



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:07 PM EDT

PDB ID : 4QOM / pdb_00004qom
Title : Bacillus pumilus catalase with pyrogallol bound
Authors : Loewen, P.C.
Deposited on : 2014-06-20
Resolution : 1.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

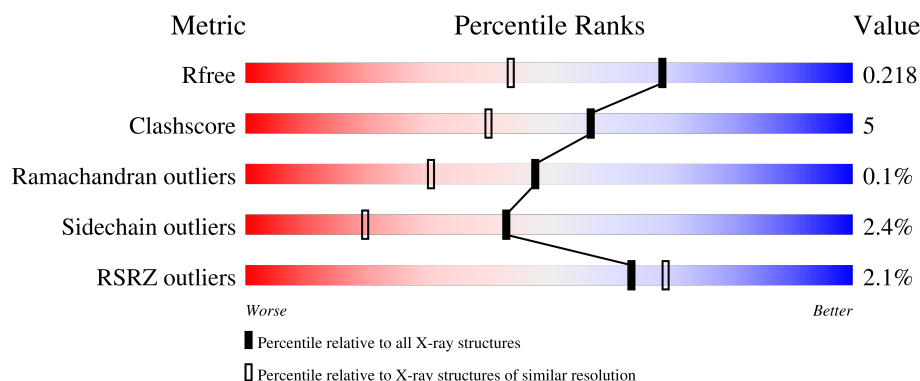
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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 $\leq 5\%$. 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	491	
1	B	491	
1	C	491	
1	D	491	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PYG	A	504	-	-	X	-
3	PYG	B	504	-	X	-	-
3	PYG	C	504	-	-	X	-
3	PYG	D	504	-	X	-	-

2 Entry composition [i](#)

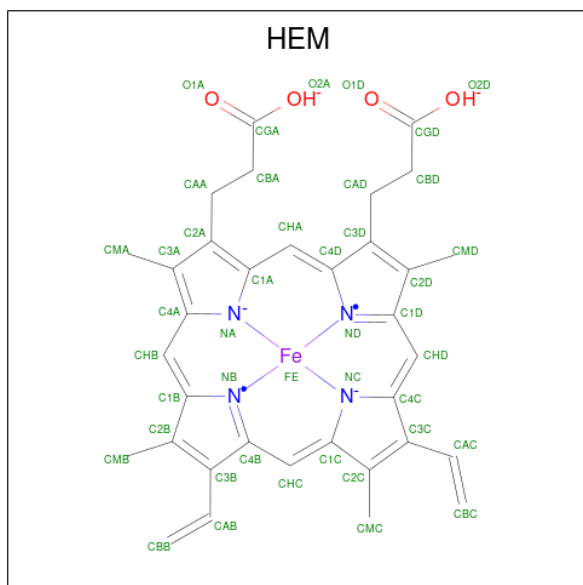
There are 6 unique types of molecules in this entry. The entry contains 17977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	5	0
			3949	2488	692	755	14			
1	B	480	Total	C	N	O	S	0	6	0
			3954	2493	691	754	16			
1	C	480	Total	C	N	O	S	0	6	0
			3962	2498	695	755	14			
1	D	480	Total	C	N	O	S	0	6	0
			3958	2494	692	758	14			

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



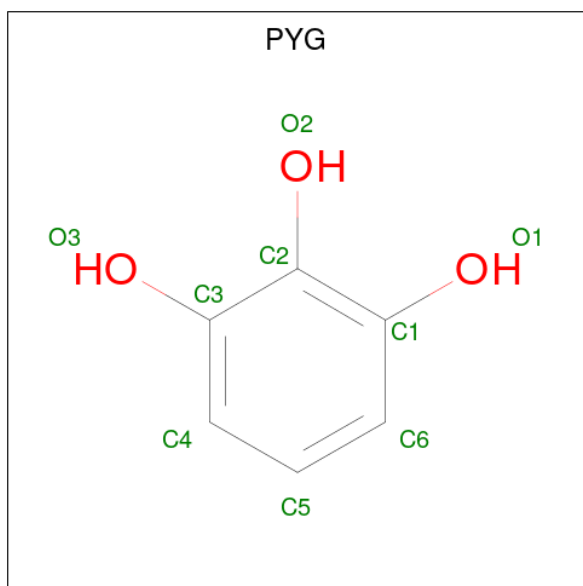
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	1
			43	34	1	4 4		
2	A	1	Total	C	Fe	N O	0	1
			43	34	1	4 4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	1

- Molecule 3 is BENZENE-1,2,3-TRIOL (CCD ID: PYG) (formula: $C_6H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	6	3		
3	A	1	Total	C	O	0	0
			9	6	3		
3	B	1	Total	C	O	0	0
			9	6	3		
3	B	1	Total	C	O	0	0
			9	6	3		
3	C	1	Total	C	O	0	0
			9	6	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			9	6	3		
3	D	1	Total	C	O	0	0
			9	6	3		
3	D	1	Total	C	O	0	0
			9	6	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	1	Total	Cl	0	0
			1	1		
4	C	2	Total	Cl	0	0
			2	2		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		

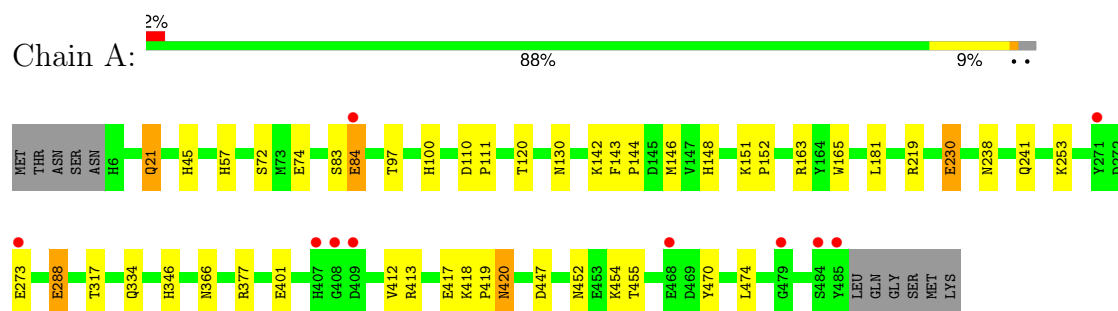
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	436	Total	O	0	0
			436	436		
6	B	424	Total	O	0	0
			424	424		
6	C	446	Total	O	0	0
			446	446		
6	D	424	Total	O	0	0
			424	424		

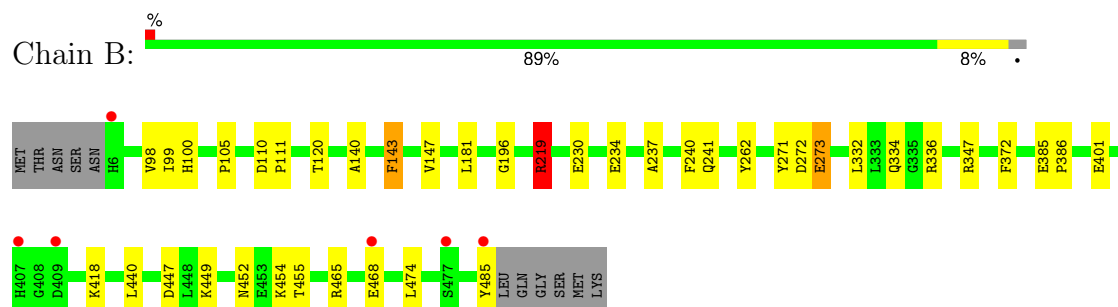
3 Residue-property plots [i](#)

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.

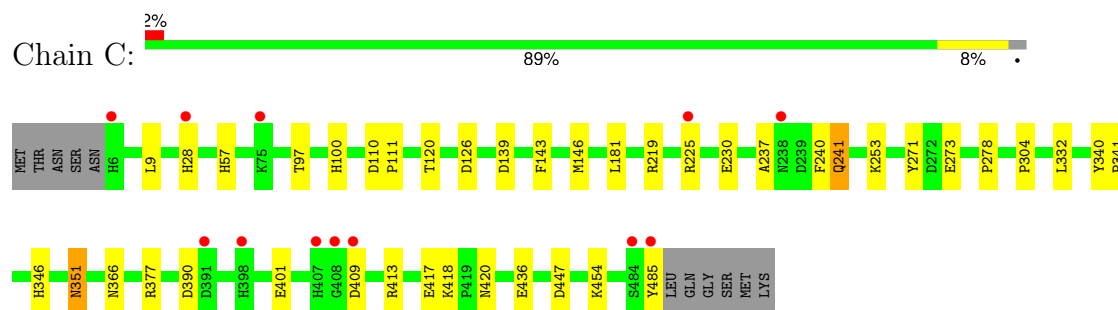
• Molecule 1: Catalase



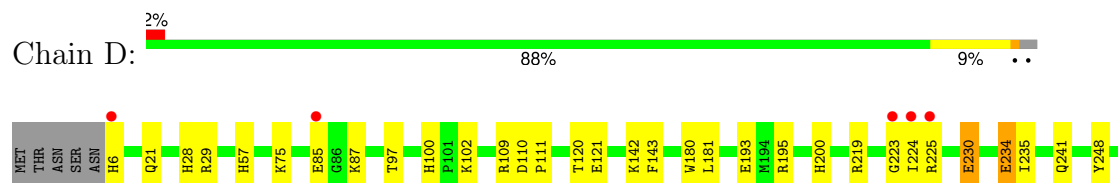
• Molecule 1: Catalase

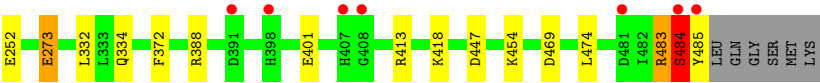


• Molecule 1: Catalase



• Molecule 1: Catalase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.85Å 109.42Å 103.37Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	103.29 – 1.65 103.29 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.8 (103.29-1.65) 96.8 (103.29-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.178 , 0.210 0.188 , 0.218	Depositor DCC
R_{free} test set	11730 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.075 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17977	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PYG, NA, CL

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	1.11	7/4068 (0.2%)	1.03	6/5516 (0.1%)
1	B	1.17	5/4075 (0.1%)	1.01	4/5524 (0.1%)
1	C	1.20	7/4080 (0.2%)	1.07	4/5531 (0.1%)
1	D	1.11	1/4076 (0.0%)	1.00	5/5526 (0.1%)
All	All	1.15	20/16299 (0.1%)	1.03	19/22097 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	PHE	C-O	-7.43	1.17	1.24
1	A	163	ARG	C-O	-6.71	1.16	1.24
1	A	148	HIS	N-CA	-6.56	1.38	1.46
1	A	165	TRP	N-CA	6.17	1.54	1.46
1	C	126	ASP	CA-C	5.87	1.59	1.52
1	B	271	TYR	C-O	-5.85	1.17	1.24
1	A	470	TYR	C-O	-5.67	1.17	1.24
1	C	366	ASN	C-O	5.59	1.30	1.23
1	C	377	ARG	N-CA	5.57	1.50	1.46
1	D	200	HIS	CA-C	-5.53	1.45	1.52
1	A	377	ARG	N-CA	5.37	1.50	1.46
1	B	196	GLY	N-CA	5.30	1.50	1.45
1	B	418	LYS	CA-CB	-5.26	1.48	1.52
1	C	418	LYS	CA-C	5.23	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	GLN	N-CA	5.15	1.52	1.46
1	C	139	ASP	C-O	-5.10	1.18	1.23
1	C	304	PRO	N-CA	-5.10	1.41	1.47
1	A	144	PRO	C-O	-5.09	1.18	1.24
1	C	346	HIS	C-O	5.07	1.29	1.24
1	B	336	ARG	CZ-NH2	-5.03	1.26	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	ARG	NE-CZ-NH1	-7.86	113.64	121.50
1	C	225	ARG	NE-CZ-NH2	7.75	126.18	119.20
1	B	219	ARG	CB-CA-C	-6.89	101.99	109.85
1	A	288	GLU	N-CA-CB	6.21	119.08	110.07
1	D	418	LYS	O-C-N	5.86	124.22	121.53
1	A	273	GLU	N-CA-C	5.84	121.12	113.30
1	C	351	ASN	N-CA-C	5.62	118.93	112.97
1	B	99	ILE	N-CA-C	5.59	117.51	111.58
1	D	248	TYR	N-CA-C	-5.31	105.49	111.28
1	A	84	GLU	N-CA-C	5.26	117.26	108.99
1	D	413	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	A	317	THR	CA-C-N	-5.21	114.25	119.56
1	A	317	THR	C-N-CA	-5.21	114.25	119.56
1	B	147	VAL	N-CA-C	5.20	115.41	110.42
1	D	483	ARG	N-CA-C	-5.14	102.44	110.10
1	C	413	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	D	469	ASP	N-CA-C	-5.10	105.80	111.36
1	A	418	LYS	CB-CA-C	-5.08	107.59	111.20
1	B	418	LYS	O-C-N	5.05	123.85	121.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	484	SER	Peptide

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	3949	0	3748	31	1
1	B	3954	0	3761	23	1
1	C	3962	0	3771	23	1
1	D	3958	0	3757	42	2
2	A	86	0	60	11	0
2	B	86	0	60	11	0
2	C	86	0	60	7	0
2	D	86	0	60	10	0
3	A	18	0	9	7	0
3	B	18	0	9	5	0
3	C	18	0	10	5	0
3	D	18	0	9	3	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	436	0	0	11	0
6	B	424	0	0	5	1
6	C	446	0	0	11	0
6	D	424	0	0	16	0
All	All	17977	0	15314	146	3

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 (146) 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)
2:A:501[A]:HEM:HMB2	2:A:501[A]:HEM:HBB2	1.33	1.08
1:C:436:GLU:OE2	6:C:743:HOH:O	1.72	1.05
1:C:454:LYS:HE3	6:C:1045:HOH:O	1.63	0.97
2:A:502[B]:HEM:HMC2	2:A:502[B]:HEM:HBC2	1.43	0.97
1:C:28:HIS:CE1	6:C:842:HOH:O	2.17	0.95
1:C:28:HIS:ND1	6:C:842:HOH:O	2.00	0.94
2:A:501[A]:HEM:HBB2	2:A:501[A]:HEM:CMB	1.96	0.90
2:B:502[B]:HEM:CMC	2:B:502[B]:HEM:HBC2	2.02	0.90
1:D:195:ARG:CD	1:D:224:ILE:HD11	2.03	0.89
1:B:449:LYS:NZ	6:B:940:HOH:O	1.94	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:ARG:HD3	1:D:224:ILE:CD1	2.07	0.84
2:C:501[A]:HEM:HMC2	2:C:501[A]:HEM:HBC2	1.61	0.80
1:C:219:ARG:HD2	6:C:728:HOH:O	1.83	0.78
2:C:501[A]:HEM:HBC2	2:C:501[A]:HEM:CMC	2.14	0.76
1:D:180:TRP:HZ3	1:D:195:ARG:HH22	1.32	0.76
1:B:372[A]:PHE:CE2	6:D:904:HOH:O	2.38	0.76
1:D:195:ARG:CG	1:D:224:ILE:HD11	2.16	0.75
2:A:501[A]:HEM:CMC	2:A:501[A]:HEM:HBC2	2.17	0.75
2:B:501[A]:HEM:HMB2	2:B:501[A]:HEM:HBB2	1.69	0.75
1:A:83:SER:OG	6:A:958:HOH:O	2.04	0.75
1:D:195:ARG:HD3	1:D:224:ILE:HD11	1.66	0.74
2:B:501[A]:HEM:HBB2	2:B:501[A]:HEM:CMB	2.17	0.72
1:D:454:LYS:HE3	6:D:997:HOH:O	1.89	0.72
1:D:85:GLU:H	1:D:85:GLU:CD	1.98	0.71
1:A:181:LEU:HD21	3:A:503:PYG:C6	2.20	0.71
1:C:219:ARG:CD	6:C:728:HOH:O	2.37	0.71
2:B:502[B]:HEM:HBC2	2:B:502[B]:HEM:HMC1	1.72	0.70
1:B:181:LEU:HD21	3:B:503:PYG:C6	2.21	0.69
1:A:452:ASN:HD22	1:A:455:THR:H	1.41	0.69
2:B:502[B]:HEM:HMC1	2:B:502[B]:HEM:CBC	2.23	0.69
1:B:100:HIS:HE1	6:C:704:HOH:O	1.76	0.68
2:A:501[A]:HEM:HMB2	2:A:501[A]:HEM:CBB	2.20	0.67
1:B:452:ASN:HD22	1:B:455:THR:H	1.43	0.67
2:A:501[A]:HEM:HBC2	2:A:501[A]:HEM:HMC2	1.77	0.66
1:D:252:GLU:OE1	6:D:675:HOH:O	2.12	0.66
1:A:45:HIS:HE1	1:C:351:ASN:OD1	1.78	0.66
1:D:181:LEU:HD21	3:D:503:PYG:C6	2.25	0.65
2:A:502[B]:HEM:HBC2	2:A:502[B]:HEM:CMC	2.21	0.65
2:B:501[A]:HEM:HMC2	2:B:501[A]:HEM:HBC2	1.79	0.64
1:B:372[A]:PHE:CD2	6:D:904:HOH:O	2.49	0.64
1:D:195:ARG:HD3	1:D:224:ILE:HD13	1.78	0.64
1:A:219:ARG:HD2	6:A:859:HOH:O	1.99	0.63
2:B:501[A]:HEM:HBC2	2:B:501[A]:HEM:CMC	2.30	0.62
1:D:195:ARG:CD	1:D:224:ILE:CD1	2.71	0.61
1:D:195:ARG:CG	1:D:224:ILE:CD1	2.78	0.61
1:D:219:ARG:CG	6:D:853:HOH:O	2.49	0.60
1:C:111:PRO:HG2	3:C:504:PYG:O1	2.01	0.60
1:D:143:PHE:CZ	3:D:504:PYG:H4	2.37	0.60
1:C:390:ASP:O	6:C:867:HOH:O	2.16	0.59
1:A:219:ARG:HD2	6:A:834:HOH:O	2.02	0.59
1:A:452:ASN:HD21	1:A:454:LYS:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ASN:HD21	1:B:454:LYS:HB3	1.67	0.58
1:A:45:HIS:HD2	6:A:686:HOH:O	1.86	0.58
1:C:181:LEU:HD21	3:C:503:PYG:C6	2.34	0.58
2:C:501[A]:HEM:HMC2	2:C:501[A]:HEM:CBC	2.34	0.57
1:C:146:MET:HE3	3:C:504:PYG:H5	1.87	0.57
1:D:234:GLU:HG2	6:D:775:HOH:O	2.04	0.57
1:D:483:ARG:O	1:D:484:SER:CB	2.50	0.57
2:D:501[A]:HEM:CMC	2:D:501[A]:HEM:HBC2	2.35	0.57
1:D:234:GLU:CG	6:D:775:HOH:O	2.52	0.56
1:A:334:GLN:HG3	6:D:884:HOH:O	2.05	0.56
2:D:502[B]:HEM:CMC	2:D:502[B]:HEM:HBC2	2.35	0.56
2:B:502[B]:HEM:HBC2	2:B:502[B]:HEM:HMC3	1.86	0.56
1:D:111:PRO:HG2	3:D:504:PYG:O1	2.05	0.55
2:D:501[A]:HEM:CMB	2:D:501[A]:HEM:HBB2	2.37	0.55
1:C:332:LEU:HD12	2:C:501[A]:HEM:HBB1	1.88	0.55
1:A:100:HIS:HE1	6:D:673:HOH:O	1.88	0.55
1:C:143:PHE:CZ	3:C:504:PYG:H4	2.42	0.55
2:A:501[A]:HEM:HMC2	2:A:501[A]:HEM:CBC	2.36	0.54
1:D:332:LEU:HD12	2:D:501[A]:HEM:HBB1	1.89	0.54
1:B:111:PRO:HG2	3:B:504:PYG:O1	2.08	0.54
2:D:501[A]:HEM:HBB2	2:D:501[A]:HEM:HMB2	1.90	0.54
6:A:803:HOH:O	1:D:100:HIS:HE1	1.92	0.53
1:A:417:GLU:HG3	1:D:28:HIS:NE2	2.24	0.52
1:A:143:PHE:CZ	3:A:504:PYG:H6	2.43	0.52
1:D:195:ARG:HG3	1:D:224:ILE:CD1	2.40	0.52
1:A:230:GLU:CG	6:A:668:HOH:O	2.58	0.51
3:A:503:PYG:O2	6:A:638:HOH:O	2.19	0.51
2:B:501[A]:HEM:HMB2	2:B:501[A]:HEM:CBB	2.39	0.51
1:A:111:PRO:HG2	3:A:504:PYG:O3	2.11	0.50
1:B:334:GLN:HG3	6:C:705:HOH:O	2.11	0.50
1:B:465:ARG:NE	6:B:929:HOH:O	2.44	0.49
6:A:978:HOH:O	1:D:334:GLN:HG3	2.12	0.49
1:B:143:PHE:CZ	3:B:504:PYG:H4	2.47	0.49
1:C:146:MET:CE	3:C:504:PYG:H5	2.43	0.49
1:A:366:ASN:HA	1:C:9[B]:LEU:HD22	1.94	0.49
1:A:219:ARG:CD	6:A:859:HOH:O	2.59	0.48
2:A:502[B]:HEM:CMB	2:A:502[B]:HEM:HBB2	2.43	0.48
1:A:412[A]:VAL:HG12	1:A:413:ARG:N	2.28	0.48
1:B:468:GLU:HG3	6:B:931:HOH:O	2.13	0.48
1:D:29:ARG:NH1	6:D:973:HOH:O	2.47	0.47
1:D:87:LYS:NZ	1:D:121:GLU:OE2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASN:CG	2:A:502[B]:HEM:HMB2	2.40	0.47
1:A:346:HIS:HE1	6:D:904:HOH:O	1.98	0.46
1:D:234:GLU:HG3	1:D:235:ILE:N	2.30	0.46
1:D:6:HIS:HA	6:D:789:HOH:O	2.14	0.46
1:D:195:ARG:HG3	1:D:224:ILE:HG12	1.97	0.46
1:A:181:LEU:HD21	3:A:503:PYG:C5	2.45	0.46
1:A:230:GLU:HG2	6:A:668:HOH:O	2.14	0.46
1:D:219:ARG:HG2	6:D:853:HOH:O	2.16	0.46
1:C:240:PHE:C	1:C:241:GLN:HG3	2.41	0.45
1:C:253:LYS:HE2	1:C:253:LYS:HB3	1.74	0.45
1:A:146:MET:HE3	3:A:504:PYG:H5	1.97	0.45
1:D:57:HIS:HA	1:D:97:THR:O	2.16	0.45
1:B:332:LEU:HD12	2:B:501[A]:HEM:HBB1	1.99	0.45
6:B:736:HOH:O	1:C:100:HIS:HE1	1.98	0.45
1:C:219:ARG:HD2	6:C:1000:HOH:O	2.16	0.45
2:A:502[B]:HEM:CMC	2:A:502[B]:HEM:CBC	2.95	0.45
2:D:501[A]:HEM:HBC2	2:D:501[A]:HEM:HMC2	1.99	0.45
1:A:72:SER:HB3	1:A:84:GLU:HA	2.00	0.44
1:A:238:ASN:ND2	6:A:1007:HOH:O	2.26	0.44
1:D:102[B]:LYS:HE3	1:D:102[B]:LYS:HB2	1.62	0.43
1:A:72:SER:OG	1:A:74:GLU:OE1	2.36	0.43
1:B:140:ALA:HA	2:B:501[A]:HEM:HBB1	2.00	0.43
6:C:1045:HOH:O	1:D:388:ARG:HD2	2.19	0.43
1:D:57:HIS:HB2	2:D:501[A]:HEM:HAD2	1.99	0.43
1:B:230:GLU:OE2	1:B:234:GLU:OE2	2.36	0.43
1:C:57:HIS:HA	1:C:97:THR:O	2.18	0.43
1:A:21:GLN:HA	1:D:142:LYS:HD3	2.01	0.42
1:D:109:ARG:NE	6:D:945:HOH:O	2.31	0.42
1:A:146:MET:CE	3:A:504:PYG:H5	2.50	0.42
1:D:483:ARG:O	1:D:484:SER:HB3	2.18	0.42
1:B:181:LEU:HD21	3:B:503:PYG:C5	2.50	0.42
1:B:272:ASP:HB2	6:B:910:HOH:O	2.18	0.42
1:C:340:TYR:HB2	1:C:341:PRO:HD3	2.01	0.42
1:B:98:VAL:HG11	3:B:504:PYG:C6	2.49	0.42
1:B:385:GLU:HA	1:B:386:PRO:C	2.45	0.41
1:A:151:LYS:O	1:A:152:PRO:C	2.61	0.41
2:C:501[A]:HEM:HBB2	2:C:501[A]:HEM:HMB2	2.02	0.41
1:A:419:PRO:O	1:A:420:ASN:C	2.63	0.41
1:D:230:GLU:CD	1:D:230:GLU:H	2.27	0.41
2:C:501[A]:HEM:HBB2	2:C:501[A]:HEM:CMB	2.51	0.41
1:D:225:ARG:HD2	6:D:961:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ALA:HB2	1:C:237:ALA:HB2	2.02	0.41
1:B:219:ARG:NH2	1:B:262:TYR:OH	2.54	0.41
1:C:271:TYR:HD1	1:C:278:PRO:HD2	1.86	0.41
2:C:502[B]:HEM:CMB	2:C:502[B]:HEM:HBB2	2.51	0.41
1:D:85:GLU:HG3	6:D:1024:HOH:O	2.19	0.41
1:A:142:LYS:HD3	1:D:21:GLN:HA	2.02	0.41
2:D:501[A]:HEM:HMC2	2:D:501[A]:HEM:CBC	2.52	0.40
2:D:502[B]:HEM:CMC	2:D:502[B]:HEM:CBC	2.99	0.40
1:D:193:GLU:HA	1:D:223:GLY:O	2.21	0.40
1:B:105:PRO:HA	1:B:240:PHE:O	2.22	0.40
1:B:347:ARG:O	1:D:372[A]:PHE:HE1	2.05	0.40
2:D:502[B]:HEM:HBC2	2:D:502[B]:HEM:HMC1	2.03	0.40
1:A:57:HIS:HA	1:A:97:THR:O	2.21	0.40

All (3) 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:B:273:GLU:OE1	1:C:417:GLU:OE2[1_455]	1.69	0.51
1:A:417:GLU:OE2	1:D:273:GLU:OE1[1_455]	2.06	0.14
1:D:225:ARG:NH1	6:B:998:HOH:O[2_655]	2.08	0.12

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	483/491 (98%)	471 (98%)	12 (2%)	0	100	100
1	B	484/491 (99%)	473 (98%)	11 (2%)	0	100	100
1	C	484/491 (99%)	471 (97%)	13 (3%)	0	100	100
1	D	484/491 (99%)	471 (97%)	12 (2%)	1 (0%)	43	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1935/1964 (98%)	1886 (98%)	48 (2%)	1 (0%)	48 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	484	SER

5.3.2 Protein sidechains ⓘ

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	426/432 (99%)	416 (98%)	10 (2%)	44 21
1	B	427/432 (99%)	417 (98%)	10 (2%)	44 21
1	C	427/432 (99%)	417 (98%)	10 (2%)	44 21
1	D	427/432 (99%)	416 (97%)	11 (3%)	40 17
All	All	1707/1728 (99%)	1666 (98%)	41 (2%)	43 20

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	120	THR
1	A	230	GLU
1	A	241	GLN
1	A	253	LYS
1	A	288	GLU
1	A	401	GLU
1	A	420	ASN
1	A	447	ASP
1	A	474	LEU
1	B	110	ASP
1	B	120	THR
1	B	219	ARG
1	B	241	GLN

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Mol	Chain	Res	Type
1	B	273	GLU
1	B	401	GLU
1	B	440	LEU
1	B	447	ASP
1	B	474	LEU
1	B	485	TYR
1	C	110	ASP
1	C	120	THR
1	C	230	GLU
1	C	241	GLN
1	C	273	GLU
1	C	401	GLU
1	C	409	ASP
1	C	420	ASN
1	C	447	ASP
1	C	485	TYR
1	D	75	LYS
1	D	110	ASP
1	D	120	THR
1	D	230	GLU
1	D	234	GLU
1	D	241	GLN
1	D	273	GLU
1	D	401	GLU
1	D	447	ASP
1	D	474	LEU
1	D	485	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	100	HIS
1	A	157	ASN
1	A	346	HIS
1	A	367	ASN
1	A	420	ASN
1	A	452	ASN
1	A	472	GLN
1	B	6	HIS
1	B	100	HIS
1	B	157	ASN

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Mol	Chain	Res	Type
1	B	346	HIS
1	B	365	HIS
1	B	398	HIS
1	B	452	ASN
1	B	472	GLN
1	C	100	HIS
1	C	157	ASN
1	C	238	ASN
1	C	241	GLN
1	C	346	HIS
1	C	365	HIS
1	C	398	HIS
1	C	407	HIS
1	C	420	ASN
1	C	472	GLN
1	D	100	HIS
1	D	157	ASN
1	D	236	GLN
1	D	346	HIS
1	D	365	HIS
1	D	367	ASN
1	D	398	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](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	501[A]	1	50,50,50	1.63	9 (18%)	67,82,82	2.21	17 (25%)
3	PYG	A	504	-	9,9,9	2.97	3 (33%)	12,12,12	1.94	3 (25%)
3	PYG	D	504	2	9,9,9	3.23	3 (33%)	12,12,12	2.97	6 (50%)
3	PYG	B	503	-	9,9,9	4.03	2 (22%)	12,12,12	2.24	4 (33%)
3	PYG	D	503	-	9,9,9	3.42	2 (22%)	12,12,12	1.71	3 (25%)
2	HEM	B	501[A]	3,1	50,50,50	1.62	12 (24%)	67,82,82	2.30	20 (29%)
2	HEM	A	502[B]	1	50,50,50	1.61	11 (22%)	67,82,82	1.93	18 (26%)
2	HEM	C	501[A]	1	50,50,50	1.50	8 (16%)	67,82,82	2.05	19 (28%)
3	PYG	A	503	-	9,9,9	3.77	2 (22%)	12,12,12	1.66	3 (25%)
2	HEM	C	502[B]	1	50,50,50	1.52	7 (14%)	67,82,82	1.84	20 (29%)
3	PYG	C	504	-	9,9,9	2.79	4 (44%)	12,12,12	2.61	3 (25%)
2	HEM	D	502[B]	1	50,50,50	1.56	9 (18%)	67,82,82	1.95	15 (22%)
2	HEM	B	502[B]	1	50,50,50	1.55	7 (14%)	67,82,82	2.01	16 (23%)
3	PYG	B	504	2	9,9,9	2.73	3 (33%)	12,12,12	3.09	6 (50%)
3	PYG	C	503	-	9,9,9	2.96	2 (22%)	12,12,12	2.34	4 (33%)
2	HEM	D	501[A]	3,1	50,50,50	1.46	5 (10%)	67,82,82	2.11	11 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	501[A]	1	-	3/14/54/54	-
3	PYG	A	504	-	-	-	0/1/1/1
3	PYG	D	504	2	-	-	0/1/1/1
3	PYG	B	503	-	-	-	0/1/1/1
3	PYG	D	503	-	-	-	0/1/1/1
2	HEM	B	501[A]	3,1	-	2/14/54/54	-
2	HEM	A	502[B]	1	-	2/14/54/54	-
2	HEM	C	501[A]	1	-	4/14/54/54	-
3	PYG	A	503	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	502[B]	1	-	2/14/54/54	-
3	PYG	C	504	-	-	-	0/1/1/1
2	HEM	D	502[B]	1	-	2/14/54/54	-
2	HEM	B	502[B]	1	-	2/14/54/54	-
3	PYG	B	504	2	-	-	0/1/1/1
3	PYG	C	503	-	-	-	0/1/1/1
2	HEM	D	501[A]	3,1	-	3/14/54/54	-

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	PYG	C3-C2	9.18	1.50	1.40
3	B	503	PYG	C3-C2	8.89	1.50	1.40
3	D	503	PYG	C3-C2	7.96	1.49	1.40
3	B	503	PYG	C1-C2	7.69	1.48	1.40
3	C	503	PYG	C3-C2	7.03	1.48	1.40
3	A	503	PYG	C1-C2	6.28	1.47	1.40
3	D	504	PYG	C1-C2	6.04	1.47	1.40
3	D	504	PYG	C3-C2	6.00	1.46	1.40
3	D	503	PYG	C1-C2	5.99	1.46	1.40
3	A	504	PYG	C3-C2	5.95	1.46	1.40
3	A	504	PYG	C1-C2	5.44	1.46	1.40
3	C	504	PYG	C1-C2	5.17	1.46	1.40
2	C	501[A]	HEM	FE-NB	5.09	2.10	1.94
3	C	504	PYG	O2-C2	-5.03	1.25	1.36
2	D	501[A]	HEM	FE-NC	5.02	2.11	1.95
2	B	502[B]	HEM	FE-NB	4.96	2.10	1.94
2	A	502[B]	HEM	FE-NB	4.87	2.09	1.94
2	C	502[B]	HEM	FE-NC	4.52	2.10	1.95
2	C	502[B]	HEM	C3C-C4C	-4.44	1.38	1.46
3	C	503	PYG	C1-C2	4.41	1.45	1.40
2	A	501[A]	HEM	FE-NC	4.41	2.09	1.95
3	B	504	PYG	C1-C2	4.41	1.45	1.40
2	A	501[A]	HEM	FE-NB	4.35	2.08	1.94
3	B	504	PYG	C3-C2	4.28	1.44	1.40
2	D	502[B]	HEM	FE-NB	4.13	2.07	1.94
2	A	501[A]	HEM	C1B-NB	-4.11	1.33	1.40
2	B	501[A]	HEM	FE-NC	4.07	2.08	1.95
2	D	501[A]	HEM	C1B-NB	-4.03	1.33	1.40
3	B	504	PYG	O2-C2	-3.99	1.27	1.36
2	A	502[B]	HEM	C1B-NB	-3.80	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501[A]	HEM	FE-NC	3.80	2.07	1.95
3	D	504	PYG	O2-C2	-3.73	1.28	1.36
2	D	502[B]	HEM	FE-NC	3.67	2.07	1.95
2	D	501[A]	HEM	FE-NB	3.53	2.05	1.94
2	C	502[B]	HEM	FE-NB	3.46	2.05	1.94
2	D	502[B]	HEM	C1B-NB	-3.40	1.34	1.40
2	B	501[A]	HEM	C1B-NB	-3.36	1.34	1.40
2	B	502[B]	HEM	FE-NC	3.36	2.06	1.95
2	B	501[A]	HEM	C4B-NB	-3.33	1.32	1.38
2	B	501[A]	HEM	FE-NB	3.33	2.05	1.94
2	D	502[B]	HEM	FE-NA	3.19	2.05	1.95
2	B	502[B]	HEM	C4B-NB	-3.14	1.32	1.38
2	A	502[B]	HEM	FE-NC	3.08	2.05	1.95
2	B	502[B]	HEM	C1B-NB	-3.02	1.35	1.40
2	C	502[B]	HEM	C4B-NB	-3.00	1.33	1.38
2	C	501[A]	HEM	C1C-C2C	-2.97	1.39	1.45
2	A	502[B]	HEM	C4D-ND	-2.95	1.35	1.40
2	A	501[A]	HEM	C4D-ND	-2.93	1.35	1.40
2	D	502[B]	HEM	CHB-C1B	2.92	1.44	1.38
3	C	504	PYG	C3-C2	2.89	1.43	1.40
2	A	502[B]	HEM	C4B-NB	-2.88	1.33	1.38
2	D	502[B]	HEM	C1C-C2C	-2.76	1.39	1.45
2	C	502[B]	HEM	C4D-C3D	2.76	1.49	1.45
2	D	501[A]	HEM	C4D-C3D	2.74	1.49	1.45
2	B	501[A]	HEM	C1C-NC	-2.69	1.34	1.39
2	A	502[B]	HEM	C1C-C2C	-2.54	1.40	1.45
2	A	502[B]	HEM	C4D-C3D	2.52	1.49	1.45
2	A	501[A]	HEM	C4B-NB	-2.52	1.33	1.38
2	A	501[A]	HEM	C1D-ND	-2.47	1.34	1.38
2	D	502[B]	HEM	C1D-ND	-2.47	1.34	1.38
2	A	501[A]	HEM	FE-NA	2.47	2.03	1.95
2	B	501[A]	HEM	C1C-C2C	-2.46	1.40	1.45
2	D	501[A]	HEM	C1C-C2C	-2.44	1.40	1.45
2	B	501[A]	HEM	C3D-C2D	-2.43	1.31	1.36
2	C	501[A]	HEM	C4D-ND	-2.39	1.36	1.40
2	C	501[A]	HEM	C1B-NB	-2.35	1.36	1.40
2	A	502[B]	HEM	FE-NA	2.34	2.02	1.95
2	C	501[A]	HEM	C3B-C4B	2.26	1.49	1.44
3	A	504	PYG	O3-C3	-2.25	1.31	1.36
2	B	501[A]	HEM	FE-NA	2.23	2.02	1.95
2	A	502[B]	HEM	O2D-CGD	-2.22	1.23	1.30
2	B	502[B]	HEM	C4D-C3D	2.22	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	HEM	O1A-CGA	2.21	1.29	1.22
2	A	502[B]	HEM	O1D-CGD	2.21	1.29	1.22
2	A	501[A]	HEM	C1C-C2C	-2.21	1.41	1.45
2	B	501[A]	HEM	C1B-C2B	-2.17	1.40	1.44
2	D	502[B]	HEM	C3C-C4C	-2.17	1.42	1.46
2	D	502[B]	HEM	C4C-NC	-2.16	1.35	1.39
2	B	501[A]	HEM	C4D-ND	-2.15	1.36	1.40
2	B	502[B]	HEM	C1C-C2C	-2.12	1.41	1.45
2	C	502[B]	HEM	C4D-ND	-2.10	1.36	1.40
2	C	501[A]	HEM	C3C-C4C	-2.09	1.42	1.46
2	C	502[B]	HEM	C1A-C2A	-2.08	1.40	1.44
2	B	501[A]	HEM	C1D-ND	-2.06	1.34	1.38
2	B	501[A]	HEM	C3C-C4C	-2.05	1.42	1.46
2	B	502[B]	HEM	O2D-CGD	-2.04	1.24	1.30
2	C	501[A]	HEM	C4D-C3D	2.02	1.48	1.45
2	A	502[B]	HEM	C1C-NC	-2.00	1.35	1.39
3	C	504	PYG	O3-C3	2.00	1.40	1.36

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501[A]	HEM	CHC-C4B-NB	7.92	132.95	124.42
2	A	501[A]	HEM	CHC-C4B-NB	7.49	132.49	124.42
3	D	504	PYG	C4-C3-C2	-7.04	112.79	120.09
2	D	501[A]	HEM	CHD-C1D-ND	6.99	131.95	124.42
3	B	504	PYG	C4-C3-C2	-6.98	112.85	120.09
2	B	501[A]	HEM	C1B-NB-C4B	6.71	113.16	105.21
2	B	501[A]	HEM	C3B-C4B-NB	-6.71	104.65	109.47
2	C	501[A]	HEM	CHC-C4B-NB	6.51	131.42	124.42
2	A	501[A]	HEM	C3B-C4B-NB	-6.29	104.95	109.47
2	A	501[A]	HEM	C1B-NB-C4B	6.18	112.52	105.21
2	D	502[B]	HEM	CHD-C1D-ND	6.03	130.91	124.42
2	B	501[A]	HEM	CHC-C4B-NB	5.84	130.71	124.42
2	D	501[A]	HEM	CHD-C1D-C2D	-5.82	115.85	125.03
2	B	501[A]	HEM	CHD-C1D-ND	5.80	130.67	124.42
2	B	501[A]	HEM	CHB-C1B-NB	5.78	131.52	124.37
2	B	502[B]	HEM	CHC-C4B-NB	5.67	130.52	124.42
2	B	502[B]	HEM	CHD-C4C-NC	5.64	130.59	124.45
2	D	501[A]	HEM	C1B-NB-C4B	5.54	111.76	105.21
2	D	501[A]	HEM	C3B-C4B-NB	-5.51	105.51	109.47
2	B	502[B]	HEM	C1B-NB-C4B	5.43	111.64	105.21
3	C	504	PYG	C4-C3-C2	-5.41	114.48	120.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502[B]	HEM	CHD-C1D-C2D	-5.36	116.57	125.03
2	C	502[B]	HEM	CHC-C4B-NB	5.35	130.18	124.42
2	D	502[B]	HEM	C1B-NB-C4B	5.18	111.34	105.21
2	A	501[A]	HEM	CHD-C1D-ND	5.08	129.89	124.42
3	C	504	PYG	C3-C2-C1	5.02	122.64	119.53
3	B	503	PYG	C6-C1-C2	-4.99	114.92	120.09
2	A	501[A]	HEM	CHB-C1B-NB	4.93	130.46	124.37
2	A	502[B]	HEM	CHC-C1C-NC	4.86	129.75	124.45
2	B	501[A]	HEM	CHA-C4D-ND	4.74	130.22	124.37
3	B	504	PYG	C3-C2-C1	4.70	122.44	119.53
2	A	502[B]	HEM	C1B-NB-C4B	4.65	110.72	105.21
3	C	503	PYG	C6-C1-C2	-4.55	115.37	120.09
2	A	501[A]	HEM	CHA-C4D-ND	4.37	129.78	124.37
2	D	502[B]	HEM	CHC-C4B-NB	4.37	129.12	124.42
2	C	501[A]	HEM	CHD-C1D-ND	4.37	129.12	124.42
2	C	502[B]	HEM	C1B-NB-C4B	4.34	110.35	105.21
2	A	502[B]	HEM	CHB-C1B-NB	4.28	129.67	124.37
3	D	504	PYG	C3-C2-C1	4.27	122.18	119.53
2	B	501[A]	HEM	CAD-C3D-C4D	4.16	131.95	124.70
2	C	501[A]	HEM	C1B-NB-C4B	4.10	110.06	105.21
2	B	502[B]	HEM	CHA-C4D-ND	4.08	129.41	124.37
3	A	504	PYG	C5-C6-C1	4.02	125.01	120.05
2	A	502[B]	HEM	CHC-C4B-NB	4.02	128.75	124.42
3	B	504	PYG	C5-C4-C3	3.98	124.96	120.05
2	D	502[B]	HEM	CHB-C1B-NB	3.92	129.22	124.37
3	B	503	PYG	O1-C1-C2	3.79	127.64	117.90
3	A	504	PYG	C6-C1-C2	-3.74	116.21	120.09
2	A	502[B]	HEM	CHA-C4D-C3D	-3.72	118.37	125.23
2	D	502[B]	HEM	CMB-C2B-C1B	-3.70	119.25	125.03
3	D	503	PYG	C6-C1-C2	-3.69	116.26	120.09
2	C	501[A]	HEM	CMB-C2B-C1B	3.60	130.66	125.03
2	B	502[B]	HEM	C4C-NC-C1C	3.58	111.66	105.82
2	A	502[B]	HEM	C4C-NC-C1C	3.56	111.63	105.82
2	A	502[B]	HEM	CHA-C4D-ND	3.56	128.77	124.37
2	B	501[A]	HEM	CHD-C1D-C2D	-3.55	119.43	125.03
2	C	502[B]	HEM	CMA-C3A-C4A	3.54	130.81	125.42
3	C	503	PYG	C3-C2-C1	3.54	121.72	119.53
2	B	501[A]	HEM	C1A-CHA-C4D	-3.53	117.95	126.25
2	B	502[B]	HEM	CHA-C4D-C3D	-3.52	118.73	125.23
3	D	504	PYG	C5-C4-C3	3.47	124.34	120.05
2	C	501[A]	HEM	C3B-C2B-C1B	3.44	108.99	106.41
3	B	504	PYG	O3-C3-C4	3.42	128.54	119.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501[A]	HEM	CAD-C3D-C4D	3.42	130.66	124.70
2	C	501[A]	HEM	CAD-CBD-CGD	-3.37	104.72	113.67
2	B	502[B]	HEM	C1A-CHA-C4D	-3.36	118.34	126.25
2	B	501[A]	HEM	CHA-C4D-C3D	-3.35	119.05	125.23
2	C	501[A]	HEM	CMB-C2B-C3B	-3.34	120.34	128.43
3	C	504	PYG	O3-C3-C4	3.30	128.21	119.36
2	A	502[B]	HEM	C3B-C4B-NB	-3.25	107.14	109.47
2	B	502[B]	HEM	C4C-C3C-C2C	3.23	109.62	106.81
2	C	502[B]	HEM	CHD-C1D-ND	3.22	127.89	124.42
2	A	502[B]	HEM	CHD-C4C-NC	3.17	127.91	124.45
2	C	501[A]	HEM	C4B-C3B-C2B	-3.09	104.44	107.28
2	A	501[A]	HEM	CHD-C1D-C2D	-3.09	120.15	125.03
3	C	503	PYG	C6-C5-C4	3.08	124.20	120.24
2	C	502[B]	HEM	C4C-C3C-C2C	3.07	109.48	106.81
2	C	501[A]	HEM	CMC-C2C-C1C	3.03	130.07	124.73
3	C	503	PYG	O1-C1-C2	3.03	125.69	117.90
2	C	501[A]	HEM	O1D-CGD-CBD	-3.01	113.55	123.09
3	B	503	PYG	C5-C6-C1	2.99	123.74	120.05
2	C	501[A]	HEM	CHA-C4D-ND	2.99	128.06	124.37
2	A	501[A]	HEM	C1C-CHC-C4B	-2.99	119.67	126.02
3	D	503	PYG	O1-C1-C2	2.98	125.57	117.90
2	C	501[A]	HEM	C4C-C3C-C2C	2.97	109.39	106.81
2	C	502[B]	HEM	CHA-C1A-NA	2.94	129.20	123.86
3	D	504	PYG	O3-C3-C4	2.94	127.25	119.36
2	D	502[B]	HEM	C3B-C4B-NB	-2.89	107.39	109.47
3	A	503	PYG	C3-C2-C1	-2.86	117.76	119.53
2	B	501[A]	HEM	CAD-C3D-C2D	-2.85	122.52	127.87
2	D	502[B]	HEM	CAA-CBA-CGA	-2.85	106.12	113.67
2	C	502[B]	HEM	CAD-CBD-CGD	2.83	121.18	113.67
3	D	504	PYG	C5-C6-C1	-2.81	116.57	120.05
2	C	502[B]	HEM	C2A-C1A-NA	-2.81	107.04	110.15
2	C	502[B]	HEM	CBD-CAD-C3D	-2.79	104.81	112.53
2	B	502[B]	HEM	C2D-C1D-ND	2.79	113.13	109.90
2	B	501[A]	HEM	O2A-CGA-CBA	2.79	122.80	114.00
2	B	502[B]	HEM	CMC-C2C-C1C	2.78	129.62	124.73
2	A	501[A]	HEM	C4C-NC-C1C	2.76	110.33	105.82
2	C	502[B]	HEM	CHD-C1D-C2D	-2.76	120.67	125.03
2	B	502[B]	HEM	C3B-C4B-NB	-2.75	107.50	109.47
2	C	501[A]	HEM	O2D-CGD-CBD	2.74	122.66	114.00
2	A	501[A]	HEM	CBB-CAB-C3B	-2.74	113.84	127.53
2	A	501[A]	HEM	CHA-C4D-C3D	-2.71	120.22	125.23
2	C	501[A]	HEM	CBA-CAA-C2A	-2.70	105.07	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502[B]	HEM	CHD-C1D-ND	2.70	127.33	124.42
2	D	502[B]	HEM	CBD-CAD-C3D	-2.66	105.17	112.53
2	C	501[A]	HEM	CHD-C1D-C2D	-2.64	120.86	125.03
2	A	502[B]	HEM	CAA-C2A-C1A	2.63	130.08	124.94
2	C	502[B]	HEM	C3C-C2C-C1C	-2.62	104.56	107.05
2	C	501[A]	HEM	CMA-C3A-C2A	2.62	131.18	125.62
2	C	502[B]	HEM	O2D-CGD-CBD	2.62	122.27	114.00
2	C	502[B]	HEM	CHB-C1B-NB	2.61	127.59	124.37
2	B	502[B]	HEM	CBD-CAD-C3D	-2.59	105.37	112.53
3	A	503	PYG	O3-C3-C2	2.59	124.56	117.90
2	A	501[A]	HEM	CHD-C4C-NC	2.57	127.25	124.45
3	A	503	PYG	O1-C1-C2	2.57	124.50	117.90
2	B	501[A]	HEM	CHD-C4C-NC	2.55	127.23	124.45
2	A	501[A]	HEM	C1A-CHA-C4D	-2.50	120.36	126.25
2	A	502[B]	HEM	CHD-C1D-C2D	-2.48	121.12	125.03
2	D	502[B]	HEM	C2B-C1B-NB	-2.47	107.00	109.84
2	A	502[B]	HEM	C3D-C4D-ND	2.45	112.86	110.17
2	A	501[A]	HEM	CHC-C1C-NC	2.44	127.11	124.45
2	C	502[B]	HEM	C3A-C4A-NA	-2.43	106.24	110.14
2	D	502[B]	HEM	O2D-CGD-CBD	2.40	121.59	114.00
3	A	504	PYG	C3-C2-C1	-2.40	118.05	119.53
2	D	501[A]	HEM	CAD-CBD-CGD	-2.40	107.31	113.67
2	C	501[A]	HEM	CHC-C4B-C3B	-2.40	120.29	125.07
2	C	502[B]	HEM	C3B-C4B-NB	-2.39	107.75	109.47
2	B	502[B]	HEM	CBC-CAC-C3C	-2.38	115.63	127.53
3	B	504	PYG	O1-C1-C6	2.37	125.73	119.36
2	C	502[B]	HEM	CMA-C3A-C2A	-2.36	120.61	125.62
2	D	501[A]	HEM	O2A-CGA-CBA	2.36	121.44	114.00
2	B	501[A]	HEM	CAD-CBD-CGD	-2.35	107.43	113.67
2	D	502[B]	HEM	C4A-C3A-C2A	2.33	109.48	106.82
2	A	502[B]	HEM	CBB-CAB-C3B	-2.31	115.96	127.53
2	A	501[A]	HEM	O1D-CGD-CBD	-2.31	115.76	123.09
2	C	502[B]	HEM	C4C-NC-C1C	2.31	109.58	105.82
2	C	502[B]	HEM	C1A-CHA-C4D	-2.30	120.83	126.25
2	B	501[A]	HEM	CHC-C1C-NC	2.30	126.95	124.45
2	C	502[B]	HEM	O2A-CGA-CBA	2.30	121.25	114.00
2	A	501[A]	HEM	C4C-C3C-C2C	2.29	108.80	106.81
2	B	501[A]	HEM	C4C-CHD-C1D	-2.29	121.16	126.02
2	D	501[A]	HEM	CBA-CAA-C2A	-2.29	106.21	112.53
2	B	501[A]	HEM	C4C-NC-C1C	2.27	109.52	105.82
2	C	501[A]	HEM	CAD-C3D-C2D	-2.26	123.64	127.87
2	D	502[B]	HEM	C2D-C1D-ND	2.25	112.51	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502[B]	HEM	CAD-CBD-CGD	2.25	119.64	113.67
3	D	504	PYG	C6-C5-C4	2.25	123.13	120.24
2	D	501[A]	HEM	CMC-C2C-C1C	2.24	128.67	124.73
2	B	502[B]	HEM	C2B-C1B-NB	-2.24	107.27	109.84
2	D	501[A]	HEM	C4C-CHD-C1D	-2.20	121.34	126.02
2	B	501[A]	HEM	O2A-CGA-O1A	-2.20	117.68	123.33
2	A	501[A]	HEM	C4D-ND-C1D	2.16	107.77	105.21
2	A	502[B]	HEM	C4C-CHD-C1D	-2.15	121.44	126.02
2	B	501[A]	HEM	C2B-C1B-NB	-2.12	107.40	109.84
2	B	502[B]	HEM	CHB-C1B-NB	2.12	126.99	124.37
3	B	504	PYG	C5-C6-C1	-2.10	117.45	120.05
3	D	503	PYG	C5-C6-C1	2.10	122.64	120.05
2	D	502[B]	HEM	C4C-CHD-C1D	-2.09	121.57	126.02
2	A	502[B]	HEM	O2D-CGD-O1D	-2.09	117.95	123.33
2	D	502[B]	HEM	CHD-C4C-NC	2.08	126.72	124.45
3	B	503	PYG	C6-C5-C4	2.08	122.92	120.24
2	B	501[A]	HEM	CHB-C1B-C2B	-2.08	121.05	126.95
2	D	501[A]	HEM	CHB-C1B-NB	2.04	126.89	124.37
2	A	502[B]	HEM	O2D-CGD-CBD	2.03	120.41	114.00
2	C	502[B]	HEM	C4A-NA-C1A	2.03	109.13	105.82
2	B	502[B]	HEM	CMC-C2C-C3C	-2.03	123.52	128.43

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	502[B]	HEM	CAA-CBA-CGA-O2A
2	B	501[A]	HEM	CAD-CBD-CGD-O1D
2	B	502[B]	HEM	CAA-CBA-CGA-O1A
2	D	502[B]	HEM	CAA-CBA-CGA-O2A
2	A	501[A]	HEM	CAD-CBD-CGD-O1D
2	B	502[B]	HEM	CAA-CBA-CGA-O2A
2	A	501[A]	HEM	CAD-CBD-CGD-O2D
2	B	501[A]	HEM	CAD-CBD-CGD-O2D
2	C	502[B]	HEM	CAA-CBA-CGA-O1A
2	D	502[B]	HEM	CAA-CBA-CGA-O1A
2	A	502[B]	HEM	CAA-CBA-CGA-O1A
2	C	501[A]	HEM	CAD-CBD-CGD-O2D
2	A	502[B]	HEM	CAA-CBA-CGA-O2A
2	D	501[A]	HEM	CAD-CBD-CGD-O2D
2	C	501[A]	HEM	CAD-CBD-CGD-O1D
2	D	501[A]	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	D	501[A]	HEM	CAA-CBA-CGA-O2A
2	C	501[A]	HEM	CAA-CBA-CGA-O2A
2	A	501[A]	HEM	CAA-CBA-CGA-O2A
2	C	501[A]	HEM	CAA-CBA-CGA-O1A

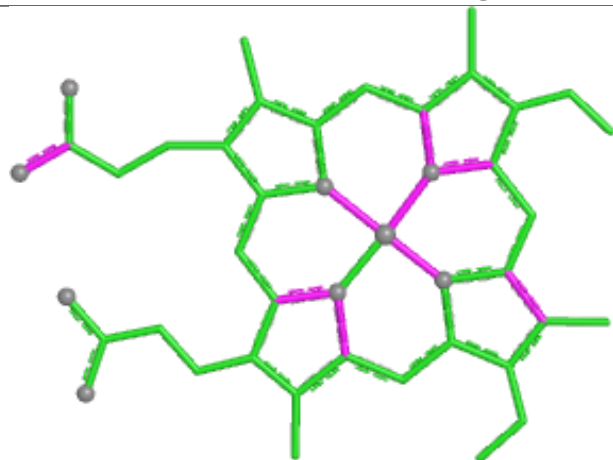
There are no ring outliers.

16 monomers are involved in 59 short contacts:

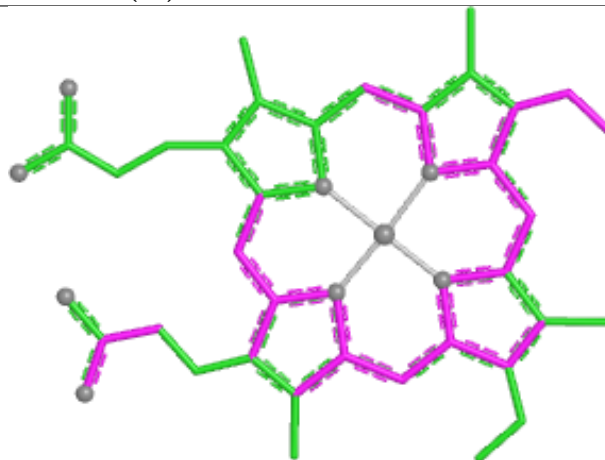
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501[A]	HEM	6	0
3	A	504	PYG	4	0
3	D	504	PYG	2	0
3	B	503	PYG	2	0
3	D	503	PYG	1	0
2	B	501[A]	HEM	7	0
2	A	502[B]	HEM	5	0
2	C	501[A]	HEM	6	0
3	A	503	PYG	3	0
2	C	502[B]	HEM	1	0
3	C	504	PYG	4	0
2	D	502[B]	HEM	3	0
2	B	502[B]	HEM	4	0
3	B	504	PYG	3	0
3	C	503	PYG	1	0
2	D	501[A]	HEM	7	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

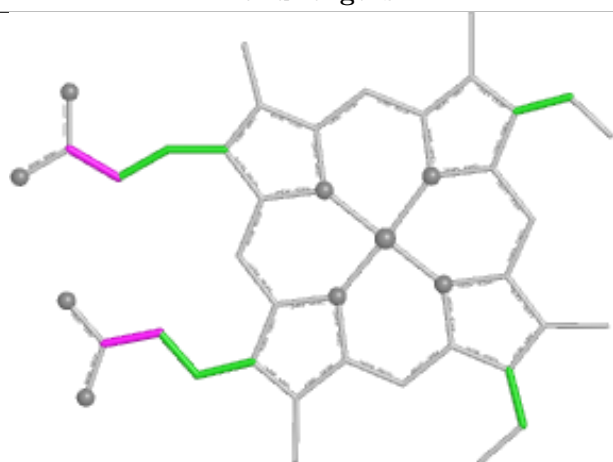
Ligand HEM A 501 (A)



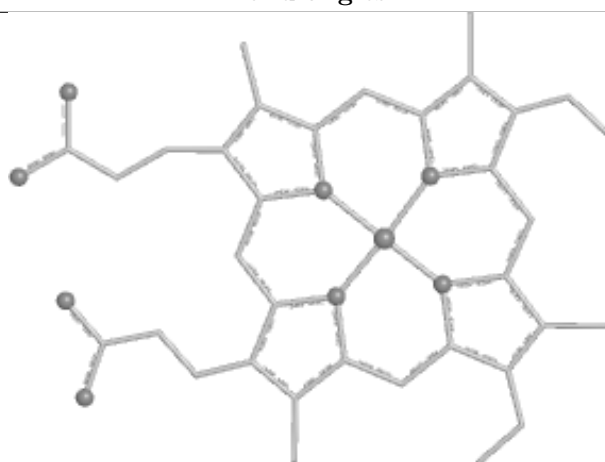
Bond lengths



Bond angles

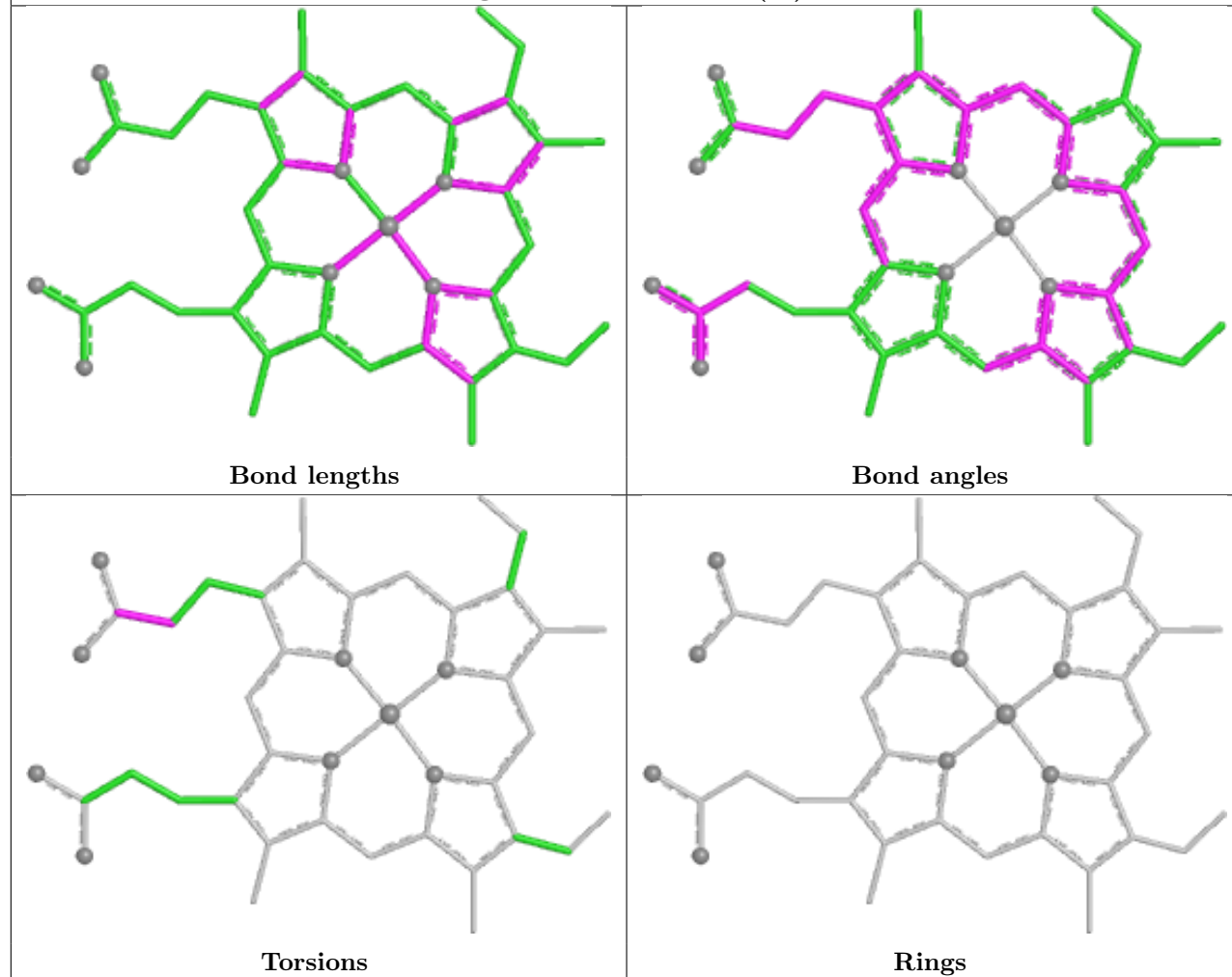


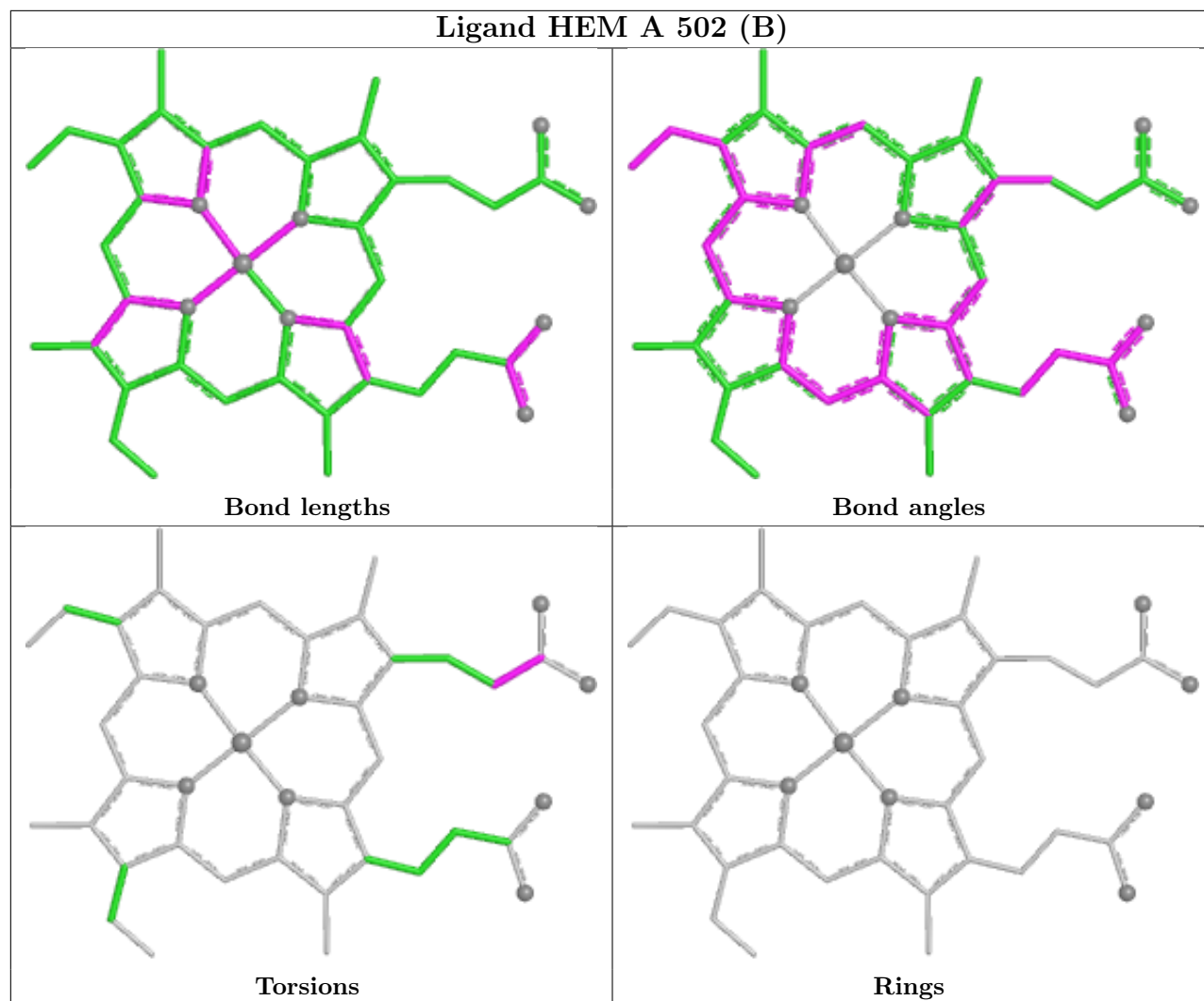
Torsions



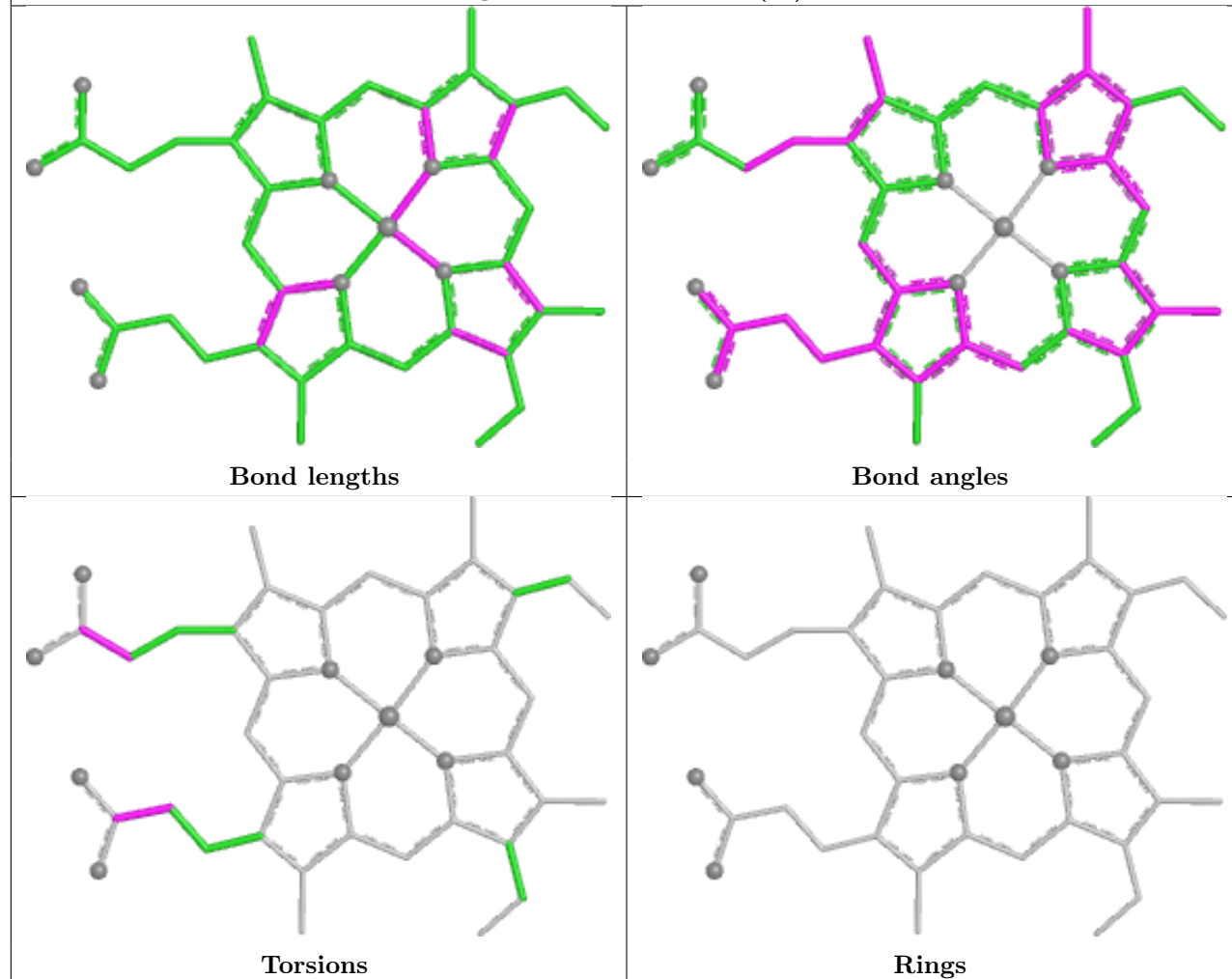
Rings

Ligand HEM B 501 (A)

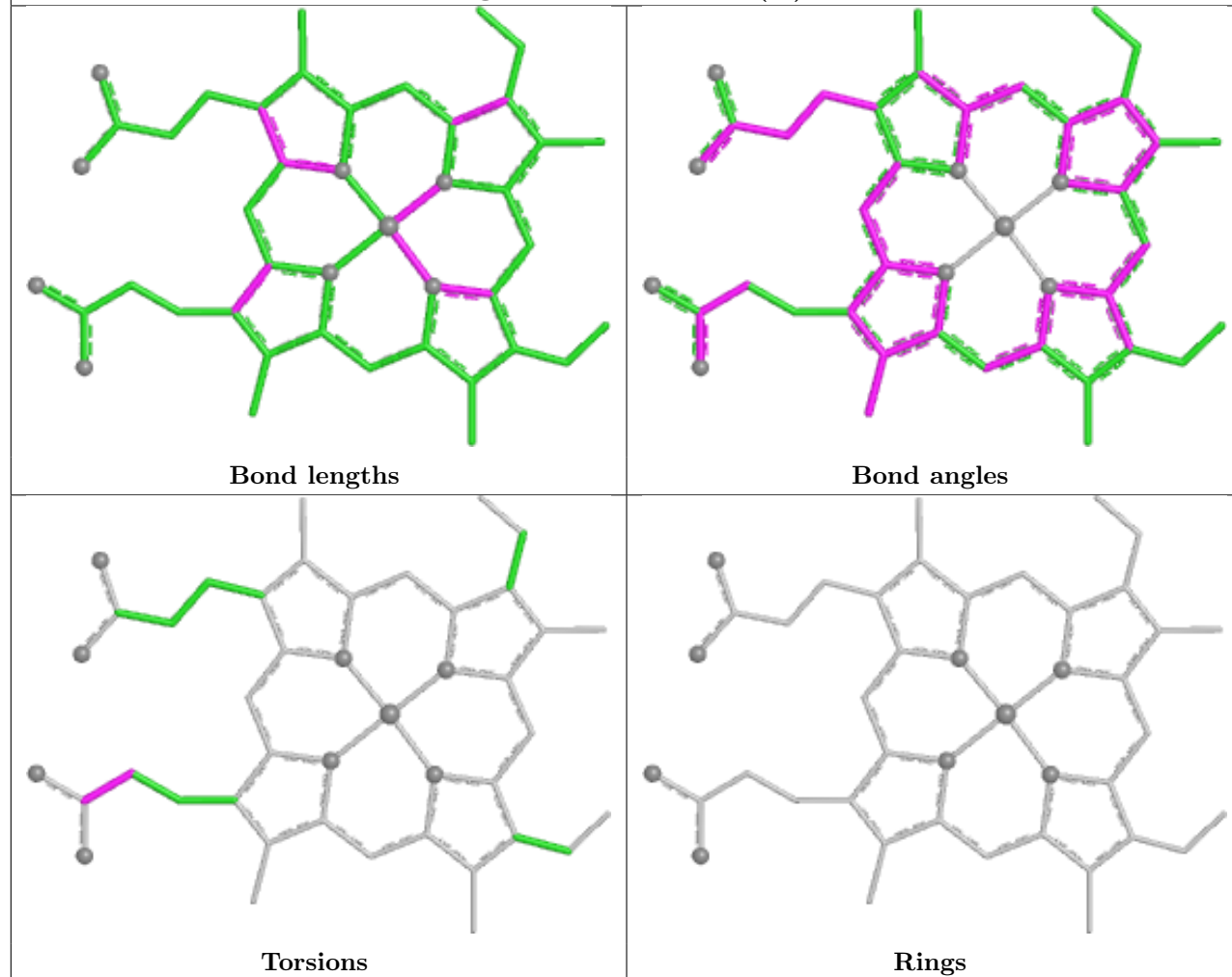




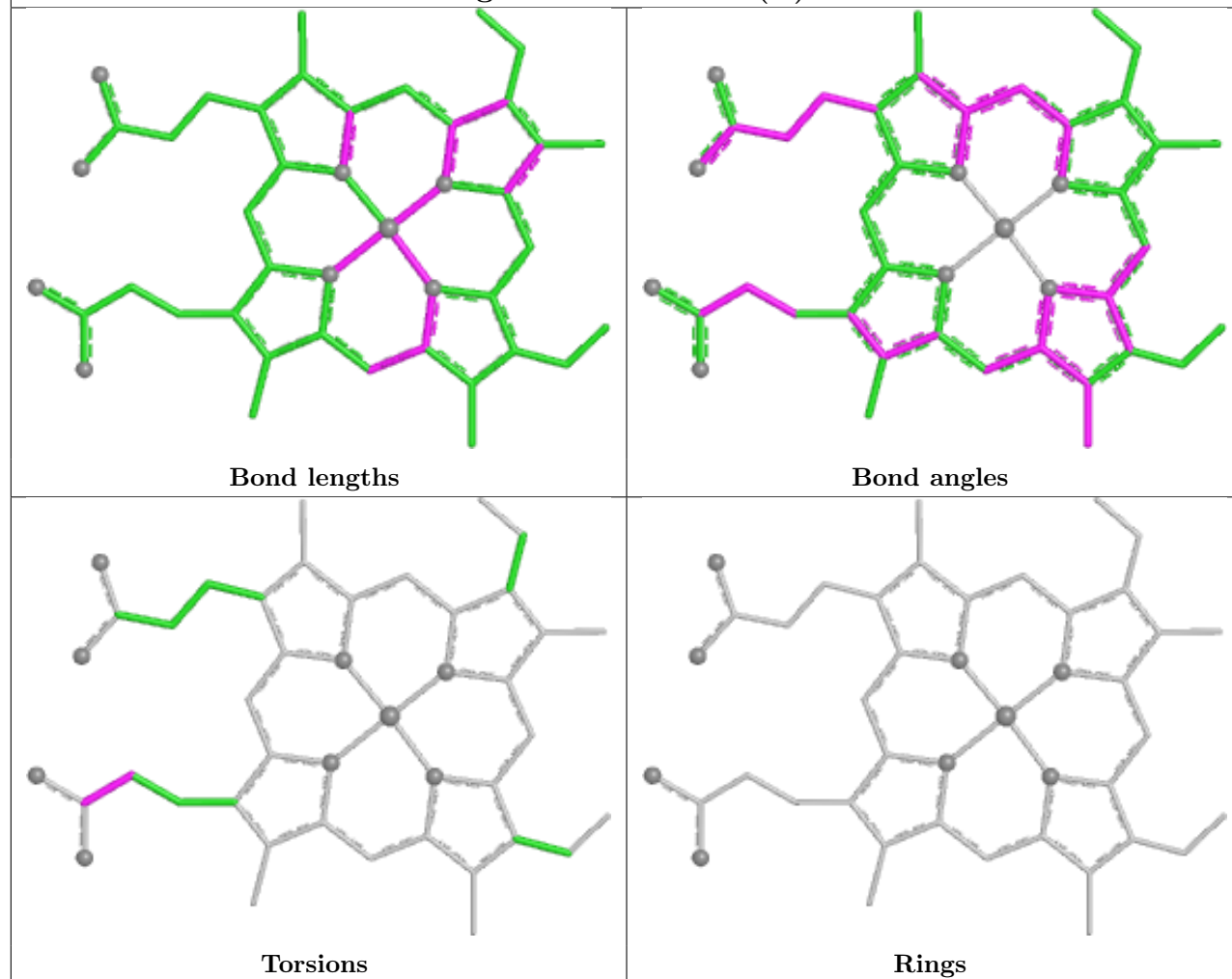
Ligand HEM C 501 (A)



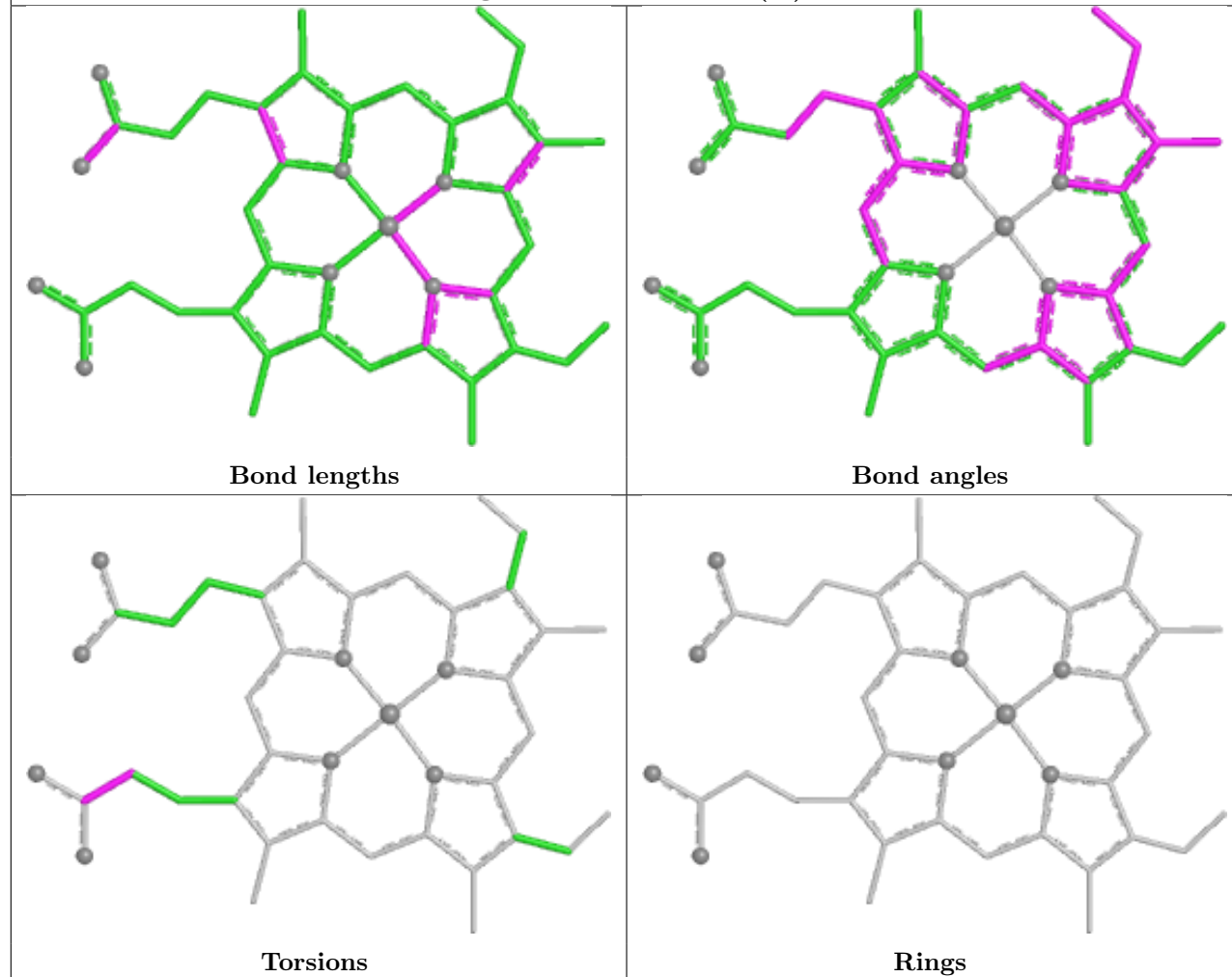
Ligand HEM C 502 (B)

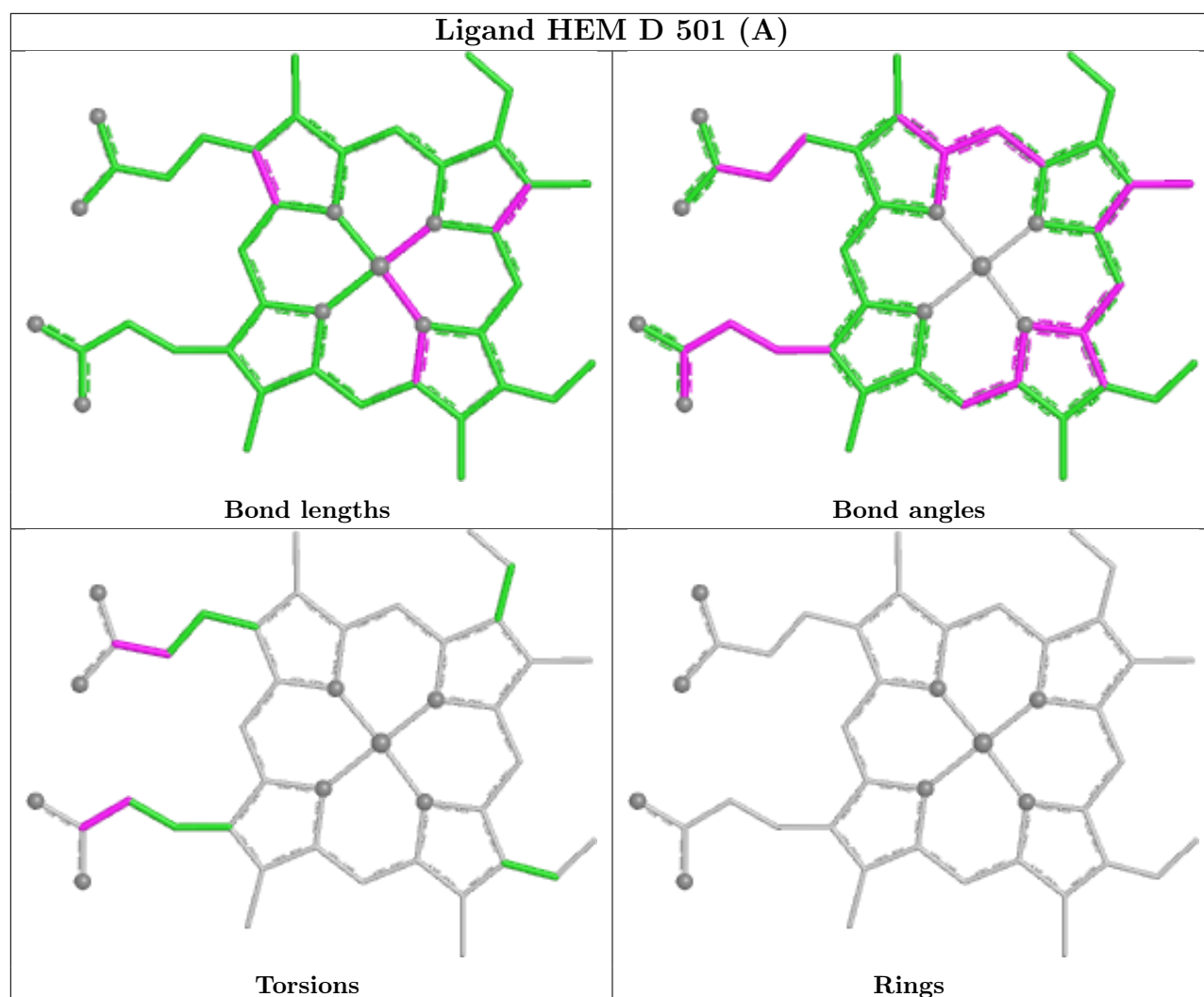


Ligand HEM D 502 (B)



Ligand HEM B 502 (B)





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	480/491 (97%)	0.26	10 (2%) 63 69	9, 23, 39, 64	5 (1%)
1	B	480/491 (97%)	0.05	6 (1%) 75 80	9, 20, 36, 60	6 (1%)
1	C	480/491 (97%)	-0.01	12 (2%) 58 64	8, 18, 34, 70	6 (1%)
1	D	480/491 (97%)	0.12	12 (2%) 58 64	7, 21, 36, 80	6 (1%)
All	All	1920/1964 (97%)	0.11	40 (2%) 63 69	7, 21, 36, 80	23 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	485	TYR	5.2
1	D	485	TYR	4.5
1	C	485	TYR	4.0
1	D	484	SER	4.0
1	B	485	TYR	3.8
1	B	6	HIS	3.7
1	C	6	HIS	3.6
1	A	484	SER	3.4
1	D	6	HIS	3.1
1	A	407	HIS	2.9
1	B	407	HIS	2.7
1	D	85	GLU	2.6
1	A	468	GLU	2.6
1	D	407	HIS	2.6
1	B	468	GLU	2.6
1	C	408	GLY	2.5
1	A	479	GLY	2.5
1	D	408	GLY	2.5
1	A	409	ASP	2.4
1	C	391	ASP	2.4
1	C	398	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	271	TYR	2.4
1	C	407	HIS	2.4
1	C	238	ASN	2.3
1	C	28	HIS	2.2
1	A	273	GLU	2.2
1	A	408	GLY	2.2
1	D	223	GLY	2.2
1	D	225	ARG	2.2
1	D	398	HIS	2.2
1	C	75	LYS	2.2
1	D	481	ASP	2.1
1	A	84	GLU	2.1
1	C	225	ARG	2.1
1	B	409	ASP	2.1
1	D	224	ILE	2.1
1	C	484	SER	2.1
1	D	391	ASP	2.1
1	B	477	SER	2.0
1	C	409	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PYG	A	503	9/9	0.84	0.12	40,42,45,48	0
3	PYG	C	503	9/9	0.84	0.13	31,33,36,39	0
3	PYG	D	503	9/9	0.84	0.14	33,35,39,41	0
3	PYG	A	504	9/9	0.90	0.11	27,34,35,36	0

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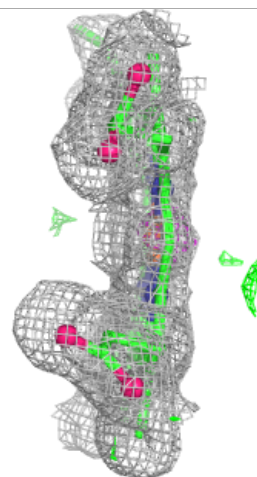
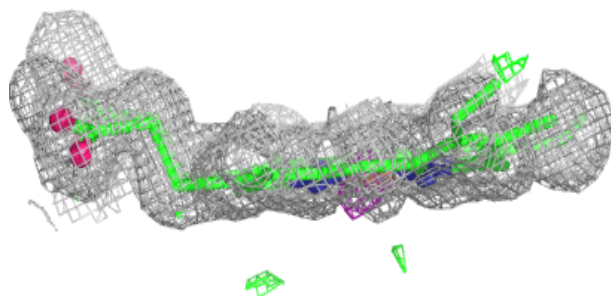
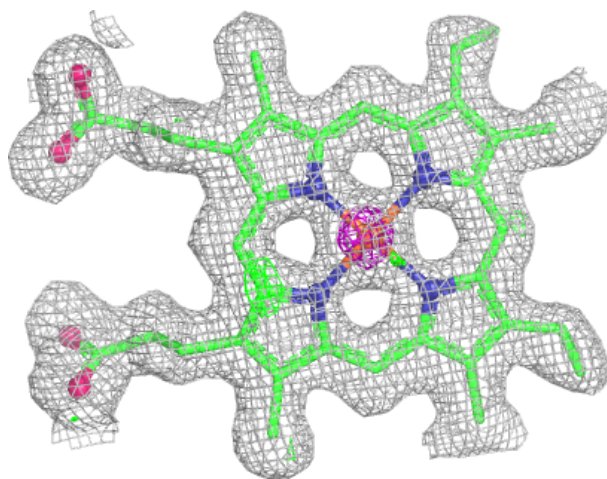
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PYG	B	504	9/9	0.90	0.12	27,31,35,35	0
3	PYG	B	503	9/9	0.91	0.11	34,39,44,50	0
3	PYG	D	504	9/9	0.91	0.10	21,32,37,38	0
3	PYG	C	504	9/9	0.93	0.09	20,28,31,32	0
2	HEM	B	501[A]	43/43	0.95	0.09	14,17,19,23	43
2	HEM	D	501[A]	43/43	0.95	0.08	14,16,19,23	43
2	HEM	A	501[A]	43/43	0.96	0.08	13,15,17,18	43
2	HEM	A	502[B]	43/43	0.96	0.09	15,16,18,20	43
5	NA	B	506	1/1	0.96	0.06	23,23,23,23	0
2	HEM	C	501[A]	43/43	0.97	0.07	11,13,14,17	43
2	HEM	C	502[B]	43/43	0.97	0.06	10,12,13,13	43
2	HEM	D	502[B]	43/43	0.98	0.06	11,12,13,13	43
4	CL	A	505	1/1	0.98	0.04	23,23,23,23	0
4	CL	C	505	1/1	0.98	0.05	23,23,23,23	0
2	HEM	B	502[B]	43/43	0.98	0.07	10,12,14,14	43
4	CL	A	506	1/1	0.99	0.03	19,19,19,19	0
4	CL	C	506	1/1	0.99	0.04	19,19,19,19	0
4	CL	D	505	1/1	0.99	0.03	18,18,18,18	0
5	NA	A	507	1/1	0.99	0.02	14,14,14,14	0
4	CL	B	505	1/1	0.99	0.03	19,19,19,19	0

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

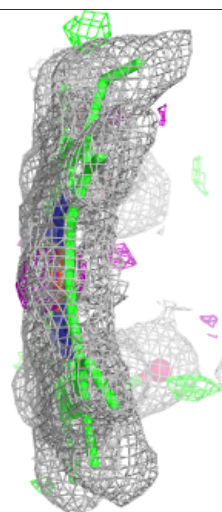
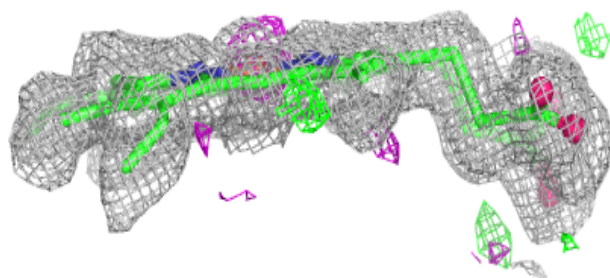
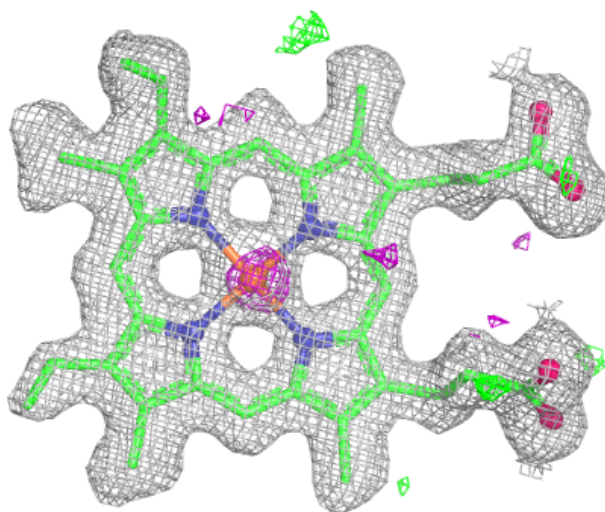
Electron density around HEM B 501 (A):

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



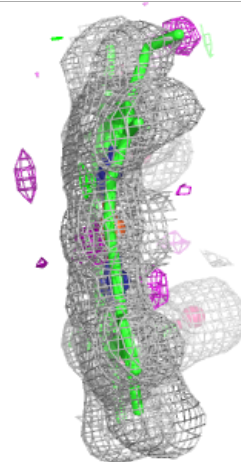
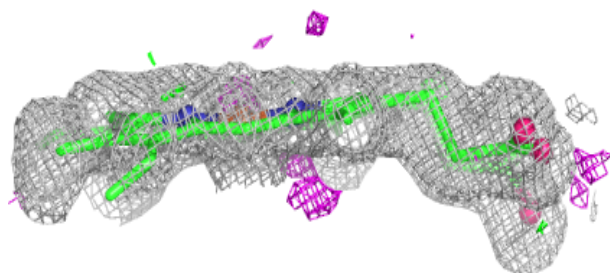
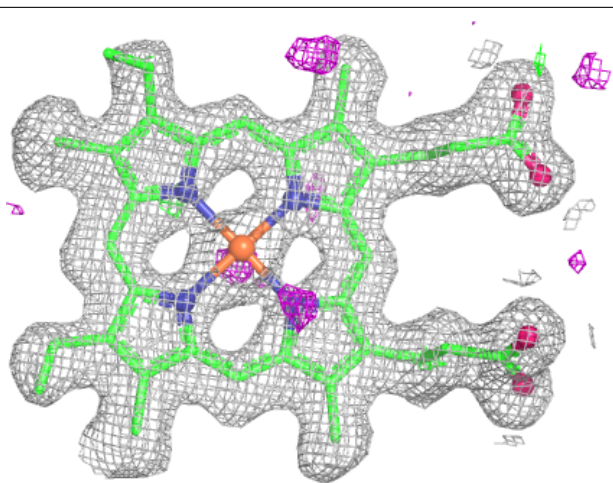
Electron density around HEM D 501 (A):

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



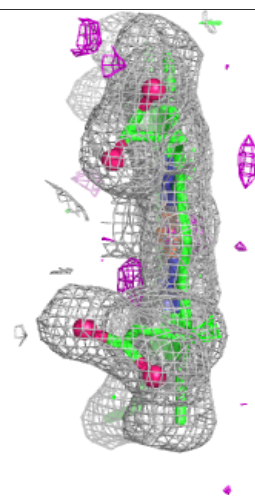
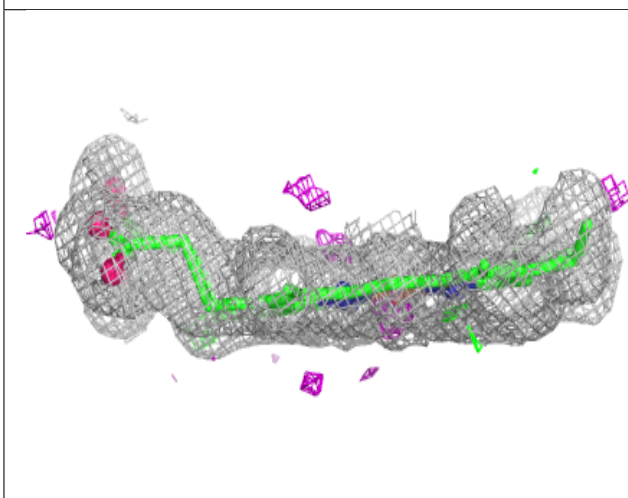
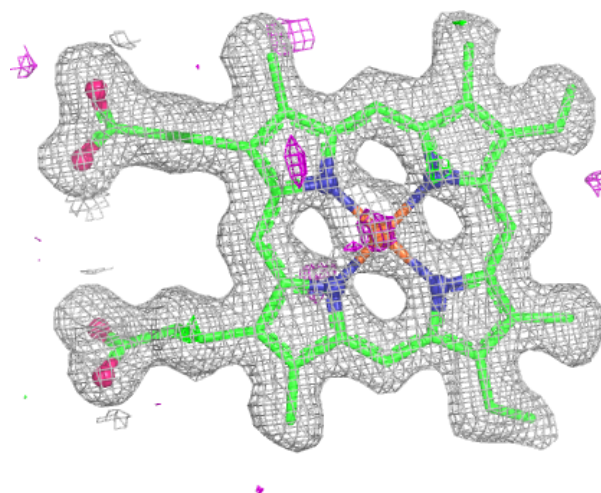
Electron density around HEM A 501 (A):

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



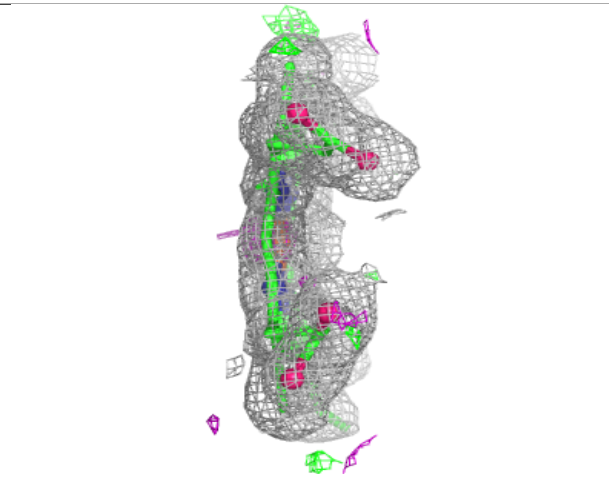
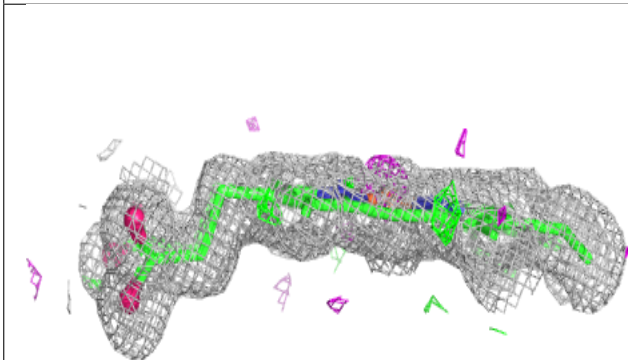
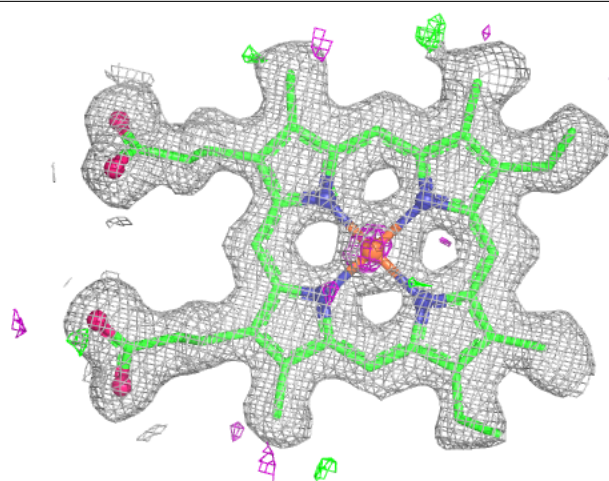
Electron density around HEM A 502 (B):

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



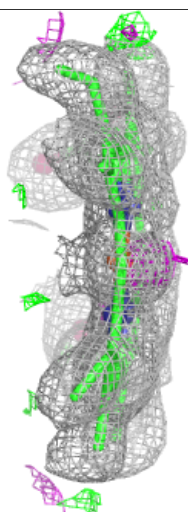
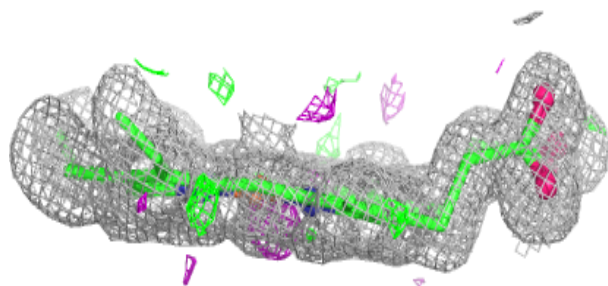
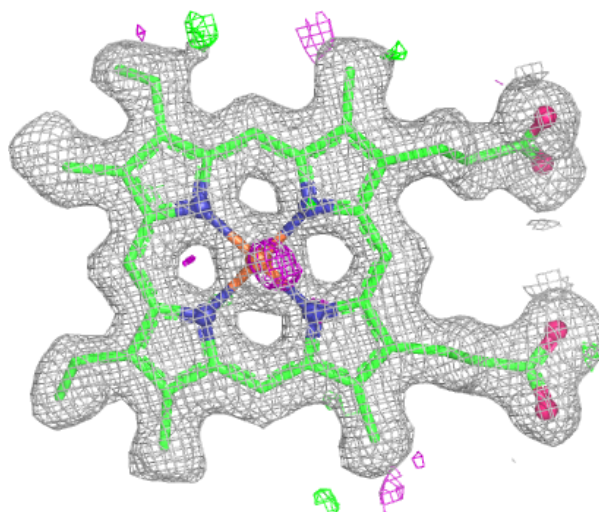
Electron density around HEM C 501 (A):

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



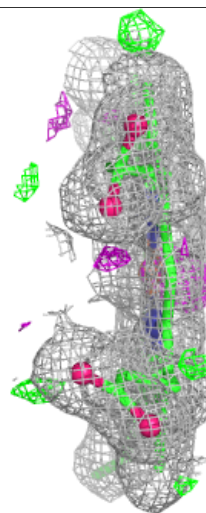
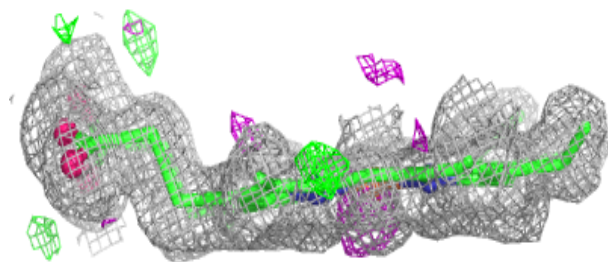
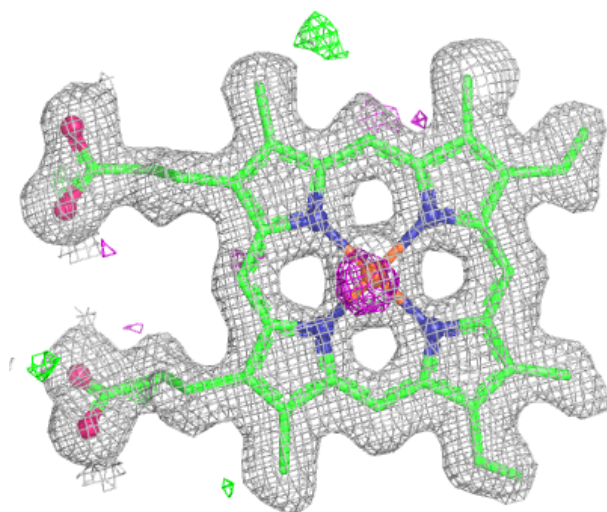
Electron density around HEM C 502 (B):

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



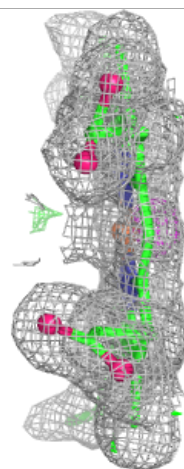
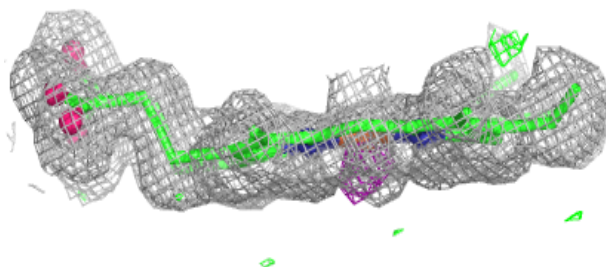
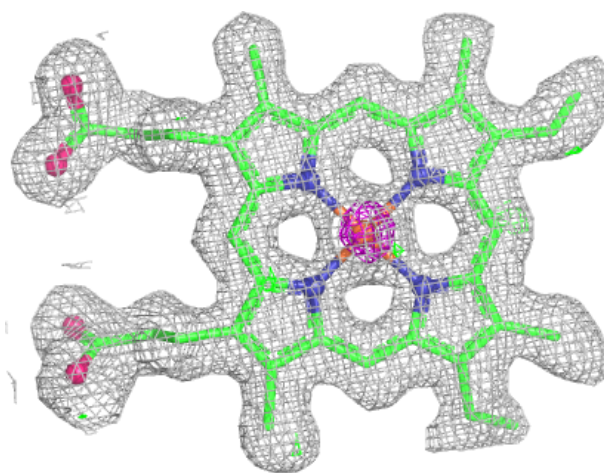
Electron density around HEM D 502 (B):

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



Electron density around HEM B 502 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.