Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:37 PM BST

PDB ID	:	6QZO
Title	:	Crystal structure of DyP-type peroxidase from Cellulomonas bogoriensis
Authors	:	Rozeboom, H.J.; Fraaije, M.W.
Deposited on	:	2019-03-12
Resolution	:	2.40 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 following versions of software and data (see references ⓘ) were used in the production of this report:

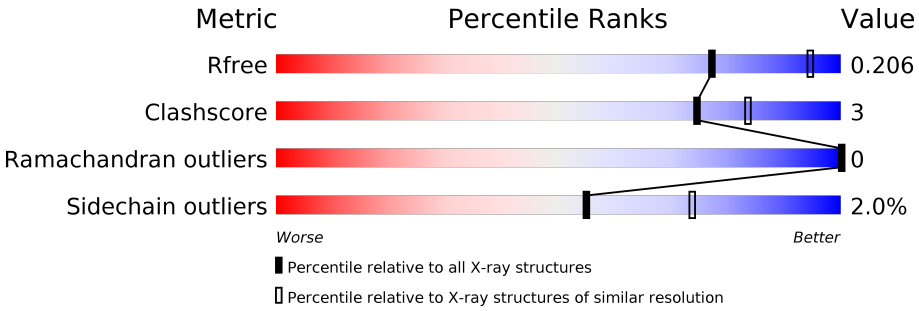
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 on 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%

Mol	Chain	Length	Quality of chain
1	A	383	86% 7% • 6%
1	B	383	87% 6% • 6%
1	C	383	87% 7% • 6%
1	D	383	88% 6% • 6%
1	E	383	89% • • 6%
1	F	383	87% 6% • 6%
1	G	383	88% 6% • 6%

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Mol	Chain	Length	Quality of chain
1	H	383	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22946 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.

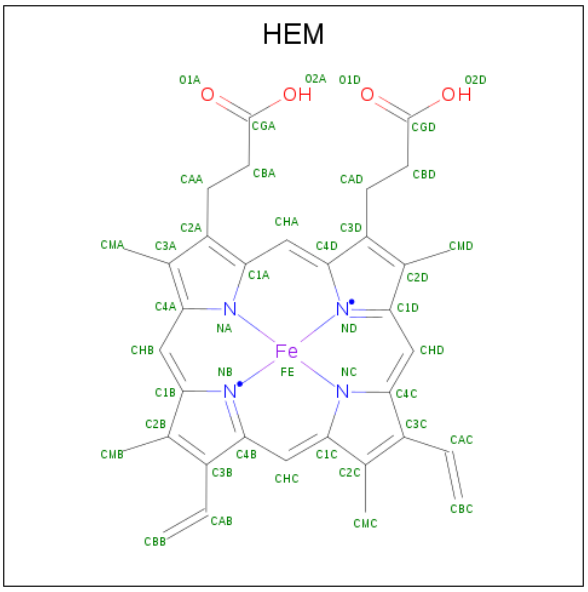
- Molecule 1 is a protein called Peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2770	1729	512	522	7			
1	B	361	Total	C	N	O	S	0	0	0
			2770	1729	512	522	7			
1	C	361	Total	C	N	O	S	0	0	0
			2770	1729	512	522	7			
1	D	361	Total	C	N	O	S	0	0	0
			2770	1729	512	522	7			
1	E	361	Total	C	N	O	S	0	0	0
			2770	1729	512	522	7			
1	F	361	Total	C	N	O	S	0	0	0
			2770	1729	512	522	7			
1	G	361	Total	C	N	O	S	0	0	0
			2770	1729	512	522	7			
1	H	361	Total	C	N	O	S	0	0	0
			2770	1729	512	522	7			

There are 8 discrepancies between the modelled and reference sequences:

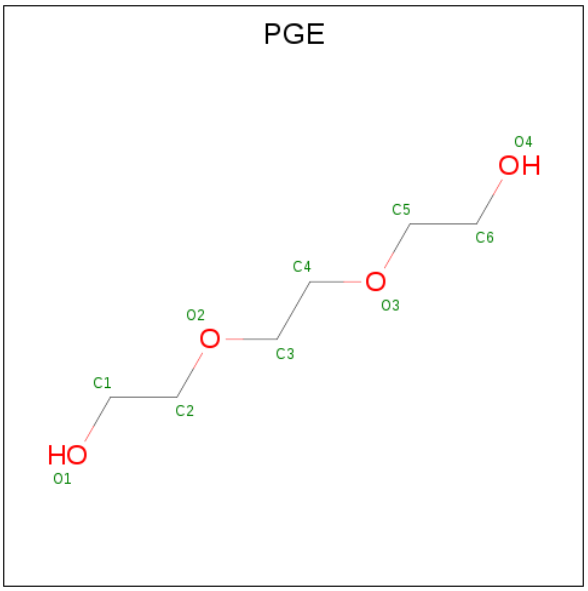
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0A0BZU2
B	1	MET	-	initiating methionine	UNP A0A0A0BZU2
C	1	MET	-	initiating methionine	UNP A0A0A0BZU2
D	1	MET	-	initiating methionine	UNP A0A0A0BZU2
E	1	MET	-	initiating methionine	UNP A0A0A0BZU2
F	1	MET	-	initiating methionine	UNP A0A0A0BZU2
G	1	MET	-	initiating methionine	UNP A0A0A0BZU2
H	1	MET	-	initiating methionine	UNP A0A0A0BZU2

- 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
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		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 10 6 4	0	0

- Molecule 4 is water.

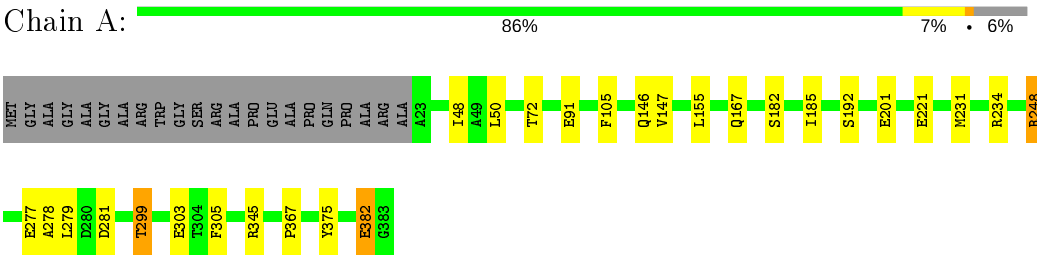
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	0	0
4	B	76	Total O 76 76	0	0
4	C	61	Total O 61 61	0	0
4	D	23	Total O 23 23	0	0
4	E	67	Total O 67 67	0	0
4	F	40	Total O 40 40	0	0
4	G	39	Total O 39 39	0	0
4	H	57	Total O 57 57	0	0

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. 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. 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.

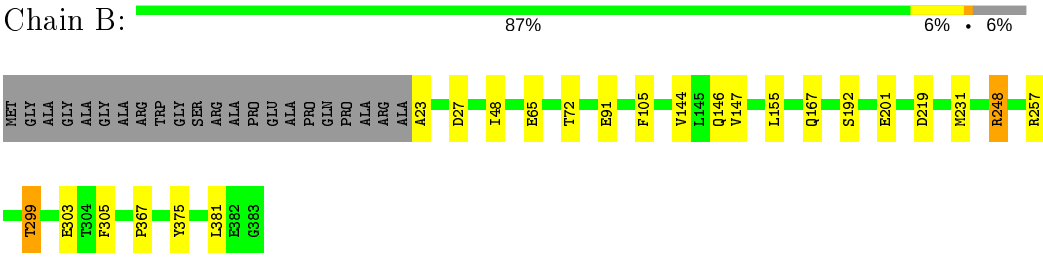
- Molecule 1: Peroxidase

Chain A:



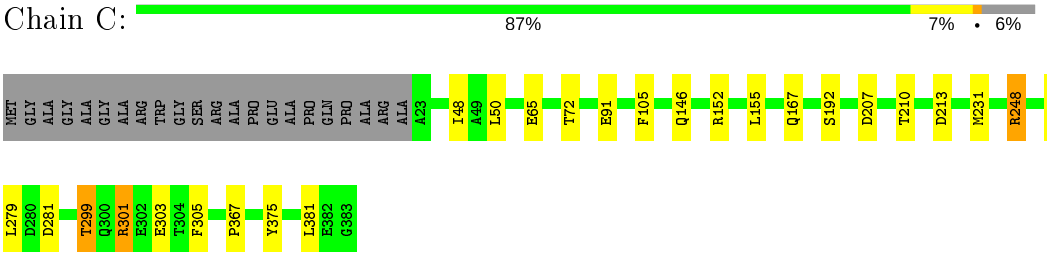
- Molecule 1: Peroxidase

Chain B:



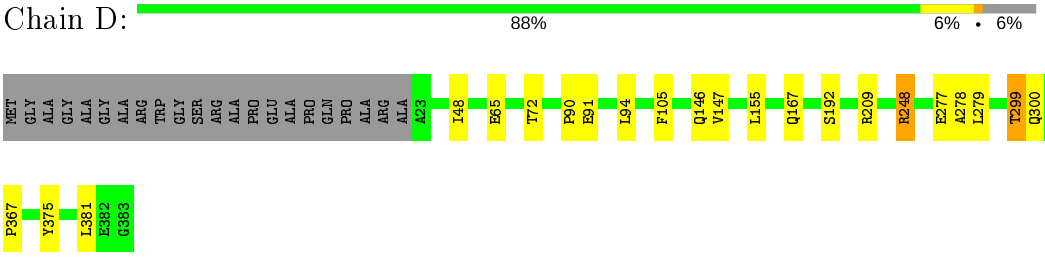
- Molecule 1: Peroxidase

Chain C:



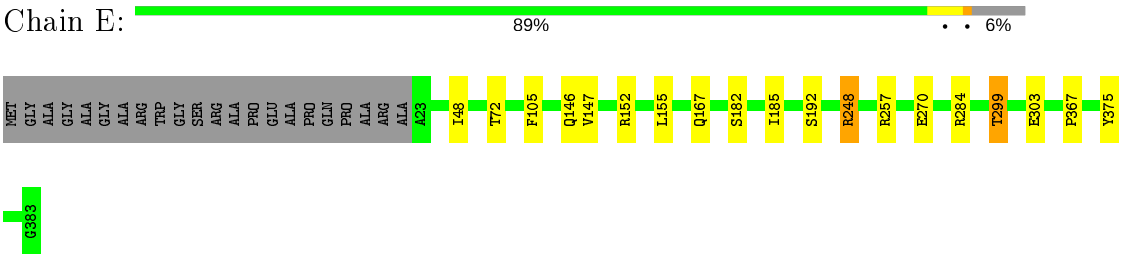
- Molecule 1: Peroxidase

Chain D:



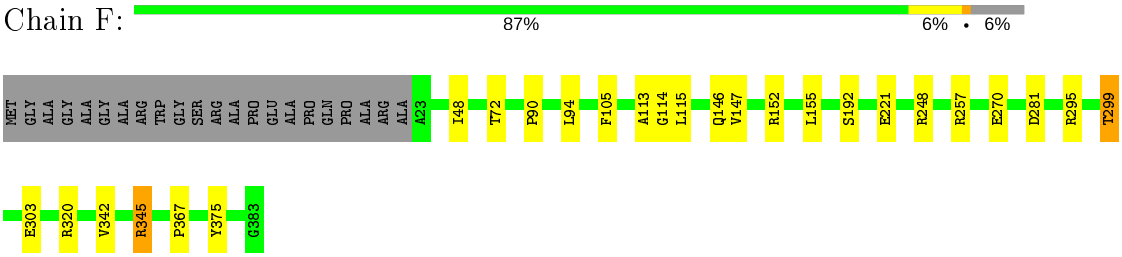
• Molecule 1: Peroxidase

Chain E:



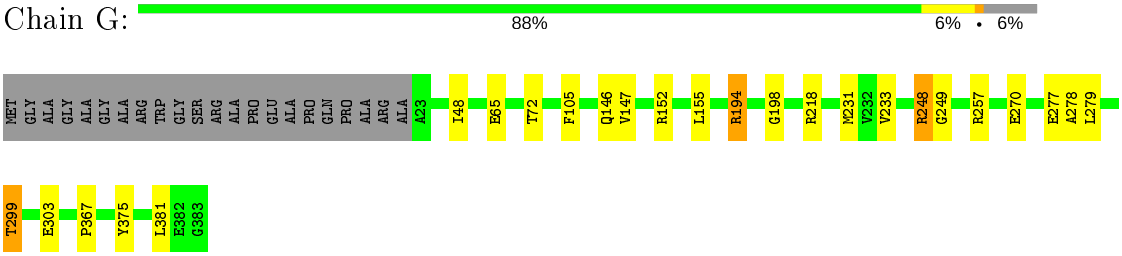
• Molecule 1: Peroxidase

Chain F:



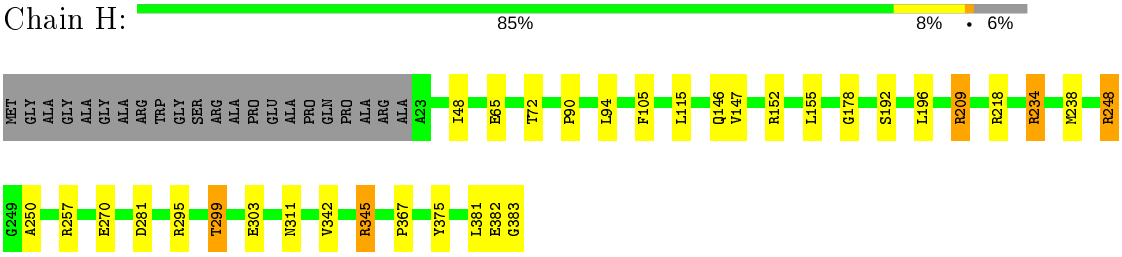
• Molecule 1: Peroxidase

Chain G:



• Molecule 1: Peroxidase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	173.99Å 173.99Å 283.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.87 – 2.40 58.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.9 (58.87-2.40) 97.9 (58.87-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.242 , 0.267 0.184 , 0.206	Depositor DCC
R_{free} test set	9263 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 1.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.468 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.509 for H, K, L 0.491 for -K, -H, -L	Depositor
Outliers	8 of 184620 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22946	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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 44.27 % 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 1.5627e-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, PGE

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	0.68	0/2838	0.85	4/3878 (0.1%)
1	B	0.69	0/2838	0.84	0/3878
1	C	0.67	0/2838	0.83	2/3878 (0.1%)
1	D	0.68	0/2838	0.82	0/3878
1	E	0.68	0/2838	0.82	1/3878 (0.0%)
1	F	0.67	0/2838	0.83	2/3878 (0.1%)
1	G	0.68	0/2838	0.84	3/3878 (0.1%)
1	H	0.68	0/2838	0.87	4/3878 (0.1%)
All	All	0.68	0/22704	0.84	16/31024 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	234	ARG	CG-CD-NE	-13.72	82.98	111.80
1	G	194	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	H	345	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	G	194	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	C	257	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	A	345	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	H	345	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	E	248	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	H	248	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	A	345	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	221	GLU	CB-CA-C	5.21	120.81	110.40
1	G	248	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	F	345	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	F	221	GLU	CB-CA-C	5.07	120.54	110.40
1	C	301	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	234	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	2770	0	2708	23	0
1	B	2770	0	2708	21	0
1	C	2770	0	2708	21	0
1	D	2770	0	2708	15	0
1	E	2770	0	2708	7	0
1	F	2770	0	2708	19	0
1	G	2770	0	2708	14	0
1	H	2770	0	2708	20	0
2	A	43	0	30	4	0
2	B	43	0	30	3	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
2	E	43	0	30	0	0
2	F	43	0	30	4	0
2	G	43	0	30	1	0
2	H	43	0	30	3	0
3	H	10	0	14	2	0
4	A	69	0	0	0	0
4	B	76	0	0	1	0
4	C	61	0	0	1	0
4	D	23	0	0	0	0
4	E	67	0	0	0	0
4	F	40	0	0	0	0
4	G	39	0	0	0	0
4	H	57	0	0	0	0
All	All	22946	0	21918	143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (143) 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:F:114:GLY:C	1:F:115:LEU:HD12	1.99	0.82
1:F:113:ALA:O	1:F:115:LEU:CD1	2.28	0.81
1:F:113:ALA:CB	1:F:115:LEU:HD13	2.14	0.77
1:C:207:ASP:HB3	1:C:210:THR:HG22	1.67	0.76
1:F:113:ALA:C	1:F:115:LEU:HD13	2.14	0.67
1:B:219:ASP:HB3	4:B:569:HOH:O	1.95	0.67
1:B:144:VAL:HG11	1:B:231:MET:HE3	1.76	0.66
1:A:48:ILE:HG12	1:A:50:LEU:HD22	1.76	0.66
1:B:144:VAL:HG11	1:B:231:MET:CE	2.26	0.65
1:F:113:ALA:C	1:F:115:LEU:CD1	2.65	0.65
1:C:207:ASP:HB3	1:C:210:THR:CG2	2.30	0.60
1:A:305:PHE:HZ	2:A:401:HEM:HBC2	1.65	0.60
1:C:277:GLU:O	1:C:279:LEU:CD1	2.50	0.59
1:H:115:LEU:HD21	1:H:383:GLY:O	2.02	0.59
1:C:91:GLU:OE2	1:D:248:ARG:NH1	2.34	0.58
1:E:299:THR:HB	1:E:303:GLU:OE1	2.03	0.58
1:G:277:GLU:O	1:G:279:LEU:CD1	2.50	0.58
1:A:277:GLU:O	1:A:279:LEU:CD1	2.50	0.58
1:D:299:THR:HB	1:D:303:GLU:OE1	2.04	0.58
1:G:299:THR:HB	1:G:303:GLU:OE1	2.04	0.58
2:F:401:HEM:HHD	2:F:401:HEM:HBC2	1.86	0.58
1:D:277:GLU:O	1:D:279:LEU:CD1	2.51	0.58
1:F:299:THR:HB	1:F:303:GLU:OE1	2.02	0.58
1:C:299:THR:HB	1:C:303:GLU:OE1	2.04	0.58
1:H:299:THR:HB	1:H:303:GLU:OE1	2.04	0.58
1:B:299:THR:HB	1:B:303:GLU:OE1	2.04	0.57
1:H:105:PHE:CE2	1:H:367:PRO:HG3	2.39	0.57
1:H:115:LEU:CD2	1:H:383:GLY:O	2.53	0.57
1:H:295:ARG:O	1:H:345:ARG:HD2	2.04	0.57
1:H:250:ALA:HB1	3:H:402:PGE:H52	1.87	0.56
1:A:299:THR:HB	1:A:303:GLU:OE1	2.04	0.56
1:F:295:ARG:O	1:F:345:ARG:HD2	2.05	0.56
1:G:105:PHE:CE2	1:G:367:PRO:HG3	2.41	0.56
1:G:65:GLU:HA	1:G:381:LEU:HD22	1.88	0.56
1:E:105:PHE:CE2	1:E:367:PRO:HG3	2.42	0.55
1:D:105:PHE:CE2	1:D:367:PRO:HG3	2.42	0.55
1:D:65:GLU:HA	1:D:381:LEU:HD22	1.89	0.55
1:F:113:ALA:HB3	1:F:115:LEU:HD13	1.88	0.55
1:A:105:PHE:CE2	1:A:367:PRO:HG3	2.42	0.54
1:B:105:PHE:CE2	1:B:367:PRO:HG3	2.42	0.54
2:G:401:HEM:HBC2	2:G:401:HEM:HHD	1.88	0.54
1:H:65:GLU:HA	1:H:381:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:PHE:CE2	1:C:367:PRO:HG3	2.43	0.53
1:C:65:GLU:HA	1:C:381:LEU:HD22	1.91	0.53
1:C:279:LEU:HD11	4:C:534:HOH:O	2.08	0.53
1:F:105:PHE:CE2	1:F:367:PRO:HG3	2.43	0.53
1:B:65:GLU:HA	1:B:381:LEU:HD22	1.91	0.52
1:D:147:VAL:HG12	1:D:155:LEU:HD12	1.92	0.52
1:A:248:ARG:NH2	1:B:91:GLU:OE2	2.37	0.51
1:H:196:LEU:HB2	1:H:238:MET:HE1	1.93	0.50
2:F:401:HEM:HMB2	2:F:401:HEM:HBB2	1.93	0.50
1:G:279:LEU:HD12	1:G:279:LEU:N	2.26	0.50
1:B:279:LEU:HB2	1:C:299:THR:HG23	1.92	0.50
1:A:147:VAL:HG12	1:A:155:LEU:HD12	1.92	0.50
2:H:401:HEM:HMB2	2:H:401:HEM:HBB2	1.92	0.50
1:F:147:VAL:HG12	1:F:155:LEU:HD12	1.94	0.49
1:B:147:VAL:HG12	1:B:155:LEU:HD12	1.94	0.49
1:A:248:ARG:HH22	1:B:91:GLU:CD	2.16	0.49
1:A:50:LEU:HD12	1:A:231:MET:HE1	1.94	0.49
1:C:207:ASP:CB	1:C:210:THR:HG22	2.39	0.49
1:D:279:LEU:N	1:D:279:LEU:HD12	2.28	0.49
1:E:147:VAL:HG12	1:E:155:LEU:HD12	1.95	0.49
1:F:113:ALA:HB1	1:F:115:LEU:HD13	1.91	0.49
1:A:279:LEU:N	1:A:279:LEU:HD12	2.28	0.48
2:B:401:HEM:HBB2	2:B:401:HEM:HMB2	1.95	0.48
1:G:147:VAL:HG12	1:G:155:LEU:HD12	1.95	0.48
1:C:279:LEU:HD12	1:C:279:LEU:N	2.28	0.48
1:G:48:ILE:HD11	1:G:146:GLN:HG3	1.95	0.48
1:F:115:LEU:HD12	1:F:115:LEU:N	2.28	0.48
1:B:144:VAL:CG1	1:B:231:MET:HE1	2.44	0.48
1:F:48:ILE:HD11	1:F:146:GLN:HG3	1.96	0.48
1:A:91:GLU:OE2	1:B:248:ARG:NH1	2.39	0.48
1:C:305:PHE:HZ	2:C:401:HEM:HBC2	1.78	0.48
1:E:48:ILE:HD11	1:E:146:GLN:HG3	1.96	0.47
1:C:213:ASP:OD1	1:C:301:ARG:NH1	2.47	0.47
1:B:144:VAL:CG1	1:B:231:MET:CE	2.92	0.47
1:H:238:MET:HE2	1:H:238:MET:HB2	1.66	0.47
1:H:48:ILE:HD11	1:H:146:GLN:HG3	1.97	0.46
1:C:48:ILE:HD11	1:C:146:GLN:HG3	1.97	0.46
1:D:278:ALA:C	1:D:279:LEU:HD12	2.36	0.46
1:A:278:ALA:C	1:A:279:LEU:HD12	2.36	0.46
1:B:48:ILE:HD11	1:B:146:GLN:HG3	1.98	0.46
1:G:278:ALA:C	1:G:279:LEU:HD12	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ALA:C	1:C:279:LEU:HD12	2.36	0.45
1:C:277:GLU:O	1:C:279:LEU:HD12	2.16	0.45
1:G:277:GLU:O	1:G:279:LEU:HD12	2.15	0.45
1:A:277:GLU:O	1:A:279:LEU:HD12	2.16	0.45
1:H:196:LEU:HB2	1:H:238:MET:CE	2.47	0.45
1:A:48:ILE:HD11	1:A:146:GLN:HG3	1.99	0.45
1:H:342:VAL:HG12	2:H:401:HEM:CBC	2.47	0.45
1:C:248:ARG:HH12	1:D:91:GLU:CD	2.20	0.44
1:D:48:ILE:HD11	1:D:146:GLN:HG3	1.99	0.44
1:H:147:VAL:HG12	1:H:155:LEU:HD12	1.98	0.44
1:A:192:SER:OG	1:A:201:GLU:O	2.35	0.44
1:G:72:THR:HG21	1:G:375:TYR:HA	1.98	0.44
1:B:305:PHE:HZ	2:B:401:HEM:HBC2	1.82	0.44
2:D:401:HEM:HMB2	2:D:401:HEM:HBB2	1.99	0.44
1:B:144:VAL:HG11	1:B:231:MET:HE1	2.00	0.44
1:H:209:ARG:N	1:H:209:ARG:HD2	2.32	0.44
1:H:90:PRO:O	1:H:94:LEU:HD13	2.17	0.44
2:A:401:HEM:HMB2	2:A:401:HEM:HBB2	2.00	0.44
1:D:277:GLU:O	1:D:279:LEU:HD12	2.17	0.44
1:B:23:ALA:N	1:B:27:ASP:OD2	2.52	0.43
2:H:401:HEM:HBC2	2:H:401:HEM:HHD	2.00	0.43
1:D:300:GLN:NE2	1:D:302:GLU:OE2	2.49	0.43
1:A:257:ARG:NH2	1:A:270:GLU:O	2.51	0.43
1:E:257:ARG:NH2	1:E:270:GLU:O	2.52	0.43
1:A:182:SER:HB2	1:A:185:ILE:HD12	2.01	0.43
1:C:72:THR:HG21	1:C:375:TYR:HA	2.00	0.43
1:A:305:PHE:CZ	2:A:401:HEM:HBC2	2.50	0.43
1:F:72:THR:HG21	1:F:375:TYR:HA	2.01	0.43
1:G:257:ARG:NH2	1:G:270:GLU:O	2.52	0.43
1:B:257:ARG:NH2	1:B:270:GLU:O	2.52	0.42
1:H:72:THR:HG21	1:H:375:TYR:HA	2.01	0.42
1:D:90:PRO:O	1:D:94:LEU:HD13	2.19	0.42
1:F:113:ALA:O	1:F:115:LEU:HD11	2.16	0.42
1:F:90:PRO:O	1:F:94:LEU:HD13	2.19	0.42
1:H:257:ARG:NH2	1:H:270:GLU:O	2.52	0.42
1:A:72:THR:HG21	1:A:375:TYR:HA	2.01	0.42
1:A:50:LEU:HD13	1:A:146:GLN:HA	2.01	0.42
1:B:299:THR:HG23	1:C:279:LEU:HB2	2.02	0.42
1:D:72:THR:HG21	1:D:375:TYR:HA	2.00	0.42
2:F:401:HEM:CMB	2:F:401:HEM:HBB2	2.49	0.42
1:F:257:ARG:NH2	1:F:270:GLU:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ARG:NH1	1:D:91:GLU:OE2	2.48	0.42
1:F:113:ALA:O	1:F:115:LEU:HD12	2.14	0.42
1:A:382:GLU:O	1:G:249:GLY:N	2.52	0.42
1:B:72:THR:HG21	1:B:375:TYR:HA	2.02	0.42
1:G:231:MET:HE2	1:G:233:VAL:CG2	2.50	0.41
2:A:401:HEM:CMB	2:A:401:HEM:HBB2	2.50	0.41
1:A:48:ILE:HG12	1:A:50:LEU:CD2	2.46	0.41
1:B:192:SER:OG	1:B:201:GLU:O	2.37	0.41
2:B:401:HEM:HHD	2:B:401:HEM:HBC2	2.01	0.41
1:E:72:THR:HG21	1:E:375:TYR:HA	2.01	0.41
1:A:48:ILE:CD1	1:A:50:LEU:HD21	2.50	0.41
2:D:401:HEM:CMB	2:D:401:HEM:HBB2	2.50	0.41
1:G:194:ARG:NH2	1:G:198:GLY:O	2.54	0.40
1:E:182:SER:HB2	1:E:185:ILE:HD12	2.03	0.40
1:F:342:VAL:HG12	2:F:401:HEM:CBC	2.51	0.40
1:H:178:GLY:HA2	1:H:311:ASN:O	2.22	0.40
1:H:250:ALA:HB1	3:H:402:PGE:H42	2.02	0.40
1:H:303:GLU:OE1	1:H:345:ARG:NH2	2.54	0.40
1:C:50:LEU:CD2	1:C:231:MET:HE1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/383 (94%)	349 (97%)	10 (3%)	0	100	100
1	B	359/383 (94%)	351 (98%)	8 (2%)	0	100	100
1	C	359/383 (94%)	350 (98%)	9 (2%)	0	100	100
1	D	359/383 (94%)	350 (98%)	9 (2%)	0	100	100
1	E	359/383 (94%)	350 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	359/383 (94%)	349 (97%)	10 (3%)	0	100	100
1	G	359/383 (94%)	349 (97%)	10 (3%)	0	100	100
1	H	359/383 (94%)	350 (98%)	9 (2%)	0	100	100
All	All	2872/3064 (94%)	2798 (97%)	74 (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	288/299 (96%)	283 (98%)	5 (2%)	60	78
1	B	288/299 (96%)	285 (99%)	3 (1%)	76	88
1	C	288/299 (96%)	281 (98%)	7 (2%)	49	68
1	D	288/299 (96%)	283 (98%)	5 (2%)	60	78
1	E	288/299 (96%)	282 (98%)	6 (2%)	53	72
1	F	288/299 (96%)	282 (98%)	6 (2%)	53	72
1	G	288/299 (96%)	284 (99%)	4 (1%)	67	82
1	H	288/299 (96%)	279 (97%)	9 (3%)	40	60
All	All	2304/2392 (96%)	2259 (98%)	45 (2%)	55	74

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	A	248	ARG
1	A	281	ASP
1	A	299	THR
1	A	382	GLU
1	B	167	GLN
1	B	248	ARG
1	B	299	THR

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Mol	Chain	Res	Type
1	C	152	ARG
1	C	155	LEU
1	C	167	GLN
1	C	192	SER
1	C	248	ARG
1	C	281	ASP
1	C	299	THR
1	D	167	GLN
1	D	192	SER
1	D	209	ARG
1	D	248	ARG
1	D	299	THR
1	E	152	ARG
1	E	167	GLN
1	E	192	SER
1	E	248	ARG
1	E	284	ARG
1	E	299	THR
1	F	152	ARG
1	F	192	SER
1	F	248	ARG
1	F	281	ASP
1	F	299	THR
1	F	320	ARG
1	G	152	ARG
1	G	218	ARG
1	G	248	ARG
1	G	299	THR
1	H	152	ARG
1	H	192	SER
1	H	209	ARG
1	H	218	ARG
1	H	234	ARG
1	H	248	ARG
1	H	281	ASP
1	H	299	THR
1	H	382	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN

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Mol	Chain	Res	Type
1	C	117	HIS
1	C	167	GLN
1	D	167	GLN
1	G	300	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)

9 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	E	401	1	27,50,50	0.97	1 (3%)	17,82,82	1.30	3 (17%)
2	HEM	G	401	1	27,50,50	0.88	1 (3%)	17,82,82	0.90	1 (5%)
2	HEM	A	401	1	27,50,50	0.94	1 (3%)	17,82,82	1.14	1 (5%)
3	PGE	H	402	-	9,9,9	0.13	0	8,8,8	0.10	0
2	HEM	H	401	1	27,50,50	0.94	1 (3%)	17,82,82	1.45	5 (29%)
2	HEM	D	401	1	27,50,50	1.02	2 (7%)	17,82,82	1.18	2 (11%)
2	HEM	F	401	1	27,50,50	0.96	2 (7%)	17,82,82	1.05	1 (5%)
2	HEM	B	401	1	27,50,50	0.93	2 (7%)	17,82,82	1.20	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	C	401	1	27,50,50	0.85	0	17,82,82	1.56	2 (11%)

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	E	401	1	-	0/6/54/54	-
2	HEM	G	401	1	-	0/6/54/54	-
2	HEM	A	401	1	-	0/6/54/54	-
3	PGE	H	402	-	-	2/7/7/7	-
2	HEM	H	401	1	-	0/6/54/54	-
2	HEM	D	401	1	-	0/6/54/54	-
2	HEM	F	401	1	-	0/6/54/54	-
2	HEM	B	401	1	-	0/6/54/54	-
2	HEM	C	401	1	-	0/6/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	HEM	C3B-C2B	-2.73	1.36	1.40
2	E	401	HEM	C3C-C2C	-2.46	1.37	1.40
2	D	401	HEM	C3B-C2B	-2.46	1.37	1.40
2	H	401	HEM	C4D-C3D	2.39	1.48	1.42
2	B	401	HEM	C3C-C2C	-2.31	1.37	1.40
2	A	401	HEM	C4D-C3D	2.28	1.47	1.42
2	B	401	HEM	C3B-C2B	-2.26	1.37	1.40
2	D	401	HEM	C4D-C3D	2.19	1.47	1.42
2	F	401	HEM	C4D-C3D	2.06	1.47	1.42
2	G	401	HEM	C4D-C3D	2.05	1.47	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	HEM	CAA-CBA-CGA	-3.75	106.39	112.67
2	H	401	HEM	CMA-C3A-C4A	-3.71	122.76	128.46
2	E	401	HEM	CBA-CAA-C2A	2.89	117.81	112.49
2	D	401	HEM	CMA-C3A-C4A	-2.77	124.20	128.46
2	B	401	HEM	CMA-C3A-C4A	-2.55	124.54	128.46
2	F	401	HEM	CMA-C3A-C4A	-2.50	124.61	128.46
2	C	401	HEM	C3C-C4C-NC	-2.37	106.47	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	HEM	C1D-C2D-C3D	2.24	108.56	107.00
2	H	401	HEM	C3C-C4C-NC	-2.22	106.75	110.94
2	E	401	HEM	C3C-C4C-NC	-2.17	106.85	110.94
2	D	401	HEM	C3C-C4C-NC	-2.14	106.89	110.94
2	H	401	HEM	CBA-CAA-C2A	2.14	116.43	112.49
2	B	401	HEM	CAA-CBA-CGA	-2.09	109.17	112.67
2	H	401	HEM	C4A-C3A-C2A	2.05	108.42	107.00
2	H	401	HEM	CMA-C3A-C2A	2.04	128.78	124.94
2	A	401	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
2	G	401	HEM	CMA-C3A-C4A	-2.02	125.36	128.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	402	PGE	C3-C4-O3-C5
3	H	402	PGE	O1-C1-C2-O2

There are no ring outliers.

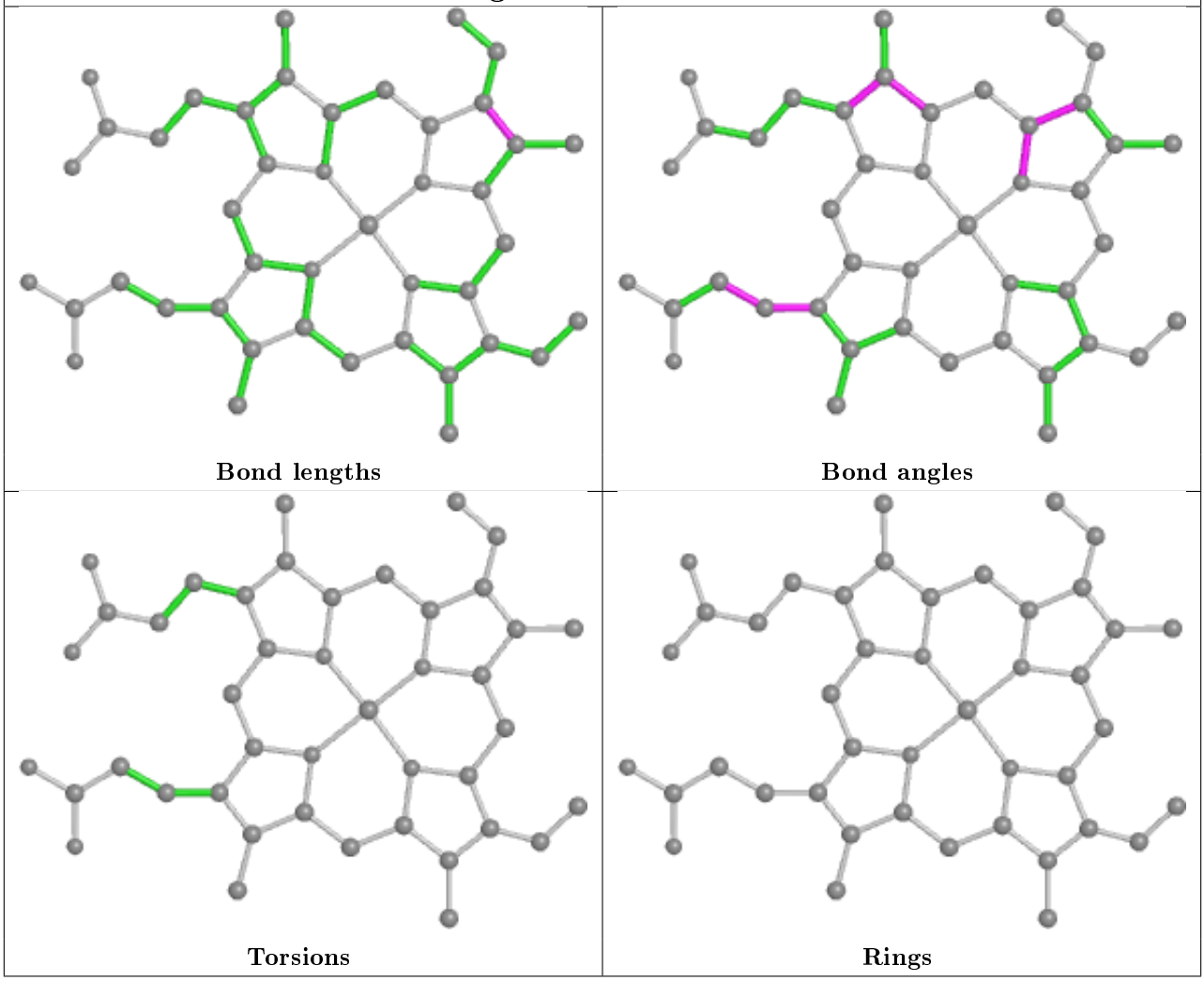
8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	401	HEM	1	0
2	A	401	HEM	4	0
3	H	402	PGE	2	0
2	H	401	HEM	3	0
2	D	401	HEM	2	0
2	F	401	HEM	4	0
2	B	401	HEM	3	0
2	C	401	HEM	1	0

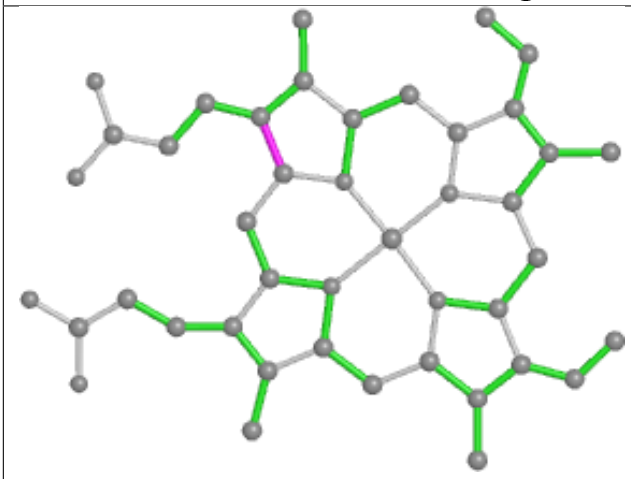
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

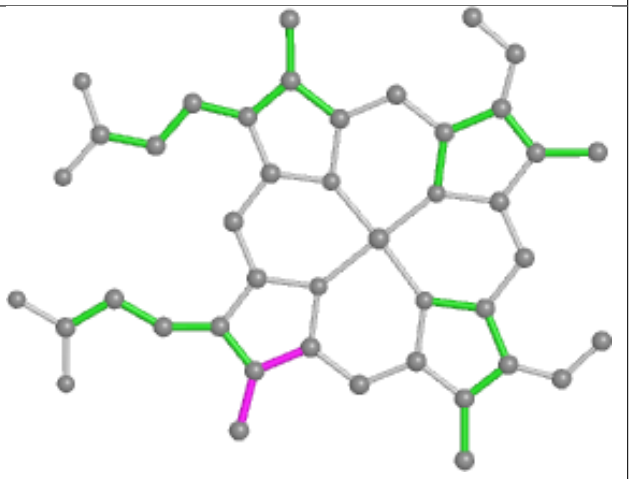
Ligand HEM E 401



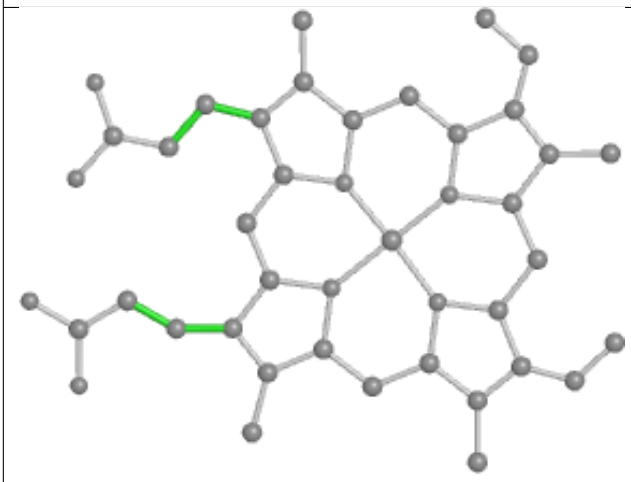
Ligand HEM G 401



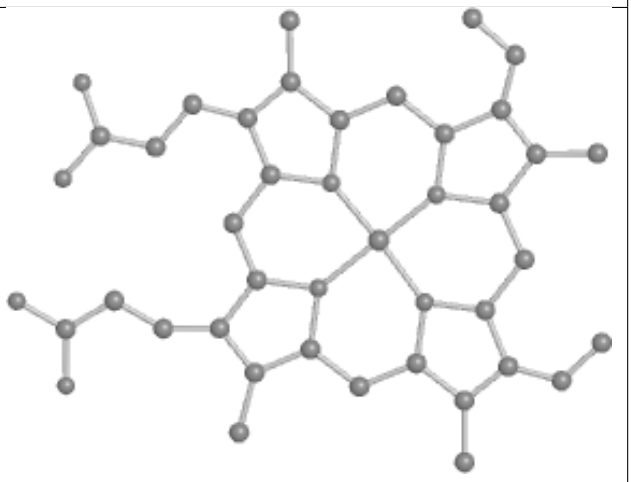
Bond lengths



Bond angles

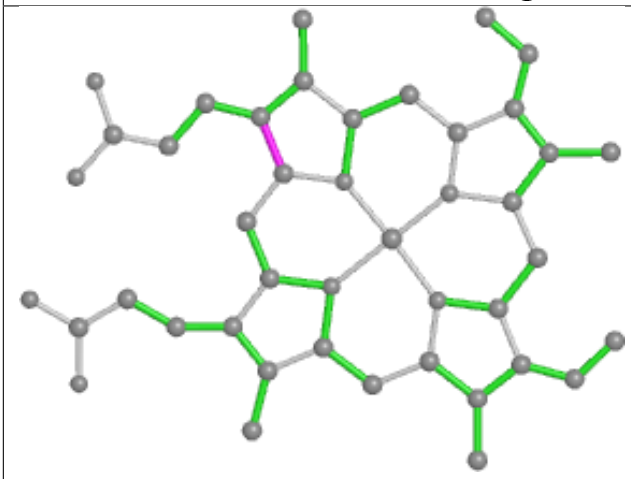


Torsions

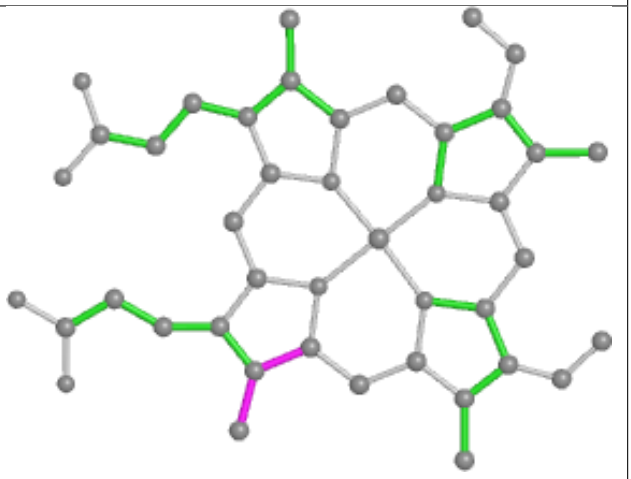


Rings

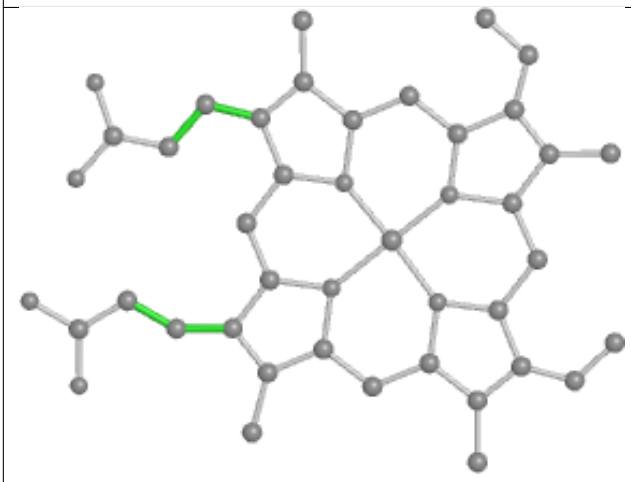
Ligand HEM A 401



Bond lengths



Bond angles



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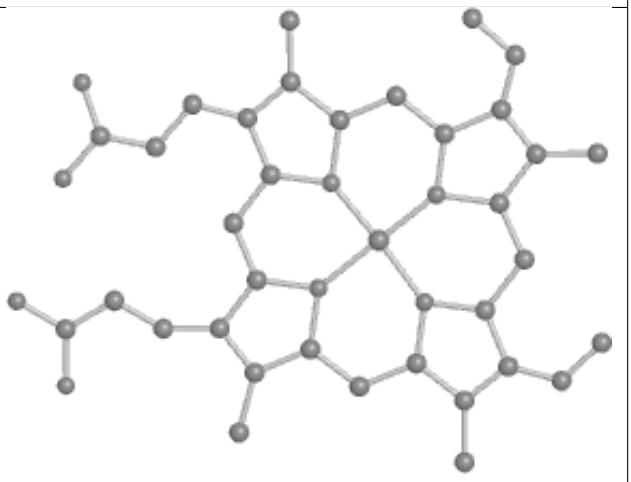

Rings

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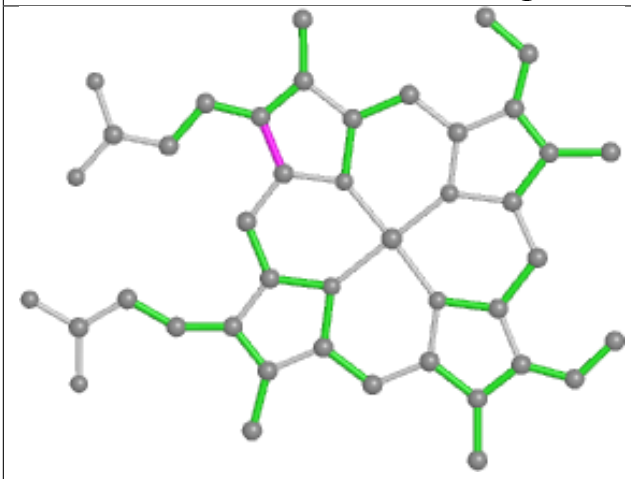
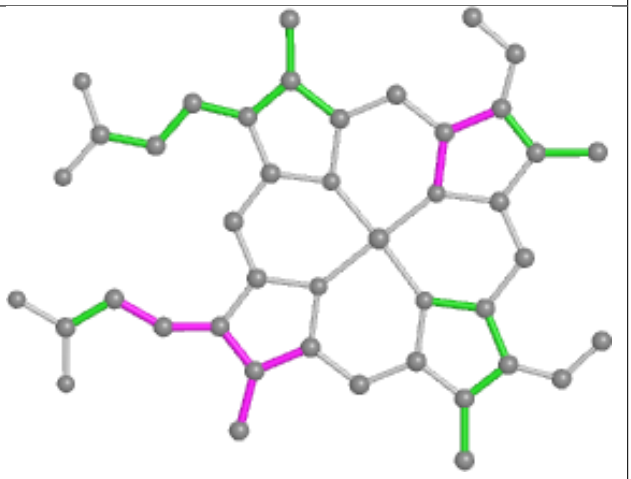
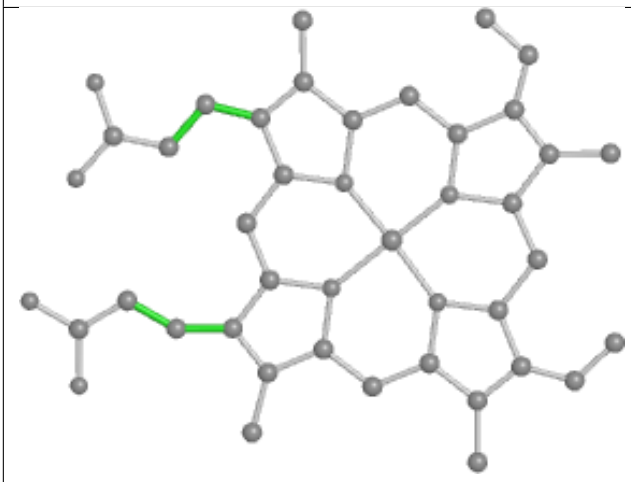


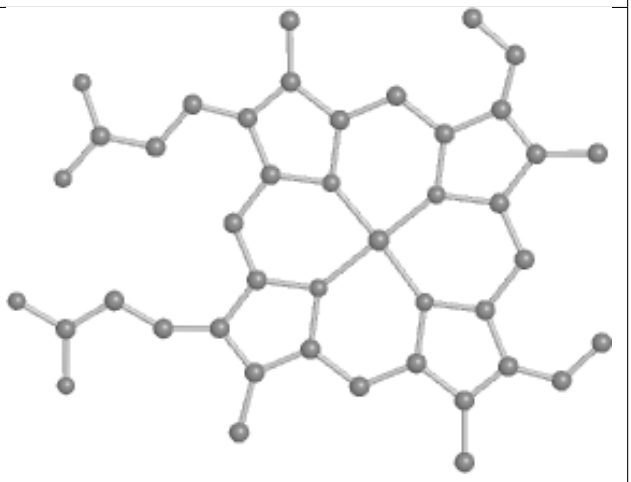
Bond lengths



Bond angles

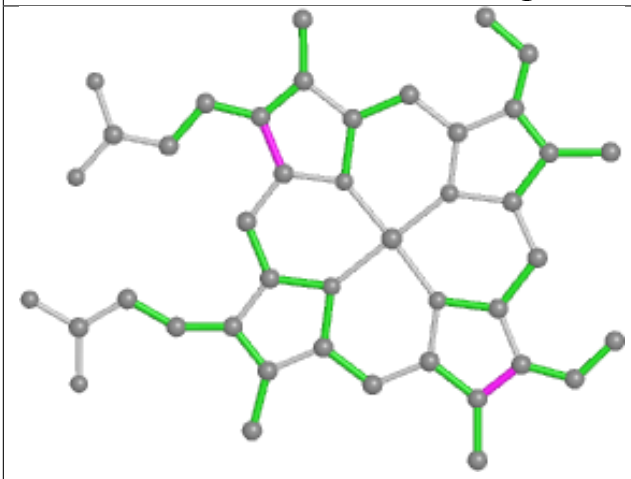


Torsions

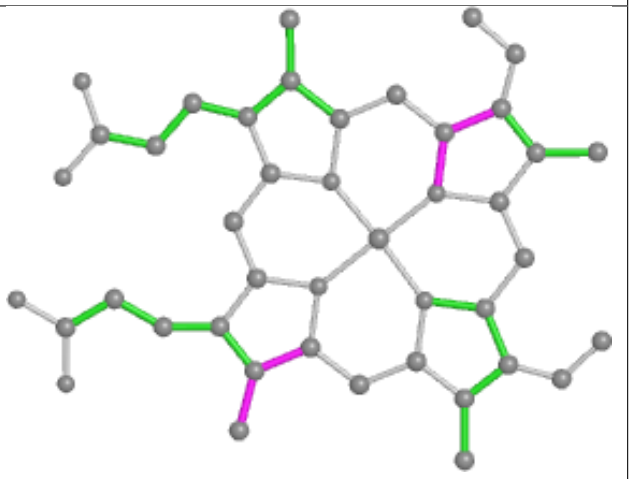


Rings

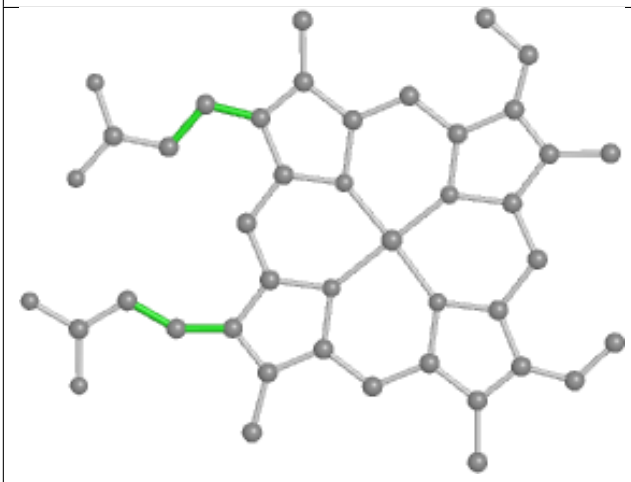
Ligand HEM D 401



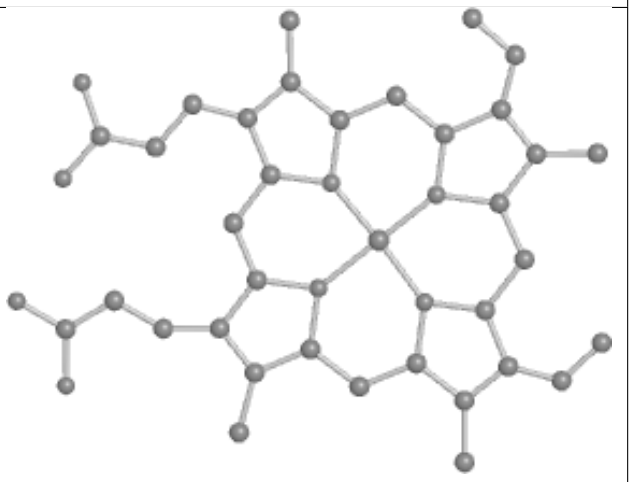
Bond lengths



Bond angles

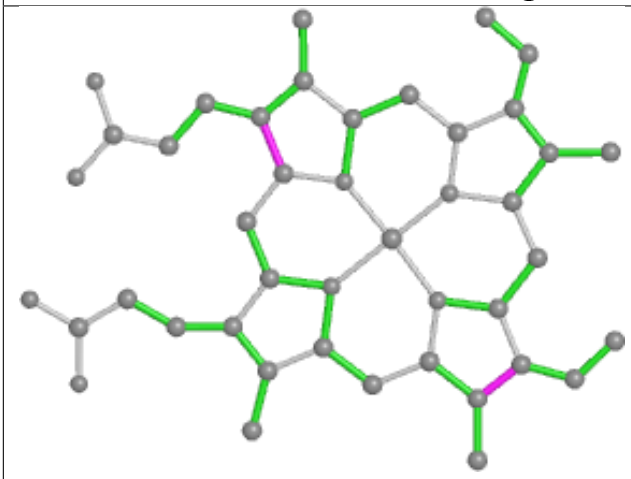


Torsions

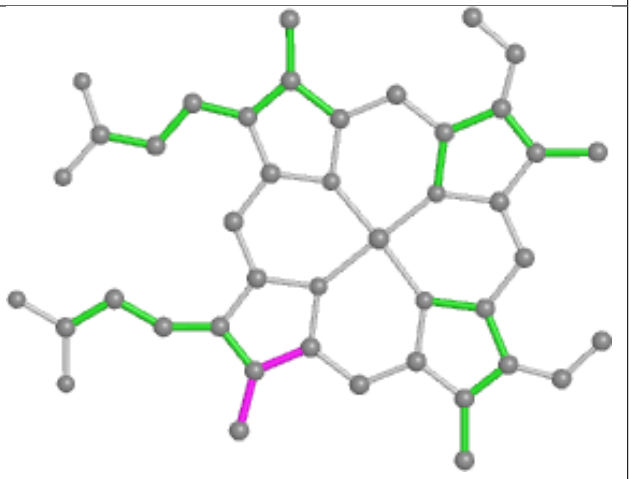


Rings

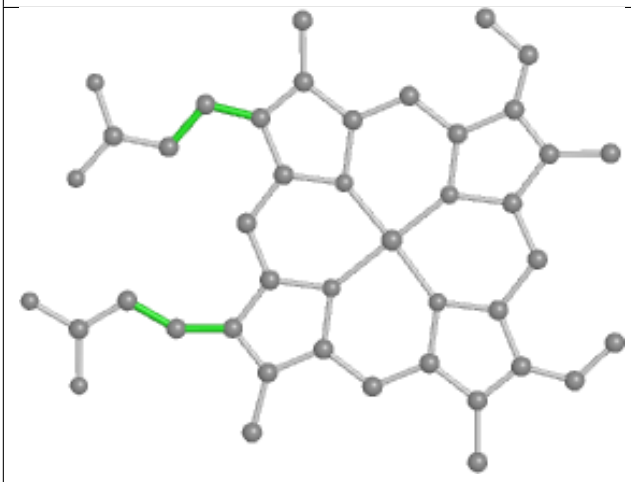
Ligand HEM F 401



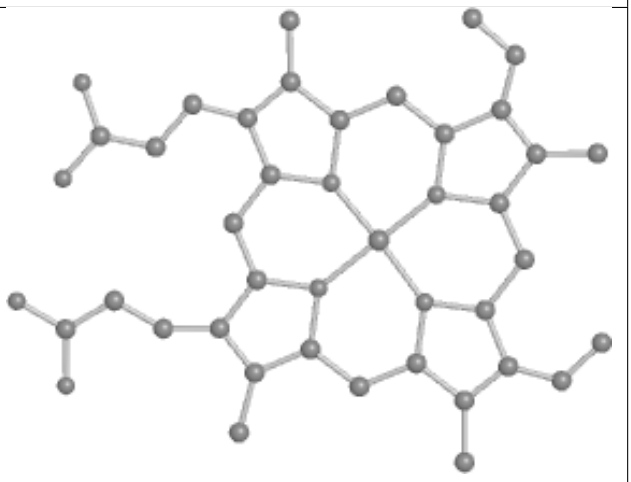
Bond lengths



Bond angles

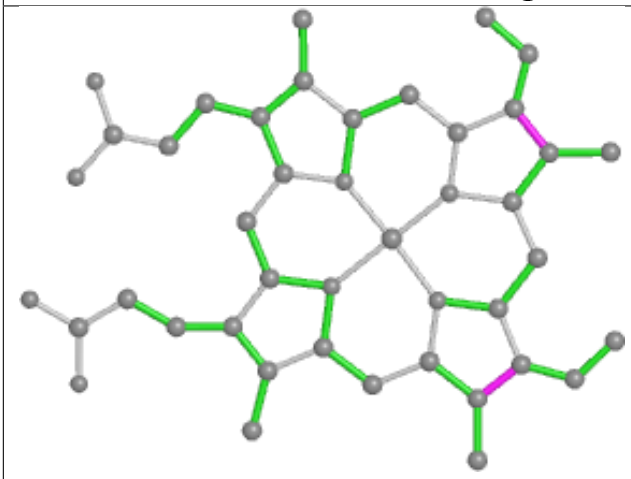


Torsions

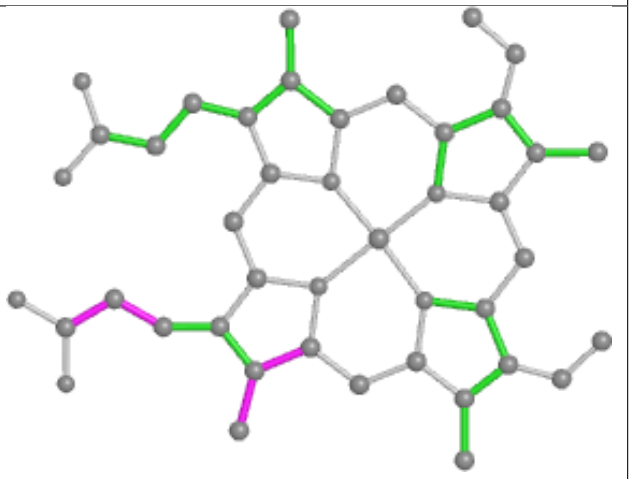


Rings

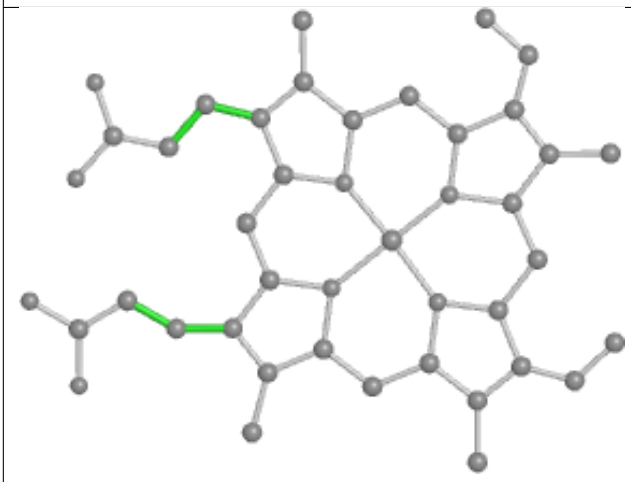
Ligand HEM B 401



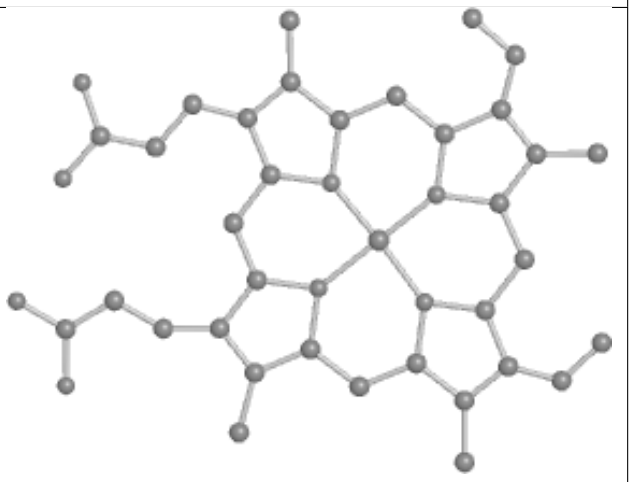
Bond lengths



Bond angles

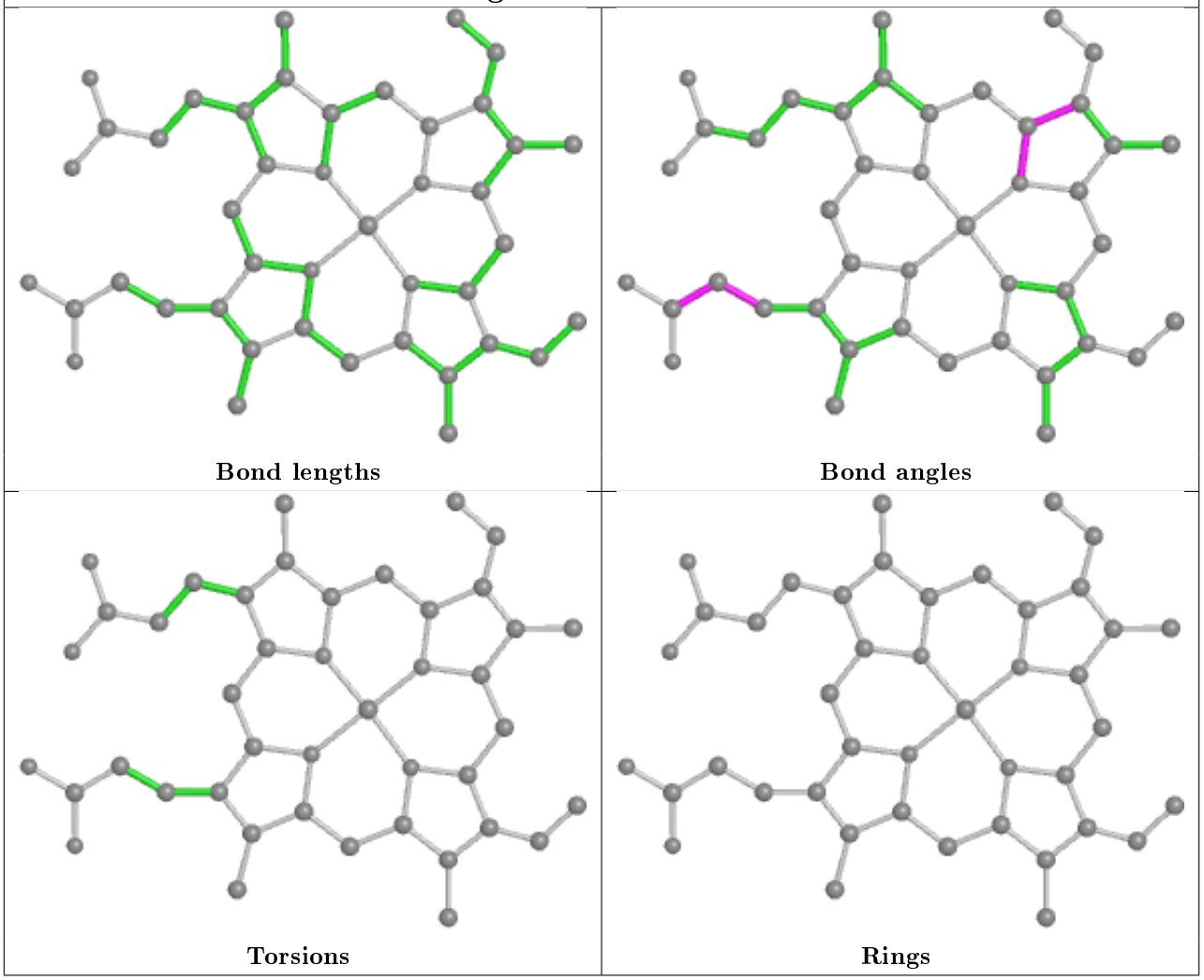


Torsions



Rings

Ligand HEM C 401



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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

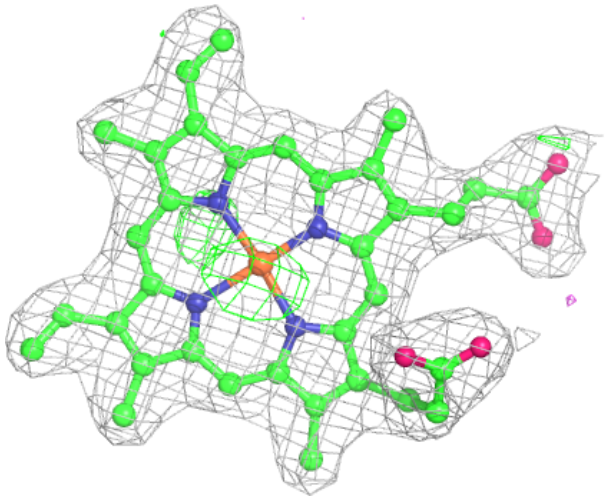
6.4 Ligands

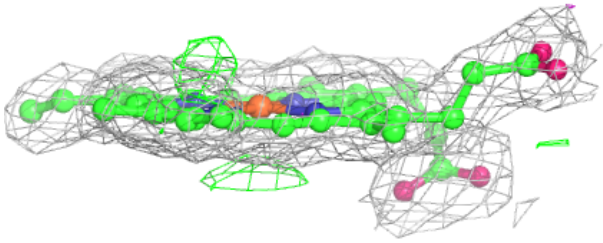
Unable to reproduce the depositors R factor - this section is therefore empty.

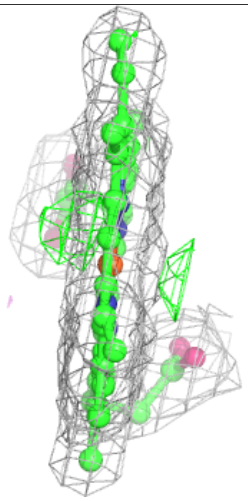
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM E 401:

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

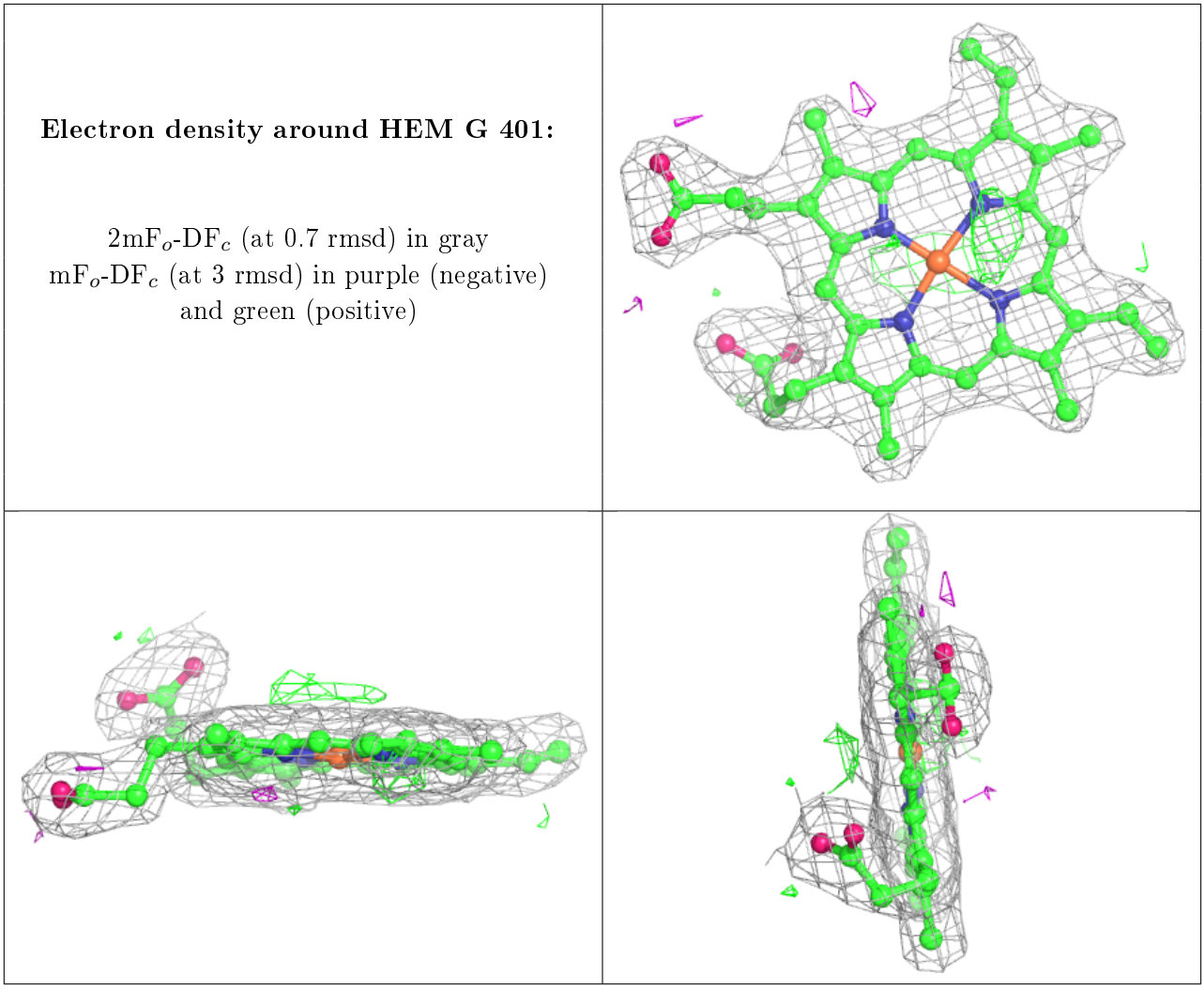






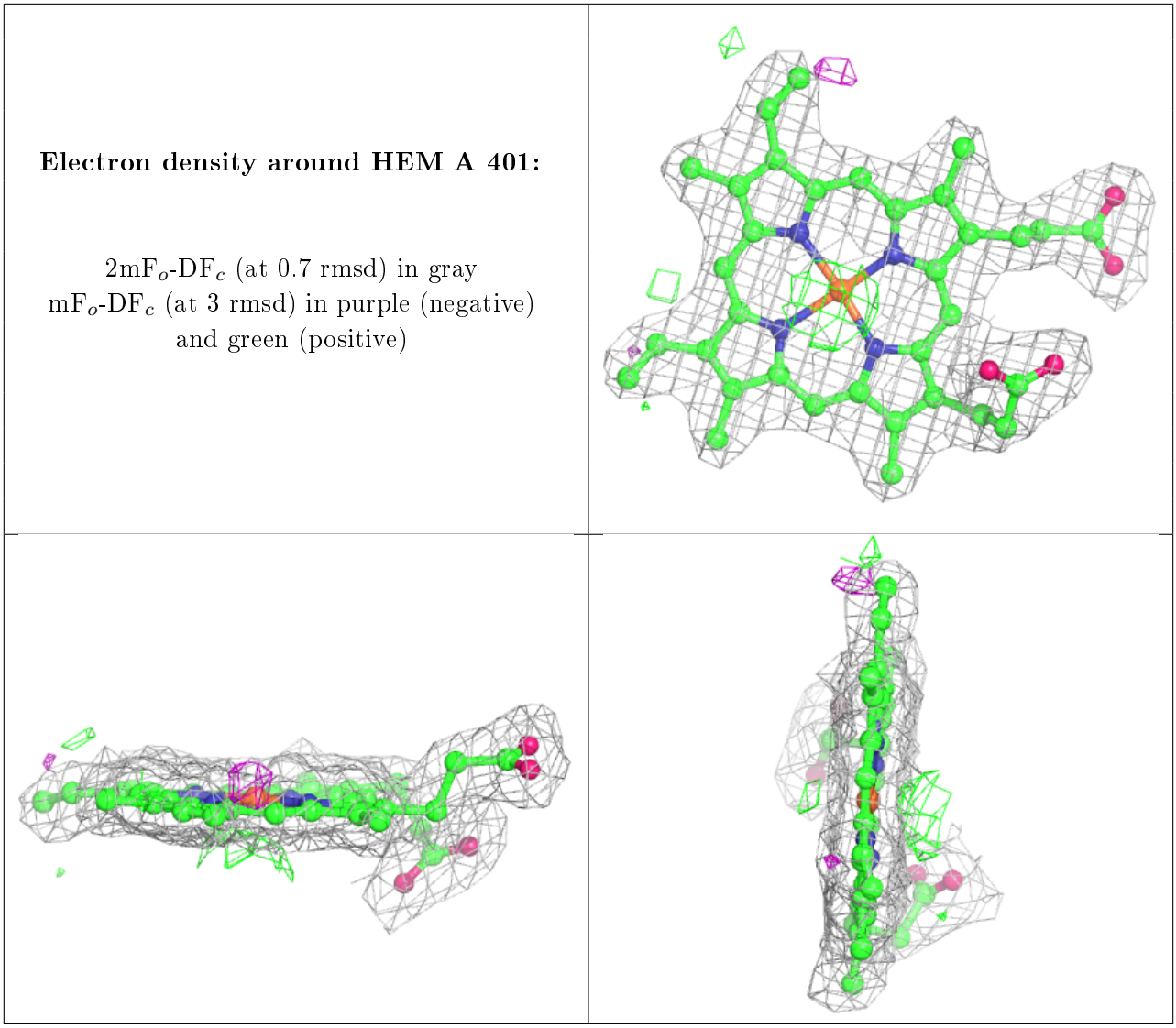
Electron density around HEM G 401:

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



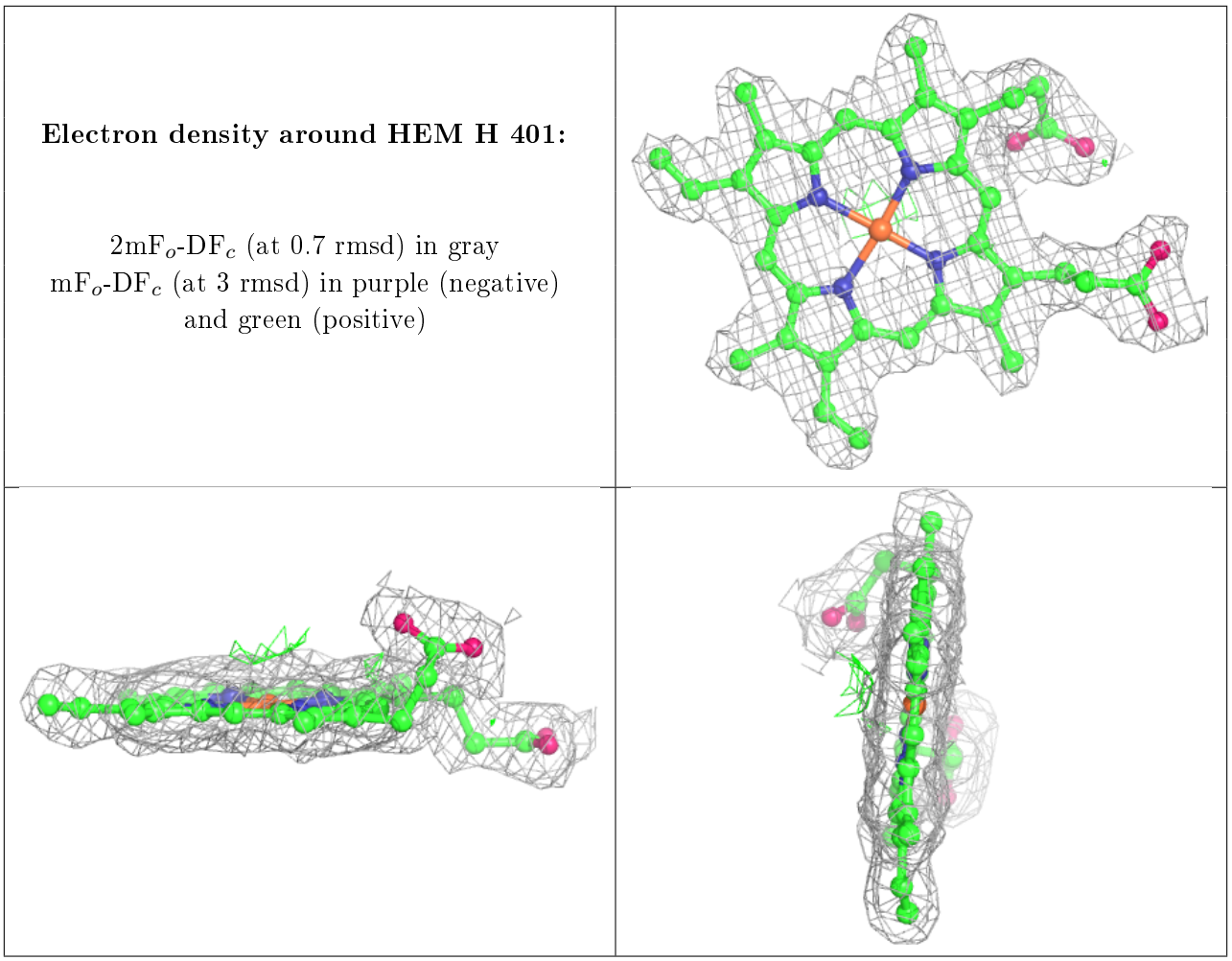
Electron density around HEM A 401:

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



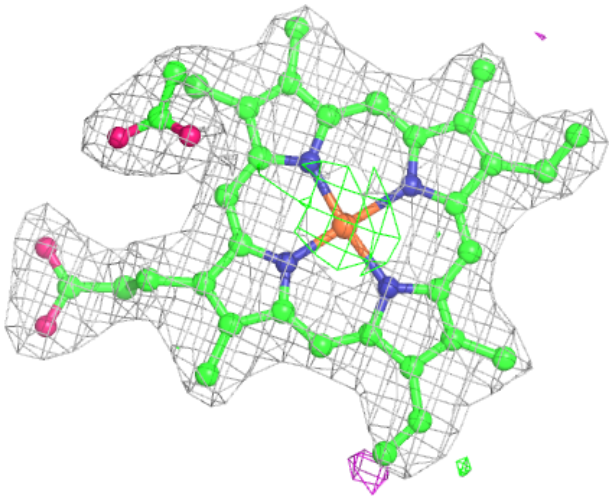
Electron density around HEM H 401:

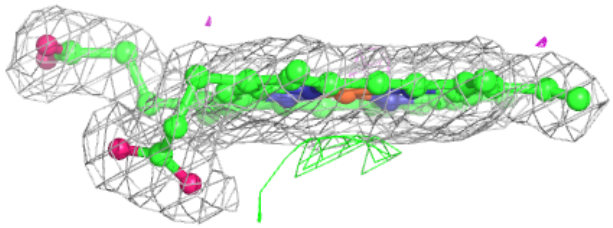
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

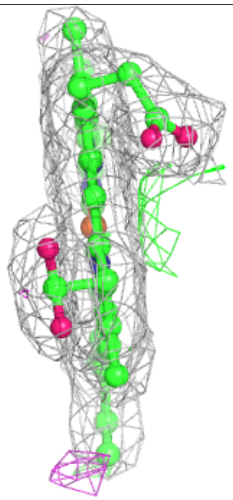


Electron density around HEM D 401:

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

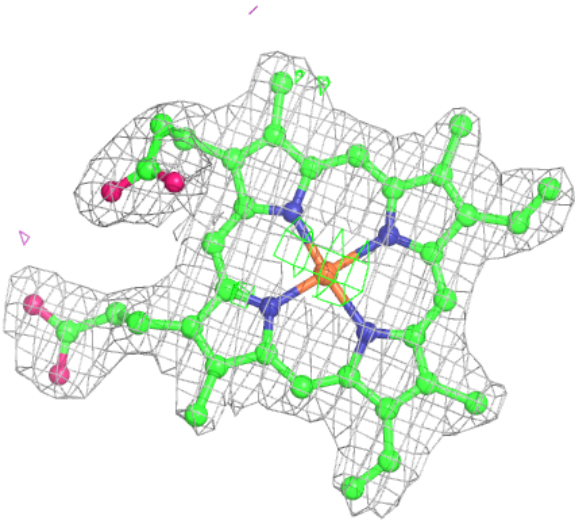


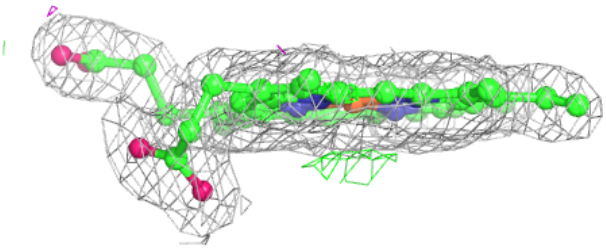


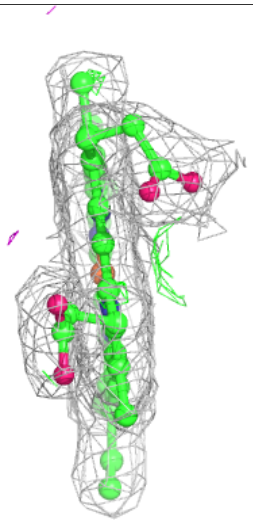


Electron density around HEM F 401:

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

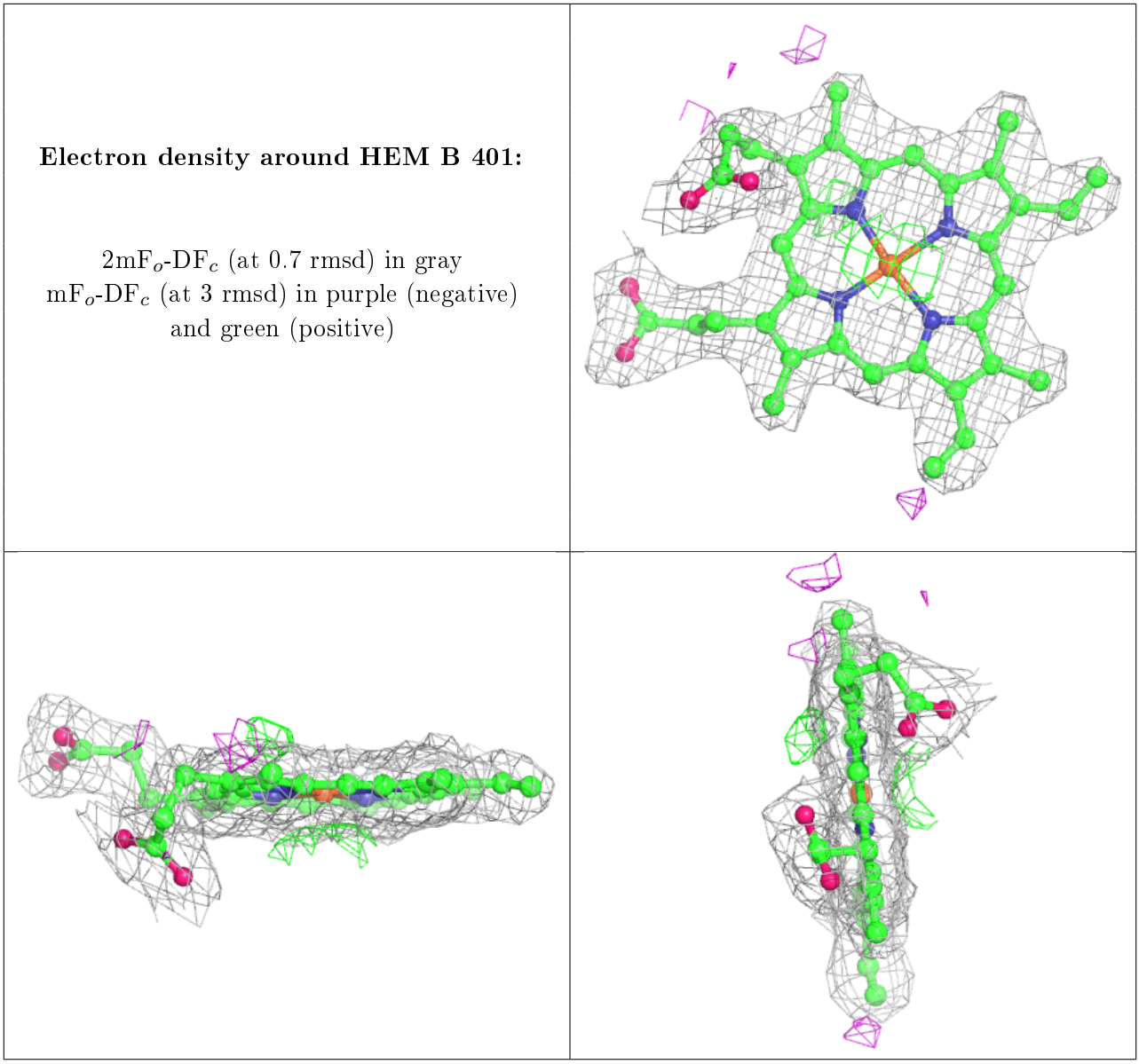






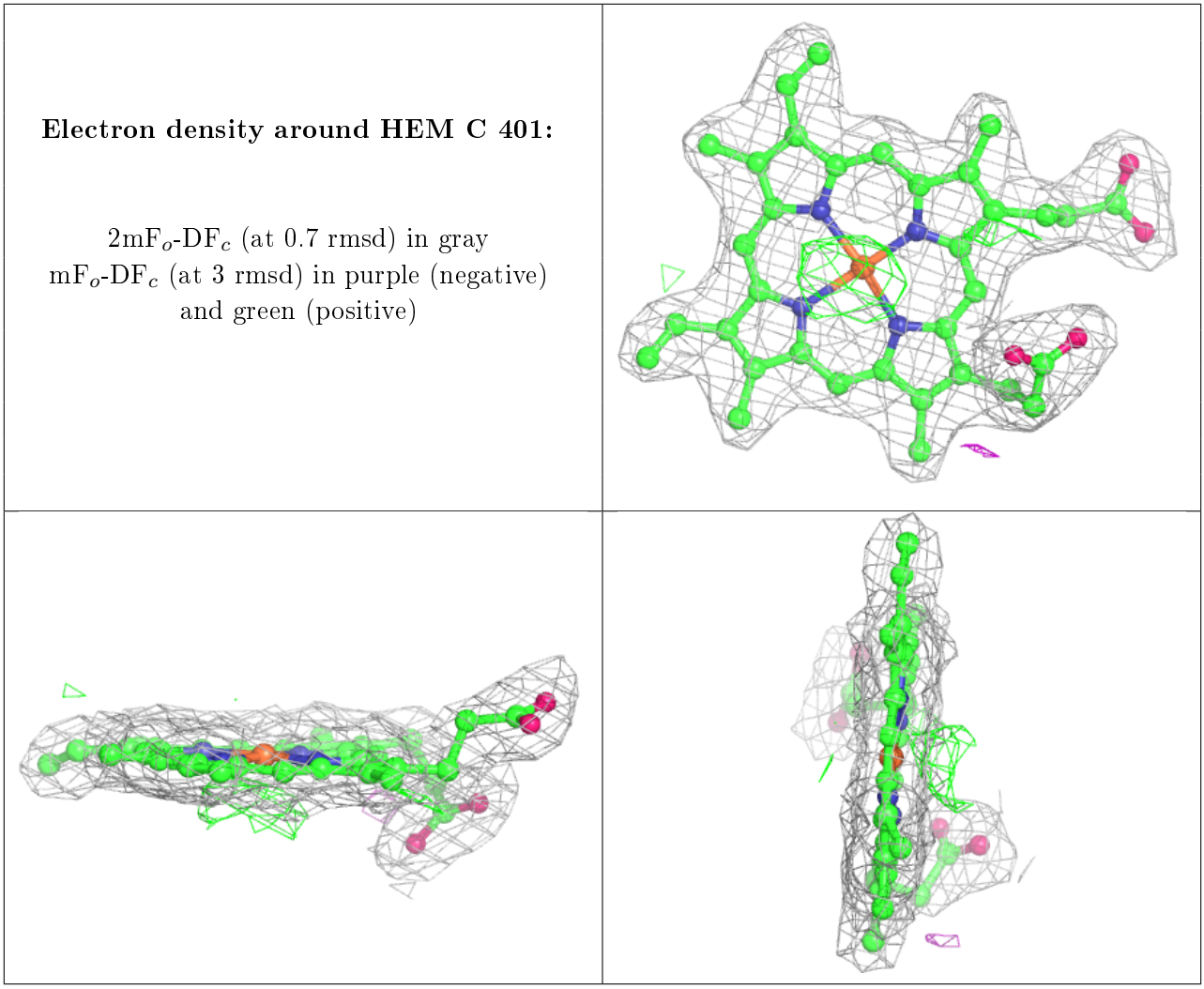
Electron density around HEM B 401:

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



Electron density around HEM C 401:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.