Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 06:34 am GMT

PDB ID	:	4V3U
Title	:	Structure of human nNOS R354A G357D mutant heme domain in complex with N-2-(2-(1H-imidazol-1-yl)pyrimidin-4-yl)ethyl-3-(pyridin-3-yl) propan-1-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2014-10-20
Resolution	:	2.30 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

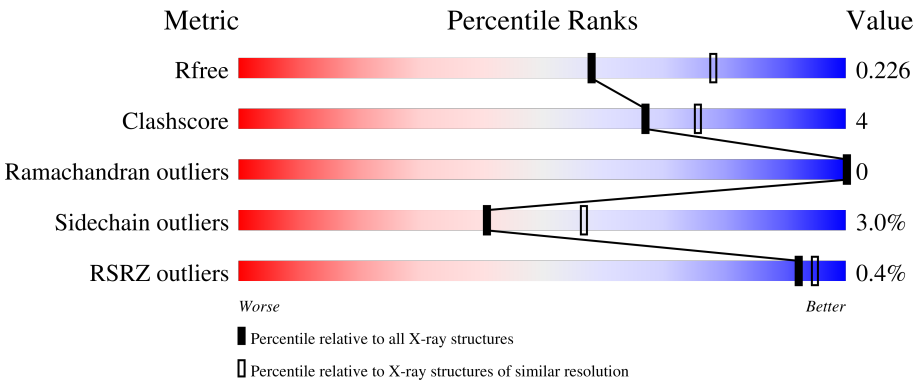
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	420	90% 10%
1	B	420	85% 13% •
1	C	420	89% 10%
1	D	420	% 83% 13% • •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14827 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.

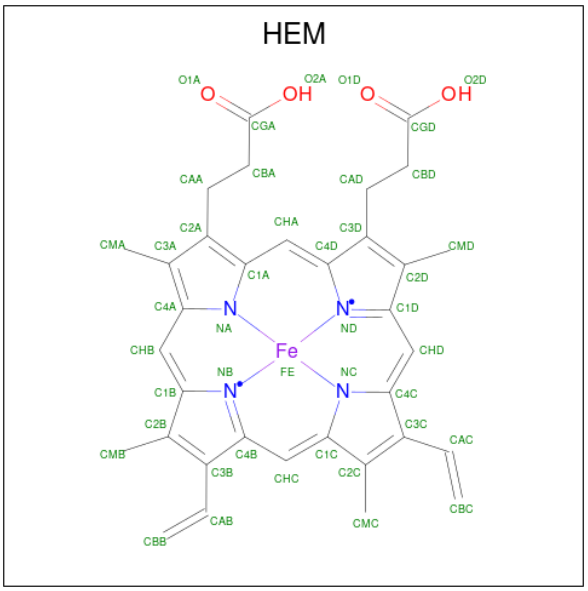
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, BRAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	3424	2188	589	625	22	0	0	0
1	B	411	3351	2147	571	611	22	0	1	0
1	C	420	3424	2188	589	625	22	0	0	0
1	D	411	3362	2154	574	612	22	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

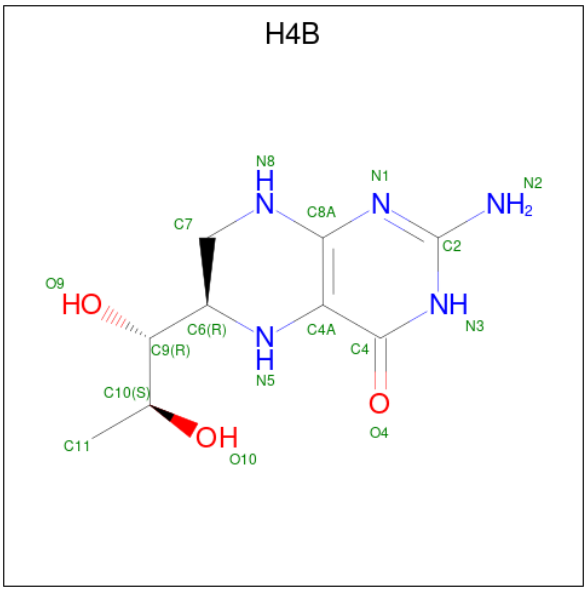
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475
C	354	ALA	ARG	engineered mutation	UNP P29475
C	357	ASP	GLY	engineered mutation	UNP P29475
D	354	ALA	ARG	engineered mutation	UNP P29475
D	357	ASP	GLY	engineered mutation	UNP P29475

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



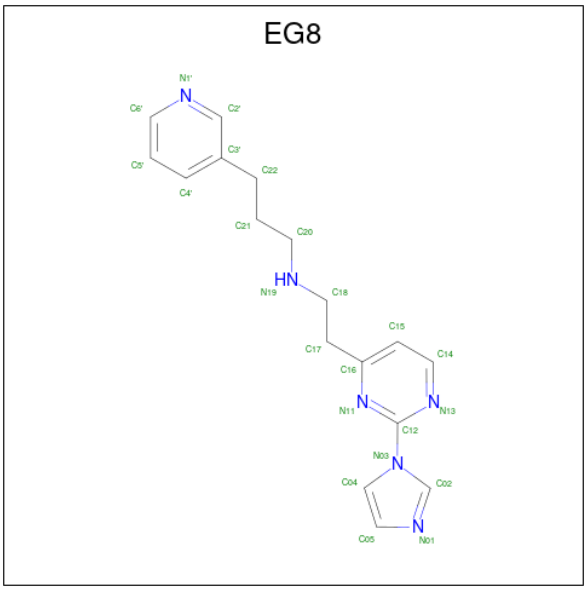
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



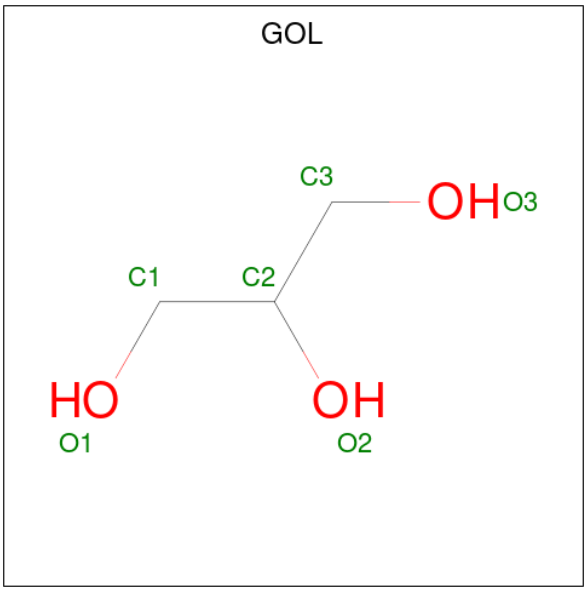
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	9	5	3	0	0
3	B	1	17	9	5	3	0	0
3	C	1	17	9	5	3	0	0
3	D	1	17	9	5	3	0	0

- Molecule 4 is N-{2-[2-(1H-imidazol-1-yl)pyrimidin-4-yl]ethyl}-3-(pyridin-3-yl)propan-1-amine (three-letter code: EG8) (formula: $C_{17}H_{20}N_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	A	1	23	17	6	0	0
4	B	1	23	17	6	0	0
4	C	1	23	17	6	0	0
4	D	1	23	17	6	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	1	1	1	0	0
			Total	Zn		
6	C	1	1	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	238	238	238	0	0
			Total	O		
7	B	205	205	205	0	0

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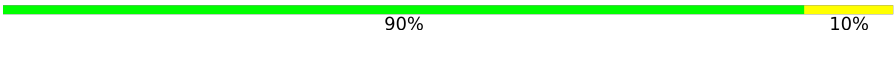
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	C	270	270	270	0	0
			Total	O		
7	D	189	189	189	0	0

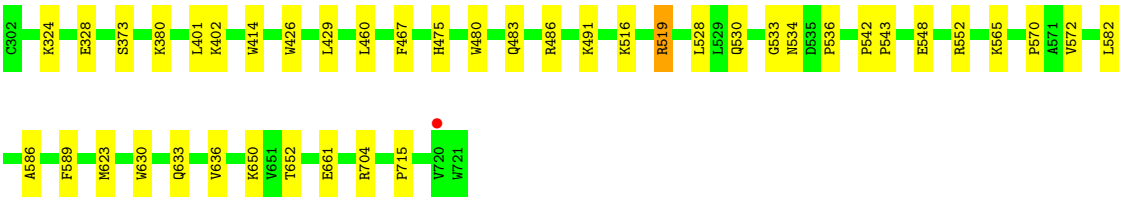
3 Residue-property plots (i)

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: NITRIC OXIDE SYNTHASE, BRAIN

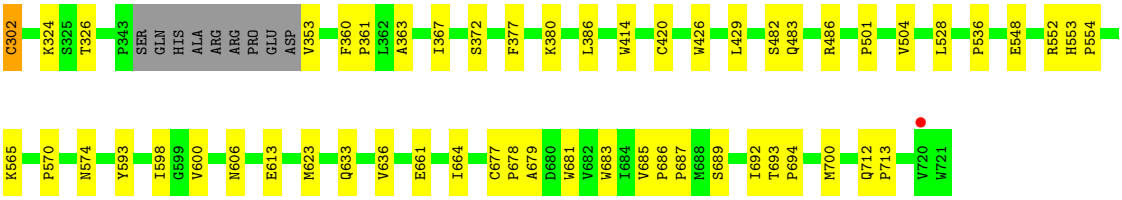
Chain A:





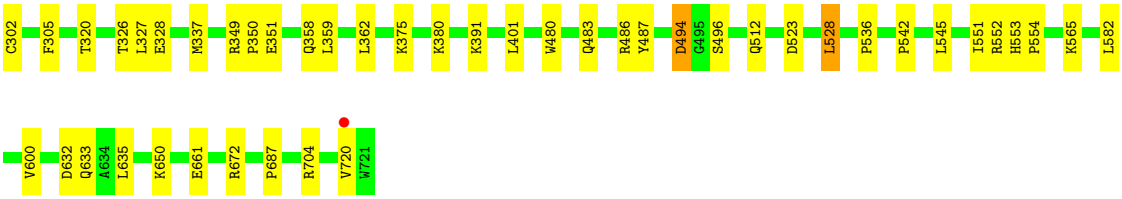
• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain B:



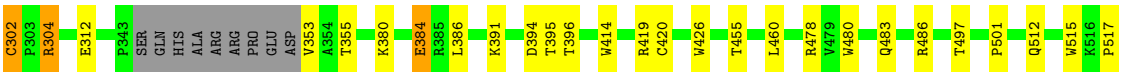
• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

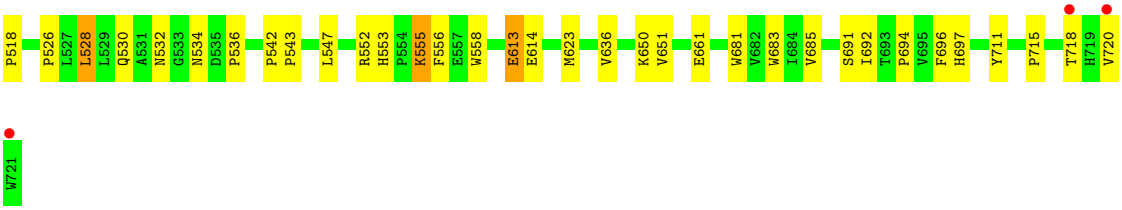
Chain C:



• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain D:




P518
P526
L527
L528
L529
Q530
A531
N532
G533
N534
D535
P536
P542
P543
L547
R552
H553
P554
K555
F556
E557
W558
E613
E614
M623
V636
K650
V651
E661
W681
V682
W683
I684
V685
S691
I692
T693
P694
V695
F696
H697
Y711
P715
T718
H719
V720
W721

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.56Å 84.63Å 167.27Å 90.00° 91.96° 90.00°	Depositor
Resolution (Å)	78.80 – 2.30 78.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (78.80-2.30) 99.5 (78.80-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.189 , 0.235 0.177 , 0.226	Depositor DCC
R_{free} test set	5420 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14827	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3409e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: H4B, ZN, EG8, GOL, 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	0.41	0/3523	0.53	0/4782
1	B	0.41	0/3450	0.54	1/4682 (0.0%)
1	C	0.42	0/3523	0.55	0/4782
1	D	0.41	0/3464	0.54	1/4700 (0.0%)
All	All	0.42	0/13960	0.54	2/18946 (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	D	302	CYS	CA-CB-SG	-5.95	103.29	114.00
1	B	302	CYS	CA-CB-SG	-5.80	103.55	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3324	22	0
1	B	3351	0	3260	31	0
1	C	3424	0	3324	23	0
1	D	3362	0	3274	29	0
2	A	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	1	0
3	C	17	0	15	0	0
3	D	17	0	15	1	0
4	A	23	0	20	2	0
4	B	23	0	20	1	0
4	C	23	0	20	0	0
4	D	23	0	20	1	0
5	A	6	0	8	1	0
5	B	6	0	8	1	0
5	C	12	0	16	0	0
5	D	6	0	8	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	238	0	0	2	0
7	B	205	0	0	0	0
7	C	270	0	0	2	0
7	D	189	0	0	0	0
All	All	14827	0	13482	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.61	0.82
1:D:528:LEU:HD22	1:D:536:PRO:HB2	1.64	0.79
2:C:750:HEM:HBC2	2:C:750:HEM:HMC2	1.72	0.71
1:C:528:LEU:HD22	1:C:536:PRO:HB2	1.73	0.70
1:D:395:THR:HG23	1:D:396:THR:HG23	1.76	0.68
2:C:750:HEM:HHC	2:C:750:HEM:HBB2	1.76	0.66
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.80	0.64
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.78	0.64
1:A:528:LEU:HD22	1:A:536:PRO:HB2	1.79	0.63
1:C:494:ASP:HB3	1:C:496:SER:H	1.63	0.62
2:D:750:HEM:HBB2	2:D:750:HEM:HHC	1.80	0.62
1:B:483:GLN:HB2	1:B:486:ARG:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:LEU:HD21	1:D:651:VAL:HG22	1.84	0.59
2:B:750:HEM:HMC2	2:B:750:HEM:HBC2	1.84	0.59
1:A:530:GLN:HG3	1:A:534:ASN:O	2.04	0.58
1:B:326:THR:HG22	1:D:304:ARG:HB3	1.84	0.58
1:A:483:GLN:HB2	1:A:486:ARG:HG3	1.86	0.58
1:D:419:ARG:NH1	1:D:711:TYR:OH	2.37	0.58
1:C:327:LEU:HB2	1:C:704:ARG:HB2	1.86	0.56
1:A:636:VAL:HG11	1:B:633:GLN:HG3	1.87	0.56
1:A:429:LEU:O	5:A:880:GOL:H11	2.07	0.55
1:C:375:LYS:NZ	7:C:2043:HOH:O	2.40	0.54
1:C:600:VAL:HG22	1:C:635:LEU:HD11	1.90	0.54
1:B:324:LYS:HA	1:D:304:ARG:HD3	1.91	0.53
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.90	0.52
1:B:420:CYS:HB2	2:B:750:HEM:ND	2.25	0.52
1:C:328:GLU:O	1:C:704:ARG:NH1	2.37	0.52
1:C:480:TRP:HB2	1:C:528:LEU:HB3	1.93	0.51
1:D:515:TRP:CE2	1:D:526:PRO:HD3	2.46	0.51
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.46	0.50
1:C:633:GLN:HG3	1:D:636:VAL:HG11	1.93	0.49
1:D:391:LYS:O	1:D:395:THR:HG22	2.12	0.49
1:A:519:ARG:NH2	7:A:2127:HOH:O	2.45	0.49
1:C:380:LYS:HD2	1:C:380:LYS:N	2.27	0.49
1:D:312[A]:GLU:HG2	1:D:697:HIS:CG	2.48	0.49
1:D:480:TRP:HB2	1:D:528:LEU:HB3	1.95	0.48
1:D:478:ARG:NH2	1:D:715:PRO:HD3	2.29	0.48
1:D:420:CYS:HB2	2:D:750:HEM:ND	2.28	0.48
1:D:414:TRP:CE3	1:D:426:TRP:HA	2.49	0.48
1:B:686:PRO:HG2	1:B:693:THR:HG21	1.96	0.48
1:C:600:VAL:HG11	1:C:687:PRO:HB2	1.94	0.48
1:B:360:PHE:HB2	1:B:361:PRO:HD3	1.95	0.47
1:C:401:LEU:HG	1:C:582:LEU:HD12	1.95	0.47
1:C:542:PRO:HD2	1:C:545:LEU:HD12	1.96	0.47
1:C:650:LYS:HD3	1:C:650:LYS:HA	1.73	0.47
2:D:750:HEM:O1D	4:D:800:EG8:N19	2.48	0.46
1:D:683:TRP:HA	3:D:760:H4B:N1	2.30	0.46
1:D:530:GLN:HG3	1:D:534:ASN:O	2.15	0.45
1:B:679:ALA:HB3	1:B:700:MET:HB3	1.98	0.45
1:D:613:GLU:HG2	1:D:623:MET:HE1	1.99	0.45
1:C:349:ARG:HB3	1:C:351:GLU:OE2	2.16	0.45
1:A:475:HIS:HA	1:A:533:GLY:HA3	1.99	0.44
1:C:551:ILE:HG12	1:C:565:LYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:O	1:A:704:ARG:HD3	2.17	0.44
1:C:358:GLN:O	1:C:362:LEU:HG	2.18	0.44
2:A:750:HEM:C1A	4:A:800:EG8:H02	2.52	0.44
1:A:480:TRP:HA	1:A:715:PRO:HG2	1.99	0.44
1:C:483:GLN:HB2	1:C:486:ARG:HG3	1.99	0.44
1:A:572:VAL:HB	1:A:589:PHE:CZ	2.53	0.44
1:B:363:ALA:O	1:B:367:ILE:HG12	2.16	0.43
1:A:548:GLU:OE1	1:A:565:LYS:HE3	2.18	0.43
1:D:553:HIS:CE1	1:D:555:LYS:HB2	2.54	0.43
1:C:635:LEU:HD22	1:D:692:ILE:HD13	2.01	0.43
1:A:633:GLN:HG2	1:B:636:VAL:HG11	1.98	0.43
1:B:483:GLN:NE2	4:B:800:EG8:H15	2.34	0.43
1:B:613:GLU:HG2	1:B:623:MET:CE	2.48	0.43
1:D:691:SER:HA	1:D:696:PHE:CG	2.54	0.43
1:B:414:TRP:CE3	1:B:426:TRP:HA	2.54	0.43
1:B:593:TYR:CD2	1:B:598:ILE:HD11	2.54	0.43
1:B:429:LEU:O	5:B:880:GOL:H32	2.19	0.43
1:A:623:MET:HA	1:A:630:TRP:CD1	2.54	0.43
1:B:372:SER:HA	1:B:377:PHE:HB2	2.00	0.43
1:D:542:PRO:HA	1:D:543:PRO:HD3	1.77	0.42
1:D:661:GLU:HG3	1:D:694:PRO:HG3	2.01	0.42
1:D:517:PRO:HA	1:D:518:PRO:HD3	1.94	0.42
1:A:570:PRO:HB2	4:A:800:EG8:N13	2.35	0.42
1:B:482:SER:HA	1:B:574:ASN:HB3	2.01	0.42
1:B:664:ILE:HG13	1:B:694:PRO:HB2	2.01	0.42
1:A:467:PHE:HB2	1:A:586:ALA:HB3	2.01	0.42
1:C:305:PHE:CD1	1:C:320:THR:HG22	2.55	0.42
1:B:600:VAL:HG11	1:B:687:PRO:HB2	2.01	0.42
1:B:548:GLU:OE1	1:B:565:LYS:HE3	2.20	0.42
1:B:570:PRO:HB3	1:B:593:TYR:CZ	2.55	0.42
1:A:460:LEU:HG	1:A:652:THR:HB	2.02	0.41
1:A:528:LEU:HD23	1:A:528:LEU:HA	1.74	0.41
1:A:401:LEU:HG	1:A:582:LEU:HD12	2.02	0.41
1:C:391:LYS:HG3	7:C:2044:HOH:O	2.19	0.41
1:D:556:PHE:HB3	1:D:558:TRP:CE2	2.56	0.41
1:A:402:LYS:NZ	7:A:2054:HOH:O	2.48	0.41
1:B:683:TRP:HA	3:B:760:H4B:N1	2.35	0.41
1:B:380:LYS:H	1:B:380:LYS:HG2	1.53	0.41
1:B:677:CYS:HA	1:B:678:PRO:HD2	1.87	0.41
1:B:685:VAL:HA	1:B:686:PRO:HD3	1.90	0.41
1:B:689:SER:HB3	1:B:692:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:GLN:HB2	1:D:486:ARG:HG3	2.03	0.41
1:A:542:PRO:HA	1:A:543:PRO:HD3	1.86	0.41
1:B:553:HIS:CG	1:B:554:PRO:HD2	2.56	0.41
1:C:349:ARG:HA	1:C:350:PRO:HD3	1.88	0.41
1:B:501:PRO:O	1:B:504:VAL:HG23	2.21	0.41
1:C:553:HIS:CG	1:C:554:PRO:HD2	2.56	0.41
1:B:712:GLN:HB2	1:B:713:PRO:HD2	2.03	0.40
1:D:380:LYS:O	1:D:384:GLU:HB2	2.21	0.40
1:D:455:THR:HA	1:D:460:LEU:HD22	2.02	0.40
1:D:497:THR:HG21	1:D:501:PRO:HA	2.03	0.40
1:D:681:TRP:CZ2	1:D:685:VAL:HG21	2.56	0.40
1:C:487:TYR:HA	1:C:523:ASP:O	2.21	0.40
1:A:480:TRP:HB2	1:A:528:LEU:HB3	2.03	0.40
1:B:681:TRP:CE2	1:B:685:VAL:HG21	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	418/420 (100%)	411 (98%)	7 (2%)	0	100	100
1	B	408/420 (97%)	399 (98%)	9 (2%)	0	100	100
1	C	418/420 (100%)	410 (98%)	8 (2%)	0	100	100
1	D	409/420 (97%)	400 (98%)	9 (2%)	0	100	100
All	All	1653/1680 (98%)	1620 (98%)	33 (2%)	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	375/375 (100%)	366 (98%)	9 (2%)	49	66
1	B	368/375 (98%)	362 (98%)	6 (2%)	62	78
1	C	375/375 (100%)	363 (97%)	12 (3%)	39	54
1	D	369/375 (98%)	352 (95%)	17 (5%)	27	38
All	All	1487/1500 (99%)	1443 (97%)	44 (3%)	41	57

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	LYS
1	A	373	SER
1	A	380	LYS
1	A	491	LYS
1	A	516	LYS
1	A	519	ARG
1	A	552	ARG
1	A	650	LYS
1	A	661	GLU
1	B	302	CYS
1	B	353	VAL
1	B	386	LEU
1	B	552	ARG
1	B	606	ASN
1	B	661	GLU
1	C	302	CYS
1	C	326	THR
1	C	337	MET
1	C	359	LEU
1	C	494	ASP
1	C	512	GLN
1	C	528	LEU
1	C	552	ARG
1	C	632	ASP

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Mol	Chain	Res	Type
1	C	661	GLU
1	C	672	ARG
1	C	720	VAL
1	D	302	CYS
1	D	304	ARG
1	D	353	VAL
1	D	355	THR
1	D	384	GLU
1	D	386	LEU
1	D	394	ASP
1	D	512	GLN
1	D	528	LEU
1	D	532	ASN
1	D	552	ARG
1	D	555	LYS
1	D	613	GLU
1	D	614	GLU
1	D	650	LYS
1	D	718	THR
1	D	720	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	512	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
3	H4B	B	760	-	16,18,18	0.89	0	11,26,26	2.64	6 (54%)
2	HEM	D	750	1,4	41,50,50	1.98	7 (17%)	45,82,82	1.74	8 (17%)
4	EG8	A	800	2	24,25,25	1.24	4 (16%)	28,31,31	2.30	10 (35%)
3	H4B	C	760	-	16,18,18	0.95	0	11,26,26	2.57	4 (36%)
2	HEM	C	750	1,4	41,50,50	1.86	4 (9%)	45,82,82	1.71	7 (15%)
4	EG8	B	800	2	24,25,25	1.16	4 (16%)	28,31,31	2.27	12 (42%)
5	GOL	C	880	-	5,5,5	0.33	0	5,5,5	0.24	0
2	HEM	B	750	1,4	41,50,50	1.96	7 (17%)	45,82,82	1.70	9 (20%)
5	GOL	D	880	-	5,5,5	0.37	0	5,5,5	0.34	0
4	EG8	D	800	2	24,25,25	1.30	4 (16%)	28,31,31	2.25	11 (39%)
5	GOL	B	880	-	5,5,5	0.41	0	5,5,5	0.61	0
3	H4B	A	760	-	16,18,18	0.96	0	11,26,26	2.70	6 (54%)
5	GOL	C	882	-	5,5,5	0.35	0	5,5,5	0.25	0
3	H4B	D	760	-	16,18,18	0.91	0	11,26,26	2.86	6 (54%)
4	EG8	C	800	2	24,25,25	1.27	4 (16%)	28,31,31	2.40	11 (39%)
2	HEM	A	750	1,4	41,50,50	1.93	6 (14%)	45,82,82	1.80	9 (20%)
5	GOL	A	880	-	5,5,5	0.42	0	5,5,5	0.52	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
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
2	HEM	D	750	1,4	-	3/12/54/54	-
4	EG8	A	800	2	-	1/9/13/13	0/3/3/3
3	H4B	C	760	-	-	0/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	750	1,4	-	1/12/54/54	-
4	EG8	B	800	2	-	1/9/13/13	0/3/3/3
5	GOL	C	880	-	-	4/4/4/4	-
2	HEM	B	750	1,4	-	3/12/54/54	-
5	GOL	D	880	-	-	2/4/4/4	-
4	EG8	D	800	2	-	2/9/13/13	0/3/3/3
5	GOL	B	880	-	-	1/4/4/4	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	GOL	C	882	-	-	3/4/4/4	-
3	H4B	D	760	-	-	0/8/17/17	0/2/2/2
4	EG8	C	800	2	-	2/9/13/13	0/3/3/3
2	HEM	A	750	1,4	-	1/12/54/54	-
5	GOL	A	880	-	-	4/4/4/4	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	750	HEM	C3D-C2D	7.94	1.53	1.36
2	B	750	HEM	C3D-C2D	7.72	1.53	1.36
2	A	750	HEM	C3D-C2D	7.72	1.53	1.36
2	C	750	HEM	C3D-C2D	7.40	1.52	1.36
2	C	750	HEM	C3C-C2C	-4.12	1.34	1.40
2	A	750	HEM	C3C-CAC	4.06	1.56	1.47
4	C	800	EG8	C04-N03	-3.93	1.33	1.39
2	D	750	HEM	C3C-CAC	3.87	1.55	1.47
4	D	800	EG8	C04-N03	-3.81	1.33	1.39
2	B	750	HEM	C3C-C2C	-3.75	1.35	1.40
2	B	750	HEM	C3C-CAC	3.67	1.55	1.47
4	B	800	EG8	C04-N03	-3.64	1.33	1.39
4	A	800	EG8	C04-N03	-3.59	1.34	1.39
2	A	750	HEM	C3C-C2C	-3.57	1.35	1.40
2	D	750	HEM	C3C-C2C	-3.51	1.35	1.40
2	C	750	HEM	C3C-CAC	3.47	1.54	1.47
2	B	750	HEM	CAB-C3B	3.21	1.56	1.47
2	D	750	HEM	CAB-C3B	3.14	1.56	1.47
2	C	750	HEM	CAB-C3B	3.03	1.55	1.47
2	A	750	HEM	CAB-C3B	2.95	1.55	1.47
4	A	800	EG8	C12-N13	2.80	1.35	1.31
4	D	800	EG8	C12-N11	2.80	1.36	1.32
4	D	800	EG8	C02-N03	-2.77	1.33	1.36
2	B	750	HEM	FE-ND	2.76	2.10	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	800	EG8	C12-N13	2.74	1.35	1.31
4	C	800	EG8	C12-N11	2.69	1.36	1.32
4	A	800	EG8	C02-N03	-2.61	1.33	1.36
4	D	800	EG8	C12-N13	2.60	1.35	1.31
4	B	800	EG8	C12-N13	2.57	1.35	1.31
2	D	750	HEM	FE-ND	2.57	2.09	1.96
4	B	800	EG8	C02-N03	-2.37	1.34	1.36
2	D	750	HEM	CMD-C2D	2.37	1.55	1.50
2	A	750	HEM	FE-ND	2.35	2.08	1.96
2	A	750	HEM	CAA-C2A	2.32	1.55	1.52
4	A	800	EG8	C12-N11	2.30	1.35	1.32
4	C	800	EG8	C02-N03	-2.27	1.34	1.36
2	B	750	HEM	CMB-C2B	2.24	1.55	1.50
2	D	750	HEM	CAA-C2A	2.19	1.55	1.52
4	B	800	EG8	C12-N11	2.12	1.35	1.32
2	B	750	HEM	CAA-C2A	2.01	1.55	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	750	HEM	C4D-ND-C1D	6.62	111.91	105.07
2	A	750	HEM	C4D-ND-C1D	6.03	111.30	105.07
2	B	750	HEM	C4D-ND-C1D	5.73	110.99	105.07
2	C	750	HEM	C4D-ND-C1D	5.61	110.87	105.07
3	C	760	H4B	C8A-C4A-C4	5.35	119.33	114.57
3	B	760	H4B	C8A-C4A-C4	5.35	119.32	114.57
4	C	800	EG8	C14-N13-C12	5.15	120.87	114.04
4	C	800	EG8	N13-C12-N11	-5.00	120.42	126.08
4	A	800	EG8	C14-N13-C12	4.99	120.65	114.04
3	D	760	H4B	C8A-C4A-C4	4.80	118.83	114.57
4	D	800	EG8	C14-N13-C12	4.59	120.12	114.04
4	C	800	EG8	N11-C12-N03	4.54	120.66	114.78
4	B	800	EG8	C14-N13-C12	4.51	120.01	114.04
3	A	760	H4B	C8A-C4A-C4	4.47	118.54	114.57
4	B	800	EG8	N13-C12-N11	-4.37	121.12	126.08
2	A	750	HEM	C4B-CHC-C1C	4.29	128.21	122.56
4	A	800	EG8	N13-C12-N11	-4.16	121.37	126.08
4	B	800	EG8	N13-C12-N03	4.12	121.20	114.81
3	A	760	H4B	C4-C4A-N5	4.06	122.53	119.12
4	B	800	EG8	C02-N03-C04	4.03	115.82	108.50
4	D	800	EG8	N13-C12-N11	-3.95	121.61	126.08
3	D	760	H4B	C4-C4A-N5	3.88	122.37	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	800	EG8	C02-N03-C04	3.86	115.50	108.50
4	A	800	EG8	C15-C14-N13	-3.79	119.25	123.96
3	D	760	H4B	N1-C2-N3	-3.76	119.52	125.42
4	D	800	EG8	N11-C12-N03	3.74	119.61	114.78
4	A	800	EG8	C02-N03-C04	3.72	115.25	108.50
4	A	800	EG8	N11-C12-N03	3.72	119.59	114.78
2	C	750	HEM	CBA-CAA-C2A	-3.64	106.42	112.62
2	C	750	HEM	C4B-CHC-C1C	3.61	127.32	122.56
3	D	760	H4B	C2-N3-C4	3.59	121.64	115.93
3	A	760	H4B	N1-C2-N3	-3.59	119.79	125.42
4	C	800	EG8	C17-C16-N11	3.51	121.17	115.95
2	A	750	HEM	C1B-NB-C4B	3.43	108.62	105.07
2	D	750	HEM	C4B-CHC-C1C	3.41	127.06	122.56
4	C	800	EG8	C02-N03-C04	3.41	114.69	108.50
4	A	800	EG8	C04-N03-C12	-3.36	121.71	125.50
3	B	760	H4B	N1-C2-N3	-3.33	120.20	125.42
4	D	800	EG8	C15-C14-N13	-3.28	119.88	123.96
4	D	800	EG8	C04-N03-C12	-3.27	121.80	125.50
3	C	760	H4B	N1-C2-N3	-3.27	120.29	125.42
2	B	750	HEM	C1B-NB-C4B	3.25	108.44	105.07
4	C	800	EG8	C15-C14-N13	-3.25	119.92	123.96
4	D	800	EG8	C17-C16-N11	3.23	120.76	115.95
4	B	800	EG8	C15-C14-N13	-3.18	120.01	123.96
2	D	750	HEM	C1B-NB-C4B	3.12	108.30	105.07
3	C	760	H4B	C2-N3-C4	3.11	120.87	115.93
4	C	800	EG8	C04-N03-C12	-3.08	122.03	125.50
3	B	760	H4B	C2-N3-C4	3.08	120.81	115.93
3	A	760	H4B	C2-N3-C4	3.07	120.80	115.93
4	C	800	EG8	C6'-N1'-C2'	3.04	122.10	116.85
2	B	750	HEM	CBA-CAA-C2A	-3.03	107.44	112.62
3	D	760	H4B	C2-N1-C8A	3.03	121.34	114.54
2	C	750	HEM	C1B-NB-C4B	2.95	108.12	105.07
2	B	750	HEM	CHC-C4B-C3B	2.95	129.09	124.57
3	B	760	H4B	C4-C4A-N5	2.95	121.59	119.12
3	A	760	H4B	C2-N1-C8A	2.94	121.13	114.54
4	A	800	EG8	C14-C15-C16	2.91	119.35	116.62
2	A	750	HEM	CBD-CAD-C3D	-2.91	104.55	112.63
4	A	800	EG8	C17-C16-N11	2.90	120.27	115.95
3	B	760	H4B	C2-N1-C8A	2.88	121.00	114.54
2	B	750	HEM	C4B-CHC-C1C	2.82	126.29	122.56
2	D	750	HEM	CBD-CAD-C3D	-2.82	104.79	112.63
3	C	760	H4B	C2-N1-C8A	2.82	120.86	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	760	H4B	N2-C2-N3	2.82	121.64	117.25
4	A	800	EG8	N13-C12-N03	2.72	119.02	114.81
4	C	800	EG8	N13-C12-N03	2.66	118.92	114.81
4	D	800	EG8	C14-C15-C16	2.65	119.11	116.62
2	A	750	HEM	CHC-C4B-C3B	2.61	128.57	124.57
2	B	750	HEM	CMD-C2D-C1D	2.60	129.00	125.04
4	D	800	EG8	N13-C12-N03	2.55	118.76	114.81
4	B	800	EG8	C02-N03-C12	-2.55	121.02	126.02
4	C	800	EG8	C14-C15-C16	2.49	118.96	116.62
2	B	750	HEM	C1D-C2D-C3D	-2.48	104.34	106.96
4	D	800	EG8	C6'-N1'-C2'	2.48	121.14	116.85
4	B	800	EG8	C14-C15-C16	2.46	118.93	116.62
2	D	750	HEM	C3B-C2B-C1B	2.44	108.30	106.49
2	D	750	HEM	CHC-C4B-C3B	2.39	128.23	124.57
4	B	800	EG8	C6'-N1'-C2'	2.39	120.97	116.85
4	C	800	EG8	C15-C16-N11	-2.35	119.43	122.41
4	B	800	EG8	C15-C16-N11	-2.33	119.45	122.41
2	A	750	HEM	CMA-C3A-C4A	-2.30	124.92	128.46
2	D	750	HEM	C1D-C2D-C3D	-2.28	104.55	106.96
2	A	750	HEM	CMD-C2D-C1D	2.25	128.46	125.04
4	B	800	EG8	N11-C12-N03	2.23	117.67	114.78
3	B	760	H4B	N2-C2-N3	2.19	120.67	117.25
3	A	760	H4B	N2-C2-N3	2.17	120.62	117.25
2	C	750	HEM	C3B-C2B-C1B	2.16	108.09	106.49
4	A	800	EG8	C15-C16-N11	-2.15	119.68	122.41
2	D	750	HEM	C3D-C4D-ND	-2.13	107.79	110.17
4	D	800	EG8	C15-C16-N11	-2.13	119.71	122.41
2	C	750	HEM	C1D-C2D-C3D	-2.12	104.73	106.96
2	B	750	HEM	C3B-C2B-C1B	2.11	108.06	106.49
2	B	750	HEM	CBD-CAD-C3D	-2.11	106.75	112.63
4	B	800	EG8	C04-N03-C12	-2.07	123.16	125.50
2	A	750	HEM	C1D-C2D-C3D	-2.06	104.79	106.96
2	C	750	HEM	CAD-CBD-CGD	-2.02	109.25	113.60
4	B	800	EG8	C05-C04-N03	-2.02	102.94	106.50
2	A	750	HEM	CBA-CAA-C2A	-2.01	109.19	112.62

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	880	GOL	C1-C2-C3-O3
5	A	880	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	800	EG8	C17-C18-N19-C20
5	A	880	GOL	O1-C1-C2-C3
5	C	880	GOL	O1-C1-C2-C3
5	C	880	GOL	C1-C2-C3-O3
5	C	882	GOL	O1-C1-C2-C3
5	D	880	GOL	C1-C2-C3-O3
4	B	800	EG8	N19-C20-C21-C22
5	A	880	GOL	O2-C2-C3-O3
5	D	880	GOL	O2-C2-C3-O3
5	C	882	GOL	O1-C1-C2-O2
2	A	750	HEM	C4B-C3B-CAB-CBB
2	B	750	HEM	C4B-C3B-CAB-CBB
2	C	750	HEM	C4B-C3B-CAB-CBB
2	D	750	HEM	C4B-C3B-CAB-CBB
4	C	800	EG8	N19-C20-C21-C22
5	C	882	GOL	O2-C2-C3-O3
5	C	880	GOL	O1-C1-C2-O2
4	D	800	EG8	C21-C22-C3'-C4'
4	C	800	EG8	C21-C22-C3'-C4'
2	B	750	HEM	CAD-CBD-CGD-O2D
2	B	750	HEM	CAD-CBD-CGD-O1D
4	A	800	EG8	C21-C22-C3'-C4'
2	D	750	HEM	CAD-CBD-CGD-O2D
5	B	880	GOL	O2-C2-C3-O3
5	C	880	GOL	O2-C2-C3-O3
2	D	750	HEM	CAD-CBD-CGD-O1D

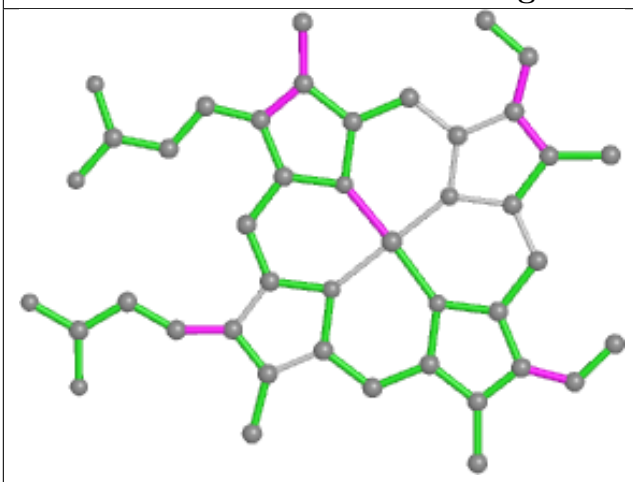
There are no ring outliers.

11 monomers are involved in 17 short contacts:

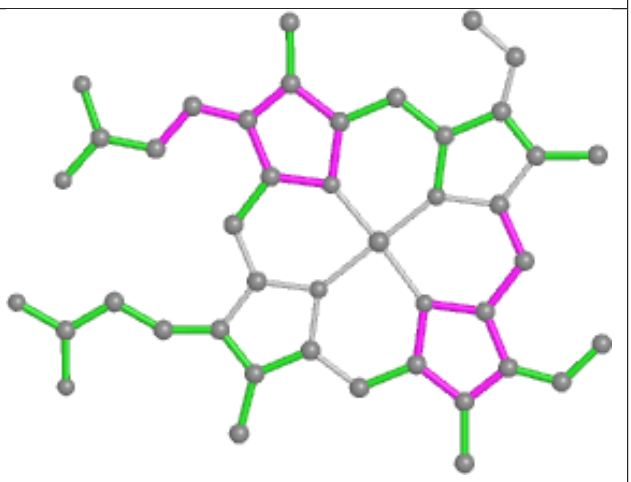
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	760	H4B	1	0
2	D	750	HEM	3	0
4	A	800	EG8	2	0
2	C	750	HEM	2	0
4	B	800	EG8	1	0
2	B	750	HEM	3	0
4	D	800	EG8	1	0
5	B	880	GOL	1	0
3	D	760	H4B	1	0
2	A	750	HEM	3	0
5	A	880	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

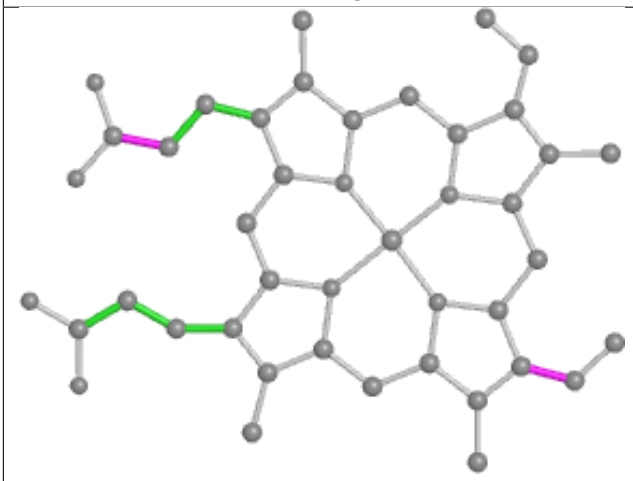
Ligand HEM D 750



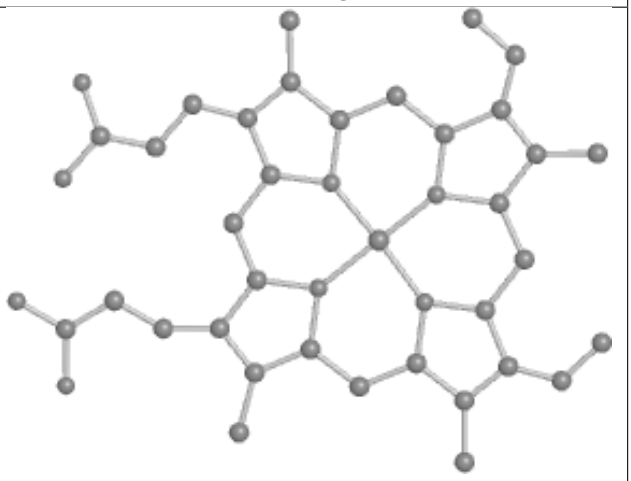
Bond lengths



Bond angles

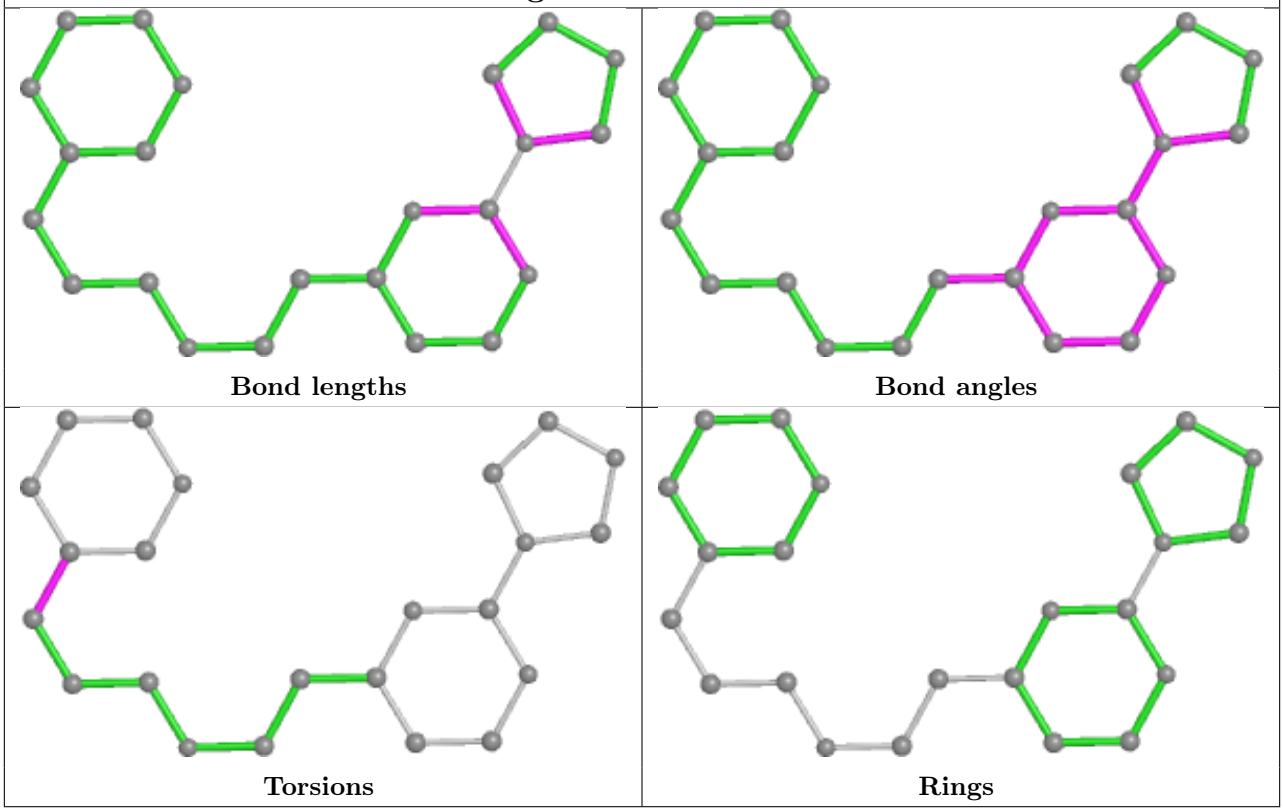


Torsions

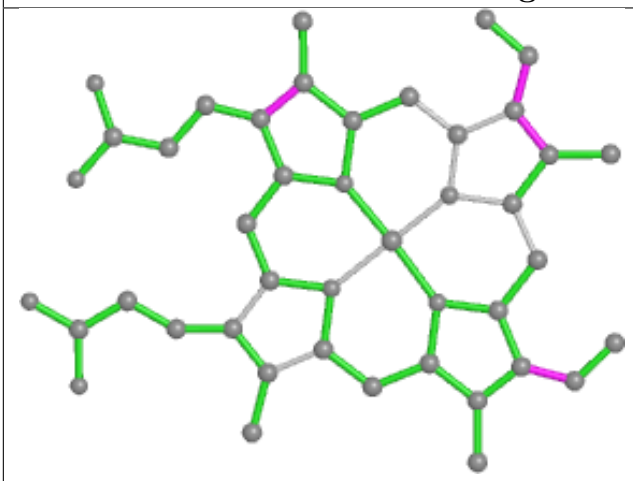


Rings

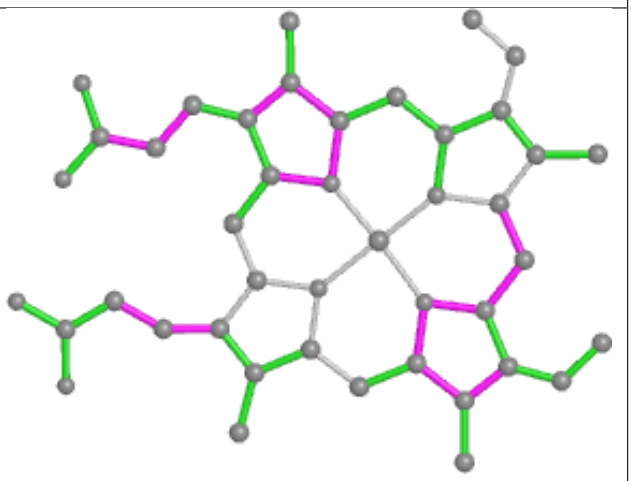
Ligand EG8 A 800



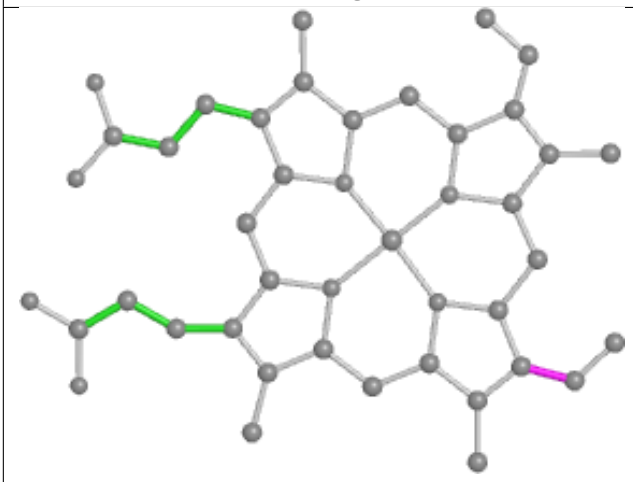
Ligand HEM C 750



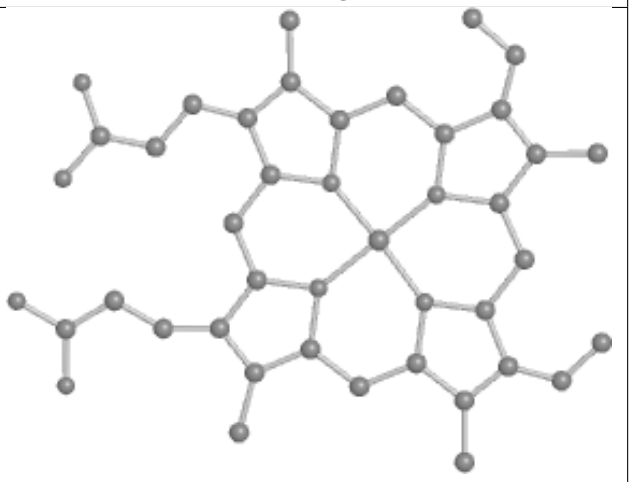
Bond lengths



Bond angles

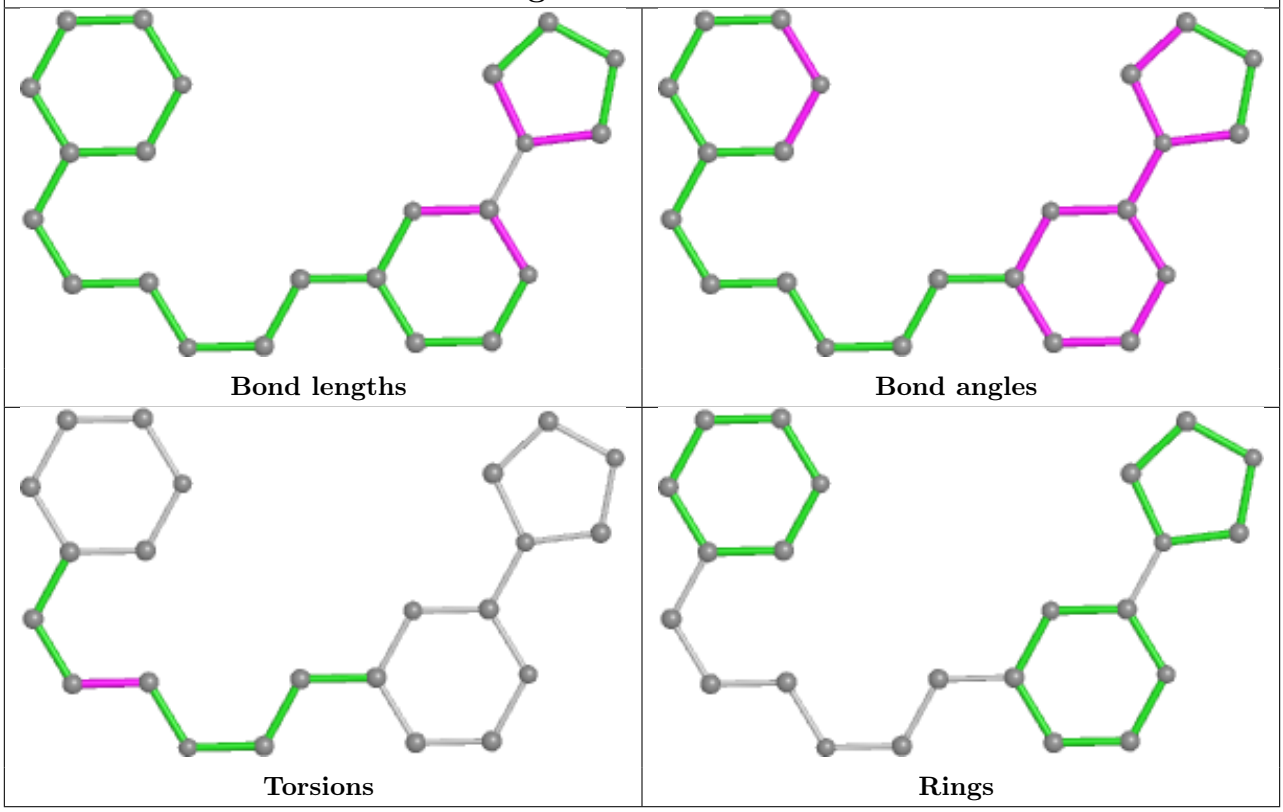


Torsions

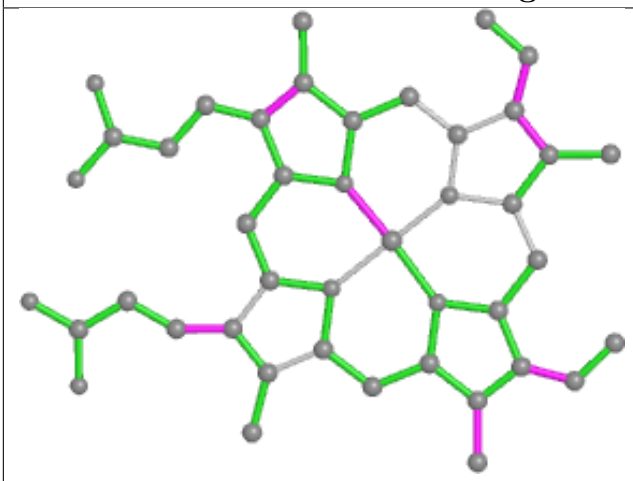


Rings

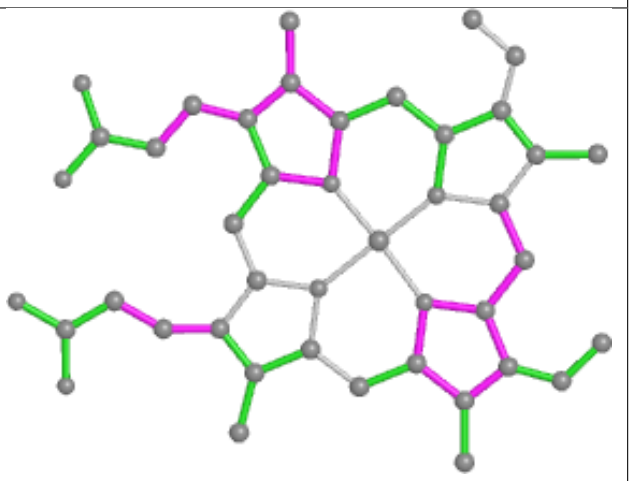
Ligand EG8 B 800



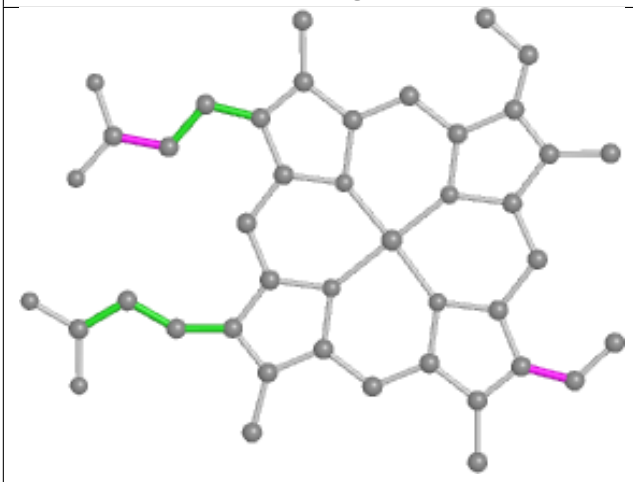
Ligand HEM B 750



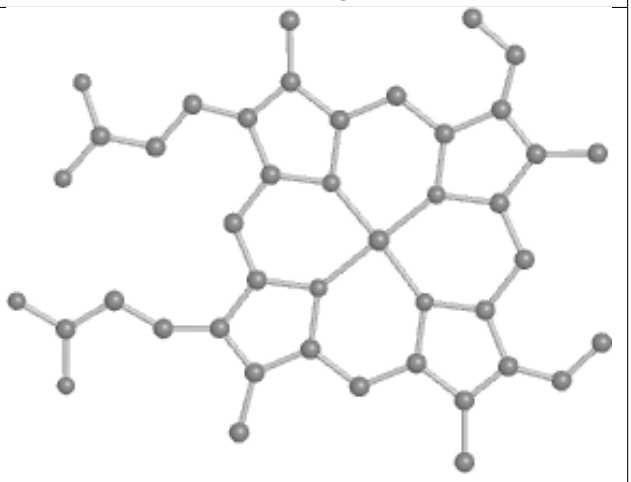
Bond lengths



Bond angles

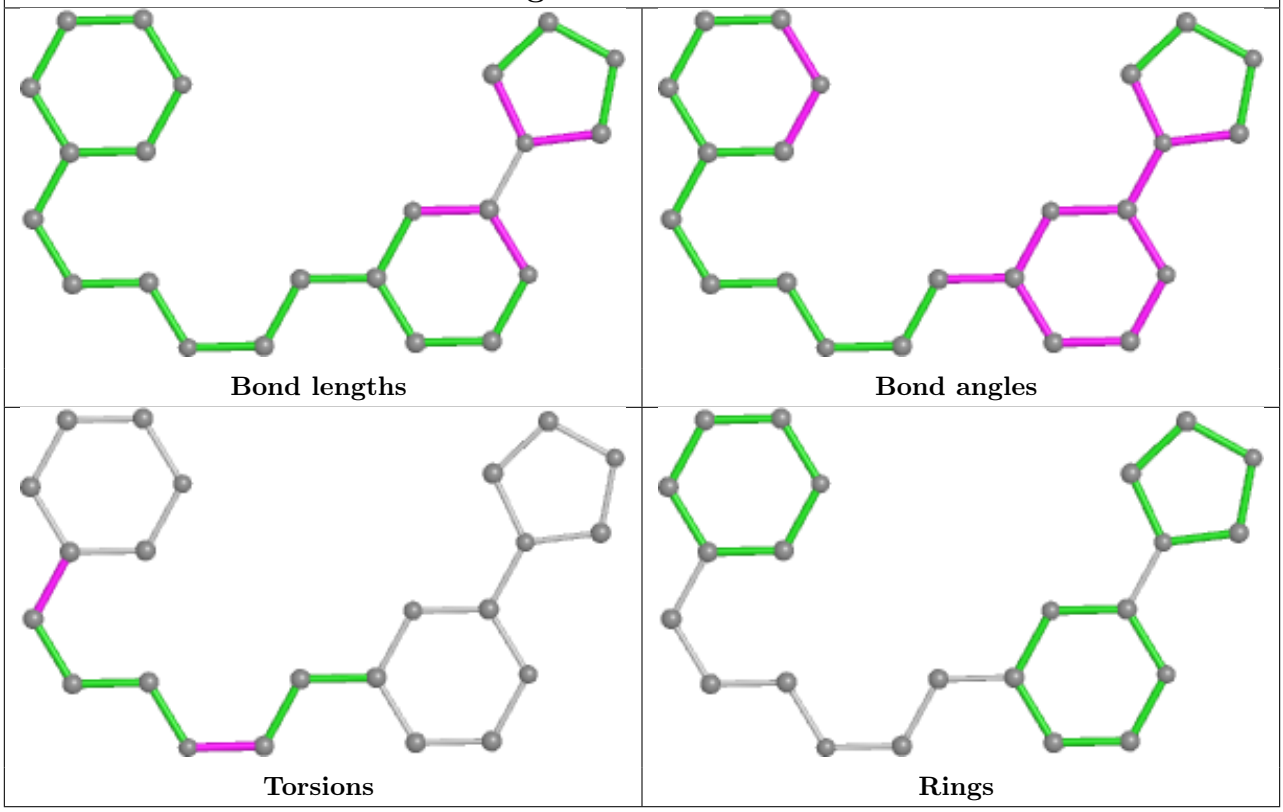


Torsions

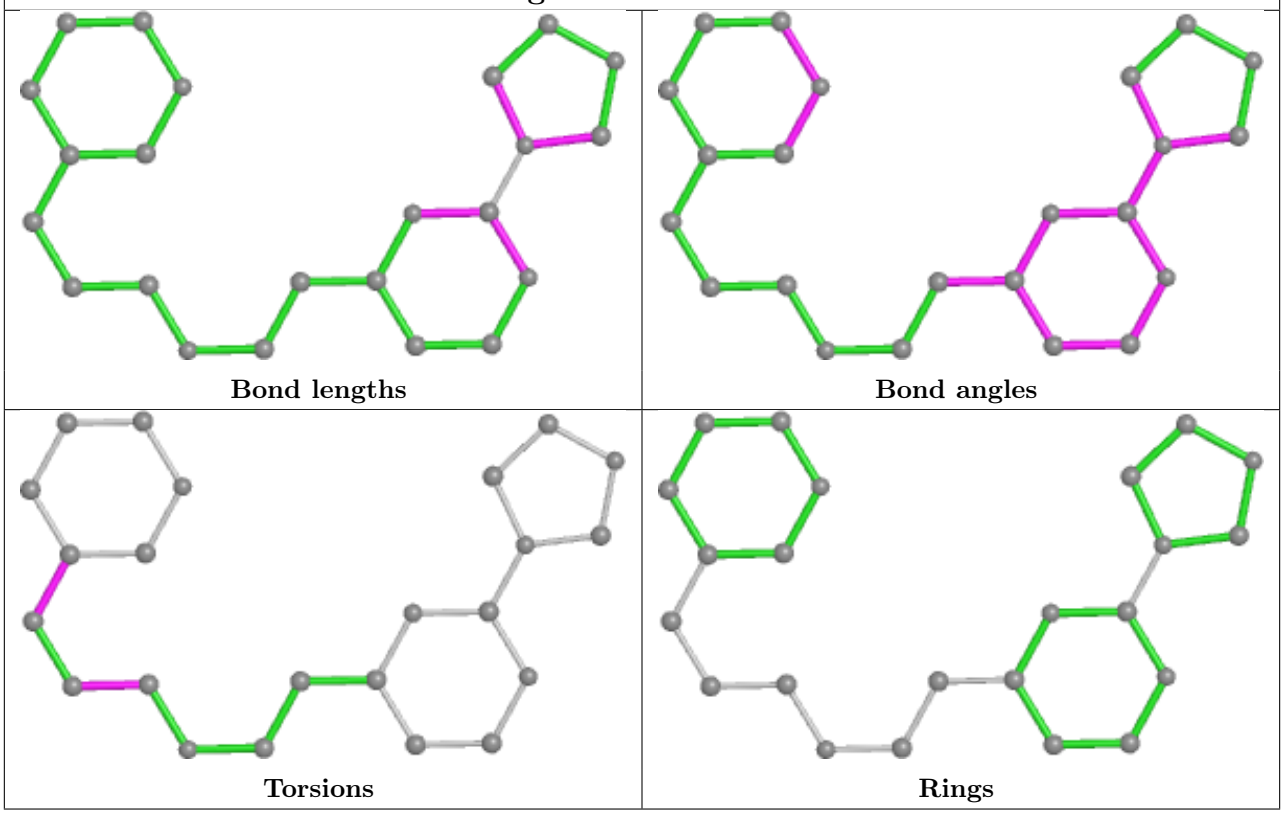


Rings

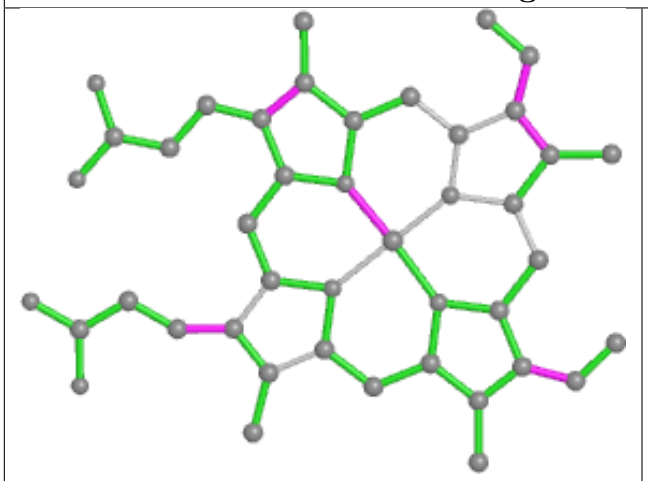
Ligand EG8 D 800



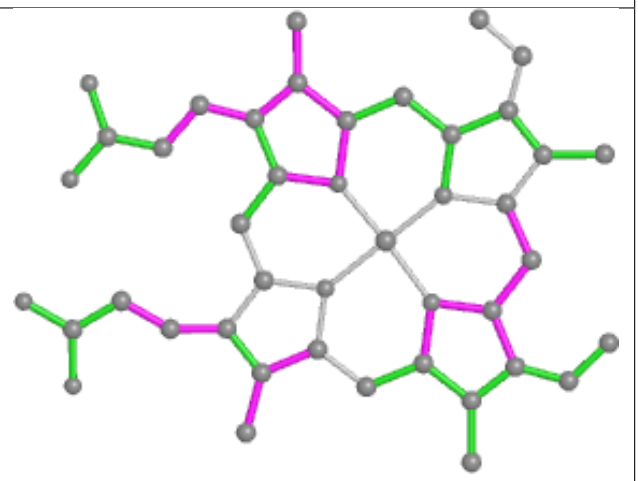
Ligand EG8 C 800



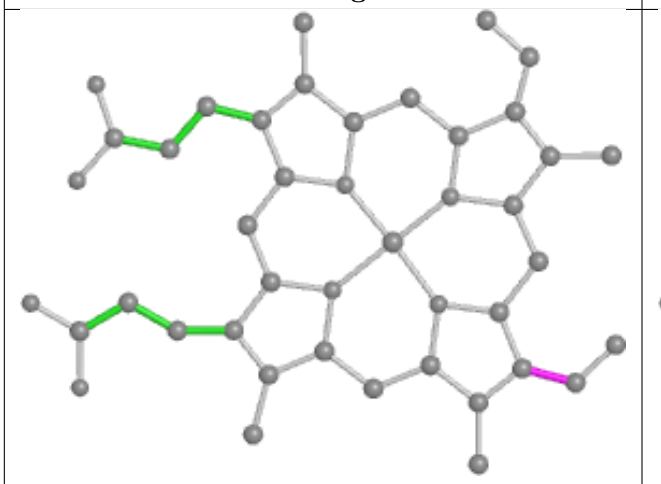
Ligand HEM A 750



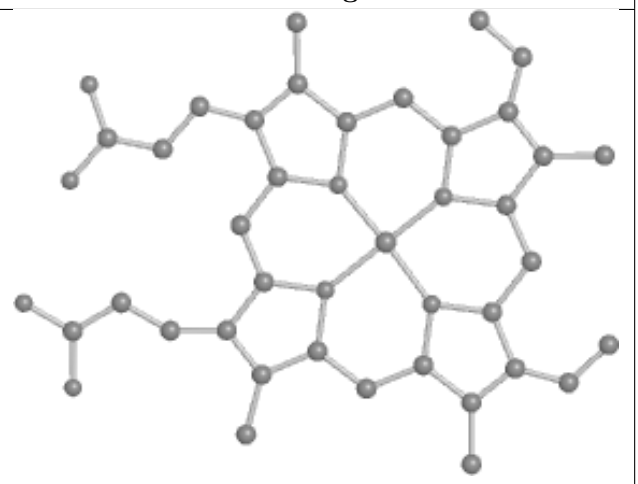
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	420/420 (100%)	-0.29	1 (0%)	95	96	19, 37, 61, 88	0
1	B	411/420 (97%)	-0.30	1 (0%)	95	96	17, 36, 65, 76	0
1	C	420/420 (100%)	-0.31	1 (0%)	95	96	18, 33, 57, 76	0
1	D	411/420 (97%)	-0.22	3 (0%)	87	91	18, 39, 69, 88	0
All	All	1662/1680 (98%)	-0.28	6 (0%)	92	95	17, 36, 64, 88	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	721	TRP	3.3
1	B	720	VAL	3.2
1	D	720	VAL	3.1
1	C	720	VAL	2.2
1	A	720	VAL	2.2
1	D	718	THR	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

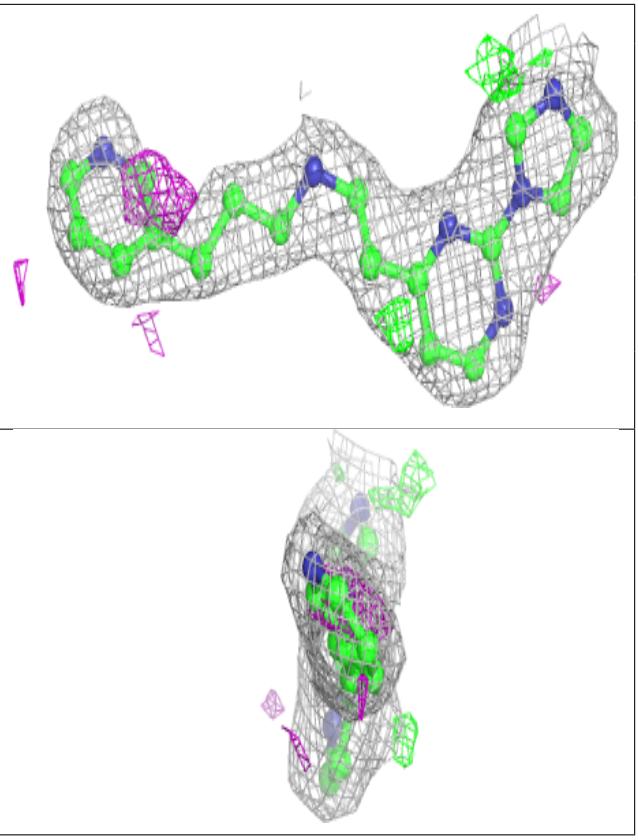
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	880	6/6	0.87	0.13	39,44,45,45	0
5	GOL	C	882	6/6	0.89	0.20	47,55,59,62	0
5	GOL	B	880	6/6	0.90	0.13	52,57,58,59	0
5	GOL	D	880	6/6	0.93	0.14	51,54,56,58	0
4	EG8	A	800	23/23	0.95	0.15	29,38,45,54	0
5	GOL	C	880	6/6	0.96	0.12	39,43,44,44	0
4	EG8	C	800	23/23	0.97	0.13	21,32,45,52	0
2	HEM	B	750	43/43	0.98	0.12	7,27,32,36	0
4	EG8	D	800	23/23	0.98	0.12	24,35,46,50	0
2	HEM	C	750	43/43	0.98	0.13	15,24,32,41	0
3	H4B	C	760	17/17	0.98	0.12	11,20,23,29	0
3	H4B	D	760	17/17	0.98	0.11	13,23,27,28	0
2	HEM	A	750	43/43	0.98	0.14	7,24,31,35	0
4	EG8	B	800	23/23	0.98	0.12	20,33,47,54	0
3	H4B	B	760	17/17	0.99	0.11	17,20,28,36	0
2	HEM	D	750	43/43	0.99	0.12	12,24,32,37	0
3	H4B	A	760	17/17	0.99	0.12	14,20,25,29	0
6	ZN	C	900	1/1	0.99	0.15	23,23,23,23	0
6	ZN	A	900	1/1	1.00	0.17	21,21,21,21	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.

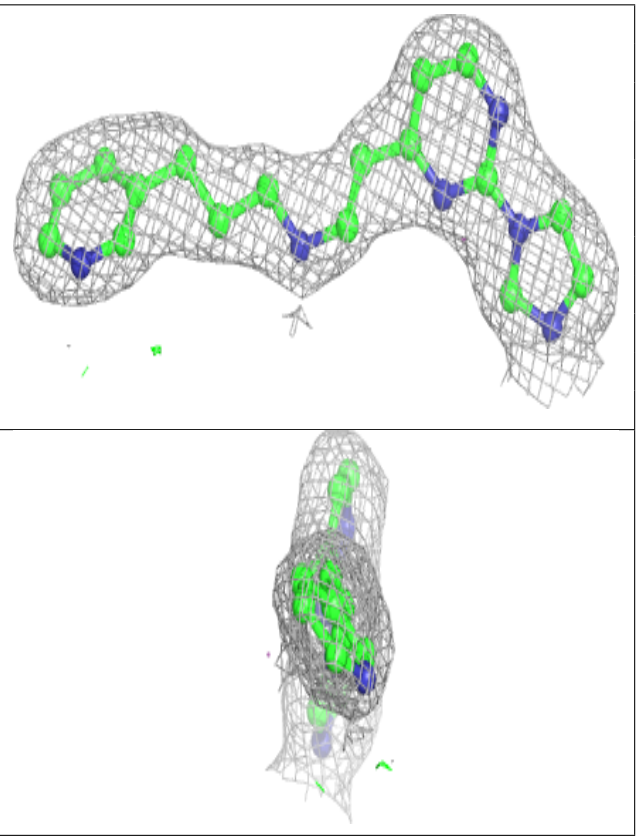
Electron density around EG8 A 800:

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



Electron density around EG8 C 800:

$2mF_o$-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 750:

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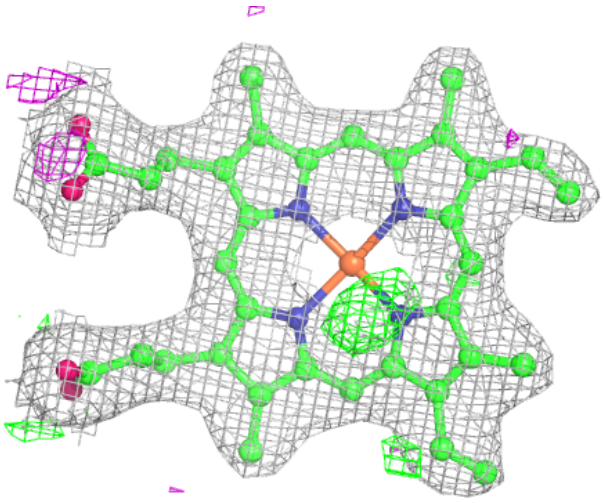
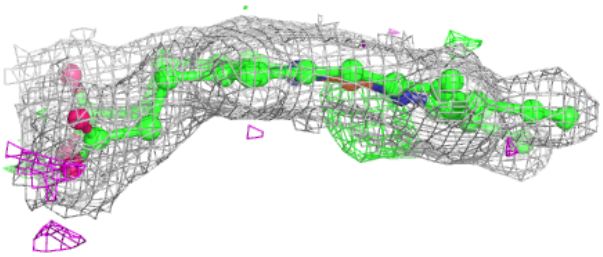
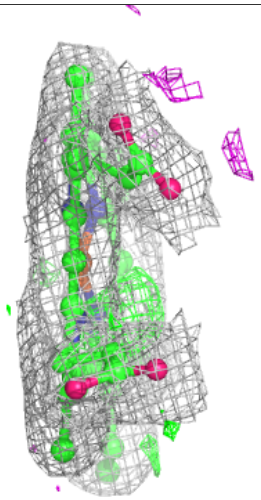
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around EG8 D 800:

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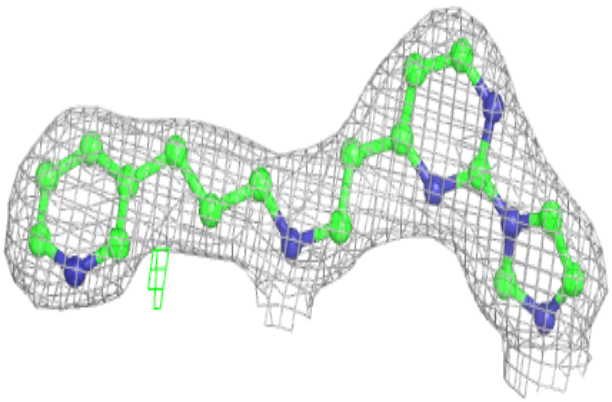
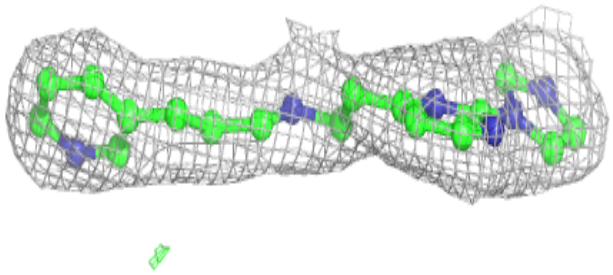
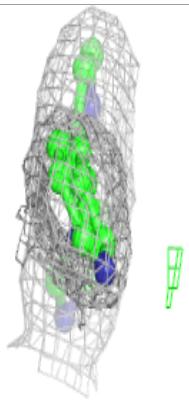
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEM C 750:

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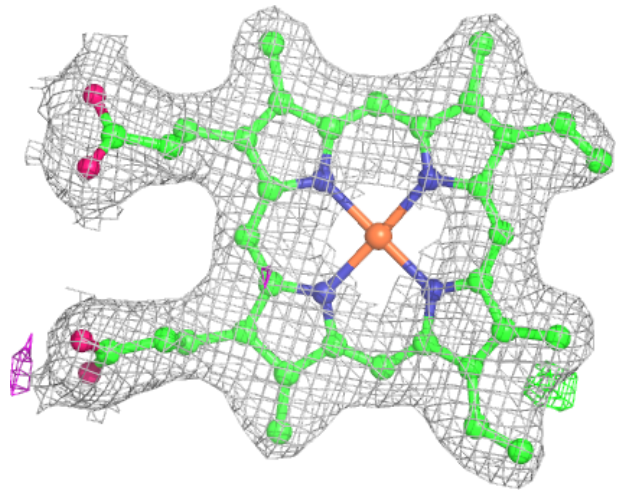
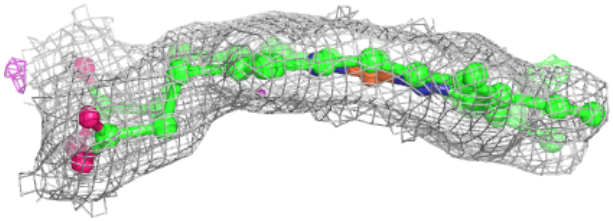
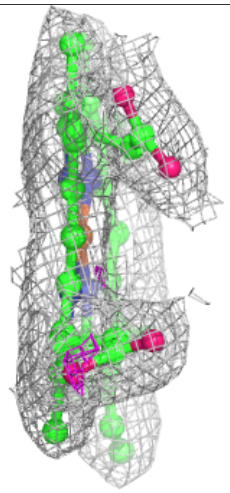
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

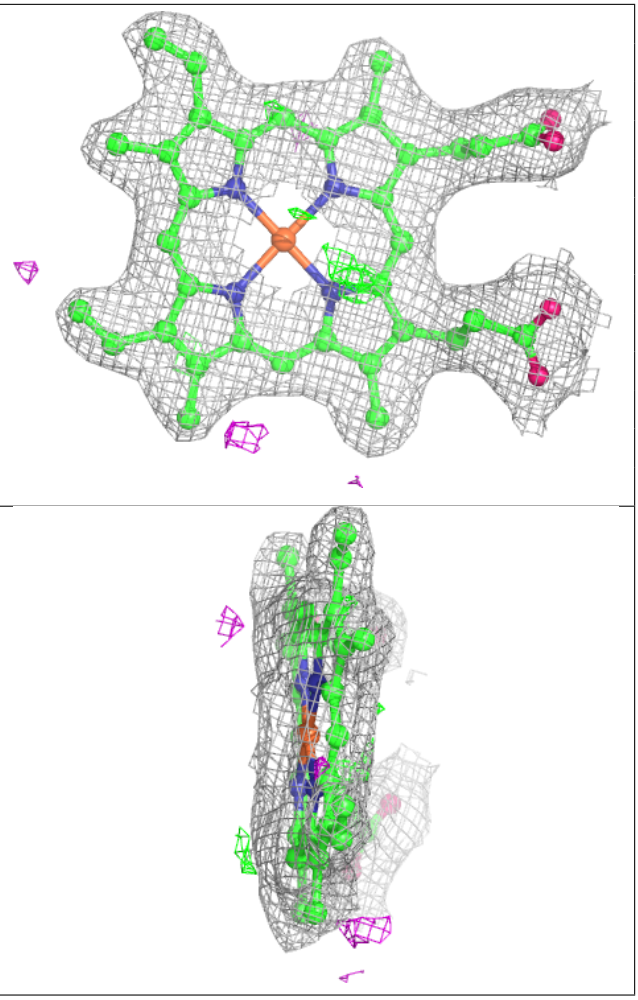






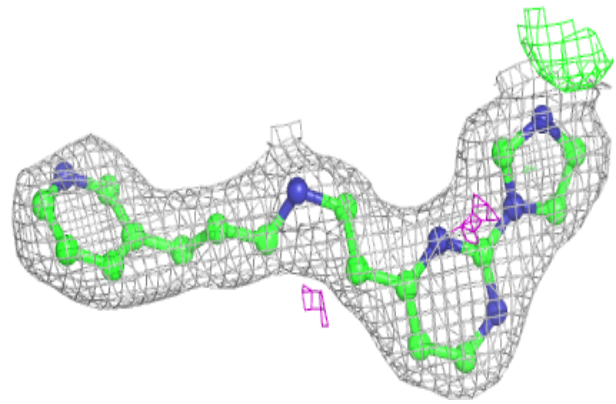
Electron density around HEM A 750:

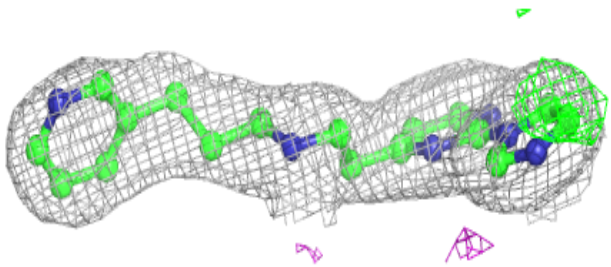
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

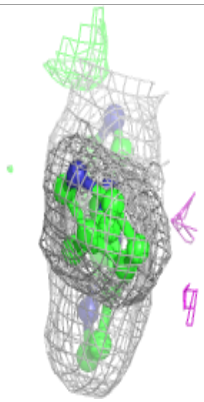


Electron density around EG8 B 800:

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

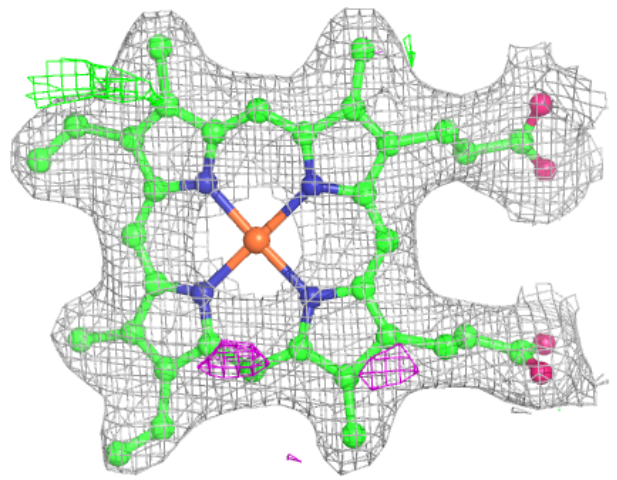


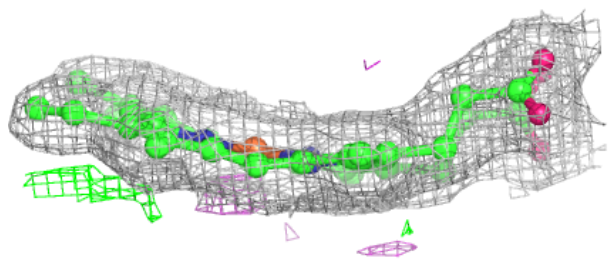


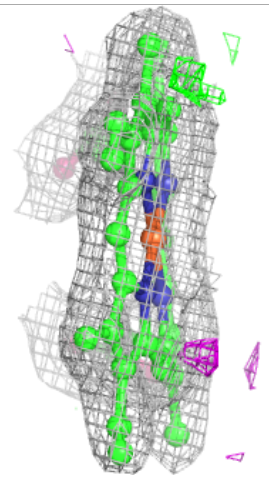


Electron density around HEM D 750:

$2mF_o$-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.