Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2023 – 08:04 AM EDT

PDB ID	:	8FBC
Title	:	Crystal structure of P450T2
Authors	:	Pereira, J.H.; Huang, J.; Keasling, J.; Adams, P.D.
Deposited on	:	2022-11-29
Resolution	:	1.53 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:

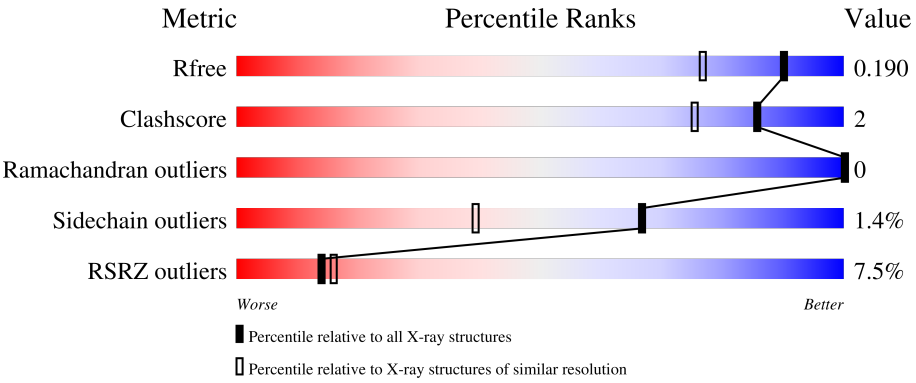
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 1.53 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}	130704	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	395	5% 92% 7% ••
1	B	395	10% 93% 5% ••

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13447 atoms, of which 6138 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	393	Total	C	H	N	O	S	0	0	0
			6146	1959	3046	549	573	19			
1	B	391	Total	C	H	N	O	S	0	0	0
			6120	1951	3032	547	571	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASP	ALA	conflict	UNP A0A3C0KFZ6
A	18	ASP	GLY	conflict	UNP A0A3C0KFZ6
A	22	SER	ALA	conflict	UNP A0A3C0KFZ6
A	47	SER	ALA	conflict	UNP A0A3C0KFZ6
A	103	MET	LEU	conflict	UNP A0A3C0KFZ6
A	111	ASP	THR	conflict	UNP A0A3C0KFZ6
A	114	LYS	ARG	conflict	UNP A0A3C0KFZ6
A	115	GLN	ASP	conflict	UNP A0A3C0KFZ6
A	120	VAL	LEU	conflict	UNP A0A3C0KFZ6
A	121	LYS	ARG	conflict	UNP A0A3C0KFZ6
A	124	LYS	GLY	conflict	UNP A0A3C0KFZ6
A	201	SER	GLU	conflict	UNP A0A3C0KFZ6
A	209	ASN	HIS	conflict	UNP A0A3C0KFZ6
A	222	ASP	GLU	conflict	UNP A0A3C0KFZ6
A	247	PHE	MET	conflict	UNP A0A3C0KFZ6
A	266	ALA	SER	conflict	UNP A0A3C0KFZ6
A	325	VAL	ALA	conflict	UNP A0A3C0KFZ6
A	329	ALA	THR	conflict	UNP A0A3C0KFZ6
A	393	LYS	ARG	conflict	UNP A0A3C0KFZ6
A	394	ALA	VAL	conflict	UNP A0A3C0KFZ6
B	16	ASP	ALA	conflict	UNP A0A3C0KFZ6
B	18	ASP	GLY	conflict	UNP A0A3C0KFZ6
B	22	SER	ALA	conflict	UNP A0A3C0KFZ6
B	47	SER	ALA	conflict	UNP A0A3C0KFZ6
B	103	MET	LEU	conflict	UNP A0A3C0KFZ6

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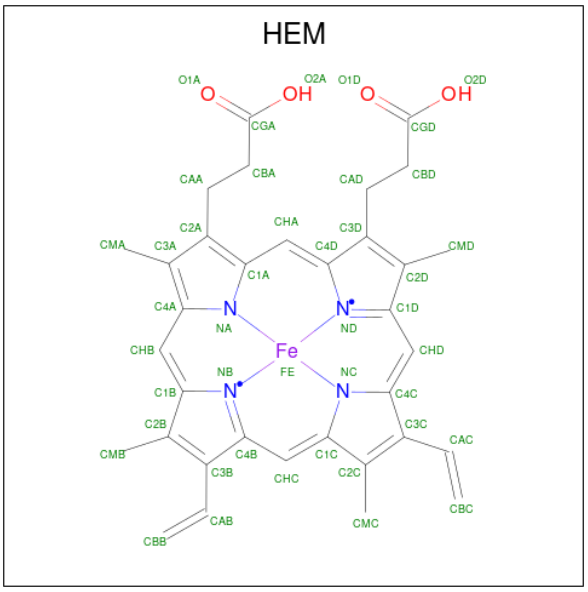
Chain	Residue	Modelled	Actual	Comment	Reference
B	111	ASP	THR	conflict	UNP A0A3C0KFZ6
B	114	LYS	ARG	conflict	UNP A0A3C0KFZ6
B	115	GLN	ASP	conflict	UNP A0A3C0KFZ6
B	120	VAL	LEU	conflict	UNP A0A3C0KFZ6
B	121	LYS	ARG	conflict	UNP A0A3C0KFZ6
B	124	LYS	GLY	conflict	UNP A0A3C0KFZ6
B	201	SER	GLU	conflict	UNP A0A3C0KFZ6
B	209	ASN	HIS	conflict	UNP A0A3C0KFZ6
B	222	ASP	GLU	conflict	UNP A0A3C0KFZ6
B	247	PHE	MET	conflict	UNP A0A3C0KFZ6
B	266	ALA	SER	conflict	UNP A0A3C0KFZ6
B	325	VAL	ALA	conflict	UNP A0A3C0KFZ6
B	329	ALA	THR	conflict	UNP A0A3C0KFZ6
B	393	LYS	ARG	conflict	UNP A0A3C0KFZ6
B	394	ALA	VAL	conflict	UNP A0A3C0KFZ6

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is water.

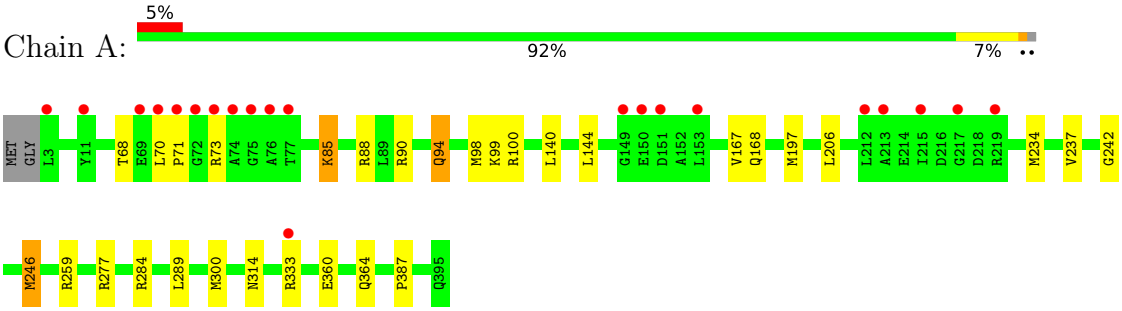
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	559	Total O 559 559	0	0
3	B	476	Total O 476 476	0	0

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.

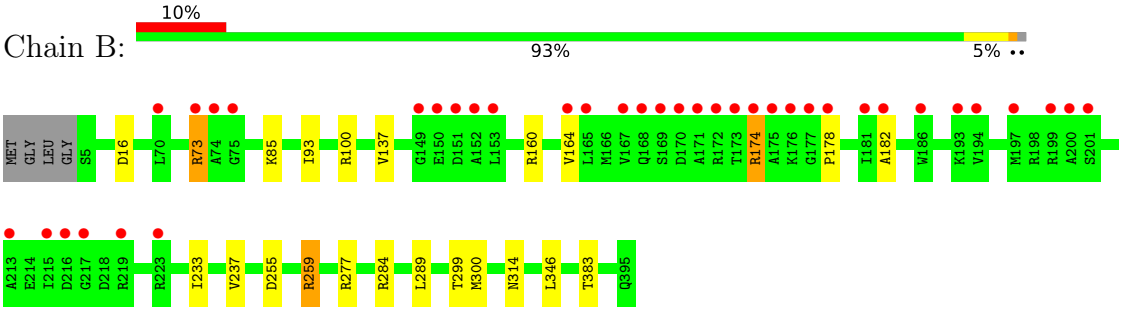
• Molecule 1: Cytochrome P450

Chain A:



• Molecule 1: Cytochrome P450

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.93Å 95.61Å 100.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.80 – 1.53 47.80 – 1.53	Depositor EDS
% Data completeness (in resolution range)	95.4 (47.80-1.53) 95.4 (47.80-1.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 1.53Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.164 , 0.191 0.163 , 0.190	Depositor DCC
R_{free} test set	1919 reflections (1.61%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13447	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3992e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 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	0.36	0/3172	0.63	1/4292 (0.0%)
1	B	0.32	0/3160	0.59	0/4276
All	All	0.34	0/6332	0.61	1/8568 (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	3
1	B	0	3
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	246	MET	CA-CB-CG	-6.66	101.97	113.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	THR	Peptide
1	A	73	ARG	Sidechain
1	A	88	ARG	Sidechain
1	B	174	ARG	Sidechain
1	B	259	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	73	ARG	Sidechain

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	3100	3046	3044	13	0
1	B	3088	3032	3030	14	0
2	A	43	30	30	0	0
2	B	43	30	30	0	0
3	A	559	0	0	2	0
3	B	476	0	0	2	0
All	All	7309	6138	6134	27	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 2.

All (27) 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:B:160:ARG:O	1:B:164:VAL:HG12	2.00	0.62
1:B:16:ASP:OD1	1:B:174:ARG:NH2	2.40	0.55
1:A:168:GLN:NE2	3:A:505:HOH:O	2.38	0.55
1:A:90:ARG:O	1:A:94:GLN:HG3	2.07	0.54
1:B:259:ARG:HH11	1:B:259:ARG:HG3	1.75	0.51
1:B:284:ARG:NH2	3:B:507:HOH:O	2.44	0.51
1:A:284:ARG:NH2	3:A:509:HOH:O	2.44	0.50
1:B:299:THR:HG23	1:B:299:THR:O	2.12	0.48
1:A:167:VAL:HG12	1:A:234:MET:SD	2.52	0.48
1:A:360:GLU:O	1:A:364:GLN:HG3	2.14	0.48
1:A:277:ARG:O	1:A:314:ASN:HB3	2.15	0.47
1:B:255:ASP:O	1:B:259:ARG:HG2	2.15	0.47
1:A:140:LEU:HD13	1:A:237:VAL:HG23	1.97	0.47
1:B:289:LEU:CD1	1:B:300:MET:HB3	2.45	0.47
1:B:277:ARG:O	1:B:314:ASN:HB3	2.16	0.44
1:A:85:LYS:HE2	1:A:85:LYS:HB2	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HA	1:A:71:PRO:HD3	1.89	0.43
1:A:289:LEU:CD1	1:A:300:MET:HB3	2.49	0.43
1:B:178:PRO:O	1:B:182:ALA:HB2	2.17	0.43
1:B:137:VAL:HG11	1:B:160:ARG:HA	2.01	0.43
1:A:144:LEU:HA	1:A:206:LEU:HB2	2.01	0.42
1:B:233:ILE:O	1:B:237:VAL:HG23	2.20	0.42
1:B:284:ARG:O	1:B:383:THR:HG23	2.20	0.42
1:A:98:MET:HE2	1:A:99:LYS:HD2	2.03	0.40
1:B:85:LYS:HG3	3:B:727:HOH:O	2.20	0.40
1:A:242:GLY:O	1:A:246:MET:HG2	2.22	0.40
1:B:93:ILE:HG21	1:B:346:LEU:HD21	2.03	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	391/395 (99%)	384 (98%)	7 (2%)	0	100	100
1	B	389/395 (98%)	376 (97%)	13 (3%)	0	100	100
All	All	780/790 (99%)	760 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	326/327 (100%)	319 (98%)	7 (2%)	53 22
1	B	325/327 (99%)	323 (99%)	2 (1%)	86 72
All	All	651/654 (100%)	642 (99%)	9 (1%)	67 39

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

Mol	Chain	Res	Type
1	A	85	LYS
1	A	94	GLN
1	A	100	ARG
1	A	197	MET
1	A	259	ARG
1	A	333	ARG
1	A	387	PRO
1	B	73	ARG
1	B	100	ARG

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

Mol	Chain	Res	Type
1	A	168	GLN
1	A	188	GLN
1	B	94	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	A	400	1,3	41,50,50	1.44	4 (9%)	45,82,82	1.60	10 (22%)
2	HEM	B	400	1,3	41,50,50	1.39	3 (7%)	45,82,82	1.38	6 (13%)

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	A	400	1,3	-	0/12/54/54	-
2	HEM	B	400	1,3	-	0/12/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	HEM	C3C-C2C	-4.21	1.34	1.40
2	A	400	HEM	C3C-C2C	-4.15	1.34	1.40
2	A	400	HEM	C3C-CAC	3.55	1.55	1.47
2	B	400	HEM	C3C-CAC	3.25	1.54	1.47
2	B	400	HEM	CAB-C3B	2.67	1.54	1.47
2	A	400	HEM	CAB-C3B	2.32	1.53	1.47
2	A	400	HEM	CAA-C2A	2.12	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	HEM	C1B-NB-C4B	3.39	108.58	105.07
2	A	400	HEM	C4D-ND-C1D	3.39	108.58	105.07
2	A	400	HEM	CMA-C3A-C4A	-3.12	123.66	128.46
2	B	400	HEM	CHC-C4B-NB	3.11	127.81	124.43
2	B	400	HEM	C1B-NB-C4B	3.05	108.23	105.07
2	B	400	HEM	CMA-C3A-C4A	-2.88	124.04	128.46
2	A	400	HEM	C3B-C2B-C1B	2.56	108.38	106.49
2	A	400	HEM	C4A-C3A-C2A	2.40	108.67	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	HEM	C4C-CHD-C1D	2.36	125.68	122.56
2	A	400	HEM	CMC-C2C-C3C	2.30	128.98	124.68
2	A	400	HEM	C2D-C1D-ND	-2.25	107.19	109.88
2	B	400	HEM	CHD-C1D-ND	2.21	126.84	124.43
2	B	400	HEM	CMC-C2C-C3C	2.17	128.73	124.68
2	A	400	HEM	C4B-CHC-C1C	2.06	125.27	122.56
2	A	400	HEM	C2B-C1B-NB	-2.05	107.41	109.84
2	B	400	HEM	C4C-CHD-C1D	2.03	125.23	122.56

There are no chirality outliers.

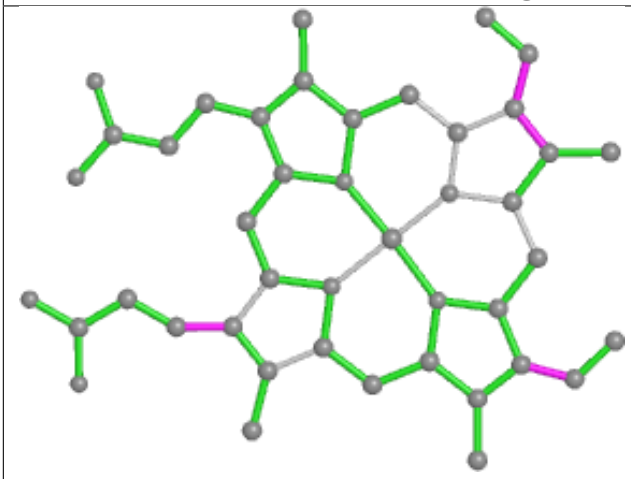
There are no torsion outliers.

There are no ring outliers.

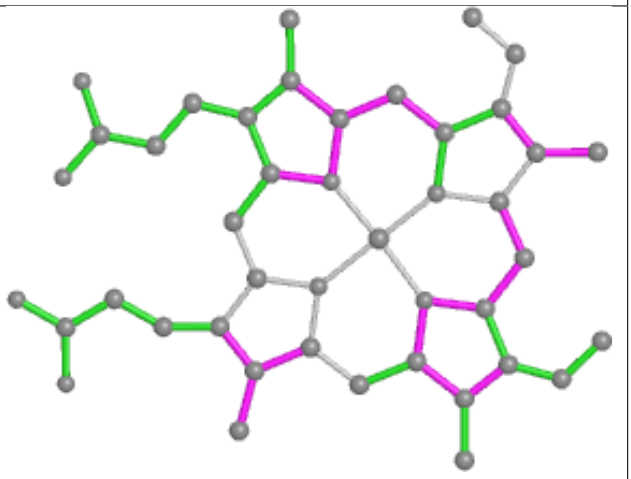
No monomer is involved in short contacts.

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.

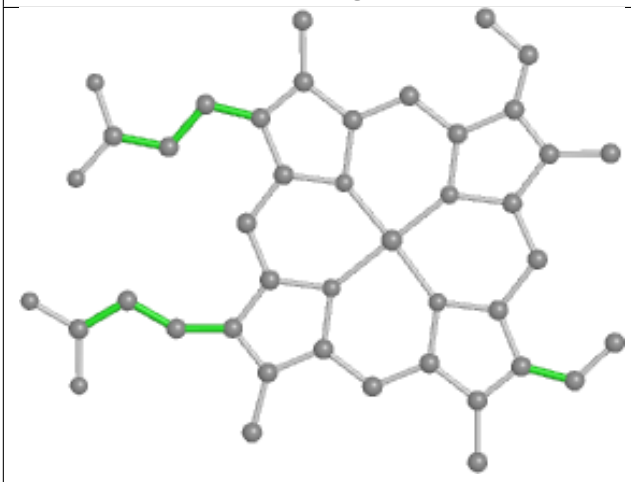
Ligand HEM A 400



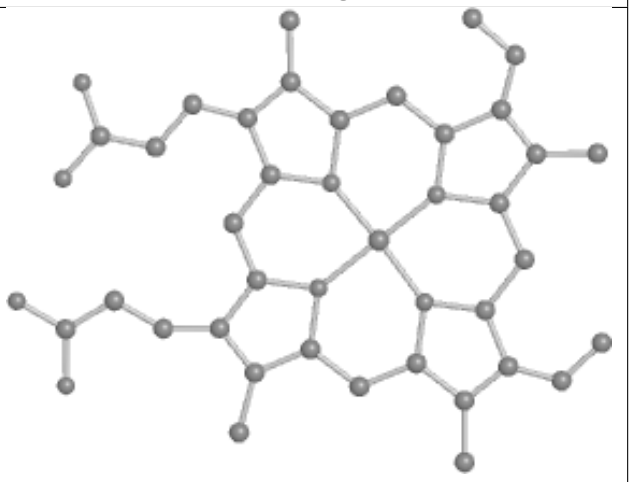
Bond lengths



Bond angles

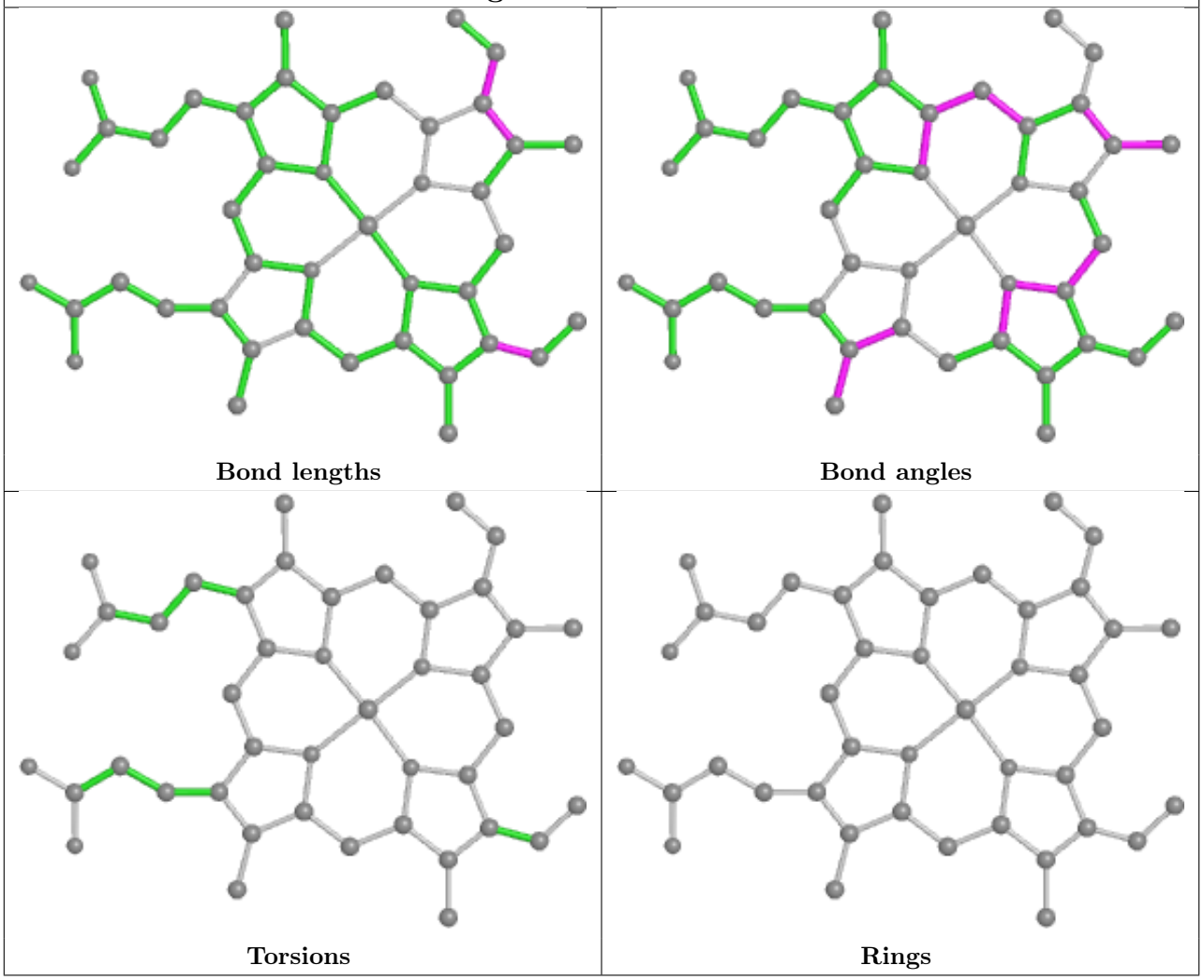


Torsions



Rings

Ligand HEM B 400



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	393/395 (99%)	-0.00	21 (5%) 26 30	11, 21, 42, 66	0
1	B	391/395 (98%)	0.15	38 (9%) 7 9	12, 23, 59, 116	0
All	All	784/790 (99%)	0.07	59 (7%) 14 16	11, 21, 52, 116	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	LEU	11.7
1	B	149	GLY	7.2
1	B	173	THR	6.9
1	B	150	GLU	6.4
1	A	72	GLY	6.3
1	B	151	ASP	6.3
1	A	3	LEU	6.0
1	A	71	PRO	5.8
1	B	200	ALA	5.8
1	A	149	GLY	5.7
1	B	171	ALA	5.7
1	B	73	ARG	5.5
1	B	174	ARG	5.5
1	A	153	LEU	5.4
1	B	172	ARG	5.3
1	B	164	VAL	5.3
1	A	74	ALA	5.2
1	B	153	LEU	4.8
1	B	170	ASP	4.7
1	B	70	LEU	4.6
1	A	151	ASP	4.5
1	B	197	MET	4.1
1	A	150	GLU	4.1
1	B	178	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	76	ALA	3.9
1	B	175	ALA	3.5
1	B	165	LEU	3.5
1	A	212	LEU	3.5
1	B	186	TRP	3.5
1	A	73	ARG	3.4
1	B	167	VAL	3.3
1	B	74	ALA	3.3
1	B	176	LYS	3.2
1	B	217	GLY	3.2
1	A	69	GLU	3.2
1	B	169	SER	3.0
1	B	194	VAL	2.9
1	A	213	ALA	2.9
1	B	215	ILE	2.8
1	B	177	GLY	2.8
1	B	216	ASP	2.7
1	A	219	ARG	2.7
1	B	201	SER	2.7
1	B	223	ARG	2.6
1	A	11	TYR	2.5
1	B	152	ALA	2.4
1	B	219	ARG	2.4
1	A	333	ARG	2.4
1	A	75	GLY	2.4
1	B	213	ALA	2.3
1	B	199	ARG	2.3
1	B	168	GLN	2.2
1	B	193	LYS	2.2
1	A	215	ILE	2.2
1	B	182	ALA	2.2
1	B	75	GLY	2.1
1	B	181	ILE	2.0
1	A	77	THR	2.0
1	A	217	GLY	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)

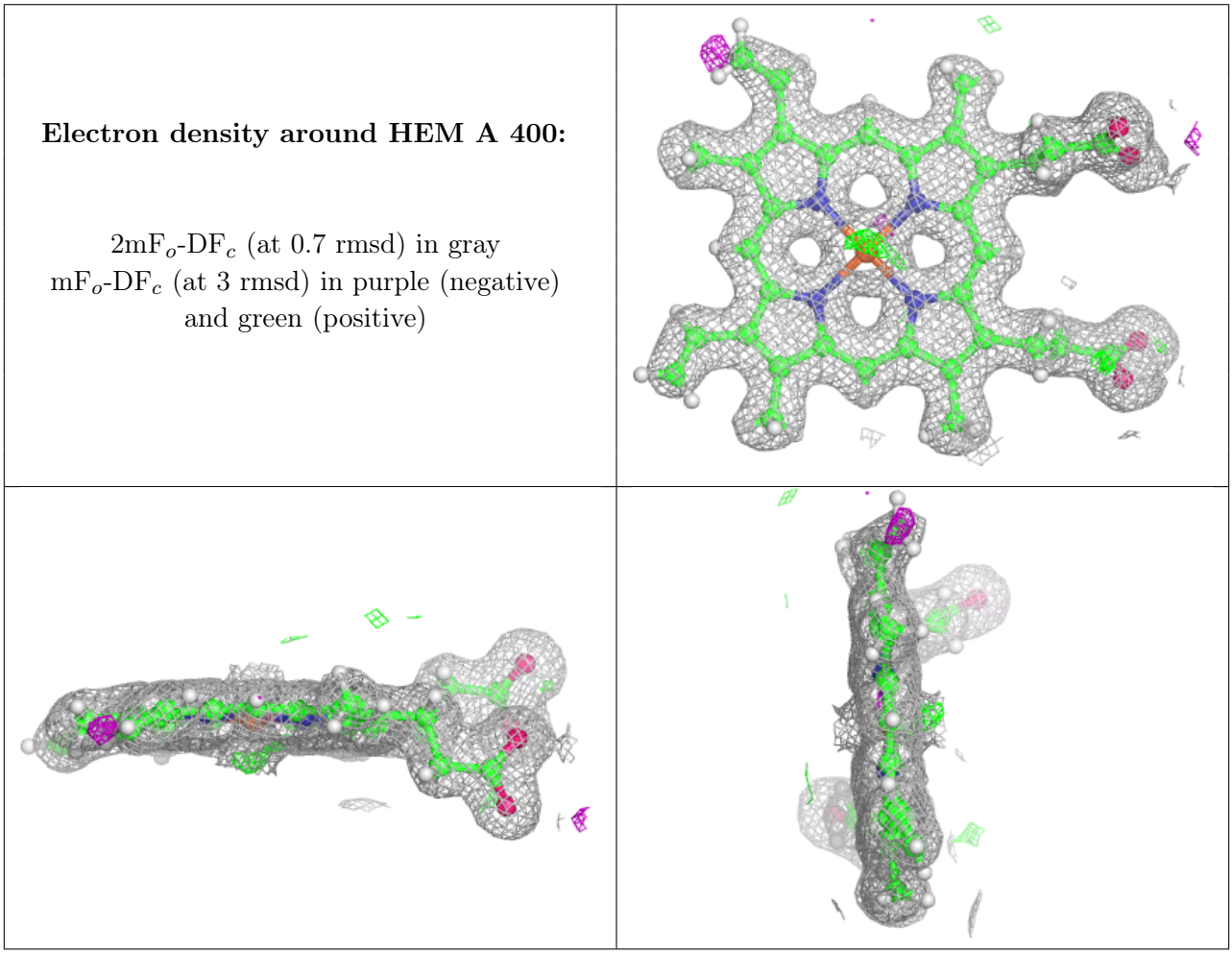
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	HEM	A	400	43/43	0.99	0.07	11,16,25,31	0
2	HEM	B	400	43/43	0.99	0.06	13,17,25,31	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.

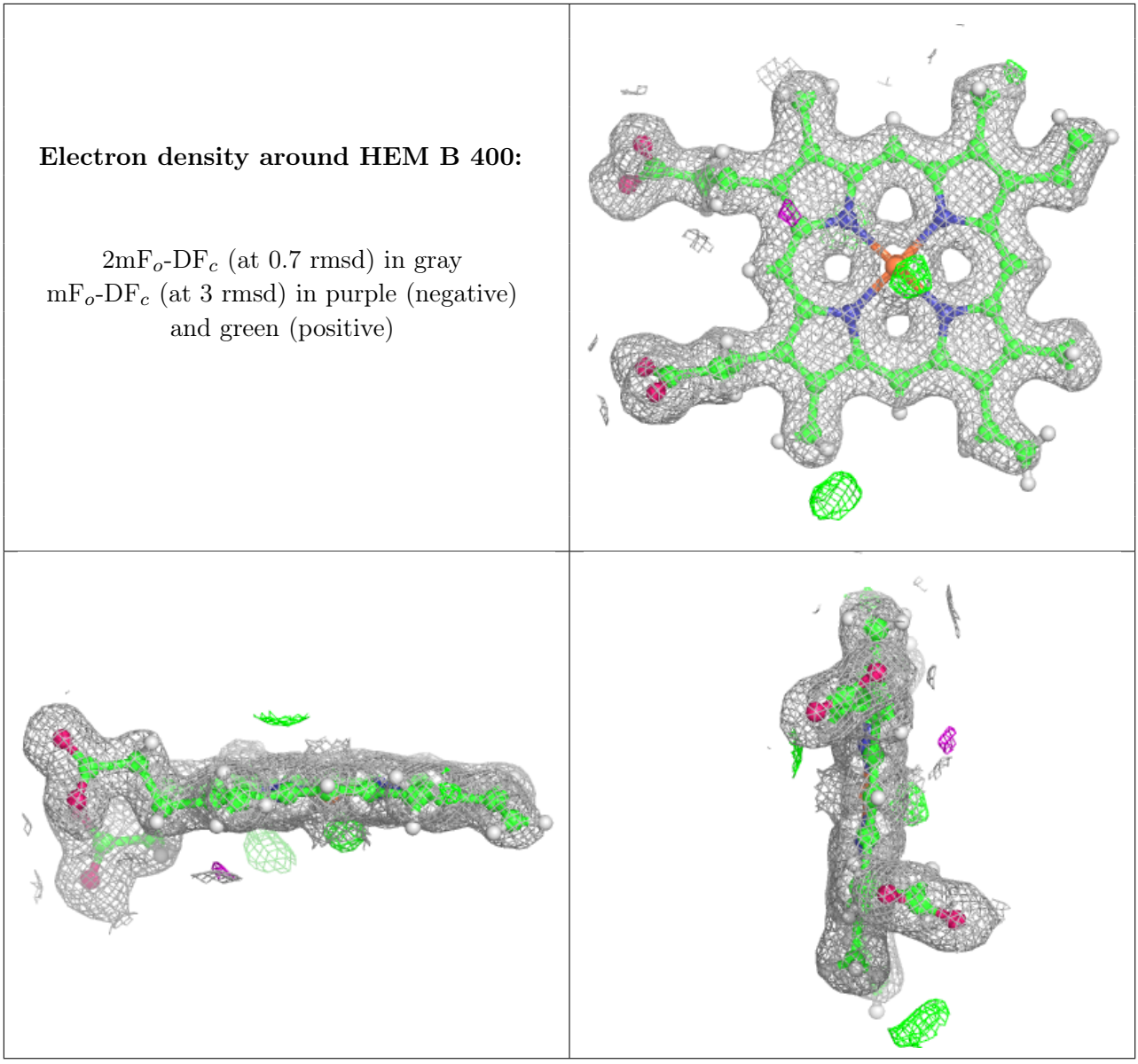
Electron density around HEM A 400:

$2mF_o$-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 400:

$2mF_o$-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.