Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2025 – 12:11 PM EST

PDB ID	:	9AZ2
Title	:	Crystal structure of PF3257 peroxidase from Pseudomonas fluorescens
Authors	:	Stogios, P.J.; Skarina, T.; Choolaei, Z.; Yakunin, A.; Savchenko, A.
Deposited on	:	2024-03-09
Resolution	:	2.52 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:

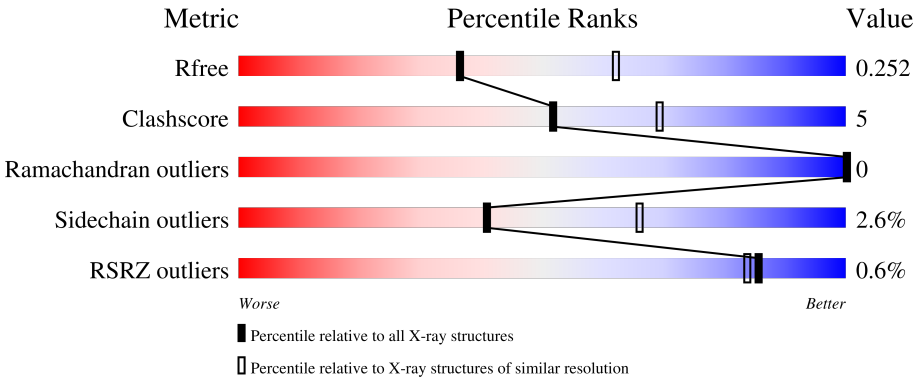
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



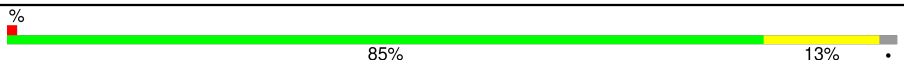
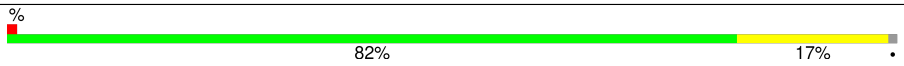
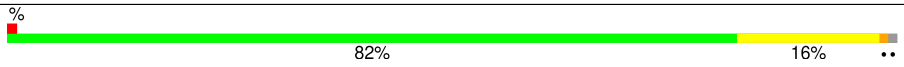
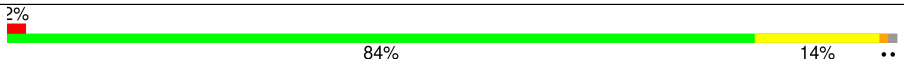
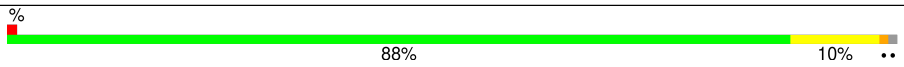
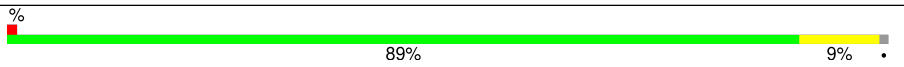
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6935 (2.54-2.50)
Clashscore	180529	7778 (2.54-2.50)
Ramachandran outliers	177936	7674 (2.54-2.50)
Sidechain outliers	177891	7676 (2.54-2.50)
RSRZ outliers	164620	6935 (2.54-2.50)

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	396	88% 10% •
1	B	396	87% 11% ••
1	C	396	87% 11% •
1	D	396	86% 13% •
1	E	396	83% 15% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	396	
1	G	396	
1	H	396	
1	I	396	
1	J	396	
1	K	396	
1	L	396	

2 Entry composition (i)

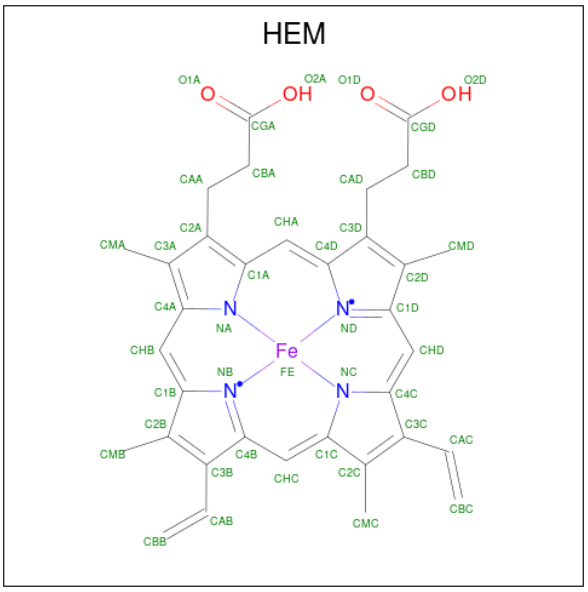
There are 4 unique types of molecules in this entry. The entry contains 38503 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Deferrochelatase.

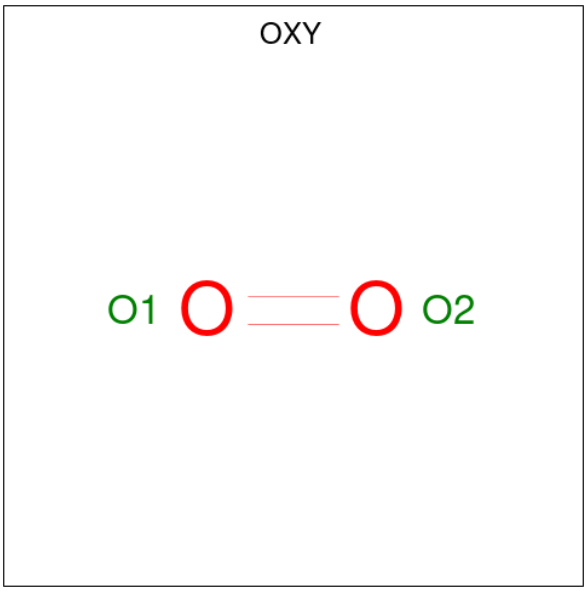
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3027	1897	546	574	10			
1	B	392	Total	C	N	O	S	0	0	0
			3041	1906	549	576	10			
1	C	390	Total	C	N	O	S	0	0	0
			3027	1897	546	574	10			
1	D	392	Total	C	N	O	S	0	0	0
			3037	1903	548	576	10			
1	E	391	Total	C	N	O	S	0	0	0
			3032	1900	547	575	10			
1	F	390	Total	C	N	O	S	0	0	0
			3025	1895	546	574	10			
1	G	387	Total	C	N	O	S	0	0	0
			3004	1881	542	571	10			
1	H	391	Total	C	N	O	S	0	0	0
			3032	1900	547	575	10			
1	I	392	Total	C	N	O	S	0	0	0
			3037	1903	548	576	10			
1	J	392	Total	C	N	O	S	0	0	0
			3037	1903	548	576	10			
1	K	392	Total	C	N	O	S	0	0	0
			3037	1903	548	576	10			
1	L	391	Total	C	N	O	S	0	0	0
			3032	1900	547	575	10			

- 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		
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		
2	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 2 2	0	0
3	B	1	Total O 2 2	0	0
3	C	1	Total O 2 2	0	0
3	D	1	Total O 2 2	0	0
3	E	1	Total O 2 2	0	0
3	F	1	Total O 2 2	0	0
3	G	1	Total O 2 2	0	0
3	H	1	Total O 2 2	0	0
3	I	1	Total O 2 2	0	0
3	J	1	Total O 2 2	0	0
3	K	1	Total O 2 2	0	0
3	L	1	Total O 2 2	0	0

- Molecule 4 is water.

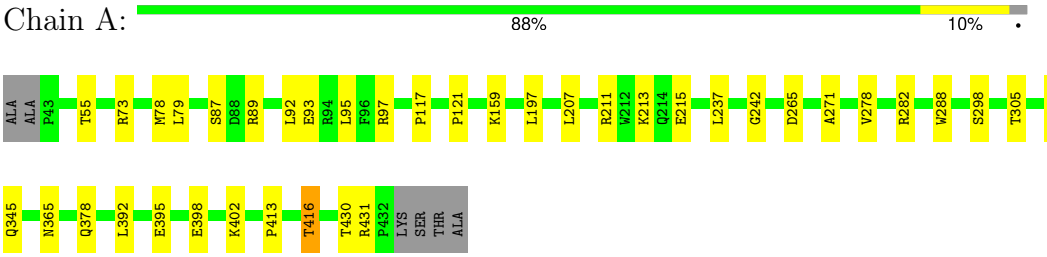
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	173	Total O 174 174	0	1
4	B	135	Total O 136 136	0	1
4	C	134	Total O 134 134	0	0
4	D	127	Total O 127 127	0	0
4	E	145	Total O 145 145	0	0
4	F	132	Total O 132 132	0	0
4	G	112	Total O 112 112	0	0
4	H	141	Total O 141 141	0	0
4	I	96	Total O 96 96	0	0
4	J	122	Total O 122 122	0	0
4	K	122	Total O 122 122	0	0
4	L	154	Total O 154 154	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.

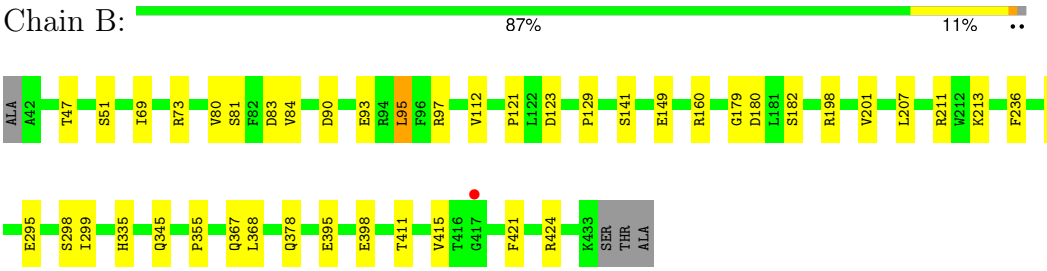
• Molecule 1: Deferrochelatase

Chain A:



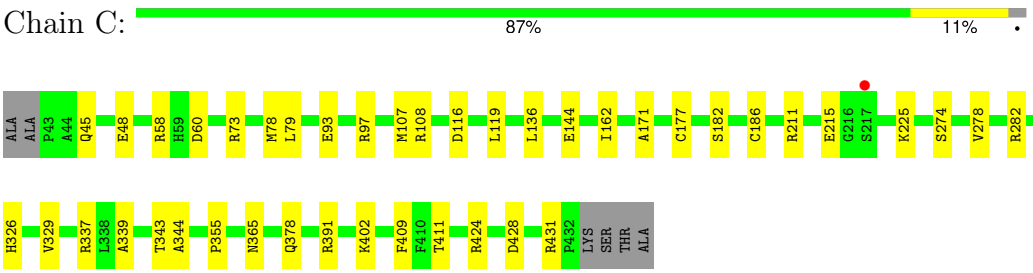
• Molecule 1: Deferrochelatase

Chain B:



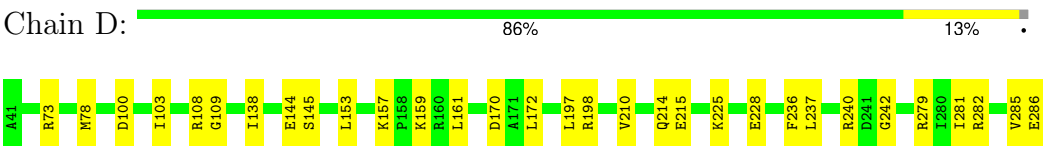
• Molecule 1: Deferrochelatase

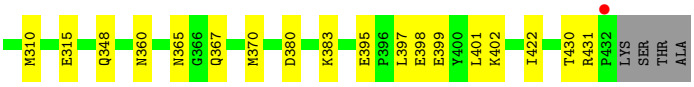
Chain C:



• Molecule 1: Deferrochelatase

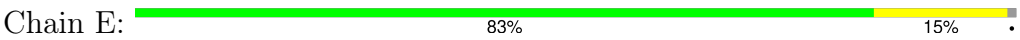
Chain D:

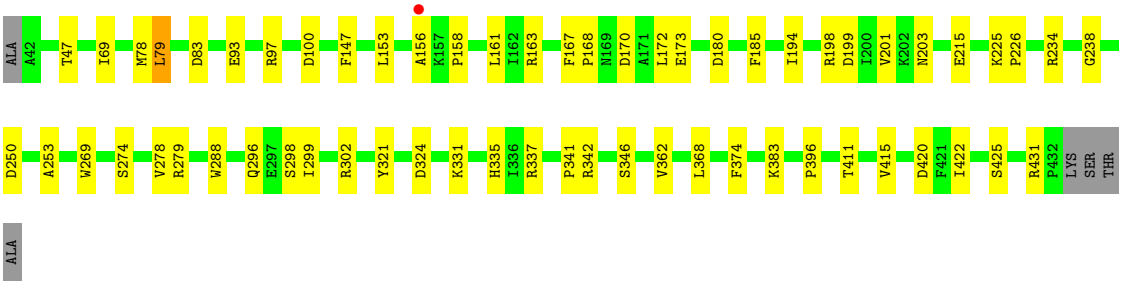




• Molecule 1: Deferrochelatase

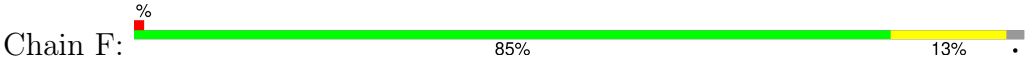
Chain E:

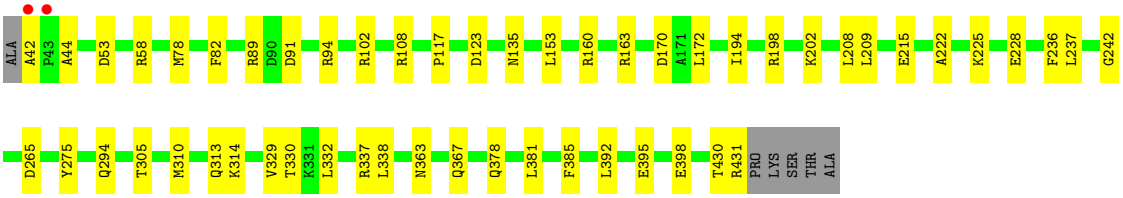




• Molecule 1: Deferrochelatase

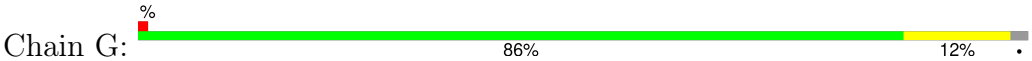
Chain F:

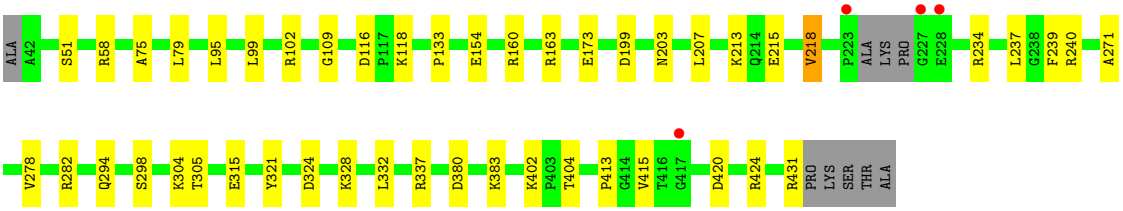




• Molecule 1: Deferrochelatase

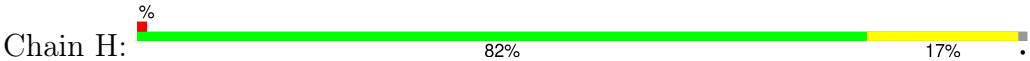
Chain G:

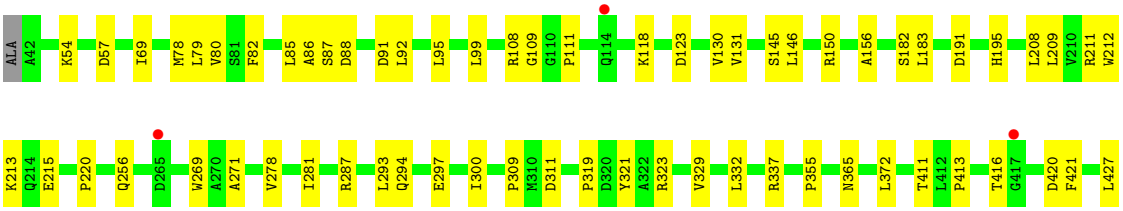


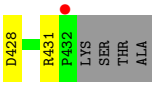


• Molecule 1: Deferrochelatase

Chain H:

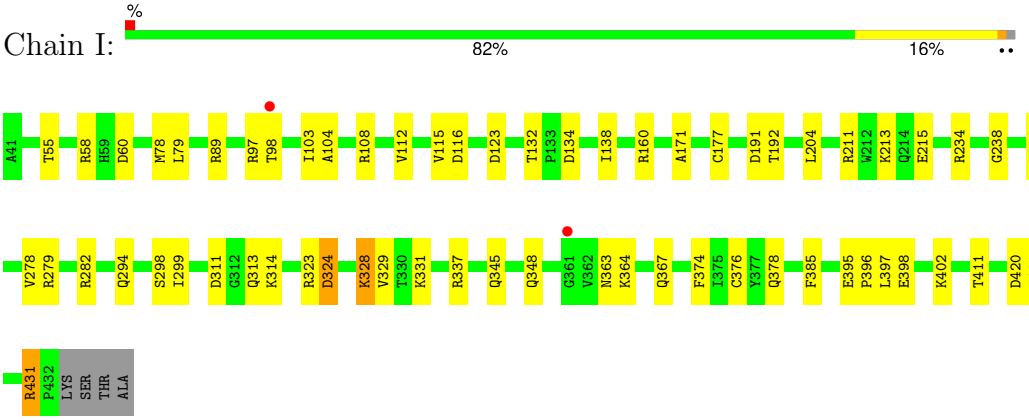






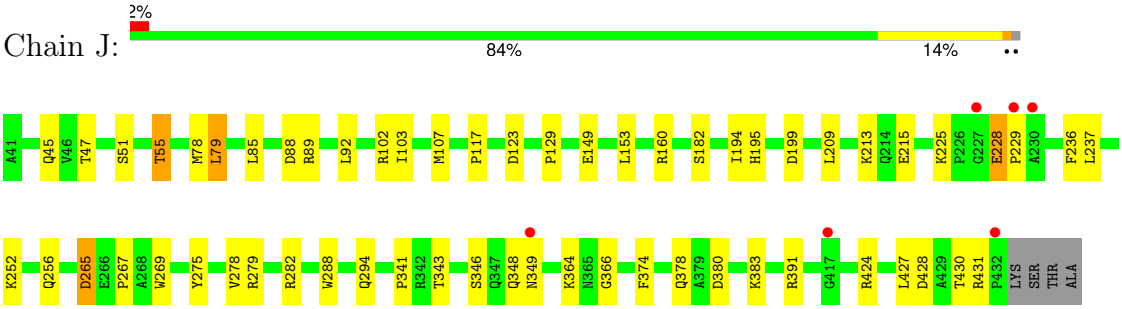
• Molecule 1: Deferrochelatase

Chain I:



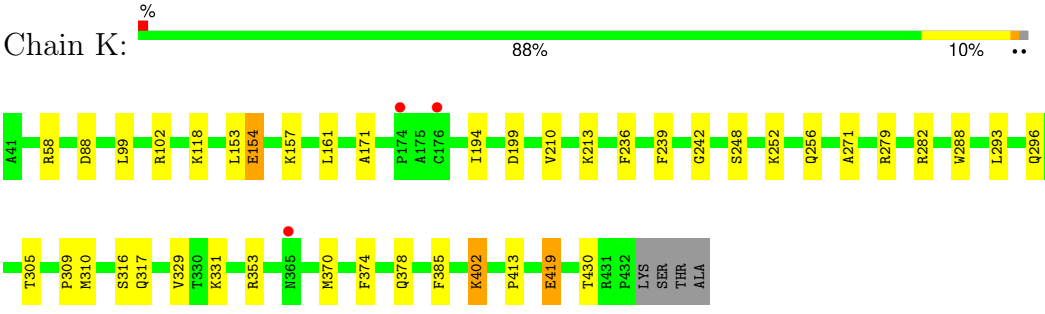
• Molecule 1: Deferrochelatase

Chain J:



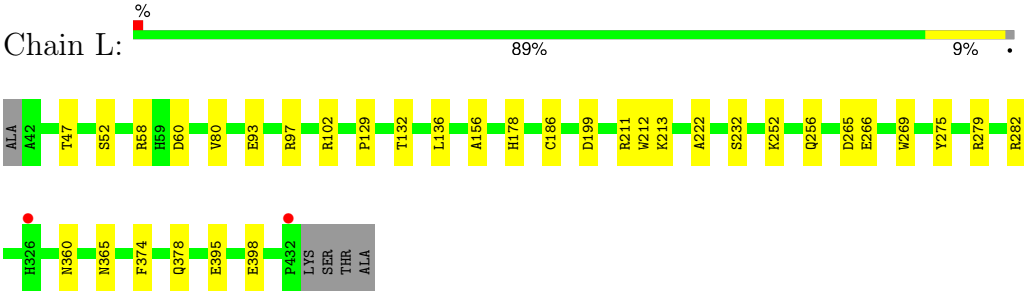
• Molecule 1: Deferrochelatase

Chain K:



• Molecule 1: Deferrochelatase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.33Å 114.75Å 143.72Å 83.31° 77.44° 86.26°	Depositor
Resolution (Å)	19.99 – 2.52 19.99 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.99-2.52) 96.8 (19.99-2.52)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.53Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.198 , 0.252 0.198 , 0.252	Depositor DCC
R_{free} test set	156539 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	38503	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OXY, 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	0.24	0/3098	0.48	0/4209
1	B	0.24	0/3112	0.48	0/4228
1	C	0.25	0/3098	0.49	0/4209
1	D	0.24	0/3108	0.49	0/4224
1	E	0.25	0/3103	0.49	0/4217
1	F	0.24	0/3095	0.48	0/4205
1	G	0.24	0/3072	0.49	0/4172
1	H	0.25	0/3103	0.49	0/4217
1	I	0.26	0/3108	0.52	2/4224 (0.0%)
1	J	0.24	0/3108	0.49	0/4224
1	K	0.25	0/3108	0.49	0/4224
1	L	0.24	0/3103	0.48	0/4217
All	All	0.25	0/37216	0.49	2/50570 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	324	ASP	CB-CG-OD1	7.98	125.48	118.30
1	I	324	ASP	CB-CG-OD2	-7.49	111.56	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3027	0	2975	29	0
1	B	3041	0	2992	29	0
1	C	3027	0	2975	22	0
1	D	3037	0	2984	36	0
1	E	3032	0	2979	39	0
1	F	3025	0	2972	33	0
1	G	3004	0	2946	28	0
1	H	3032	0	2979	36	0
1	I	3037	0	2984	36	1
1	J	3037	0	2984	37	0
1	K	3037	0	2984	28	1
1	L	3032	0	2979	26	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
2	C	43	0	30	1	0
2	D	43	0	30	4	0
2	E	43	0	30	4	0
2	F	43	0	30	4	0
2	G	43	0	30	1	0
2	H	43	0	30	2	0
2	I	43	0	30	3	0
2	J	43	0	30	1	0
2	K	43	0	30	3	0
2	L	43	0	30	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	1	0
3	L	2	0	0	0	0
4	A	174	0	0	2	0
4	B	136	0	0	2	0
4	C	134	0	0	3	1
4	D	127	0	0	0	0
4	E	145	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	132	0	0	2	0
4	G	112	0	0	1	0
4	H	141	0	0	4	1
4	I	96	0	0	2	0
4	J	122	0	0	2	0
4	K	122	0	0	1	0
4	L	154	0	0	3	0
All	All	38503	0	36093	365	2

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 5.

All (365) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:HD22	1:A:278:VAL:HG11	1.64	0.80
1:E:78:MET:HG3	1:E:215:GLU:HG2	1.64	0.79
1:D:281:ILE:HG21	2:D:501:HEM:HBB1	1.66	0.77
1:D:287:ARG:NH2	1:D:399:GLU:O	2.18	0.76
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.67	0.76
2:I:501:HEM:HBC2	2:I:501:HEM:HHD	1.70	0.74
1:J:228:GLU:HG3	1:J:229:PRO:HD2	1.70	0.73
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.71	0.72
2:H:501:HEM:HBB2	2:H:501:HEM:HHC	1.71	0.72
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.68	0.72
1:J:364:LYS:H	1:J:364:LYS:HD2	1.55	0.72
1:D:236:PHE:O	1:E:198:ARG:NH2	2.25	0.70
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.73	0.70
1:I:345:GLN:OE1	1:I:345:GLN:N	2.20	0.69
1:G:234:ARG:NH2	1:G:304:LYS:O	2.26	0.69
1:B:198:ARG:NH1	1:K:236:PHE:O	2.24	0.69
2:K:501:HEM:HHC	2:K:501:HEM:HBB2	1.75	0.66
1:I:58:ARG:NH2	1:I:60:ASP:OD1	2.22	0.66
1:C:58:ARG:NH2	1:C:60:ASP:OD1	2.28	0.66
1:F:117:PRO:HB2	1:J:294:GLN:HG3	1.79	0.65
1:K:298:SER:HB2	1:K:331:LYS:HD3	1.79	0.64
1:C:45:GLN:HB2	1:C:48:GLU:HG3	1.80	0.63
1:H:294:GLN:NE2	4:H:605:HOH:O	2.28	0.63
1:K:171:ALA:HB3	1:K:402:LYS:HD3	1.80	0.63
1:F:198:ARG:NH1	1:J:236:PHE:O	2.29	0.62
1:H:281:ILE:HG21	2:H:501:HEM:HBB1	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:NH2	1:A:430:THR:OG1	2.33	0.62
1:I:115:VAL:HG22	1:I:116:ASP:H	1.62	0.62
1:F:160:ARG:HH12	1:F:265:ASP:HB3	1.64	0.62
1:I:279:ARG:HB2	1:I:374:PHE:HB3	1.82	0.62
1:B:93:GLU:OE2	1:B:97:ARG:NH1	2.34	0.61
1:D:153:LEU:HD23	1:D:430:THR:HG21	1.82	0.61
1:D:285:VAL:HG11	1:D:370:MET:HE1	1.83	0.60
1:D:197:LEU:HD21	1:E:368:LEU:HD11	1.83	0.60
1:G:75:ALA:HA	1:G:218:VAL:HG12	1.83	0.60
1:H:109:GLY:HA2	1:H:131:VAL:HG12	1.84	0.60
1:A:89:ARG:HH12	1:A:431:ARG:HG2	1.67	0.59
1:F:242:GLY:HA3	1:J:47:THR:HG21	1.85	0.59
1:A:73:ARG:NH2	1:L:47:THR:O	2.36	0.59
1:L:213:LYS:NZ	4:L:605:HOH:O	2.35	0.59
1:E:156:ALA:O	1:E:269:TRP:NE1	2.31	0.59
1:B:73:ARG:HH21	1:B:355:PRO:HD2	1.68	0.59
1:J:102:ARG:NH2	4:J:606:HOH:O	2.36	0.58
1:L:93:GLU:OE2	1:L:97:ARG:NH1	2.35	0.58
1:H:85:LEU:HD11	1:H:209:LEU:HB2	1.86	0.58
2:E:501:HEM:HBB2	2:E:501:HEM:HMB2	1.84	0.58
1:D:395:GLU:HG2	1:D:398:GLU:HG3	1.86	0.58
1:K:353:ARG:NH1	3:K:502:OXY:O2	2.35	0.58
1:B:213:LYS:NZ	4:B:614:HOH:O	2.37	0.58
1:J:279:ARG:HB2	1:J:374:PHE:HB3	1.85	0.58
1:D:170:ASP:HB3	1:D:172:LEU:HD13	1.85	0.57
1:D:236:PHE:CZ	1:E:194:ILE:HD13	2.39	0.57
1:F:313:GLN:HG3	1:F:314:LYS:HG3	1.86	0.57
1:J:89:ARG:HH22	1:J:430:THR:HG23	1.69	0.57
1:J:380:ASP:HB3	1:J:383:LYS:HB2	1.86	0.57
1:E:156:ALA:HB1	1:E:269:TRP:CD1	2.40	0.57
1:E:279:ARG:HB2	1:E:374:PHE:HB3	1.87	0.57
1:B:95:LEU:HD12	1:B:207:LEU:HB3	1.87	0.56
1:E:288:TRP:O	1:E:296:GLN:NE2	2.38	0.56
1:E:158:PRO:HB2	1:E:161:LEU:HB2	1.87	0.56
1:G:240:ARG:NH1	1:G:315:GLU:OE1	2.32	0.56
1:J:79:LEU:HD22	1:J:278:VAL:HG11	1.87	0.56
1:I:428:ASP:HA	1:I:431:ARG:HG2	1.86	0.56
1:E:79:LEU:HD22	1:E:278:VAL:HG11	1.86	0.56
1:H:80:VAL:HG13	1:H:213:LYS:HB3	1.87	0.56
1:H:431:ARG:NH1	4:H:610:HOH:O	2.39	0.56
1:D:397:LEU:HG	1:D:401:LEU:HD11	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:160:ARG:NH1	1:J:265:ASP:OD1	2.30	0.55
1:G:154:GLU:N	1:G:154:GLU:OE1	2.34	0.55
1:H:79:LEU:HD22	1:H:278:VAL:HG11	1.88	0.55
1:H:211:ARG:HG2	1:H:212:TRP:CD1	2.41	0.55
1:A:211:ARG:NH2	4:A:612:HOH:O	2.40	0.55
1:D:100:ASP:HB2	1:D:422:ILE:HG22	1.89	0.55
1:D:236:PHE:HZ	1:E:194:ILE:HD13	1.72	0.55
1:F:385:PHE:HE1	2:F:501:HEM:HBB2	1.72	0.55
1:C:108:ARG:NH1	4:C:607:HOH:O	2.37	0.55
1:I:78:MET:HB2	1:I:215:GLU:HG2	1.88	0.55
1:E:341:PRO:HD2	1:E:346:SER:HB2	1.88	0.55
1:I:177:CYS:O	1:I:211:ARG:NH1	2.40	0.55
1:B:95:LEU:HB2	1:B:207:LEU:HD13	1.89	0.55
1:J:153:LEU:HD23	1:J:430:THR:HG21	1.88	0.54
1:K:419:GLU:CD	1:K:419:GLU:H	2.10	0.54
1:L:266:GLU:OE2	1:L:275:TYR:OH	2.24	0.54
1:A:55:THR:HG21	1:L:222:ALA:HB2	1.90	0.54
1:B:47:THR:HG21	1:K:242:GLY:HA3	1.90	0.54
1:E:321:TYR:CE2	1:E:342:ARG:HG3	2.43	0.54
1:C:424:ARG:NH1	4:C:614:HOH:O	2.41	0.54
1:E:324:ASP:O	1:E:337:ARG:NH2	2.31	0.54
1:K:88:ASP:OD1	1:K:88:ASP:N	2.41	0.54
1:A:117:PRO:HB2	1:L:294:GLN:HB3	1.90	0.53
1:I:324:ASP:HB2	1:I:328:LYS:H	1.73	0.53
1:I:324:ASP:OD1	1:I:337:ARG:NH1	2.34	0.53
1:J:92:LEU:HD23	1:J:427:LEU:HD21	1.91	0.53
1:C:93:GLU:OE2	1:C:97:ARG:NH1	2.42	0.53
1:F:225:LYS:HB2	1:F:228:GLU:HG3	1.91	0.53
1:C:78:MET:HG3	1:C:215:GLU:HG2	1.89	0.53
1:H:123:ASP:OD2	1:H:195:HIS:NE2	2.38	0.53
1:H:287:ARG:NH2	4:H:603:HOH:O	2.27	0.53
1:K:302:ARG:HH21	1:K:309:PRO:HD3	1.74	0.53
1:I:252:LYS:O	1:I:256:GLN:HG3	2.10	0.52
1:J:364:LYS:HD2	1:J:364:LYS:N	2.22	0.52
1:K:385:PHE:HE1	2:K:501:HEM:HAB	1.72	0.52
1:E:234:ARG:NH1	1:E:238:GLY:O	2.41	0.52
1:F:170:ASP:HB3	1:F:172:LEU:HG	1.91	0.52
1:F:294:GLN:HG3	1:J:117:PRO:HB2	1.91	0.52
1:B:141:SER:HB2	1:B:182:SER:HB3	1.92	0.52
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.92	0.52
1:H:211:ARG:HG2	1:H:212:TRP:HD1	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:LEU:HD22	1:G:278:VAL:HG11	1.90	0.52
1:A:93:GLU:OE2	1:A:97:ARG:NH1	2.41	0.52
1:G:102:ARG:NH2	4:G:607:HOH:O	2.39	0.52
1:A:339:ALA:HB2	1:A:392:LEU:HD21	1.91	0.51
1:I:299:ILE:HG12	1:I:396:PRO:HB2	1.90	0.51
1:A:237:LEU:HD22	2:A:501:HEM:HBC1	1.92	0.51
2:E:501:HEM:HMC1	2:E:501:HEM:HBC2	1.91	0.51
1:E:302:ARG:NH2	4:E:607:HOH:O	2.43	0.51
1:F:338:LEU:HB2	1:F:392:LEU:HD23	1.93	0.51
1:B:395:GLU:HG2	1:B:398:GLU:HG3	1.93	0.51
1:B:83:ASP:OD1	1:B:211:ARG:NH1	2.43	0.51
1:I:395:GLU:HG2	1:I:398:GLU:HG3	1.92	0.51
1:I:431:ARG:HA	1:I:431:ARG:NE	2.26	0.51
1:L:265:ASP:OD1	1:L:265:ASP:N	2.43	0.51
1:A:305:THR:HG23	1:L:129:PRO:HG3	1.92	0.50
1:C:310:MET:HB3	1:C:329:VAL:HG12	1.92	0.50
1:B:69:ILE:HD11	1:B:411:THR:HG21	1.93	0.50
1:C:339:ALA:O	1:C:391:ARG:NH2	2.39	0.50
1:H:311:ASP:HB3	1:H:329:VAL:HG11	1.93	0.50
1:L:279:ARG:HB2	1:L:374:PHE:HB3	1.93	0.50
2:F:501:HEM:HBC2	2:F:501:HEM:HMC1	1.94	0.50
1:J:103:ILE:O	1:J:107:MET:HG3	2.12	0.50
1:A:242:GLY:HA3	1:L:47:THR:HG21	1.94	0.50
1:E:274:SER:O	1:E:411:THR:N	2.41	0.50
1:K:302:ARG:NH2	1:K:317:GLN:O	2.45	0.50
2:K:501:HEM:HBC2	2:K:501:HEM:HMC1	1.92	0.50
1:L:80:VAL:HG13	1:L:213:LYS:HG3	1.93	0.50
1:I:112:VAL:HG11	1:I:123:ASP:HB2	1.94	0.50
1:F:91:ASP:OD1	1:F:94:ARG:NH2	2.45	0.50
1:F:222:ALA:HB2	1:J:55:THR:HG21	1.94	0.50
1:I:213:LYS:NZ	4:I:618:HOH:O	2.44	0.50
1:J:364:LYS:H	1:J:364:LYS:CD	2.23	0.50
2:L:501:HEM:HBB2	2:L:501:HEM:HMB2	1.92	0.50
1:D:214:GLN:NE2	1:D:360:ASN:OD1	2.40	0.50
1:D:242:GLY:HA3	1:E:47:THR:HG21	1.94	0.50
2:G:501:HEM:HMB2	2:G:501:HEM:HBB2	1.94	0.49
1:I:234:ARG:NH1	1:I:238:GLY:O	2.45	0.49
1:A:95:LEU:HB2	1:A:207:LEU:HD13	1.95	0.49
1:A:78:MET:HE1	1:A:197:LEU:HB2	1.95	0.49
1:A:395:GLU:HG2	1:A:398:GLU:HG3	1.94	0.49
1:G:213:LYS:NZ	1:G:215:GLU:OE2	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:THR:O	1:A:416:THR:OG1	2.27	0.49
1:J:85:LEU:HD11	1:J:209:LEU:HB2	1.94	0.49
1:F:275:TYR:HB3	1:F:381:LEU:HD13	1.94	0.49
1:D:210:VAL:HG21	1:E:368:LEU:HD21	1.93	0.49
1:H:111:PRO:HA	1:H:130:VAL:HA	1.93	0.49
1:L:178:HIS:HB2	1:L:211:ARG:NH2	2.27	0.49
1:F:332:LEU:HA	1:F:337:ARG:HD3	1.95	0.49
1:L:58:ARG:NH1	1:L:60:ASP:OD1	2.40	0.49
1:H:86:ALA:HB1	1:H:91:ASP:HB3	1.93	0.49
1:J:343:THR:OG1	1:J:346:SER:OG	2.21	0.49
1:D:225:LYS:HB2	1:D:228:GLU:HB2	1.95	0.49
1:J:78:MET:HB2	1:J:215:GLU:HG2	1.95	0.49
1:H:95:LEU:HD21	1:H:208:LEU:HD21	1.94	0.48
1:H:78:MET:HB2	1:H:215:GLU:HG2	1.95	0.48
1:C:97:ARG:NH2	4:C:619:HOH:O	2.46	0.48
1:G:116:ASP:OD2	1:G:118:LYS:HB3	2.14	0.48
1:H:54:LYS:HB2	1:H:57:ASP:OD2	2.13	0.48
1:D:78:MET:HB2	1:D:215:GLU:HG2	1.95	0.48
1:E:69:ILE:HD11	1:E:411:THR:HG21	1.95	0.48
1:B:121:PRO:HG3	1:K:293:LEU:HB2	1.96	0.48
1:C:79:LEU:CD2	1:C:278:VAL:HG11	2.43	0.48
1:D:159:LYS:HA	1:D:159:LYS:HD3	1.58	0.48
2:A:501:HEM:HBB1	4:A:623:HOH:O	2.14	0.48
1:G:239:PHE:CE1	1:G:304:LYS:HG3	2.49	0.48
1:G:324:ASP:O	1:G:337:ARG:NH2	2.47	0.48
1:H:332:LEU:HA	1:H:337:ARG:HD3	1.96	0.48
1:J:160:ARG:HB2	1:J:275:TYR:CZ	2.49	0.47
1:L:213:LYS:HB3	1:L:213:LYS:HE2	1.60	0.47
1:I:58:ARG:HG3	1:I:58:ARG:HH11	1.79	0.47
1:I:89:ARG:HE	1:I:431:ARG:NH2	2.12	0.47
1:I:395:GLU:HG3	1:I:397:LEU:H	1.79	0.47
1:E:225:LYS:HB3	1:E:226:PRO:HD2	1.95	0.47
1:G:332:LEU:HA	1:G:337:ARG:HD2	1.96	0.47
1:H:191:ASP:OD1	4:H:601:HOH:O	2.20	0.47
1:K:302:ARG:NH1	4:K:604:HOH:O	2.30	0.47
1:F:237:LEU:HG	2:F:501:HEM:HBC1	1.96	0.47
1:H:92:LEU:HD23	1:H:427:LEU:HD21	1.96	0.47
1:K:154:GLU:CD	1:K:154:GLU:H	2.17	0.47
1:K:288:TRP:O	1:K:296:GLN:NE2	2.48	0.47
1:D:287:ARG:HG3	1:D:290:ARG:HH21	1.78	0.47
1:F:209:LEU:HD11	1:J:366:GLY:HA3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:501:HEM:HBB2	2:J:501:HEM:HMB2	1.96	0.47
1:A:237:LEU:HG	1:A:288:TRP:CE2	2.50	0.47
1:E:415:VAL:HG13	1:E:420:ASP:HB3	1.97	0.47
1:H:146:LEU:HA	1:H:150:ARG:HH21	1.80	0.47
1:A:159:LYS:HE2	1:A:159:LYS:HB3	1.57	0.47
1:A:265:ASP:OD1	1:A:265:ASP:N	2.48	0.47
1:G:102:ARG:HD2	1:G:203:ASN:HD22	1.79	0.47
1:J:424:ARG:NH1	4:J:616:HOH:O	2.47	0.47
1:G:118:LYS:HB2	1:G:118:LYS:HE2	1.56	0.47
1:B:282:ARG:HH22	1:B:367:GLN:HG3	1.79	0.46
1:D:285:VAL:HB	1:E:198:ARG:NH1	2.30	0.46
1:L:102:ARG:NH2	4:L:620:HOH:O	2.44	0.46
1:H:118:LYS:HD3	1:H:118:LYS:HA	1.84	0.46
1:H:428:ASP:O	1:H:431:ARG:HG2	2.15	0.46
1:A:213:LYS:NZ	1:L:360:ASN:O	2.45	0.46
1:H:321:TYR:CZ	1:H:337:ARG:HG3	2.51	0.46
1:F:310:MET:HB2	1:F:329:VAL:HG12	1.96	0.46
2:E:501:HEM:HBD1	2:E:501:HEM:HHA	1.97	0.46
1:K:279:ARG:HB2	1:K:374:PHE:HB3	1.98	0.46
1:A:271:ALA:O	1:A:413:PRO:HB3	2.15	0.46
1:B:281:ILE:HG21	2:B:501:HEM:HBB1	1.97	0.46
1:E:199:ASP:O	1:E:203:ASN:ND2	2.47	0.46
1:F:58:ARG:HG3	1:F:58:ARG:HH11	1.81	0.46
1:E:83:ASP:HA	1:E:180:ASP:HB2	1.98	0.46
1:H:82:PHE:HE1	1:H:183:LEU:HB2	1.80	0.46
1:G:321:TYR:CE2	1:G:337:ARG:HG3	2.51	0.46
1:C:73:ARG:NH1	1:C:355:PRO:O	2.48	0.45
1:E:299:ILE:HG12	1:E:396:PRO:HB2	1.97	0.45
1:H:69:ILE:HD11	1:H:411:THR:HG21	1.97	0.45
1:B:112:VAL:HG11	1:B:123:ASP:HB2	1.98	0.45
1:E:100:ASP:HB2	1:E:422:ILE:HG22	1.97	0.45
1:F:305:THR:HG23	1:J:129:PRO:HG3	1.99	0.45
1:J:349:ASN:HD21	1:J:391:ARG:HH12	1.63	0.45
1:K:252:LYS:O	1:K:256:GLN:HG3	2.17	0.45
1:L:132:THR:OG1	4:L:601:HOH:O	2.20	0.45
1:D:210:VAL:HG11	1:E:362:VAL:HG11	1.98	0.45
1:F:153:LEU:HD23	1:F:430:THR:HG21	1.98	0.45
1:L:102:ARG:HD3	1:L:199:ASP:OD1	2.16	0.45
1:A:121:PRO:HG3	1:L:293:LEU:HB2	1.99	0.45
1:G:173:GLU:OE1	1:G:404:THR:HB	2.17	0.45
1:H:420:ASP:OD1	1:H:421:PHE:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:102:ARG:NH2	1:K:199:ASP:OD2	2.47	0.45
1:I:104:ALA:O	1:I:108:ARG:HB3	2.16	0.45
1:L:395:GLU:HG2	1:L:398:GLU:HG3	1.98	0.45
1:B:274:SER:O	1:B:411:THR:N	2.48	0.45
1:B:295:GLU:HG2	1:B:299:ILE:HD11	1.98	0.45
1:B:415:VAL:HG11	1:B:421:PHE:C	2.37	0.45
1:L:211:ARG:HG2	1:L:212:TRP:CD1	2.52	0.45
1:B:80:VAL:HG13	1:B:213:LYS:HB2	1.99	0.44
1:C:177:CYS:O	1:C:211:ARG:NH1	2.50	0.44
1:E:170:ASP:HB3	1:E:172:LEU:HG	2.00	0.44
1:H:146:LEU:HA	1:H:150:ARG:NH2	2.32	0.44
1:C:321:TYR:CZ	1:C:337:ARG:HG3	2.53	0.44
1:D:157:LYS:HE2	1:D:161:LEU:O	2.17	0.44
1:F:236:PHE:CZ	1:J:194:ILE:HD13	2.52	0.44
1:F:385:PHE:HE1	2:F:501:HEM:CBB	2.29	0.44
1:J:341:PRO:HD2	1:J:346:SER:HB3	1.99	0.44
1:A:282:ARG:HB3	1:A:402:LYS:HB3	1.98	0.44
1:E:321:TYR:CD2	1:E:342:ARG:HG3	2.52	0.44
1:B:73:ARG:NH2	4:B:618:HOH:O	2.42	0.44
1:E:78:MET:HB3	1:E:185:PHE:HB2	1.99	0.44
1:G:237:LEU:O	1:G:304:LYS:NZ	2.50	0.44
1:J:149:GLU:OE1	1:J:149:GLU:N	2.42	0.44
1:B:81:SER:OG	1:B:179:GLY:HA3	2.17	0.44
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	2.00	0.44
1:I:374:PHE:CE2	2:I:501:HEM:HBB2	2.53	0.44
1:D:170:ASP:OD2	1:D:279:ARG:NH1	2.47	0.44
1:I:79:LEU:HD22	1:I:278:VAL:HG11	1.99	0.44
1:L:211:ARG:HG2	1:L:212:TRP:HD1	1.83	0.44
1:C:274:SER:O	1:C:411:THR:N	2.50	0.44
1:C:343:THR:HG22	1:C:344:ALA:N	2.33	0.44
1:D:109:GLY:O	1:G:58:ARG:NH2	2.33	0.43
1:D:237:LEU:HG	1:D:288:TRP:CE2	2.53	0.43
1:E:147:PHE:HD2	1:E:153:LEU:O	2.00	0.43
1:K:239:PHE:HE2	1:K:288:TRP:HZ2	1.65	0.43
1:H:309:PRO:HB3	1:H:319:PRO:HG3	2.00	0.43
1:F:363:ASN:OD1	1:F:367:GLN:N	2.46	0.43
1:K:157:LYS:HE2	1:K:161:LEU:O	2.19	0.43
1:G:102:ARG:HD3	1:G:199:ASP:OD1	2.18	0.43
1:K:153:LEU:HA	1:K:430:THR:HG21	2.00	0.43
1:G:109:GLY:HA3	1:G:133:PRO:HD3	2.01	0.43
1:J:237:LEU:HD22	1:J:288:TRP:CD1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:ARG:HA	1:E:201:VAL:HG22	2.01	0.43
1:G:99:LEU:HD23	1:G:99:LEU:HA	1.91	0.43
1:J:267:PRO:HB2	1:J:269:TRP:CD1	2.53	0.43
1:F:313:GLN:CG	1:F:314:LYS:HG3	2.49	0.43
1:G:102:ARG:HD2	1:G:203:ASN:ND2	2.34	0.43
1:H:156:ALA:HB1	1:H:269:TRP:NE1	2.34	0.43
1:F:82:PHE:HB3	1:F:208:LEU:HD22	2.01	0.43
1:H:293:LEU:O	1:H:297:GLU:HG3	2.19	0.43
1:H:355:PRO:HB2	1:H:372:LEU:HD11	2.00	0.43
1:F:102:ARG:NH2	4:F:623:HOH:O	2.51	0.43
1:B:282:ARG:HH22	1:B:367:GLN:CG	2.32	0.43
1:D:286:GLU:O	1:D:290:ARG:HG3	2.19	0.43
1:D:365:ASN:OD1	1:D:365:ASN:N	2.51	0.43
1:I:58:ARG:HG3	1:I:58:ARG:NH1	2.34	0.43
1:L:156:ALA:HB1	1:L:269:TRP:NE1	2.34	0.43
1:I:103:ILE:HG23	1:I:138:ILE:HB	2.00	0.42
1:K:271:ALA:O	1:K:413:PRO:HB3	2.19	0.42
1:F:330:THR:O	1:F:337:ARG:NH1	2.52	0.42
1:G:271:ALA:O	1:G:413:PRO:HB3	2.18	0.42
1:L:80:VAL:HG22	1:L:213:LYS:HG3	2.01	0.42
1:B:236:PHE:CZ	1:K:194:ILE:HD13	2.53	0.42
1:B:335:HIS:CD2	2:B:501:HEM:NA	2.87	0.42
1:C:428:ASP:O	1:C:431:ARG:HD2	2.19	0.42
1:F:42:ALA:O	1:F:44:ALA:N	2.48	0.42
1:F:395:GLU:HG2	1:F:398:GLU:HG3	2.02	0.42
1:I:420:ASP:OD1	1:I:421:PHE:N	2.52	0.42
1:L:252:LYS:O	1:L:256:GLN:HG2	2.20	0.42
1:A:237:LEU:HD22	2:A:501:HEM:CBC	2.49	0.42
1:B:198:ARG:HD2	1:K:370:MET:SD	2.59	0.42
1:A:78:MET:CE	1:A:197:LEU:HB2	2.49	0.42
1:C:136:LEU:HA	1:C:186:CYS:O	2.18	0.42
1:C:107:MET:HG2	1:C:136:LEU:O	2.20	0.42
1:C:171:ALA:HB2	1:C:402:LYS:HE3	2.01	0.42
1:D:73:ARG:HE	1:D:73:ARG:HB3	1.68	0.42
1:D:103:ILE:HG23	1:D:138:ILE:HB	2.01	0.42
1:I:55:THR:HB	1:I:132:THR:OG1	2.20	0.42
1:I:134:ASP:HB3	1:I:192:THR:HG21	2.02	0.42
1:I:274:SER:O	1:I:411:THR:N	2.52	0.42
1:A:402:LYS:HA	1:A:402:LYS:HD3	1.75	0.42
1:C:116:ASP:HB3	1:C:119:LEU:HG	2.02	0.42
1:D:402:LYS:HD3	1:D:402:LYS:HA	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:PHE:HB3	1:E:168:PRO:HD2	2.02	0.42
1:E:173:GLU:OE1	4:E:601:HOH:O	2.22	0.42
1:I:171:ALA:HB2	1:I:402:LYS:HE3	2.01	0.42
1:I:345:GLN:O	1:I:348:GLN:HG2	2.20	0.42
1:J:348:GLN:OE1	1:J:383:LYS:HE2	2.19	0.42
1:C:144:GLU:HG3	1:C:162:ILE:HA	2.00	0.42
1:F:78:MET:HB2	1:F:215:GLU:HG2	2.01	0.42
1:G:380:ASP:HB3	1:G:383:LYS:HB2	2.02	0.42
1:I:98:THR:OG1	1:I:204:LEU:HD21	2.19	0.42
1:G:294:GLN:O	1:G:298:SER:OG	2.32	0.41
1:G:415:VAL:HG23	1:G:420:ASP:HB3	2.01	0.41
1:H:150:ARG:HE	1:H:150:ARG:HB2	1.75	0.41
1:F:89:ARG:NH1	1:F:430:THR:OG1	2.53	0.41
1:F:163:ARG:NH1	4:F:602:HOH:O	2.27	0.41
1:D:281:ILE:CG2	2:D:501:HEM:HBB1	2.45	0.41
1:D:370:MET:HB3	1:D:370:MET:HE2	1.94	0.41
1:I:311:ASP:HB3	1:I:329:VAL:HG11	2.01	0.41
1:B:84:VAL:HG23	1:B:180:ASP:HB3	2.02	0.41
1:B:129:PRO:HB3	1:K:305:THR:HG23	2.02	0.41
1:A:92:LEU:HD12	1:A:95:LEU:HD23	2.02	0.41
1:A:213:LYS:NZ	1:A:215:GLU:OE2	2.47	0.41
1:G:95:LEU:HB2	1:G:207:LEU:HD13	2.01	0.41
1:G:402:LYS:HA	1:G:402:LYS:HD3	1.79	0.41
1:G:328:LYS:HD3	1:G:328:LYS:HA	1.88	0.41
2:L:501:HEM:HMC1	2:L:501:HEM:HBC2	2.03	0.41
1:D:380:ASP:HB3	1:D:383:LYS:HB3	2.02	0.41
1:F:194:ILE:HD13	1:J:236:PHE:CZ	2.56	0.41
1:I:385:PHE:HE1	2:I:501:HEM:CBB	2.34	0.41
1:J:102:ARG:HD3	1:J:199:ASP:OD1	2.20	0.41
1:J:123:ASP:OD1	1:J:195:HIS:NE2	2.54	0.41
1:K:310:MET:HB2	1:K:329:VAL:HG12	2.03	0.41
1:E:93:GLU:OE2	1:E:97:ARG:NH1	2.54	0.41
1:H:99:LEU:HD23	1:H:99:LEU:HA	1.94	0.41
1:H:300:ILE:HD13	1:H:300:ILE:HA	1.94	0.41
1:A:333:ASP:OD1	1:A:333:ASP:N	2.55	0.40
1:B:198:ARG:HA	1:B:201:VAL:HG22	2.02	0.40
1:C:182:SER:HB3	1:C:409:PHE:CD2	2.55	0.40
1:D:240:ARG:NH1	1:D:315:GLU:OE1	2.46	0.40
1:D:289:ASP:OD1	1:E:198:ARG:NH1	2.53	0.40
1:K:302:ARG:NH2	1:K:309:PRO:HD3	2.36	0.40
1:J:428:ASP:OD1	1:J:431:ARG:NH1	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:LEU:HA	1:L:186:CYS:O	2.22	0.40
1:E:250:ASP:HB3	1:E:253:ALA:HB3	2.04	0.40
1:E:335:HIS:CD2	2:E:501:HEM:ND	2.90	0.40
1:I:89:ARG:HE	1:I:431:ARG:CZ	2.34	0.40
1:K:99:LEU:HD23	1:K:99:LEU:HA	1.93	0.40
1:B:368:LEU:HD21	1:K:210:VAL:HG21	2.03	0.40
1:D:365:ASN:OD1	1:D:367:GLN:HG2	2.21	0.40
1:H:271:ALA:O	1:H:413:PRO:HB3	2.22	0.40
1:I:323:ARG:NH2	4:I:610:HOH:O	2.36	0.40
1:I:363:ASN:HB2	1:I:367:GLN:O	2.21	0.40
1:J:252:LYS:O	1:J:256:GLN:HG3	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:97:ARG:O	1:K:118:LYS:NZ[1_655]	2.07	0.13
4:C:682:HOH:O	4:H:614:HOH:O[1_655]	2.18	0.02

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	388/396 (98%)	375 (97%)	13 (3%)	0	100	100
1	B	390/396 (98%)	375 (96%)	15 (4%)	0	100	100
1	C	388/396 (98%)	378 (97%)	10 (3%)	0	100	100
1	D	390/396 (98%)	373 (96%)	17 (4%)	0	100	100
1	E	389/396 (98%)	376 (97%)	13 (3%)	0	100	100
1	F	388/396 (98%)	375 (97%)	13 (3%)	0	100	100
1	G	383/396 (97%)	368 (96%)	15 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	389/396 (98%)	373 (96%)	16 (4%)	0	100	100
1	I	390/396 (98%)	373 (96%)	17 (4%)	0	100	100
1	J	390/396 (98%)	375 (96%)	15 (4%)	0	100	100
1	K	390/396 (98%)	375 (96%)	15 (4%)	0	100	100
1	L	389/396 (98%)	376 (97%)	13 (3%)	0	100	100
All	All	4664/4752 (98%)	4492 (96%)	172 (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	327/330 (99%)	321 (98%)	6 (2%)	54	77
1	B	328/330 (99%)	318 (97%)	10 (3%)	36	61
1	C	327/330 (99%)	321 (98%)	6 (2%)	54	77
1	D	327/330 (99%)	319 (98%)	8 (2%)	44	68
1	E	327/330 (99%)	320 (98%)	7 (2%)	48	72
1	F	326/330 (99%)	319 (98%)	7 (2%)	48	72
1	G	324/330 (98%)	316 (98%)	8 (2%)	42	67
1	H	327/330 (99%)	317 (97%)	10 (3%)	35	59
1	I	327/330 (99%)	313 (96%)	14 (4%)	25	45
1	J	327/330 (99%)	315 (96%)	12 (4%)	29	52
1	K	327/330 (99%)	318 (97%)	9 (3%)	38	63
1	L	327/330 (99%)	321 (98%)	6 (2%)	54	77
All	All	3921/3960 (99%)	3818 (97%)	103 (3%)	41	66

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	298	SER
1	A	345	GLN
1	A	365	ASN
1	A	378	GLN
1	A	416	THR
1	B	51	SER
1	B	90	ASP
1	B	95	LEU
1	B	149	GLU
1	B	160	ARG
1	B	282	ARG
1	B	298	SER
1	B	345	GLN
1	B	378	GLN
1	B	424	ARG
1	C	225	LYS
1	C	282	ARG
1	C	310	MET
1	C	326	HIS
1	C	365	ASN
1	C	378	GLN
1	D	108	ARG
1	D	144	GLU
1	D	145	SER
1	D	198	ARG
1	D	282	ARG
1	D	310	MET
1	D	348	GLN
1	D	431	ARG
1	E	79	LEU
1	E	163	ARG
1	E	298	SER
1	E	331	LYS
1	E	383	LYS
1	E	425	SER
1	E	431	ARG
1	F	53	ASP
1	F	108	ARG
1	F	123	ASP
1	F	135	ASN
1	F	202	LYS
1	F	378	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	431	ARG
1	G	51	SER
1	G	160	ARG
1	G	163	ARG
1	G	218	VAL
1	G	282	ARG
1	G	305	THR
1	G	424	ARG
1	G	431	ARG
1	H	87	SER
1	H	88	ASP
1	H	108	ARG
1	H	145	SER
1	H	182	SER
1	H	220	PRO
1	H	256	GLN
1	H	323	ARG
1	H	365	ASN
1	H	416	THR
1	I	160	ARG
1	I	191	ASP
1	I	282	ARG
1	I	294	GLN
1	I	298	SER
1	I	313	GLN
1	I	314	LYS
1	I	328	LYS
1	I	331	LYS
1	I	364	LYS
1	I	376	CYS
1	I	378	GLN
1	I	425	SER
1	I	431	ARG
1	J	45	GLN
1	J	51	SER
1	J	55	THR
1	J	79	LEU
1	J	88	ASP
1	J	182	SER
1	J	213	LYS
1	J	225	LYS
1	J	228	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	265	ASP
1	J	282	ARG
1	J	378	GLN
1	K	58	ARG
1	K	154	GLU
1	K	213	LYS
1	K	248	SER
1	K	282	ARG
1	K	316	SER
1	K	378	GLN
1	K	402	LYS
1	K	419	GLU
1	L	52	SER
1	L	232	SER
1	L	282	ARG
1	L	298	SER
1	L	365	ASN
1	L	378	GLN

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

Mol	Chain	Res	Type
1	E	255	GLN
1	J	64	GLN
1	J	272	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	OXY	B	502	-	1,1,1	0.16	0	-		
2	HEM	E	501	1	42,50,50	1.49	5 (11%)	46,82,82	1.65	11 (23%)
3	OXY	L	502	2	1,1,1	0.16	0	-		
2	HEM	H	501	1,3	42,50,50	1.47	5 (11%)	46,82,82	1.58	11 (23%)
2	HEM	L	501	1,3	42,50,50	1.48	6 (14%)	46,82,82	1.34	8 (17%)
2	HEM	I	501	1,3	42,50,50	1.54	5 (11%)	46,82,82	1.45	8 (17%)
3	OXY	A	502	2	1,1,1	0.16	0	-		
3	OXY	I	502	2	1,1,1	0.17	0	-		
3	OXY	J	502	2	1,1,1	0.17	0	-		
3	OXY	F	502	-	1,1,1	0.17	0	-		
2	HEM	F	501	1	42,50,50	1.46	5 (11%)	46,82,82	1.40	8 (17%)
2	HEM	B	501	1	42,50,50	1.47	4 (9%)	46,82,82	1.54	11 (23%)
3	OXY	D	502	-	1,1,1	0.16	0	-		
2	HEM	A	501	1,3	42,50,50	1.48	4 (9%)	46,82,82	1.57	9 (19%)
3	OXY	G	502	2	1,1,1	0.17	0	-		
3	OXY	C	502	-	1,1,1	0.16	0	-		
2	HEM	D	501	1	42,50,50	1.47	6 (14%)	46,82,82	1.56	10 (21%)
2	HEM	J	501	1,3	42,50,50	1.48	5 (11%)	46,82,82	1.41	8 (17%)
2	HEM	K	501	1,3	42,50,50	1.47	4 (9%)	46,82,82	1.58	10 (21%)
2	HEM	C	501	1	42,50,50	1.48	4 (9%)	46,82,82	1.57	9 (19%)
2	HEM	G	501	1,3	42,50,50	1.53	6 (14%)	46,82,82	1.35	6 (13%)
3	OXY	K	502	2	1,1,1	0.16	0	-		
3	OXY	E	502	-	1,1,1	0.17	0	-		
3	OXY	H	502	2	1,1,1	0.16	0	-		

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	501	1	-	2/12/54/54	-
2	HEM	I	501	1,3	-	4/12/54/54	-
2	HEM	J	501	1,3	-	2/12/54/54	-
2	HEM	K	501	1,3	-	5/12/54/54	-
2	HEM	L	501	1,3	-	4/12/54/54	-
2	HEM	F	501	1	-	2/12/54/54	-
2	HEM	C	501	1	-	3/12/54/54	-
2	HEM	G	501	1,3	-	2/12/54/54	-
2	HEM	H	501	1,3	-	3/12/54/54	-
2	HEM	B	501	1	-	5/12/54/54	-
2	HEM	A	501	1,3	-	3/12/54/54	-
2	HEM	D	501	1	-	3/12/54/54	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	501	HEM	C3C-C2C	-4.81	1.33	1.40
2	A	501	HEM	C3C-C2C	-3.94	1.35	1.40
2	H	501	HEM	C3C-C2C	-3.91	1.35	1.40
2	B	501	HEM	C3C-C2C	-3.90	1.35	1.40
2	F	501	HEM	C3C-C2C	-3.90	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.88	1.35	1.40
2	L	501	HEM	C3C-C2C	-3.88	1.35	1.40
2	G	501	HEM	C3C-C2C	-3.88	1.35	1.40
2	E	501	HEM	C3C-C2C	-3.86	1.35	1.40
2	D	501	HEM	C3C-C2C	-3.80	1.35	1.40
2	K	501	HEM	C3C-C2C	-3.78	1.35	1.40
2	J	501	HEM	C3C-C2C	-3.77	1.35	1.40
2	K	501	HEM	C3C-CAC	3.59	1.55	1.47
2	E	501	HEM	C3C-CAC	3.58	1.55	1.47
2	A	501	HEM	C3C-CAC	3.57	1.55	1.47
2	J	501	HEM	C3C-CAC	3.53	1.55	1.47
2	F	501	HEM	C3C-CAC	3.52	1.55	1.47
2	L	501	HEM	C3C-CAC	3.50	1.55	1.47
2	B	501	HEM	C3C-CAC	3.49	1.55	1.47
2	D	501	HEM	C3C-CAC	3.48	1.55	1.47
2	C	501	HEM	C3C-CAC	3.47	1.55	1.47
2	I	501	HEM	C3C-CAC	3.45	1.55	1.47
2	G	501	HEM	C3C-CAC	3.45	1.55	1.47
2	H	501	HEM	C3C-CAC	3.45	1.55	1.47
2	I	501	HEM	C3C-C4C	3.40	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	HEM	CAB-C3B	3.12	1.55	1.47
2	J	501	HEM	CAB-C3B	3.12	1.55	1.47
2	L	501	HEM	CAB-C3B	3.09	1.55	1.47
2	E	501	HEM	CAB-C3B	3.04	1.55	1.47
2	C	501	HEM	CAB-C3B	2.94	1.55	1.47
2	F	501	HEM	CAB-C3B	2.89	1.55	1.47
2	B	501	HEM	CAB-C3B	2.88	1.55	1.47
2	E	501	HEM	C3C-C4C	2.87	1.45	1.41
2	K	501	HEM	CAB-C3B	2.86	1.55	1.47
2	H	501	HEM	CAB-C3B	2.85	1.55	1.47
2	K	501	HEM	C3C-C4C	2.84	1.45	1.41
2	A	501	HEM	C3C-C4C	2.84	1.45	1.41
2	D	501	HEM	CAB-C3B	2.83	1.54	1.47
2	A	501	HEM	CAB-C3B	2.82	1.54	1.47
2	G	501	HEM	C3C-C4C	2.80	1.45	1.41
2	I	501	HEM	CAB-C3B	2.77	1.54	1.47
2	F	501	HEM	C3C-C4C	2.75	1.45	1.41
2	L	501	HEM	C3C-C4C	2.65	1.45	1.41
2	J	501	HEM	C3C-C4C	2.65	1.45	1.41
2	D	501	HEM	C3C-C4C	2.60	1.45	1.41
2	B	501	HEM	C3C-C4C	2.54	1.45	1.41
2	H	501	HEM	C3C-C4C	2.54	1.45	1.41
2	C	501	HEM	C3C-C4C	2.54	1.45	1.41
2	G	501	HEM	FE-ND	2.32	2.11	1.98
2	L	501	HEM	CMB-C2B	2.14	1.55	1.50
2	E	501	HEM	CMB-C2B	2.13	1.55	1.50
2	J	501	HEM	CMB-C2B	2.13	1.55	1.50
2	G	501	HEM	CMB-C2B	2.11	1.55	1.50
2	F	501	HEM	CMB-C2B	2.10	1.55	1.50
2	L	501	HEM	CMD-C2D	2.10	1.55	1.50
2	I	501	HEM	CMB-C2B	2.04	1.55	1.50
2	H	501	HEM	CMD-C2D	2.02	1.54	1.50
2	D	501	HEM	CMD-C2D	2.00	1.54	1.50
2	D	501	HEM	CMB-C2B	2.00	1.54	1.50

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	HEM	CAD-C3D-C4D	3.54	130.87	124.70
2	E	501	HEM	CAD-C3D-C2D	-3.25	121.77	127.87
2	E	501	HEM	C4C-CHD-C1D	3.04	126.58	122.56
2	A	501	HEM	C4B-CHC-C1C	3.04	126.56	122.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	C4C-CHD-C1D	3.03	126.56	122.56
2	H	501	HEM	C4C-CHD-C1D	3.03	126.55	122.56
2	J	501	HEM	C4C-CHD-C1D	2.99	126.50	122.56
2	D	501	HEM	C4C-CHD-C1D	2.93	126.42	122.56
2	K	501	HEM	C4B-CHC-C1C	2.93	126.42	122.56
2	K	501	HEM	C3B-C4B-NB	-2.92	107.37	109.47
2	I	501	HEM	C4C-CHD-C1D	2.87	126.35	122.56
2	K	501	HEM	C4C-CHD-C1D	2.87	126.35	122.56
2	C	501	HEM	C3B-C2B-C1B	2.86	108.56	106.41
2	D	501	HEM	C3B-C4B-NB	-2.85	107.42	109.47
2	E	501	HEM	C4D-ND-C1D	2.85	108.58	105.21
2	B	501	HEM	C4B-CHC-C1C	2.85	126.31	122.56
2	A	501	HEM	C4C-CHD-C1D	2.82	126.28	122.56
2	B	501	HEM	C3B-C4B-NB	-2.82	107.44	109.47
2	A	501	HEM	C3B-C2B-C1B	2.78	108.50	106.41
2	E	501	HEM	CHD-C1D-ND	2.75	127.40	124.44
2	H	501	HEM	C3B-C4B-NB	-2.75	107.50	109.47
2	B	501	HEM	C3B-C2B-C1B	2.74	108.47	106.41
2	D	501	HEM	C4B-CHC-C1C	2.74	126.17	122.56
2	I	501	HEM	C4B-CHC-C1C	2.74	126.17	122.56
2	K	501	HEM	C3B-C2B-C1B	2.73	108.46	106.41
2	H	501	HEM	C3B-C2B-C1B	2.72	108.45	106.41
2	A	501	HEM	C3B-C4B-NB	-2.72	107.52	109.47
2	L	501	HEM	C4C-CHD-C1D	2.71	126.13	122.56
2	H	501	HEM	C4B-CHC-C1C	2.70	126.12	122.56
2	B	501	HEM	C4C-CHD-C1D	2.65	126.05	122.56
2	G	501	HEM	C4C-CHD-C1D	2.64	126.05	122.56
2	C	501	HEM	C3B-C4B-NB	-2.63	107.58	109.47
2	D	501	HEM	C3B-C2B-C1B	2.59	108.36	106.41
2	F	501	HEM	C4C-CHD-C1D	2.58	125.96	122.56
2	C	501	HEM	C4B-CHC-C1C	2.56	125.94	122.56
2	H	501	HEM	C1B-NB-C4B	2.55	108.23	105.21
2	K	501	HEM	C1B-NB-C4B	2.54	108.21	105.21
2	F	501	HEM	C4D-ND-C1D	2.54	108.21	105.21
2	I	501	HEM	C4D-ND-C1D	2.54	108.21	105.21
2	E	501	HEM	C3D-C4D-ND	-2.53	107.40	110.17
2	B	501	HEM	C1B-NB-C4B	2.52	108.19	105.21
2	C	501	HEM	C1B-NB-C4B	2.51	108.18	105.21
2	A	501	HEM	C1B-NB-C4B	2.50	108.17	105.21
2	I	501	HEM	CHC-C4B-NB	2.48	127.11	124.44
2	K	501	HEM	C4D-ND-C1D	2.46	108.13	105.21
2	J	501	HEM	C4D-ND-C1D	2.46	108.12	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	HEM	C1B-NB-C4B	2.46	108.12	105.21
2	C	501	HEM	C4D-ND-C1D	2.44	108.10	105.21
2	H	501	HEM	C4D-ND-C1D	2.43	108.08	105.21
2	J	501	HEM	C4B-CHC-C1C	2.41	125.74	122.56
2	A	501	HEM	C4D-ND-C1D	2.40	108.06	105.21
2	L	501	HEM	C4B-CHC-C1C	2.40	125.72	122.56
2	C	501	HEM	C4A-C3A-C2A	2.37	108.65	107.00
2	E	501	HEM	C4B-CHC-C1C	2.33	125.63	122.56
2	D	501	HEM	C4D-ND-C1D	2.31	107.95	105.21
2	G	501	HEM	C4B-CHC-C1C	2.31	125.60	122.56
2	I	501	HEM	C1B-NB-C4B	2.28	107.91	105.21
2	B	501	HEM	CHC-C4B-C3B	2.26	128.03	124.57
2	L	501	HEM	C4D-ND-C1D	2.26	107.88	105.21
2	J	501	HEM	C3D-C4D-ND	-2.26	107.69	110.17
2	C	501	HEM	CHC-C4B-C3B	2.26	128.03	124.57
2	I	501	HEM	C3D-C4D-ND	-2.26	107.69	110.17
2	H	501	HEM	C3D-C4D-ND	-2.25	107.70	110.17
2	E	501	HEM	C1D-C2D-C3D	2.25	109.34	106.98
2	C	501	HEM	C3D-C4D-ND	-2.24	107.71	110.17
2	J	501	HEM	C1B-NB-C4B	2.24	107.86	105.21
2	E	501	HEM	C2D-C1D-ND	-2.23	107.32	109.90
2	F	501	HEM	C3D-C4D-ND	-2.23	107.72	110.17
2	L	501	HEM	C1B-NB-C4B	2.22	107.84	105.21
2	H	501	HEM	CHC-C4B-C3B	2.22	127.97	124.57
2	F	501	HEM	C1B-NB-C4B	2.22	107.83	105.21
2	L	501	HEM	C4A-C3A-C2A	2.21	108.54	107.00
2	H	501	HEM	CMA-C3A-C4A	-2.21	125.22	128.46
2	F	501	HEM	C4B-CHC-C1C	2.20	125.46	122.56
2	K	501	HEM	CBA-CAA-C2A	-2.20	108.85	112.54
2	D	501	HEM	C3D-C4D-ND	-2.19	107.77	110.17
2	B	501	HEM	C4D-ND-C1D	2.18	107.79	105.21
2	G	501	HEM	CMC-C2C-C3C	2.18	129.03	124.68
2	G	501	HEM	CBA-CAA-C2A	-2.18	108.88	112.54
2	D	501	HEM	C4A-C3A-C2A	2.17	108.51	107.00
2	A	501	HEM	CMC-C2C-C3C	2.16	129.01	124.68
2	D	501	HEM	CHC-C4B-C3B	2.14	127.85	124.57
2	A	501	HEM	C3D-C4D-ND	-2.14	107.82	110.17
2	F	501	HEM	CMC-C2C-C3C	2.14	128.96	124.68
2	H	501	HEM	C4A-C3A-C2A	2.14	108.48	107.00
2	E	501	HEM	CMC-C2C-C3C	2.14	128.95	124.68
2	G	501	HEM	C4A-C3A-C2A	2.13	108.48	107.00
2	K	501	HEM	C3D-C4D-ND	-2.12	107.85	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	501	HEM	C4A-C3A-C2A	2.11	108.47	107.00
2	G	501	HEM	C4D-ND-C1D	2.10	107.69	105.21
2	E	501	HEM	C1B-NB-C4B	2.10	107.69	105.21
2	F	501	HEM	CHD-C1D-ND	2.10	126.69	124.44
2	K	501	HEM	CHC-C4B-C3B	2.09	127.77	124.57
2	D	501	HEM	CMA-C3A-C4A	-2.09	125.40	128.46
2	B	501	HEM	C4A-C3A-C2A	2.06	108.43	107.00
2	L	501	HEM	CMC-C2C-C3C	2.06	128.80	124.68
2	L	501	HEM	C3B-C2B-C1B	2.05	107.95	106.41
2	B	501	HEM	CBA-CAA-C2A	-2.04	109.11	112.54
2	I	501	HEM	CHD-C1D-ND	2.03	126.62	124.44
2	J	501	HEM	CMC-C2C-C3C	2.03	128.74	124.68
2	B	501	HEM	CMA-C3A-C4A	-2.03	125.48	128.46
2	F	501	HEM	C2D-C1D-ND	-2.02	107.57	109.90
2	A	501	HEM	CHC-C4B-C3B	2.02	127.66	124.57
2	J	501	HEM	C3B-C2B-C1B	2.02	107.92	106.41
2	K	501	HEM	C2D-C1D-ND	-2.01	107.58	109.90
2	I	501	HEM	C2D-C1D-ND	-2.01	107.58	109.90
2	B	501	HEM	C3D-C4D-ND	-2.01	107.97	110.17
2	L	501	HEM	CMA-C3A-C4A	-2.01	125.51	128.46
2	H	501	HEM	CMC-C2C-C3C	2.01	128.70	124.68

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	501	HEM	C2D-C3D-CAD-CBD
2	E	501	HEM	C4D-C3D-CAD-CBD
2	B	501	HEM	C4B-C3B-CAB-CBB
2	I	501	HEM	C2B-C3B-CAB-CBB
2	A	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
2	H	501	HEM	C4B-C3B-CAB-CBB
2	I	501	HEM	C4B-C3B-CAB-CBB
2	K	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	CAD-CBD-CGD-O1D
2	J	501	HEM	CAA-CBA-CGA-O1A
2	G	501	HEM	CAA-CBA-CGA-O2A
2	L	501	HEM	CAA-CBA-CGA-O2A
2	K	501	HEM	CAA-CBA-CGA-O1A
2	I	501	HEM	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	501	HEM	CAA-CBA-CGA-O1A
2	H	501	HEM	CAA-CBA-CGA-O2A
2	K	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O2D
2	I	501	HEM	CAD-CBD-CGD-O2D
2	J	501	HEM	CAA-CBA-CGA-O2A
2	K	501	HEM	CAA-CBA-CGA-O2A
2	L	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O1A
2	H	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O2D
2	K	501	HEM	CAD-CBD-CGD-O2D
2	L	501	HEM	CAD-CBD-CGD-O2D
2	F	501	HEM	CAD-CBD-CGD-O2D
2	F	501	HEM	CAD-CBD-CGD-O1D
2	L	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

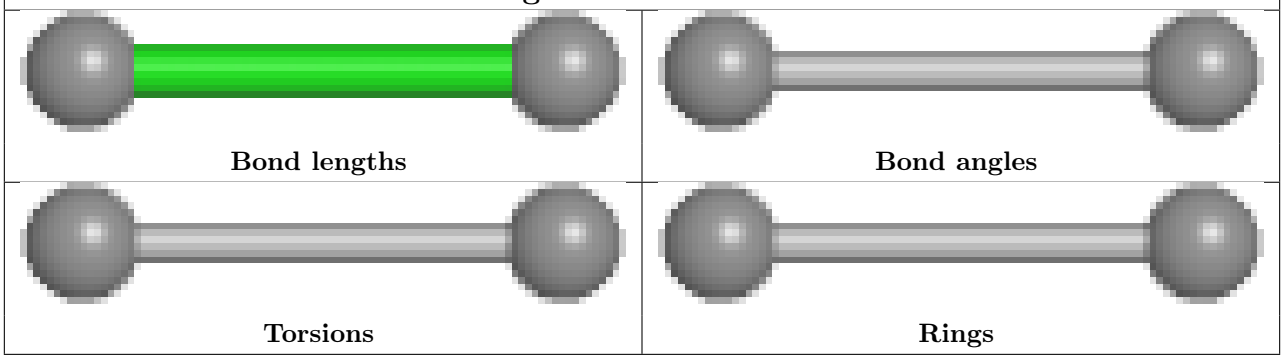
13 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	HEM	4	0
2	H	501	HEM	2	0
2	L	501	HEM	2	0
2	I	501	HEM	3	0
2	F	501	HEM	4	0
2	B	501	HEM	3	0
2	A	501	HEM	5	0
2	D	501	HEM	4	0
2	J	501	HEM	1	0
2	K	501	HEM	3	0
2	C	501	HEM	1	0
2	G	501	HEM	1	0
3	K	502	OXY	1	0

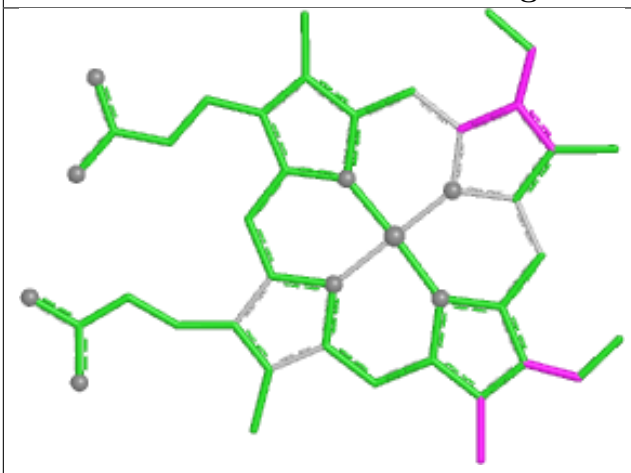
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

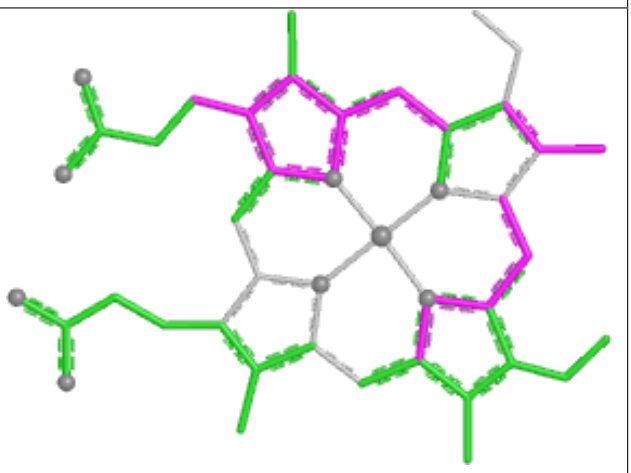
Ligand OXY B 502



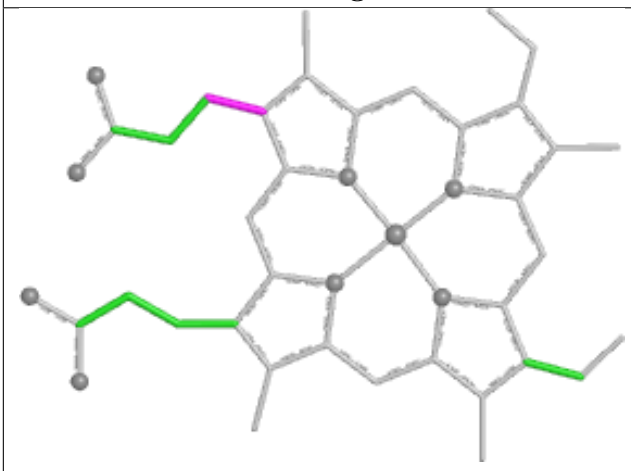
Ligand HEM E 501



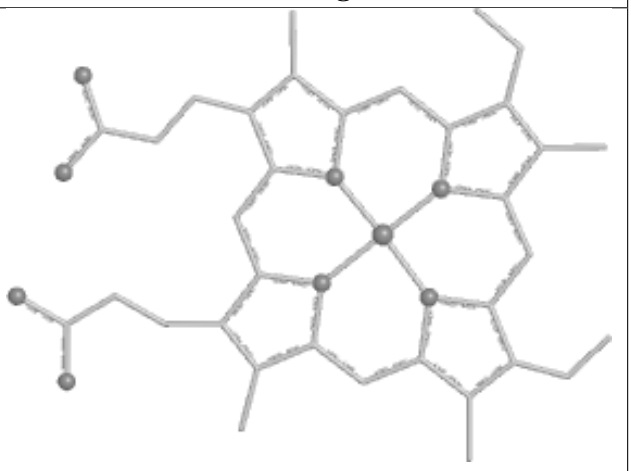
Bond lengths



Bond angles

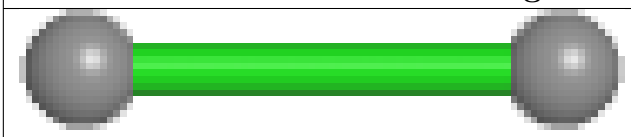


Torsions



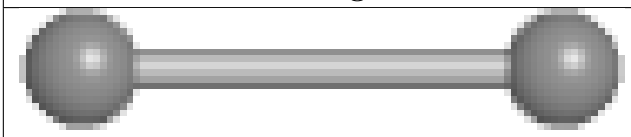
Rings

Ligand OXY L 502

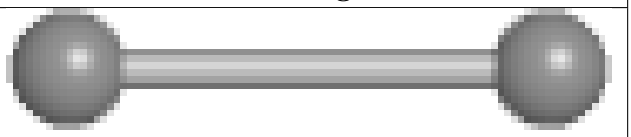


Bond lengths

Bond angles

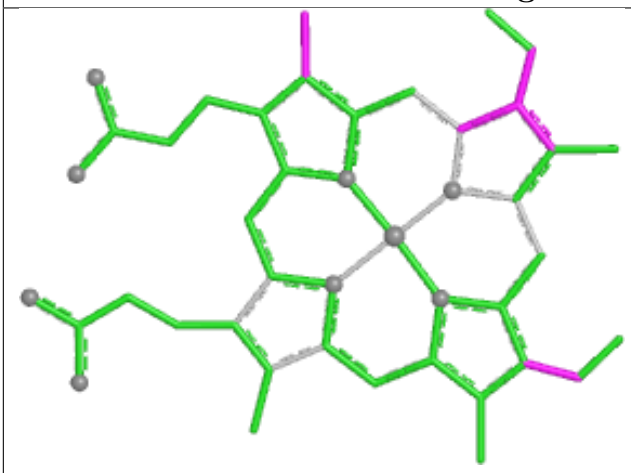


Torsions

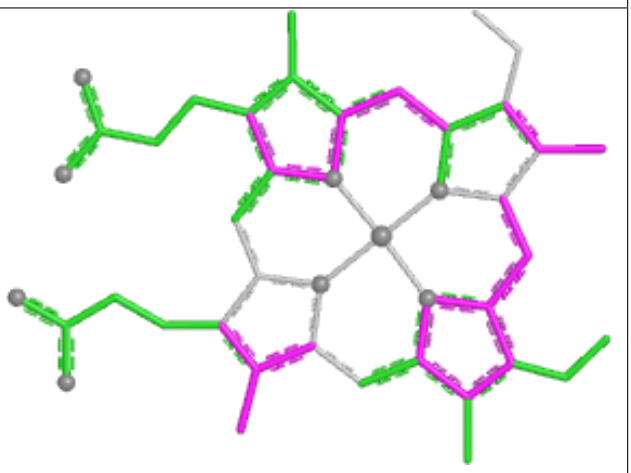


Rings

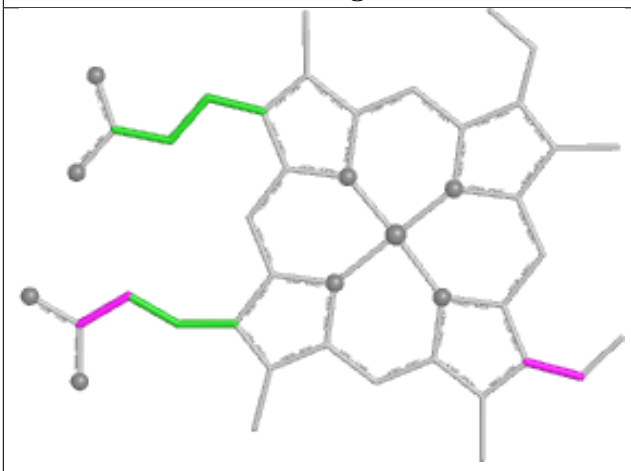
Ligand HEM H 501



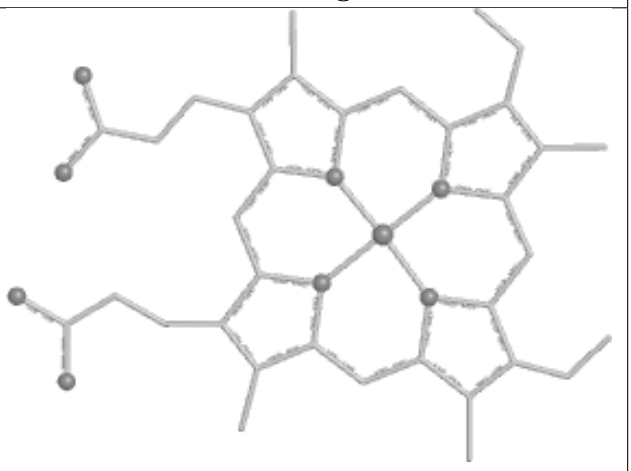
Bond lengths



Bond angles

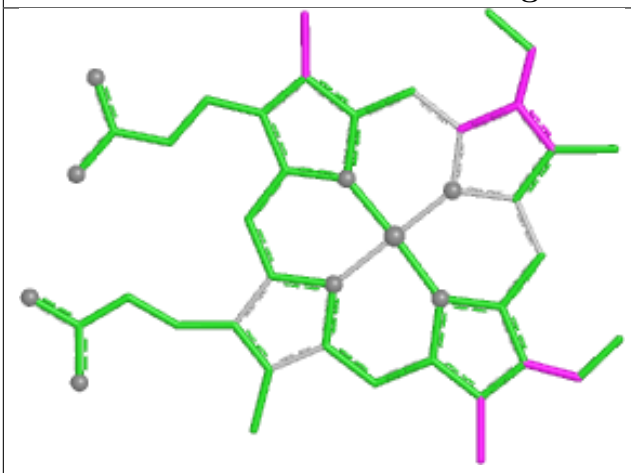


Torsions

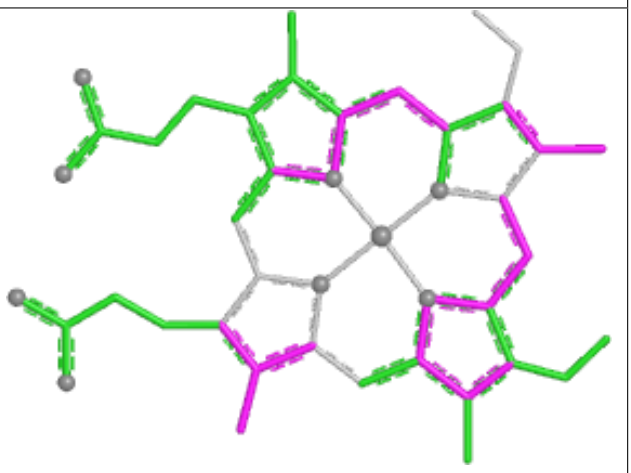


Rings

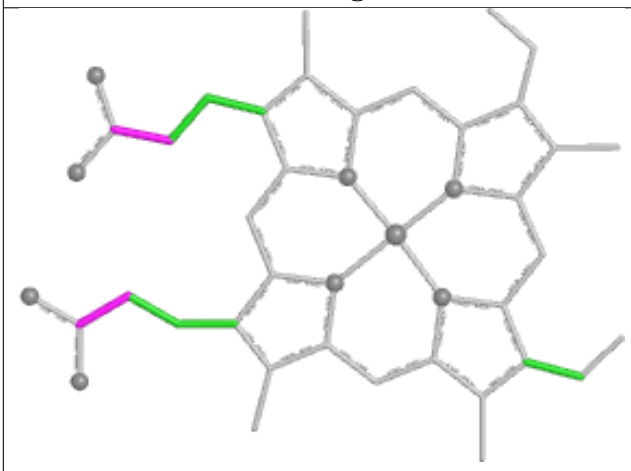
Ligand HEM L 501



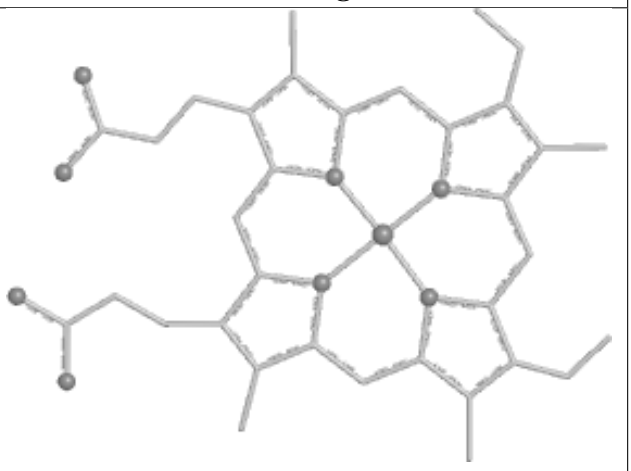
Bond lengths



Bond angles

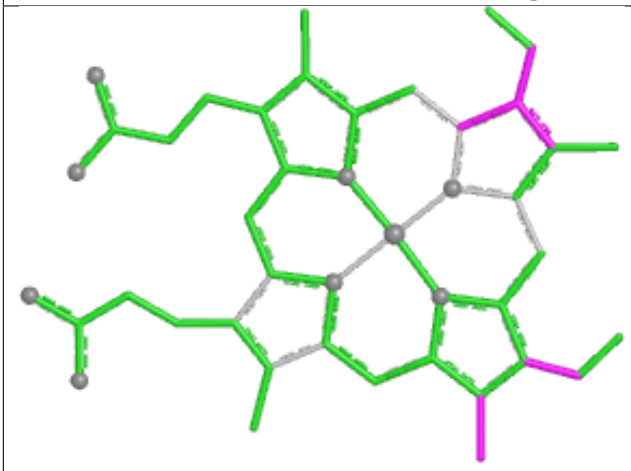


Torsions

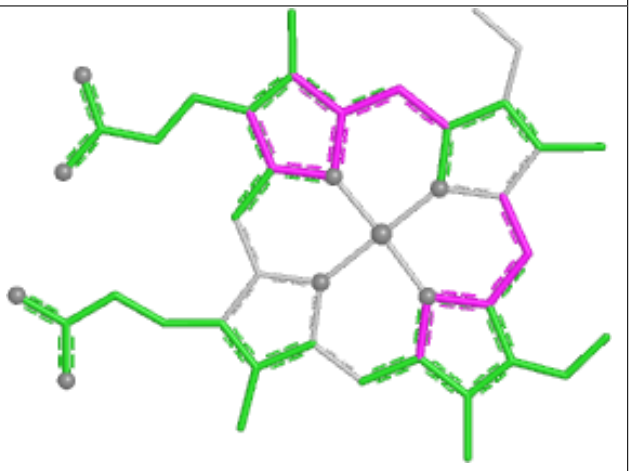


Rings

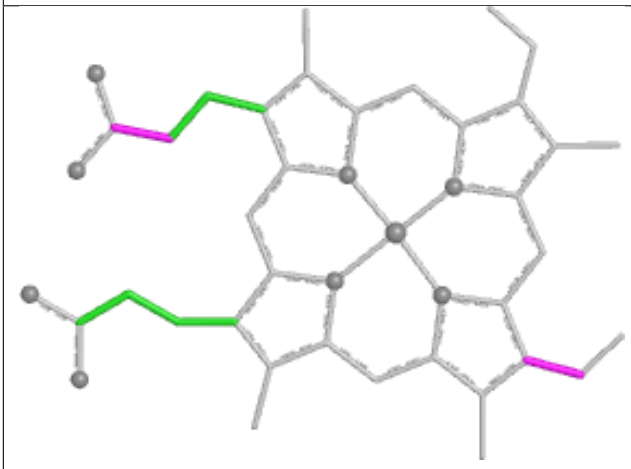
Ligand HEM I 501



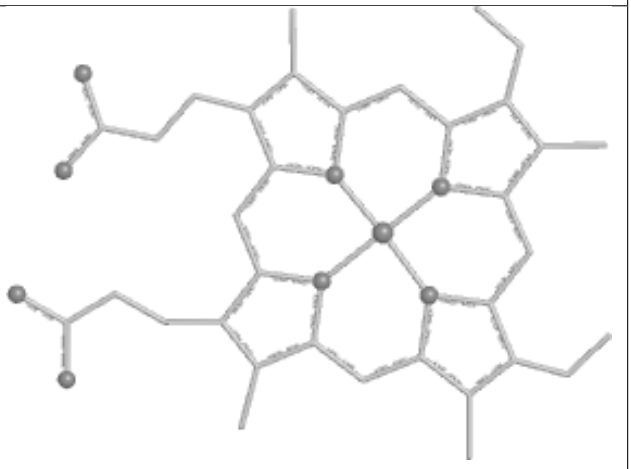
Bond lengths



Bond angles

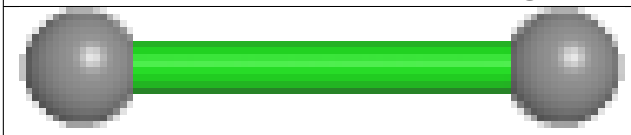


Torsions



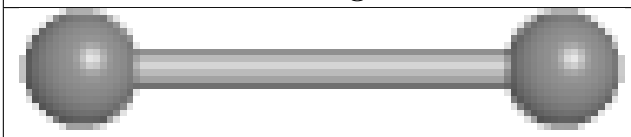
Rings

Ligand OXY A 502

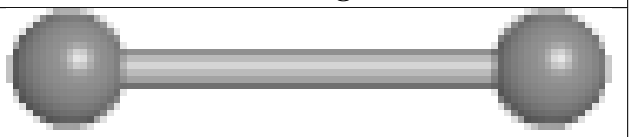


Bond lengths

Bond angles

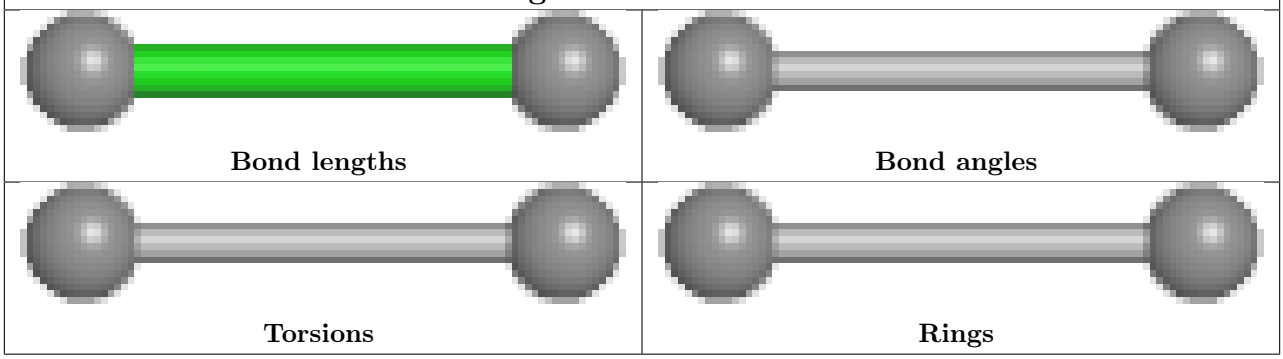


Torsions

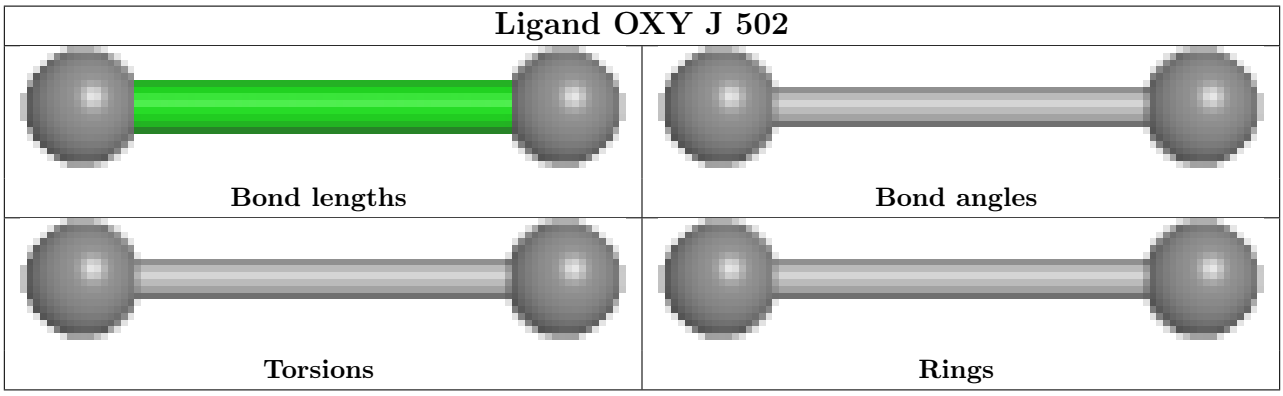


Rings

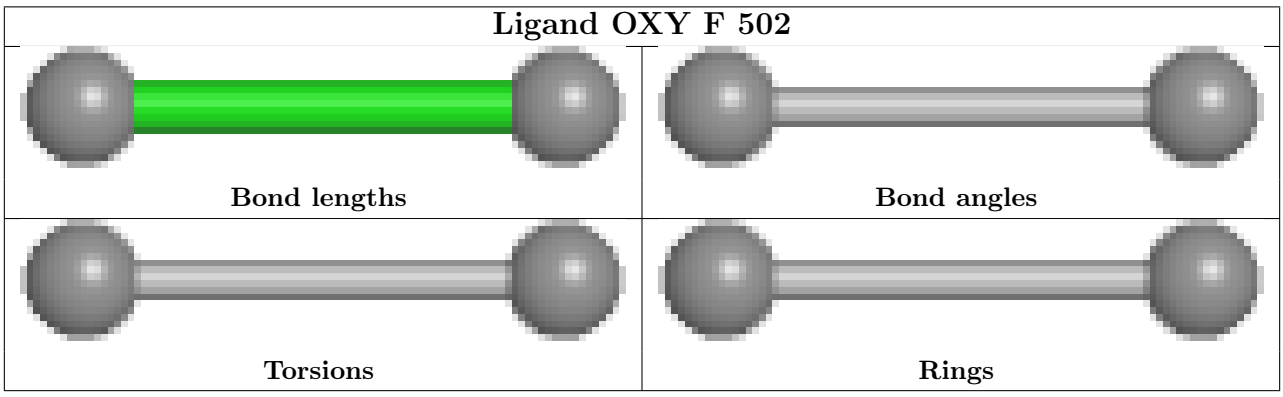
Ligand OXY I 502



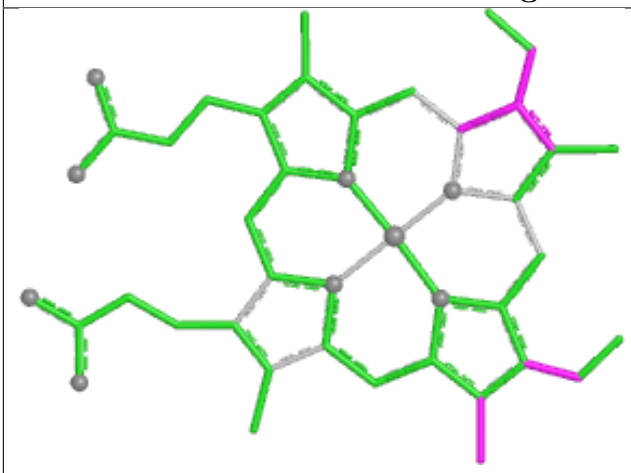
Ligand OXY J 502



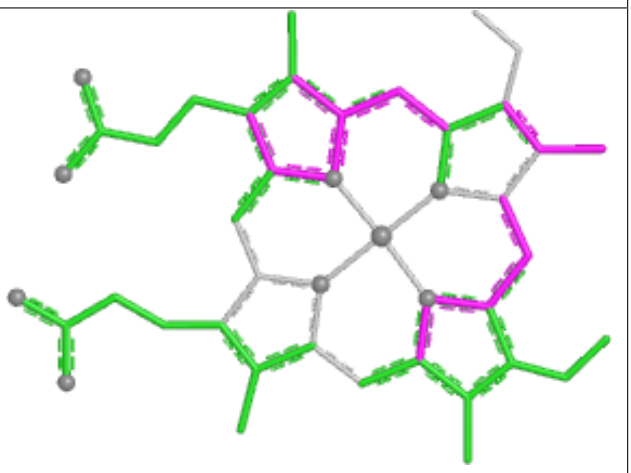
Ligand OXY F 502



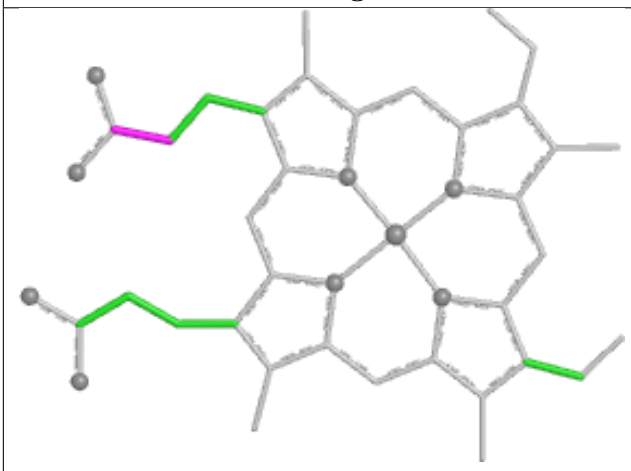
Ligand HEM F 501



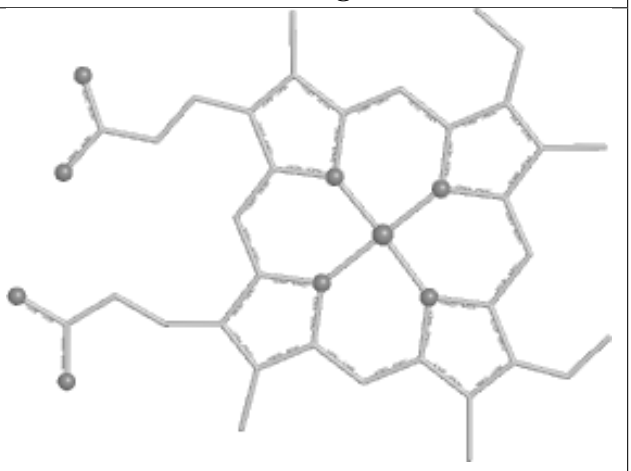
Bond lengths



Bond angles

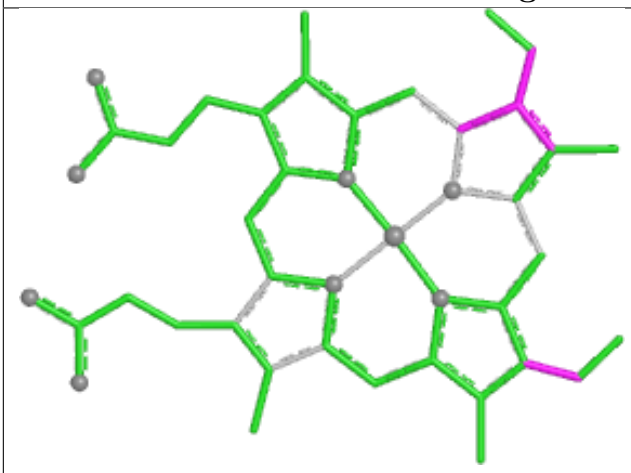


Torsions

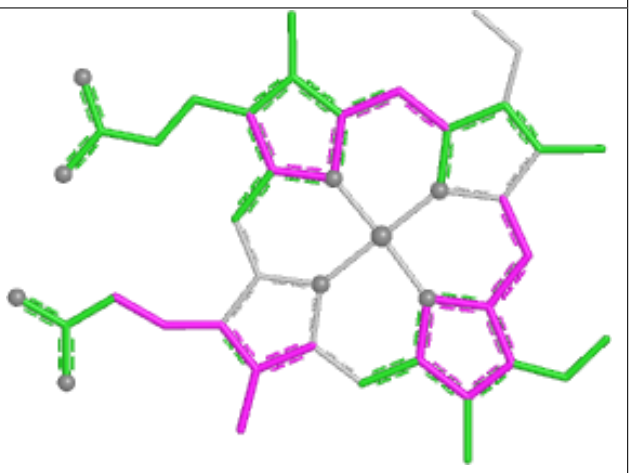


Rings

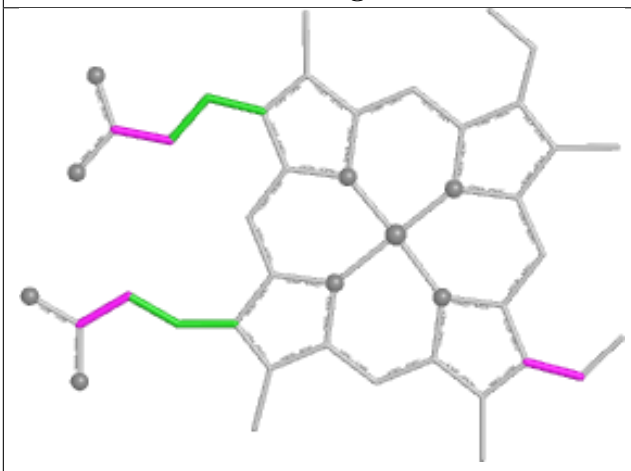
Ligand HEM B 501



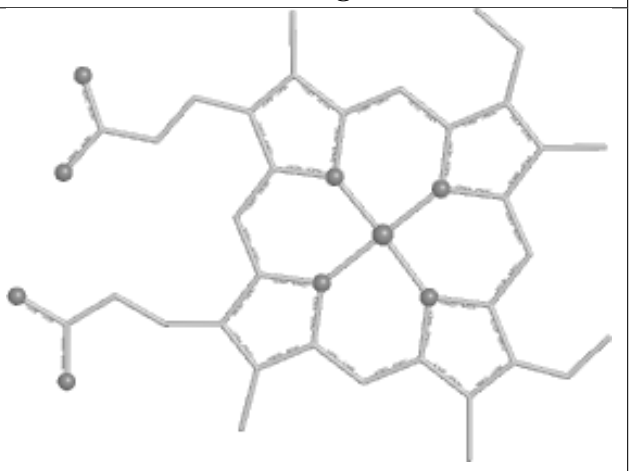
Bond lengths



Bond angles

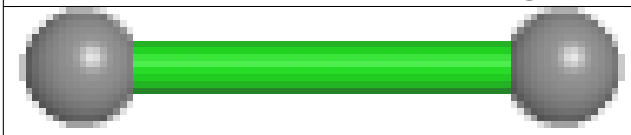


Torsions



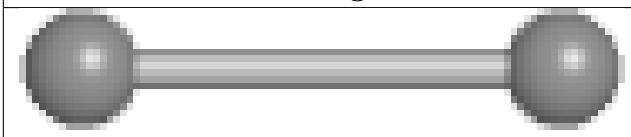
Rings

Ligand OXY D 502

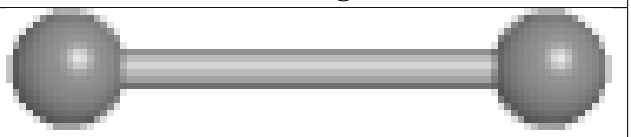


Bond lengths

Bond angles

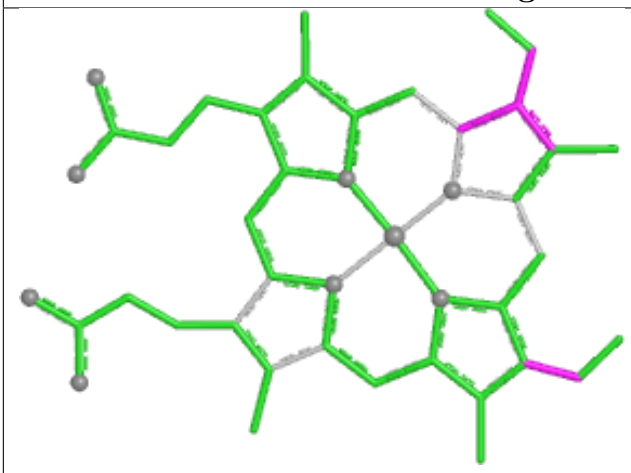


Torsions

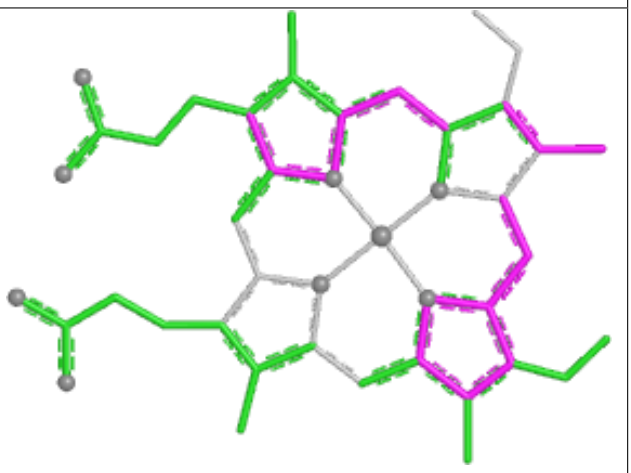


Rings

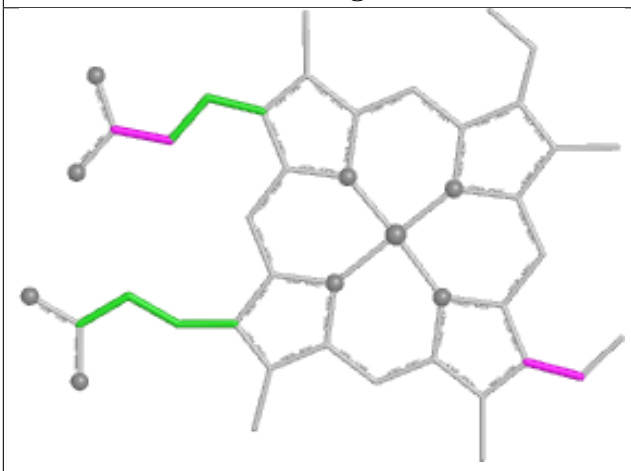
Ligand HEM A 501



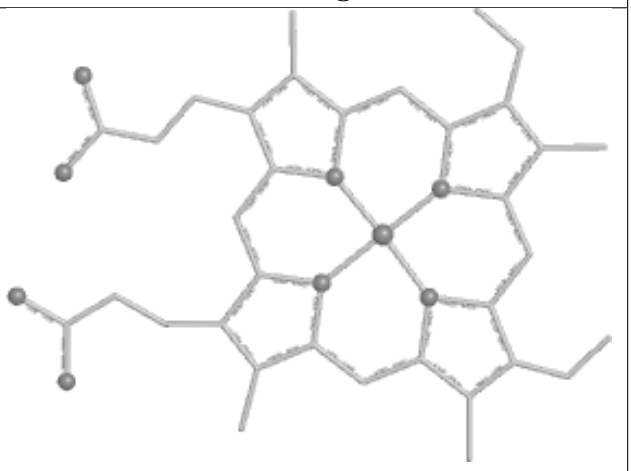
Bond lengths



Bond angles

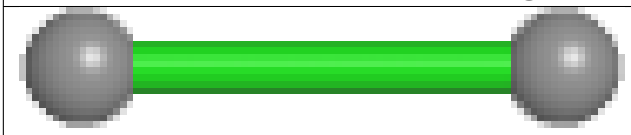


Torsions



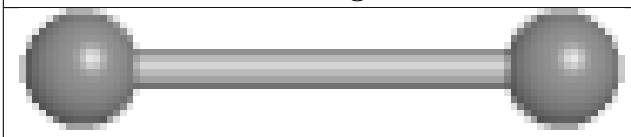
Rings

Ligand OXY G 502

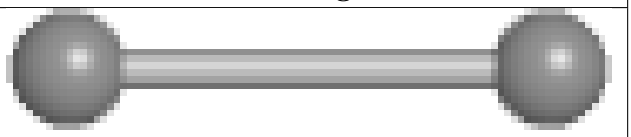


Bond lengths

Bond angles

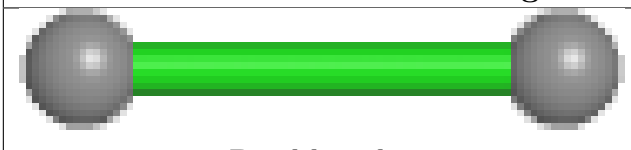


Torsions

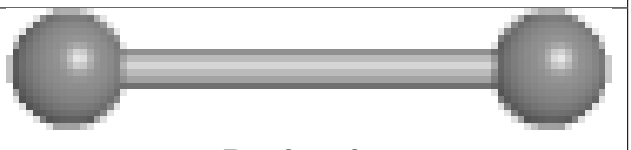


Rings

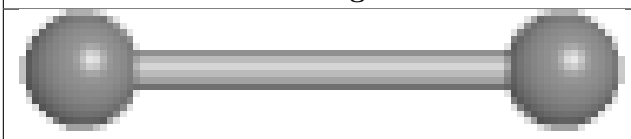
Ligand OXY C 502



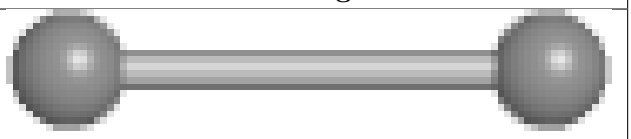
Bond lengths



Bond angles

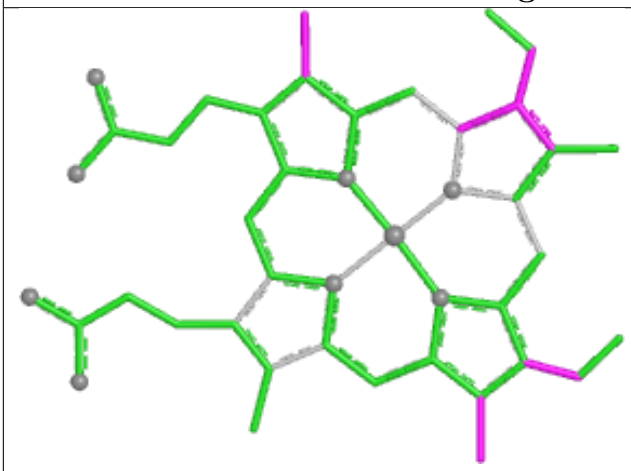


Torsions

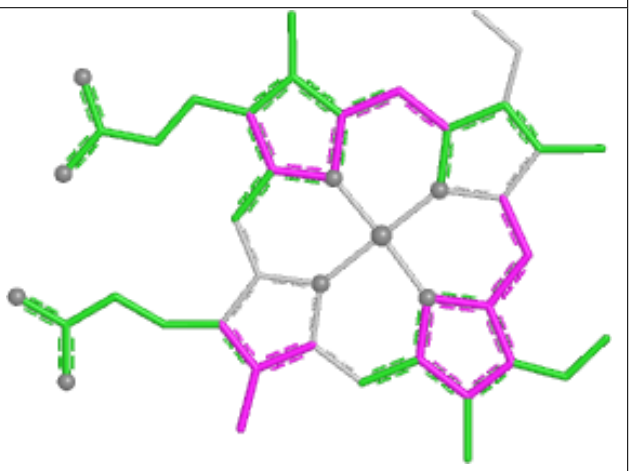


Rings

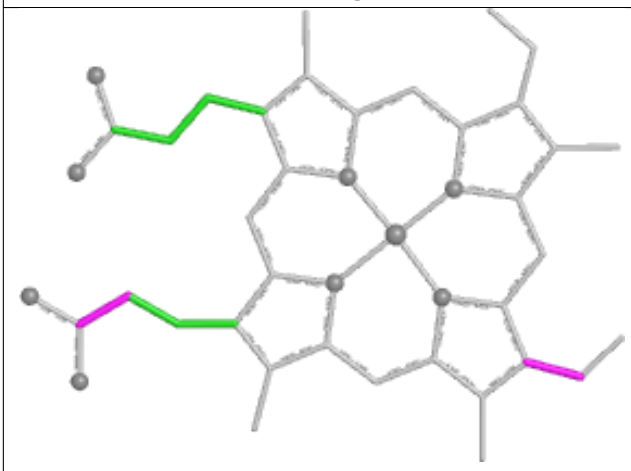
Ligand HEM D 501



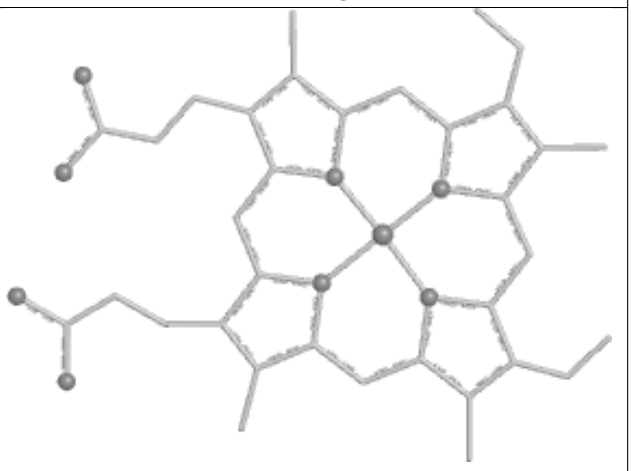
Bond lengths



Bond angles

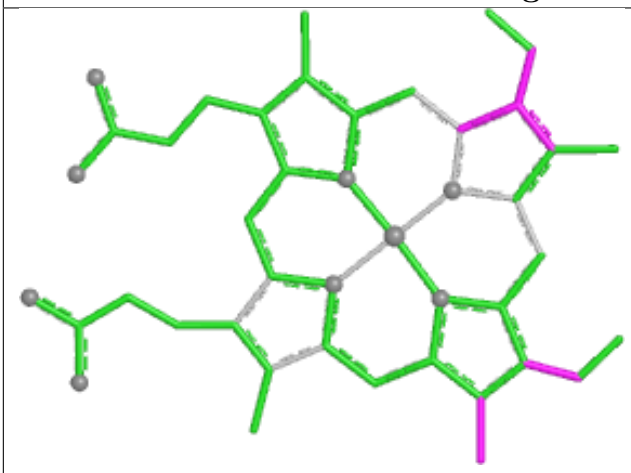


Torsions

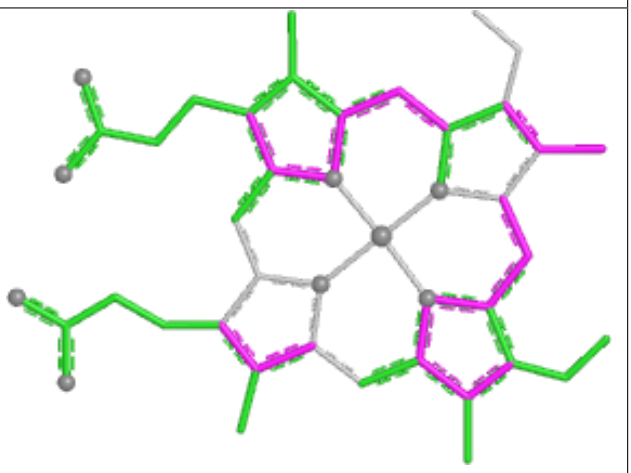


Rings

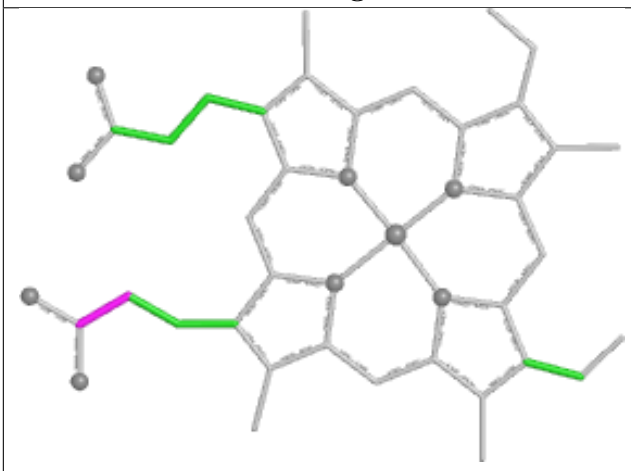
Ligand HEM J 501



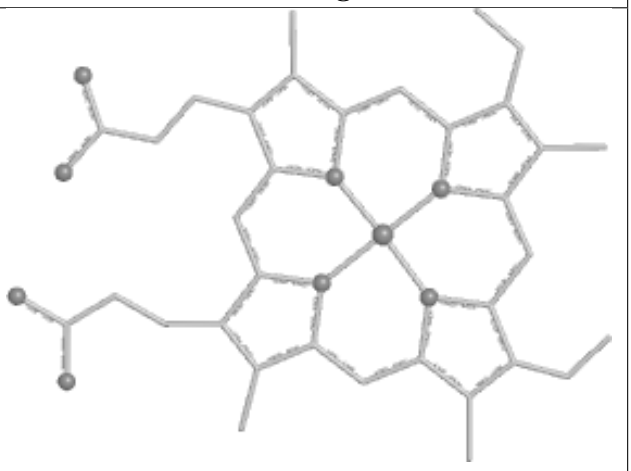
Bond lengths



Bond angles

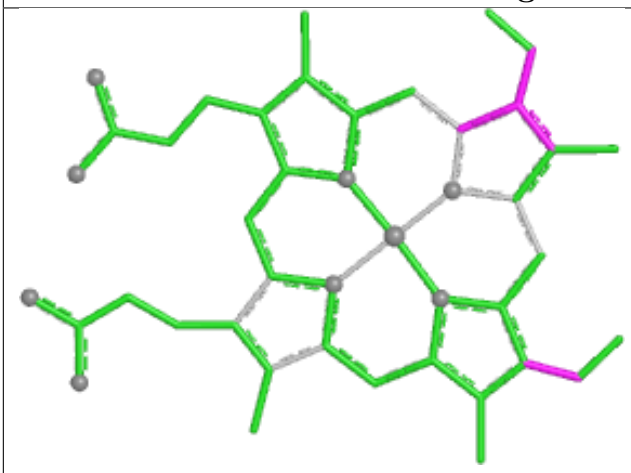


Torsions

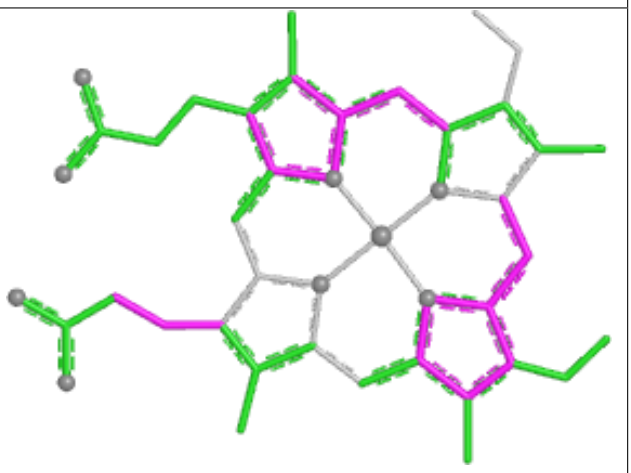


Rings

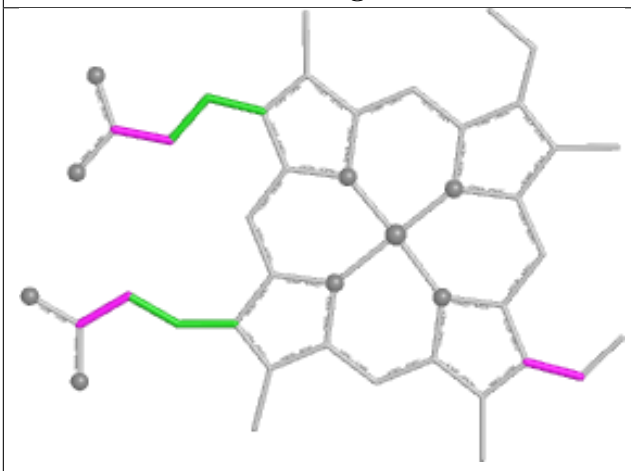
Ligand HEM K 501



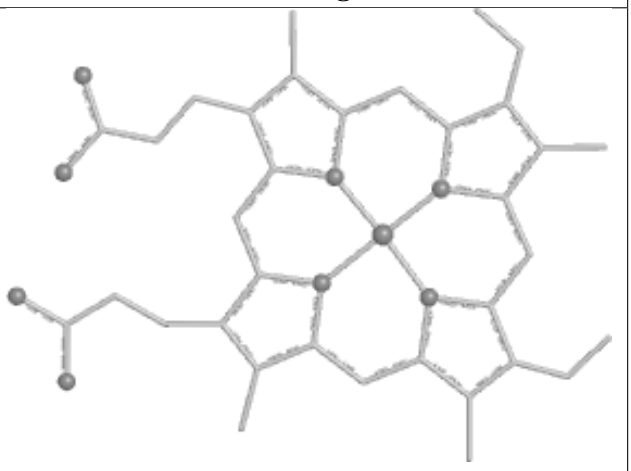
Bond lengths



Bond angles

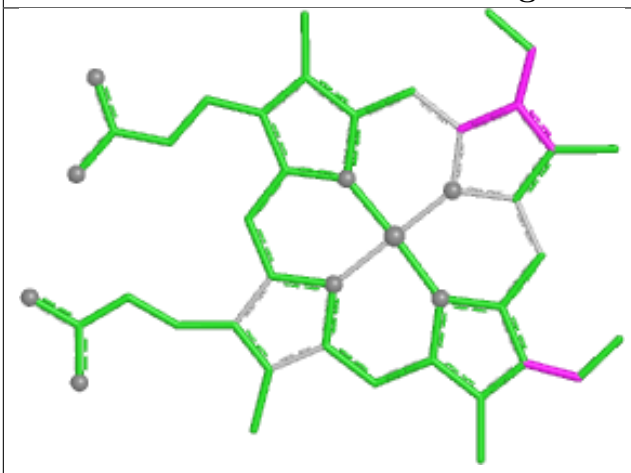


Torsions

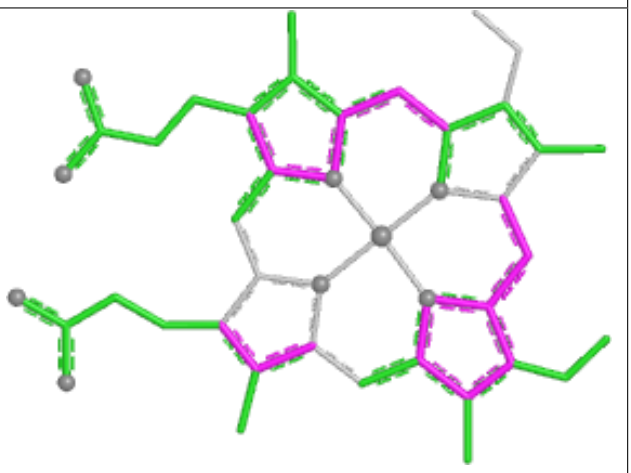


Rings

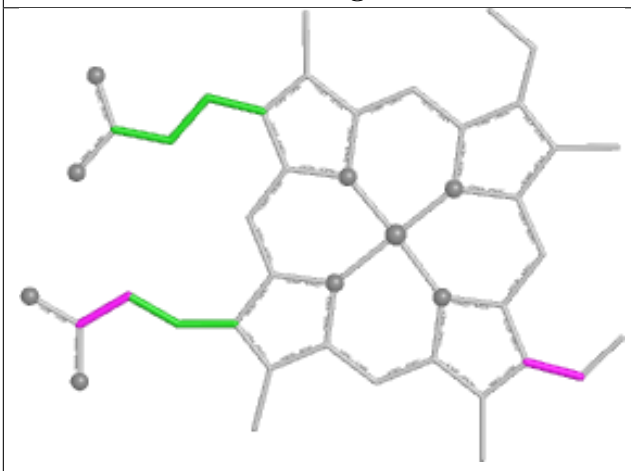
Ligand HEM C 501



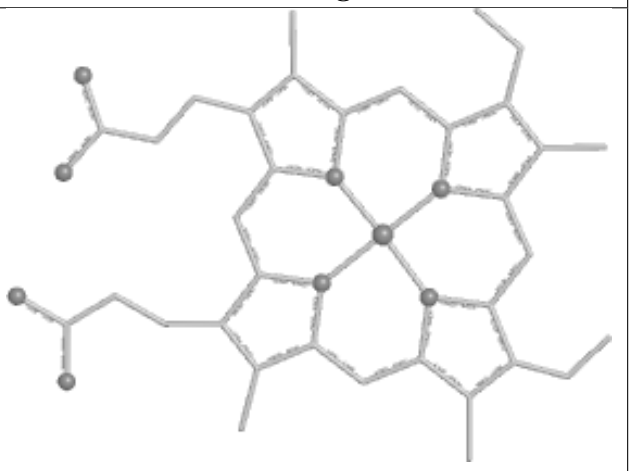
Bond lengths



Bond angles

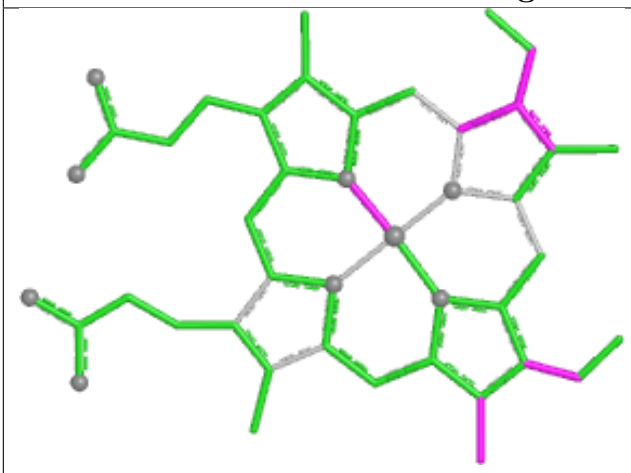


Torsions

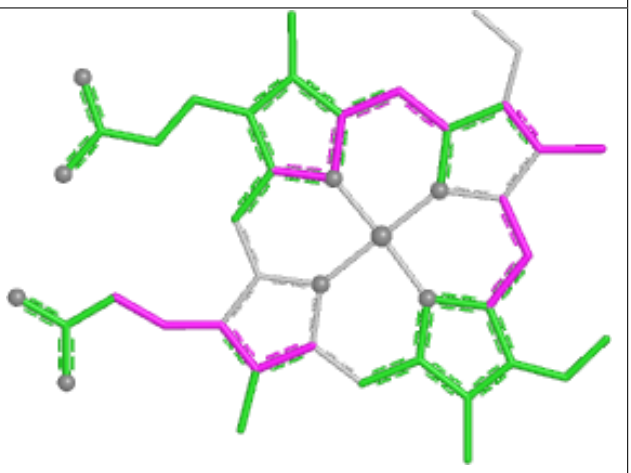


Rings

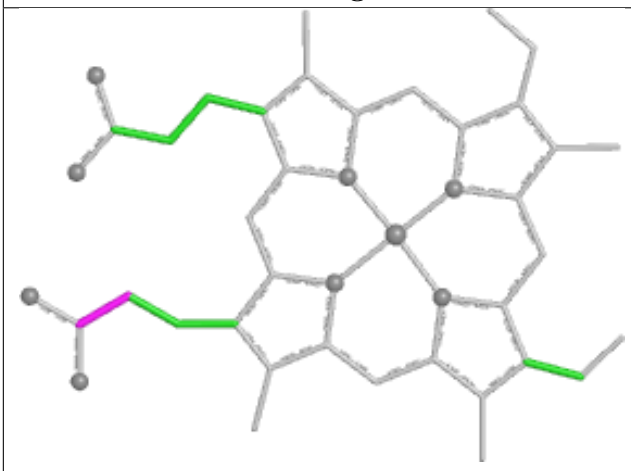
Ligand HEM G 501



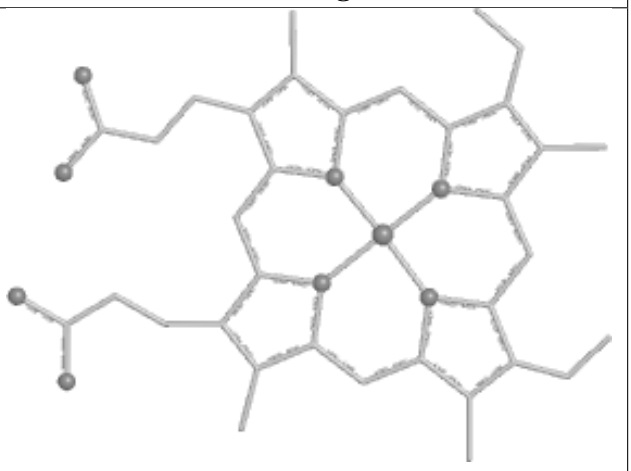
Bond lengths



Bond angles

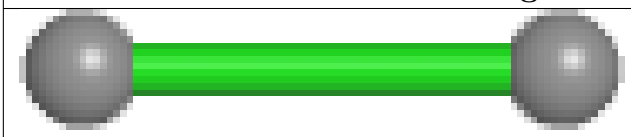


Torsions



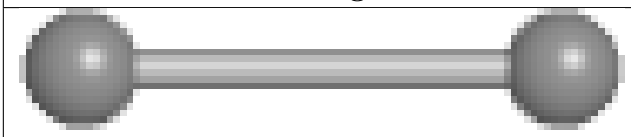
Rings

Ligand OXY K 502

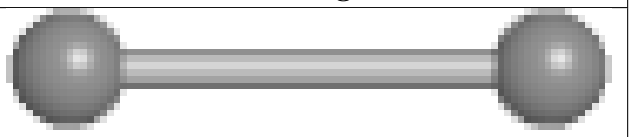


Bond lengths

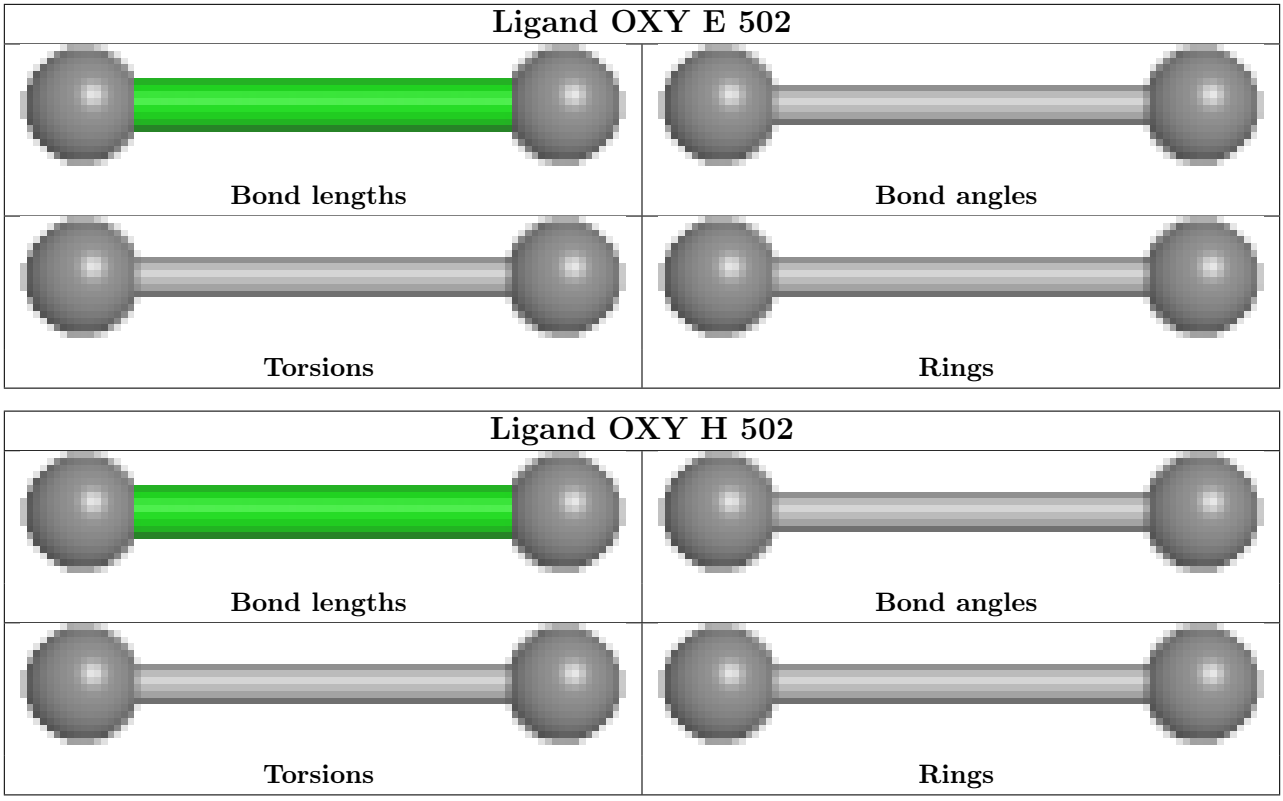
Bond angles



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	390/396 (98%)	-0.45	0	100	100	19, 30, 47, 67	0
1	B	392/396 (98%)	-0.28	1 (0%)	90	89	23, 35, 58, 108	0
1	C	390/396 (98%)	-0.27	1 (0%)	90	89	22, 35, 56, 81	0
1	D	392/396 (98%)	-0.24	1 (0%)	90	89	23, 37, 60, 80	0
1	E	391/396 (98%)	-0.29	1 (0%)	90	89	21, 35, 56, 88	0
1	F	390/396 (98%)	-0.30	2 (0%)	87	86	22, 36, 53, 92	0
1	G	387/396 (97%)	-0.12	4 (1%)	79	77	29, 41, 59, 91	0
1	H	391/396 (98%)	-0.18	4 (1%)	79	77	25, 38, 65, 98	0
1	I	392/396 (98%)	-0.19	2 (0%)	87	86	26, 40, 60, 92	0
1	J	392/396 (98%)	-0.20	6 (1%)	71	69	26, 37, 60, 117	0
1	K	392/396 (98%)	-0.14	3 (0%)	82	81	25, 41, 69, 95	0
1	L	391/396 (98%)	-0.28	2 (0%)	87	86	21, 37, 59, 97	0
All	All	4690/4752 (98%)	-0.24	27 (0%)	85	84	19, 37, 60, 117	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	417	GLY	5.1
1	C	217	SER	3.9
1	F	42	ALA	3.7
1	H	432	PRO	3.3
1	G	223	PRO	3.2
1	L	432	PRO	3.0
1	E	156	ALA	2.8
1	L	326	HIS	2.6
1	K	365	ASN	2.6
1	B	417	GLY	2.5
1	J	229	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	417	GLY	2.4
1	F	43	PRO	2.4
1	H	417	GLY	2.4
1	J	432	PRO	2.4
1	H	114	GLN	2.3
1	H	265	ASP	2.2
1	J	230	ALA	2.2
1	K	176	CYS	2.2
1	K	174	PRO	2.2
1	J	349	ASN	2.2
1	G	228	GLU	2.1
1	G	227	GLY	2.1
1	I	361	GLY	2.1
1	D	432	PRO	2.1
1	J	227	GLY	2.1
1	I	98	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OXY	G	502	2/2	0.81	0.09	34,34,34,44	0
3	OXY	I	502	2/2	0.85	0.09	38,38,38,39	0
2	HEM	L	501	43/43	0.88	0.12	26,35,43,72	0
3	OXY	K	502	2/2	0.89	0.08	33,33,33,36	0
2	HEM	B	501	43/43	0.91	0.10	21,26,31,63	0
2	HEM	G	501	43/43	0.91	0.10	29,33,39,63	0
3	OXY	L	502	2/2	0.91	0.07	32,32,32,35	0

Continued on next page...

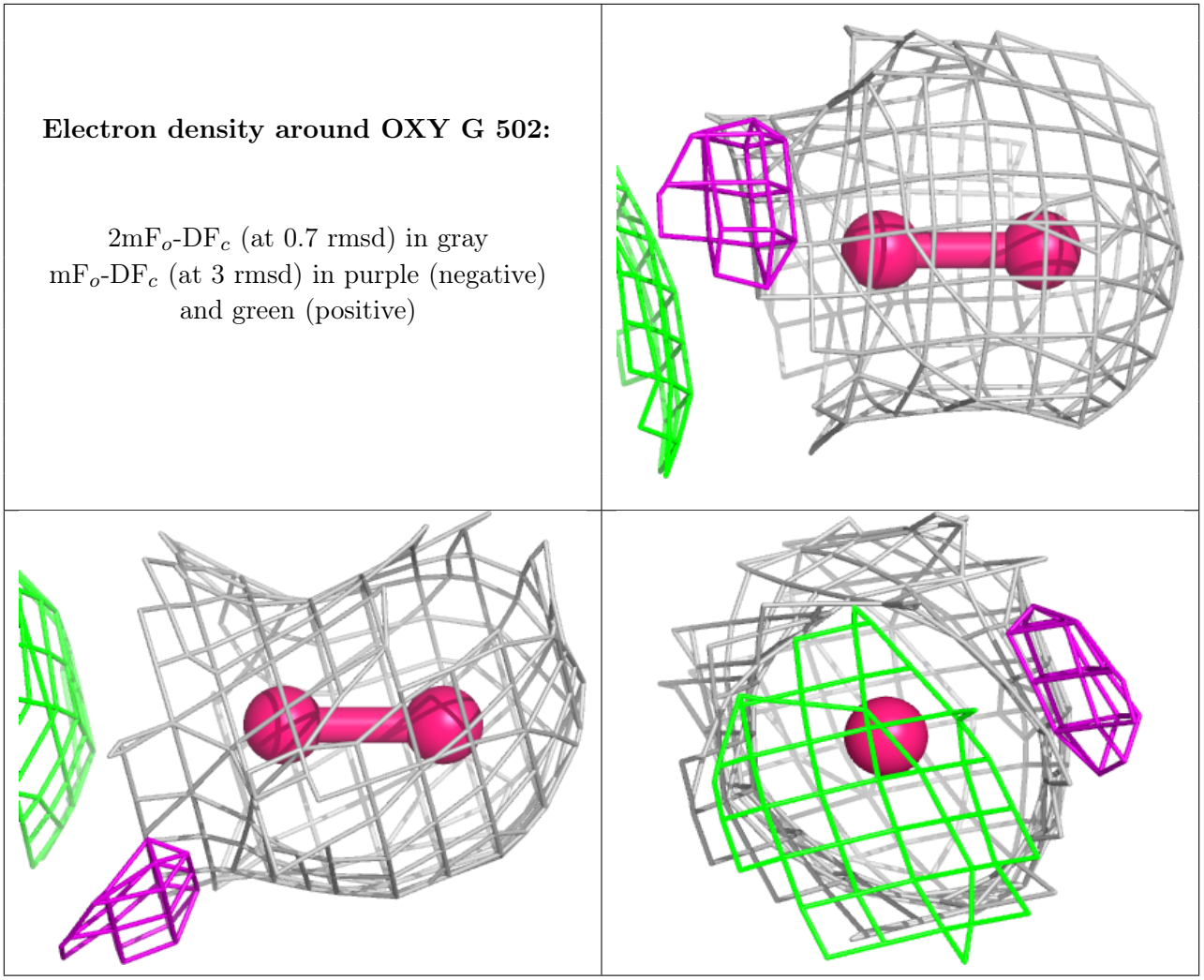
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	A	501	43/43	0.93	0.09	16,21,24,47	0
2	HEM	I	501	43/43	0.93	0.11	31,36,39,53	0
2	HEM	D	501	43/43	0.93	0.10	26,31,34,57	0
3	OXY	E	502	2/2	0.93	0.07	26,26,26,28	0
3	OXY	F	502	2/2	0.94	0.06	26,26,26,29	0
2	HEM	F	501	43/43	0.94	0.10	24,28,35,36	0
3	OXY	H	502	2/2	0.94	0.07	27,27,27,27	0
3	OXY	A	502	2/2	0.94	0.07	20,20,20,20	0
3	OXY	B	502	2/2	0.94	0.06	27,27,27,30	0
2	HEM	K	501	43/43	0.94	0.10	27,33,38,51	0
2	HEM	J	501	43/43	0.95	0.08	20,28,33,42	0
2	HEM	E	501	43/43	0.95	0.09	25,30,37,41	0
3	OXY	C	502	2/2	0.96	0.06	28,28,28,30	0
2	HEM	H	501	43/43	0.96	0.08	23,27,31,36	0
3	OXY	J	502	2/2	0.97	0.07	25,25,25,29	0
3	OXY	D	502	2/2	0.97	0.05	28,28,28,31	0
2	HEM	C	501	43/43	0.97	0.07	20,28,35,37	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.

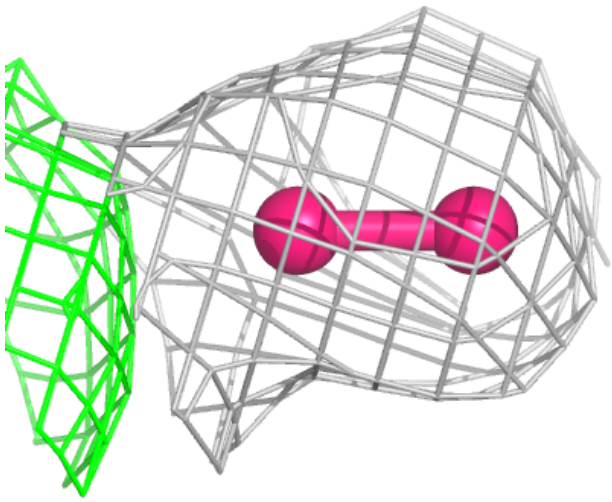
Electron density around OXY G 502:

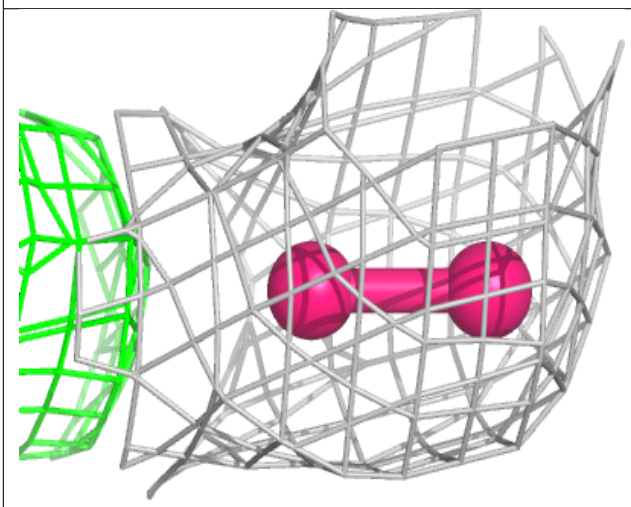
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

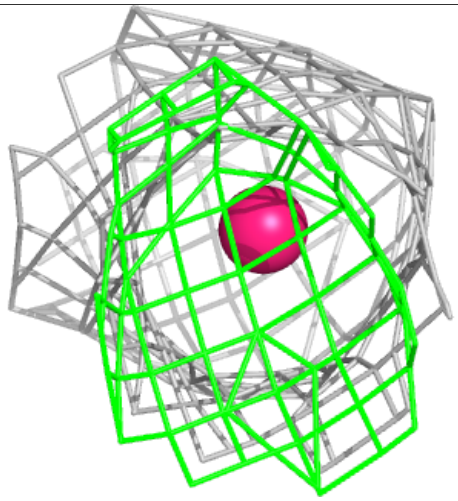


Electron density around OXY I 502:

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

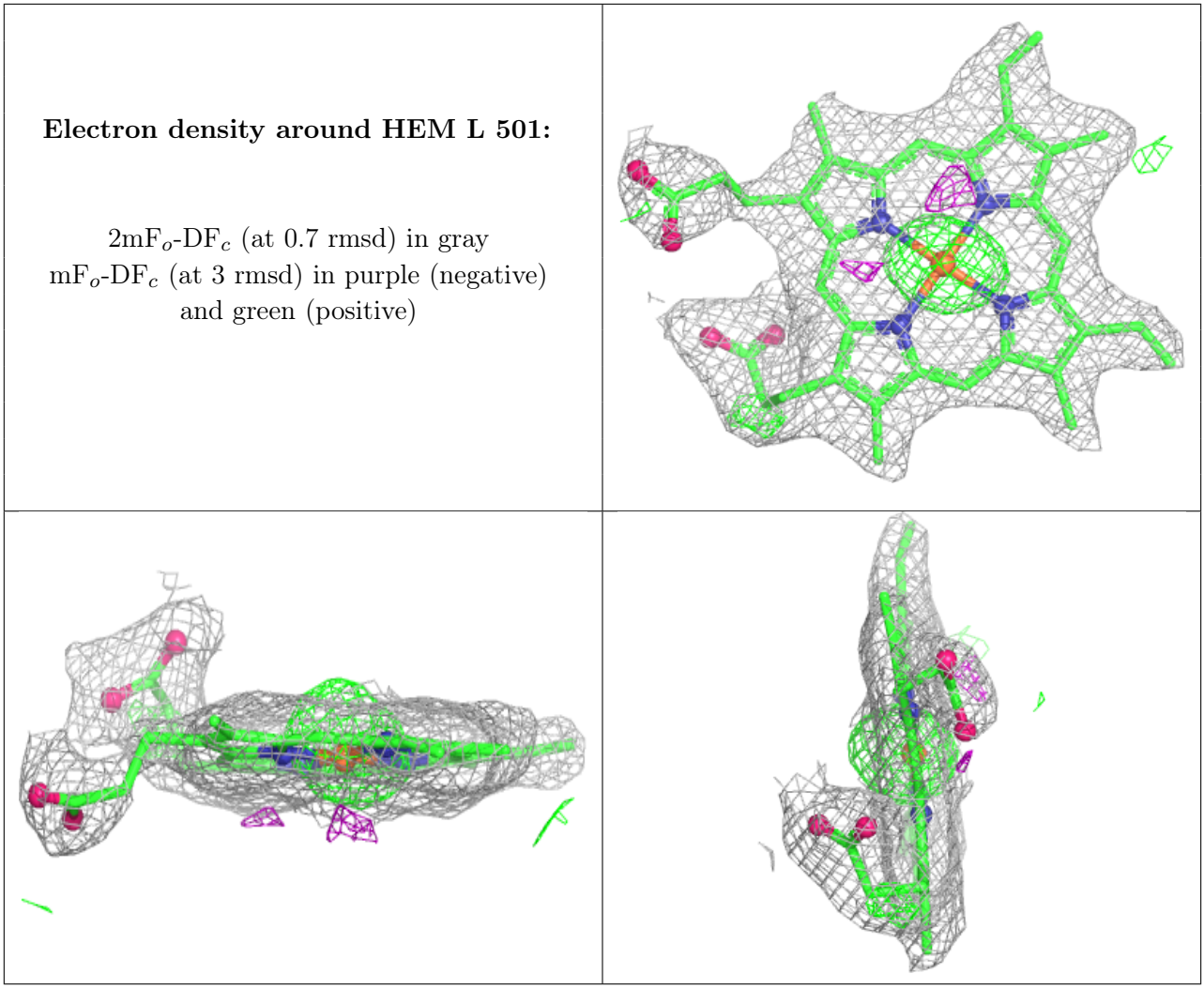






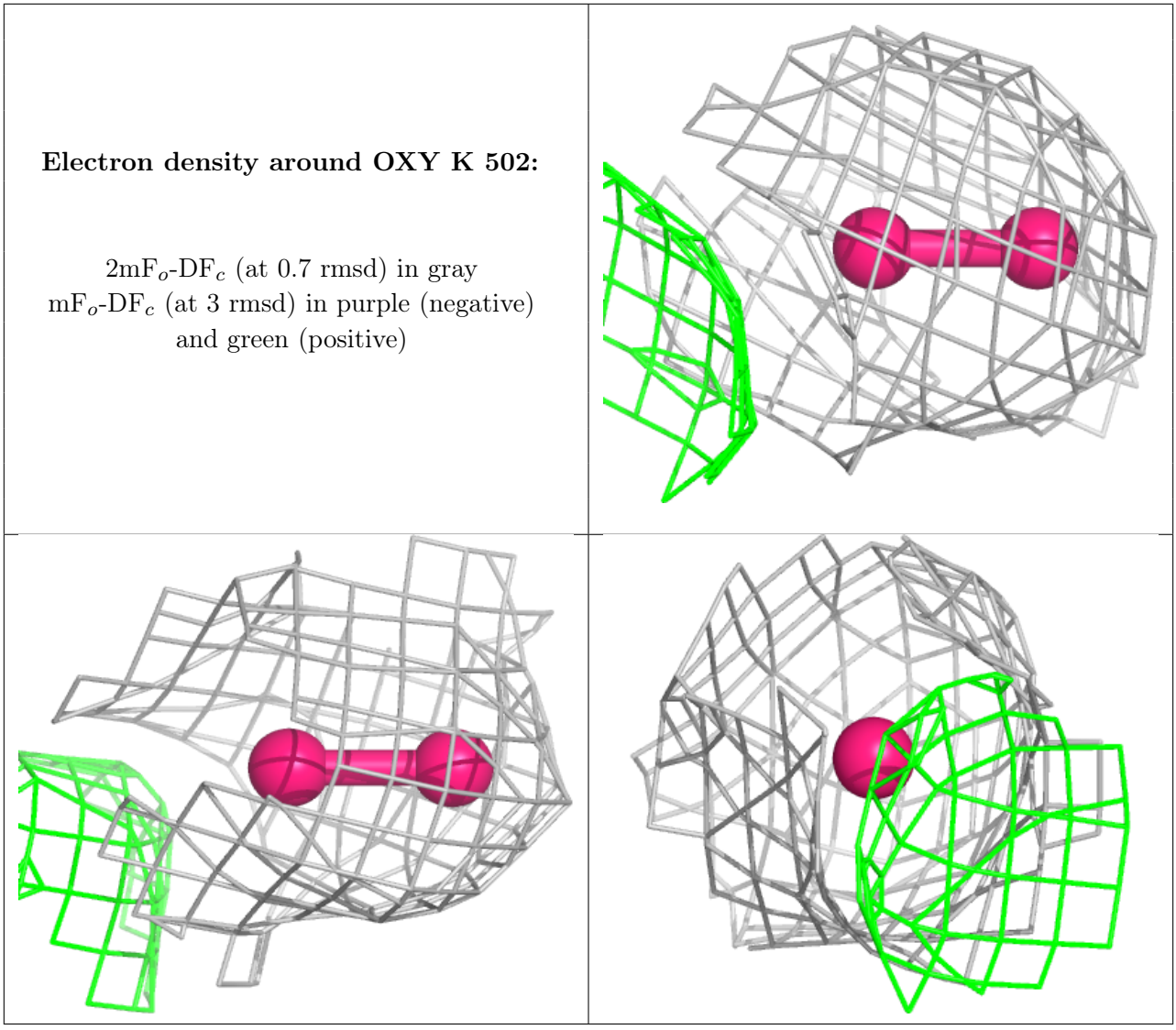
Electron density around HEM L 501:

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



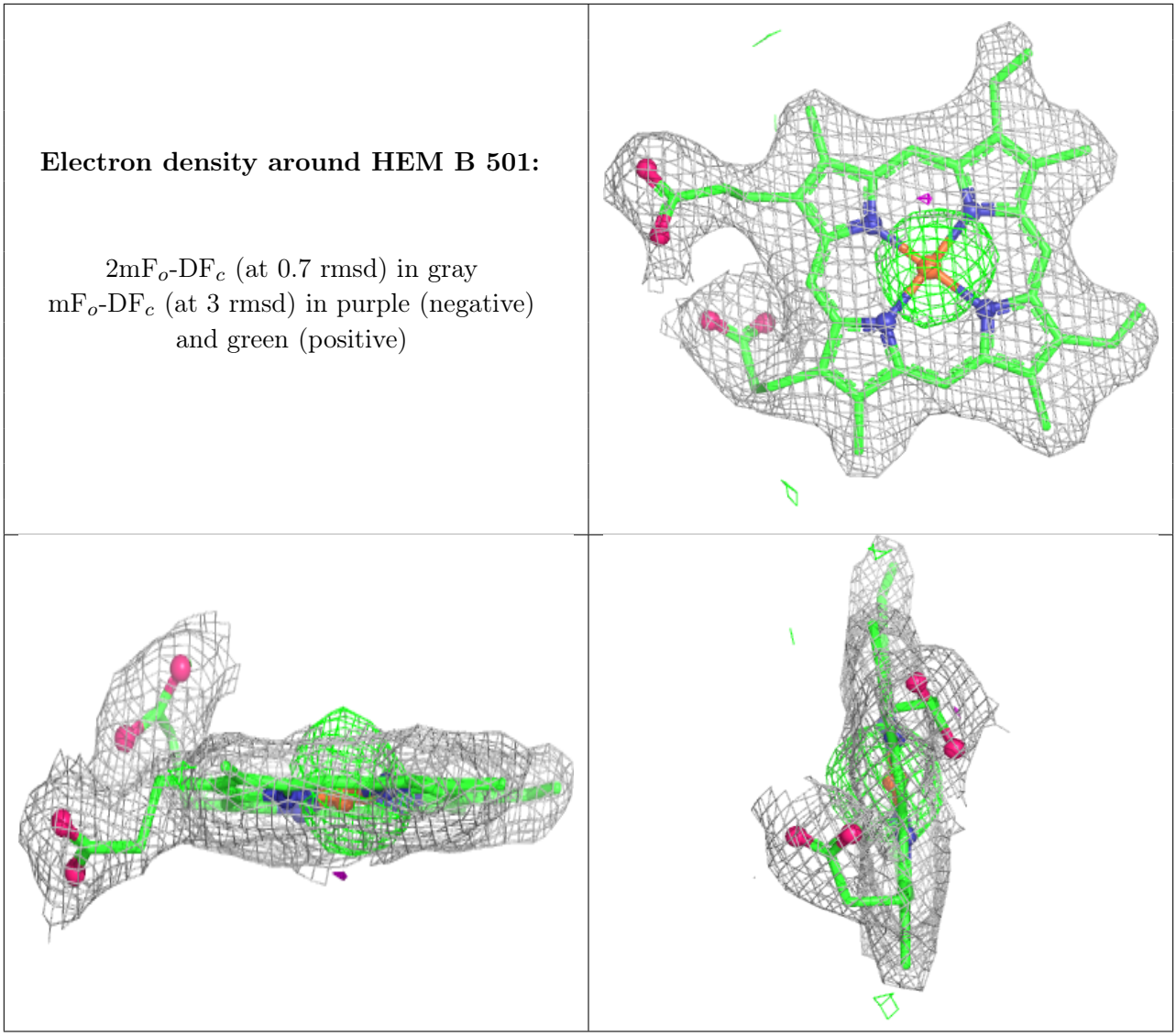
Electron density around OXY K 502:

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



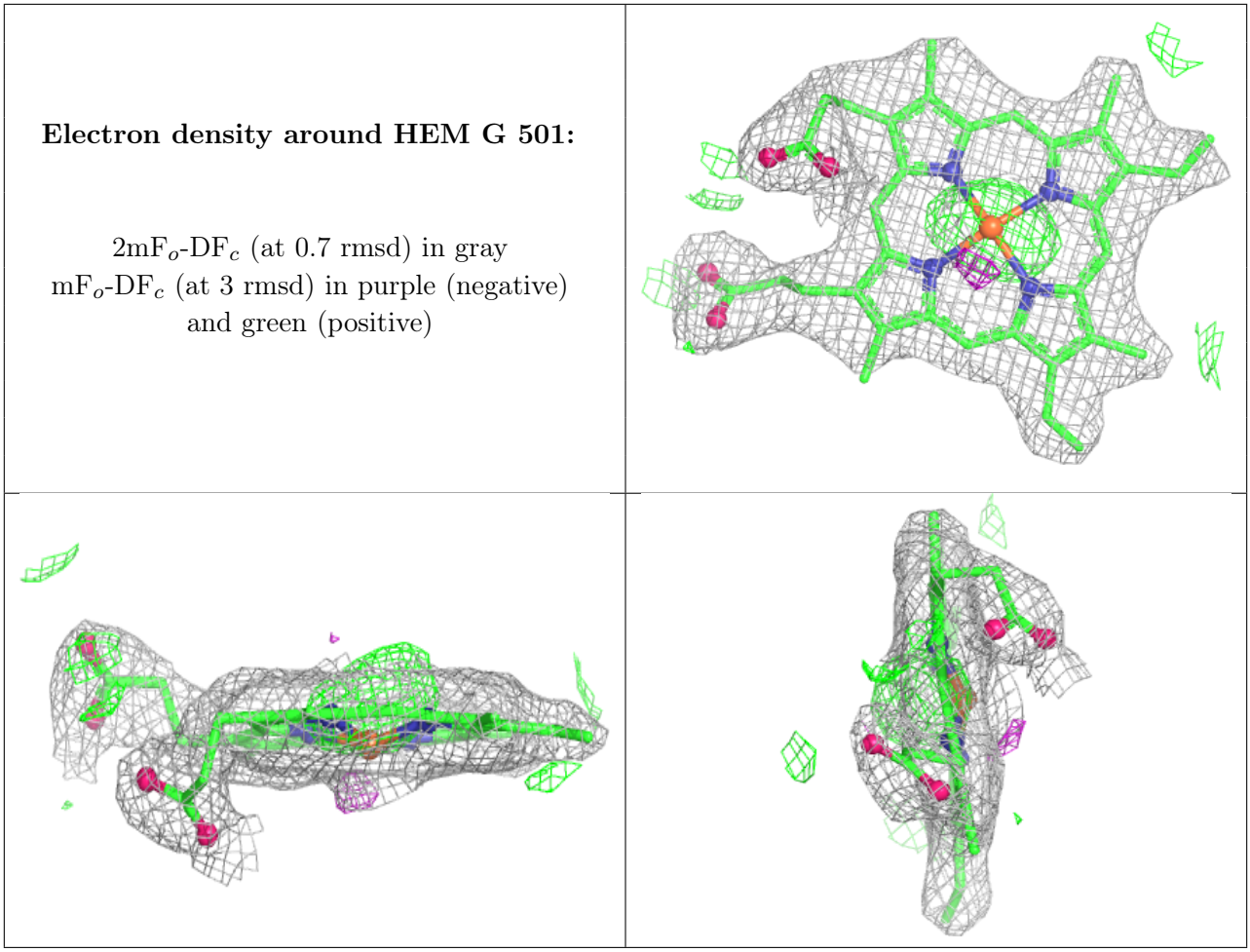
Electron density around HEM B 501:

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



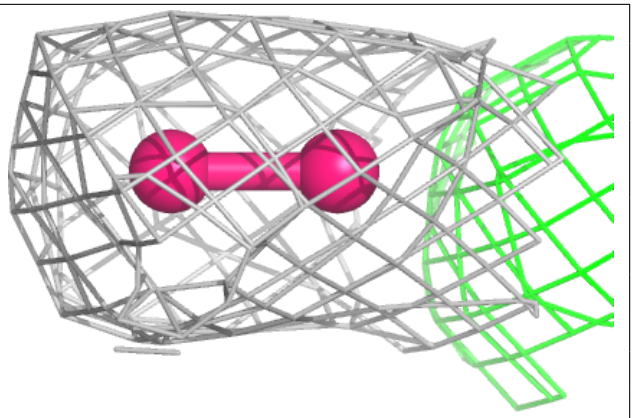
Electron density around HEM G 501:

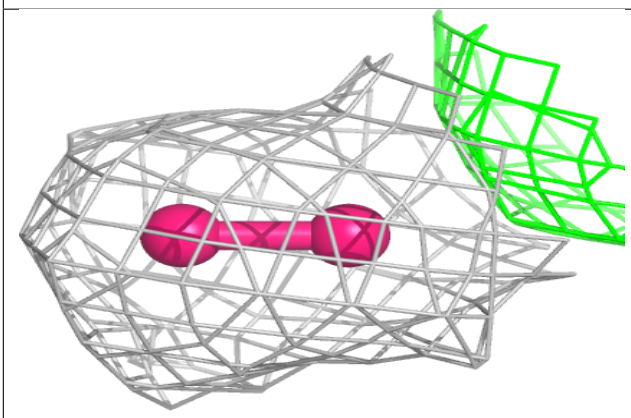
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

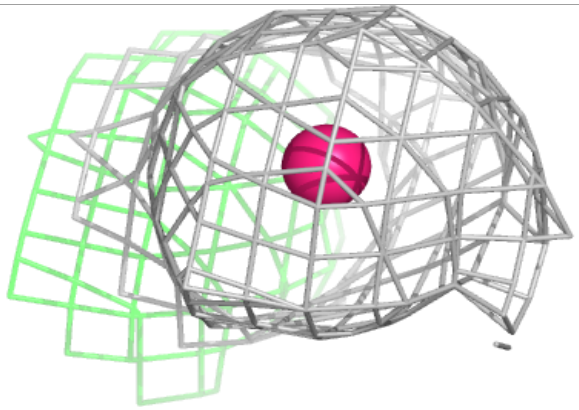


Electron density around OXY L 502:

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

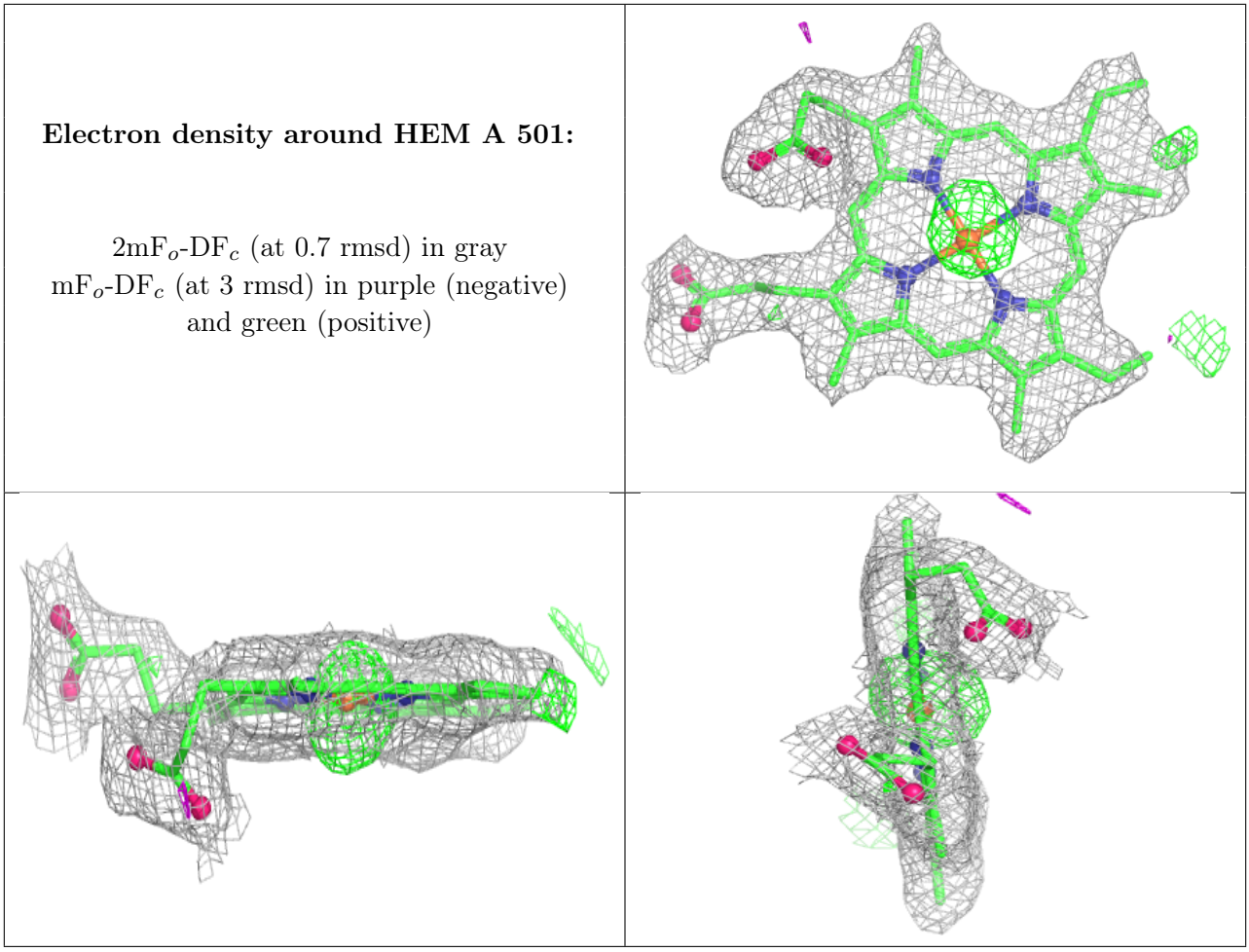






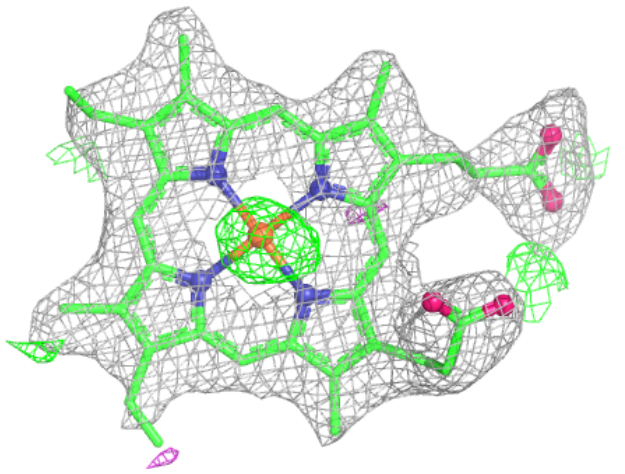
Electron density around HEM A 501:

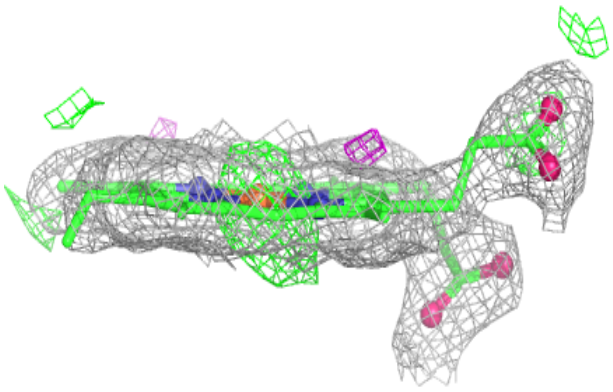
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

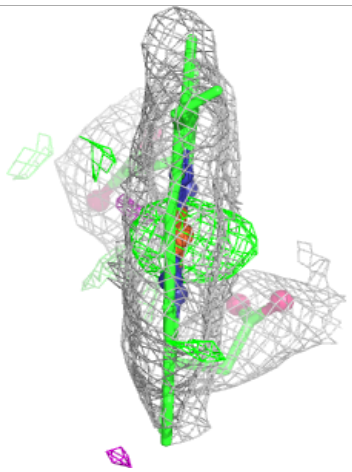


Electron density around HEM I 501:

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

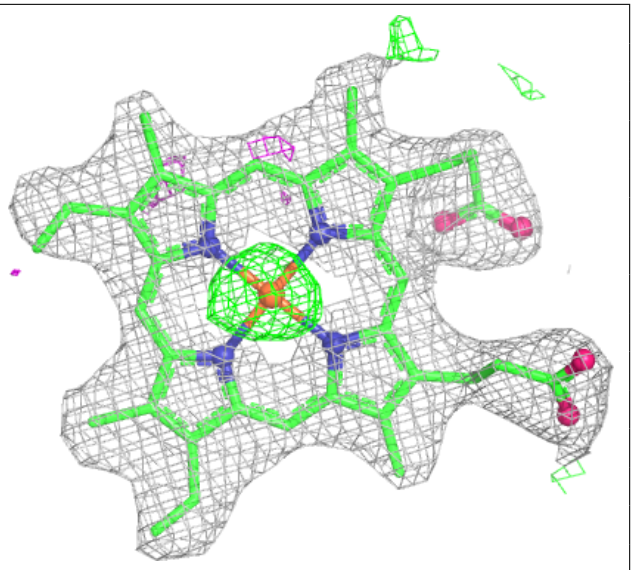


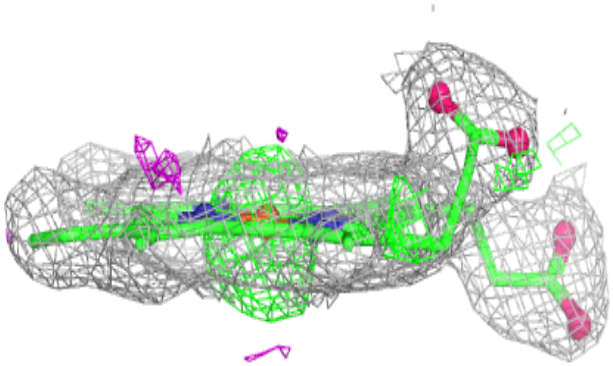


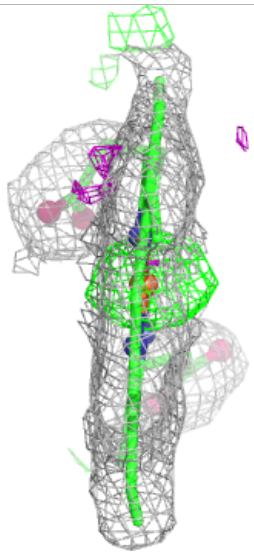


Electron density around HEM D 501:

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

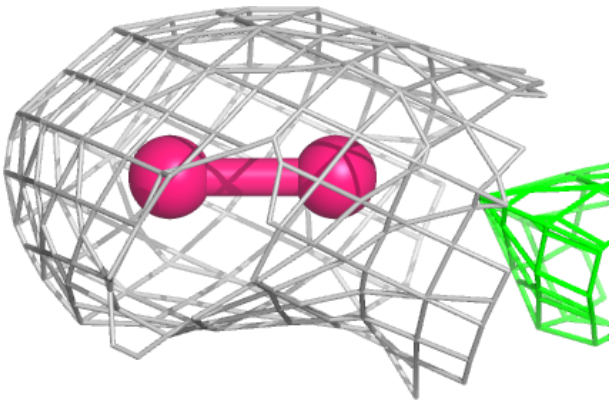


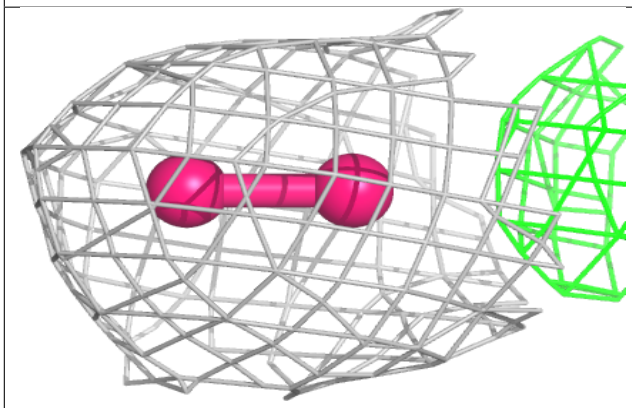


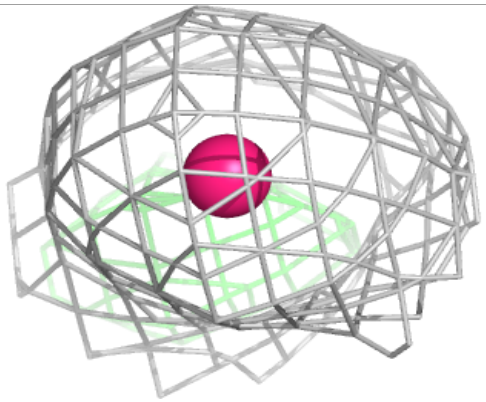


Electron density around OXY E 502:

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

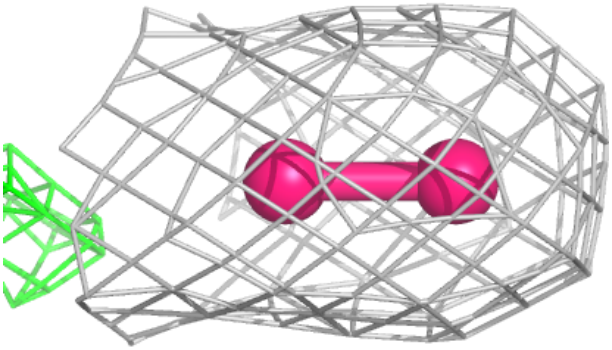


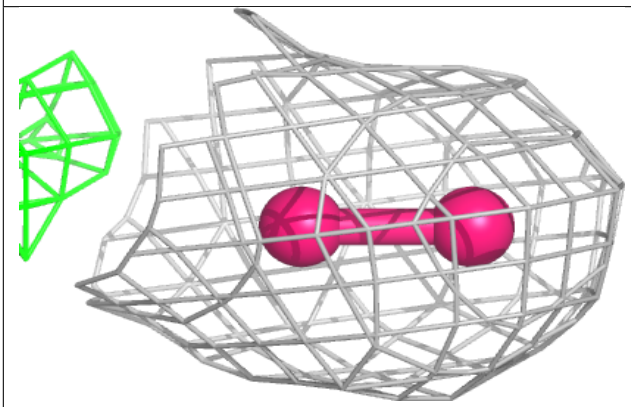


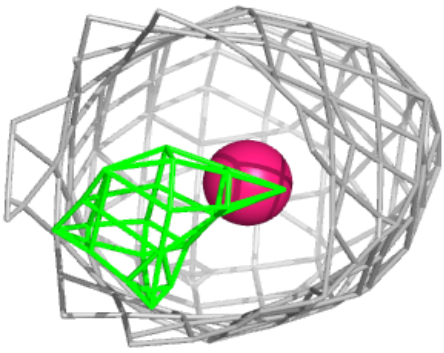


Electron density around OXY F 502:

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

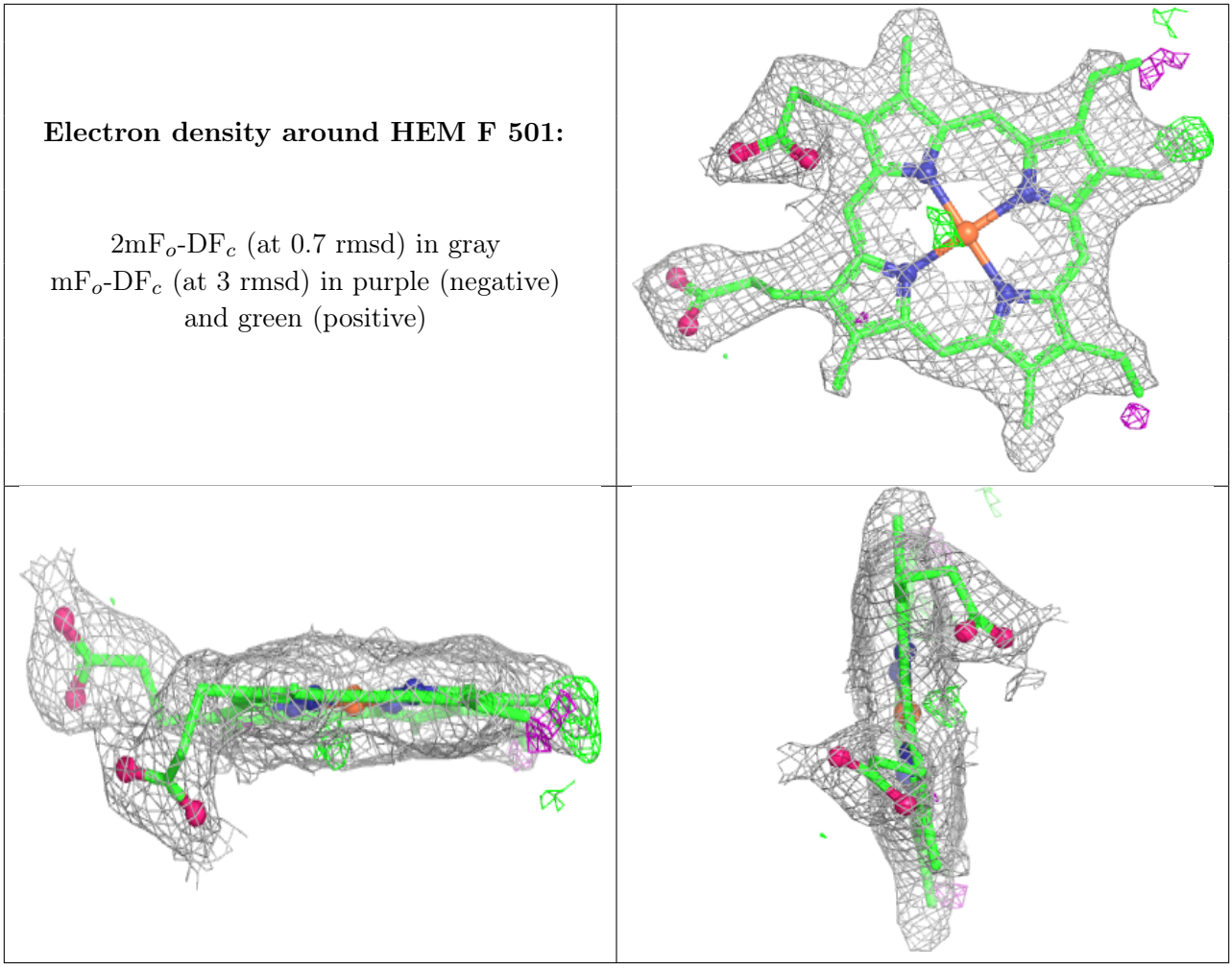






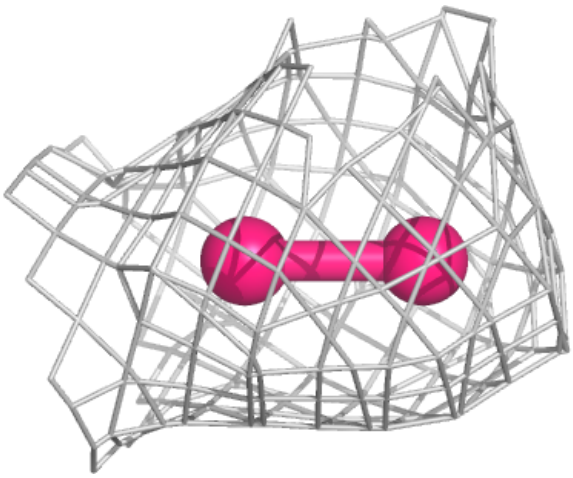
Electron density around HEM F 501:

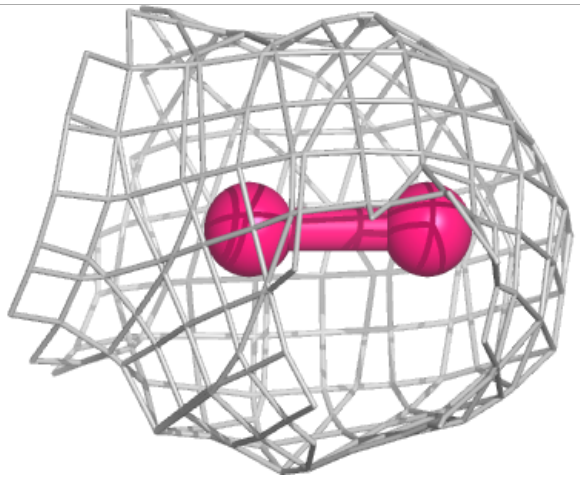
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

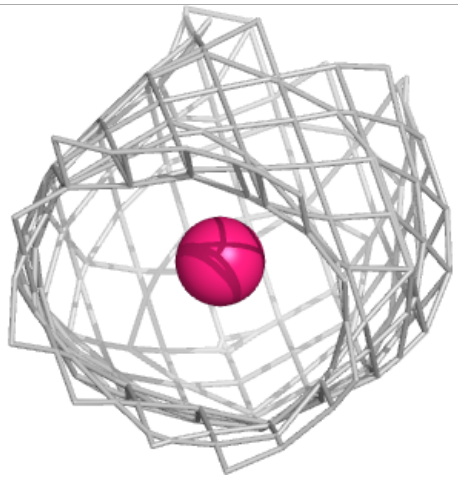


Electron density around OXY H 502:

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

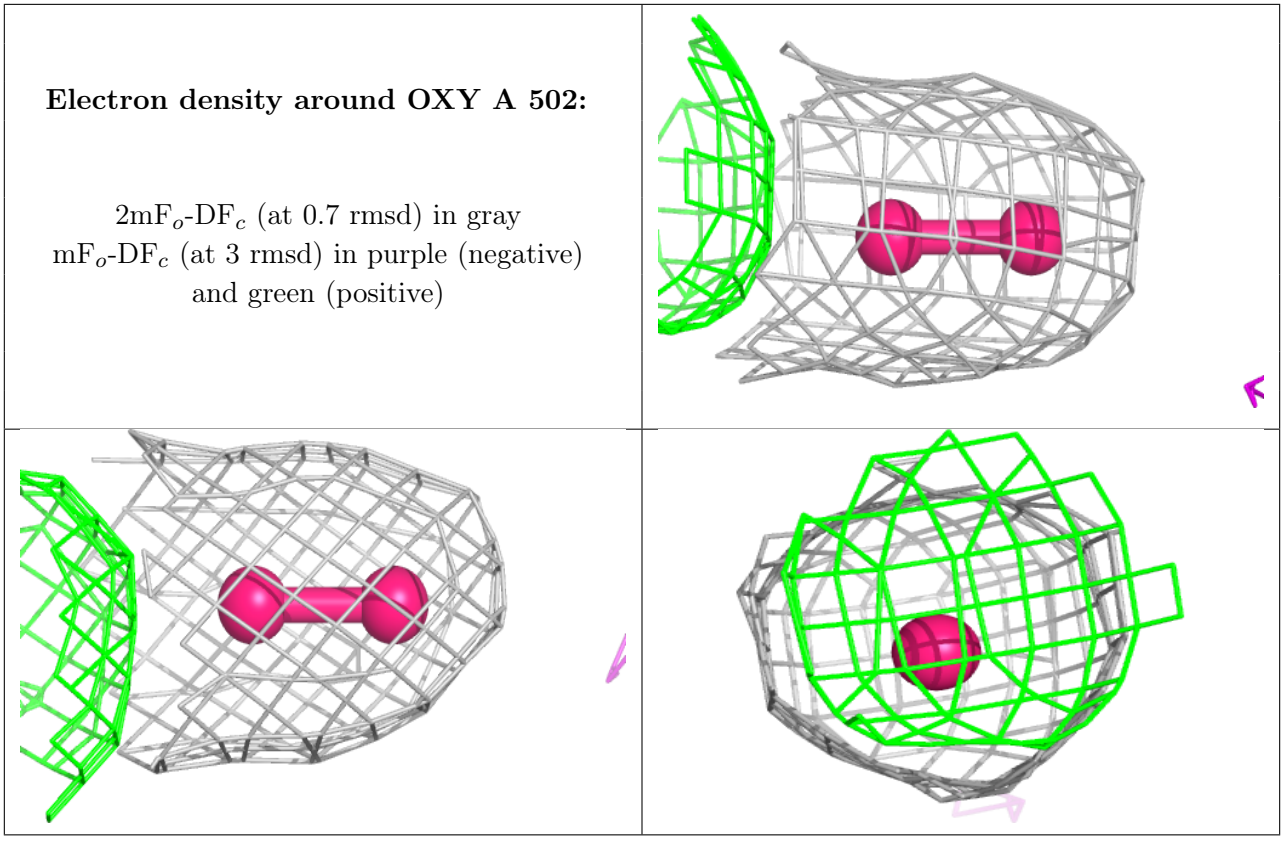






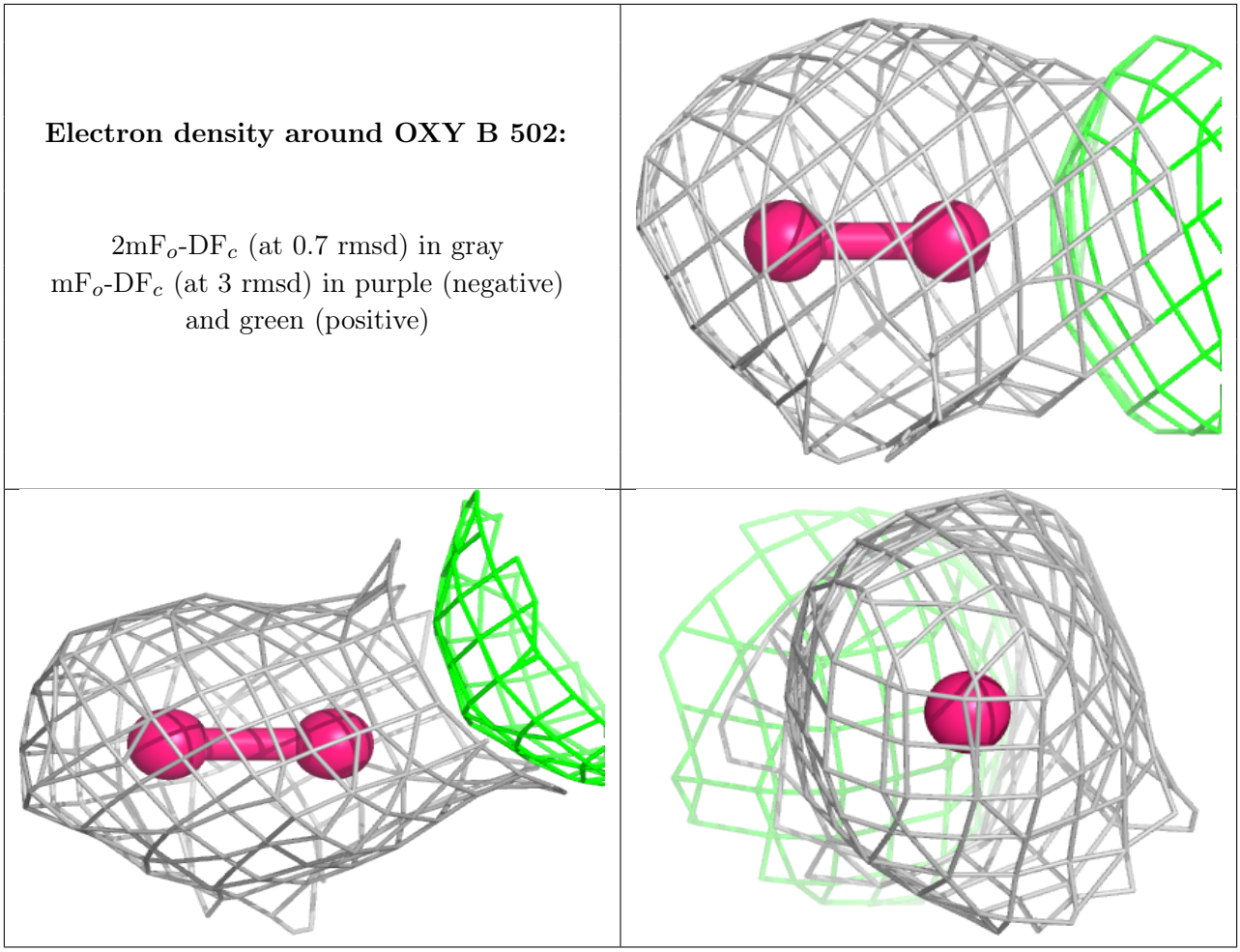
Electron density around OXY A 502:

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



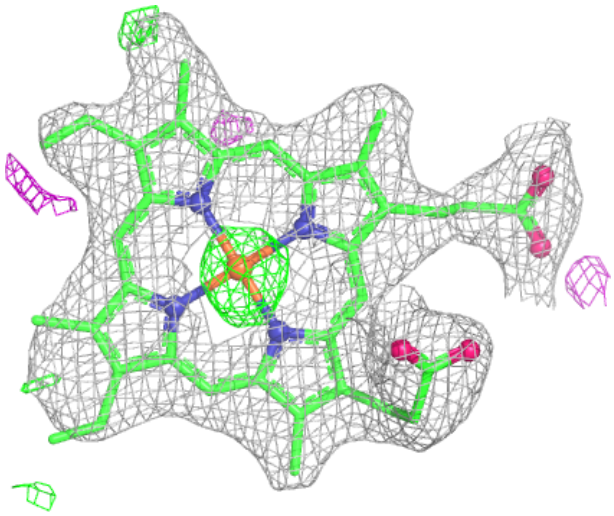
Electron density around OXY B 502:

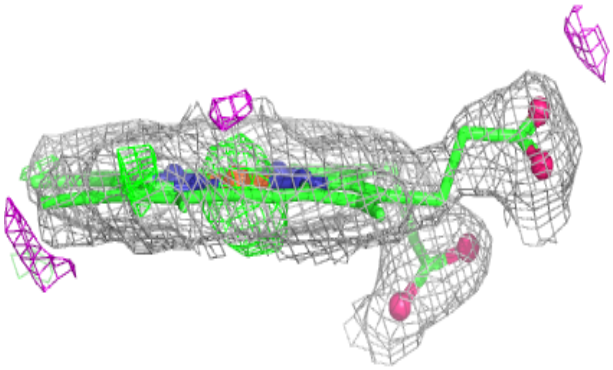
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

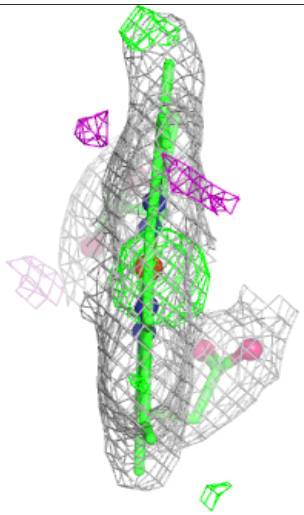


Electron density around HEM K 501:

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

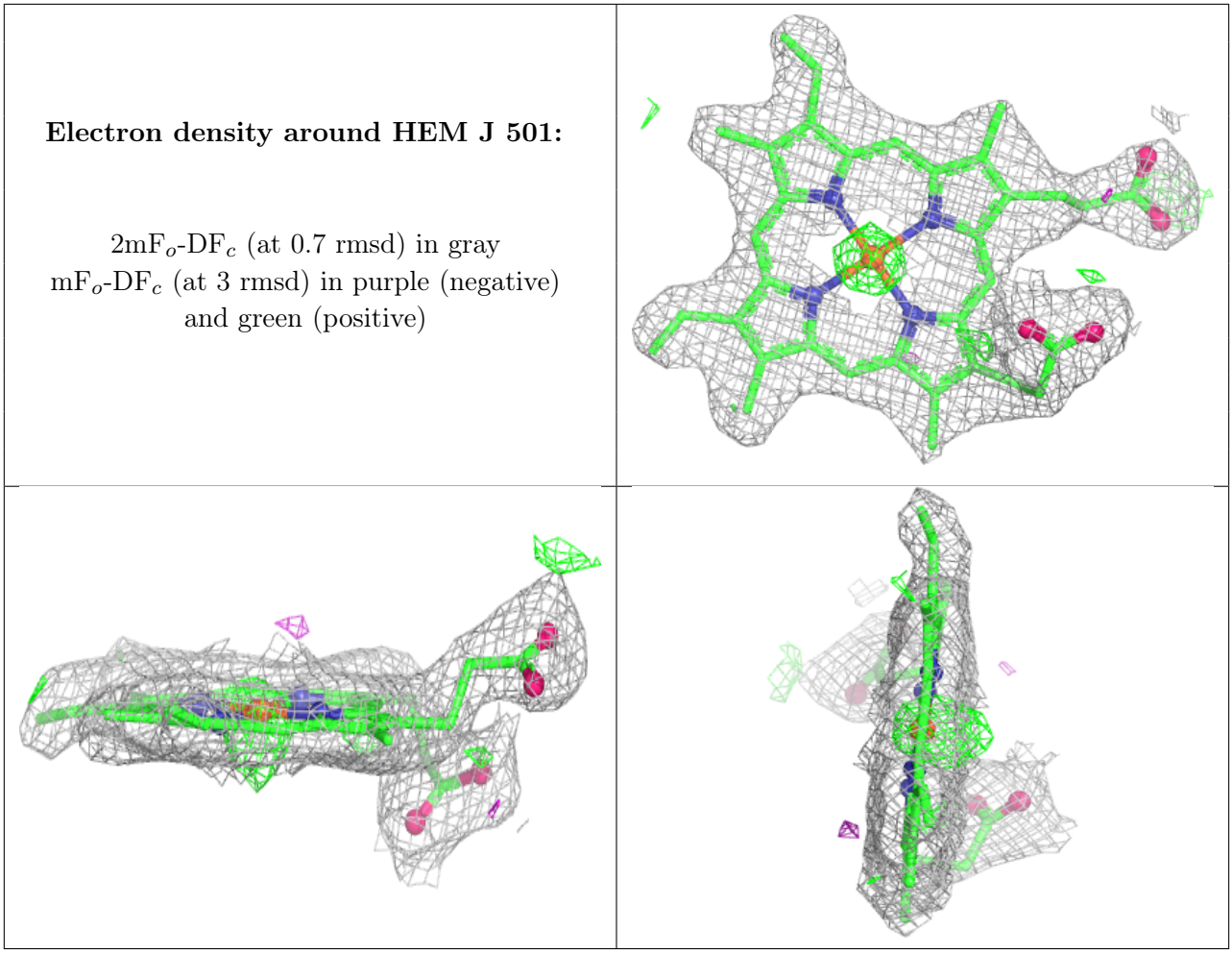






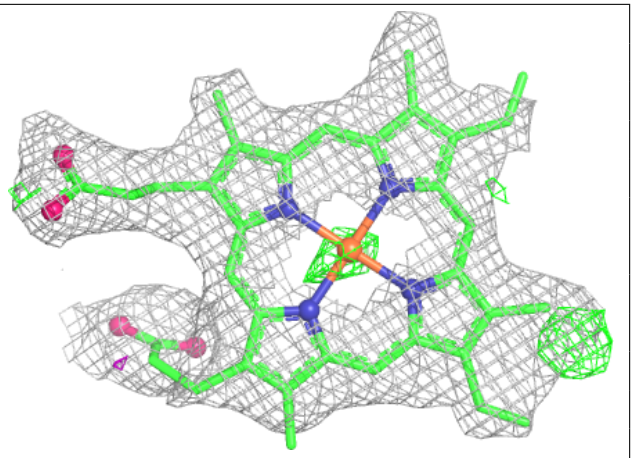
Electron density around HEM J 501:

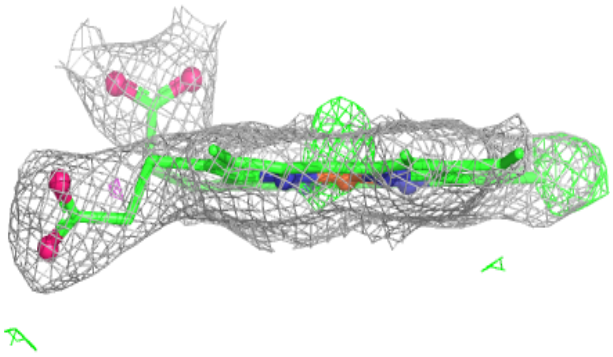
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

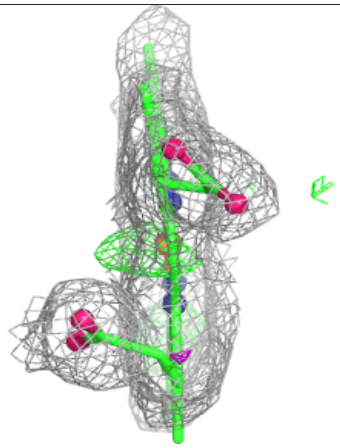


Electron density around HEM E 501:

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

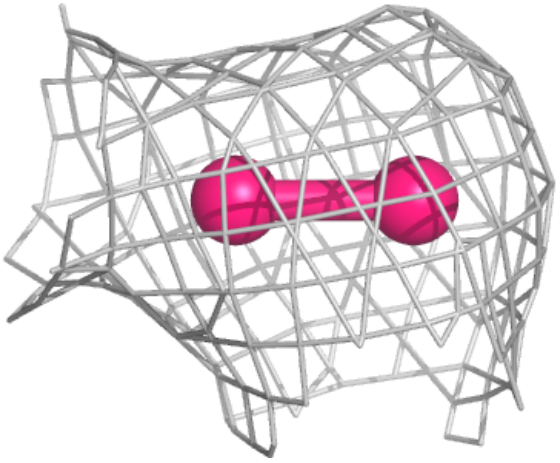


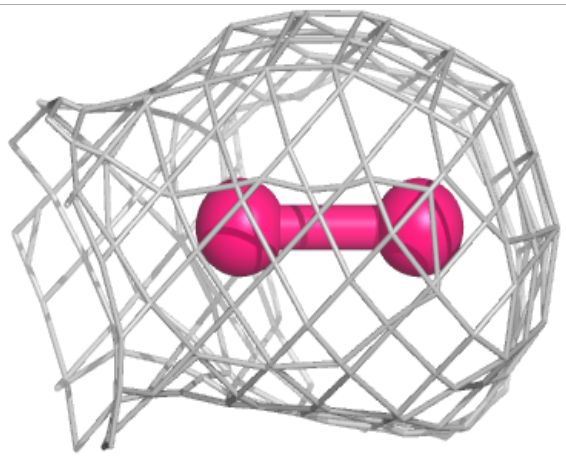


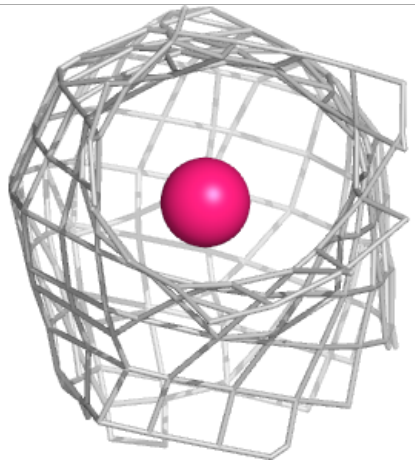


Electron density around OXY C 502:

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

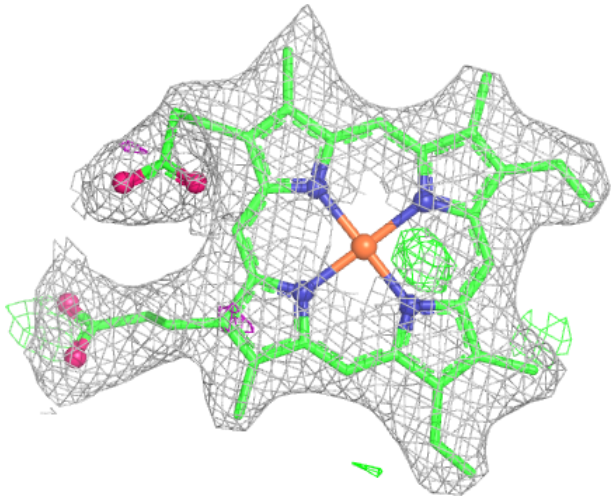


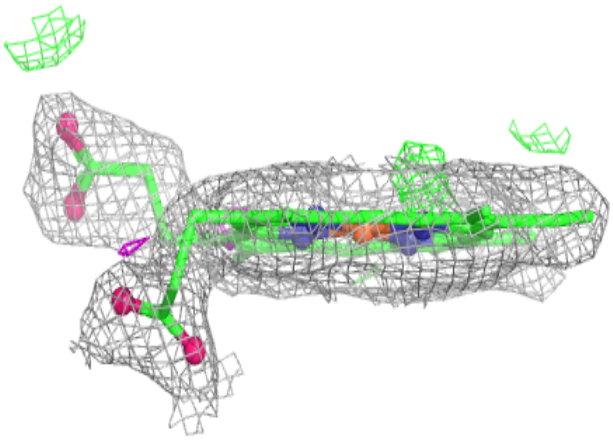


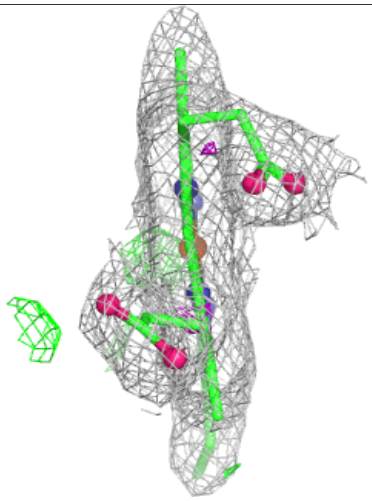


Electron density around HEM H 501:

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

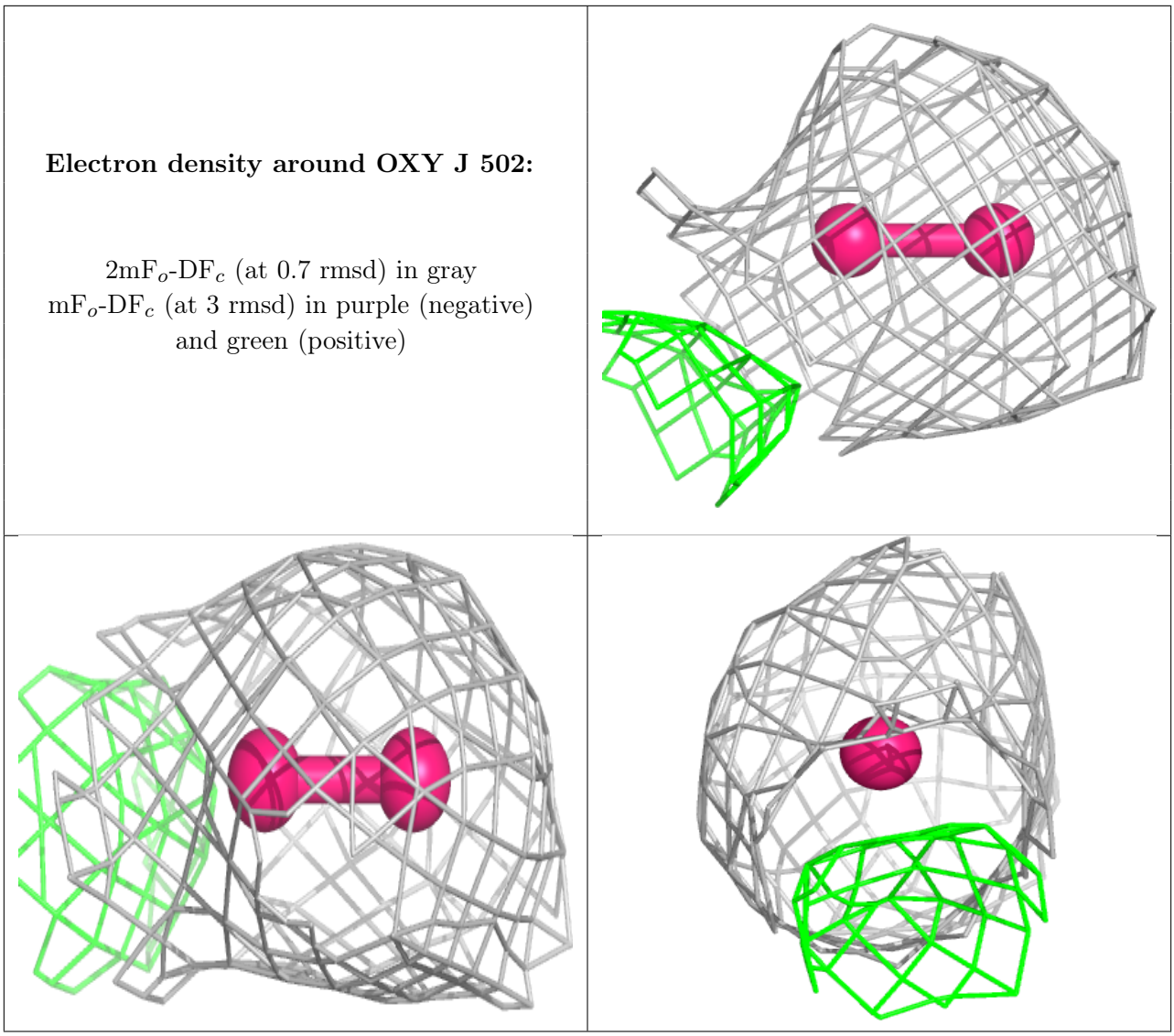






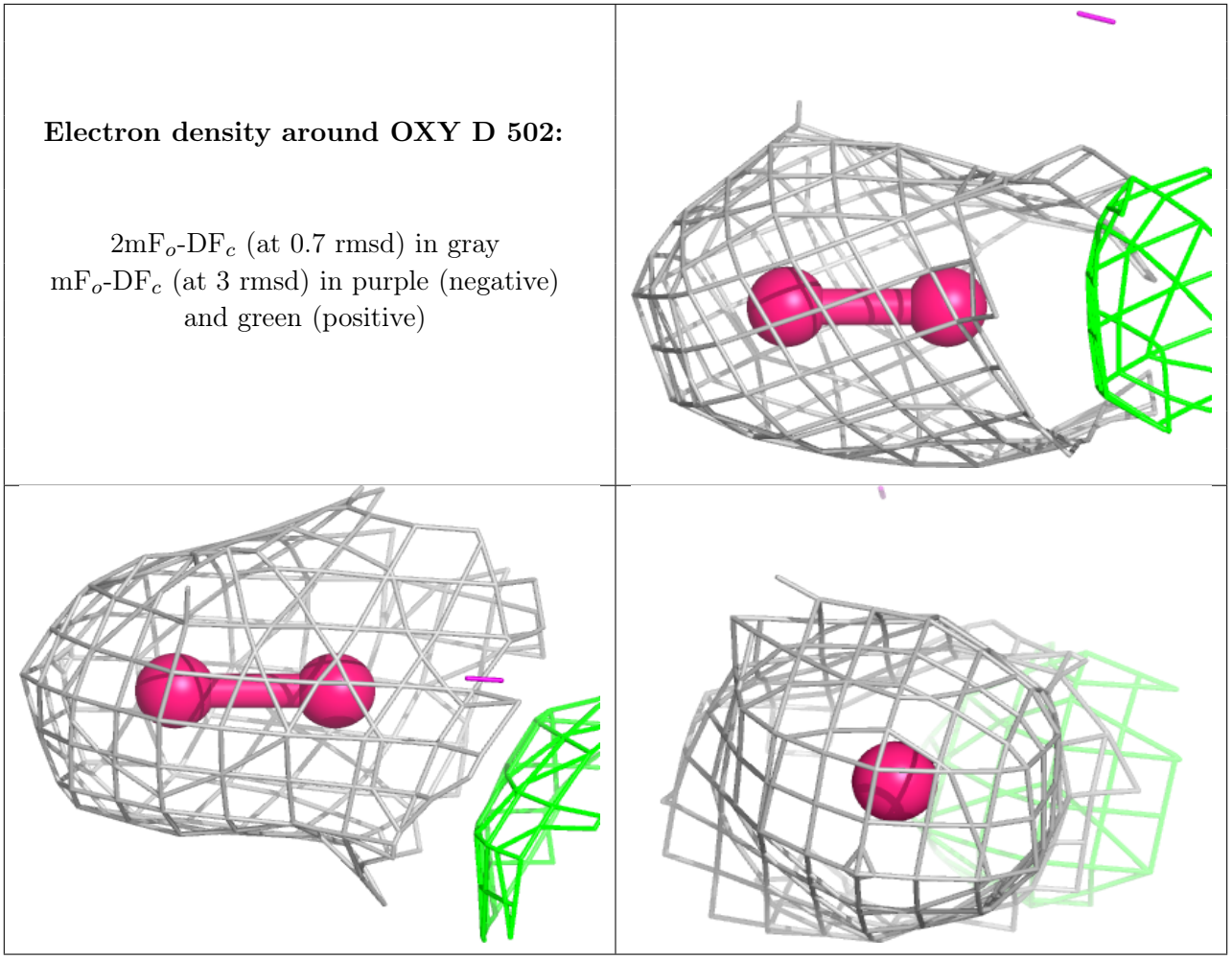
Electron density around OXY J 502:

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



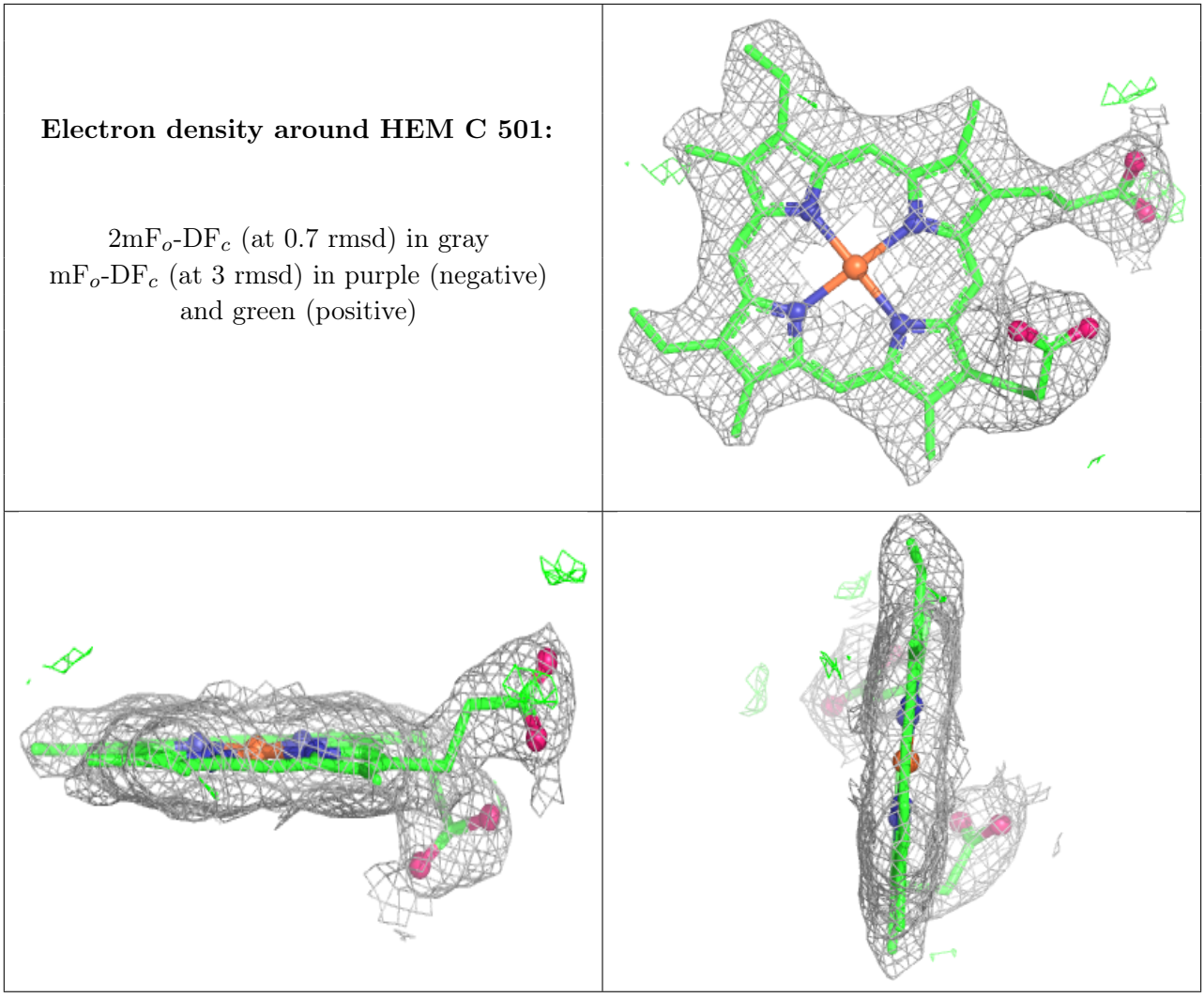
Electron density around OXY D 502:

$2mF_o$-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 501:

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



6.5 Other polymers

There are no such residues in this entry.