



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:07 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 Full wwPDB X-ray Structure Validation 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

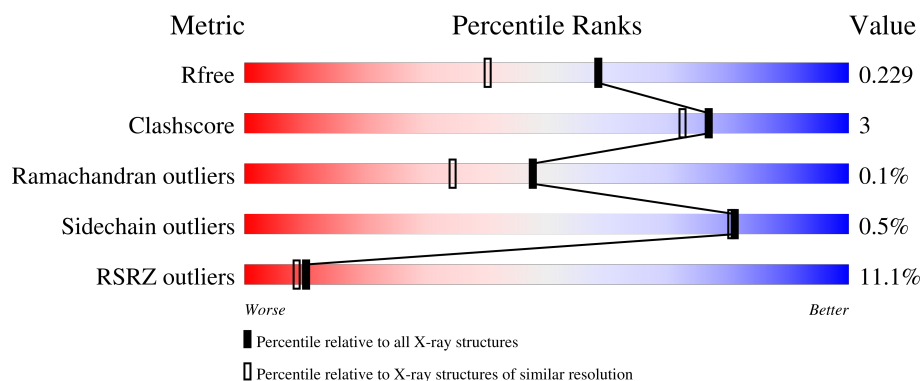
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

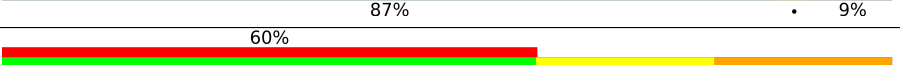
The reported resolution of this entry is 1.79 Å.

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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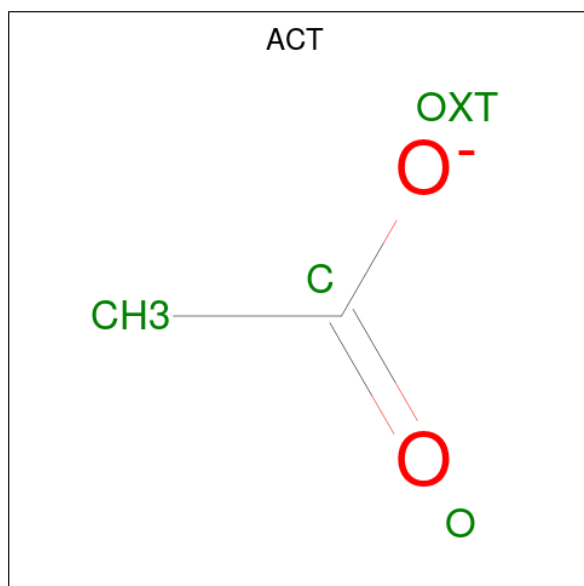
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	expression tag	UNP A0A3E2YLT4
B	-17	SER	-	expression tag	UNP A0A3E2YLT4
B	-16	HIS	-	expression tag	UNP A0A3E2YLT4
B	-15	HIS	-	expression tag	UNP A0A3E2YLT4
B	-14	HIS	-	expression tag	UNP A0A3E2YLT4
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: $C_2H_3O_2$).



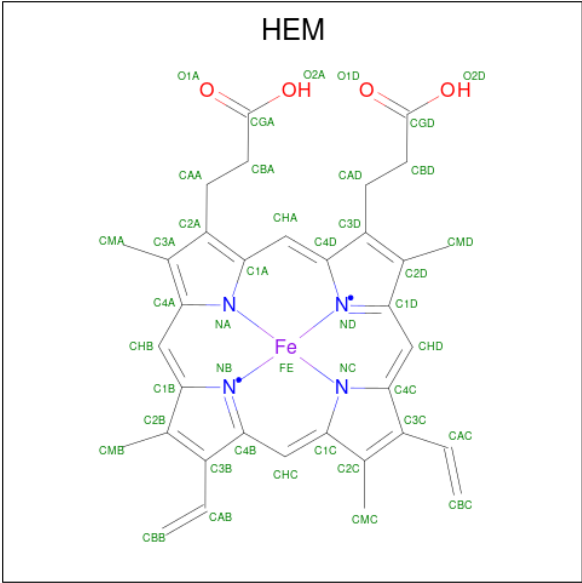
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	1
			14	4	6	4		

- 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: C₃₄H₃₂FeN₄O₄).



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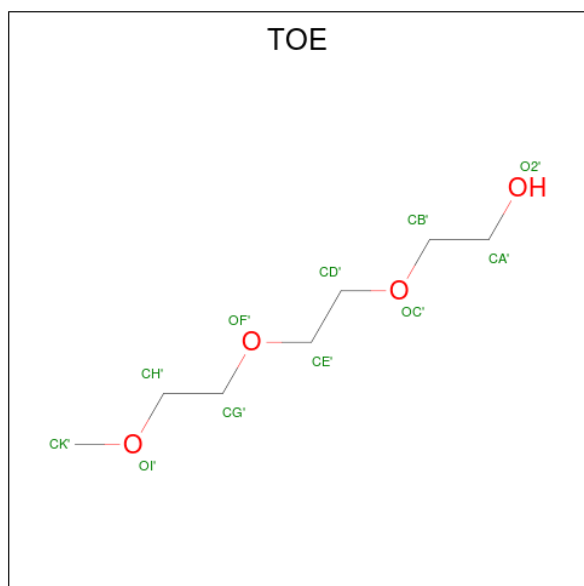
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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

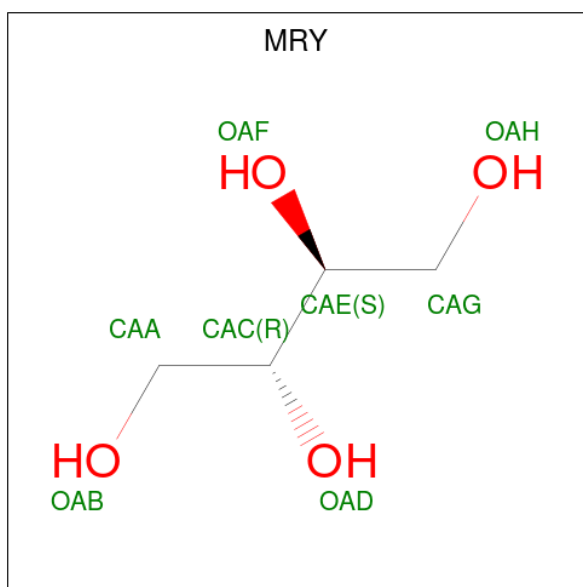
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Na	0	0
			3	3		
6	B	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		

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



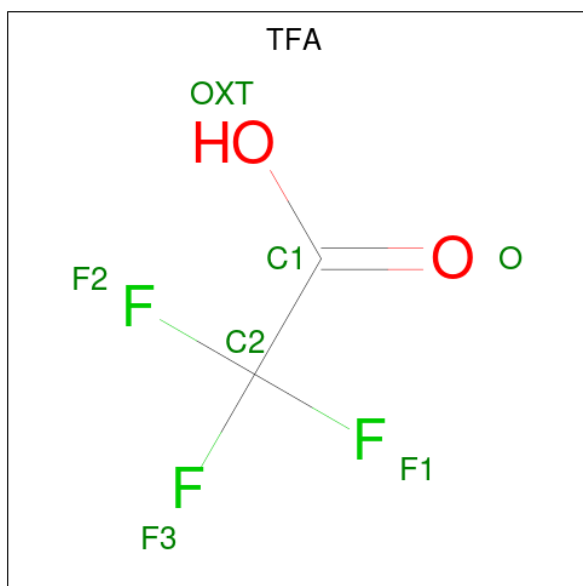
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			27	7	16	4		

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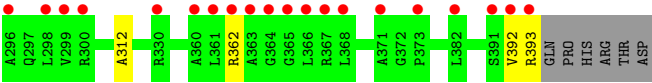
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	F	O	0	0
			7	2	3	2		

- 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 1: Cytochrome P450-SU1





● 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.

All (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:HH1C	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
1:B:267:ASP:OD2	1:B:362:ARG:NH2	2.35	0.58
5:B:404:HEM:HBC2	5:B:404:HEM:CMC	2.36	0.54
5:A:406:HEM:HBB2	5:A:406:HEM:HMB2	1.90	0.53
1:B:163:GLN:NE2	10:B:504:HOH:O	2.41	0.52
5:C:401:HEM:HMB2	5:C:401:HEM:HBB2	1.91	0.52
1:C:72:ILE:HG13	1:C:74:VAL:HG23	1.93	0.51
1:A:253:ARG:NH2	10:A:504:HOH:O	2.43	0.51
1:A:343:ALA:HB1	3:A:402:ACT:H1	1.94	0.50
1:B:104:GLU:OE1	8:B:403:MRY:OAB	2.29	0.50
5:C:401:HEM:CMC	5:C:401:HEM:HBC2	2.43	0.49
1:A:97:LEU:C	1:A:97:LEU:HD23	2.38	0.48
5:C:401:HEM:HBB2	5:C:401:HEM:CMB	2.43	0.48
5:A:406:HEM:HBB2	5:A:406:HEM:CMB	2.44	0.47
5:A:406:HEM:HBC2	5:A:406:HEM:CMC	2.45	0.47
1:A:218:GLN:O	1:A:219:ASP:HB3	2.15	0.47
1:B:199:LEU:HD21	1:B:229:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:O	1:A:252:VAL:HG13	2.16	0.46
1:A:52:TYR:HA	1:A:312:ALA:HB1	1.97	0.46
5:A:406:HEM:HBC2	5:A:406:HEM:HMC1	1.98	0.46
1:A:331:ARG:CZ	1:A:331:ARG:HB2	2.45	0.45
1:C:52:TYR:HA	1:C:312:ALA:HB1	1.98	0.45
1:C:69:PHE:CE1	1:C:287:VAL:HG13	2.52	0.45
1:B:15:ASP:HB3	1:B:18:ALA:HB2	1.99	0.45
7:B:402:TOE:H2	10:B:670:HOH:O	2.17	0.45
1:C:97:LEU:C	1:C:97:LEU:HD23	2.42	0.45
1:C:267:ASP:OD1	1:C:362:ARG:NH2	2.47	0.45
1:A:114:PHE:CE1	1:A:146:THR:HG23	2.51	0.45
5:C:401:HEM:HBC2	5:C:401:HEM:HMC1	1.99	0.45
1:B:30:ARG:NH1	10:B:511:HOH:O	2.50	0.44
5:B:404:HEM:HBB2	5:B:404:HEM:CHC	2.44	0.44
1:B:203:ASP:OD1	1:B:204:GLU:N	2.51	0.44
1:C:230:ARG:NH2	9:C:403:TFA:O	2.52	0.43
1:C:126:SER:HA	1:C:392:VAL:HG11	2.01	0.42
1:B:367:ARG:HG2	1:B:393:ARG:HD2	2.01	0.42
1:B:239:SER:HB3	5:B:404:HEM:C3B	2.54	0.42
1:B:203:ASP:OD1	1:B:205:ARG:N	2.51	0.42
1:A:84[B]:GLN:HE21	2:D:4:LEU:HD13	1.85	0.41
1:A:218:GLN:O	1:A:219:ASP:CB	2.67	0.41
1:B:72:ILE:HG13	1:B:74:VAL:HG23	2.00	0.41
1:C:392:VAL:O	1:C:393:ARG:HG3	2.20	0.41
1:C:62:THR:HA	1:C:65:PHE:O	2.21	0.41
1:B:154:PRO:HA	1:B:155:PRO:HD3	2.00	0.41
1:B:347:ALA:O	1:B:351:THR:HG23	2.21	0.41
5:B:404:HEM:HHC	5:B:404:HEM:CBB	2.47	0.41
1:B:52:TYR:HA	1:B:312:ALA:HB1	2.01	0.40
1:B:214:ALA:HB2	8:B:403:MRY:CAA	2.51	0.40
1:A:199:LEU:HD21	1:A:229:LEU:CD1	2.52	0.40
1:B:235:ALA:HB1	10:B:572:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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	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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	-

All (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
5	A	406	HEM	CAB-C3B	2.95	1.55	1.47
5	C	401	HEM	FE-ND	2.92	2.03	1.94
5	C	401	HEM	CAB-C3B	2.92	1.55	1.47
5	B	404	HEM	CAC-C3C	2.90	1.55	1.47
5	A	406	HEM	FE-NA	2.86	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	401	HEM	CAC-C3C	2.82	1.54	1.47
5	A	406	HEM	CAC-C3C	2.81	1.54	1.47
5	B	404	HEM	CAB-C3B	2.71	1.54	1.47
5	A	406	HEM	FE-ND	2.64	2.03	1.94
5	A	406	HEM	FE-NC	2.45	2.03	1.95
5	C	401	HEM	FE-NC	2.26	2.02	1.95
5	A	406	HEM	CMC-C2C	2.15	1.55	1.50
5	C	401	HEM	CMC-C2C	2.12	1.55	1.50
5	B	404	HEM	FE-NA	2.11	2.02	1.95
5	C	401	HEM	CMB-C2B	2.08	1.55	1.50
5	B	404	HEM	CMC-C2C	2.05	1.55	1.50
5	B	404	HEM	FE-NB	2.05	2.01	1.94
5	B	404	HEM	CMA-C3A	2.04	1.55	1.50
5	C	401	HEM	CMA-C3A	2.01	1.54	1.50

All (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
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
5	B	404	HEM	C2A-C1A-NA	-2.49	107.39	110.15
3	B	405[B]	ACT	O-C-CH3	-2.48	112.36	122.53
5	A	406	HEM	C4D-ND-C1D	2.45	108.11	105.21
5	B	404	HEM	CAA-CBA-CGA	-2.42	107.24	113.67
5	C	401	HEM	C1B-NB-C4B	2.38	108.03	105.21
5	C	401	HEM	C4D-ND-C1D	2.34	107.97	105.21
5	B	404	HEM	C3D-C4D-ND	-2.33	107.61	110.17
5	B	404	HEM	CHD-C1D-ND	2.31	126.91	124.42
5	B	404	HEM	C1B-NB-C4B	2.27	107.89	105.21
5	B	404	HEM	C3B-C4B-NB	-2.25	107.85	109.47
5	B	404	HEM	C3B-C2B-C1B	2.24	108.09	106.41
5	A	406	HEM	CAD-CBD-CGD	-2.18	107.89	113.67
5	A	406	HEM	C1B-NB-C4B	2.16	107.76	105.21
3	B	401	ACT	O-C-CH3	-2.12	113.85	122.53
5	C	401	HEM	CAD-CBD-CGD	-2.07	108.17	113.67
9	C	402	TFA	OXT-C1-C2	2.05	120.60	112.58
5	C	401	HEM	C3D-C4D-ND	-2.03	107.95	110.17
5	A	406	HEM	C3D-C4D-ND	-2.03	107.95	110.17
5	C	401	HEM	C3B-C2B-C1B	2.01	107.92	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	406	HEM	C3B-C2B-C1B	2.01	107.92	106.41

There are no chirality outliers.

All (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
8	B	403	MRY	OAB-CAA-CAC-CAE
4	A	403	PG4	O2-C3-C4-O3
7	B	402	TOE	OF'-CG'-CH'-OI'
4	A	403	PG4	O1-C1-C2-O2
4	A	403	PG4	C8-C7-O4-C6
7	B	402	TOE	OC'-CD'-CE'-OF'
7	B	402	TOE	O2'-CA'-CB'-OC'
4	A	403	PG4	C4-C3-O2-C2
7	B	402	TOE	CG'-CH'-OI'-CK'
7	B	402	TOE	CE'-CD'-OC'-CB'
5	B	404	HEM	CAA-CBA-CGA-O1A
5	C	401	HEM	CAD-CBD-CGD-O2D
5	A	406	HEM	CAD-CBD-CGD-O2D
5	C	401	HEM	CAD-CBD-CGD-O1D
5	A	406	HEM	CAD-CBD-CGD-O1D
7	B	402	TOE	CH'-CG'-OF'-CE'
5	B	404	HEM	CAA-CBA-CGA-O2A
5	B	404	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

8 monomers are involved in 20 short contacts:

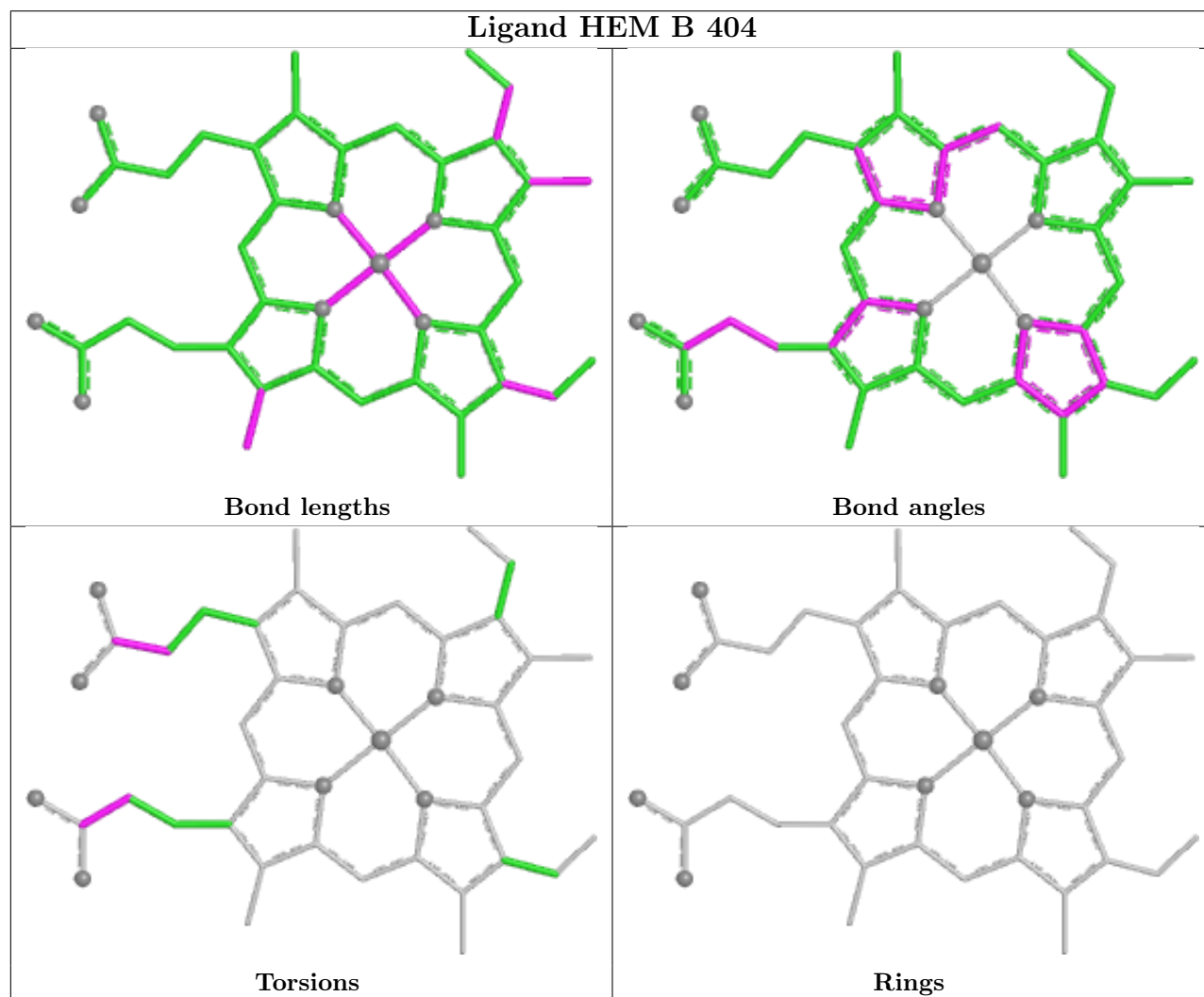
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	404	HEM	6	0
3	A	402	ACT	1	0
5	A	406	HEM	4	0
8	B	403	MRY	2	0
5	C	401	HEM	4	0
7	B	402	TOE	1	0
9	C	403	TFA	1	0

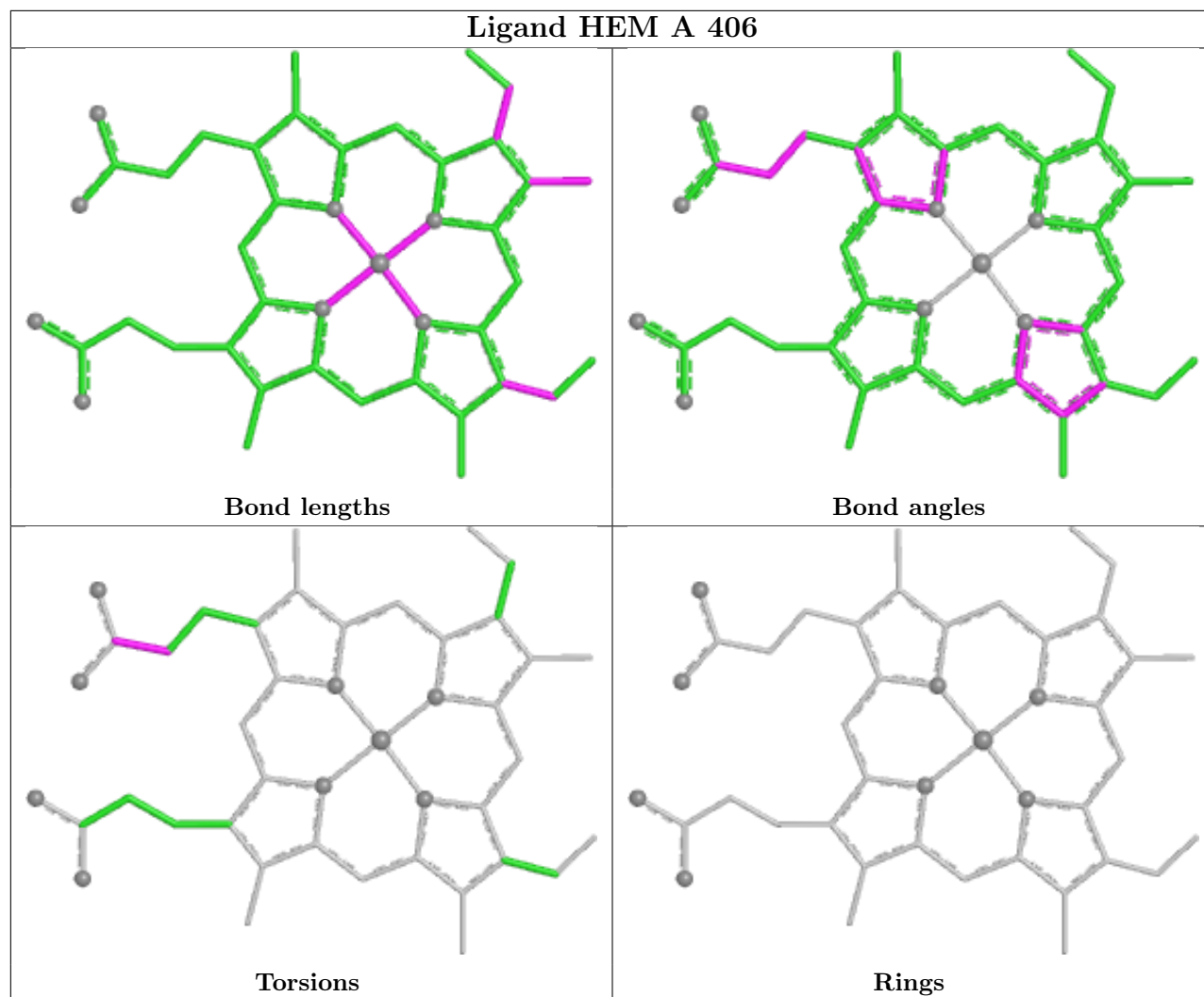
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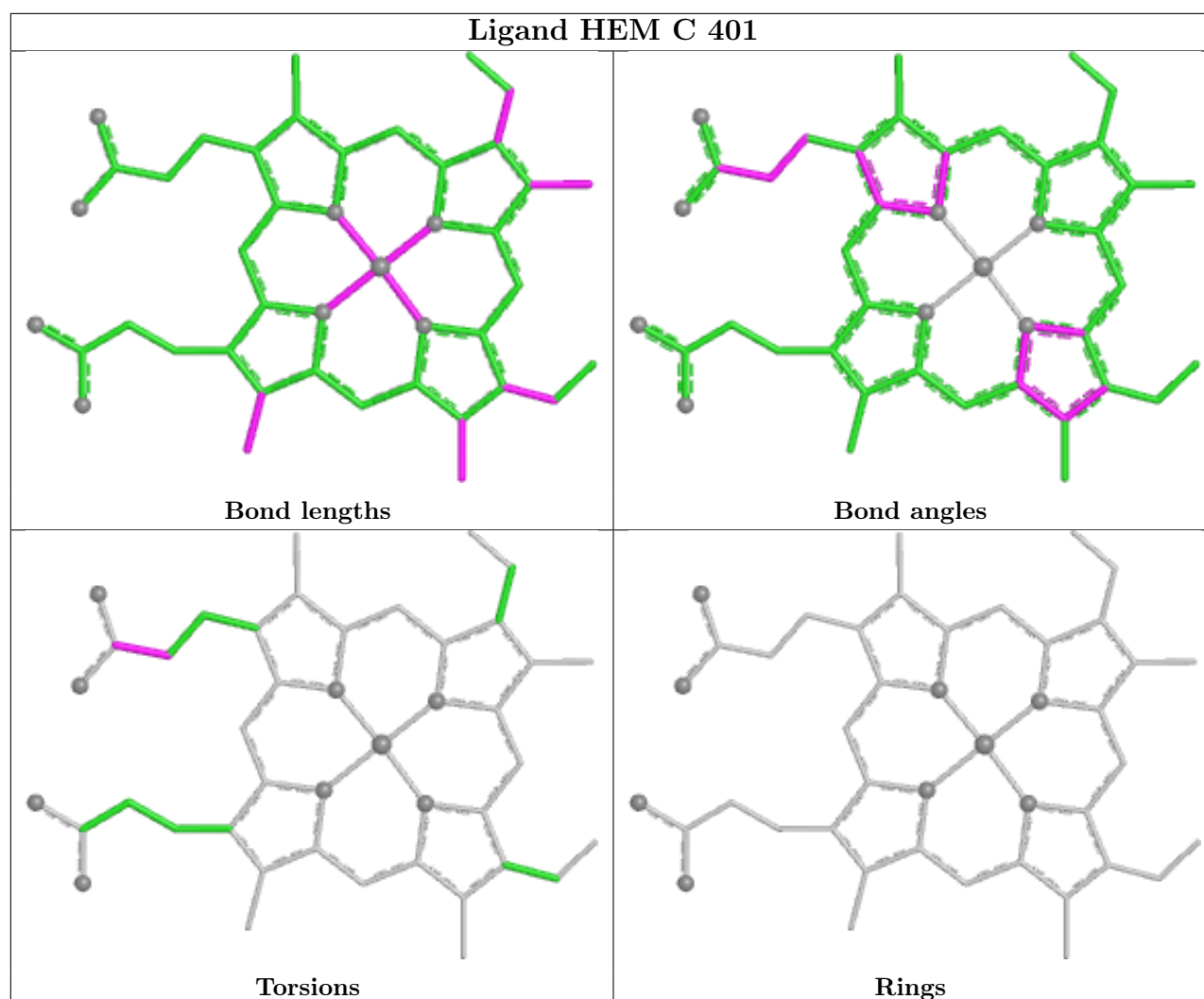
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ACT	1	0

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.







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%)

All (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
1	A	74	VAL	4.5
1	A	76	ILE	4.4
1	C	266	ALA	4.3
1	C	123	ALA	4.3
1	C	122	LEU	4.1
1	C	392	VAL	4.1
1	C	44	LEU	4.0
1	A	43	PHE	3.9
1	A	69	PHE	3.9
1	A	217	ALA	3.8
1	C	361	LEU	3.8
1	C	262	ALA	3.8
1	C	12	PRO	3.8
1	C	128	GLN	3.8
1	C	393	ARG	3.7
1	B	13	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	81	LEU	3.6
1	A	366	LEU	3.6
1	C	76	ILE	3.6
1	A	365	GLY	3.6
1	C	366	LEU	3.6
1	C	119	ALA	3.6
1	C	69	PHE	3.5
1	C	219	ASP	3.5
1	C	74	VAL	3.5
1	A	79	THR	3.5
1	C	125	LEU	3.4
1	C	107	LEU	3.4
1	B	393	ARG	3.4
1	C	298	LEU	3.3
1	B	12	PRO	3.3
1	A	127	GLY	3.2
1	C	43	PHE	3.2
1	A	89	PRO	3.2
1	A	216	ARG	3.1
1	C	296	ALA	3.1
1	B	164	TRP	3.1
1	C	118	ALA	3.1
1	C	289	VAL	3.1
2	D	4	LEU	3.1
1	C	221	PRO	3.0
2	D	5	HIS	3.0
1	A	205	ARG	3.0
1	B	69	PHE	2.9
1	C	73	ASP	2.9
1	C	371	ALA	2.8
1	C	364	GLY	2.8
1	A	220	VAL	2.8
1	C	368	LEU	2.8
1	A	218	GLN	2.8
1	A	219	ASP	2.8
1	C	126	SER	2.7
1	C	220	VAL	2.7
1	A	164	TRP	2.7
1	C	363	ALA	2.7
1	C	263	THR	2.6
1	B	203	ASP	2.6
1	C	35	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	103	HIS	2.5
1	A	77	PRO	2.5
1	C	77	PRO	2.5
1	C	217	ALA	2.5
1	C	391	SER	2.5
1	A	262	ALA	2.5
1	C	127	GLY	2.5
1	C	264	ARG	2.5
1	C	81	LEU	2.4
1	A	215	ALA	2.4
1	A	222	ALA	2.4
1	C	72	ILE	2.4
1	A	39[A]	HIS	2.4
1	C	115	ALA	2.4
1	C	75	GLU	2.4
1	C	112	GLN	2.4
1	C	110	VAL	2.4
1	B	295	GLY	2.3
1	C	290	ARG	2.3
1	C	362	ARG	2.3
1	C	65	PHE	2.3
1	A	72	ILE	2.3
1	A	126	SER	2.3
1	A	203	ASP	2.3
1	A	159	ALA	2.3
1	C	116	ALA	2.3
1	A	75	GLU	2.3
1	A	80	GLN	2.3
1	C	367	ARG	2.3
1	C	40	TRP	2.2
1	C	360	ALA	2.2
1	C	111	ARG	2.2
1	C	258	LEU	2.2
1	A	161	PHE	2.2
1	A	236	GLY	2.2
1	C	265	ASP	2.2
1	A	125	LEU	2.2
1	B	290	ARG	2.2
1	C	261	PRO	2.2
1	B	296	ALA	2.2
1	C	291	ASP	2.2
1	C	218	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	130	GLY	2.2
1	A	367	ARG	2.2
1	B	103	HIS	2.2
1	C	330	ARG	2.2
1	C	300	ARG	2.1
1	A	364	GLY	2.1
1	C	299	VAL	2.1
1	C	225	LEU	2.1
1	C	79	THR	2.1
1	C	117	ILE	2.1
1	C	382	LEU	2.1
1	C	88	PRO	2.1
1	C	293	PRO	2.1
1	C	47	TRP	2.1
1	A	201	GLU	2.0
1	C	64	ASN	2.0
1	A	195	VAL	2.0
2	D	2	ARG	2.0
1	A	352	LEU	2.0
1	C	373	PRO	2.0
1	B	104	GLU	2.0
1	A	393	ARG	2.0
1	B	76	ILE	2.0

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.

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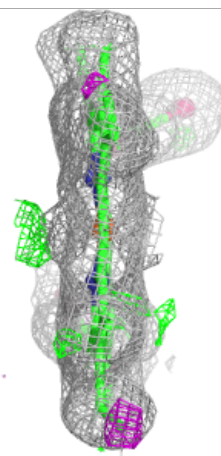
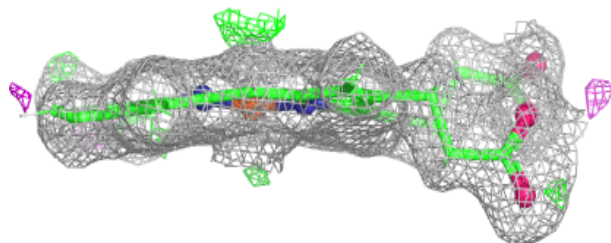
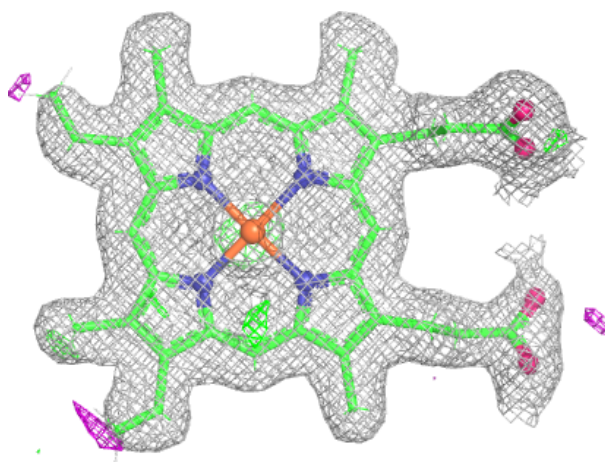
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	B	405[A]	4/4	0.72	0.17	35,39,42,42	7
3	ACT	B	405[B]	4/4	0.72	0.17	30,37,42,42	7
3	ACT	B	401	4/4	0.75	0.18	42,51,53,55	0
3	ACT	A	402	4/4	0.79	0.15	41,50,51,52	0
3	ACT	A	405	4/4	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.

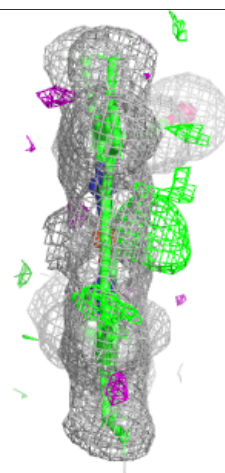
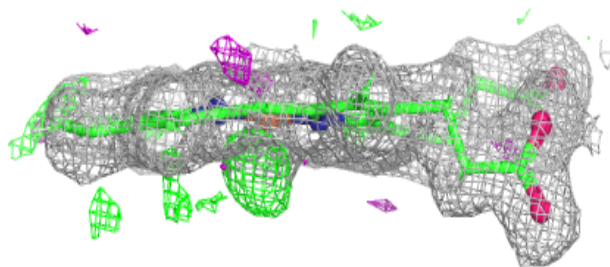
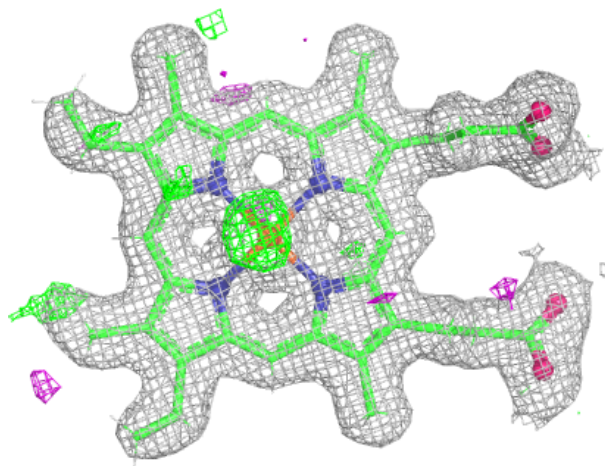
Electron density around HEM C 401:

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



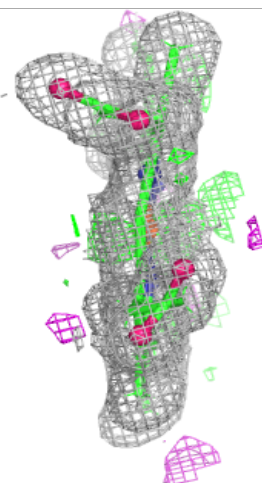
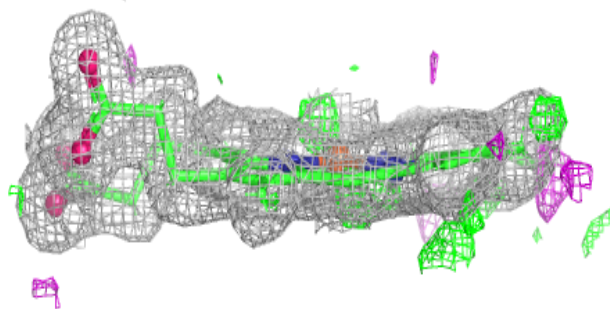
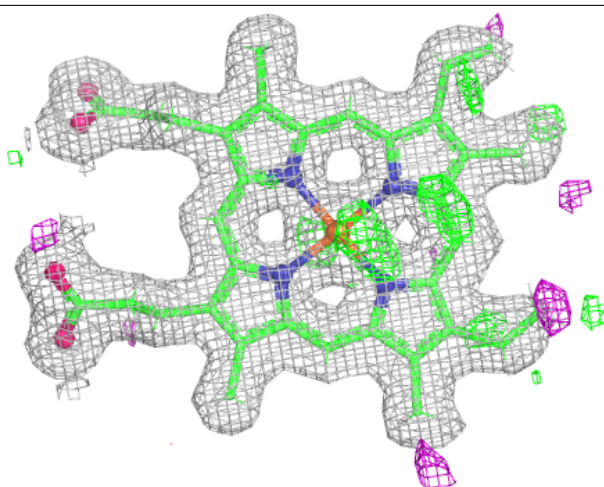
Electron density around HEM A 406:

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



Electron density around HEM B 404:

$2mF_o-DF_c$ (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.