Full wwPDB X-ray Structure Validation Report (i)

Apr 15, 2025 – 01:08 pm BST

PDB ID	:	9FON / pdb_00009fon
Title	:	Cocrystal structure of Drosophila melangaster TDO with Compound 128
Authors	:	Wicki, M.; Mac Sweeney, A.
Deposited on	:	2024-06-12
Resolution	:	2.12 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 (i) 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 (i)) were used in the production of this report:

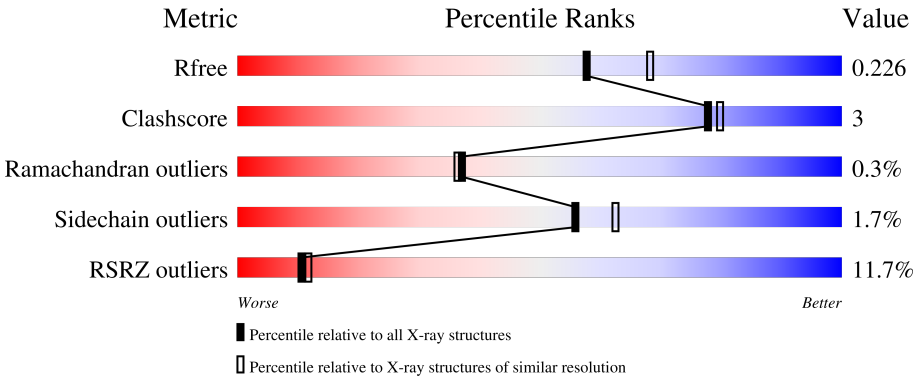
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.12 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}	164625	7689 (2.14-2.10)
Clashscore	180529	8431 (2.14-2.10)
Ramachandran outliers	177936	8366 (2.14-2.10)
Sidechain outliers	177891	8367 (2.14-2.10)
RSRZ outliers	164620	7689 (2.14-2.10)

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 <=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	365	7% 87% 6% 7%
1	B	365	15% 88% 6% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5650 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

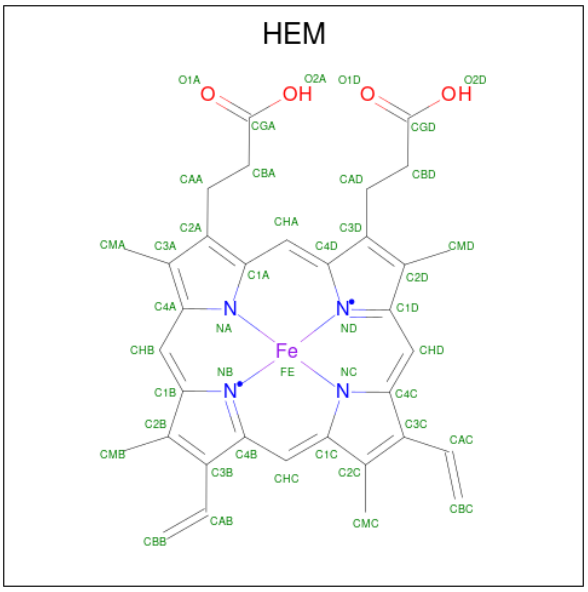
- Molecule 1 is a protein called Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	1	0
			2729	1756	461	500	12			
1	B	344	Total	C	N	O	S	0	0	0
			2681	1732	450	488	11			

There are 18 discrepancies between the modelled and reference sequences:

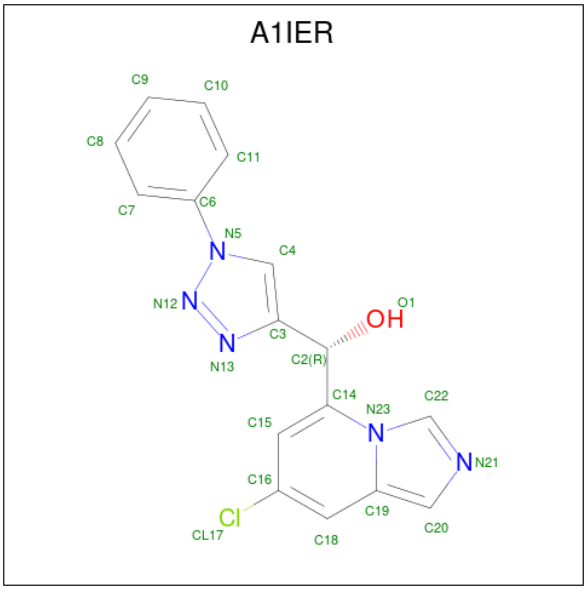
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP P20351
A	380	LEU	-	expression tag	UNP P20351
A	381	GLU	-	expression tag	UNP P20351
A	382	HIS	-	expression tag	UNP P20351
A	383	HIS	-	expression tag	UNP P20351
A	384	HIS	-	expression tag	UNP P20351
A	385	HIS	-	expression tag	UNP P20351
A	386	HIS	-	expression tag	UNP P20351
A	387	HIS	-	expression tag	UNP P20351
B	23	MET	-	initiating methionine	UNP P20351
B	380	LEU	-	expression tag	UNP P20351
B	381	GLU	-	expression tag	UNP P20351
B	382	HIS	-	expression tag	UNP P20351
B	383	HIS	-	expression tag	UNP P20351
B	384	HIS	-	expression tag	UNP P20351
B	385	HIS	-	expression tag	UNP P20351
B	386	HIS	-	expression tag	UNP P20351
B	387	HIS	-	expression tag	UNP P20351

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is ({R})-(7-chloranylimidazo[1,5-a]pyridin-5-yl)-(1-phenyl-1,2,3-triazol-4-yl)methanol (CCD ID: A1IER) (formula: $C_{16}H_{12}ClN_5O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			23	16	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			23	16	1	5	1		

- Molecule 4 is water.

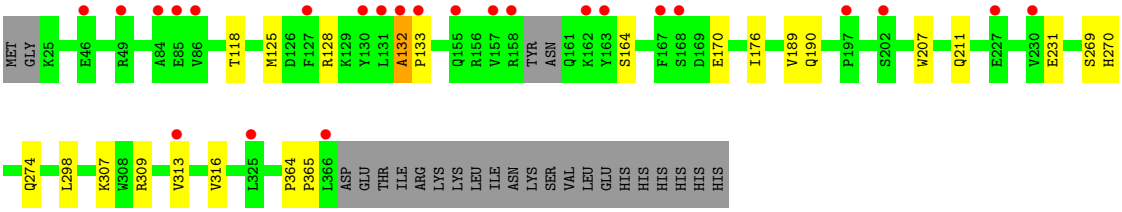
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	58	Total	O	0	0
			58	58		

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.

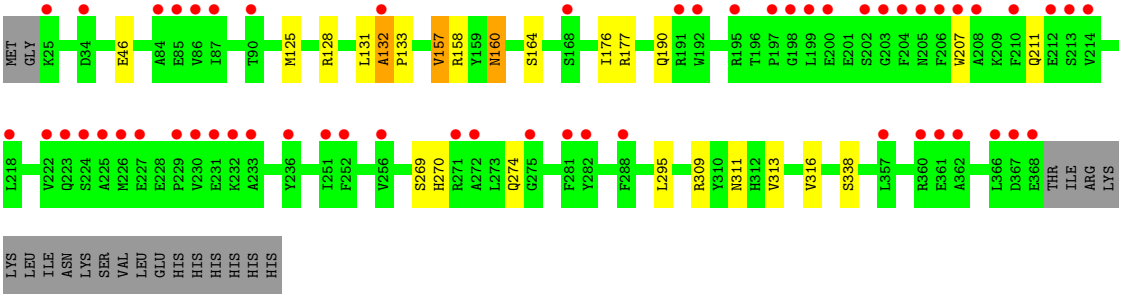
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain A:



• Molecule 1: Tryptophan 2,3-dioxygenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.54Å 119.54Å 101.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.13 – 2.12 39.13 – 2.12	Depositor EDS
% Data completeness (in resolution range)	87.9 (39.13-2.12) 87.9 (39.13-2.12)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.12Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.231 , 0.257 0.226 , 0.226	Depositor DCC
R_{free} test set	7894 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5650	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: A1IER, 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	0.39	0/2787	0.51	0/3774
1	B	0.40	0/2741	0.51	0/3724
All	All	0.40	0/5528	0.51	0/7498

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

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	2729	0	2618	15	0
1	B	2681	0	2516	15	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
3	A	23	0	0	0	0
3	B	23	0	0	0	0
4	A	50	0	0	0	0
4	B	58	0	0	0	0
All	All	5650	0	5194	29	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 (29) 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:132:ALA:HB3	1:A:133:PRO:HD3	1.67	0.77
1:B:132:ALA:HB3	1:B:133:PRO:HD3	1.69	0.75
1:A:125:MET:HA	1:A:128:ARG:HD3	1.70	0.73
1:B:125:MET:HA	1:B:128:ARG:HD3	1.74	0.70
1:A:132:ALA:HB3	1:A:133:PRO:CD	2.33	0.58
1:B:132:ALA:HB3	1:B:133:PRO:CD	2.33	0.58
1:A:132:ALA:CB	1:A:133:PRO:HD3	2.32	0.58
1:B:132:ALA:CB	1:B:133:PRO:HD3	2.34	0.57
1:B:157:VAL:HG11	1:B:338:SER:OG	2.04	0.57
1:A:309:ARG:O	1:A:313:VAL:HG23	2.05	0.56
1:B:309:ARG:O	1:B:313:VAL:HG23	2.07	0.54
1:B:164:SER:HB3	1:B:176:ILE:HG21	1.94	0.50
1:A:164:SER:HB3	1:A:176:ILE:HG21	1.94	0.49
1:A:132:ALA:CB	1:A:133:PRO:CD	2.92	0.48
1:A:307:LYS:NZ	1:B:311:ASN:HD21	2.13	0.47
1:A:207:TRP:O	1:A:211:GLN:HG3	2.16	0.46
1:A:270:HIS:O	1:A:274:GLN:HG3	2.15	0.46
1:B:207:TRP:O	1:B:211:GLN:HG3	2.16	0.46
1:A:190:GLN:HE21	1:A:269:SER:H	1.64	0.46
1:B:190:GLN:HE21	1:B:269:SER:H	1.63	0.44
1:B:158:ARG:HD3	1:B:160:ASN:O	2.18	0.44
1:B:270:HIS:O	1:B:274:GLN:HG3	2.17	0.44
1:B:132:ALA:CB	1:B:133:PRO:CD	2.93	0.43
1:B:316:VAL:HG22	2:B:401:HEM:C1B	2.54	0.42
1:A:189:VAL:HG21	1:A:298:LEU:HD11	2.01	0.42
1:A:364:PRO:HA	1:A:365:PRO:HD3	1.95	0.42
1:A:316:VAL:HG22	2:A:401:HEM:C1B	2.55	0.41
1:B:190:GLN:NE2	1:B:269:SER:H	2.19	0.40
1:A:316:VAL:HG22	2:A:401:HEM:CHB	2.51	0.40

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	337/365 (92%)	330 (98%)	6 (2%)	1 (0%)	37	36
1	B	342/365 (94%)	334 (98%)	7 (2%)	1 (0%)	37	36
All	All	679/730 (93%)	664 (98%)	13 (2%)	2 (0%)	37	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ALA
1	B	132	ALA

5.3.2 Protein sidechains (i)

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	280/337 (83%)	277 (99%)	3 (1%)	70	76
1	B	264/337 (78%)	258 (98%)	6 (2%)	45	50
All	All	544/674 (81%)	535 (98%)	9 (2%)	56	62

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	THR
1	A	170	GLU
1	A	231	GLU
1	B	46	GLU
1	B	131	LEU
1	B	157	VAL
1	B	160	ASN
1	B	177	ARG
1	B	295	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	205	ASN
1	A	292	HIS
1	A	311	ASN
1	B	112	GLN
1	B	190	GLN
1	B	292	HIS
1	B	311	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	B	401	1,3	41,50,50	0.92	2 (4%)	45,82,82	1.13	4 (8%)
3	A1IER	A	402	2	20,26,26	1.11	2 (10%)	20,37,37	1.04	1 (5%)
2	HEM	A	401	1,3	41,50,50	0.92	2 (4%)	45,82,82	1.15	4 (8%)
3	A1IER	B	402	2	20,26,26	1.41	3 (15%)	20,37,37	1.05	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	401	1,3	-	3/12/54/54	-
3	A1IER	A	402	2	-	2/8/12/12	0/4/4/4
2	HEM	A	401	1,3	-	2/12/54/54	-
3	A1IER	B	402	2	-	2/8/12/12	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	A1IER	C18-C19	3.84	1.43	1.40
2	A	401	HEM	CHB-C1B	2.92	1.42	1.35
2	B	401	HEM	CHB-C1B	2.70	1.41	1.35
3	B	402	A1IER	C3-N13	2.54	1.37	1.34
3	B	402	A1IER	C15-C14	-2.25	1.36	1.38
3	A	402	A1IER	C3-N13	2.20	1.37	1.34
2	B	401	HEM	C1B-NB	-2.14	1.36	1.40
2	A	401	HEM	C1B-NB	-2.12	1.36	1.40
3	A	402	A1IER	C15-C16	2.06	1.41	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	HEM	C4C-CHD-C1D	3.71	127.46	122.56
2	B	401	HEM	C4C-CHD-C1D	3.53	127.21	122.56
2	B	401	HEM	C4B-CHC-C1C	3.43	127.08	122.56
2	A	401	HEM	C4B-CHC-C1C	3.13	126.69	122.56
3	A	402	A1IER	C16-C15-C14	2.58	121.21	118.18
2	A	401	HEM	CMC-C2C-C3C	2.57	129.48	124.68
3	B	402	A1IER	C16-C15-C14	2.44	121.05	118.18
2	B	401	HEM	CMC-C2C-C3C	2.41	129.19	124.68
2	B	401	HEM	CMA-C3A-C4A	-2.13	125.19	128.46
2	A	401	HEM	CMA-C3A-C4A	-2.12	125.21	128.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1IER	C15-C14-C2-O1

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Mol	Chain	Res	Type	Atoms
3	B	402	A1IER	C15-C14-C2-O1
2	B	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAD-CBD-CGD-O2D
3	A	402	A1IER	N23-C14-C2-O1
3	B	402	A1IER	N23-C14-C2-O1

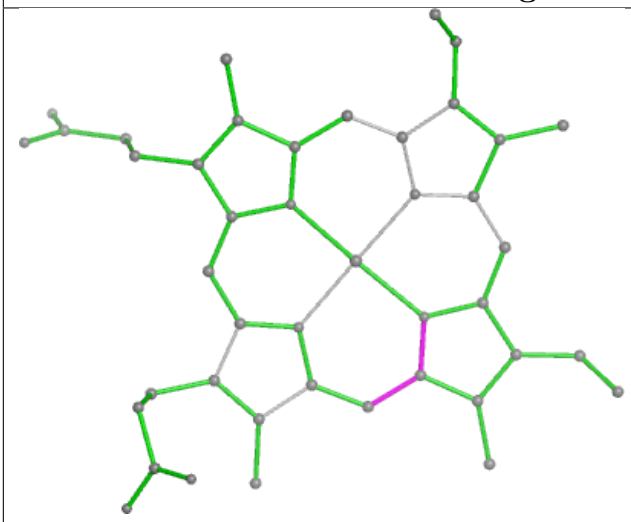
There are no ring outliers.

2 monomers are involved in 3 short contacts:

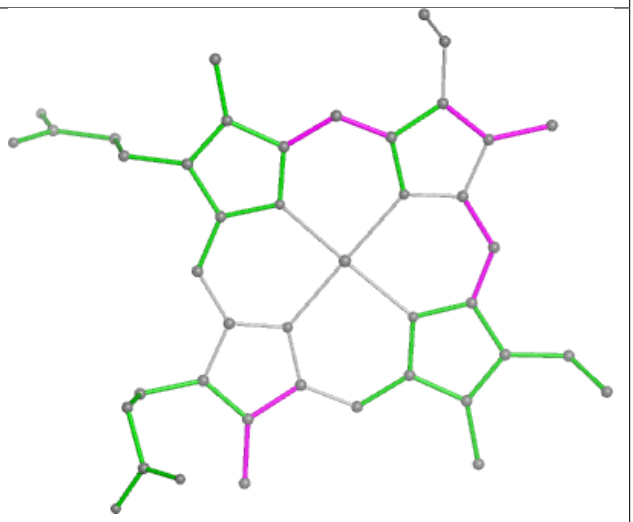
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HEM	1	0
2	A	401	HEM	2	0

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 then 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.

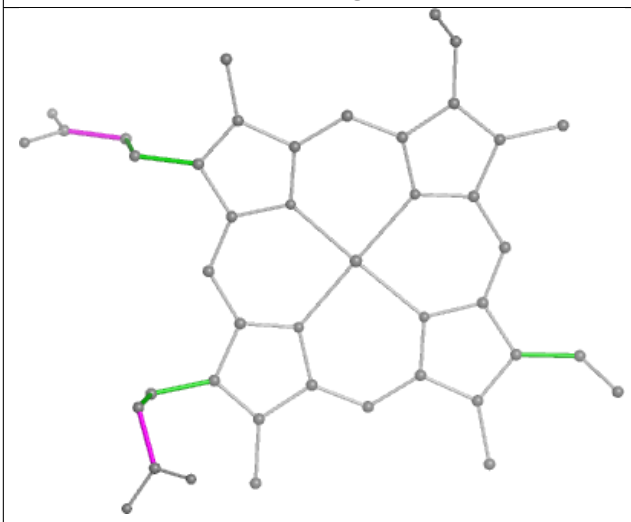
Ligand HEM B 401



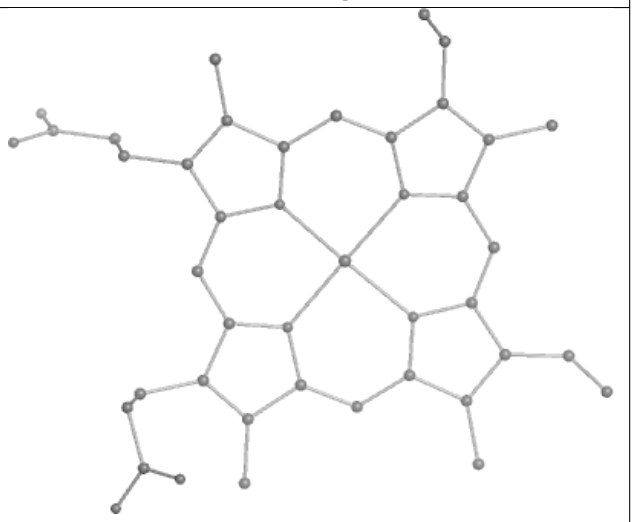
Bond lengths



Bond angles

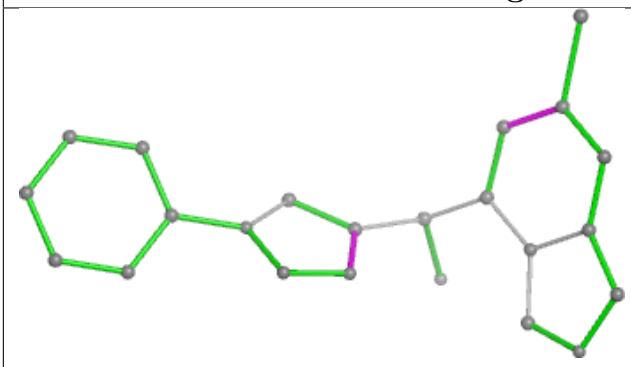


Torsions

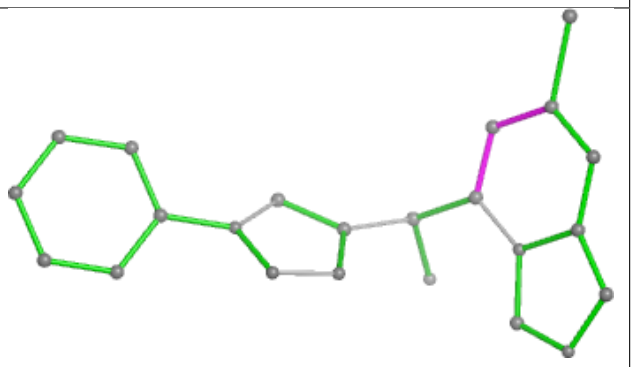


Rings

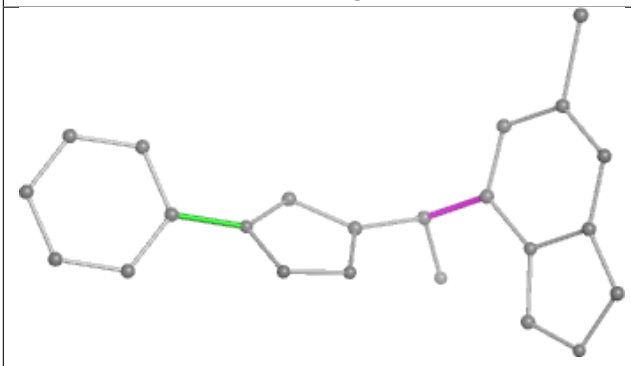
Ligand A1IER A 402



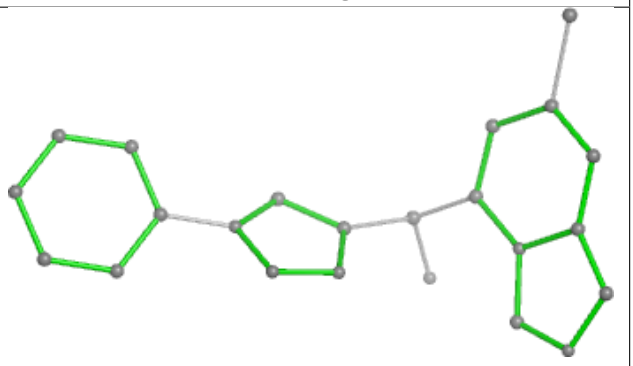
Bond lengths



Bond angles

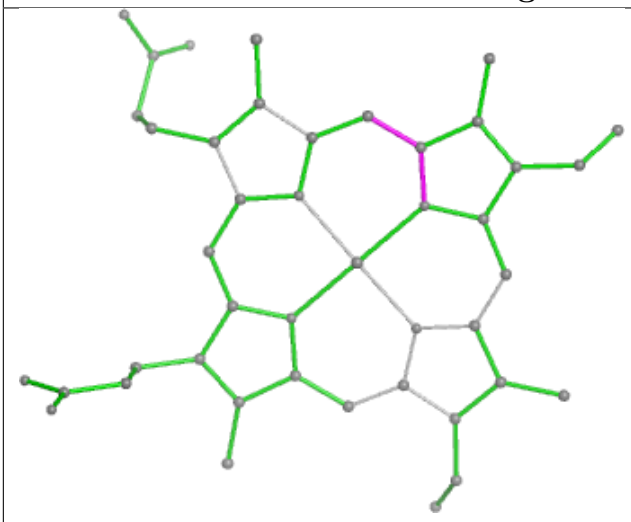


Torsions

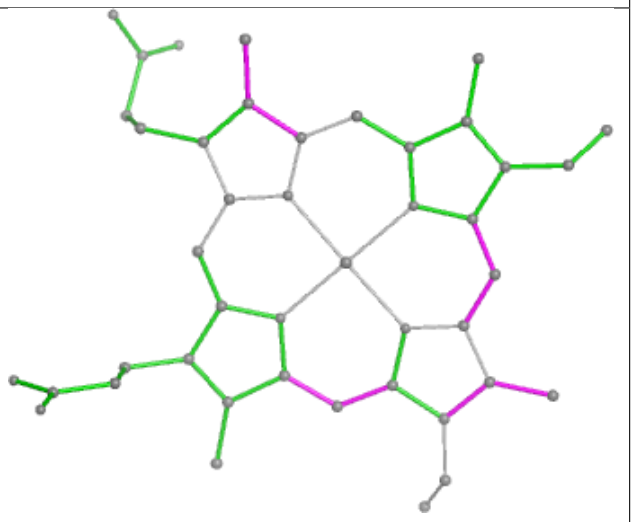


Rings

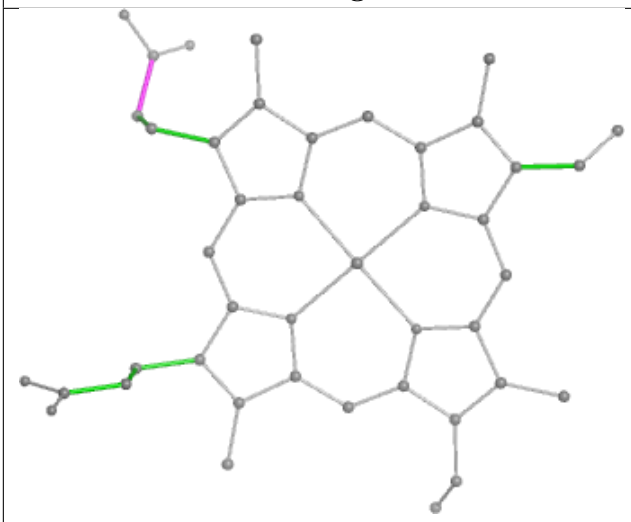
Ligand HEM A 401



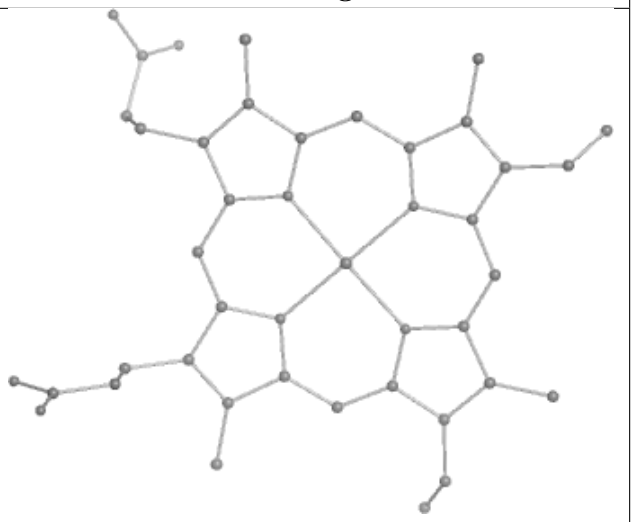
Bond lengths



Bond angles

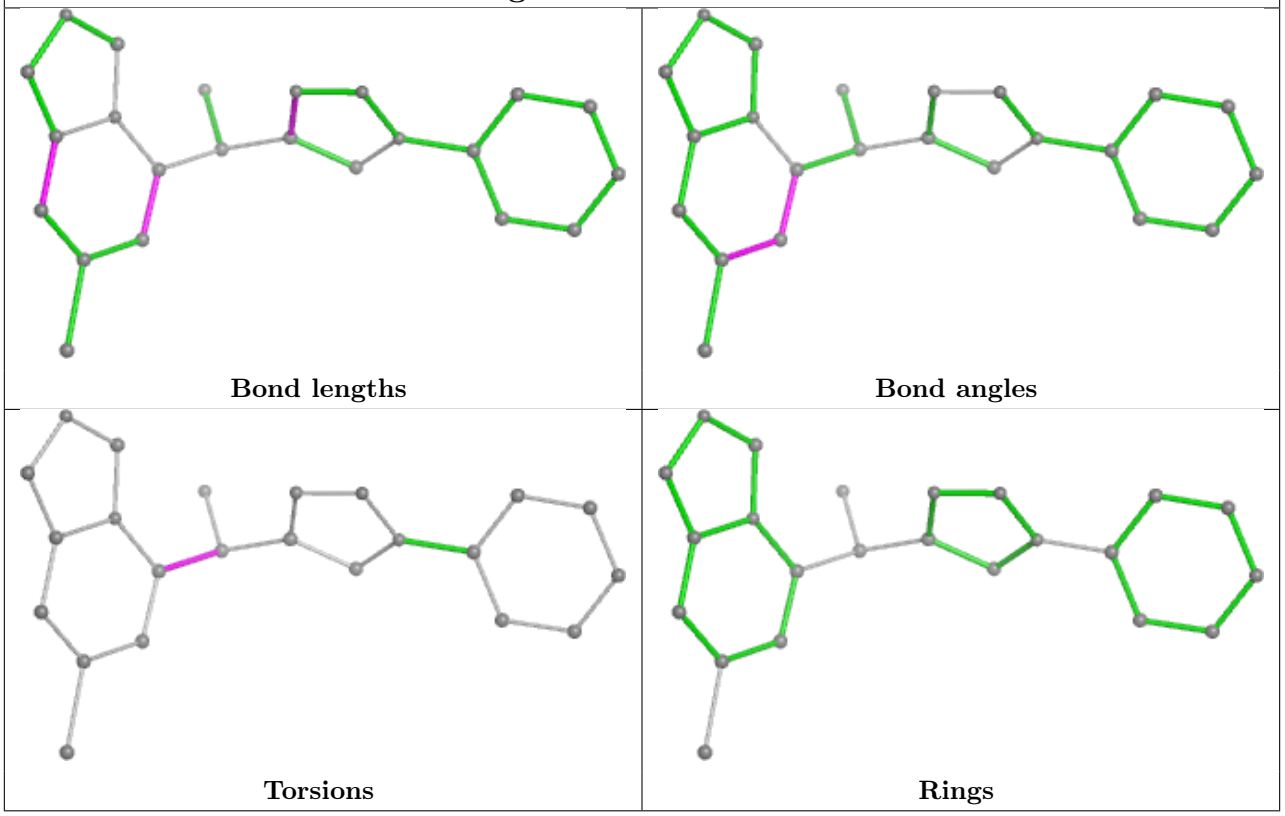


Torsions



Rings

Ligand A1IER B 402



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, 95^{th} 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	340/365 (93%)	0.41	24 (7%) 23 26	16, 44, 67, 76	1 (0%)
1	B	344/365 (94%)	0.85	56 (16%) 5 6	23, 49, 81, 96	0
All	All	684/730 (93%)	0.64	80 (11%) 10 12	16, 46, 75, 96	1 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	GLU	4.6
1	B	199	LEU	4.5
1	B	86	VAL	4.0
1	B	132	ALA	4.0
1	B	87	ILE	4.0
1	A	157	VAL	3.9
1	B	222	VAL	3.8
1	B	203	GLY	3.7
1	B	226	MET	3.7
1	B	206	PHE	3.5
1	B	202	SER	3.4
1	B	252	PHE	3.2
1	B	205	ASN	3.2
1	A	197	PRO	3.2
1	B	361	GLU	3.2
1	B	232	LYS	3.1
1	B	197	PRO	3.1
1	B	207	TRP	3.1
1	A	366	LEU	3.0
1	B	225	ALA	3.0
1	A	85	GLU	3.0
1	B	256	VAL	2.8
1	A	49	ARG	2.8
1	B	191	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	366	LEU	2.8
1	B	227	GLU	2.8
1	A	132	ALA	2.7
1	B	233	ALA	2.7
1	B	204	PHE	2.7
1	A	168	SER	2.7
1	B	230	VAL	2.7
1	B	210	PHE	2.7
1	A	167	PHE	2.6
1	A	158	ARG	2.6
1	B	25	LYS	2.5
1	A	86	VAL	2.5
1	B	281	PHE	2.5
1	B	224	SER	2.5
1	B	272	ALA	2.5
1	B	200	GLU	2.5
1	A	133	PRO	2.4
1	B	192	TRP	2.4
1	B	85	GLU	2.4
1	B	282	TYR	2.4
1	B	168	SER	2.4
1	A	202	SER	2.4
1	B	288	PHE	2.3
1	B	236	TYR	2.3
1	B	360	ARG	2.3
1	B	229	PRO	2.3
1	B	90	THR	2.3
1	B	214	VAL	2.3
1	B	198	GLY	2.3
1	B	212	GLU	2.2
1	A	130	TYR	2.2
1	B	367	ASP	2.2
1	B	195	ARG	2.2
1	B	231	GLU	2.2
1	A	84	ALA	2.2
1	A	162	LYS	2.2
1	B	213	SER	2.1
1	A	155	GLN	2.1
1	A	131	LEU	2.1
1	A	325	LEU	2.1
1	B	218	LEU	2.1
1	B	357	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	223	GLN	2.1
1	A	46	GLU	2.1
1	B	271	ARG	2.1
1	A	127	PHE	2.1
1	B	34	ASP	2.1
1	B	84	ALA	2.1
1	B	275	GLY	2.1
1	A	227	GLU	2.1
1	A	163	TYR	2.0
1	A	230	VAL	2.0
1	B	251	ILE	2.0
1	B	208	ALA	2.0
1	B	362	ALA	2.0
1	A	313	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

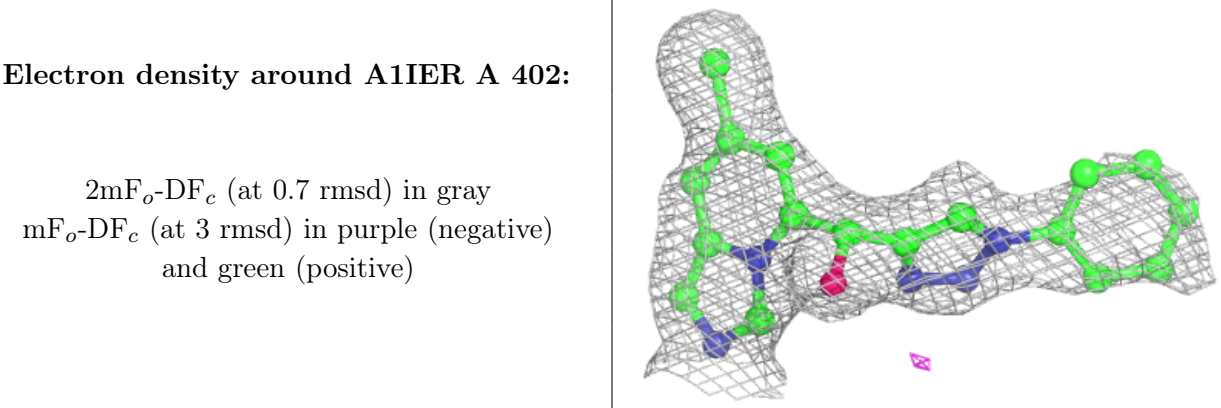
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	A1IER	A	402	23/23	0.89	0.12	55,58,64,64	0
3	A1IER	B	402	23/23	0.95	0.08	32,34,36,36	0
2	HEM	A	401	43/43	0.96	0.09	41,43,51,54	0
2	HEM	B	401	43/43	0.98	0.06	28,30,35,38	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.

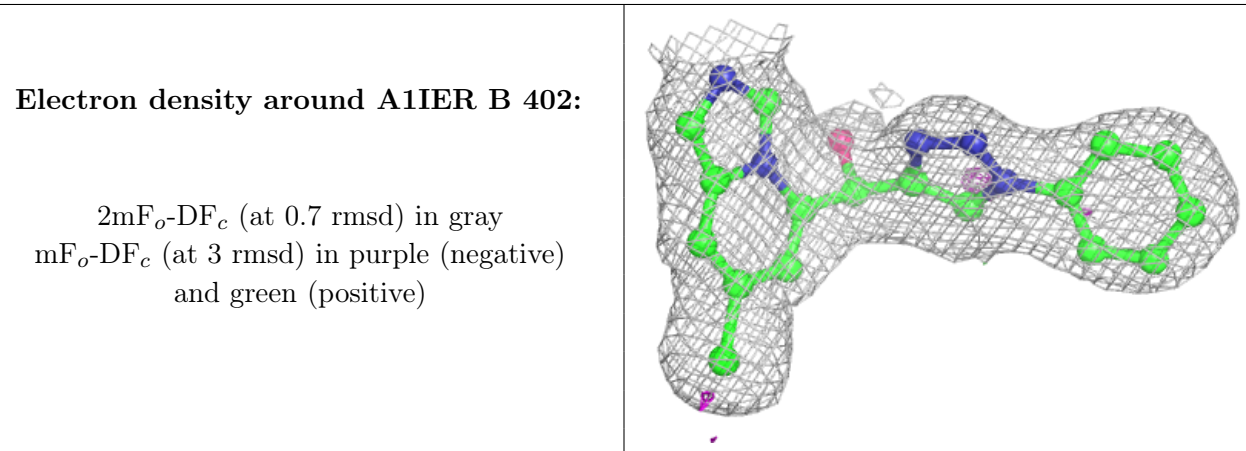
Electron density around A1IER A 402:

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



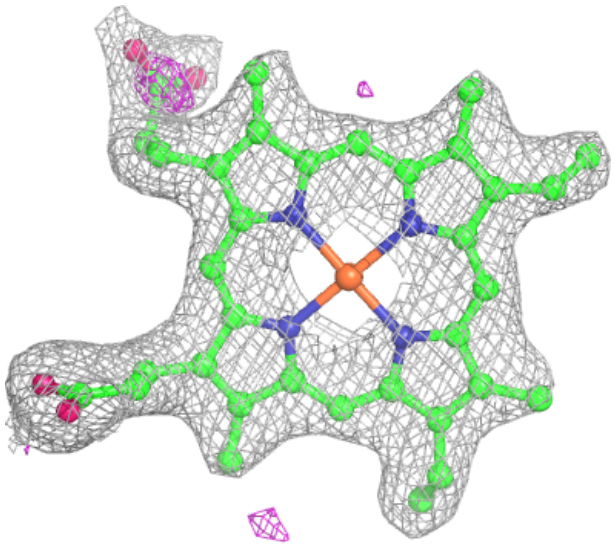
Electron density around A1IER B 402:

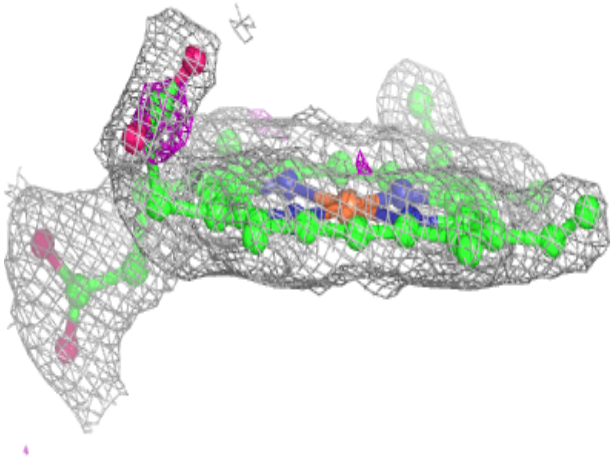
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

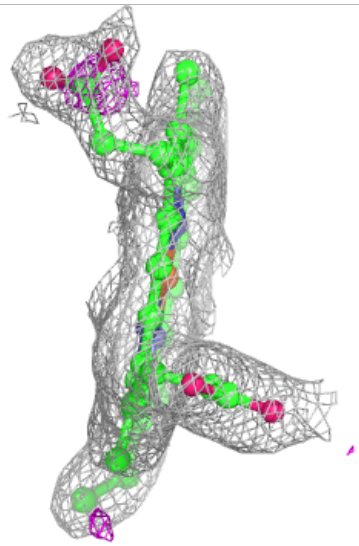


Electron density around HEM A 401:

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

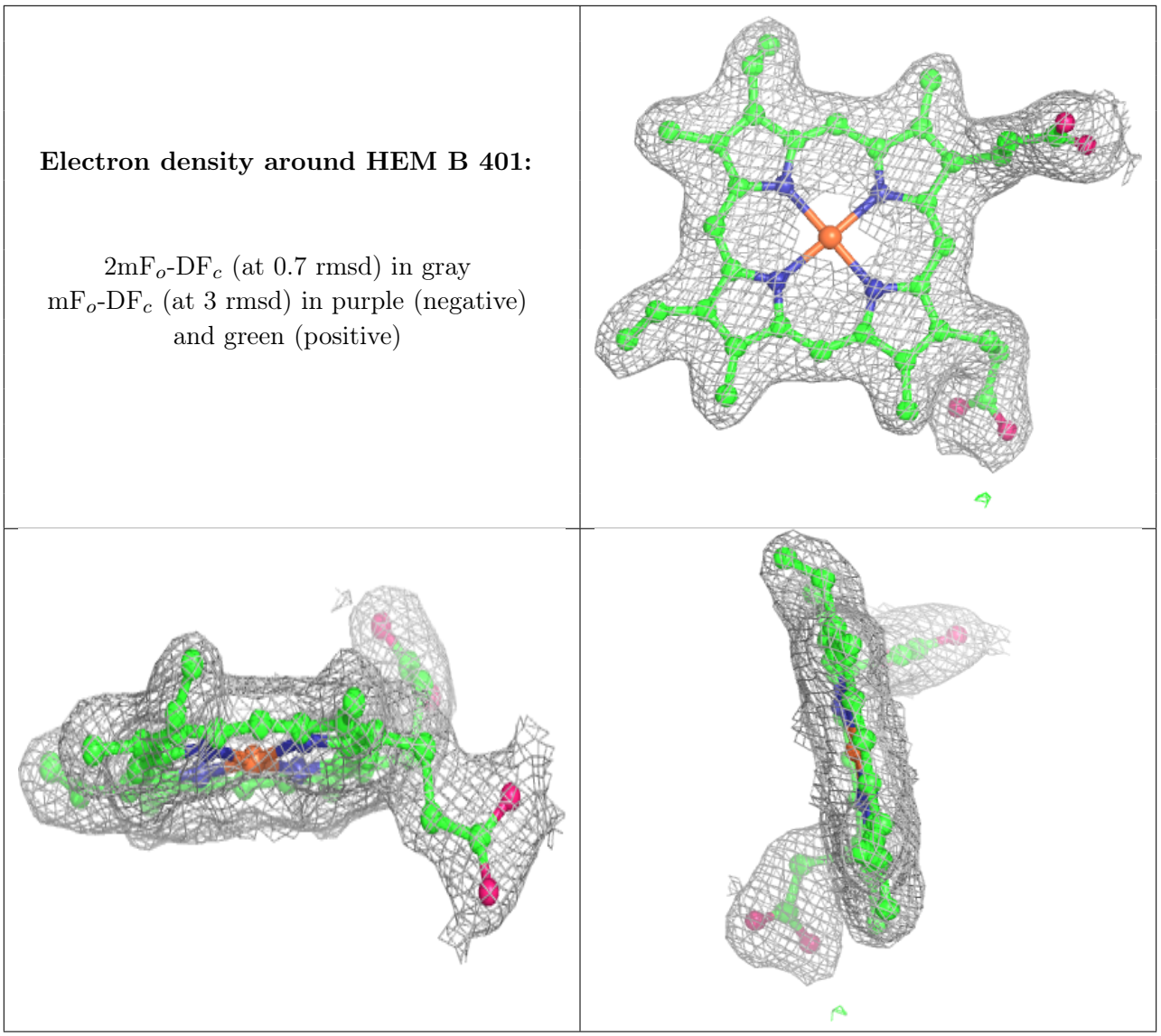






Electron density around HEM B 401:

$2mF_o$-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.