP A0A3E2YLT4
B	-1	HIS	-	expression tag	UNP A0A3E2YLT4
B	0	MET	-	expression tag	UNP A0A3E2YLT4
C	-20	MET	-	initiating methionine	UNP A0A3E2YLT4
C	-19	GLY	-	expression tag	UNP A0A3E2YLT4
C	-18	SER	-	expression tag	UNP A0A3E2YLT4
C	-17	SER	-	expression tag	UNP A0A3E2YLT4
C	-16	HIS	-	expression tag	UNP A0A3E2YLT4
C	-15	HIS	-	expression tag	UNP A0A3E2YLT4
C	-14	HIS	-	expression tag	UNP A0A3E2YLT4
C	-13	HIS	-	expression tag	UNP A0A3E2YLT4
C	-12	HIS	-	expression tag	UNP A0A3E2YLT4
C	-11	HIS	-	expression tag	UNP A0A3E2YLT4
C	-10	SER	-	expression tag	UNP A0A3E2YLT4
C	-9	SER	-	expression tag	UNP A0A3E2YLT4
C	-8	GLY	-	expression tag	UNP A0A3E2YLT4
C	-7	LEU	-	expression tag	UNP A0A3E2YLT4
C	-6	VAL	-	expression tag	UNP A0A3E2YLT4
C	-5	PRO	-	expression tag	UNP A0A3E2YLT4
C	-4	ARG	-	expression tag	UNP A0A3E2YLT4
C	-3	GLY	-	expression tag	UNP A0A3E2YLT4
C	-2	SER	-	expression tag	UNP A0A3E2YLT4
C	-1	HIS	-	expression tag	UNP A0A3E2YLT4
C	0	MET	-	expression tag	UNP A0A3E2YLT4

- Molecule 2 is a protein called MET-ARG-TYR-LEU-HIS.

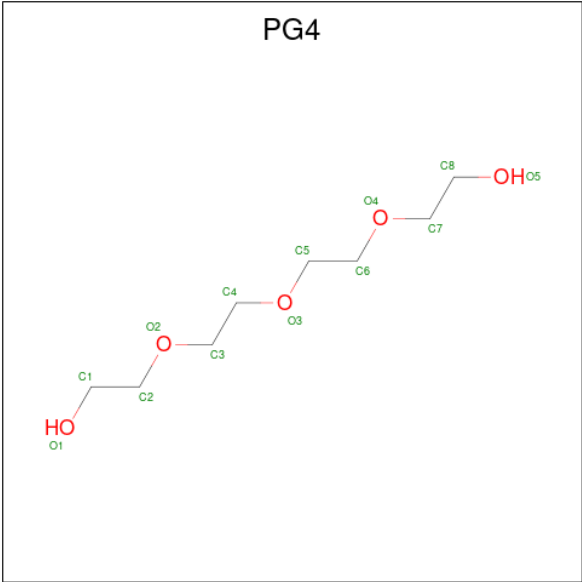
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	5	Total	C	H	N	O	S	0	0
			101	32	51	10	7	1		0

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



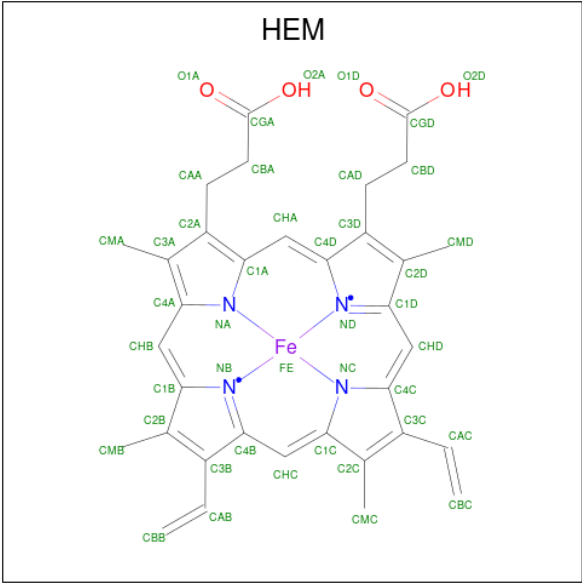
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	1
			14	4	6	4		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
5	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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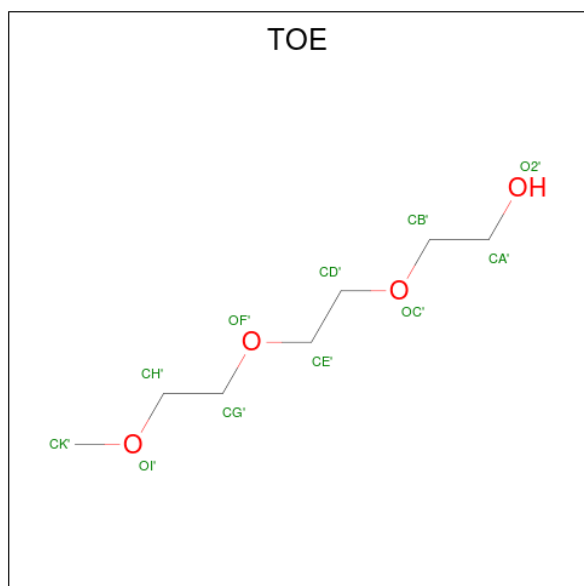
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

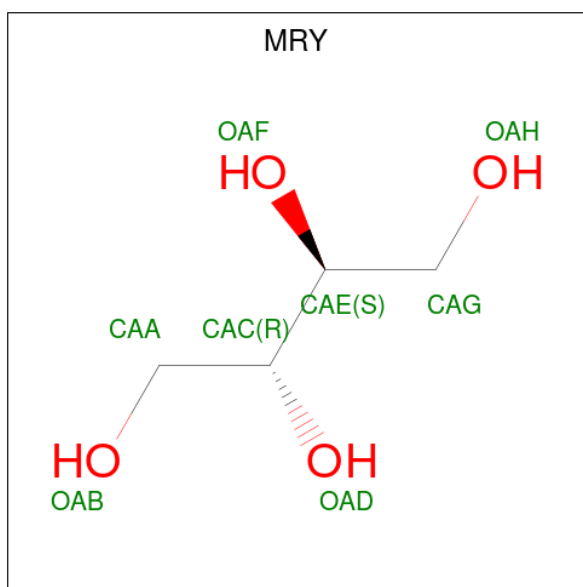
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Na	0	0
			3	3		
6	B	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		

- Molecule 7 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (CCD ID: TOE) (formula: C₇H₁₆O₄).



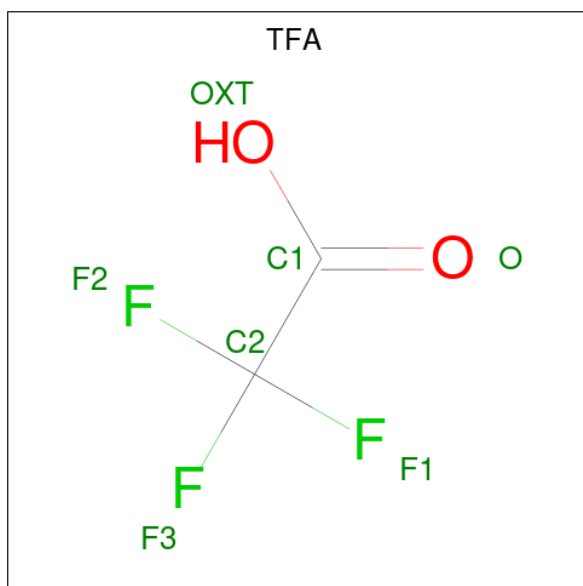
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			27	7	16	4		

- Molecule 8 is MESO-ERYTHRITOL (CCD ID: MRY) (formula: C₄H₁₀O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			18	4	10	4		

- Molecule 9 is trifluoroacetic acid (CCD ID: TFA) (formula: $C_2HF_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	F	O	0	0
			7	2	3	2		
9	B	1	Total	C	F	O	0	0
			7	2	3	2		
9	C	1	Total	C	F	O	0	0
			7	2	3	2		

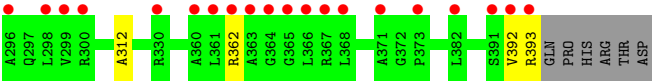
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	F	O	0	0
			7	2	3	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	201	Total	O	0	0
			201	201		
10	B	271	Total	O	0	0
			271	271		
10	C	148	Total	O	0	0
			148	148		
10	D	3	Total	O	0	0
			3	3		



● Molecule 2: MET-ARG-TYR-LEU-HIS



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.67Å 95.61Å 105.76Å 90.00° 92.71° 90.00°	Depositor
Resolution (Å)	47.80 – 1.79 47.80 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.80-1.79) 99.1 (47.80-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.199 , 0.229 0.199 , 0.229	Depositor DCC
R_{free} test set	5635 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18649	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: ACT, HEM, PG4, TFA, NA, TOE, MRY

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	0.14	0/3011	0.35	0/4109
1	B	0.13	0/2979	0.35	0/4065
1	C	0.14	0/2996	0.34	0/4087
2	D	0.10	0/51	0.23	0/65
All	All	0.14	0/9037	0.35	0/12326

There are no bond length outliers.

There are no bond angle outliers.

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	2919	2925	2900	13	0
1	B	2915	2925	2923	17	0
1	C	2926	2938	2931	9	0
2	D	50	51	51	2	0
3	A	16	12	12	2	0
3	B	12	9	9	0	0
4	A	13	18	18	0	0
5	A	43	30	30	4	0
5	B	43	30	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	43	30	30	4	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	B	11	16	16	1	0
8	B	8	10	10	2	0
9	B	14	0	0	0	0
9	C	14	0	0	1	0
10	A	201	0	0	1	0
10	B	271	0	0	4	0
10	C	148	0	0	0	0
10	D	3	0	0	0	0
All	All	9655	8994	8960	53	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 3.

The worst 5 of 53 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:A:325:VAL:H	3:A:401:ACT:H1	1.52	0.75
5:B:404:HEM:HBB2	5:B:404:HEM:HHC	1.74	0.70
5:B:404:HEM:HMC2	5:B:404:HEM:HBC2	1.75	0.68
1:B:111:ARG:HG3	1:B:352:LEU:HD11	1.81	0.63
1:A:235:ALA:HB2	2:D:5:HIS:CD2	2.36	0.61

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	384/420 (91%)	379 (99%)	4 (1%)	1 (0%)	36	25
1	B	381/420 (91%)	378 (99%)	3 (1%)	0	100	100
1	C	383/420 (91%)	377 (98%)	6 (2%)	0	100	100
2	D	3/5 (60%)	3 (100%)	0	0	100	100
All	All	1151/1265 (91%)	1137 (99%)	13 (1%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	ASP

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	298/325 (92%)	296 (99%)	2 (1%)	76	73
1	B	295/325 (91%)	295 (100%)	0	100	100
1	C	297/325 (91%)	296 (100%)	1 (0%)	86	86
2	D	5/5 (100%)	4 (80%)	1 (20%)	1	0
All	All	895/980 (91%)	891 (100%)	4 (0%)	81	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ARG
1	A	264	ARG
1	C	13	ILE
2	D	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	HIS

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Mol	Chain	Res	Type
1	B	103	HIS
1	B	282	GLN

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 ⓘ

Of 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	A	404	-	3,3,3	1.48	0	3,3,3	2.00	1 (33%)
5	HEM	B	404	10,1	50,50,50	1.40	8 (16%)	67,82,82	1.22	8 (11%)
3	ACT	A	402	-	3,3,3	1.55	0	3,3,3	1.40	0
3	ACT	B	405[A]	-	3,3,3	1.48	0	3,3,3	1.87	1 (33%)
5	HEM	A	406	10,1	50,50,50	1.39	7 (14%)	67,82,82	1.08	5 (7%)
3	ACT	B	405[B]	-	3,3,3	1.48	0	3,3,3	1.81	1 (33%)
8	MRY	B	403	-	7,7,7	0.50	0	8,8,8	1.01	0
9	TFA	B	406	-	6,6,6	1.04	0	9,9,9	0.99	0
3	ACT	A	405	-	3,3,3	1.49	0	3,3,3	1.85	1 (33%)
5	HEM	C	401	1	50,50,50	1.42	9 (18%)	67,82,82	1.10	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TOE	B	402	-	10,10,10	0.30	0	9,9,9	0.40	0
9	TFA	B	407	-	6,6,6	1.09	0	9,9,9	1.00	0
9	TFA	C	403	-	6,6,6	1.12	0	9,9,9	1.00	0
4	PG4	A	403	-	12,12,12	0.12	0	11,11,11	0.57	0
3	ACT	B	401	-	3,3,3	1.52	0	3,3,3	1.54	1 (33%)
9	TFA	C	402	-	6,6,6	1.05	0	9,9,9	1.02	1 (11%)
3	ACT	A	401	-	3,3,3	1.43	0	3,3,3	1.90	1 (33%)

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
5	HEM	B	404	10,1	-	3/14/54/54	-
5	HEM	A	406	10,1	-	2/14/54/54	-
8	MRY	B	403	-	-	6/8/8/8	-
9	TFA	B	406	-	-	0/6/6/6	-
9	TFA	B	407	-	-	0/6/6/6	-
5	HEM	C	401	1	-	2/14/54/54	-
7	TOE	B	402	-	-	6/8/8/8	-
4	PG4	A	403	-	-	4/10/10/10	-
9	TFA	C	403	-	-	0/6/6/6	-
9	TFA	C	402	-	-	0/6/6/6	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	401	HEM	FE-NA	4.15	2.08	1.95
5	B	404	HEM	FE-NC	3.95	2.08	1.95
5	B	404	HEM	FE-ND	3.83	2.06	1.94
5	A	406	HEM	FE-NB	3.79	2.06	1.94
5	C	401	HEM	FE-NB	3.11	2.04	1.94

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404	ACT	O-C-CH3	-2.72	111.38	122.53
3	A	401	ACT	O-C-CH3	-2.59	111.90	122.53
3	B	405[A]	ACT	O-C-CH3	-2.56	112.04	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	405	ACT	O-C-CH3	-2.53	112.17	122.53
5	B	404	HEM	C4D-ND-C1D	2.52	108.19	105.21

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	403	MRY	OAB-CAA-CAC-OAD
8	B	403	MRY	CAA-CAC-CAE-OAF
8	B	403	MRY	CAA-CAC-CAE-CAG
8	B	403	MRY	OAD-CAC-CAE-OAF
8	B	403	MRY	OAD-CAC-CAE-CAG

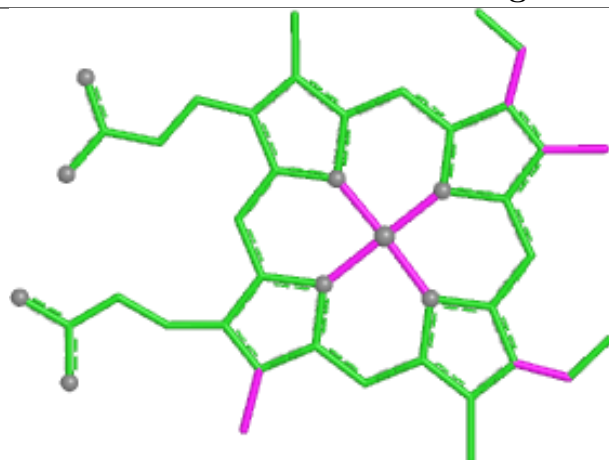
There are no ring outliers.

8 monomers are involved in 20 short contacts:

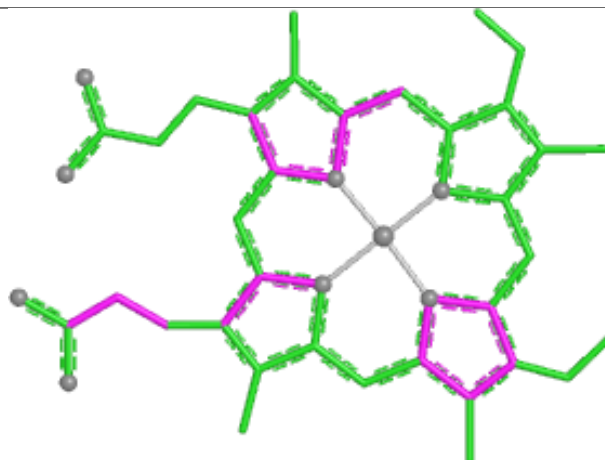
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	404	HEM	6	0
3	A	402	ACT	1	0
5	A	406	HEM	4	0
8	B	403	MRY	2	0
5	C	401	HEM	4	0
7	B	402	TOE	1	0
9	C	403	TFA	1	0
3	A	401	ACT	1	0

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.

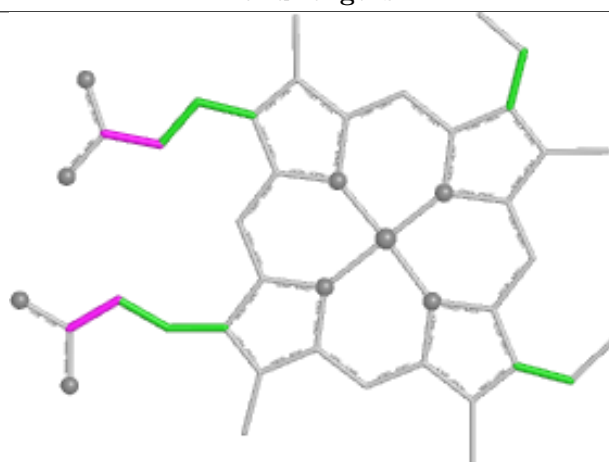
Ligand HEM B 404



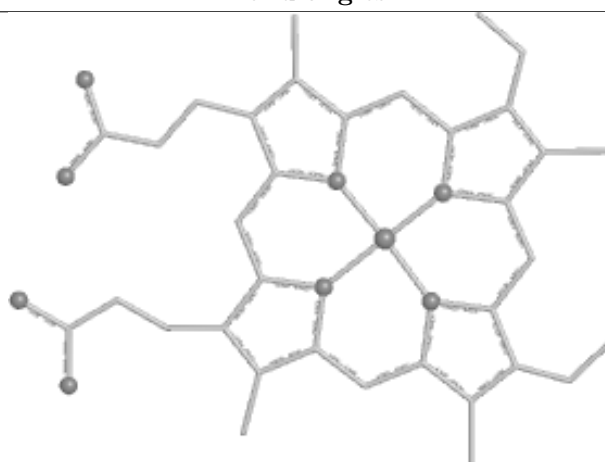
Bond lengths



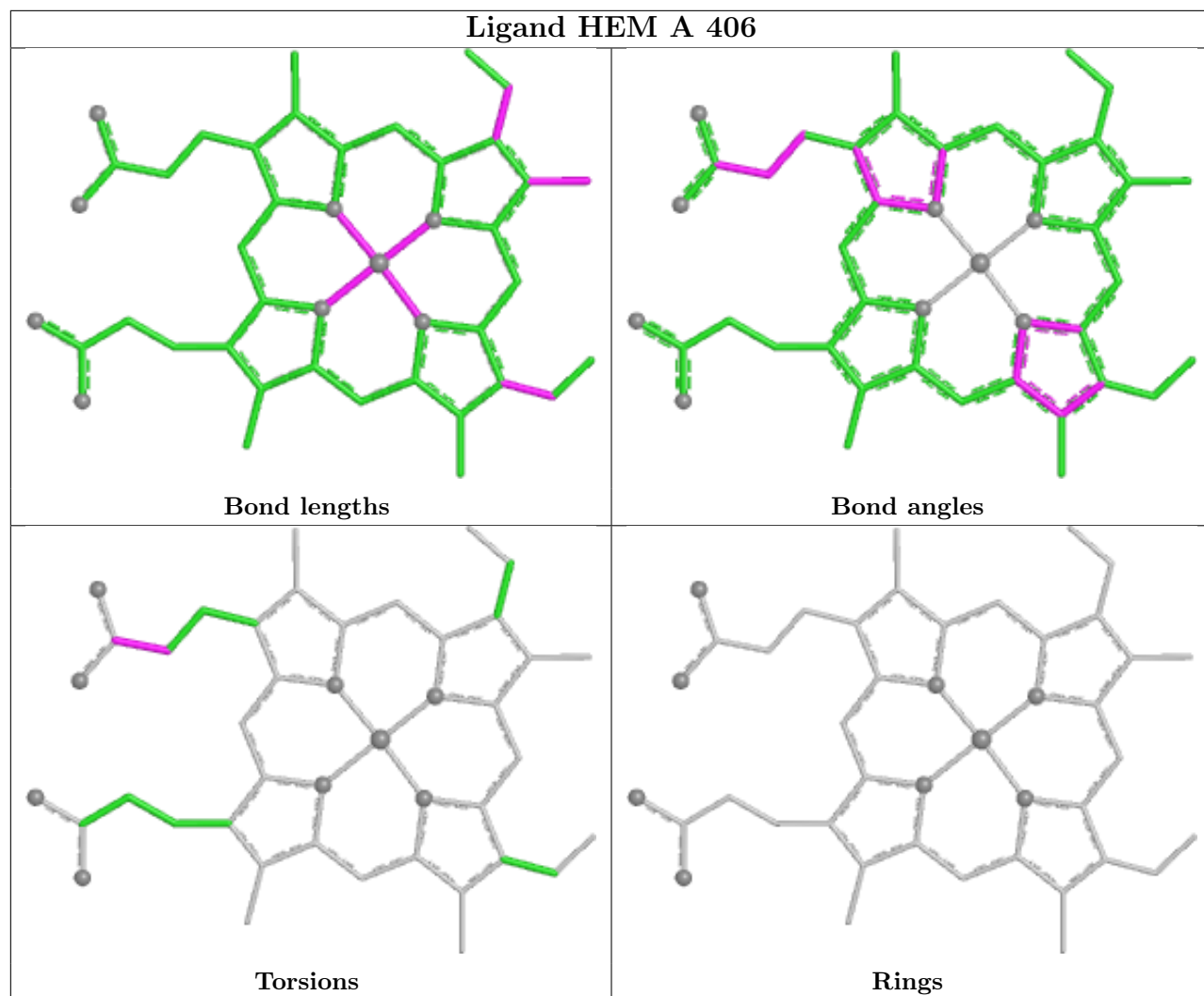
Bond angles

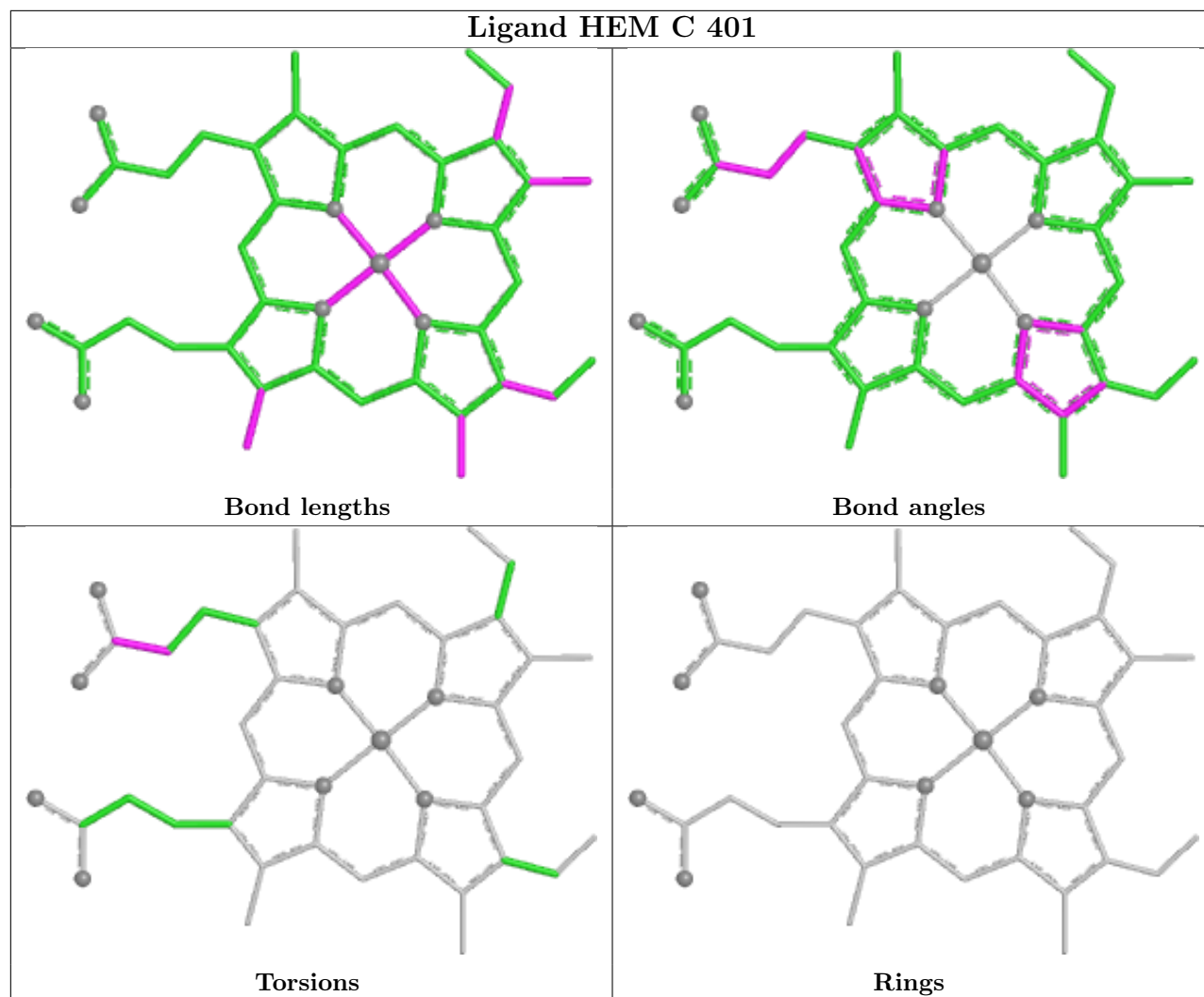


Torsions



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	380/420 (90%)	0.56	39 (10%) 12 10	12, 32, 65, 92	3 (0%)
1	B	382/420 (90%)	0.26	12 (3%) 51 51	18, 30, 55, 72	1 (0%)
1	C	382/420 (90%)	1.05	74 (19%) 3 2	17, 46, 80, 106	2 (0%)
2	D	5/5 (100%)	2.17	3 (60%) 0 0	42, 43, 51, 63	0
All	All	1149/1265 (90%)	0.63	128 (11%) 10 8	12, 36, 72, 106	6 (0%)

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	PRO	6.1
1	A	44	LEU	5.5
1	C	365	GLY	5.2
1	C	13	ILE	5.2
1	A	14	TYR	4.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

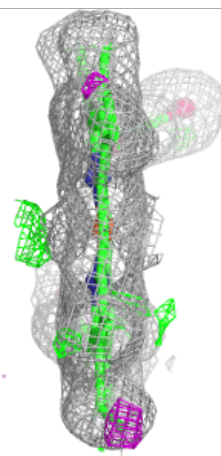
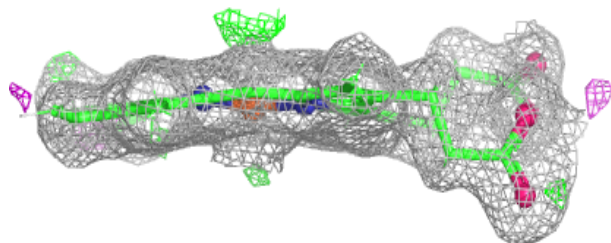
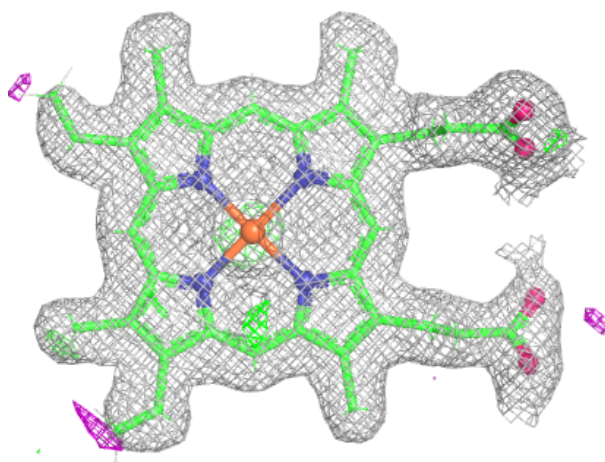
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	ACT	B	405[A]	4/4	0.72	0.17	35,39,42,42	7
3	ACT	B	405[B]	4/4	0.72	0.17	30,37,42,42	7
3	ACT	B	401	4/4	0.75	0.18	42,51,53,55	0
3	ACT	A	402	4/4	0.79	0.15	41,50,51,52	0
3	ACT	A	405	4/4	0.81	0.14	35,38,42,45	7
4	PG4	A	403	13/13	0.81	0.17	34,45,60,69	31
7	TOE	B	402	11/11	0.81	0.18	30,45,54,56	27
8	MRY	B	403	8/8	0.81	0.14	37,46,62,75	0
9	TFA	B	407	7/7	0.82	0.19	42,54,62,68	0
9	TFA	C	403	7/7	0.83	0.29	81,88,99,104	0
3	ACT	A	404	4/4	0.84	0.13	46,55,56,63	0
9	TFA	B	406	7/7	0.84	0.16	32,51,59,64	0
9	TFA	C	402	7/7	0.86	0.15	29,48,55,67	0
6	NA	A	408	1/1	0.89	0.15	55,55,55,55	0
3	ACT	A	401	4/4	0.90	0.13	19,23,39,40	0
6	NA	A	409	1/1	0.91	0.10	51,51,51,51	0
6	NA	A	407	1/1	0.93	0.13	43,43,43,43	0
6	NA	C	404	1/1	0.94	0.09	50,50,50,50	0
6	NA	B	408	1/1	0.95	0.09	51,51,51,51	0
5	HEM	C	401	43/43	0.97	0.08	20,28,37,44	0
5	HEM	A	406	43/43	0.98	0.07	14,21,35,46	0
5	HEM	B	404	43/43	0.98	0.07	12,20,29,31	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.

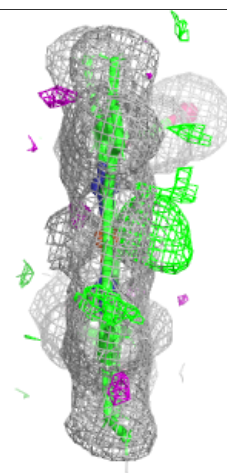
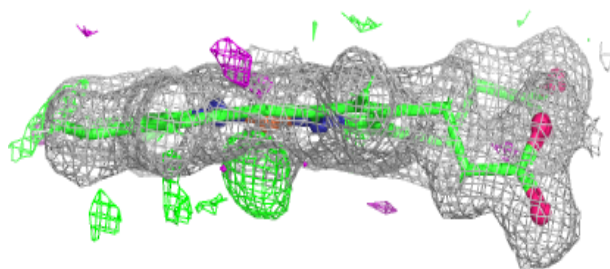
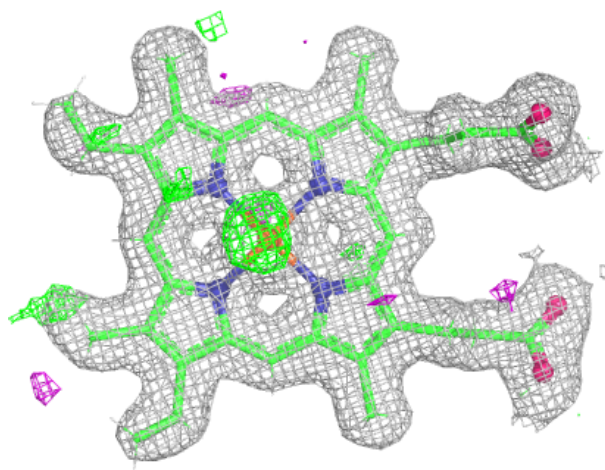
Electron density around HEM C 401:

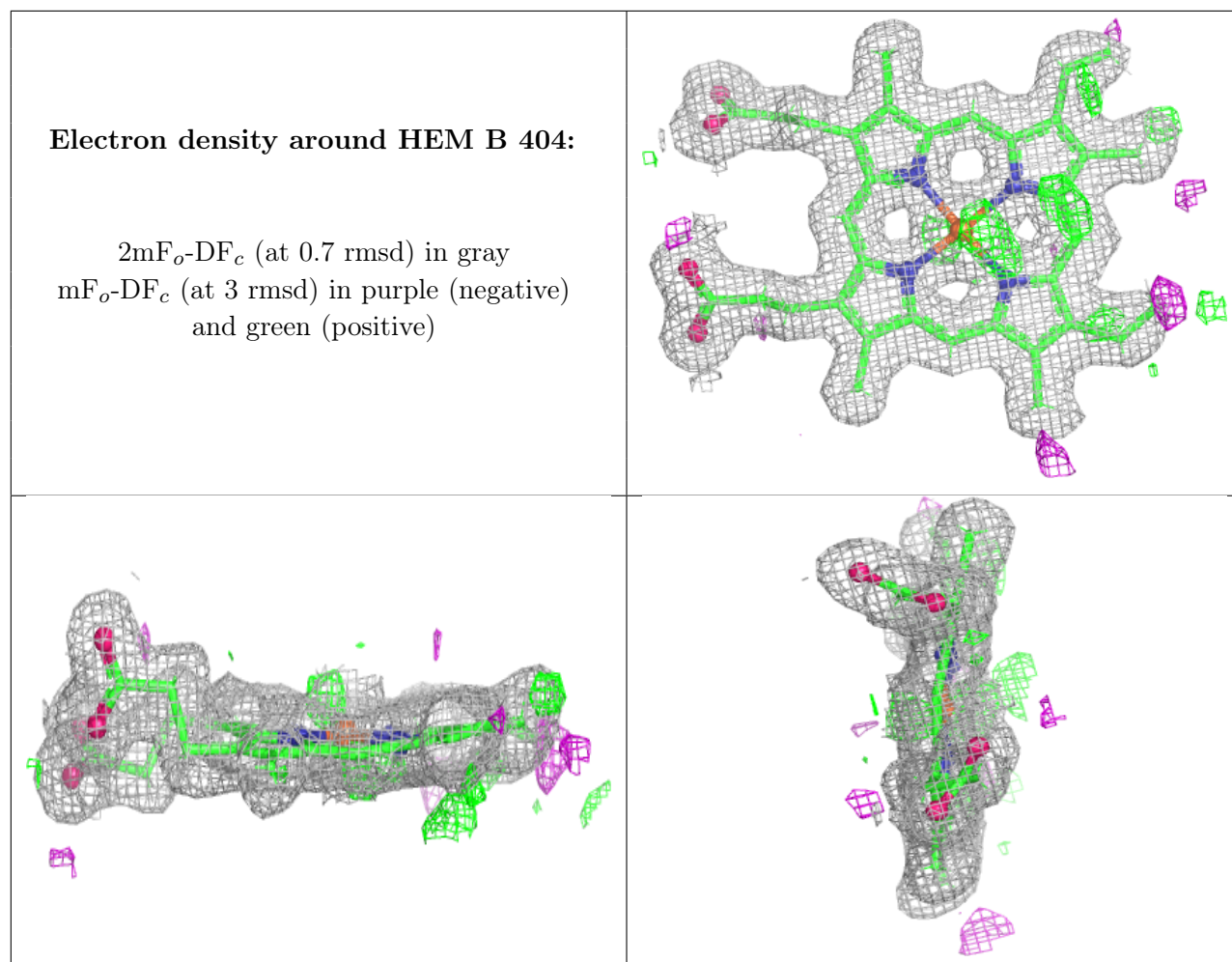
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 406:

$2mF_o-DF_c$ (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.