wwPDB X-ray Structure Validation Summary Report (i)

Sep 20, 2023 – 11:06 AM EDT

PDB ID	:	5IRQ
Title	:	Human cytochrome P450 17A1 bound to inhibitors (R)- and (S)- orteronel
Authors	:	Scott, E.E.; Petrunak, E.M.
Deposited on	:	2016-03-14
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

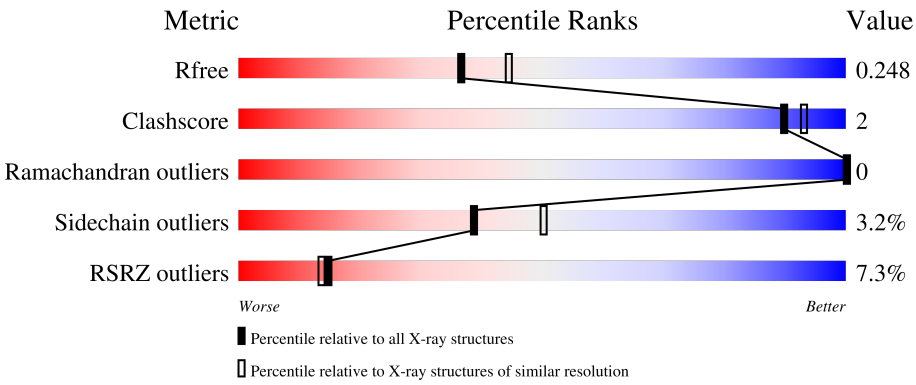
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	494	5%, 88%, 6%, 6%
1	B	494	4%, 90%, •, 5%
1	C	494	7%, 89%, 6%, •
1	D	494	11%, 86%, 8%, 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31054 atoms, of which 15364 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 Steroid 17-alpha-hydroxylase/17,20 lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	466	7503	2384	3787	643	674	15	0	0	0
1	B	467	7519	2389	3794	645	676	15	0	0	0
1	C	472	7567	2404	3815	650	683	15	0	0	0
1	D	465	7488	2380	3780	641	672	15	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression tag	UNP P05093
A	511	HIS	-	expression tag	UNP P05093
A	512	HIS	-	expression tag	UNP P05093
B	19	MET	-	expression tag	UNP P05093
B	20	ALA	-	expression tag	UNP P05093
B	21	LYS	-	expression tag	UNP P05093
B	22	LYS	-	expression tag	UNP P05093
B	23	THR	-	expression tag	UNP P05093
B	509	HIS	-	expression tag	UNP P05093
B	510	HIS	-	expression tag	UNP P05093
B	511	HIS	-	expression tag	UNP P05093
B	512	HIS	-	expression tag	UNP P05093
C	19	MET	-	expression tag	UNP P05093
C	20	ALA	-	expression tag	UNP P05093
C	21	LYS	-	expression tag	UNP P05093

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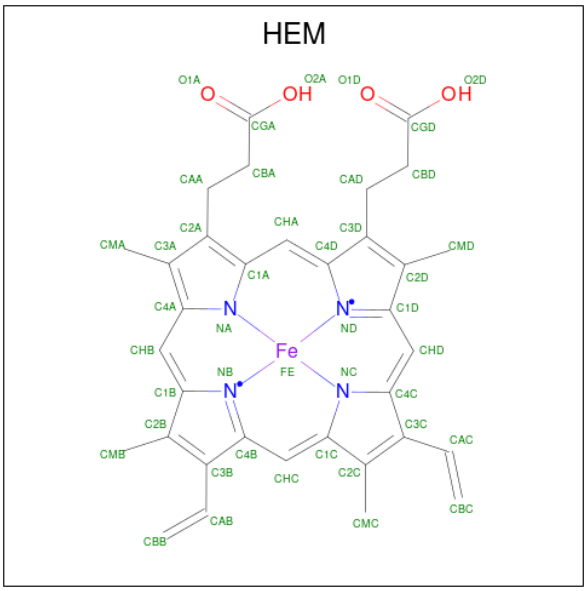
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LYS	-	expression tag	UNP P05093
C	23	THR	-	expression tag	UNP P05093
C	509	HIS	-	expression tag	UNP P05093
C	510	HIS	-	expression tag	UNP P05093
C	511	HIS	-	expression tag	UNP P05093
C	512	HIS	-	expression tag	UNP P05093
D	19	MET	-	expression tag	UNP P05093
D	20	ALA	-	expression tag	UNP P05093
D	21	LYS	-	expression tag	UNP P05093
D	22	LYS	-	expression tag	UNP P05093
D	23	THR	-	expression tag	UNP P05093
D	509	HIS	-	expression tag	UNP P05093
D	510	HIS	-	expression tag	UNP P05093
D	511	HIS	-	expression tag	UNP P05093
D	512	HIS	-	expression tag	UNP P05093

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



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

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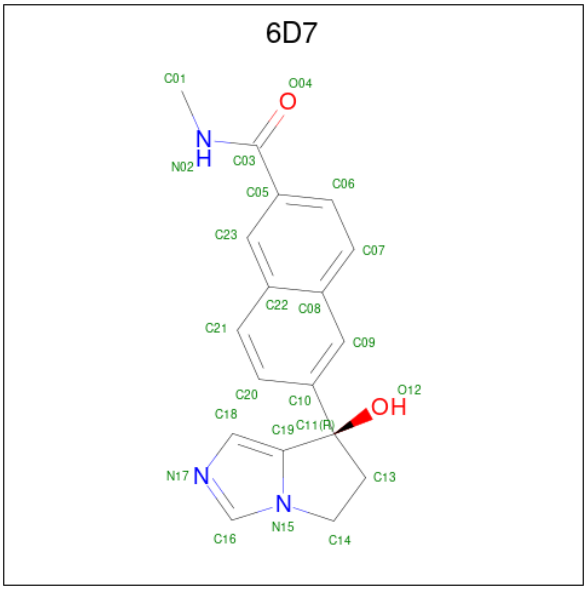
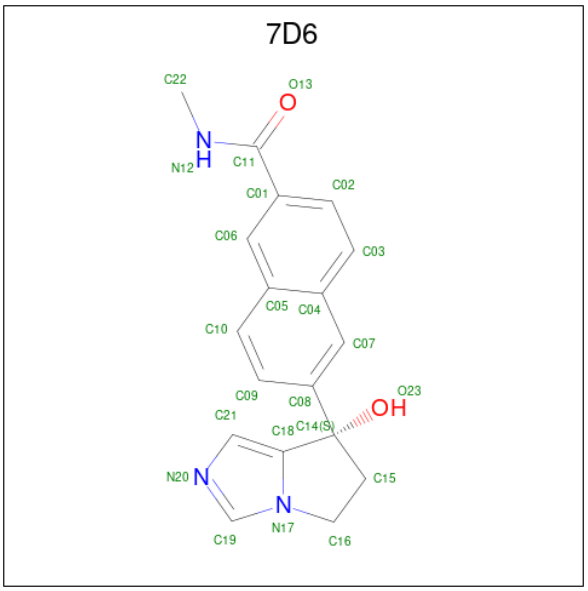
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
2	D	1	73	34	1	30	4	4	0	0

- Molecule 3 is (R)-orteronel (three-letter code: 6D7) (formula: $C_{18}H_{17}N_3O_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O			
3	A	1	40	18	17	3	2		0	0
3	B	1	40	18	17	3	2		0	0

- Molecule 4 is (S)-orteronel (three-letter code: 7D6) (formula: $C_{18}H_{17}N_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	C	1	40	18	17	3	2	0	0
			Total	C	H	N	O		
4	D	1	40	18	17	3	2	0	0

- Molecule 5 is water.

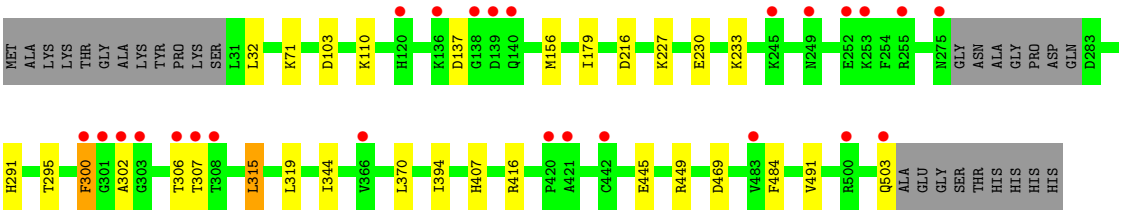
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	148	148	148	0	0
			Total	O		
5	B	143	143	143	0	0
			Total	O		
5	C	135	135	135	0	0
			Total	O		
5	D	99	99	99	0	0

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.

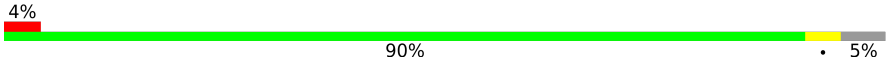
• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

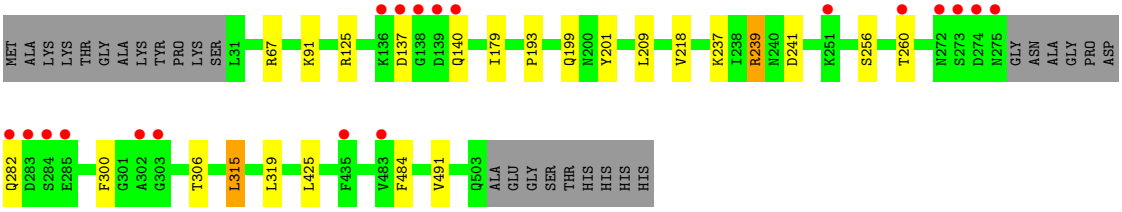
Chain A:



• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

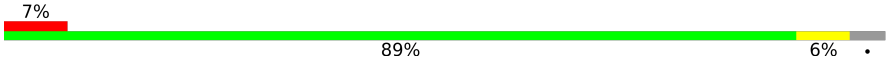
Chain B:

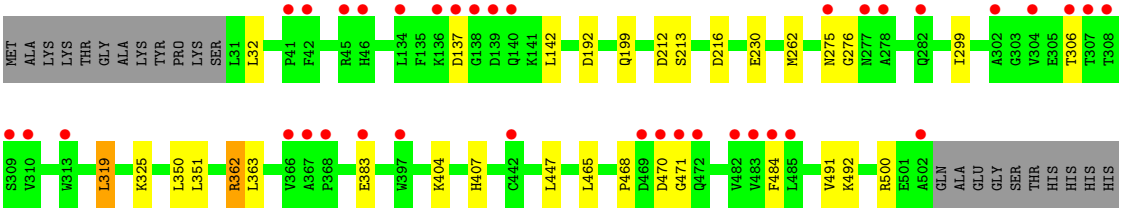




• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

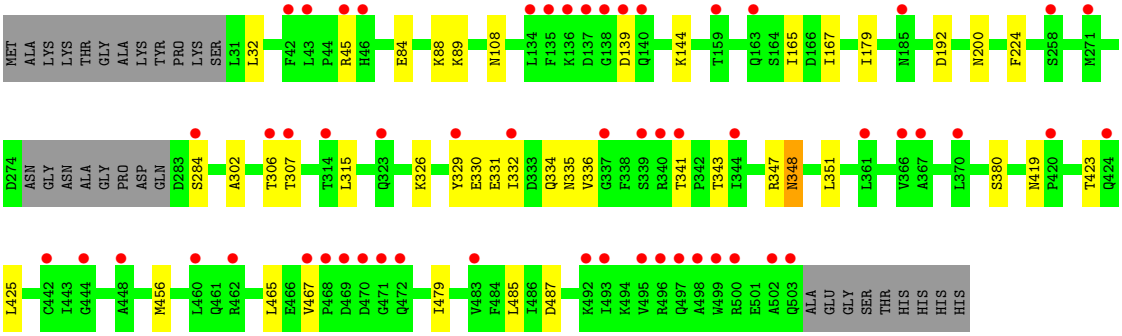
Chain C:





• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain D:


MET
ALA
LYS
LYS
THR
GLY
ALA
LYS
TYR
PRO
LYS
SER
L31
L32
F42
L43
P44
R45
H46
E84
K88
K89
N108
L134
F135
K136
D137
G138
D139
Q140
K144
T159
Q163
S164
I165
D166
I167
I179
N185
D192
N200
F224
S258
M271
D274
ASN
GLY
ASN
ALA
GLY
PRO
ASP
GLN
D283
S284
A302
T306
T307
T314
L315
Q323
K326
Y329
E330
E331
I332
D333
Q334
N335
V336
G337
F338
S339
R340
T341
P342
T343
I344
R347
N348
L351
L361
V366
A367
L370
S380
N419
P420
T423
Q424
L425
C442
I443
G444
A448
M456
L460
Q461
R462
L465
E466
V467
P468
D469
D470
G471
Q472
I479
V483
F484
L485
I486
D487
K492
I493
K494
V495
R496
Q497
A498
W499
R500
E501
A502
Q503
ALA
GLU
GLY
SER
THR
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.17Å 153.20Å 168.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.28 – 2.20 39.28 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.28-2.20) 99.8 (39.28-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10pre_2124: ???)	Depositor
R, R_{free}	0.201 , 0.249 0.202 , 0.248	Depositor DCC
R_{free} test set	5915 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31054	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 7D6, HEM, 6D7

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	0.26	0/3796	0.42	0/5139
1	B	0.28	1/3805 (0.0%)	0.43	0/5151
1	C	0.26	0/3834	0.43	0/5193
1	D	0.28	1/3788 (0.0%)	0.44	0/5128
All	All	0.27	2/15223 (0.0%)	0.43	0/20611

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	VAL	C-N	8.01	1.49	1.34
1	D	224	PHE	C-N	6.25	1.46	1.34

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	3716	3787	3786	16	0
1	B	3725	3794	3793	11	0
1	C	3752	3815	3815	12	0
1	D	3708	3780	3779	14	0
2	A	43	30	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	30	30	2	0
2	C	43	30	30	1	0
2	D	43	30	30	2	0
3	A	23	17	0	0	0
3	B	23	17	0	0	0
4	C	23	17	0	0	0
4	D	23	17	0	0	0
5	A	148	0	0	5	0
5	B	143	0	0	4	0
5	C	135	0	0	2	0
5	D	99	0	0	2	0
All	All	15690	15364	15293	55	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.

The worst 5 of 55 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:D:326:LYS:NZ	1:D:330:GLU:OE2	2.07	0.87
1:A:445:GLU:OE2	1:A:449:ARG:NH2	2.22	0.73
1:D:192:ASP:OD2	5:D:701:HOH:O	2.10	0.68
1:B:425:LEU:O	5:B:701:HOH:O	2.10	0.68
1:A:295:THR:OG1	5:A:701:HOH:O	2.13	0.67

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	462/494 (94%)	449 (97%)	13 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	463/494 (94%)	449 (97%)	14 (3%)	0	100	100
1	C	470/494 (95%)	447 (95%)	23 (5%)	0	100	100
1	D	461/494 (93%)	438 (95%)	23 (5%)	0	100	100
All	All	1856/1976 (94%)	1783 (96%)	73 (4%)	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	416/436 (95%)	406 (98%)	10 (2%)	49	62
1	B	417/436 (96%)	407 (98%)	10 (2%)	49	62
1	C	419/436 (96%)	406 (97%)	13 (3%)	40	51
1	D	415/436 (95%)	395 (95%)	20 (5%)	25	32
All	All	1667/1744 (96%)	1614 (97%)	53 (3%)	39	50

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	383	GLU
1	D	108	ASN
1	D	425	LEU
1	C	404	LYS
1	C	500	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	B	291	HIS

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)

8 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	$\#\|Z\| > 2$
4	7D6	C	601	2	20,26,26	2.67	7 (35%)	29,39,39	1.59	3 (10%)
3	6D7	B	601	2	20,26,26	5.98	14 (70%)	29,39,39	2.00	6 (20%)
2	HEM	A	600	3	41,50,50	1.46	4 (9%)	45,82,82	1.57	7 (15%)
2	HEM	B	600	3	41,50,50	1.48	5 (12%)	45,82,82	1.60	7 (15%)
3	6D7	A	601	2	20,26,26	5.96	14 (70%)	29,39,39	2.00	6 (20%)
4	7D6	D	601	2	20,26,26	2.70	7 (35%)	29,39,39	1.52	3 (10%)
2	HEM	C	600	4	41,50,50	1.46	4 (9%)	45,82,82	1.62	8 (17%)
2	HEM	D	602	4	41,50,50	1.47	5 (12%)	45,82,82	1.65	9 (20%)

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	7D6	C	601	2	-	0/12/24/24	0/4/4/4
3	6D7	B	601	2	-	0/12/24/24	0/4/4/4
2	HEM	A	600	3	-	0/12/54/54	-
2	HEM	B	600	3	-	1/12/54/54	-
3	6D7	A	601	2	-	0/12/24/24	0/4/4/4
4	7D6	D	601	2	-	0/12/24/24	0/4/4/4
2	HEM	C	600	4	-	3/12/54/54	-
2	HEM	D	602	4	-	4/12/54/54	-

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	6D7	C09-C10	9.69	1.55	1.38
3	B	601	6D7	C09-C10	9.65	1.55	1.38
3	B	601	6D7	C03-N02	9.04	1.45	1.33
3	A	601	6D7	C06-C05	8.95	1.54	1.39
3	B	601	6D7	C06-C05	8.91	1.54	1.39

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	6D7	C16-N15-C19	-6.18	107.96	110.81
3	A	601	6D7	C16-N15-C19	-5.91	108.09	110.81
4	C	601	7D6	C19-N17-C18	-5.48	108.29	110.81
4	D	601	7D6	C19-N17-C18	-5.38	108.33	110.81
3	A	601	6D7	O12-C11-C10	-4.43	101.83	110.68

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	HEM	C4B-C3B-CAB-CBB
2	C	600	HEM	C4B-C3B-CAB-CBB
2	D	602	HEM	CAA-CBA-CGA-O2A
2	D	602	HEM	C4B-C3B-CAB-CBB
2	D	602	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	1	0

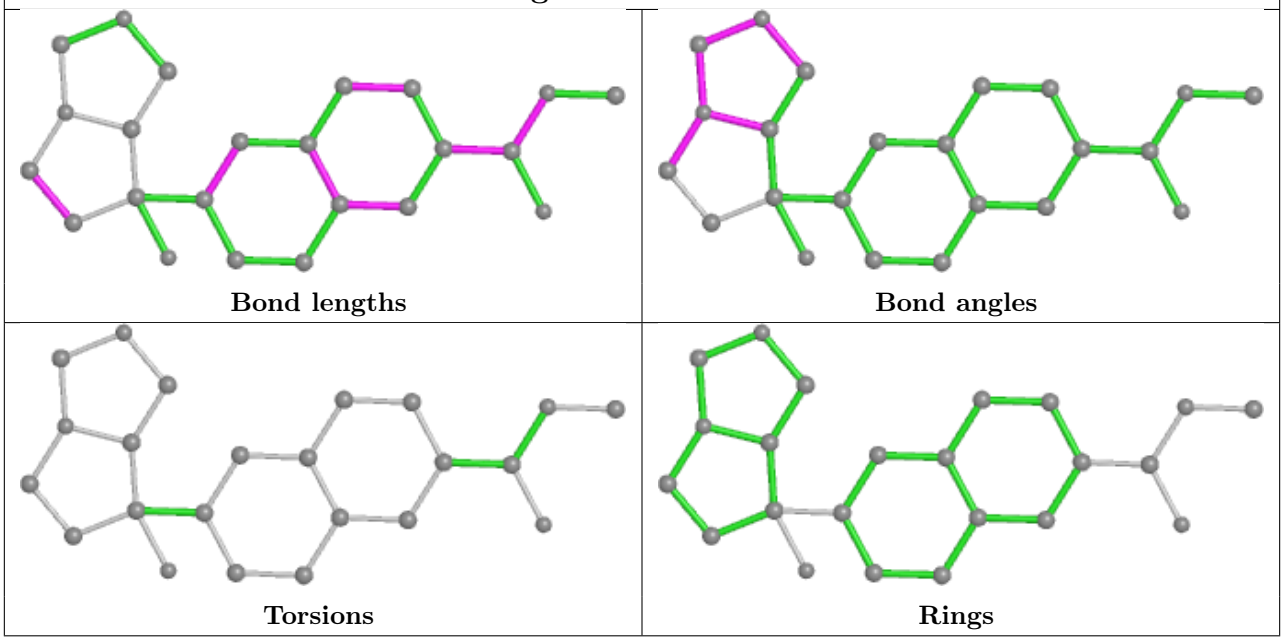
Continued on next page...

Continued from previous page...

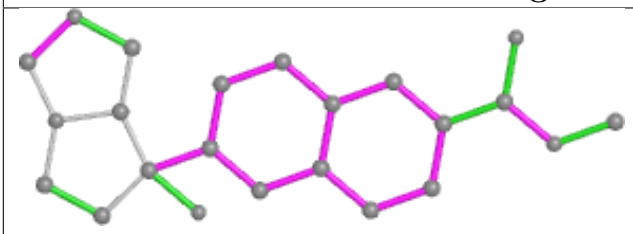
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	HEM	2	0
2	C	600	HEM	1	0
2	D	602	HEM	2	0

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.

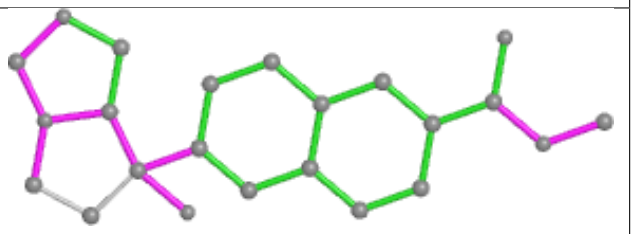
Ligand 7D6 C 601



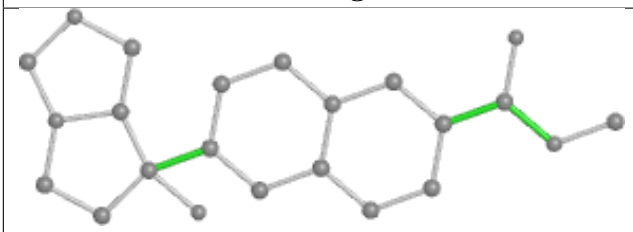
Ligand 6D7 B 601



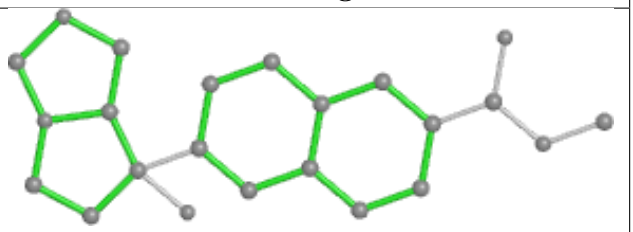
Bond lengths



Bond angles

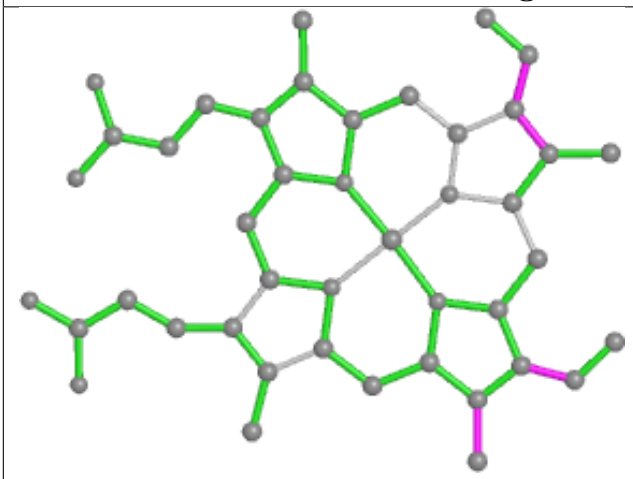


Torsions

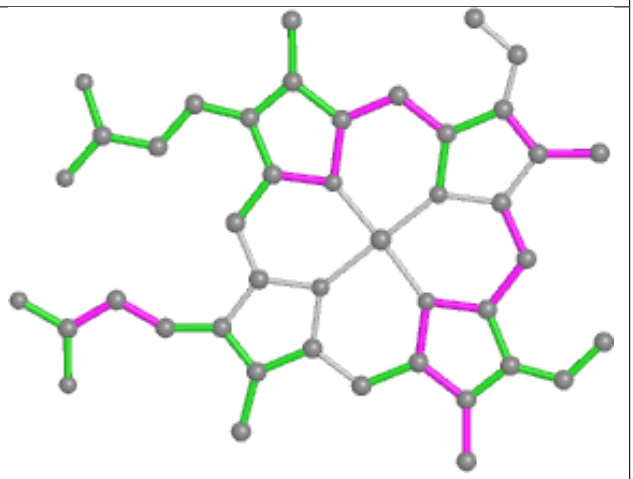


Rings

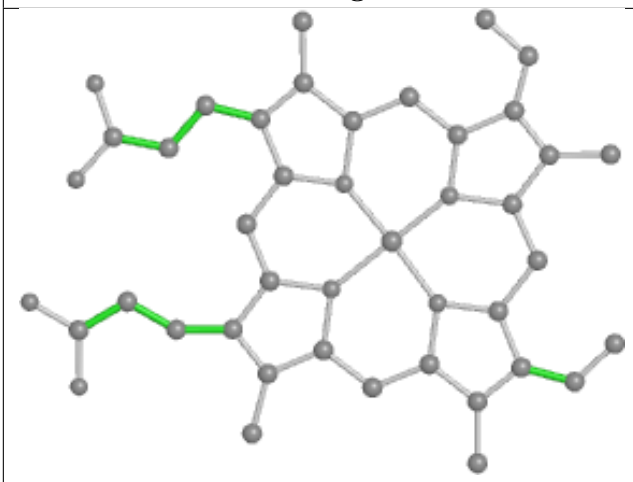
Ligand HEM A 600



Bond lengths



Bond angles



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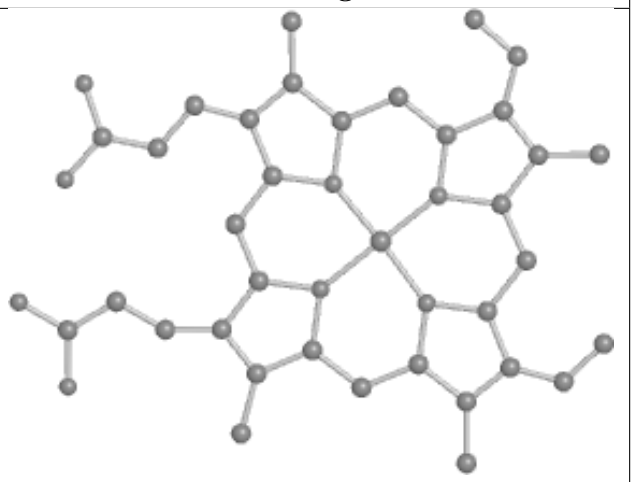
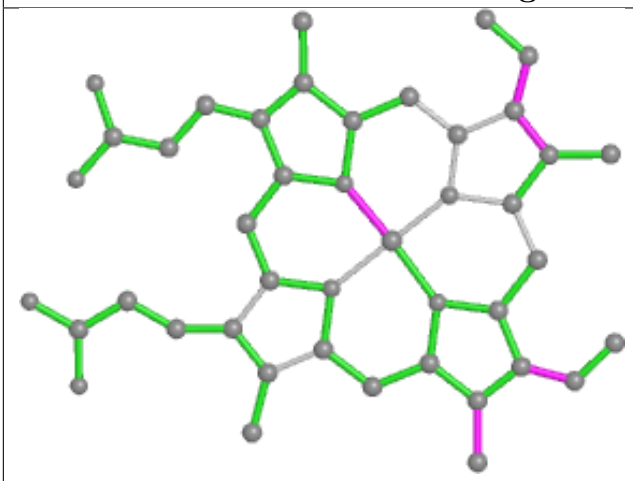
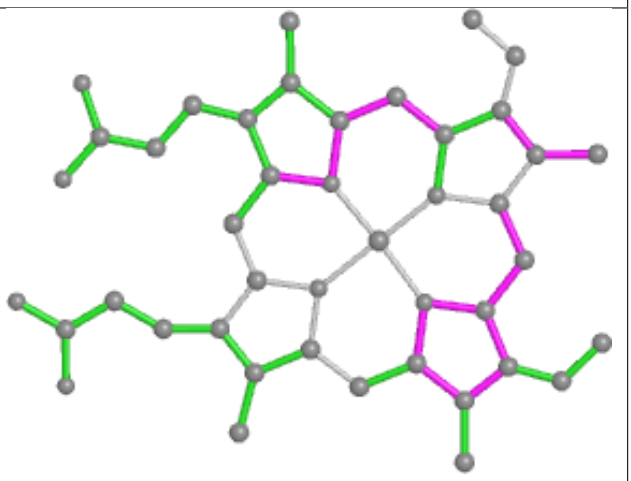


Rings

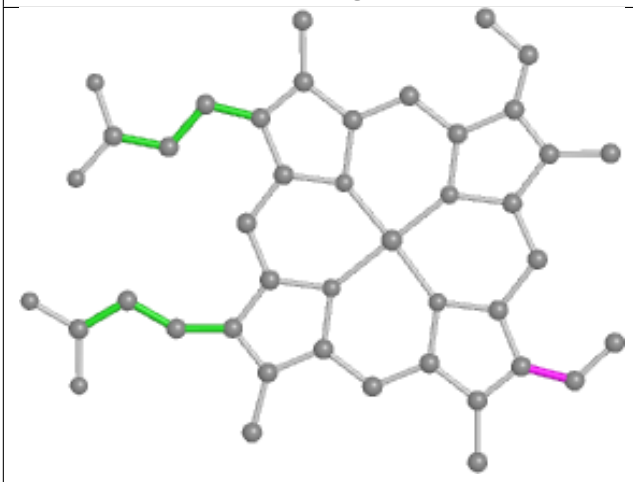
Ligand HEM B 600



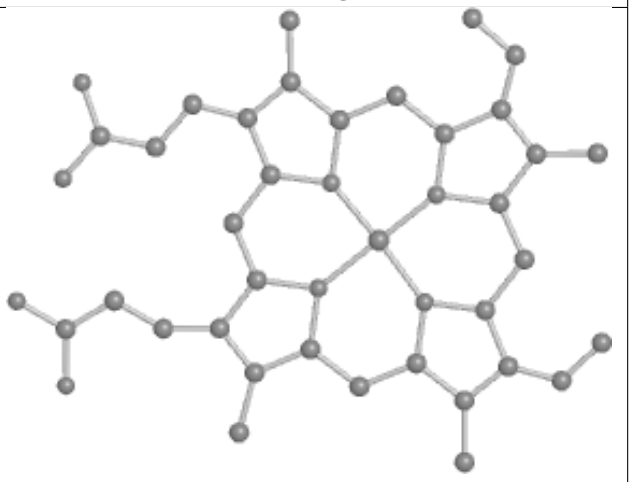
Bond lengths



Bond angles

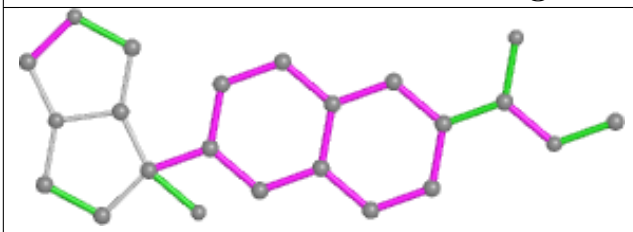


Torsions

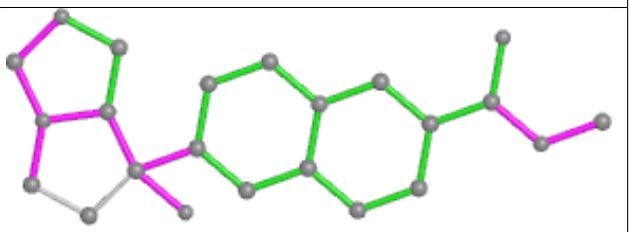


Rings

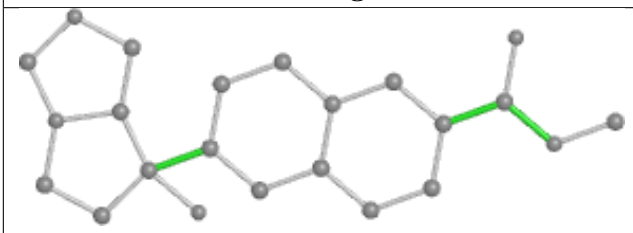
Ligand 6D7 A 601



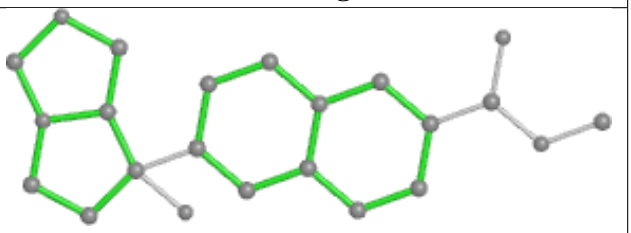
Bond lengths



Bond angles

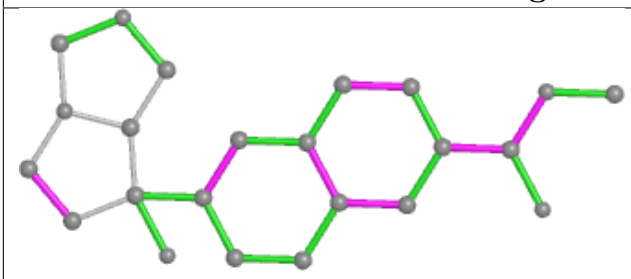


Torsions



Rings

Ligand 7D6 D 601



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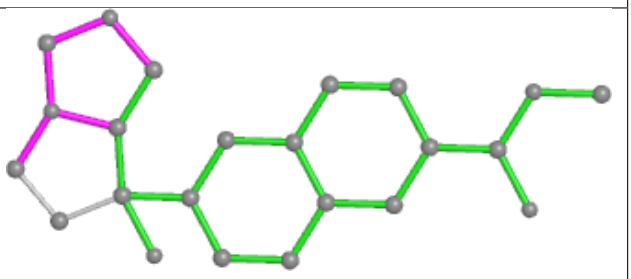

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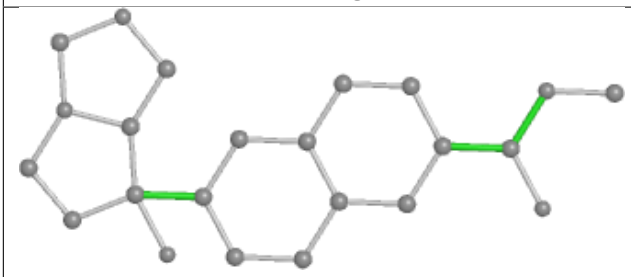

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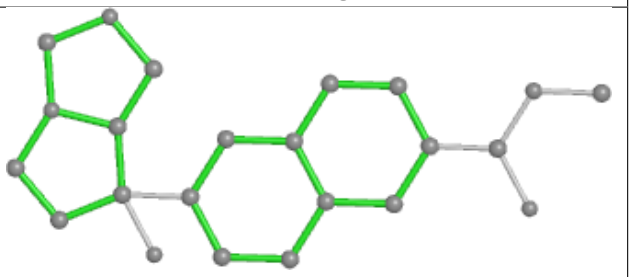
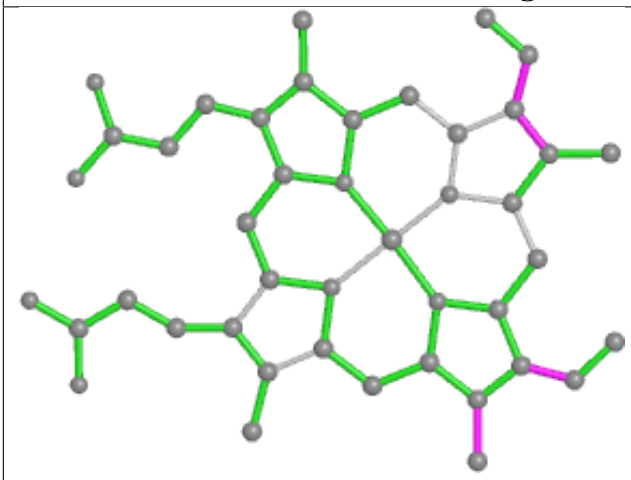


Rings

Ligand HEM C 600



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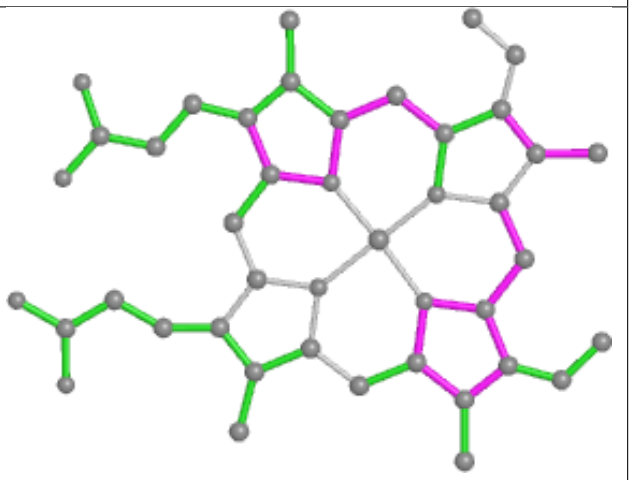
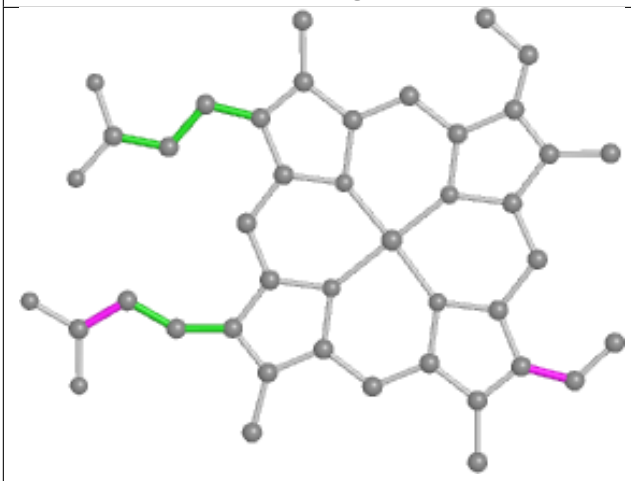


Bond angles



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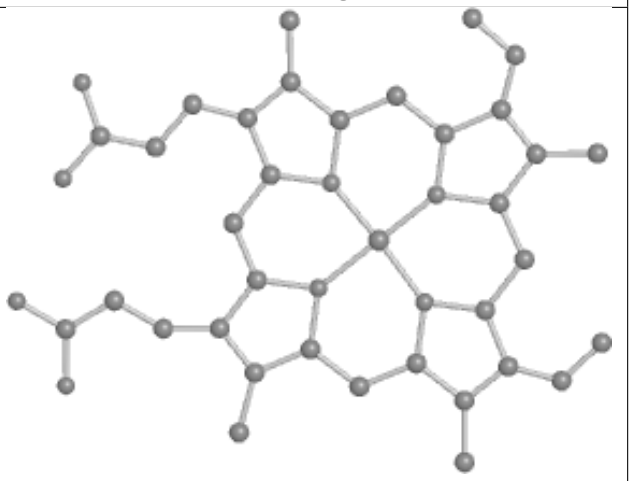
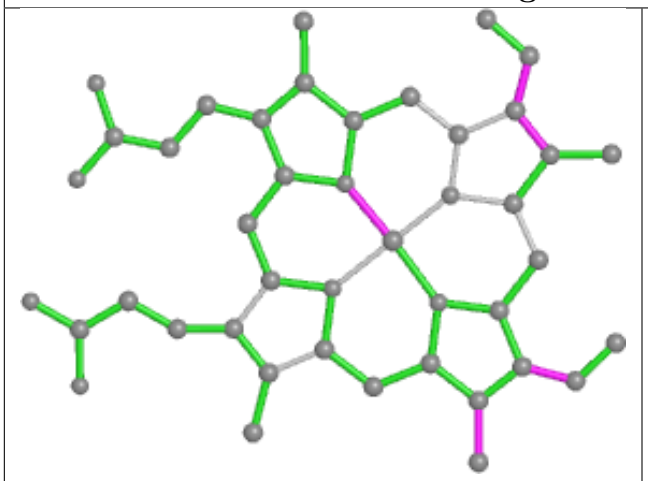


Rings

Ligand HEM D 602



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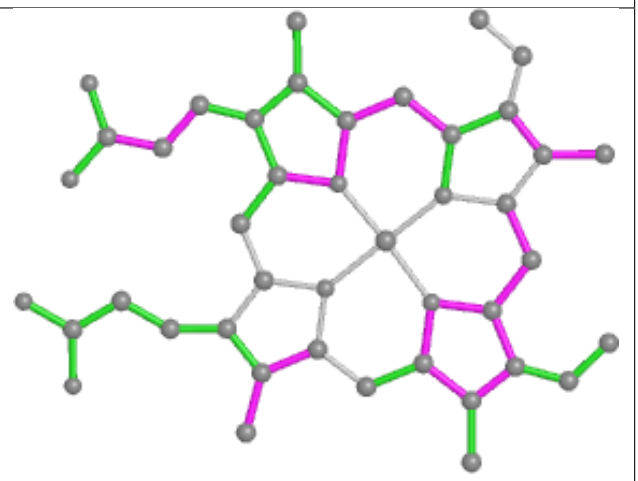
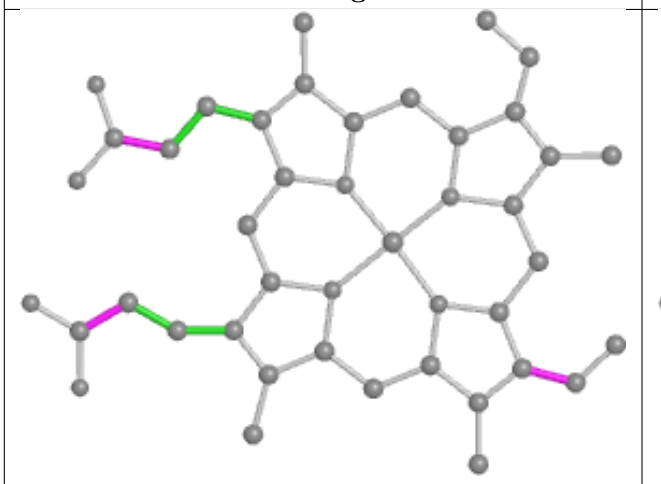
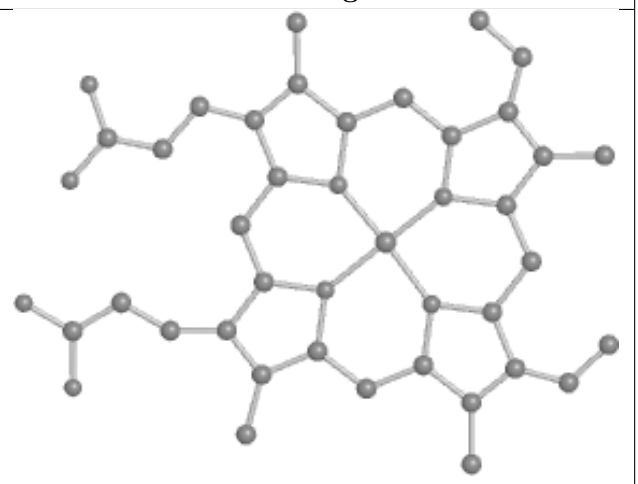


Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	466/494 (94%)	0.17	25 (5%)	25	24	28, 40, 71, 112	0
1	B	467/494 (94%)	0.18	19 (4%)	37	35	29, 41, 71, 127	0
1	C	472/494 (95%)	0.28	37 (7%)	13	11	28, 41, 74, 109	0
1	D	465/494 (94%)	0.61	56 (12%)	4	3	28, 48, 90, 122	0
All	All	1870/1976 (94%)	0.31	137 (7%)	15	14	28, 42, 81, 127	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	139	ASP	8.2
1	B	139	ASP	7.0
1	D	499	TRP	6.9
1	C	139	ASP	6.7
1	D	503	GLN	6.0

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)

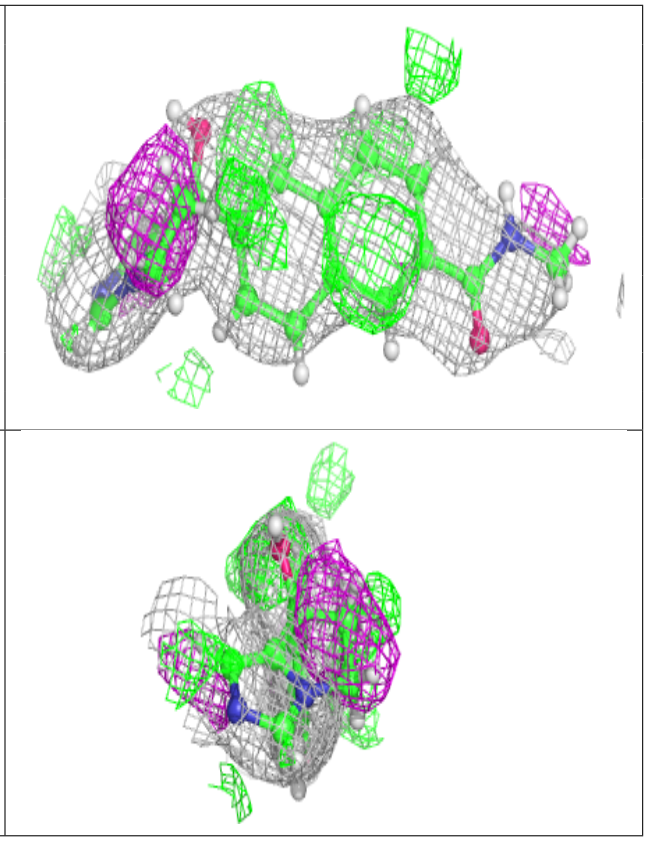
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	6D7	A	601	23/23	0.73	0.40	30,48,78,79	0
3	6D7	B	601	23/23	0.73	0.39	33,50,69,76	0
4	7D6	C	601	23/23	0.91	0.26	30,43,58,59	0
4	7D6	D	601	23/23	0.91	0.22	32,46,56,61	0
2	HEM	D	602	43/43	0.96	0.25	24,39,54,65	0
2	HEM	C	600	43/43	0.97	0.26	19,31,42,50	0
2	HEM	A	600	43/43	0.97	0.25	20,35,50,60	0
2	HEM	B	600	43/43	0.98	0.28	26,37,50,58	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.

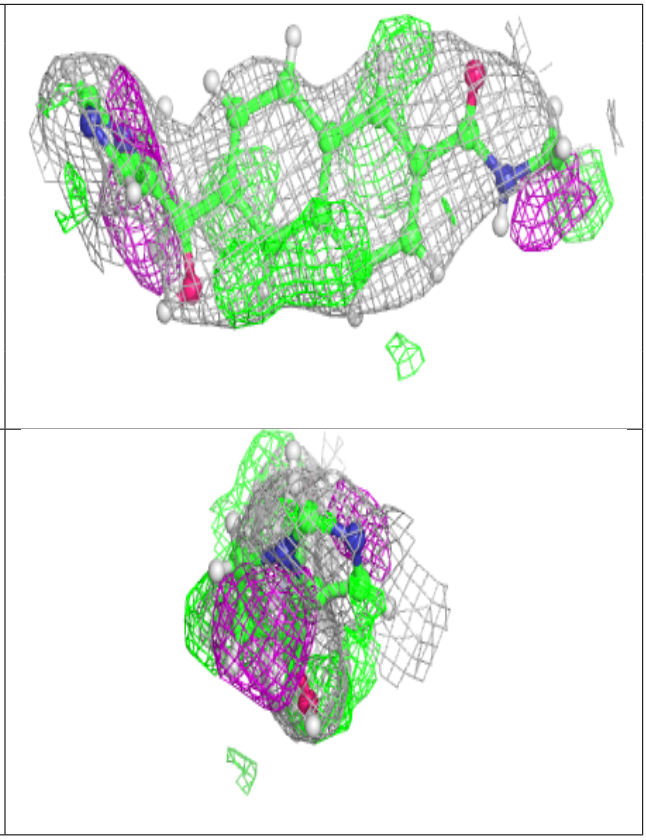
Electron density around 6D7 A 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



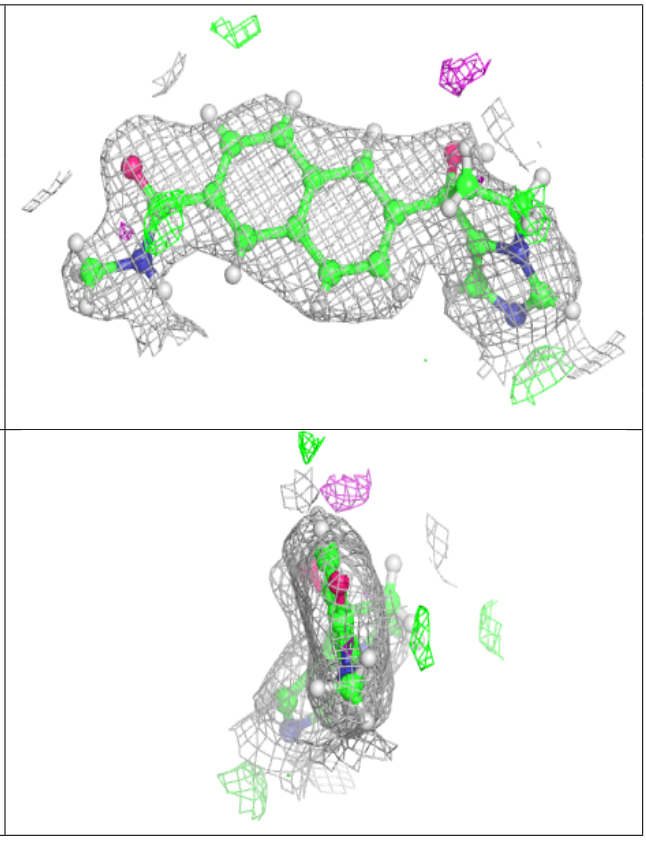
Electron density around 6D7 B 601:

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



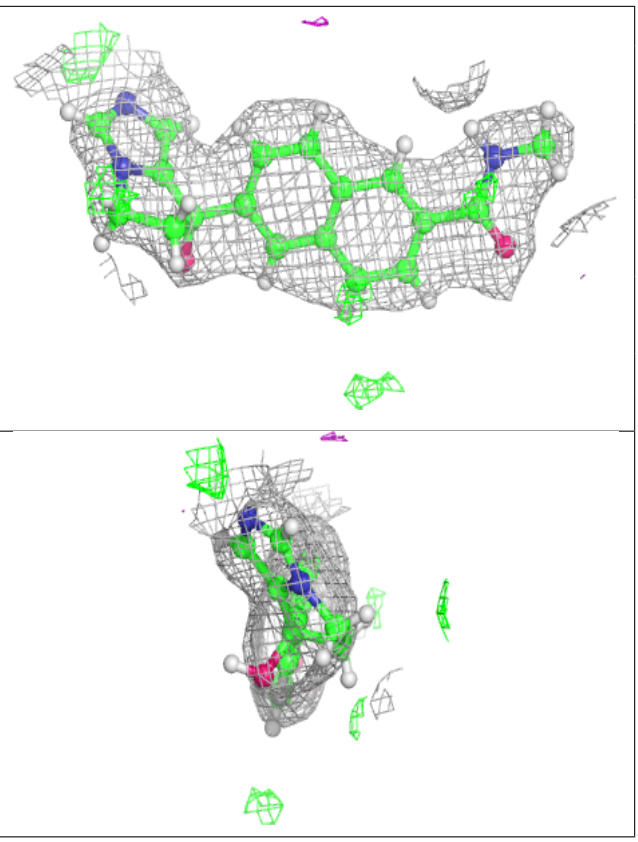
Electron density around 7D6 C 601:

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



Electron density around 7D6 D 601:

$2mF_o$-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 D 602:

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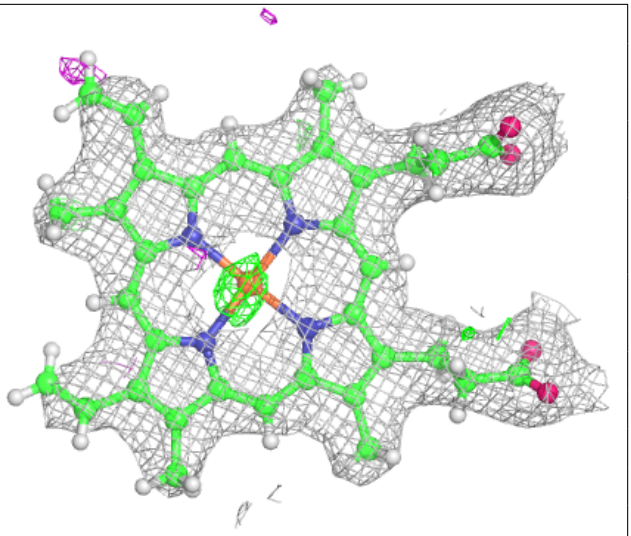
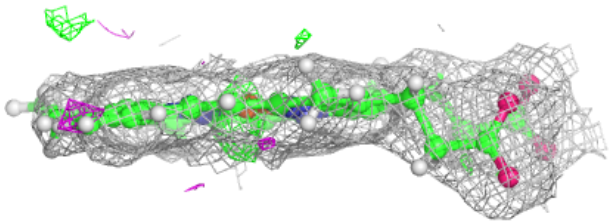
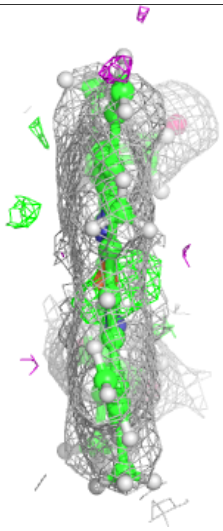
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEM C 600:

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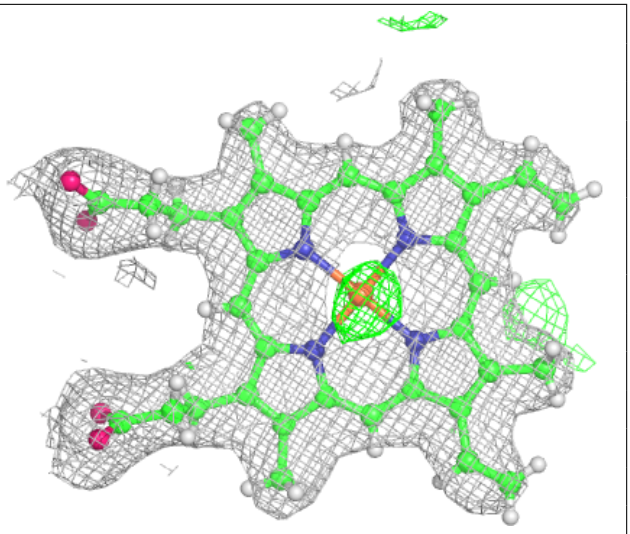
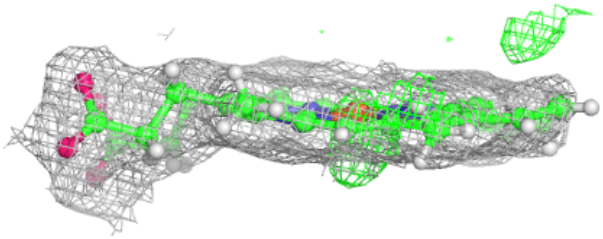
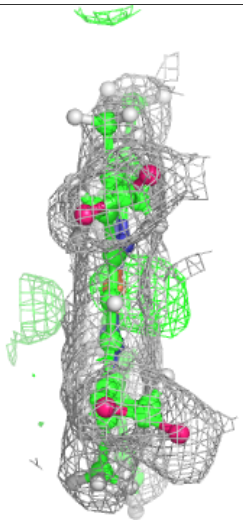
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

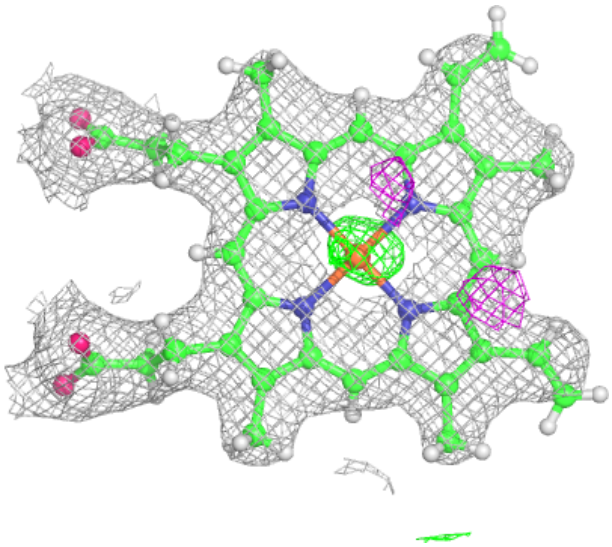


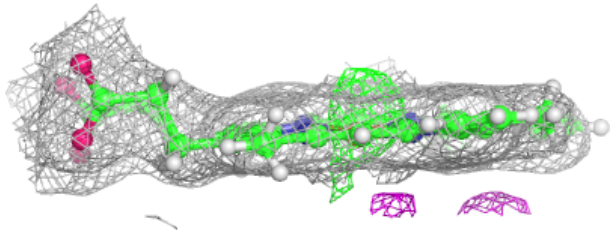


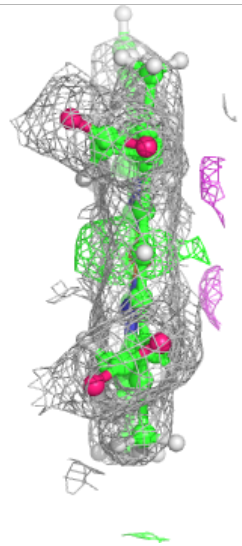


Electron density around HEM A 600:

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

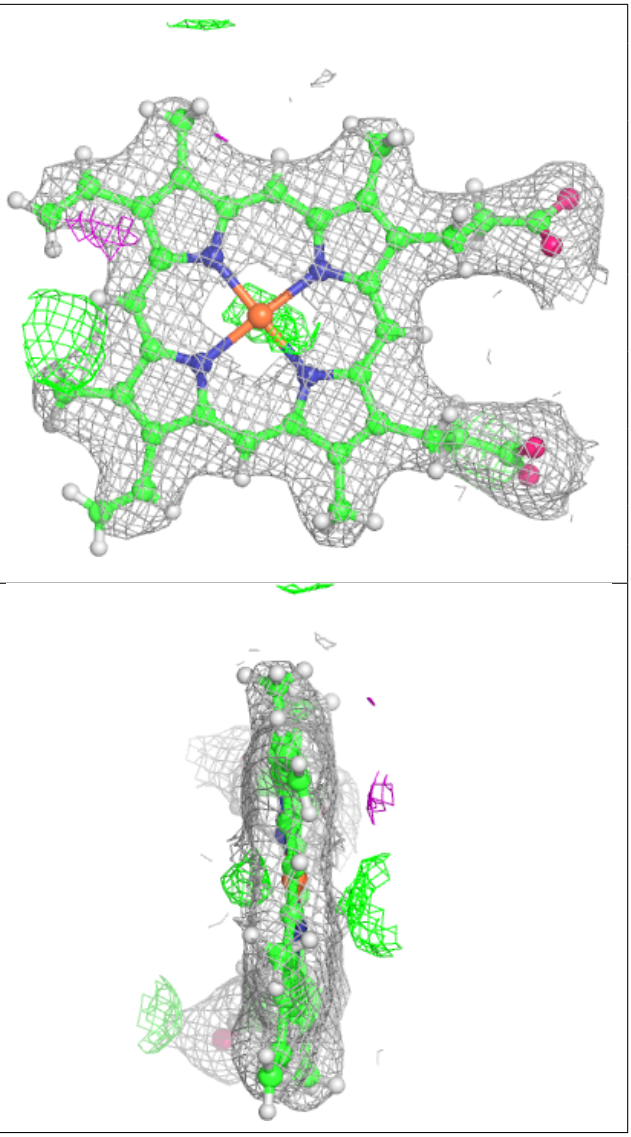






Electron density around HEM B 600:

$2mF_o$-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.