



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:28 AM UTC

PDB ID : 9BW8 / pdb_00009bw8
Title : Structure of P450Blt from Micromonospora sp. MW-13 in Complex with Fluorinated Biarylthide
Authors : Hansen, M.H.; Cryle, M.J.; Zhao, Y.
Deposited on : 2024-05-21
Resolution : 1.86 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

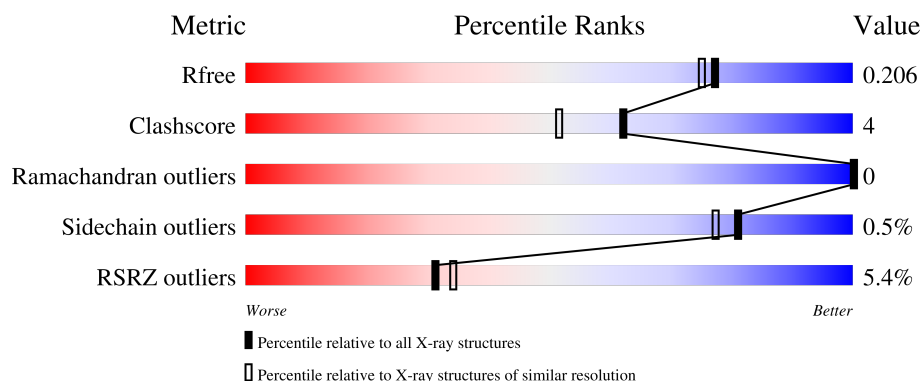
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	3% 85% 5% 10%
1	B	420	2% 85% 6% 9%
1	C	420	9% 82% 8% 9%
2	E	5	80% 40% 60%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18331 atoms, of which 8928 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	378	Total	C	H	N	O	S	0	4	0
			5795	1820	2903	546	522	4			
1	B	382	Total	C	H	N	O	S	0	4	0
			5865	1838	2939	555	529	4			
1	C	382	Total	C	H	N	O	S	0	6	0
			5883	1843	2948	557	531	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

Continued on next page...

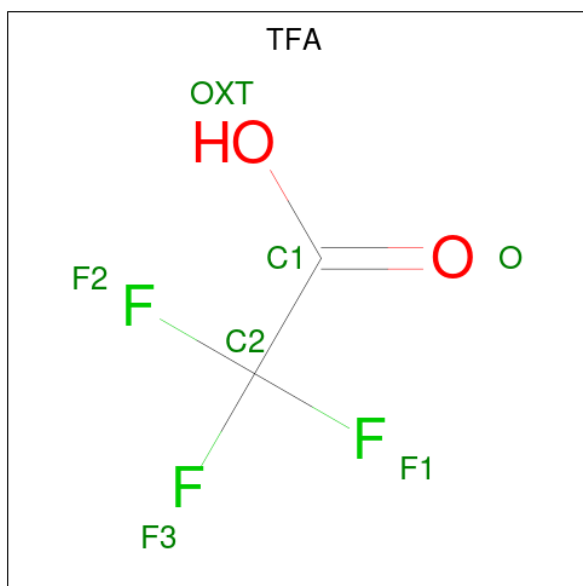
Continued from previous page...

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 Fluorinated Biarylilide.

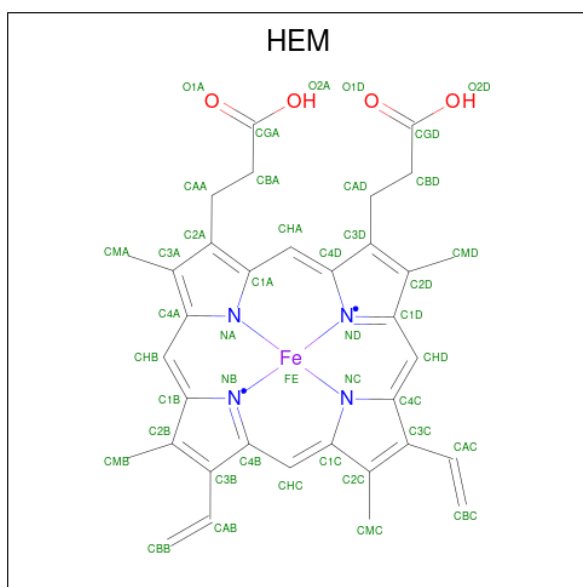
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	E	5	Total	C	F	H	N	O	S	0	0	0
			99	32	1	48	10	7	1			

- Molecule 3 is trifluoroacetic acid (CCD ID: TFA) (formula: $C_2HF_3O_2$).



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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

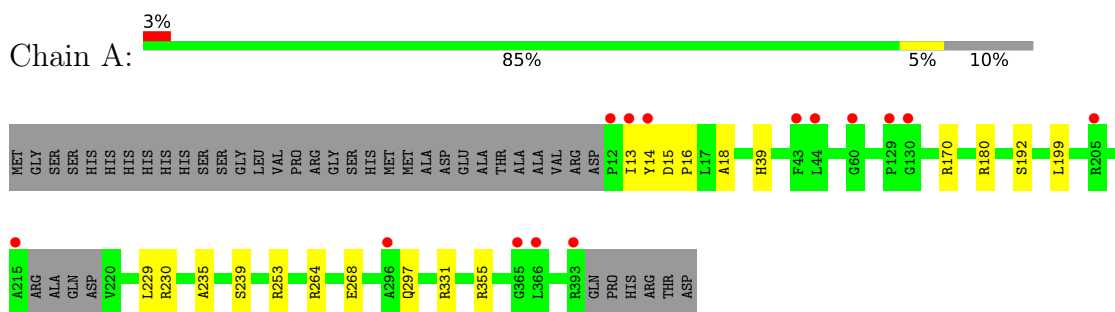
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	140	Total	O	0	0
			140	140		
6	B	193	Total	O	0	0
			193	193		
6	C	98	Total	O	0	0
			98	98		
6	E	3	Total	O	0	0
			3	3		

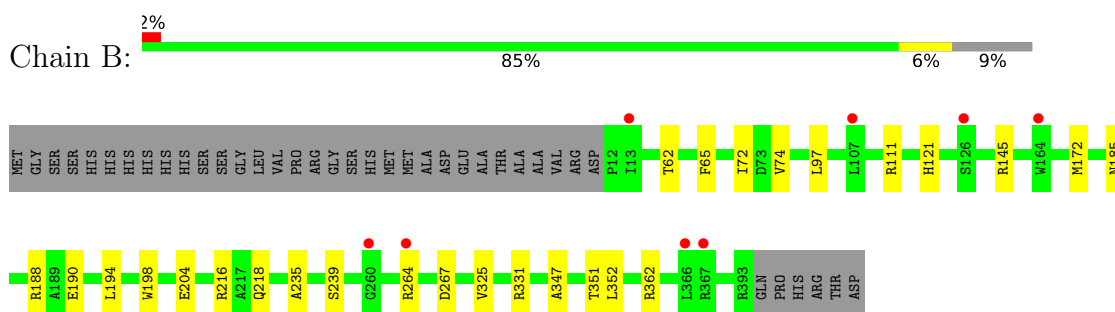
3 Residue-property plots [i](#)

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.

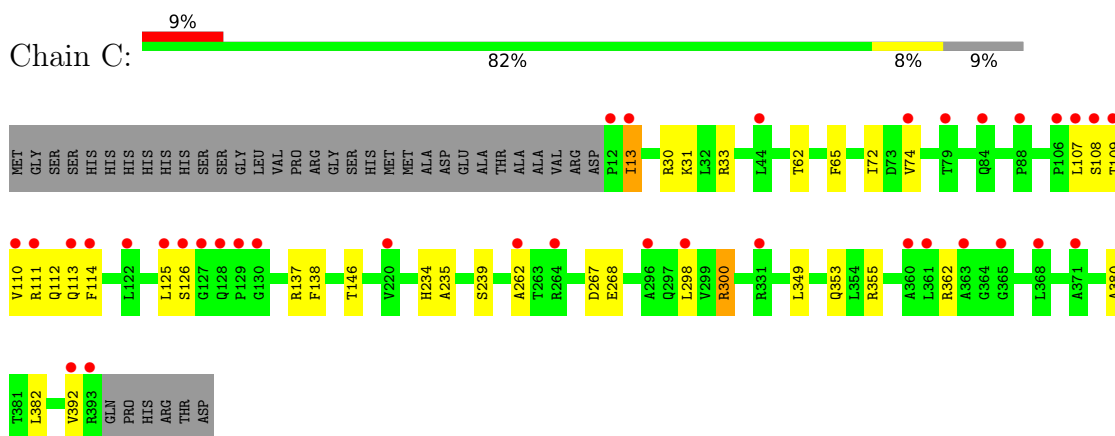
- Molecule 1: Cytochrome P450-SU1



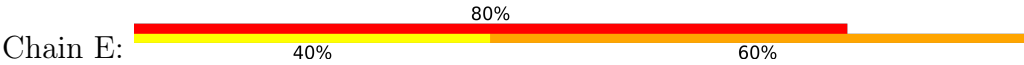
- Molecule 1: Cytochrome P450-SU1



- Molecule 1: Cytochrome P450-SU1



- Molecule 2: Fluorinated Biarylthide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.91Å 94.15Å 105.00Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	46.73 – 1.86 46.73 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.73-1.86) 98.9 (46.73-1.86)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.178 , 0.207 0.178 , 0.206	Depositor DCC
R_{free} test set	5168 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18331	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/2978	0.67	0/4064
1	B	0.56	0/3005	0.72	0/4099
1	C	0.49	0/3020	0.70	1/4119 (0.0%)
2	E	3.69	5/37 (13.5%)	2.08	2/44 (4.5%)
All	All	0.57	5/9040 (0.1%)	0.71	3/12326 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	ARG	NE-CZ	13.14	1.47	1.33
2	E	4	LEU	C-N	9.18	1.46	1.33
2	E	2	ARG	CZ-NH1	8.81	1.45	1.32
2	E	1	MET	C-N	8.03	1.44	1.33
2	E	2	ARG	CZ-NH2	-5.12	1.26	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	ARG	NE-CZ-NH2	7.08	125.57	119.20
1	C	300	ARG	CG-CD-NE	-5.42	100.08	112.00
2	E	1	MET	CG-SD-CE	5.14	112.20	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	GLN	Mainchain

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	2892	2903	2885	12	0
1	B	2926	2939	2926	20	0
1	C	2935	2948	2929	30	2
2	E	51	48	49	6	0
3	A	14	0	0	0	0
3	B	14	0	0	1	0
3	C	7	0	0	0	0
4	A	43	30	30	5	0
4	B	43	30	30	4	0
4	C	43	30	30	3	0
5	A	1	0	0	0	0
6	A	140	0	0	1	0
6	B	193	0	0	6	1
6	C	98	0	0	1	0
6	E	3	0	0	3	0
All	All	9403	8928	8879	73	3

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

All (73) 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)
4:B:403:HEM:HMC2	4:B:403:HEM:HBC2	1.45	0.99
1:B:111:ARG:HG3	1:B:352:LEU:HD11	1.53	0.89
1:C:125:LEU:HD21	1:C:137:ARG:HB3	1.55	0.89
4:C:402:HEM:HBB2	4:C:402:HEM:HMB2	1.60	0.81
4:A:403:HEM:HMB2	4:A:403:HEM:HBB2	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:MET:SD	6:B:693:HOH:O	2.43	0.76
4:B:403:HEM:HBC2	4:B:403:HEM:CMC	2.16	0.75
1:A:192:SER:OG	1:A:230:ARG:NH1	2.20	0.74
2:E:3:YOF:OH	6:E:101:HOH:O	2.08	0.70
1:B:267:ASP:OD2	1:B:362:ARG:NH2	2.25	0.69
1:A:15:ASP:HB3	1:A:18:ALA:HB2	1.76	0.67
4:A:403:HEM:HBC2	4:A:403:HEM:HMC2	1.76	0.66
1:B:204:GLU:OE2	6:B:503:HOH:O	2.13	0.66
1:A:13:ILE:HD11	1:A:39[A]:HIS:NE2	2.10	0.66
4:A:403:HEM:HBB2	4:A:403:HEM:CMB	2.29	0.62
4:C:402:HEM:HBB2	4:C:402:HEM:CMB	2.30	0.61
1:C:235:ALA:HB1	6:E:101:HOH:O	2.00	0.61
1:C:298:LEU:HD23	1:C:300:ARG:NH2	2.17	0.60
1:C:114:PHE:CE1	1:C:146:THR:HG23	2.37	0.59
1:A:13:ILE:HD12	1:A:13:ILE:H	1.66	0.59
2:E:3:YOF:N	6:E:102:HOH:O	2.32	0.59
1:C:31:LYS:NZ	6:C:503:HOH:O	2.36	0.58
1:C:126:SER:HA	1:C:392:VAL:HG11	1.87	0.56
1:C:267:ASP:OD2	1:C:362:ARG:NH2	2.25	0.56
1:C:108:SER:HA	1:C:111:ARG:NE	2.21	0.56
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.35	0.54
1:C:110:VAL:HG11	1:C:349:LEU:CD2	2.38	0.53
1:C:108:SER:O	1:C:112:GLN:HG3	2.08	0.53
1:C:382:LEU:HD11	2:E:3:YOF:F	2.01	0.52
1:A:331:ARG:CZ	1:A:331:ARG:HB2	2.40	0.51
1:B:190:GLU:OE2	6:B:504:HOH:O	2.19	0.50
1:C:13:ILE:HD12	1:C:13:ILE:O	2.11	0.50
4:B:403:HEM:HHC	4:B:403:HEM:CBB	2.42	0.49
1:C:62:THR:HA	1:C:65:PHE:O	2.13	0.49
1:A:239:SER:HB3	4:A:403:HEM:C2C	2.48	0.49
1:C:268:GLU:HG3	1:C:355:ARG:HH22	1.76	0.48
1:C:108:SER:CB	1:C:111:ARG:NH2	2.77	0.48
1:C:380:ALA:HB1	2:E:1:MET:CE	2.44	0.48
1:C:239:SER:HB3	4:C:402:HEM:C2C	2.50	0.47
1:B:216:ARG:NH2	6:B:502:HOH:O	2.11	0.47
1:B:325:VAL:HB	3:B:401:TFA:OXT	2.14	0.47
1:C:72:ILE:HG13	1:C:74:VAL:HG23	1.96	0.46
1:C:109:THR:O	1:C:113:GLN:HG3	2.16	0.46
1:B:331:ARG:CZ	1:B:331:ARG:HB2	2.46	0.45
1:A:235:ALA:HB1	6:A:580:HOH:O	2.17	0.45
1:C:30:ARG:HG3	1:C:33[B]:ARG:NH2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:C	1:B:97:LEU:HD23	2.43	0.44
1:B:218:GLN:NE2	6:B:501:HOH:O	2.10	0.44
1:B:121:HIS:NE2	1:B:145:ARG:HD3	2.32	0.44
1:A:268:GLU:HB2	1:A:355:ARG:HH22	1.83	0.43
1:B:62:THR:HA	1:B:65:PHE:O	2.18	0.43
1:B:239:SER:HB3	4:B:403:HEM:C3B	2.54	0.43
1:C:114:PHE:CE2	1:C:353:GLN:HB2	2.53	0.43
4:A:403:HEM:HMB2	4:A:403:HEM:CBB	2.42	0.43
1:C:234:HIS:ND1	2:E:5:HIS:ND1	2.67	0.43
1:A:199:LEU:HD21	1:A:229:LEU:CD1	2.49	0.42
1:B:267:ASP:CG	1:B:362:ARG:HH22	2.26	0.42
1:A:170[B]:ARG:O	1:A:180:ARG:HD3	2.19	0.42
1:C:268:GLU:CB	1:C:355:ARG:HH22	2.32	0.42
1:C:125:LEU:HD11	1:C:138:PHE:HB2	2.01	0.41
1:C:268:GLU:HB2	1:C:355:ARG:HH22	1.84	0.41
1:C:107:LEU:HD23	1:C:107:LEU:HA	1.89	0.41
1:C:267:ASP:CG	1:C:362:ARG:HH22	2.21	0.41
1:A:14:TYR:CD1	1:A:14:TYR:C	2.99	0.41
1:B:235:ALA:HB1	6:B:597:HOH:O	2.20	0.41
1:B:347:ALA:O	1:B:351:THR:HG23	2.21	0.41
1:C:108:SER:HA	1:C:111:ARG:CZ	2.51	0.41
1:B:194:LEU:HG	1:B:198:TRP:CZ2	2.56	0.41
1:B:72:ILE:HG13	1:B:74:VAL:HG23	2.02	0.40
1:B:111:ARG:HH12	1:B:264:ARG:HH21	1.68	0.40
1:A:14:TYR:HE1	1:A:16:PRO:HA	1.86	0.40
1:C:235:ALA:HB2	2:E:5:HIS:CD2	2.57	0.40
1:C:268:GLU:HG3	1:C:355:ARG:NH2	2.36	0.40

All (3) 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:C:262:ALA:O	1:C:300:ARG:HH22[2_546]	1.49	0.11
6:B:654:HOH:O	6:B:672:HOH:O[2_545]	2.16	0.04
1:C:262:ALA:O	1:C:300:ARG:NH2[2_546]	2.18	0.02

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	378/420 (90%)	374 (99%)	4 (1%)	0	100	100
1	B	384/420 (91%)	380 (99%)	4 (1%)	0	100	100
1	C	386/420 (92%)	382 (99%)	4 (1%)	0	100	100
2	E	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1150/1265 (91%)	1138 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	295/325 (91%)	293 (99%)	2 (1%)	76	70
1	B	298/325 (92%)	298 (100%)	0	100	100
1	C	300/325 (92%)	299 (100%)	1 (0%)	86	85
2	E	4/4 (100%)	3 (75%)	1 (25%)	0	0
All	All	897/979 (92%)	893 (100%)	4 (0%)	81	82

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

Mol	Chain	Res	Type
1	A	253	ARG
1	A	264	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	13	ILE
2	E	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	163	GLN
1	A	292	GLN
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 ⓘ

1 non-standard protein/DNA/RNA residue is 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	YOF	E	3	2	12,13,14	0.55	0	10,17,19	1.14	1 (10%)

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	YOF	E	3	2	-	1/5/6/8	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	YOF	CD2-CE2-CZ	-2.24	118.26	120.50

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	3	YOF	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	YOF	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
4	HEM	C	402	6,1	50,50,50	1.35	7 (14%)	67,82,82	1.13	5 (7%)
4	HEM	A	403	6,1	50,50,50	1.49	8 (16%)	67,82,82	1.41	8 (11%)
3	TFA	A	402	-	6,6,6	1.21	0	9,9,9	0.97	0
4	HEM	B	403	6,1	50,50,50	1.50	6 (12%)	67,82,82	1.90	14 (20%)
3	TFA	C	401	5	6,6,6	1.15	0	9,9,9	1.70	4 (44%)
3	TFA	B	401	-	6,6,6	1.03	0	9,9,9	1.52	2 (22%)
3	TFA	B	402	-	6,6,6	1.01	0	9,9,9	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TFA	A	401	-	6,6,6	1.01	0	9,9,9	0.97	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
4	HEM	C	402	6,1	-	2/14/54/54	-
4	HEM	A	403	6,1	-	2/14/54/54	-
3	TFA	A	402	-	-	0/6/6/6	-
4	HEM	B	403	6,1	-	3/14/54/54	-
3	TFA	C	401	5	-	0/6/6/6	-
3	TFA	B	401	-	-	0/6/6/6	-
3	TFA	B	402	-	-	0/6/6/6	-
3	TFA	A	401	-	-	0/6/6/6	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	HEM	FE-ND	4.95	2.10	1.94
4	A	403	HEM	FE-NA	3.84	2.07	1.95
4	C	402	HEM	FE-ND	3.20	2.04	1.94
4	A	403	HEM	FE-NC	3.00	2.05	1.95
4	A	403	HEM	C1A-NA	-2.98	1.34	1.39
4	C	402	HEM	CMC-C2C	2.82	1.56	1.50
4	A	403	HEM	CMC-C2C	2.81	1.56	1.50
4	B	403	HEM	CMB-C2B	2.75	1.56	1.50
4	B	403	HEM	CMA-C3A	2.72	1.56	1.50
4	C	402	HEM	CAB-C3B	2.64	1.54	1.47
4	C	402	HEM	CAC-C3C	2.50	1.54	1.47
4	B	403	HEM	CMD-C2D	2.49	1.55	1.50
4	B	403	HEM	FE-NB	2.49	2.02	1.94
4	C	402	HEM	C3C-C2C	-2.38	1.32	1.37
4	A	403	HEM	CMB-C2B	2.33	1.55	1.50
4	C	402	HEM	FE-NB	2.30	2.02	1.94
4	A	403	HEM	C2A-C3A	-2.17	1.33	1.38
4	B	403	HEM	CMC-C2C	2.15	1.55	1.50
4	C	402	HEM	CMB-C2B	2.06	1.55	1.50
4	A	403	HEM	CAC-C3C	2.02	1.52	1.47
4	A	403	HEM	C3B-C2B	-2.01	1.33	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	HEM	C3B-C4B-NB	-5.63	105.42	109.47
4	B	403	HEM	CHC-C4B-NB	5.29	130.12	124.42
4	A	403	HEM	CHD-C4C-NC	4.69	129.56	124.45
4	B	403	HEM	C4B-C3B-C2B	4.32	111.25	107.28
4	B	403	HEM	C4D-ND-C1D	4.08	110.04	105.21
4	B	403	HEM	CHD-C4C-NC	3.95	128.75	124.45
4	B	403	HEM	CMB-C2B-C1B	3.55	130.57	125.03
3	B	401	TFA	F1-C2-C1	-3.40	99.76	111.90
4	B	403	HEM	C4C-C3C-C2C	3.31	109.68	106.81
4	B	403	HEM	C1B-NB-C4B	3.25	109.06	105.21
4	B	403	HEM	CAA-CBA-CGA	-2.97	105.78	113.67
4	B	403	HEM	CHC-C1C-NC	-2.94	121.25	124.45
4	A	403	HEM	CHC-C4B-NB	2.66	127.28	124.42
4	A	403	HEM	CMA-C3A-C2A	2.64	131.21	125.62
4	C	402	HEM	CHD-C4C-NC	2.56	127.24	124.45
4	A	403	HEM	CMB-C2B-C1B	2.54	129.01	125.03
4	C	402	HEM	C4C-C3C-C2C	2.53	109.01	106.81
4	A	403	HEM	CHA-C4D-ND	2.50	127.46	124.37
4	C	402	HEM	CHA-C4D-ND	2.49	127.45	124.37
4	B	403	HEM	C3D-C4D-ND	-2.48	107.45	110.17
4	A	403	HEM	CMA-C3A-C4A	-2.44	121.71	125.42
3	C	401	TFA	F3-C2-F1	-2.43	95.72	106.20
4	C	402	HEM	CHC-C1C-NC	2.43	127.09	124.45
4	B	403	HEM	C2D-C1D-ND	-2.41	107.12	109.90
3	C	401	TFA	F2-C2-F1	2.38	116.47	106.20
3	C	401	TFA	OXT-C1-C2	2.35	121.76	112.58
4	B	403	HEM	C1C-CHC-C4B	-2.34	121.04	126.02
3	B	401	TFA	F2-C2-F1	2.33	116.23	106.20
4	A	403	HEM	C4B-C3B-C2B	2.31	109.41	107.28
4	A	403	HEM	C4C-NC-C1C	2.28	109.54	105.82
4	C	402	HEM	C1B-NB-C4B	2.18	107.78	105.21
3	C	401	TFA	OXT-C1-O	-2.10	117.15	123.86
4	B	403	HEM	CHD-C1D-C2D	2.07	128.29	125.03

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	HEM	CAA-CBA-CGA-O1A
4	B	403	HEM	CAA-CBA-CGA-O2A
4	A	403	HEM	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

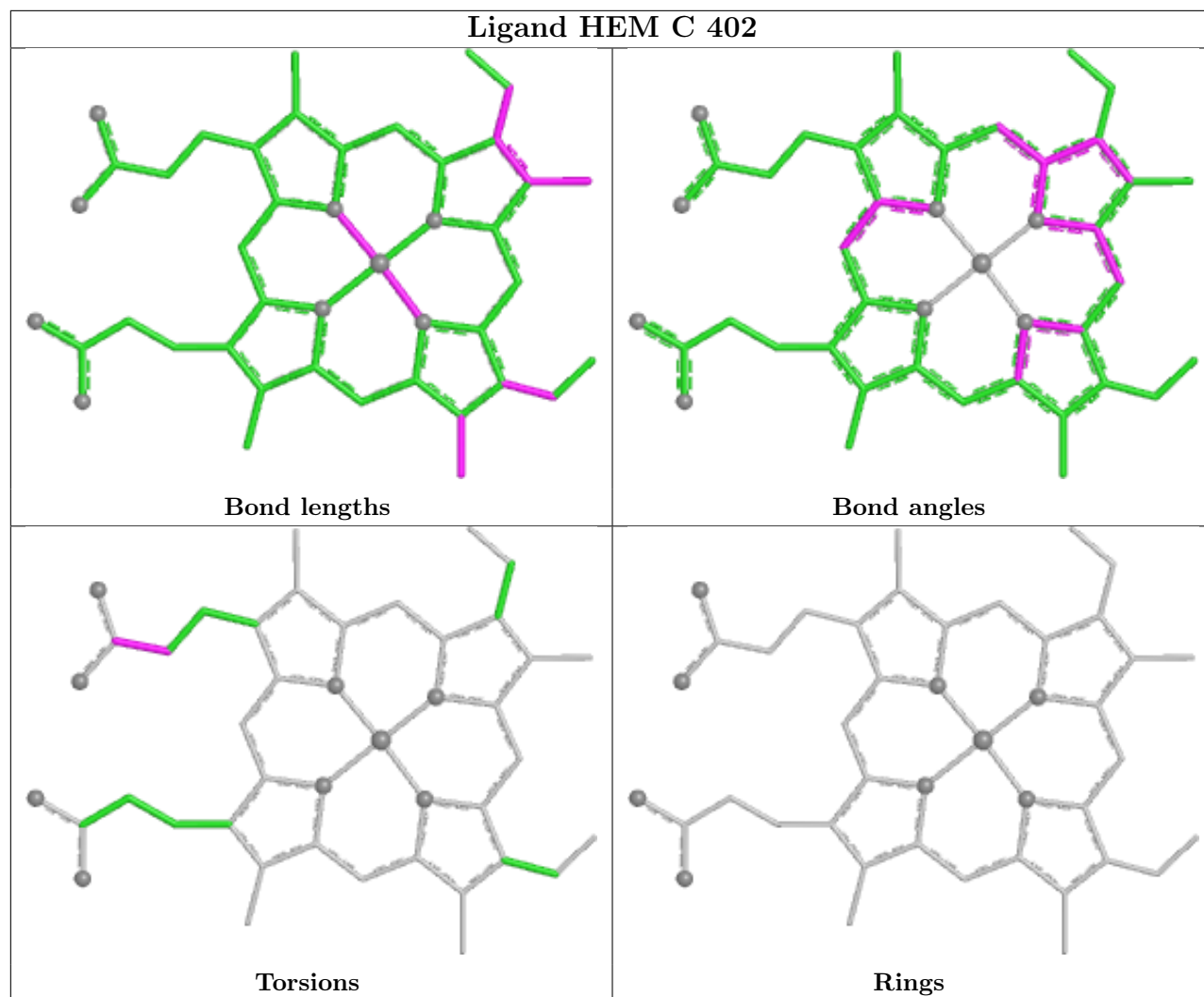
Mol	Chain	Res	Type	Atoms
4	C	402	HEM	CAD-CBD-CGD-O2D
4	C	402	HEM	CAD-CBD-CGD-O1D
4	A	403	HEM	CAD-CBD-CGD-O1D
4	B	403	HEM	CAD-CBD-CGD-O2D

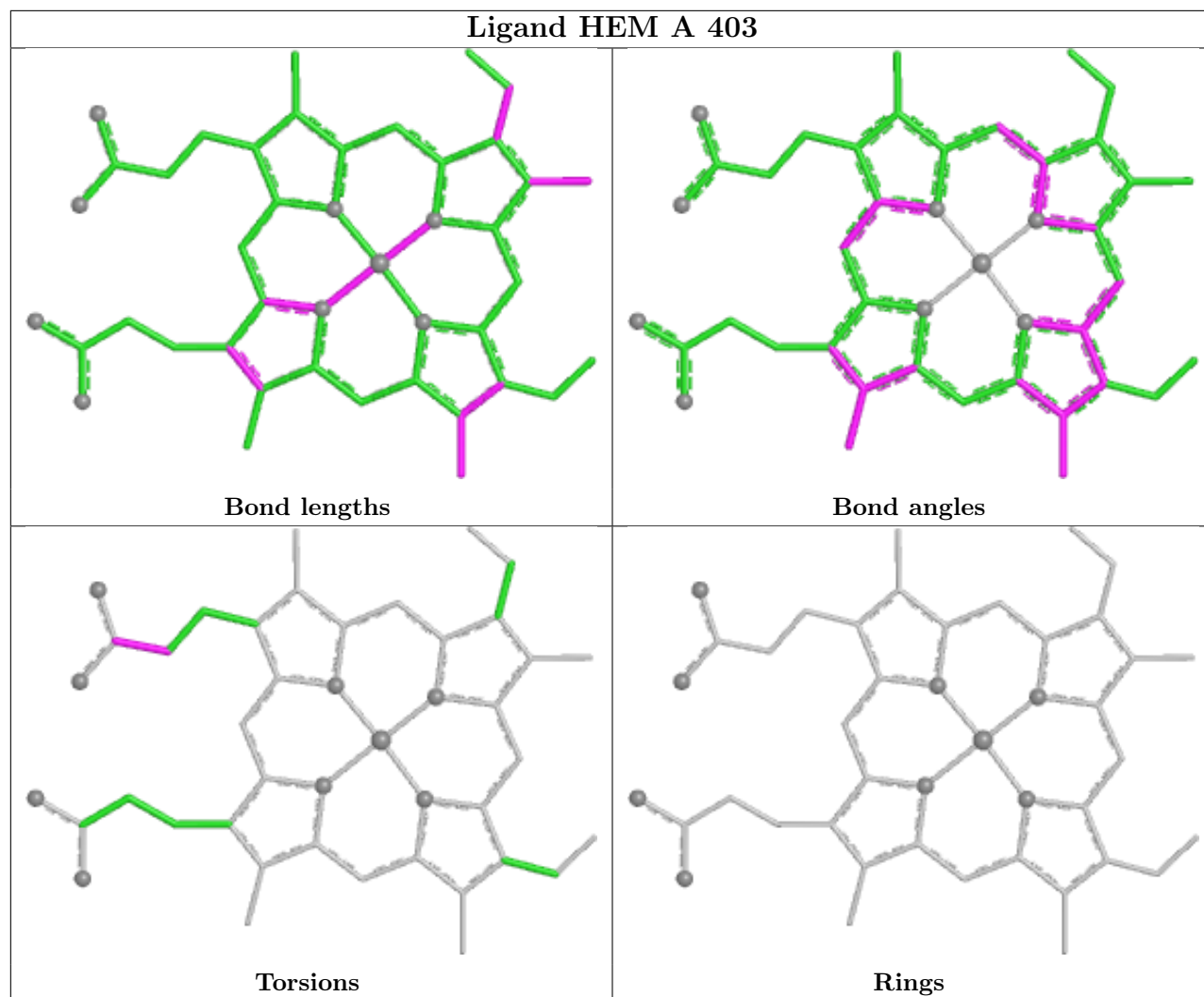
There are no ring outliers.

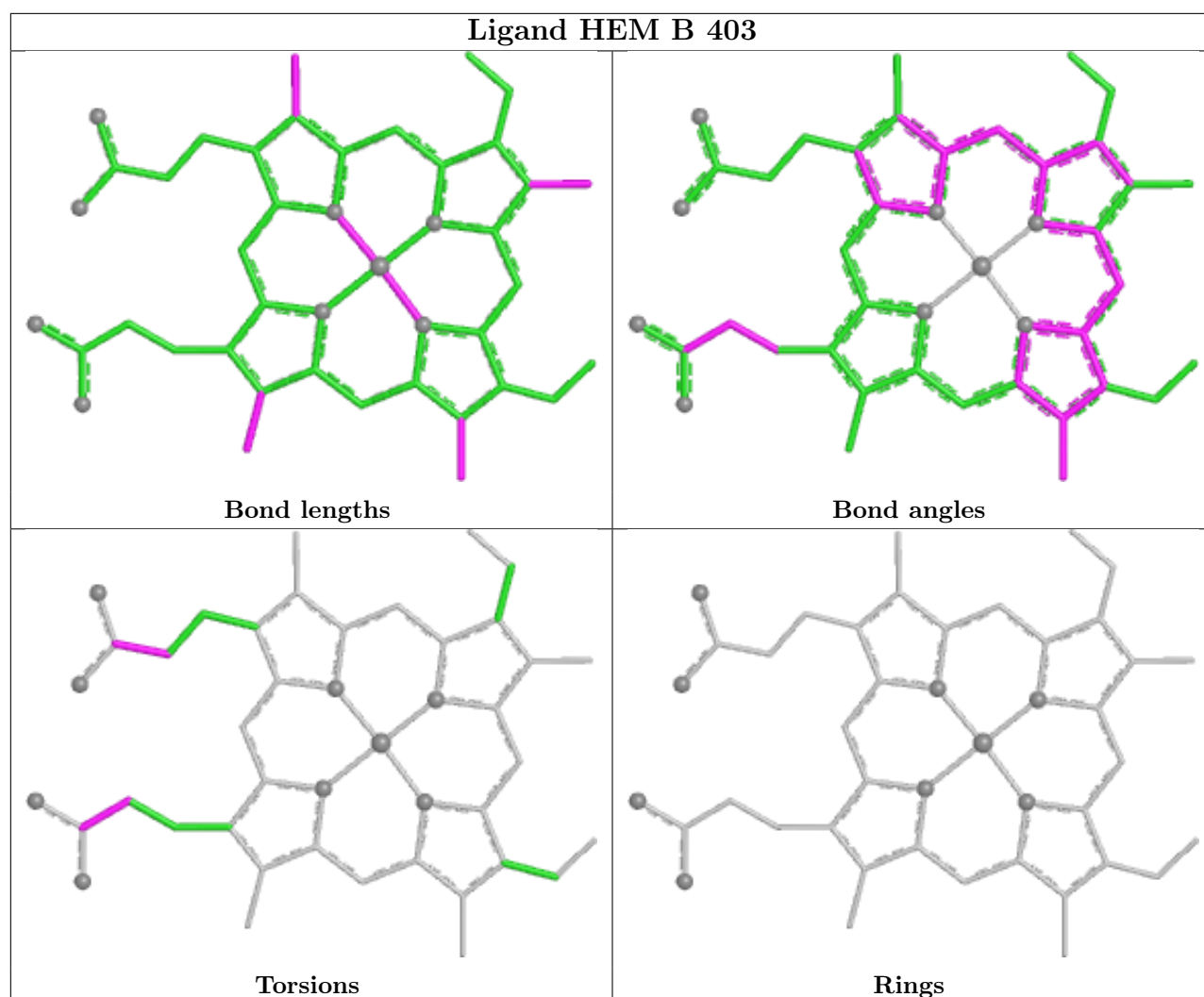
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	HEM	3	0
4	A	403	HEM	5	0
4	B	403	HEM	4	0
3	B	401	TFA	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	378/420 (90%)	0.05	14 (3%) 45 49	19, 43, 84, 154	2 (0%)
1	B	382/420 (90%)	-0.14	8 (2%) 63 67	16, 39, 69, 102	2 (0%)
1	C	382/420 (90%)	0.53	36 (9%) 14 14	21, 53, 101, 142	3 (0%)
2	E	4/5 (80%)	3.21	4 (100%) 0 0	59, 67, 69, 69	4 (100%)
All	All	1146/1265 (90%)	0.16	62 (5%) 31 34	16, 45, 88, 154	11 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	VAL	7.8
1	C	114	PHE	6.1
1	C	125	LEU	5.5
1	C	113	GLN	5.0
1	C	107	LEU	4.9
1	C	111	ARG	4.6
2	E	5	HIS	4.5
1	A	215	ALA	4.0
1	A	13	ILE	3.8
1	C	109	THR	3.7
1	A	14	TYR	3.5
1	C	108	SER	3.4
1	A	205	ARG	3.4
2	E	4	LEU	3.3
1	B	13	ILE	3.3
1	C	363	ALA	3.1
1	A	129	PRO	3.1
1	C	129	PRO	3.0
2	E	2	ARG	2.9
1	C	106	PRO	2.9
1	C	368	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	262	ALA	2.8
1	C	264	ARG	2.8
1	C	44	LEU	2.7
1	C	127	GLY	2.7
1	C	298	LEU	2.7
1	C	130	GLY	2.7
1	B	366	LEU	2.7
1	C	331	ARG	2.6
1	C	13	ILE	2.6
1	C	74	VAL	2.6
1	C	122	LEU	2.6
1	C	128	GLN	2.6
1	B	164	TRP	2.6
1	C	360	ALA	2.6
1	A	365	GLY	2.5
1	C	84[A]	GLN	2.5
1	A	12	PRO	2.4
1	C	296	ALA	2.4
1	C	361	LEU	2.4
1	B	264	ARG	2.4
1	A	130	GLY	2.3
1	A	393	ARG	2.3
1	C	393	ARG	2.3
1	B	126	SER	2.3
1	B	367	ARG	2.3
1	C	79	THR	2.3
1	A	366	LEU	2.3
1	C	12	PRO	2.2
1	C	392	VAL	2.2
1	C	365	GLY	2.2
1	C	126	SER	2.2
2	E	1	MET	2.1
1	C	88	PRO	2.1
1	B	260	GLY	2.1
1	C	220	VAL	2.1
1	B	107	LEU	2.1
1	A	296	ALA	2.1
1	C	371	ALA	2.1
1	A	60	GLY	2.0
1	A	44	LEU	2.0
1	A	43	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	YOF	E	3	13/14	0.82	0.14	52,62,69,78	21

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

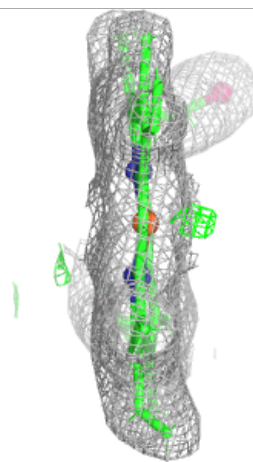
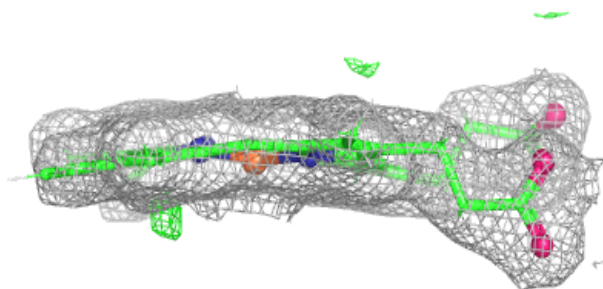
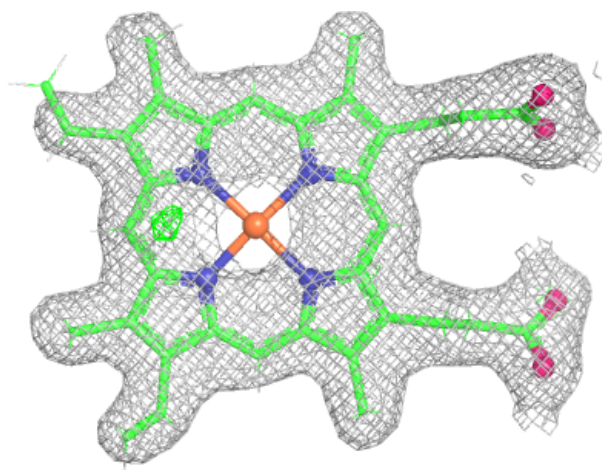
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TFA	B	401	7/7	0.81	0.18	55,56,72,72	0
3	TFA	B	402	7/7	0.84	0.15	84,87,98,115	0
3	TFA	A	402	7/7	0.85	0.12	70,75,80,85	0
3	TFA	C	401	7/7	0.88	0.14	39,47,65,69	0
3	TFA	A	401	7/7	0.90	0.17	39,48,58,62	7
5	NA	A	404	1/1	0.93	0.20	69,69,69,69	0
4	HEM	C	402	43/43	0.98	0.06	31,37,49,65	0
4	HEM	A	403	43/43	0.98	0.06	22,30,41,49	0
4	HEM	B	403	43/43	0.99	0.05	22,27,35,45	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.

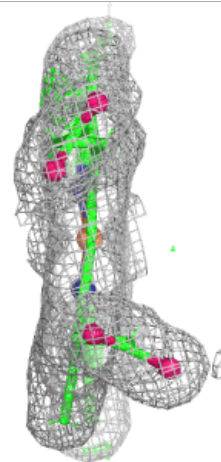
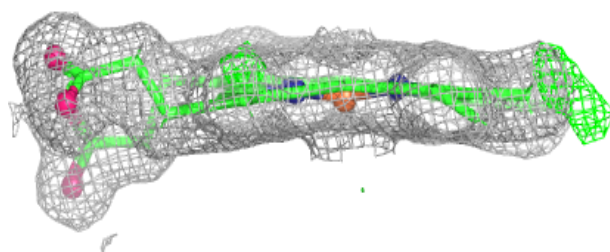
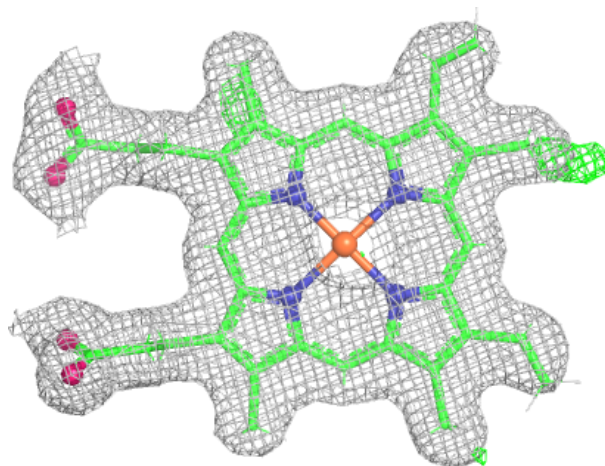
Electron density around HEM C 402:

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



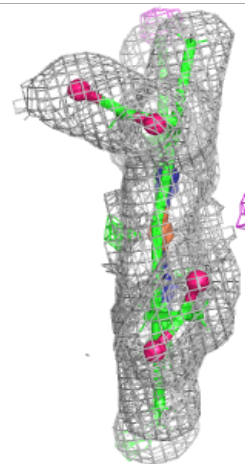
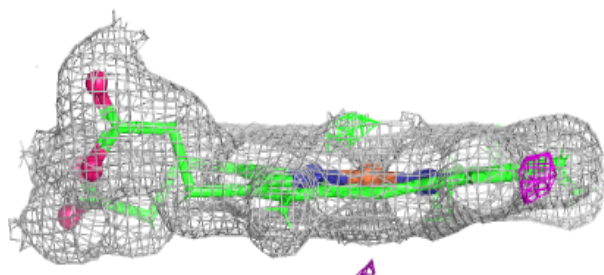
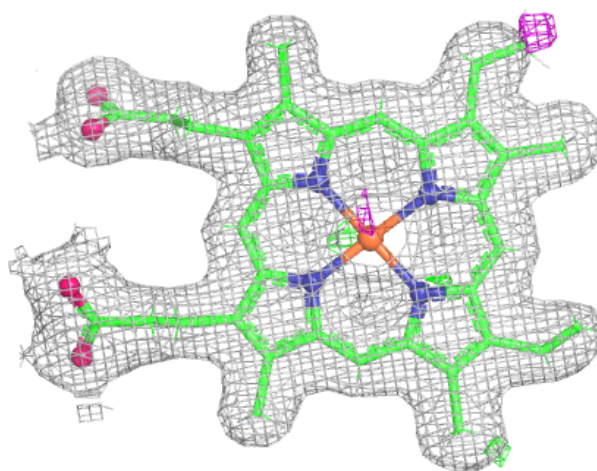
Electron density around HEM A 403:

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



Electron density around HEM B 403:

$2mF_o-DF_c$ (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.