Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 05:05 AM EDT

PDB ID	:	7SV2
Title	:	Human Cytochrome P450 (CYP) 3A5 ternary complex with azamulin
Authors	:	Hsu, M.; Johnson, E.F.
Deposited on	:	2021-11-18
Resolution	:	2.46 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:

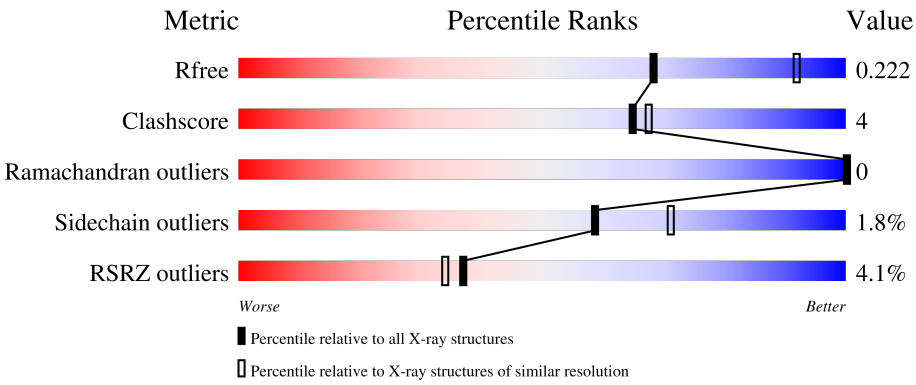
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	480	2%, 87%, 9%, •
1	B	480	4%, 82%, 14%, • •
1	C	480	4%, 85%, 10%, • 5%
1	D	480	5%, 79%, 11%, 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15215 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 Cytochrome P450 3A5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3738	2430	619	672	17	0	0	0
1	B	465	3737	2431	618	671	17	0	0	0
1	C	456	3659	2381	600	661	17	0	0	0
1	D	438	3517	2296	578	626	17	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

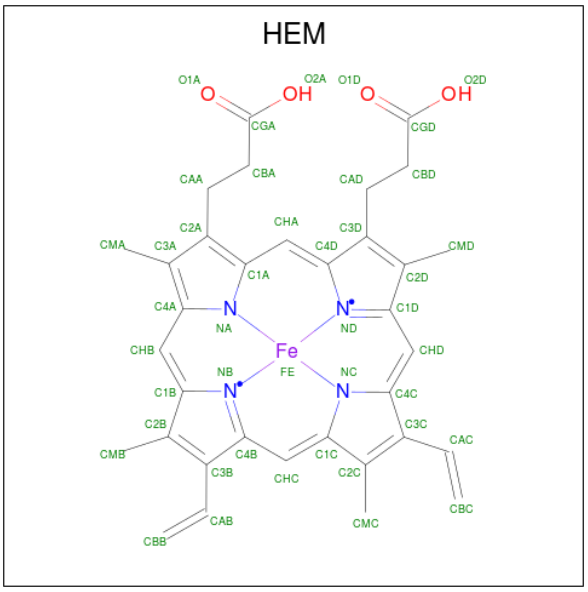
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP P20815
A	23	ALA	-	expression tag	UNP P20815
A	498	HIS	-	expression tag	UNP P20815
A	499	HIS	-	expression tag	UNP P20815
A	500	HIS	-	expression tag	UNP P20815
A	501	HIS	-	expression tag	UNP P20815
B	22	MET	-	initiating methionine	UNP P20815
B	23	ALA	-	expression tag	UNP P20815
B	498	HIS	-	expression tag	UNP P20815
B	499	HIS	-	expression tag	UNP P20815
B	500	HIS	-	expression tag	UNP P20815
B	501	HIS	-	expression tag	UNP P20815
C	22	MET	-	initiating methionine	UNP P20815
C	23	ALA	-	expression tag	UNP P20815
C	498	HIS	-	expression tag	UNP P20815
C	499	HIS	-	expression tag	UNP P20815
C	500	HIS	-	expression tag	UNP P20815
C	501	HIS	-	expression tag	UNP P20815
D	22	MET	-	initiating methionine	UNP P20815
D	23	ALA	-	expression tag	UNP P20815
D	498	HIS	-	expression tag	UNP P20815

Continued on next page...

Continued from previous page...

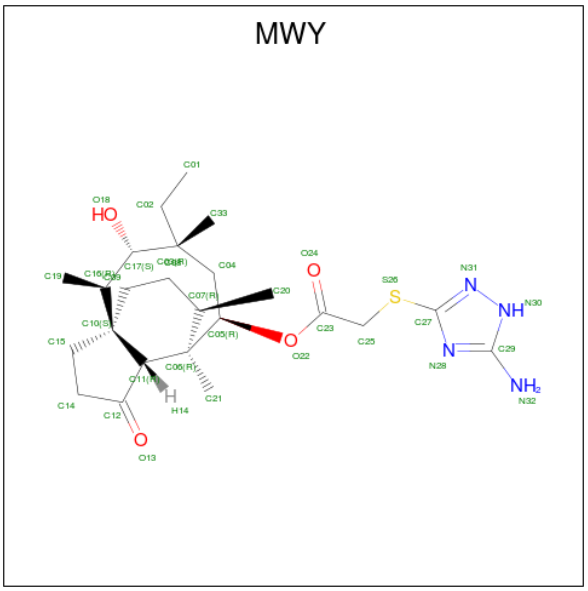
Chain	Residue	Modelled	Actual	Comment	Reference
D	499	HIS	-	expression tag	UNP P20815
D	500	HIS	-	expression tag	UNP P20815
D	501	HIS	-	expression tag	UNP P20815

- 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	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (3aS,4R,5S,6R,8R,9R,9aR,10R)-6-ethyl-5-hydroxy-4,6,9,10-tetramethyl-1-oxo decahydro-3a,9-propanocyclopenta[8]annulen-8-yl [(5-amino-1H-1,2,4-triazol-3-yl)sulfanyl]acetate (three-letter code: MWY) (formula: $C_{24}H_{38}N_4O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	33	24	4	4	1	0	0
			Total	C	N	O	S		
3	A	1	33	24	4	4	1	0	0
			Total	C	N	O	S		
3	B	1	33	24	4	4	1	0	0
			Total	C	N	O	S		
3	B	1	33	24	4	4	1	0	0
			Total	C	N	O	S		
3	C	1	33	24	4	4	1	0	0
			Total	C	N	O	S		
3	C	1	33	24	4	4	1	0	0
			Total	C	N	O	S		
3	D	1	33	24	4	4	1	0	0
			Total	C	N	O	S		
3	D	1	33	24	4	4	1	0	0

- Molecule 4 is water.

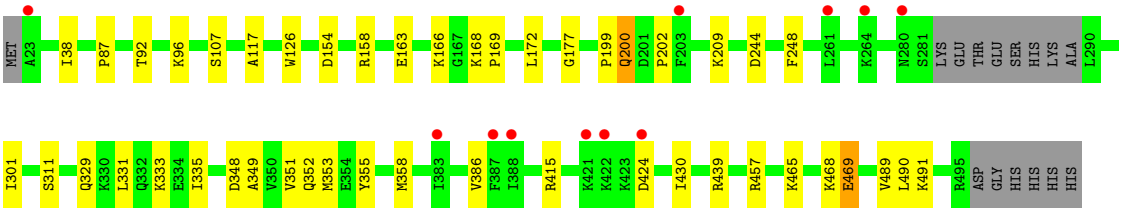
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	47	47	47	0	0
			Total	O		
4	B	32	32	32	0	0
			Total	O		
4	C	25	25	25	0	0
			Total	O		
4	D	24	24	24	0	0

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.

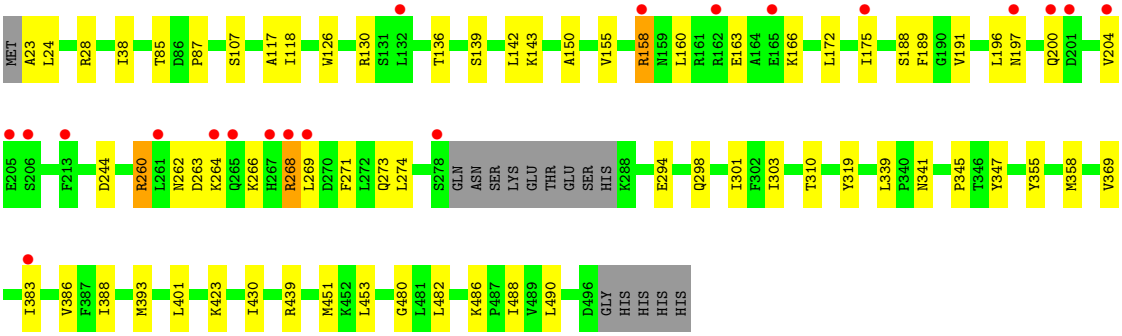
• Molecule 1: Cytochrome P450 3A5

Chain A:



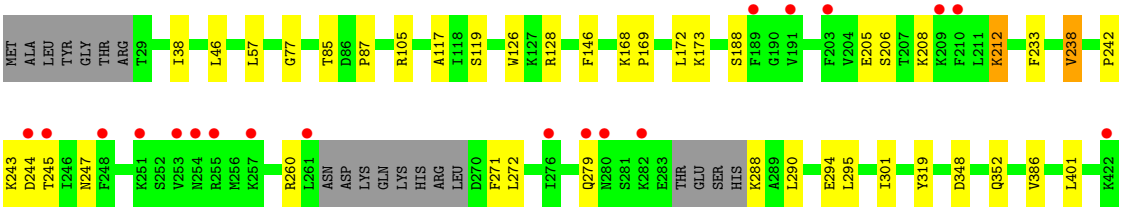
• Molecule 1: Cytochrome P450 3A5

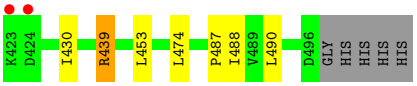
Chain B:



• Molecule 1: Cytochrome P450 3A5

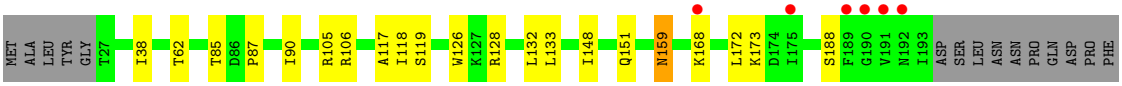
Chain C:

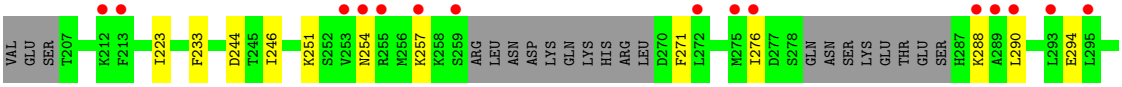


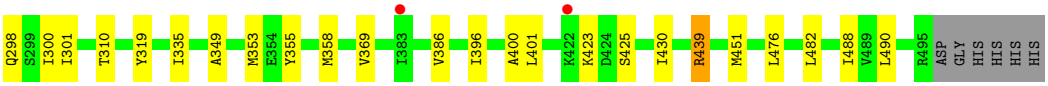


• Molecule 1: Cytochrome P450 3A5

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	104.79Å 134.30Å 275.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.44 – 2.46 39.44 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.44-2.46) 98.2 (39.44-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.188 , 0.223 0.187 , 0.222	Depositor DCC
R_{free} test set	4058 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15215	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: MWY, 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	0.26	0/3828	0.47	0/5182
1	B	0.26	0/3827	0.47	0/5180
1	C	0.26	0/3746	0.46	0/5070
1	D	0.26	0/3601	0.47	0/4871
All	All	0.26	0/15002	0.47	0/20303

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3738	0	3833	27	0
1	B	3737	0	3836	33	0
1	C	3659	0	3750	30	0
1	D	3517	0	3623	34	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
3	A	66	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	66	0	0	1	0
3	C	66	0	0	3	0
3	D	66	0	0	3	0
4	A	47	0	0	0	0
4	B	32	0	0	0	0
4	C	25	0	0	0	0
4	D	24	0	0	0	0
All	All	15215	0	15162	125	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 4.

All (125) 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:268:ARG:HD2	1:B:273:GLN:HB2	1.68	0.75
1:C:87:PRO:HG3	1:C:430:ILE:HD11	1.68	0.74
1:D:188:SER:HA	1:D:271:PHE:HB2	1.69	0.73
1:D:87:PRO:HG3	1:D:430:ILE:HD11	1.74	0.68
1:D:117:ALA:HB1	1:D:301:ILE:HG13	1.78	0.65
1:A:87:PRO:HG3	1:A:430:ILE:HD11	1.78	0.65
1:C:119:SER:O	3:C:603:MWY:N32	2.32	0.63
1:C:243:LYS:O	1:C:247:ASN:ND2	2.32	0.63
1:B:339:LEU:HD11	1:B:345:PRO:HB3	1.81	0.62
1:C:117:ALA:HB1	1:C:301:ILE:HG13	1.82	0.61
1:A:117:ALA:HB1	1:A:301:ILE:HG13	1.82	0.61
1:B:38:ILE:HD11	1:B:386:VAL:HG21	1.86	0.58
1:B:85:THR:HB	1:B:401:LEU:HD21	1.86	0.57
1:B:260:ARG:HG3	1:B:268:ARG:NH2	2.20	0.56
1:D:369:VAL:HA	1:D:482:LEU:HB3	1.88	0.56
1:A:349:ALA:O	1:A:353:MET:HG3	2.06	0.56
1:C:38:ILE:HD11	1:C:386:VAL:HG21	1.89	0.55
1:C:244:ASP:OD1	1:C:245:THR:N	2.39	0.55
1:A:209:LYS:HE3	1:A:244:ASP:HB3	1.88	0.55
1:C:146:PHE:HE2	1:C:453:LEU:HD11	1.71	0.55
1:A:154:ASP:OD1	1:A:457:ARG:NH1	2.26	0.54
1:D:172:LEU:HD11	1:D:490:LEU:HD12	1.90	0.54
1:A:202:PRO:HB2	1:A:248:PHE:CZ	2.43	0.53
1:D:319:TYR:HB2	1:D:488:ILE:HD13	1.90	0.53
1:D:85:THR:HB	1:D:401:LEU:HD21	1.91	0.53
1:B:117:ALA:HB1	1:B:301:ILE:HG13	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:ILE:HD11	1:D:386:VAL:HG21	1.91	0.53
1:B:136:THR:HG23	1:B:274:LEU:HD22	1.91	0.52
1:D:128:ARG:NH1	1:D:288:LYS:O	2.43	0.52
1:D:246:ILE:HD13	1:D:300:ILE:HG21	1.92	0.52
1:B:319:TYR:HB2	1:B:488:ILE:HD13	1.91	0.52
1:B:172:LEU:HD11	1:B:490:LEU:HD12	1.91	0.52
1:B:139:SER:HA	1:B:142:LEU:HB3	1.91	0.52
1:B:188:SER:HA	1:B:271:PHE:HB2	1.91	0.51
1:A:335:ILE:HA	1:A:353:MET:HE1	1.93	0.51
1:D:223:ILE:HD11	1:D:233:PHE:HD2	1.76	0.51
1:C:128:ARG:NH2	1:C:294:GLU:OE2	2.44	0.50
1:B:155:VAL:HG13	1:B:158:ARG:HH12	1.76	0.50
1:B:294:GLU:O	1:B:298:GLN:HG2	2.11	0.50
1:B:262:ASN:OD1	1:B:263:ASP:N	2.45	0.50
1:A:126:TRP:CZ2	1:A:439:ARG:HD2	2.46	0.50
1:A:38:ILE:HD11	1:A:386:VAL:HG21	1.92	0.50
1:C:279:GLN:NE2	1:C:290:LEU:O	2.30	0.49
1:C:188:SER:HA	1:C:271:PHE:HB2	1.94	0.49
1:A:199:PRO:O	1:A:200:GLN:HB3	2.13	0.49
1:A:166:LYS:HG3	1:A:168:LYS:H	1.77	0.49
1:C:233:PHE:HB3	1:C:238:VAL:HG22	1.95	0.49
1:A:92:THR:HA	1:A:96:LYS:HB2	1.95	0.48
1:C:272:LEU:HD12	1:C:295:LEU:HD21	1.94	0.48
1:A:169:PRO:HB2	1:A:489:VAL:HG12	1.96	0.48
1:B:143:LYS:HE2	1:B:347:TYR:CD2	2.49	0.48
1:B:355:TYR:HD1	1:B:358:MET:HE3	1.79	0.48
1:D:349:ALA:O	1:D:353:MET:HG3	2.14	0.48
1:C:242:PRO:HG2	1:C:245:THR:HB	1.96	0.48
1:B:369:VAL:HA	1:B:482:LEU:HB3	1.96	0.47
1:B:155:VAL:HA	1:B:158:ARG:NH2	2.30	0.47
1:D:423:LYS:HD3	1:D:423:LYS:HA	1.68	0.47
1:D:106:ARG:O	3:D:603:MWY:N30	2.47	0.47
1:D:62:THR:HG22	1:D:400:ALA:HA	1.96	0.47
1:D:148:ILE:O	1:D:151:GLN:HG2	2.14	0.47
1:B:150:ALA:HA	1:B:453:LEU:HD11	1.97	0.46
1:D:355:TYR:HD1	1:D:358:MET:HE3	1.79	0.46
1:A:169:PRO:HB2	1:A:489:VAL:CG1	2.45	0.46
1:B:189:PHE:HB2	1:B:191:VAL:HG12	1.97	0.46
1:B:87:PRO:HG3	1:B:430:ILE:HD11	1.97	0.46
1:C:173:LYS:HE3	1:C:487:PRO:HB3	1.98	0.46
1:D:294:GLU:O	1:D:298:GLN:HG2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:TYR:HD1	1:A:358:MET:HE3	1.81	0.46
1:B:126:TRP:CZ2	1:B:439:ARG:HD2	2.51	0.45
1:D:246:ILE:HG23	1:D:300:ILE:HD13	1.98	0.45
1:C:146:PHE:CE2	1:C:453:LEU:HD11	2.50	0.45
1:A:168:LYS:HD2	1:A:168:LYS:HA	1.72	0.45
1:B:118:ILE:HD11	1:B:130:ARG:HD2	1.98	0.45
1:C:168:LYS:HD3	1:C:169:PRO:O	2.17	0.45
1:D:310:THR:HG23	1:D:451:MET:HG2	1.98	0.45
1:A:465:LYS:HE3	1:A:491:LYS:HD2	1.98	0.45
1:B:393:MET:HE3	1:B:393:MET:HB2	1.82	0.45
1:C:319:TYR:CZ	1:C:474:LEU:HB2	2.52	0.45
3:C:602:MWY:C12	3:C:602:MWY:C08	2.94	0.45
1:A:172:LEU:HD11	1:A:490:LEU:HD12	1.99	0.45
1:C:208:LYS:O	1:C:212:LYS:HE2	2.17	0.44
1:A:351:VAL:HG23	1:A:352:GLN:HG3	1.99	0.44
1:B:189:PHE:CE2	1:B:303:ILE:HD11	2.51	0.44
1:B:480:GLY:HA2	3:B:603:MWY:C15	2.47	0.44
1:C:172:LEU:HD11	1:C:490:LEU:HD12	1.99	0.44
1:D:254:ASN:HA	1:D:257:LYS:HG2	1.99	0.44
1:C:126:TRP:CZ2	1:C:439:ARG:HD2	2.52	0.44
1:C:46:LEU:O	1:C:77:GLY:HA2	2.18	0.44
1:C:57:LEU:HA	1:C:57:LEU:HD23	1.86	0.44
1:A:163:GLU:O	1:A:166:LYS:HG2	2.18	0.43
1:D:335:ILE:HA	1:D:353:MET:HE1	2.00	0.43
1:B:310:THR:HG23	1:B:451:MET:HG2	2.00	0.43
1:A:335:ILE:HG12	1:A:353:MET:HE1	2.01	0.43
1:C:85:THR:HB	1:C:401:LEU:HD21	2.01	0.43
1:A:331:LEU:O	1:A:335:ILE:HG13	2.19	0.43
1:B:423:LYS:HA	1:B:423:LYS:HD3	1.81	0.43
1:A:177:GLY:HA2	1:A:311:SER:OG	2.19	0.42
1:C:128:ARG:NH1	1:C:288:LYS:O	2.53	0.42
1:A:329:GLN:O	1:A:333:LYS:HG2	2.20	0.42
1:A:468:LYS:HG2	1:A:469:GLU:HG2	1.99	0.42
1:C:319:TYR:HB2	1:C:488:ILE:HD13	2.02	0.42
1:D:119:SER:O	3:D:603:MWY:N32	2.52	0.42
1:C:206:SER:HB3	1:C:245:THR:HG23	2.01	0.42
1:C:348:ASP:O	1:C:352:GLN:HG2	2.19	0.42
1:D:335:ILE:HG12	1:D:353:MET:HE1	2.01	0.42
1:B:269:LEU:HD12	1:B:274:LEU:HD11	2.01	0.42
1:D:276:ILE:HD13	1:D:276:ILE:HA	1.83	0.42
1:D:118:ILE:HD12	1:D:133:LEU:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:HD2	1:A:169:PRO:HD2	2.01	0.42
1:D:159:ASN:N	1:D:159:ASN:HD22	2.18	0.42
1:C:105:ARG:HB2	3:C:603:MWY:C29	2.50	0.41
1:B:23:ALA:O	1:B:28:ARG:NH1	2.53	0.41
1:D:173:LYS:HE3	1:D:173:LYS:HB2	1.87	0.41
1:B:160:LEU:HA	1:B:175:ILE:HD13	2.03	0.41
1:B:383:ILE:HB	1:B:388:ILE:HD13	2.03	0.41
1:A:166:LYS:HG3	1:A:168:LYS:HB2	2.02	0.41
1:C:188:SER:O	1:C:272:LEU:HB2	2.20	0.41
1:C:260:ARG:NH2	1:C:272:LEU:HD23	2.35	0.41
1:D:476:LEU:HD13	1:D:482:LEU:HD11	2.03	0.41
1:D:105:ARG:HB2	3:D:603:MWY:C29	2.51	0.41
1:B:163:GLU:HA	1:B:166:LYS:HD3	2.03	0.40
1:D:126:TRP:CZ2	1:D:439:ARG:HD2	2.56	0.40
1:D:132:LEU:HD13	1:D:290:LEU:HD23	2.03	0.40
1:D:251:LYS:HB3	1:D:251:LYS:HE3	1.91	0.40
1:D:90:ILE:HG23	1:D:396:ILE:HG12	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	461/480 (96%)	447 (97%)	14 (3%)	0	100	100
1	B	461/480 (96%)	446 (97%)	15 (3%)	0	100	100
1	C	450/480 (94%)	438 (97%)	12 (3%)	0	100	100
1	D	430/480 (90%)	415 (96%)	15 (4%)	0	100	100
All	All	1802/1920 (94%)	1746 (97%)	56 (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	421/434 (97%)	414 (98%)	7 (2%)	60	73
1	B	420/434 (97%)	406 (97%)	14 (3%)	38	49
1	C	413/434 (95%)	409 (99%)	4 (1%)	76	84
1	D	395/434 (91%)	390 (99%)	5 (1%)	69	79
All	All	1649/1736 (95%)	1619 (98%)	30 (2%)	59	71

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	SER
1	A	158	ARG
1	A	200	GLN
1	A	348	ASP
1	A	415	ARG
1	A	424	ASP
1	A	469	GLU
1	B	24	LEU
1	B	107	SER
1	B	158	ARG
1	B	196	LEU
1	B	197	ASN
1	B	200	GLN
1	B	204	VAL
1	B	244	ASP
1	B	260	ARG
1	B	264	LYS
1	B	266	LYS
1	B	268	ARG
1	B	341	ASN
1	B	486	LYS
1	C	205	GLU
1	C	212	LYS
1	C	238	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	439	ARG
1	D	159	ASN
1	D	168	LYS
1	D	244	ASP
1	D	425	SER
1	D	439	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	GLN
1	B	192	ASN
1	B	197	ASN
1	B	237	ASN
1	C	247	ASN
1	C	329	GLN
1	D	78	GLN
1	D	159	ASN
1	D	254	ASN
1	D	384	ASN
1	D	483	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)

12 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	$\#\|Z\| > 2$
3	MWY	B	602	-	32,36,36	0.38	0	41,57,57	0.49	0
3	MWY	A	603	-	32,36,36	0.42	0	41,57,57	0.61	1 (2%)
3	MWY	A	602	-	32,36,36	0.47	1 (3%)	41,57,57	0.51	0
2	HEM	C	601	1	41,50,50	1.29	4 (9%)	45,82,82	1.82	9 (20%)
3	MWY	B	603	-	32,36,36	0.54	0	41,57,57	0.91	1 (2%)
3	MWY	D	603	-	32,36,36	0.39	0	41,57,57	0.57	0
3	MWY	C	603	-	32,36,36	0.38	0	41,57,57	0.54	0
2	HEM	A	601	1	41,50,50	1.30	4 (9%)	45,82,82	1.75	11 (24%)
3	MWY	C	602	-	32,36,36	0.60	0	41,57,57	0.72	0
3	MWY	D	602	-	32,36,36	0.34	0	41,57,57	0.49	0
2	HEM	D	601	1	41,50,50	1.30	4 (9%)	45,82,82	1.77	11 (24%)
2	HEM	B	601	1	41,50,50	1.30	4 (9%)	45,82,82	1.83	10 (22%)

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
3	MWY	B	602	-	-	0/9/73/73	0/4/4/4
3	MWY	A	603	-	-	0/9/73/73	0/4/4/4
3	MWY	A	602	-	-	1/9/73/73	0/4/4/4
2	HEM	C	601	1	-	3/12/54/54	-
3	MWY	B	603	-	-	0/9/73/73	1/4/4/4
3	MWY	D	603	-	-	0/9/73/73	0/4/4/4
3	MWY	C	603	-	-	0/9/73/73	0/4/4/4
2	HEM	A	601	1	-	3/12/54/54	-
3	MWY	C	602	-	-	1/9/73/73	1/4/4/4
3	MWY	D	602	-	-	1/9/73/73	0/4/4/4
2	HEM	D	601	1	-	2/12/54/54	-
2	HEM	B	601	1	-	2/12/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C1B-NB	-3.34	1.34	1.40
2	A	601	HEM	C1B-NB	-3.30	1.34	1.40
2	C	601	HEM	C1B-NB	-3.28	1.34	1.40
2	D	601	HEM	C1B-NB	-3.15	1.34	1.40
2	B	601	HEM	C4D-ND	-2.98	1.35	1.40
2	D	601	HEM	C4D-ND	-2.94	1.35	1.40
2	D	601	HEM	FE-NB	2.91	2.11	1.96
2	A	601	HEM	FE-NB	2.90	2.11	1.96
2	C	601	HEM	C4D-ND	-2.89	1.35	1.40
2	A	601	HEM	C4D-ND	-2.89	1.35	1.40
2	B	601	HEM	FE-NB	2.86	2.11	1.96
2	C	601	HEM	FE-NB	2.84	2.10	1.96
2	D	601	HEM	CHB-C1B	2.18	1.40	1.35
3	A	602	MWY	C04-C03	2.17	1.58	1.55
2	B	601	HEM	CHB-C1B	2.14	1.40	1.35
2	A	601	HEM	CHB-C1B	2.12	1.40	1.35
2	C	601	HEM	CHB-C1B	2.10	1.40	1.35

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	HEM	CHC-C4B-NB	4.89	129.74	124.43
2	C	601	HEM	CHC-C4B-NB	4.83	129.68	124.43
2	D	601	HEM	CHC-C4B-NB	4.69	129.52	124.43
2	A	601	HEM	CHC-C4B-NB	4.50	129.32	124.43
2	D	601	HEM	CHD-C1D-ND	4.45	129.27	124.43
2	C	601	HEM	CHD-C1D-ND	4.44	129.26	124.43
2	B	601	HEM	CHD-C1D-ND	4.36	129.17	124.43
2	A	601	HEM	CHD-C1D-ND	4.18	128.97	124.43
2	C	601	HEM	C1B-NB-C4B	3.74	108.94	105.07
2	C	601	HEM	CHB-C1B-NB	3.68	128.93	124.38
2	A	601	HEM	C1B-NB-C4B	3.67	108.86	105.07
2	B	601	HEM	C1B-NB-C4B	3.60	108.79	105.07
2	D	601	HEM	CHA-C4D-ND	3.55	128.77	124.38
2	A	601	HEM	CHB-C1B-NB	3.53	128.75	124.38
2	B	601	HEM	CHB-C1B-NB	3.53	128.74	124.38
2	B	601	HEM	CHA-C4D-ND	3.52	128.73	124.38
2	D	601	HEM	C1B-NB-C4B	3.50	108.69	105.07
2	D	601	HEM	CHB-C1B-NB	3.47	128.67	124.38
2	A	601	HEM	CHA-C4D-ND	3.42	128.60	124.38
2	C	601	HEM	CHA-C4D-ND	3.40	128.58	124.38
2	C	601	HEM	CHD-C1D-C2D	-2.89	120.47	124.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	HEM	CHD-C1D-C2D	-2.81	120.58	124.98
2	B	601	HEM	CHD-C1D-C2D	-2.72	120.73	124.98
2	A	601	HEM	CHD-C1D-C2D	-2.61	120.90	124.98
3	B	603	MWY	C08-C07-C06	2.45	113.78	111.37
2	B	601	HEM	CMC-C2C-C3C	2.42	129.20	124.68
2	B	601	HEM	CHA-C4D-C3D	-2.30	121.00	125.33
2	A	601	HEM	CHA-C4D-C3D	-2.24	121.13	125.33
2	D	601	HEM	CHA-C4D-C3D	-2.20	121.19	125.33
2	B	601	HEM	C4B-C3B-C2B	-2.17	105.39	107.11
2	C	601	HEM	CHB-C1B-C2B	-2.16	120.74	126.72
3	A	603	MWY	C33-C03-C17	-2.16	104.41	108.73
2	C	601	HEM	CHA-C4D-C3D	-2.15	121.29	125.33
2	A	601	HEM	CHB-C1B-C2B	-2.13	120.84	126.72
2	B	601	HEM	CHB-C1B-C2B	-2.11	120.88	126.72
2	D	601	HEM	CHB-C1B-C2B	-2.10	120.92	126.72
2	A	601	HEM	O2D-CGD-CBD	2.08	120.72	114.03
2	A	601	HEM	O2A-CGA-CBA	2.07	120.68	114.03
2	D	601	HEM	O2A-CGA-CBA	2.06	120.64	114.03
2	D	601	HEM	O2D-CGD-CBD	2.05	120.62	114.03
2	A	601	HEM	C4B-C3B-C2B	-2.05	105.49	107.11
2	D	601	HEM	C4D-ND-C1D	2.04	107.18	105.07
2	C	601	HEM	O2D-CGD-CBD	2.03	120.54	114.03

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	MWY	C23-C25-S26-C27
3	A	602	MWY	C23-C25-S26-C27
3	D	602	MWY	O22-C23-C25-S26
2	A	601	HEM	CAA-CBA-CGA-O2A
2	C	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAD-CBD-CGD-O2D
2	C	601	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAD-CBD-CGD-O1D
2	C	601	HEM	CAD-CBD-CGD-O2D
2	D	601	HEM	CAD-CBD-CGD-O2D
2	D	601	HEM	CAD-CBD-CGD-O1D

All (2) ring outliers are listed below:

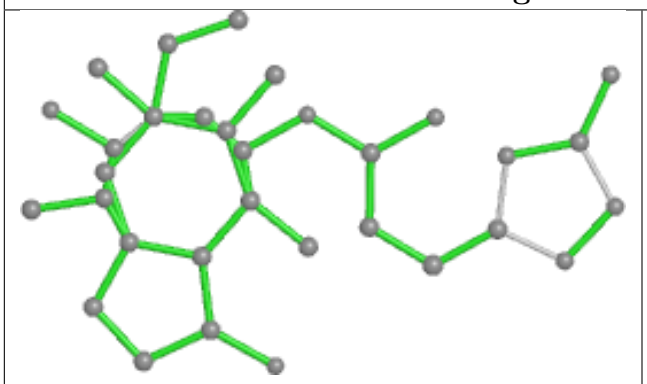
Mol	Chain	Res	Type	Atoms
3	B	603	MWY	C06-C07-C08-C09-C10-C11
3	C	602	MWY	C06-C07-C08-C09-C10-C11

4 monomers are involved in 7 short contacts:

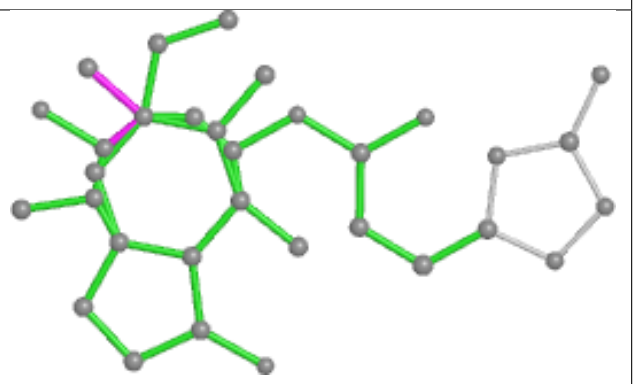
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	MWY	1	0
3	D	603	MWY	3	0
3	C	603	MWY	2	0
3	C	602	MWY	1	0

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 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.

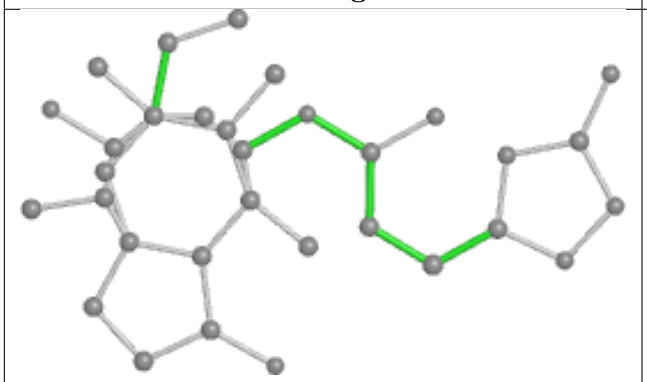
Ligand MWY A 603



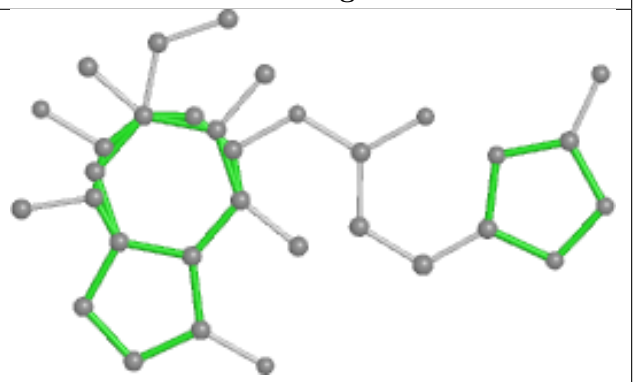
Bond lengths



Bond angles

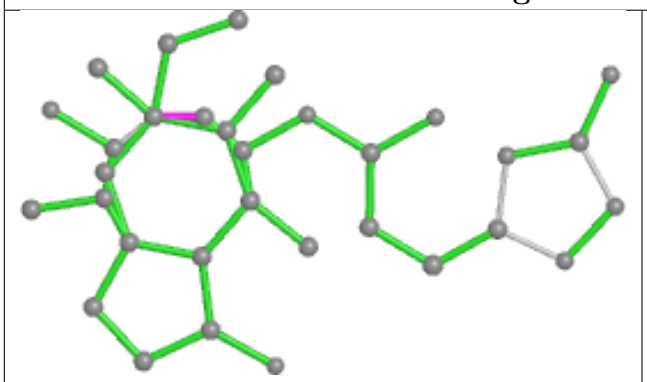


Torsions

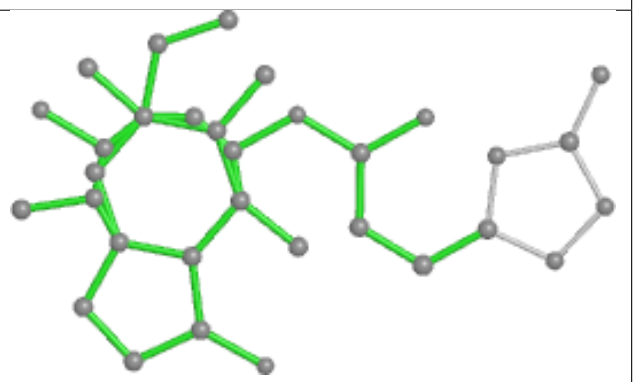


Rings

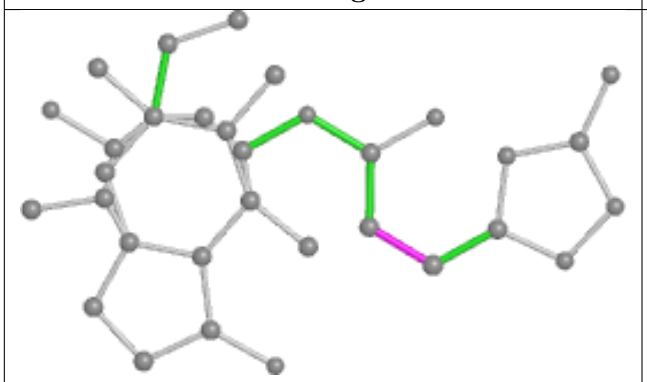
Ligand MWY A 602



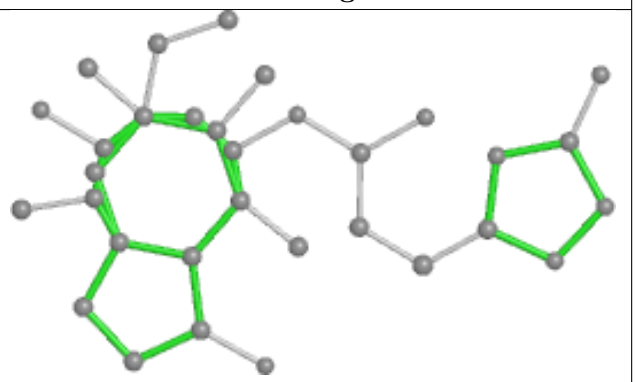
Bond lengths



Bond angles

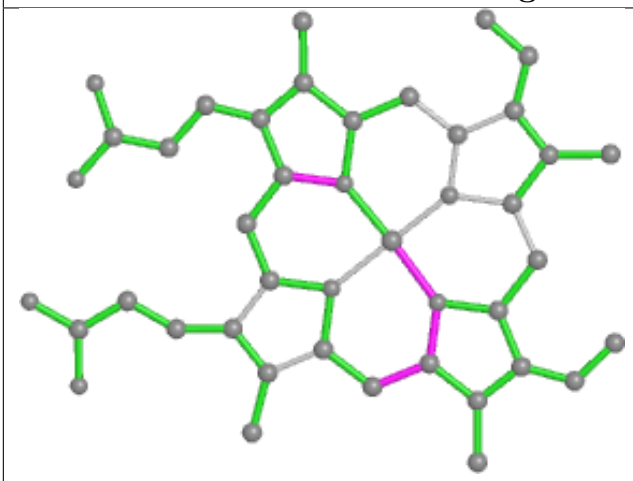


Torsions

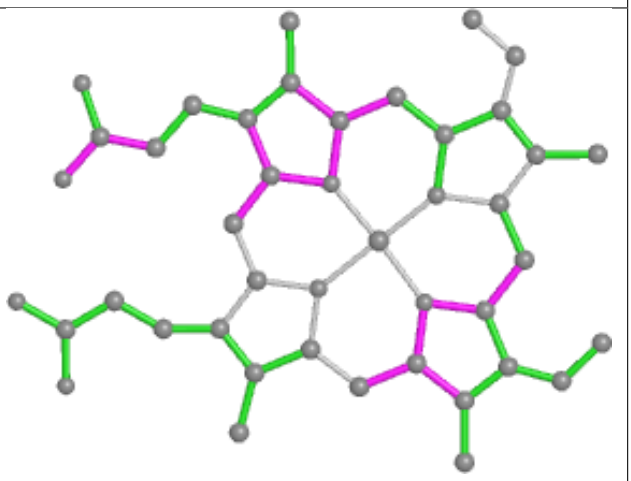


Rings

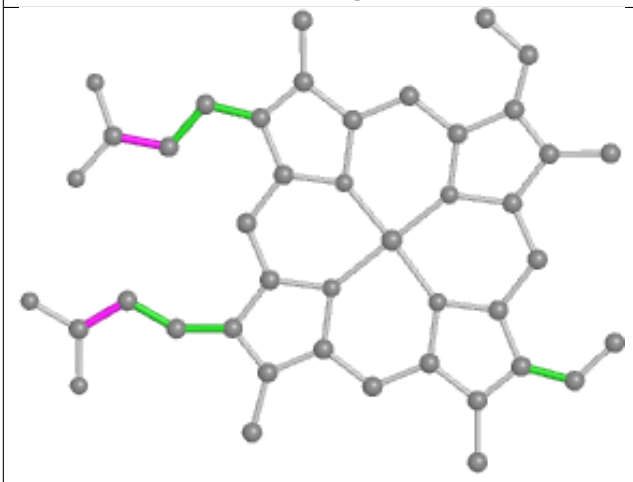
Ligand HEM C 601



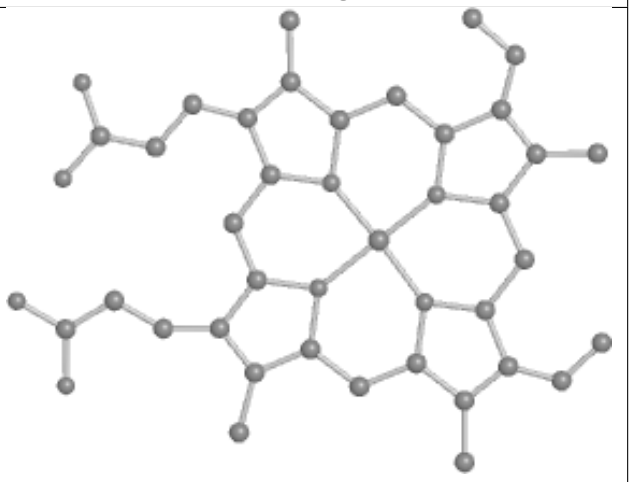
Bond lengths



Bond angles

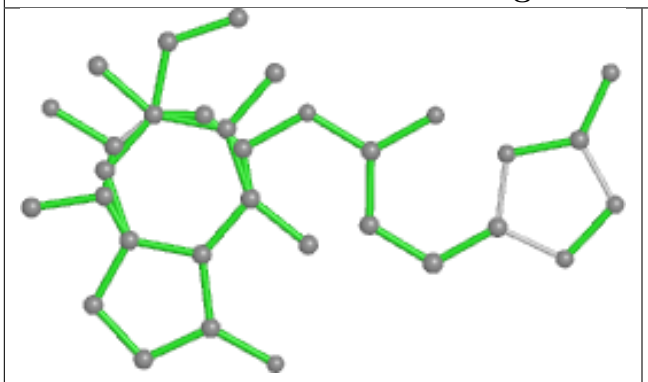


Torsions

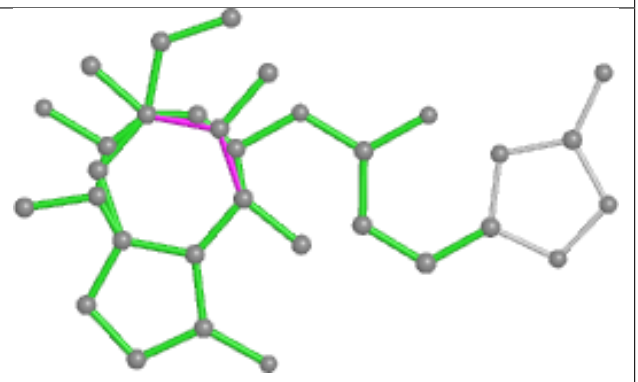


Rings

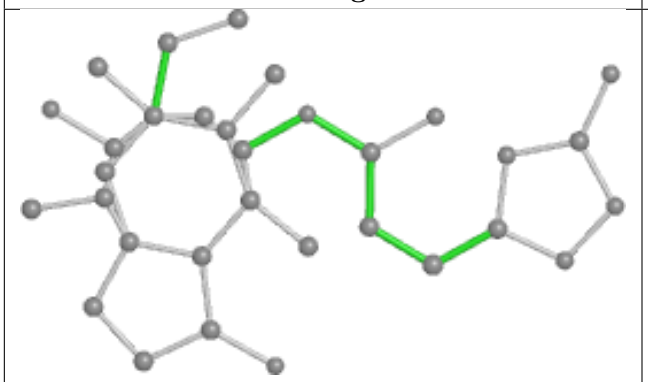
Ligand MWY B 603



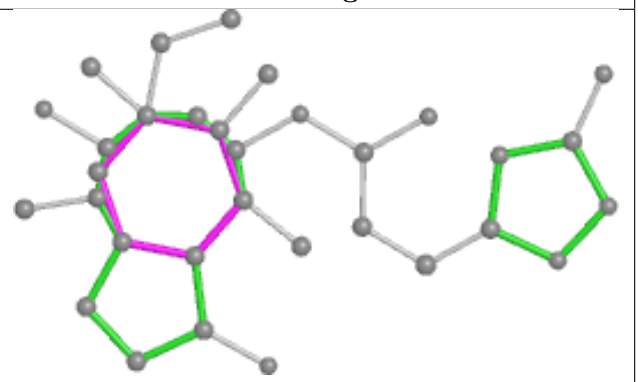
Bond lengths



Bond angles

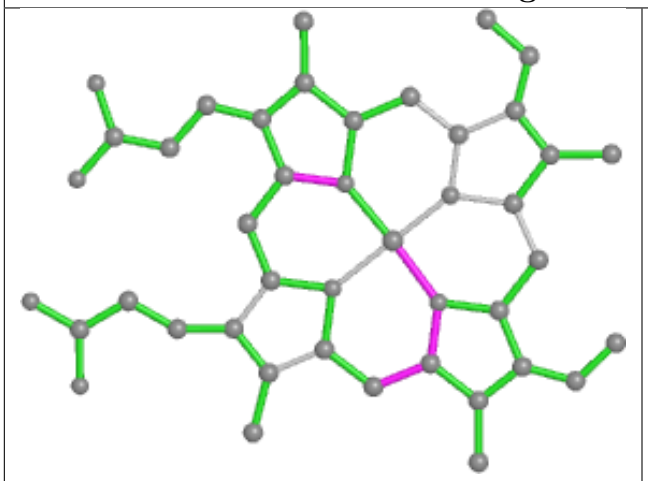


Torsions

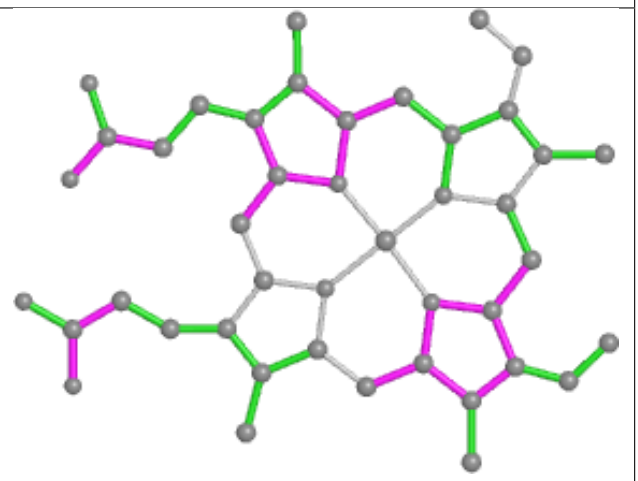


Rings

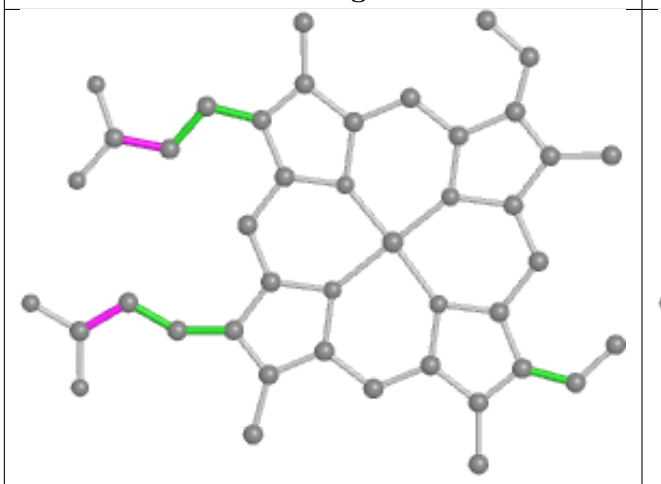
Ligand HEM A 601



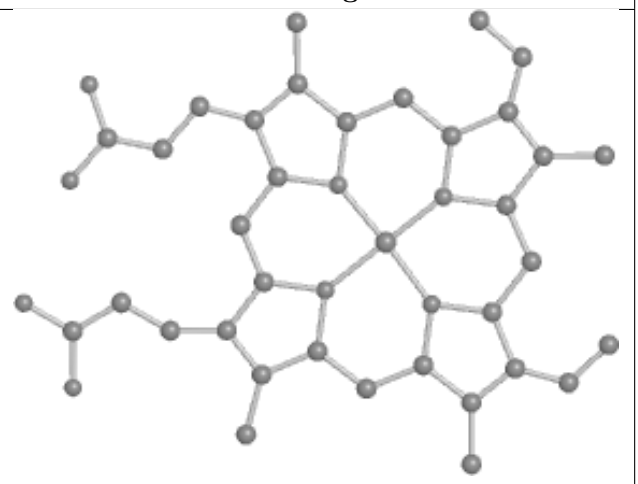
Bond lengths



Bond angles

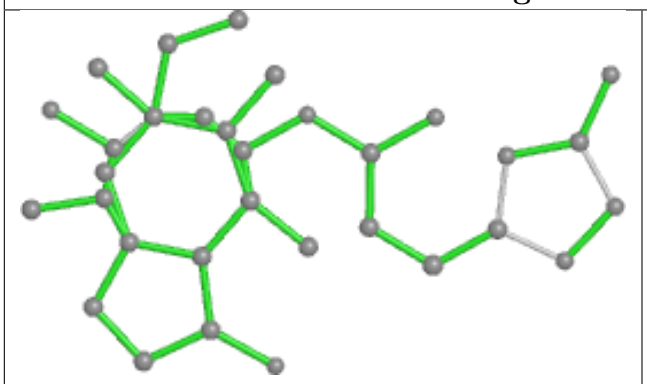


Torsions

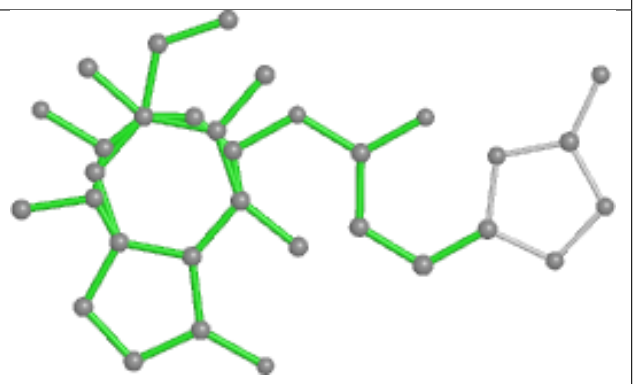


Rings

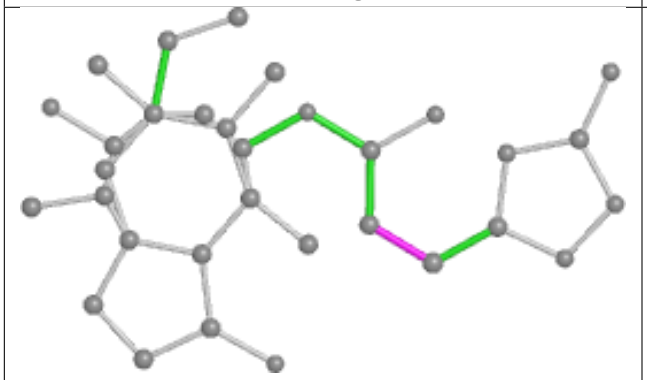
Ligand MWY C 602



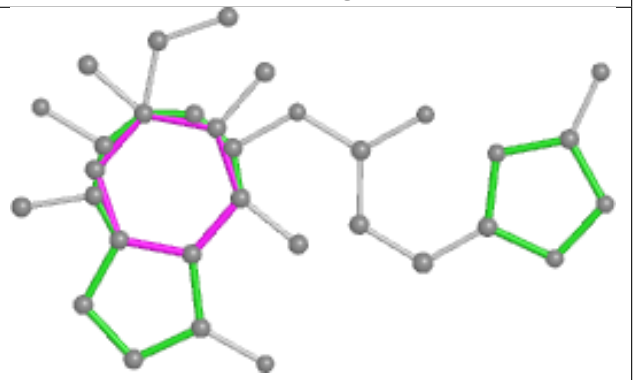
Bond lengths



Bond angles

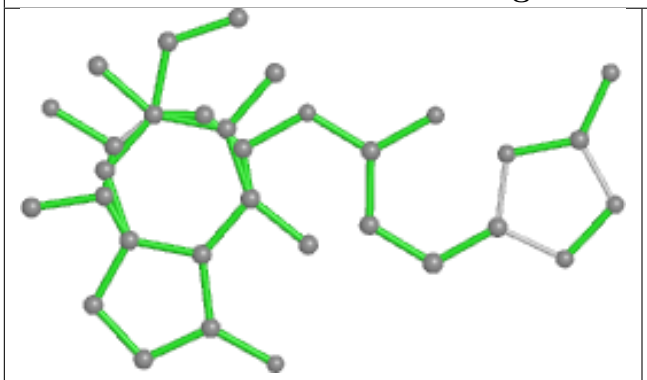


Torsions

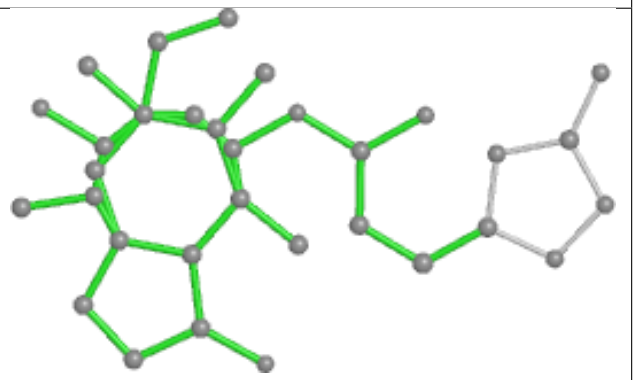


Rings

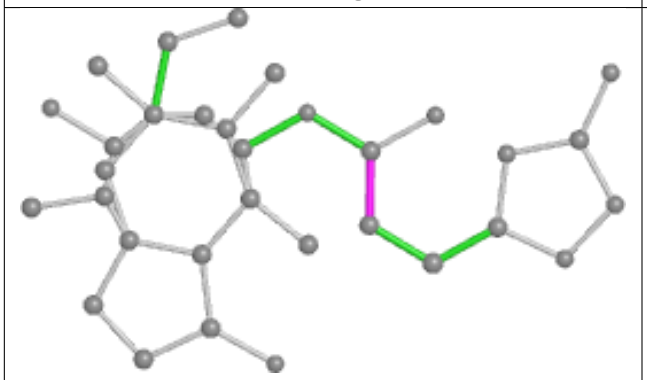
Ligand MWY D 602



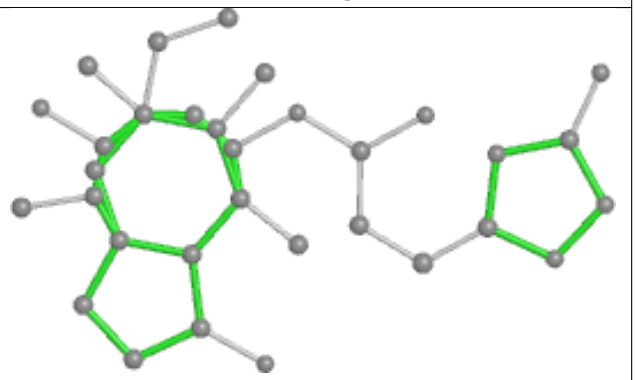
Bond lengths



Bond angles

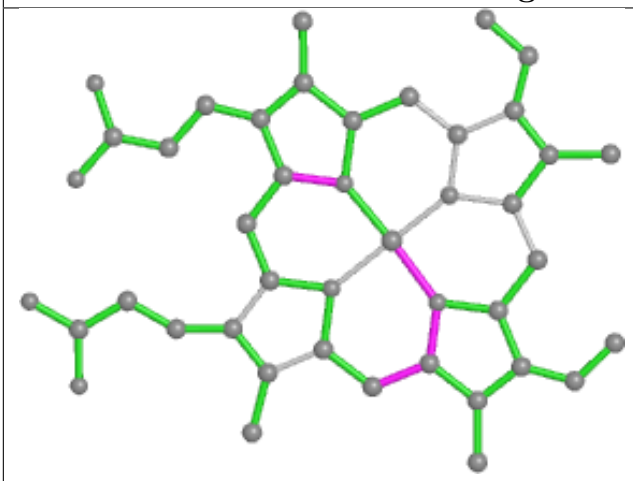


Torsions

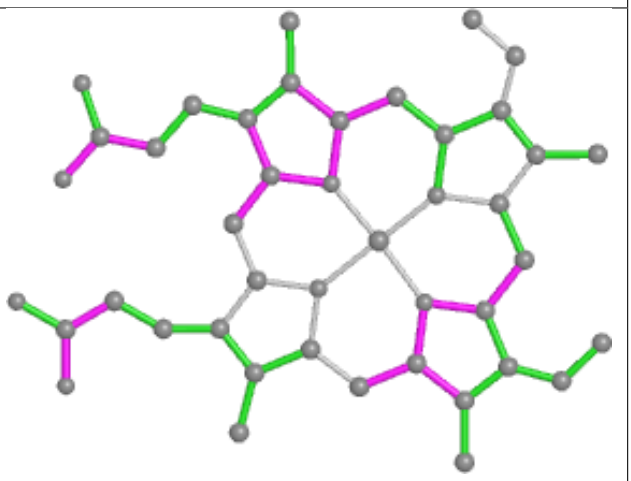


Rings

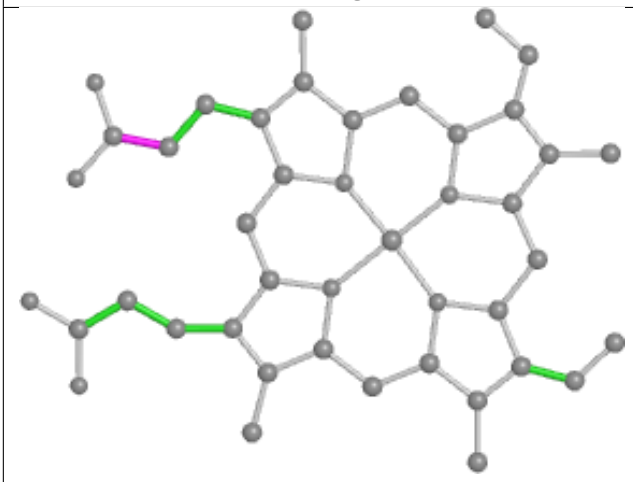
Ligand HEM D 601



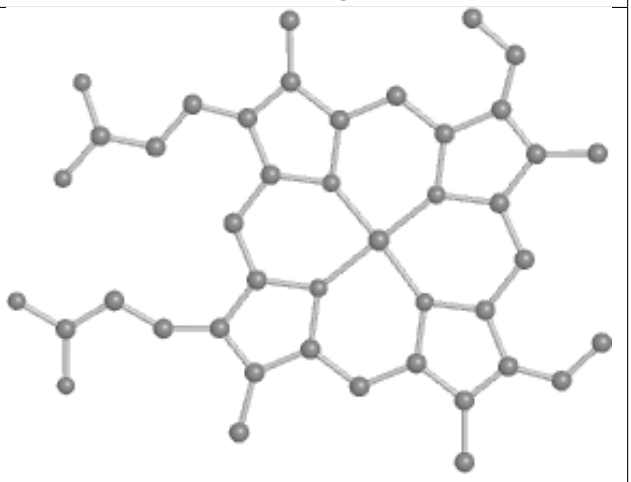
Bond lengths



Bond angles

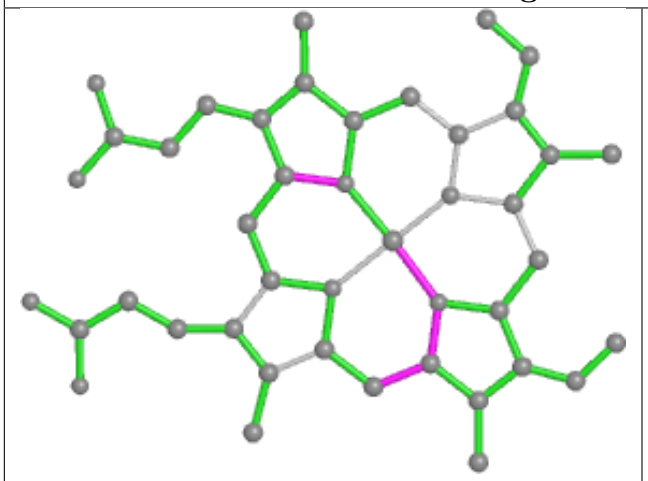


Torsions

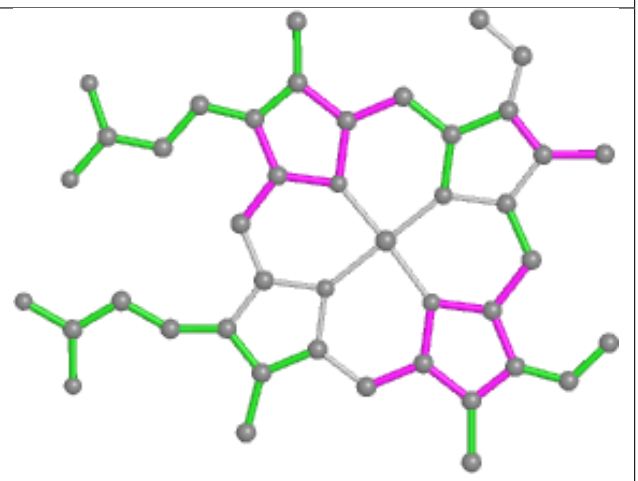


Rings

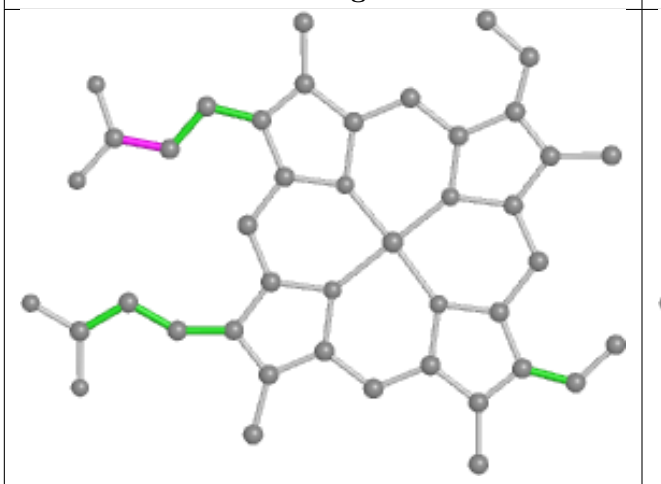
Ligand HEM B 601



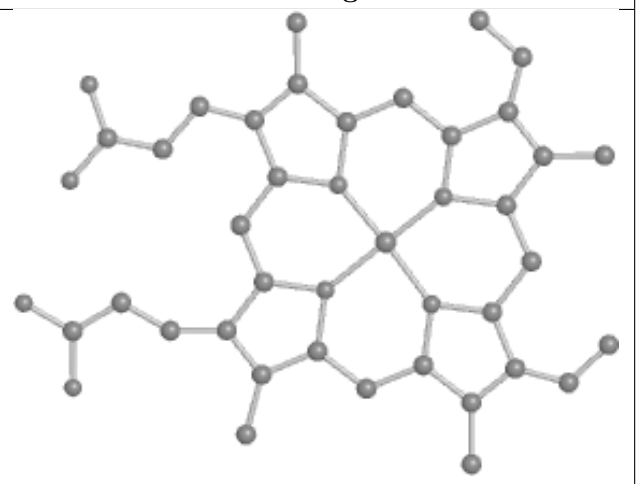
Bond lengths



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	465/480 (96%)	-0.17	11 (2%)	59	54	34, 52, 84, 112	0
1	B	465/480 (96%)	0.09	20 (4%)	35	32	38, 61, 116, 235	0
1	C	456/480 (95%)	0.01	21 (4%)	32	30	37, 61, 123, 186	0
1	D	438/480 (91%)	0.05	23 (5%)	26	23	33, 59, 104, 128	0
All	All	1824/1920 (95%)	-0.01	75 (4%)	37	34	33, 57, 108, 235	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	PHE	12.2
1	B	265	GLN	11.8
1	D	213	PHE	6.6
1	D	189	PHE	6.5
1	D	192	ASN	6.2
1	C	203	PHE	5.8
1	A	23	ALA	5.4
1	B	264	LYS	5.2
1	C	244	ASP	5.0
1	D	212	LYS	4.7
1	A	424	ASP	4.5
1	C	253	VAL	4.4
1	D	289	ALA	4.3
1	D	168	LYS	4.1
1	D	253	VAL	4.1
1	C	422	LYS	4.0
1	A	383	ILE	3.9
1	C	191	VAL	3.7
1	C	424	ASP	3.7
1	B	278	SER	3.6
1	D	383	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	279	GLN	3.5
1	B	383	ILE	3.5
1	A	264	LYS	3.4
1	D	275	MET	3.3
1	C	280	ASN	3.3
1	A	387	PHE	3.3
1	C	261	LEU	3.2
1	C	255	ARG	3.2
1	A	422	LYS	3.1
1	D	290	LEU	3.1
1	B	267	HIS	3.1
1	D	257	LYS	3.1
1	B	269	LEU	3.0
1	C	257	LYS	2.9
1	C	254	ASN	2.9
1	D	422	LYS	2.8
1	B	197	ASN	2.8
1	A	421	LYS	2.8
1	D	288	LYS	2.7
1	D	295	LEU	2.7
1	B	204	VAL	2.6
1	D	259	SER	2.6
1	A	280	ASN	2.6
1	D	190	GLY	2.6
1	A	388	ILE	2.6
1	B	206	SER	2.5
1	C	423	LYS	2.5
1	A	261	LEU	2.5
1	B	132	LEU	2.5
1	C	209	LYS	2.5
1	D	272	LEU	2.5
1	B	162	ARG	2.5
1	D	293	LEU	2.5
1	C	210	PHE	2.4
1	D	276	ILE	2.4
1	C	251	LYS	2.3
1	D	254	ASN	2.3
1	B	165	GLU	2.3
1	B	261	LEU	2.2
1	B	200	GLN	2.2
1	B	201	ASP	2.2
1	C	276	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	191	VAL	2.2
1	B	205	GLU	2.2
1	B	268	ARG	2.1
1	B	158	ARG	2.1
1	B	175	ILE	2.1
1	C	282	LYS	2.1
1	D	175	ILE	2.0
1	C	189	PHE	2.0
1	C	245	THR	2.0
1	B	213	PHE	2.0
1	D	255	ARG	2.0
1	A	203	PHE	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, 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	MWY	B	602	33/33	0.89	0.23	43,52,77,77	0
3	MWY	D	602	33/33	0.90	0.21	42,51,78,83	0
3	MWY	C	603	33/33	0.92	0.16	38,44,56,66	0
3	MWY	C	602	33/33	0.92	0.15	37,47,68,72	0
3	MWY	D	603	33/33	0.94	0.14	42,47,56,57	0
3	MWY	A	602	33/33	0.95	0.14	35,42,57,58	0
3	MWY	B	603	33/33	0.95	0.16	41,53,58,59	0
3	MWY	A	603	33/33	0.95	0.18	32,41,48,49	0
2	HEM	B	601	43/43	0.97	0.20	34,46,52,62	0
2	HEM	D	601	43/43	0.98	0.17	32,42,51,56	0
2	HEM	A	601	43/43	0.98	0.15	28,34,45,52	0

Continued on next page...

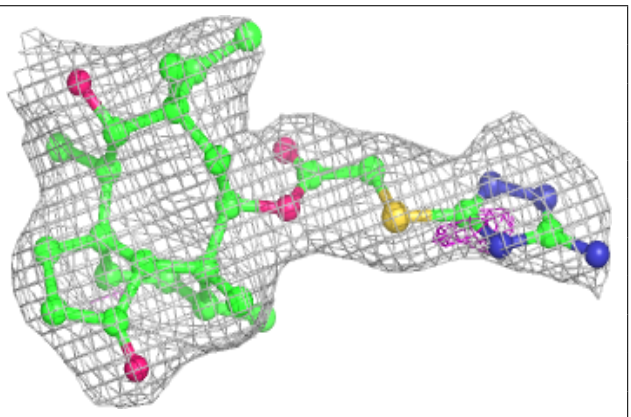
Continued from previous page...

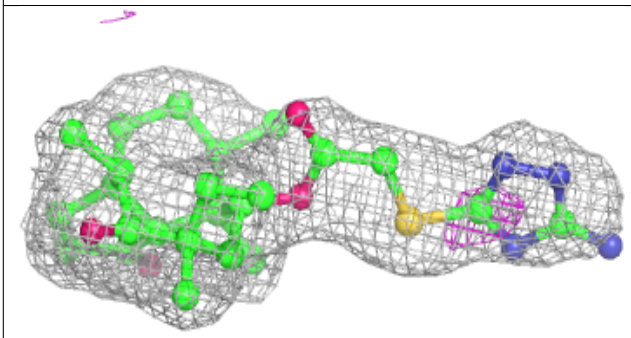
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	C	601	43/43	0.98	0.14	31,39,47,50	0

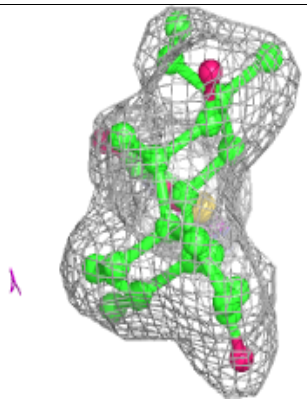
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MWY D 602:

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

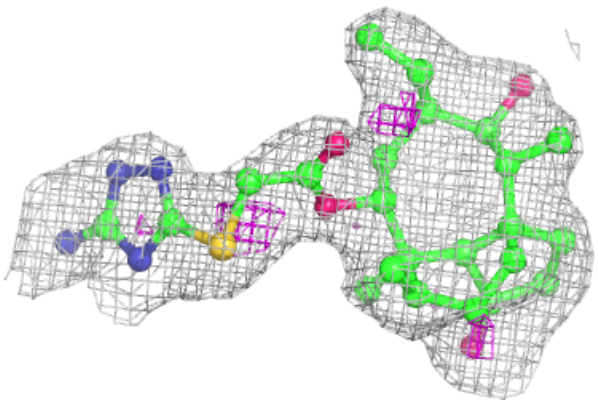


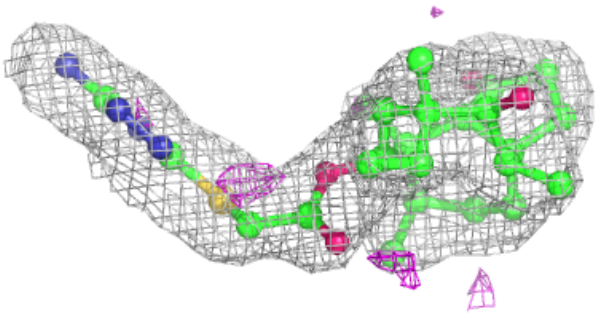


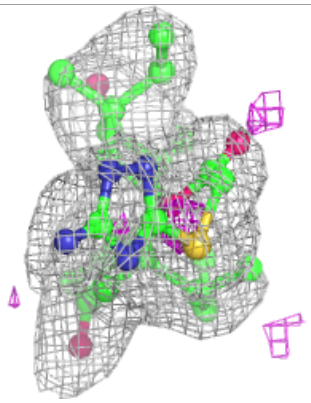


Electron density around MWY C 602:

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

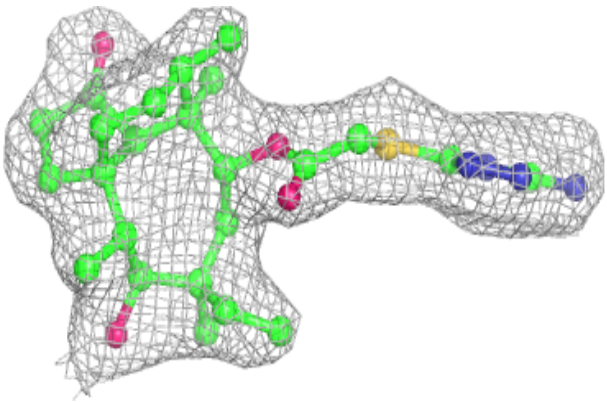


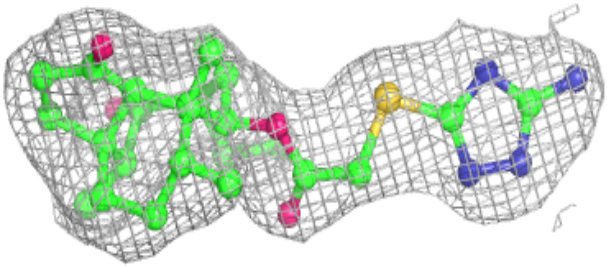




Electron density around MWY A 602:

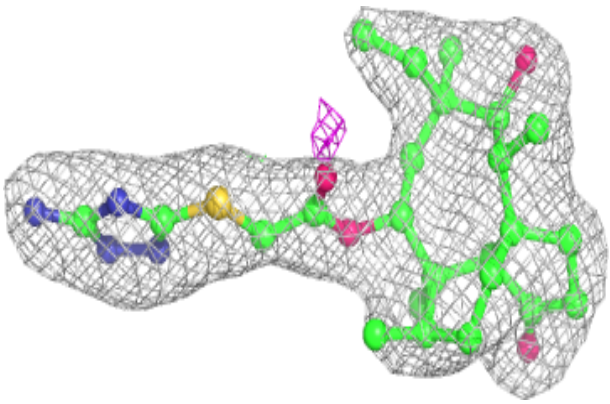
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

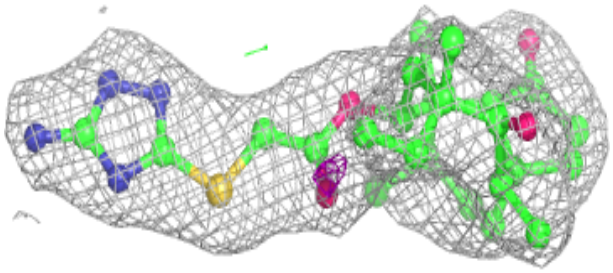


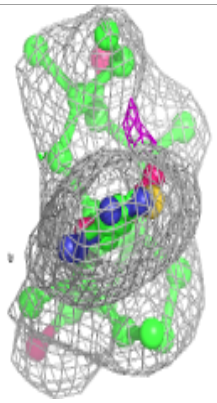


Electron density around MWY B 603:

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

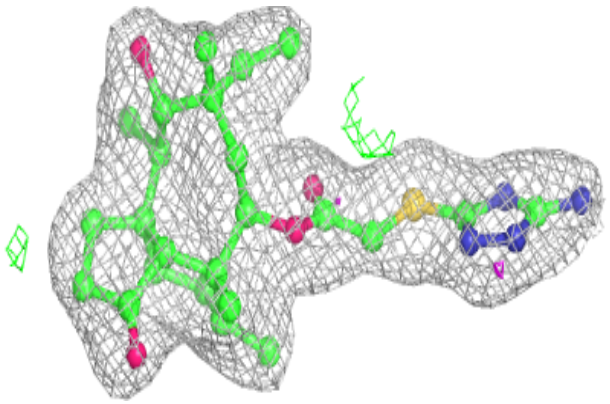


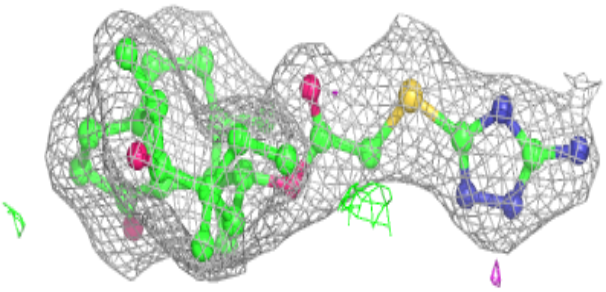


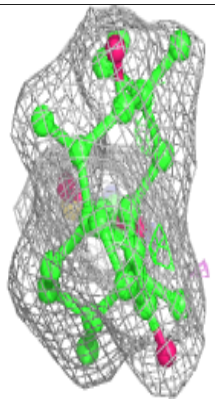


Electron density around MWY A 603:

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

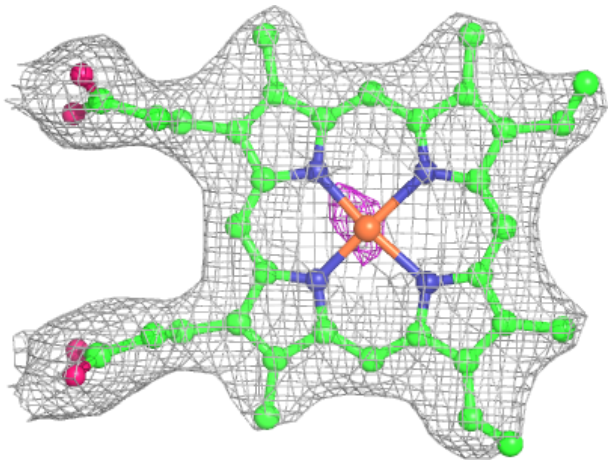


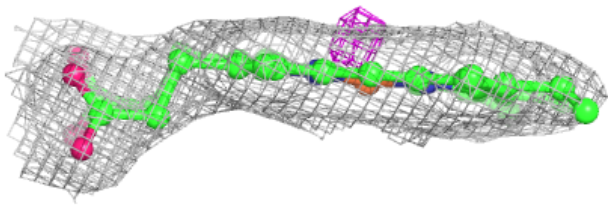


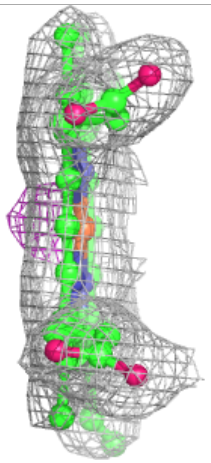


Electron density around HEM B 601:

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

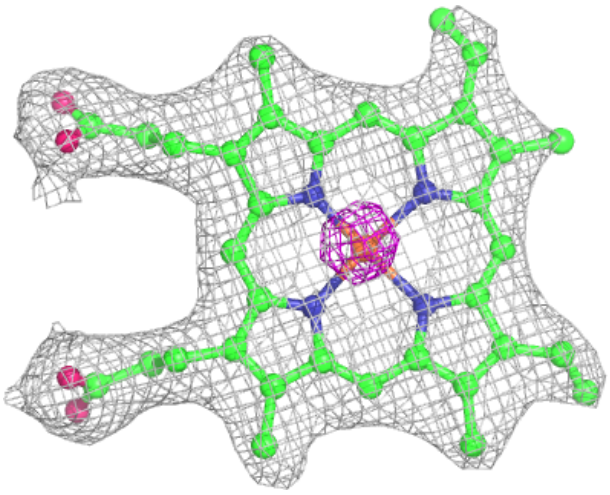


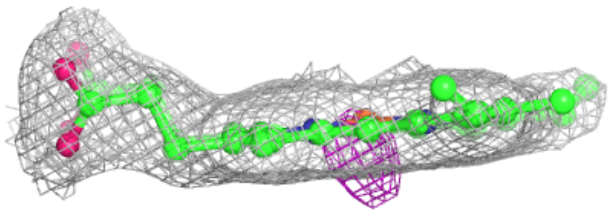


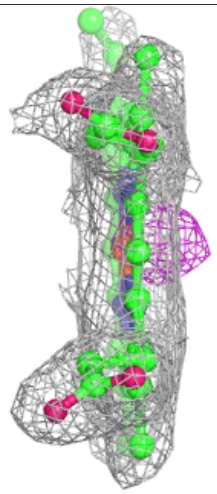


Electron density around HEM D 601:

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

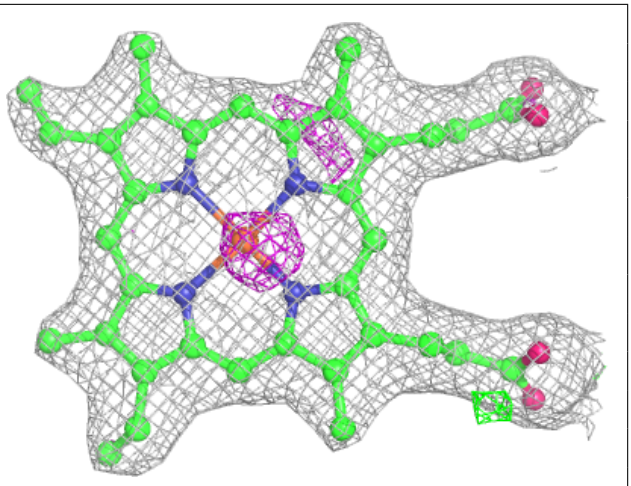


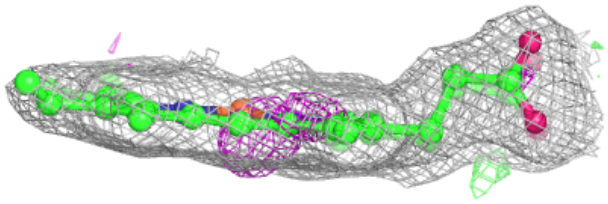


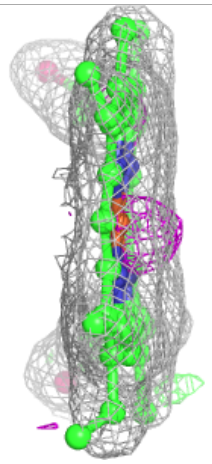


Electron density around HEM A 601:

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

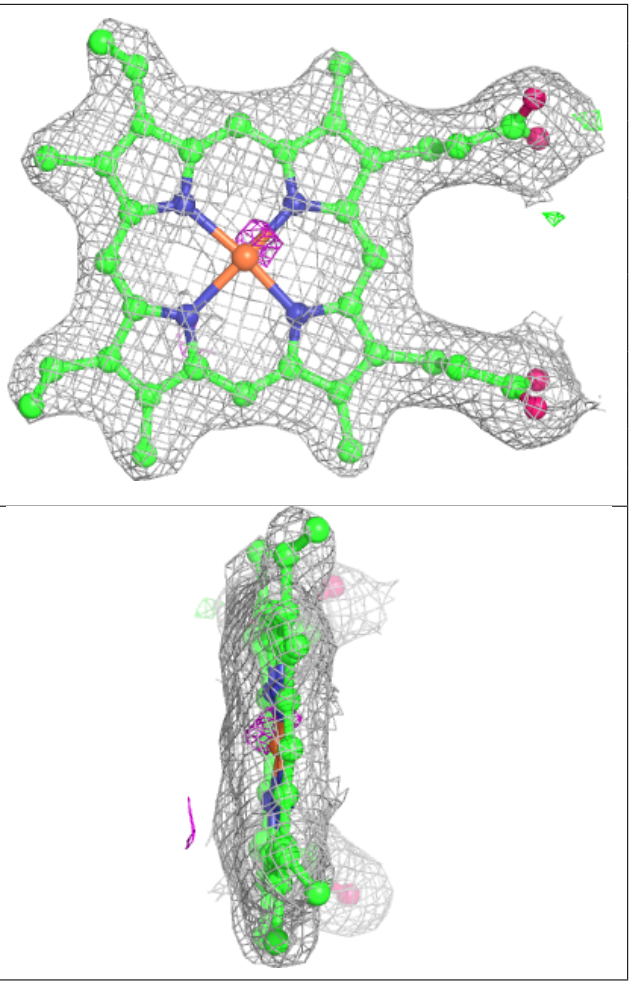






Electron density around HEM C 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.