Full wwPDB X-ray Structure Validation Report ⓘ

Apr 23, 2025 – 06:40 PM EDT

PDB ID	:	9CW8 / pdb_00009cw8
Title	:	Structure of human endothelial nitric oxide synthase heme domain bound with 3-(6-amino-4-methylpyridin-2-yl)-5-((methylamino)methyl)benzonitrile dihydrochloride
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2024-07-29
Resolution	:	1.92 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:

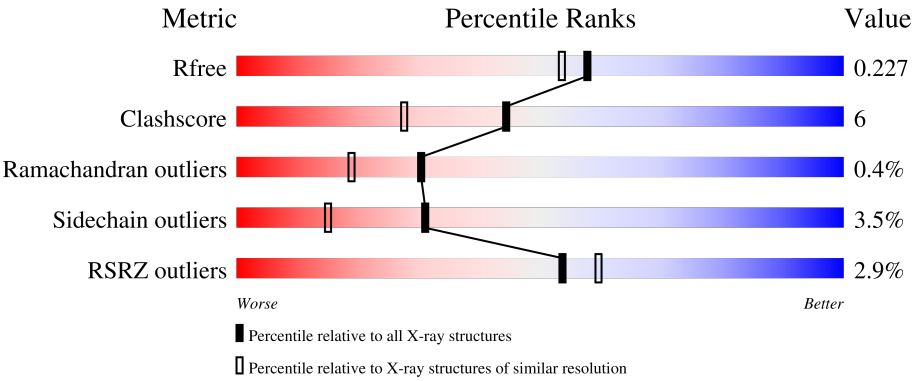
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 1.92 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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	440	6% 75% 14% • 9%
1	B	440	2% 81% 10% 9%
1	C	440	2% 78% 12% • 8%
1	D	440	% 82% 9% 9%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14141 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.

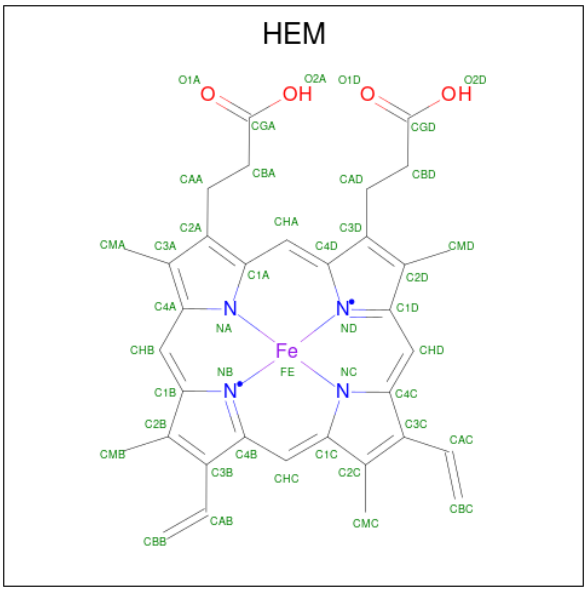
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	1	0
			3218	2049	568	585	16			
1	B	401	Total	C	N	O	S	0	3	0
			3211	2045	564	586	16			
1	C	403	Total	C	N	O	S	0	1	0
			3223	2052	569	586	16			
1	D	402	Total	C	N	O	S	0	0	0
			3211	2044	567	584	16			

There are 4 discrepancies between the modelled and reference sequences:

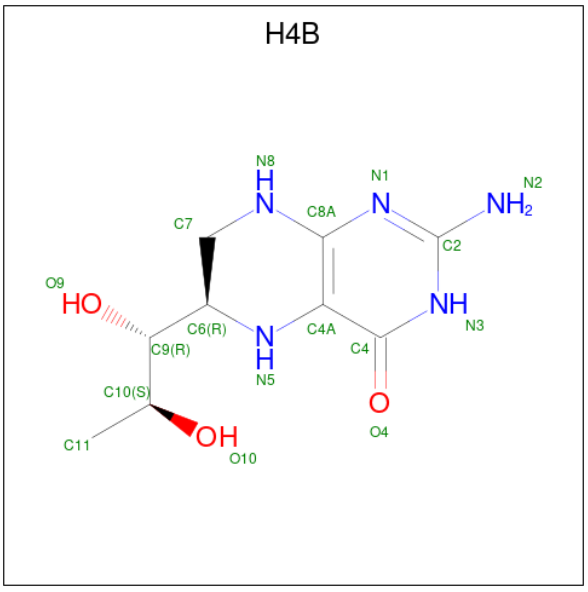
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



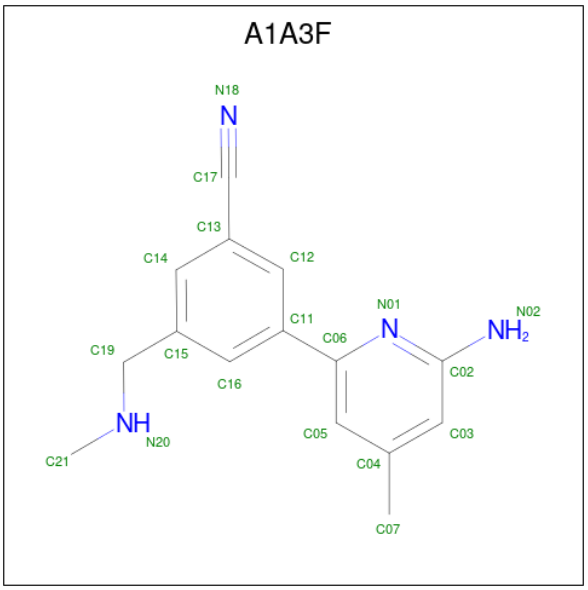
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



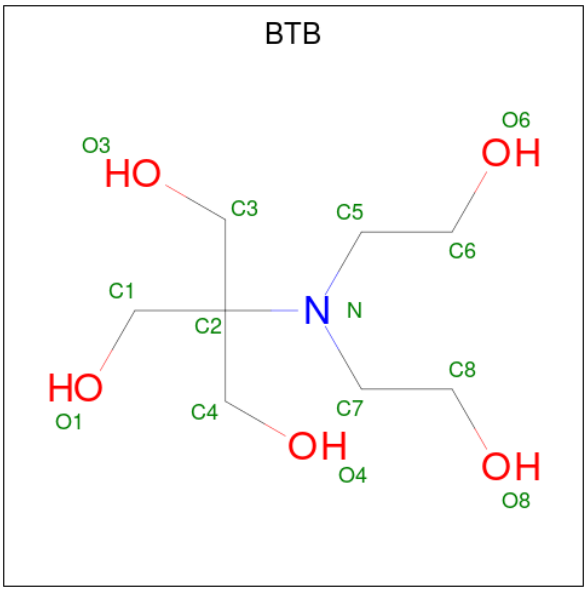
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0
3	C	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is (3P)-3-(6-amino-4-methylpyridin-2-yl)-5-[(methylamino)methyl]benzonitrile (CCD ID: A1A3F) (formula: $C_{15}H_{16}N_4$) (labeled as "Ligand of Interest" by depositor).



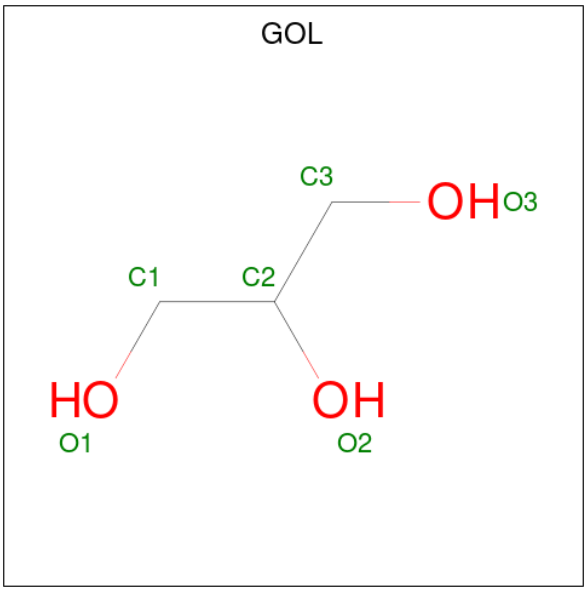
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 19 15 4	0	0
4	B	1	Total C N 19 15 4	0	0
4	C	1	Total C N 19 15 4	0	0
4	D	1	Total C N 19 15 4	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 8 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Gd 1 1	0	0
8	B	2	Total Gd 2 2	0	0
8	D	1	Total Gd 1 1	0	0

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 10 is water.

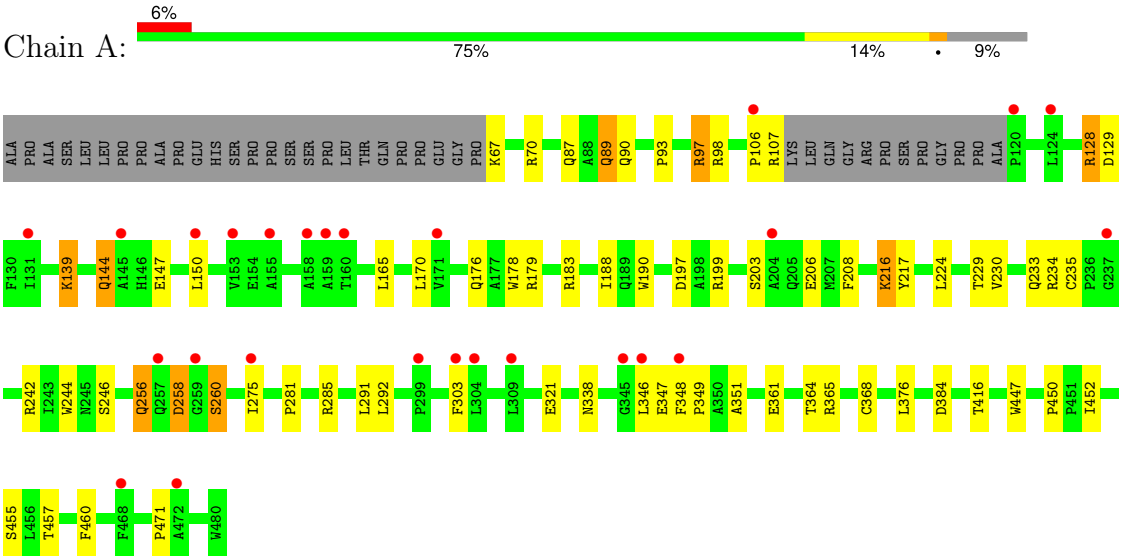
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	146	Total O 146 146	0	0
10	B	218	Total O 218 218	0	0
10	C	150	Total O 150 150	0	0
10	D	256	Total O 256 256	0	0

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.

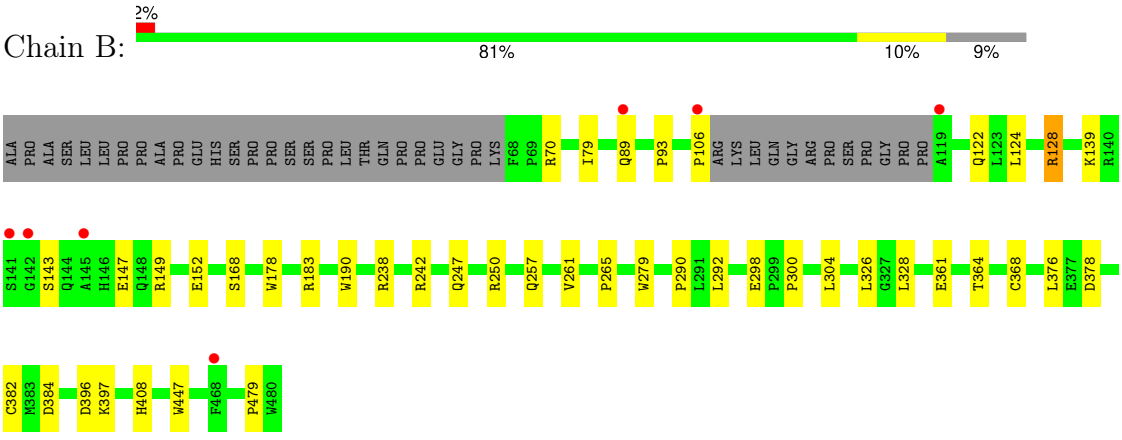
• Molecule 1: Nitric oxide synthase, endothelial

Chain A:



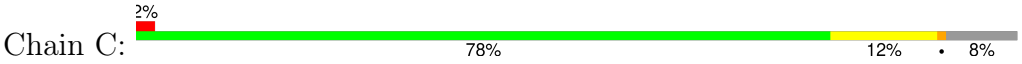
• Molecule 1: Nitric oxide synthase, endothelial

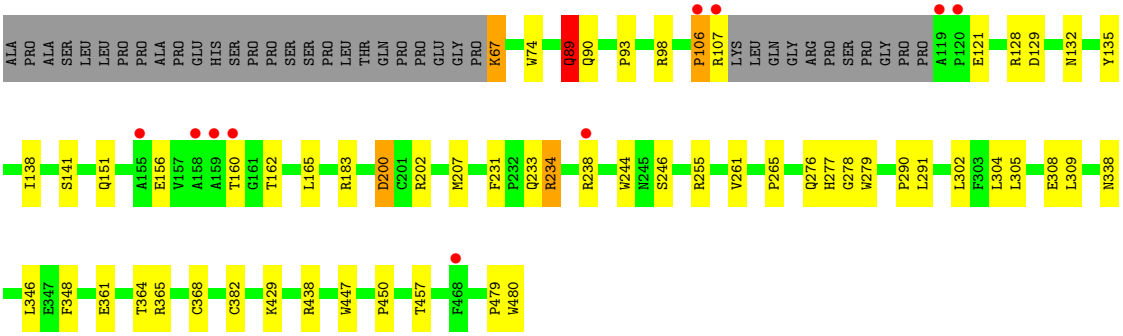
Chain B:



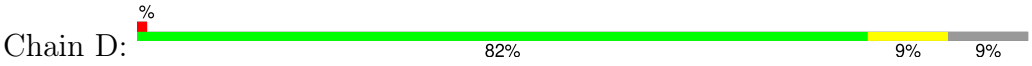
• Molecule 1: Nitric oxide synthase, endothelial

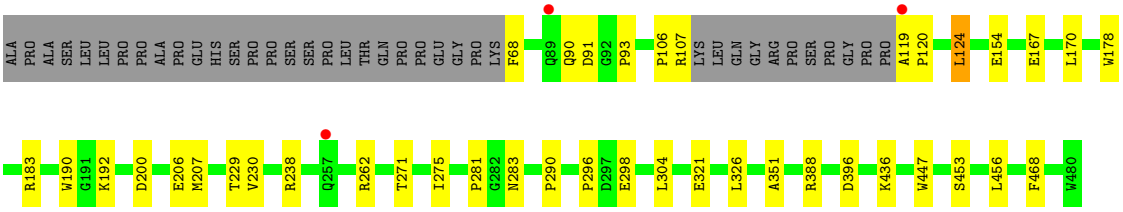
Chain C:





• Molecule 1: Nitric oxide synthase, endothelial





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.24Å 152.04Å 107.73Å 90.00° 90.57° 90.00°	Depositor
Resolution (Å)	46.73 – 1.92 46.73 – 1.92	Depositor EDS
% Data completeness (in resolution range)	94.3 (46.73-1.92) 98.2 (46.73-1.92)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.193 , 0.232 0.188 , 0.227	Depositor DCC
R_{free} test set	7309 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.097 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14141	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GD, GOL, ZN, CL, H4B, BTB, A1A3F, 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	0.35	0/3313	0.56	0/4512
1	B	0.42	0/3312	0.58	0/4514
1	C	0.36	0/3318	0.56	0/4520
1	D	0.43	0/3303	0.59	0/4501
All	All	0.39	0/13246	0.57	0/18047

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3218	0	3125	40	0
1	B	3211	0	3114	34	0
1	C	3223	0	3129	33	0
1	D	3211	0	3111	24	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
2	C	43	0	30	5	0
2	D	43	0	30	3	0
3	A	17	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	1	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	19	0	0	2	0
4	B	19	0	0	2	0
4	C	19	0	0	1	0
4	D	19	0	0	1	0
5	A	42	0	56	5	0
5	B	42	0	55	8	0
5	C	28	0	36	7	0
5	D	28	0	36	5	0
6	A	12	0	15	0	0
6	B	6	0	8	0	0
6	C	18	0	24	0	0
6	D	6	0	8	1	0
7	A	1	0	0	1	0
7	B	1	0	0	1	0
7	C	1	0	0	0	0
7	D	1	0	0	1	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	146	0	0	3	0
10	B	218	0	0	4	0
10	C	150	0	0	2	0
10	D	256	0	0	5	0
All	All	14141	0	12897	156	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 6.

All (156) 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)
4:D:503:A1A3F:N20	7:D:507:CL:CL	2.42	0.89
5:C:504:BTB:O3	10:C:601:HOH:O	2.04	0.74
4:A:503:A1A3F:N20	7:A:508:CL:CL	2.59	0.72
4:B:503:A1A3F:N20	7:B:507:CL:CL	2.59	0.71
1:D:183:ARG:HB2	2:D:501:HEM:HBD2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:NH2	10:A:603:HOH:O	2.25	0.69
1:C:129:ASP:HA	1:C:132:ASN:HD22	1.56	0.69
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.76	0.68
1:D:167:GLU:OE2	10:D:601:HOH:O	2.12	0.67
1:C:382:CYS:HA	5:C:504:BTB:H12	1.74	0.67
1:B:298:GLU:CD	5:B:505:BTB:H42	2.15	0.66
1:A:233:GLN:NE2	10:A:601:HOH:O	2.19	0.66
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.78	0.66
1:C:128:ARG:O	1:C:132:ASN:ND2	2.29	0.66
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.79	0.65
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.78	0.65
1:A:242:ARG:HD2	1:A:349:PRO:HB2	1.78	0.65
5:B:505:BTB:O3	5:B:505:BTB:O8	2.15	0.65
1:A:321:GLU:H	1:A:321:GLU:CD	2.00	0.64
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.81	0.63
1:B:149:ARG:NH1	1:B:152:GLU:OE2	2.33	0.61
1:A:93:PRO:HB3	1:A:106:PRO:HB2	1.82	0.61
1:B:183:ARG:HB2	2:B:501:HEM:CBD	2.30	0.61
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.83	0.61
1:C:93:PRO:HB3	1:C:106:PRO:HB2	1.83	0.60
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.14	0.60
1:B:397:LYS:NZ	10:B:604:HOH:O	2.35	0.60
1:B:70:ARG:HD2	1:B:79:ILE:HD13	1.85	0.59
1:D:124:LEU:HD11	1:D:154:GLU:HG3	1.85	0.58
1:C:160:THR:HG23	1:C:162:THR:H	1.68	0.58
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.84	0.58
1:A:128:ARG:HH11	1:A:128:ARG:HB2	1.68	0.58
1:B:292:LEU:HD22	1:B:300:PRO:HB2	1.86	0.57
1:C:183:ARG:HB2	2:C:501:HEM:CBD	2.34	0.57
1:D:183:ARG:HB2	2:D:501:HEM:CBD	2.34	0.57
1:D:68:PHE:N	10:D:604:HOH:O	2.37	0.56
1:D:298:GLU:OE2	5:D:505:BTB:H52	2.06	0.56
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.87	0.56
1:B:298:GLU:OE1	5:B:505:BTB:H72	2.06	0.56
1:D:107:ARG:NH1	10:D:609:HOH:O	2.39	0.55
5:D:505:BTB:H61	5:D:505:BTB:H32	1.87	0.55
5:B:509:BTB:O6	5:B:509:BTB:O1	2.22	0.55
1:D:90:GLN:HB3	1:D:468:PHE:CD1	2.41	0.55
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.42	0.55
5:C:505:BTB:O4	5:C:505:BTB:O1	2.23	0.55
5:C:504:BTB:O8	5:C:504:BTB:H62	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.43	0.54
1:D:91:ASP:OD1	10:D:602:HOH:O	2.18	0.54
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.90	0.54
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.89	0.54
1:B:124:LEU:HB3	1:B:128:ARG:HH12	1.72	0.53
1:D:238:ARG:HG3	1:D:296:PRO:HB3	1.91	0.53
1:A:256:GLN:NE2	1:A:260:SER:O	2.41	0.53
1:A:256:GLN:C	1:A:258:ASP:H	2.12	0.53
1:A:183:ARG:HB2	2:A:501:HEM:CBD	2.39	0.52
1:B:408:HIS:ND1	10:B:603:HOH:O	2.34	0.52
1:C:165:LEU:HG	1:C:346:LEU:HD12	1.91	0.52
1:B:183:ARG:HB2	2:B:501:HEM:HBD2	1.92	0.51
1:C:246:SER:HA	1:C:338:ASN:HB3	1.91	0.51
1:B:250:ARG:NH2	10:B:605:HOH:O	2.39	0.51
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.24	0.51
1:A:89:GLN:HG3	1:A:90:GLN:N	2.26	0.51
1:C:200:ASP:OD1	1:C:200:ASP:N	2.42	0.51
1:C:74:TRP:HB3	6:D:506:GOL:H11	1.93	0.51
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.47	0.50
1:A:216:LYS:HG3	1:A:217:TYR:N	2.26	0.50
1:C:479:PRO:HD2	1:C:480:TRP:CZ3	2.47	0.49
5:A:505:BTB:O4	5:A:505:BTB:O3	2.22	0.49
1:C:244:TRP:CD1	1:C:479:PRO:HG2	2.47	0.49
1:B:447:TRP:HA	3:B:502:H4B:N1	2.28	0.48
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.48	0.48
1:D:388:ARG:CZ	1:D:388:ARG:HB2	2.43	0.48
1:A:361:GLU:OE2	4:A:503:A1A3F:N02	2.47	0.48
1:B:298:GLU:HG2	10:B:677:HOH:O	2.13	0.48
1:A:384:ASP:OD1	5:A:504:BTB:O3	2.33	0.47
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.97	0.47
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.32	0.47
1:C:234:ARG:HA	1:C:238:ARG:NH2	2.29	0.47
1:D:447:TRP:HA	3:D:502:H4B:N1	2.29	0.47
1:B:298:GLU:OE1	5:B:505:BTB:H42	2.15	0.47
1:A:176:GLN:HB2	1:A:471:PRO:HG2	1.98	0.46
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.48	0.46
1:D:283:ASN:ND2	10:D:613:HOH:O	2.43	0.46
1:B:361:GLU:OE2	4:B:503:A1A3F:N02	2.48	0.46
1:A:183:ARG:HB2	2:A:501:HEM:HBD1	1.98	0.46
1:D:119:ALA:N	1:D:120:PRO:HD3	2.30	0.46
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:GLU:OE2	4:C:503:A1A3F:N02	2.48	0.46
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.98	0.46
1:A:224:LEU:HB2	1:A:416:THR:HB	1.98	0.46
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.55	0.46
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.98	0.46
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.51	0.45
5:A:506:BTB:H11	5:A:506:BTB:H51	1.45	0.45
1:B:382:CYS:SG	5:C:504:BTB:H42	2.57	0.45
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.81	0.45
1:C:429:LYS:HA	1:C:429:LYS:HD2	1.71	0.45
5:D:505:BTB:O4	5:D:505:BTB:O1	2.18	0.45
1:D:271:THR:O	1:D:275:ILE:HG12	2.17	0.45
1:A:208:PHE:CE1	1:A:303:PHE:HB3	2.51	0.45
5:A:505:BTB:H11	5:A:505:BTB:H51	1.49	0.45
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.33	0.45
1:B:384:ASP:OD2	5:B:509:BTB:H31	2.17	0.45
1:B:93:PRO:HG3	1:B:106:PRO:HB3	1.98	0.44
1:C:156:GLU:O	1:C:160:THR:HG22	2.17	0.44
1:D:93:PRO:HB3	1:D:106:PRO:HB2	2.00	0.44
1:D:229:THR:O	1:D:351:ALA:HA	2.17	0.44
1:A:170:LEU:HD11	1:A:230:VAL:HG11	2.00	0.44
1:A:170:LEU:HD11	1:A:230:VAL:HG21	1.99	0.44
1:B:250:ARG:HD2	1:B:250:ARG:HA	1.73	0.44
1:C:67:LYS:HA	1:C:67:LYS:HD3	1.82	0.44
1:B:364:THR:O	1:B:368:CYS:HB2	2.18	0.44
5:D:505:BTB:H72	5:D:505:BTB:H11	1.78	0.43
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.49	0.43
1:A:246:SER:HA	1:A:338:ASN:HB3	2.00	0.43
1:A:229:THR:O	1:A:351:ALA:HA	2.19	0.43
1:B:261:VAL:HG11	1:B:265:PRO:HA	2.01	0.43
1:C:276:GLN:O	1:C:278:GLY:N	2.46	0.43
1:A:364:THR:HG21	1:A:452:ILE:HG23	2.00	0.43
1:C:291:LEU:HD11	1:C:305:LEU:HD21	2.01	0.43
1:D:183:ARG:HD3	1:D:447:TRP:CD2	2.54	0.43
1:C:90:GLN:NE2	10:C:608:HOH:O	2.43	0.43
5:B:509:BTB:H42	5:B:509:BTB:H51	1.49	0.42
1:C:233:GLN:O	1:C:238:ARG:NH2	2.52	0.42
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.54	0.42
1:D:170:LEU:HD11	1:D:230:VAL:HG11	2.01	0.42
1:A:197:ASP:OD2	1:A:199:ARG:NH2	2.44	0.42
1:D:453:SER:HB3	1:D:456:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ARG:O	10:A:602:HOH:O	2.22	0.42
2:C:501:HEM:HBB2	2:C:501:HEM:CHC	2.46	0.42
1:A:147:GLU:OE1	1:A:147:GLU:N	2.43	0.42
1:A:244:TRP:HB2	1:A:292:LEU:HB2	2.02	0.42
1:C:364:THR:O	1:C:368:CYS:HB2	2.20	0.42
1:A:165:LEU:HG	1:A:346:LEU:HD12	2.03	0.41
1:B:143:SER:O	1:B:147:GLU:HG2	2.19	0.41
1:A:450:PRO:HG2	1:A:457:THR:HG21	2.02	0.41
1:B:279:TRP:CG	1:B:290:PRO:HG3	2.56	0.41
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.93	0.41
5:B:505:BTB:H42	5:B:505:BTB:H72	1.96	0.41
1:B:326:LEU:HB3	1:B:328:LEU:HG	2.02	0.41
1:B:93:PRO:HB3	1:B:106:PRO:HB3	2.01	0.41
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.61	0.41
1:C:261:VAL:HG11	1:C:265:PRO:HA	2.02	0.41
1:B:183:ARG:HD3	1:B:447:TRP:CD2	2.55	0.41
5:A:505:BTB:H41	5:A:505:BTB:H72	1.44	0.41
1:B:378:ASP:OD1	5:C:504:BTB:O4	2.39	0.41
1:A:89:GLN:CG	1:A:90:GLN:N	2.84	0.41
1:A:139:LYS:HE3	1:A:139:LYS:HB2	1.67	0.41
1:B:290:PRO:HB3	1:B:304:LEU:HD23	2.03	0.41
1:C:183:ARG:HB2	2:C:501:HEM:HBD1	2.02	0.41
1:C:89:GLN:H	1:C:89:GLN:HG2	1.52	0.40
1:C:135:TYR:HA	1:C:138:ILE:HG12	2.03	0.40
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.55	0.40
1:C:290:PRO:HB3	1:C:304:LEU:HD12	2.04	0.40
1:A:455:SER:HA	1:A:460:PHE:CG	2.57	0.40
5:C:505:BTB:H32	5:C:505:BTB:H52	1.84	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	399/440 (91%)	383 (96%)	14 (4%)	2 (0%)	25 13
1	B	400/440 (91%)	393 (98%)	6 (2%)	1 (0%)	37 26
1	C	400/440 (91%)	390 (98%)	7 (2%)	3 (1%)	16 6
1	D	398/440 (90%)	386 (97%)	12 (3%)	0	100 100
All	All	1597/1760 (91%)	1552 (97%)	39 (2%)	6 (0%)	30 19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	B	89	GLN
1	C	89	GLN
1	A	203	SER
1	C	277	HIS
1	C	106	PRO

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	343/373 (92%)	325 (95%)	18 (5%)	19 7
1	B	343/373 (92%)	335 (98%)	8 (2%)	45 30
1	C	343/373 (92%)	329 (96%)	14 (4%)	26 11
1	D	341/373 (91%)	332 (97%)	9 (3%)	41 26
All	All	1370/1492 (92%)	1321 (96%)	49 (4%)	31 14

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LYS
1	A	87	GLN
1	A	89	GLN
1	A	97	ARG
1	A	107	ARG

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Mol	Chain	Res	Type
1	A	128	ARG
1	A	129	ASP
1	A	139	LYS
1	A	144	GLN
1	A	188	ILE
1	A	206	GLU
1	A	216	LYS
1	A	235	CYS
1	A	256	GLN
1	A	258	ASP
1	A	260	SER
1	A	285	ARG
1	A	291	LEU
1	B	122	GLN
1	B	128	ARG
1	B	139	LYS
1	B	168[A]	SER
1	B	168[B]	SER
1	B	238	ARG
1	B	257	GLN
1	B	396	ASP
1	C	67	LYS
1	C	89	GLN
1	C	98	ARG
1	C	107	ARG
1	C	121	GLU
1	C	141	SER
1	C	151	GLN
1	C	200	ASP
1	C	202	ARG
1	C	234	ARG
1	C	255	ARG
1	C	308	GLU
1	C	309	LEU
1	C	438	ARG
1	D	124	LEU
1	D	192	LYS
1	D	200	ASP
1	D	206	GLU
1	D	207	MET
1	D	262	ARG
1	D	326	LEU

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Mol	Chain	Res	Type
1	D	396	ASP
1	D	436	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 10 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
5	BTB	A	506	-	13,13,13	0.44	0	7,16,16	0.63	0
6	GOL	C	508	-	5,5,5	0.83	0	5,5,5	0.99	0
2	HEM	C	501	1	42,50,50	1.46	6 (14%)	46,82,82	1.76	9 (19%)
6	GOL	A	511	-	5,5,5	1.36	1 (20%)	5,5,5	1.62	1 (20%)
3	H4B	D	502	-	16,18,18	0.74	0	14,26,26	2.38	4 (28%)
3	H4B	B	502	-	16,18,18	0.76	0	14,26,26	2.55	6 (42%)
3	H4B	C	502	-	16,18,18	0.84	0	14,26,26	2.50	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	A1A3F	C	503	-	20,20,20	1.69	1 (5%)	26,27,27	2.20	9 (34%)
4	A1A3F	D	503	-	20,20,20	1.64	1 (5%)	26,27,27	1.29	3 (11%)
2	HEM	B	501	1	42,50,50	1.46	5 (11%)	46,82,82	1.47	5 (10%)
6	GOL	C	507	-	5,5,5	0.85	0	5,5,5	1.04	0
5	BTB	A	504	8	13,13,13	0.45	0	7,16,16	1.24	1 (14%)
2	HEM	D	501	1	42,50,50	1.50	5 (11%)	46,82,82	1.46	7 (15%)
4	A1A3F	B	503	-	20,20,20	1.80	1 (5%)	26,27,27	1.28	3 (11%)
6	GOL	A	507	-	5,5,5	0.74	0	5,5,5	1.12	1 (20%)
5	BTB	B	509	-	13,13,13	0.59	0	7,16,16	0.78	0
5	BTB	D	504	8	13,13,13	0.42	0	7,16,16	0.99	1 (14%)
5	BTB	D	505	-	13,13,13	0.74	0	7,16,16	1.49	1 (14%)
3	H4B	A	502	-	16,18,18	0.89	0	14,26,26	2.33	4 (28%)
6	GOL	B	506	-	5,5,5	0.79	0	5,5,5	1.02	0
6	GOL	D	506	-	5,5,5	1.15	0	5,5,5	0.81	0
5	BTB	C	504	8	13,13,13	0.45	0	7,16,16	1.13	1 (14%)
4	A1A3F	A	503	-	20,20,20	1.64	1 (5%)	26,27,27	1.86	5 (19%)
2	HEM	A	501	1	42,50,50	1.51	6 (14%)	46,82,82	1.59	11 (23%)
5	BTB	B	505	-	13,13,13	0.44	0	7,16,16	0.96	0
5	BTB	C	505	-	13,13,13	0.35	0	7,16,16	0.37	0
5	BTB	B	504	8	13,13,13	0.45	0	7,16,16	0.57	0
6	GOL	C	506	-	5,5,5	0.76	0	5,5,5	1.05	0
5	BTB	A	505	-	13,13,13	0.43	0	7,16,16	0.92	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
5	BTB	A	506	-	-	14/21/21/21	-
6	GOL	C	508	-	-	4/4/4/4	-
2	HEM	C	501	1	-	2/12/54/54	-
6	GOL	A	511	-	-	3/4/4/4	-
3	H4B	D	502	-	-	1/8/17/17	0/2/2/2
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
4	A1A3F	C	503	-	-	0/9/9/9	0/2/2/2
4	A1A3F	D	503	-	-	5/9/9/9	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	501	1	-	1/12/54/54	-
6	GOL	C	507	-	-	2/4/4/4	-
5	BTB	A	504	8	-	4/21/21/21	-
2	HEM	D	501	1	-	2/12/54/54	-
4	A1A3F	B	503	-	-	5/9/9/9	0/2/2/2
6	GOL	A	507	-	-	2/4/4/4	-
5	BTB	B	509	-	-	14/21/21/21	-
5	BTB	D	504	8	-	4/21/21/21	-
5	BTB	D	505	-	-	8/21/21/21	-
3	H4B	A	502	-	-	3/8/17/17	0/2/2/2
6	GOL	B	506	-	-	2/4/4/4	-
6	GOL	D	506	-	-	3/4/4/4	-
5	BTB	C	504	8	-	2/21/21/21	-
4	A1A3F	A	503	-	-	4/9/9/9	0/2/2/2
2	HEM	A	501	1	-	2/12/54/54	-
5	BTB	B	505	-	-	11/21/21/21	-
5	BTB	C	505	-	-	5/21/21/21	-
5	BTB	B	504	8	-	3/21/21/21	-
6	GOL	C	506	-	-	3/4/4/4	-
5	BTB	A	505	-	-	11/21/21/21	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	A1A3F	C13-C17	-7.42	1.28	1.44
4	A	503	A1A3F	C13-C17	-7.07	1.29	1.44
4	D	503	A1A3F	C13-C17	-6.99	1.29	1.44
4	C	503	A1A3F	C13-C17	-6.89	1.30	1.44
2	D	501	HEM	C3C-C2C	-5.32	1.33	1.40
2	B	501	HEM	C3C-C2C	-4.08	1.34	1.40
2	A	501	HEM	C3C-C2C	-3.75	1.35	1.40
2	B	501	HEM	C3C-CAC	3.43	1.55	1.47
2	C	501	HEM	C3C-CAC	3.39	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.28	1.35	1.40
2	A	501	HEM	C3C-CAC	3.24	1.54	1.47
2	C	501	HEM	CAB-C3B	3.17	1.55	1.47
2	D	501	HEM	C3C-CAC	3.16	1.54	1.47
2	A	501	HEM	CAB-C3B	3.15	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CAB-C3B	3.00	1.55	1.47
2	A	501	HEM	C3C-C4C	2.94	1.45	1.41
2	B	501	HEM	C3C-C4C	2.93	1.45	1.41
2	D	501	HEM	CAB-C3B	2.58	1.54	1.47
2	C	501	HEM	C3C-C4C	2.56	1.45	1.41
2	D	501	HEM	C3C-C4C	2.51	1.45	1.41
2	A	501	HEM	FE-NB	2.35	2.11	1.98
6	A	511	GOL	O2-C2	-2.27	1.36	1.43
2	C	501	HEM	CMB-C2B	2.03	1.54	1.50
2	D	501	HEM	C3D-C2D	-2.03	1.32	1.36
2	B	501	HEM	CMB-C2B	2.03	1.54	1.50
2	C	501	HEM	CHA-C4D	2.01	1.39	1.34
2	A	501	HEM	CMB-C2B	2.00	1.54	1.50

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	503	A1A3F	C06-N01-C02	6.15	122.34	118.52
4	A	503	A1A3F	C06-N01-C02	6.00	122.24	118.52
3	D	502	H4B	C8A-C4A-C4	5.67	119.66	114.50
3	A	502	H4B	C8A-C4A-C4	5.65	119.64	114.50
3	C	502	H4B	C8A-C4A-C4	5.59	119.59	114.50
3	B	502	H4B	C8A-C4A-C4	5.08	119.12	114.50
2	C	501	HEM	CBA-CAA-C2A	-4.46	105.03	112.54
2	C	501	HEM	C4B-CHC-C1C	4.44	128.41	122.56
2	B	501	HEM	CBA-CAA-C2A	-4.43	105.09	112.54
4	A	503	A1A3F	C13-C17-N18	-4.12	167.70	177.87
3	C	502	H4B	C2-N3-C4	4.01	121.54	115.96
4	C	503	A1A3F	C13-C17-N18	-4.01	167.98	177.87
2	A	501	HEM	C4B-CHC-C1C	3.83	127.62	122.56
3	B	502	H4B	N1-C2-N3	-3.80	119.65	125.48
3	B	502	H4B	C2-N3-C4	3.78	121.21	115.96
3	D	502	H4B	C2-N3-C4	3.64	121.03	115.96
4	C	503	A1A3F	C14-C13-C17	3.55	124.34	119.55
2	D	501	HEM	CBD-CAD-C3D	-3.54	102.74	112.53
2	D	501	HEM	CBA-CAA-C2A	-3.52	106.61	112.54
4	B	503	A1A3F	C11-C06-N01	3.52	121.12	116.04
3	A	502	H4B	C2-N3-C4	3.44	120.75	115.96
3	C	502	H4B	N1-C2-N3	-3.44	120.21	125.48
3	A	502	H4B	N1-C2-N3	-3.38	120.30	125.48
3	D	502	H4B	N1-C2-N3	-3.37	120.32	125.48
2	C	501	HEM	C3B-C4B-NB	-3.36	107.06	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	H4B	C11-C10-C9	-3.23	108.16	112.11
4	B	503	A1A3F	C05-C06-C11	-3.14	117.57	121.82
4	D	503	A1A3F	C06-N01-C02	3.11	120.45	118.52
4	C	503	A1A3F	C11-C06-N01	3.11	120.53	116.04
4	C	503	A1A3F	C12-C13-C17	-2.98	115.54	119.55
4	C	503	A1A3F	C05-C06-N01	-2.97	118.90	122.34
2	C	501	HEM	C3D-C4D-ND	-2.96	106.92	110.17
4	D	503	A1A3F	C11-C06-N01	2.96	120.31	116.04
6	A	511	GOL	O1-C1-C2	-2.89	97.36	110.38
2	B	501	HEM	C3B-C2B-C1B	2.86	108.56	106.41
3	B	502	H4B	C2-N1-C8A	2.81	121.28	114.59
2	A	501	HEM	C3B-C2B-C1B	2.77	108.49	106.41
2	B	501	HEM	C4B-CHC-C1C	2.76	126.20	122.56
2	D	501	HEM	CMC-C2C-C3C	2.74	130.17	124.68
4	A	503	A1A3F	C05-C06-N01	-2.68	119.23	122.34
2	A	501	HEM	C4D-ND-C1D	2.67	108.37	105.21
3	B	502	H4B	N2-C2-N3	2.67	121.23	117.22
2	A	501	HEM	C1B-NB-C4B	2.64	108.34	105.21
4	A	503	A1A3F	C11-C06-N01	2.64	119.86	116.04
5	D	505	BTB	C6-C5-N	2.63	121.85	111.59
3	A	502	H4B	C2-N1-C8A	2.62	120.81	114.59
2	A	501	HEM	C3B-C4B-NB	-2.52	107.66	109.47
4	C	503	A1A3F	C13-C14-C15	-2.49	117.79	120.28
3	D	502	H4B	C2-N1-C8A	2.47	120.45	114.59
5	A	504	BTB	O3-C3-C2	2.44	117.14	111.40
4	B	503	A1A3F	C06-N01-C02	2.43	120.03	118.52
2	C	501	HEM	C1B-NB-C4B	2.40	108.06	105.21
2	C	501	HEM	CAD-C3D-C2D	-2.40	123.37	127.87
2	B	501	HEM	CAD-C3D-C2D	-2.36	123.44	127.87
4	A	503	A1A3F	N02-C02-N01	2.36	120.39	116.59
4	D	503	A1A3F	C05-C06-C11	-2.36	118.61	121.82
3	C	502	H4B	C2-N1-C8A	2.33	120.13	114.59
4	C	503	A1A3F	N02-C02-N01	2.31	120.30	116.59
2	C	501	HEM	CMC-C2C-C3C	2.29	129.25	124.68
2	C	501	HEM	C4D-ND-C1D	2.28	107.91	105.21
2	D	501	HEM	C3B-C2B-C1B	2.27	108.12	106.41
2	A	501	HEM	C3D-C4D-ND	-2.26	107.69	110.17
2	A	501	HEM	C4A-C3A-C2A	2.26	108.57	107.00
5	D	504	BTB	O4-C4-C2	-2.25	106.11	111.40
5	C	504	BTB	O3-C3-C2	2.24	116.66	111.40
2	D	501	HEM	C4B-CHC-C1C	2.24	125.51	122.56
2	D	501	HEM	CMA-C3A-C4A	-2.19	125.25	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C2D-C1D-ND	-2.19	107.37	109.90
2	A	501	HEM	CHC-C4B-C3B	2.19	127.91	124.57
4	C	503	A1A3F	C19-C15-C14	-2.17	116.00	120.63
2	D	501	HEM	C3D-C4D-ND	-2.12	107.84	110.17
6	A	507	GOL	C3-C2-C1	-2.09	104.14	111.80
2	B	501	HEM	CMC-C2C-C3C	2.06	128.80	124.68
2	A	501	HEM	CBA-CAA-C2A	-2.03	109.12	112.54
2	A	501	HEM	CMC-C2C-C3C	2.03	128.75	124.68
3	C	502	H4B	O10-C10-C9	-2.02	106.42	109.77
2	C	501	HEM	C3B-C2B-C1B	2.02	107.93	106.41

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	A1A3F	C15-C19-N20-C21
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C4-C2-N-C5
5	A	505	BTB	C4-C2-N-C7
5	A	506	BTB	O1-C1-C2-N
5	A	506	BTB	C1-C2-C3-O3
5	A	506	BTB	C4-C2-C3-O3
5	A	506	BTB	N-C2-C3-O3
5	A	506	BTB	C1-C2-N-C5
5	A	506	BTB	C1-C2-N-C7
5	A	506	BTB	C3-C2-N-C5
5	A	506	BTB	C3-C2-N-C7
5	A	506	BTB	C4-C2-N-C5
5	A	506	BTB	C4-C2-N-C7
5	B	504	BTB	O1-C1-C2-C3
5	B	504	BTB	O1-C1-C2-C4
5	B	504	BTB	O1-C1-C2-N
5	B	505	BTB	C1-C2-C3-O3
5	B	505	BTB	C4-C2-C3-O3
5	B	505	BTB	N-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	B	505	BTB	C1-C2-N-C5
5	B	505	BTB	C1-C2-N-C7
5	B	505	BTB	C3-C2-N-C5
5	B	505	BTB	C3-C2-N-C7
5	B	505	BTB	C4-C2-N-C5
5	B	505	BTB	C4-C2-N-C7
5	B	509	BTB	O1-C1-C2-C4
5	B	509	BTB	C1-C2-C3-O3
5	B	509	BTB	C4-C2-C3-O3
5	B	509	BTB	N-C2-C3-O3
5	B	509	BTB	C3-C2-C4-O4
5	B	509	BTB	C1-C2-N-C5
5	B	509	BTB	C1-C2-N-C7
5	B	509	BTB	C3-C2-N-C5
5	B	509	BTB	C3-C2-N-C7
5	B	509	BTB	C4-C2-N-C5
5	B	509	BTB	C4-C2-N-C7
5	C	505	BTB	O1-C1-C2-C3
5	C	505	BTB	O1-C1-C2-C4
5	C	505	BTB	O1-C1-C2-N
5	D	504	BTB	O1-C1-C2-C3
5	D	504	BTB	O1-C1-C2-C4
5	D	504	BTB	O1-C1-C2-N
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C1-C2-C4-O4
5	D	505	BTB	C3-C2-C4-O4
5	D	505	BTB	N-C2-C4-O4
5	D	505	BTB	C6-C5-N-C2
6	B	506	GOL	O1-C1-C2-C3
6	C	506	GOL	O1-C1-C2-C3
6	C	507	GOL	O1-C1-C2-C3
6	C	508	GOL	O1-C1-C2-O2
6	C	508	GOL	O1-C1-C2-C3
6	D	506	GOL	O1-C1-C2-C3
5	C	505	BTB	N-C5-C6-O6
5	B	509	BTB	N-C5-C6-O6
6	A	507	GOL	C1-C2-C3-O3
6	A	511	GOL	C1-C2-C3-O3
6	C	508	GOL	C1-C2-C3-O3
5	A	505	BTB	N-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
5	B	505	BTB	N-C5-C6-O6
6	A	511	GOL	O2-C2-C3-O3
6	C	506	GOL	O1-C1-C2-O2
6	C	507	GOL	O1-C1-C2-O2
5	B	505	BTB	N-C7-C8-O8
3	B	502	H4B	C7-C6-C9-O9
5	A	505	BTB	N-C5-C6-O6
6	B	506	GOL	O1-C1-C2-O2
6	D	506	GOL	O1-C1-C2-O2
5	A	506	BTB	N-C7-C8-O8
5	C	504	BTB	C4-C2-C3-O3
6	A	511	GOL	O1-C1-C2-O2
6	C	508	GOL	O2-C2-C3-O3
2	B	501	HEM	C3D-CAD-CBD-CGD
2	D	501	HEM	C3D-CAD-CBD-CGD
2	A	501	HEM	C2A-CAA-CBA-CGA
5	C	505	BTB	C6-C5-N-C7
6	D	506	GOL	O2-C2-C3-O3
2	C	501	HEM	C3D-CAD-CBD-CGD
2	A	501	HEM	C1A-C2A-CAA-CBA
5	A	506	BTB	O1-C1-C2-C4
5	D	504	BTB	C3-C2-C4-O4
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C7
6	A	507	GOL	O2-C2-C3-O3
6	C	506	GOL	O2-C2-C3-O3
3	B	502	H4B	C7-C6-C9-C10
4	D	503	A1A3F	N01-C06-C11-C12
4	D	503	A1A3F	N01-C06-C11-C16
5	D	505	BTB	N-C5-C6-O6
4	B	503	A1A3F	N01-C06-C11-C16
4	A	503	A1A3F	N01-C06-C11-C12
4	A	503	A1A3F	N01-C06-C11-C16
4	B	503	A1A3F	C05-C06-C11-C16
3	A	502	H4B	C7-C6-C9-C10
4	A	503	A1A3F	C05-C06-C11-C16
4	A	503	A1A3F	C05-C06-C11-C12
4	D	503	A1A3F	C05-C06-C11-C16
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
4	B	503	A1A3F	N01-C06-C11-C12
4	D	503	A1A3F	C05-C06-C11-C12

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Mol	Chain	Res	Type	Atoms
3	D	502	H4B	C7-C6-C9-O9
5	A	506	BTB	C3-C2-C4-O4
4	D	503	A1A3F	C14-C13-C17-N18
3	A	502	H4B	N5-C6-C9-O9
3	B	502	H4B	N5-C6-C9-O9
3	A	502	H4B	C7-C6-C9-O9
5	A	504	BTB	N-C2-C3-O3
5	A	506	BTB	N-C2-C4-O4
5	B	509	BTB	O1-C1-C2-N
5	B	509	BTB	N-C2-C4-O4
4	B	503	A1A3F	C05-C06-C11-C12
5	C	504	BTB	N-C7-C8-O8

There are no ring outliers.

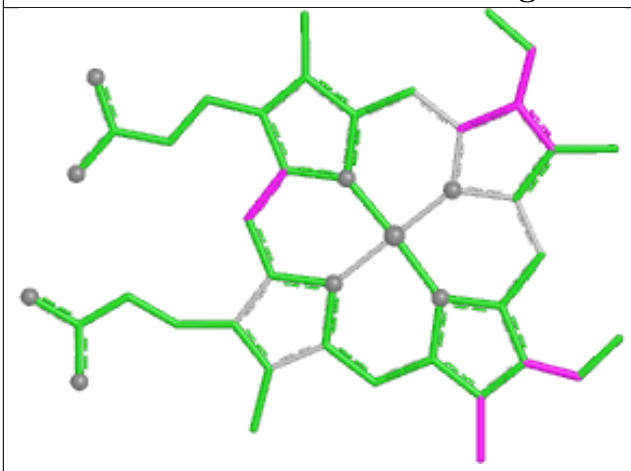
22 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	506	BTB	1	0
2	C	501	HEM	5	0
3	D	502	H4B	1	0
3	B	502	H4B	1	0
3	C	502	H4B	1	0
4	C	503	A1A3F	1	0
4	D	503	A1A3F	1	0
2	B	501	HEM	4	0
5	A	504	BTB	1	0
2	D	501	HEM	3	0
4	B	503	A1A3F	2	0
5	B	509	BTB	3	0
5	D	504	BTB	1	0
5	D	505	BTB	4	0
3	A	502	H4B	1	0
6	D	506	GOL	1	0
5	C	504	BTB	5	0
4	A	503	A1A3F	2	0
2	A	501	HEM	3	0
5	B	505	BTB	5	0
5	C	505	BTB	2	0
5	A	505	BTB	3	0

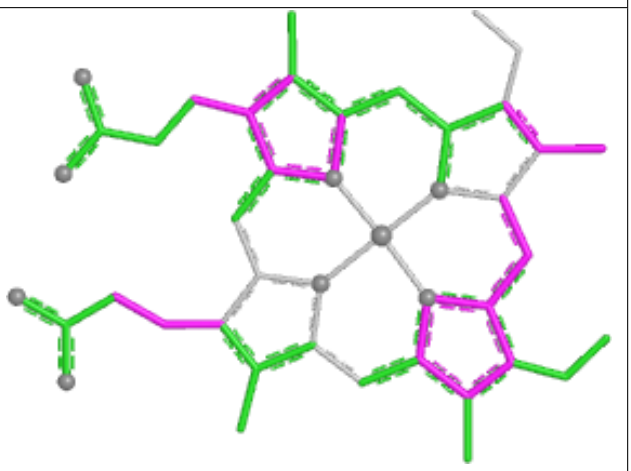
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

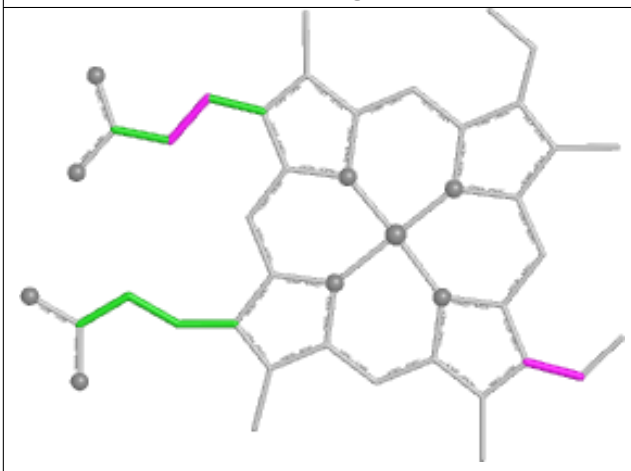
Ligand HEM C 501



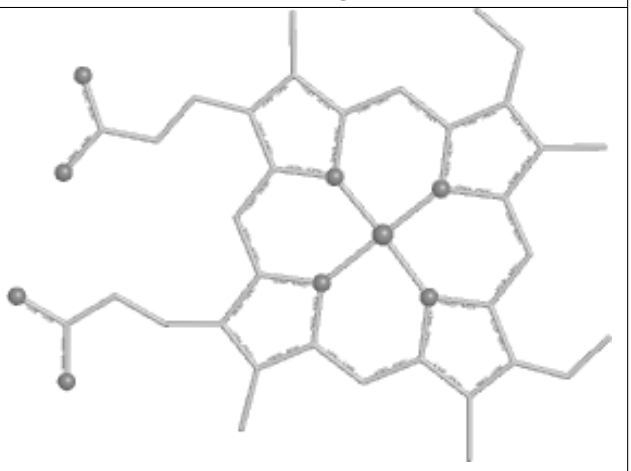
Bond lengths



Bond angles

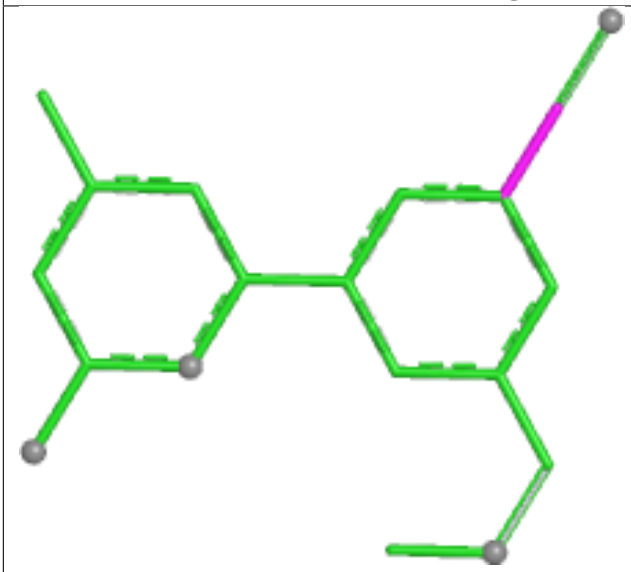


Torsions

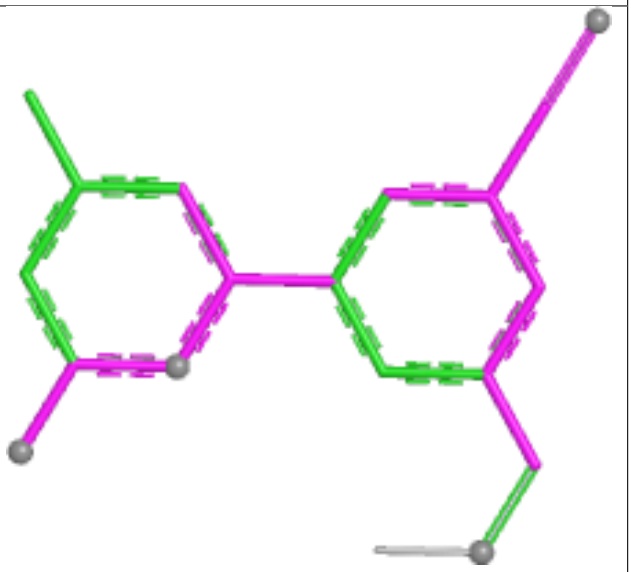


Rings

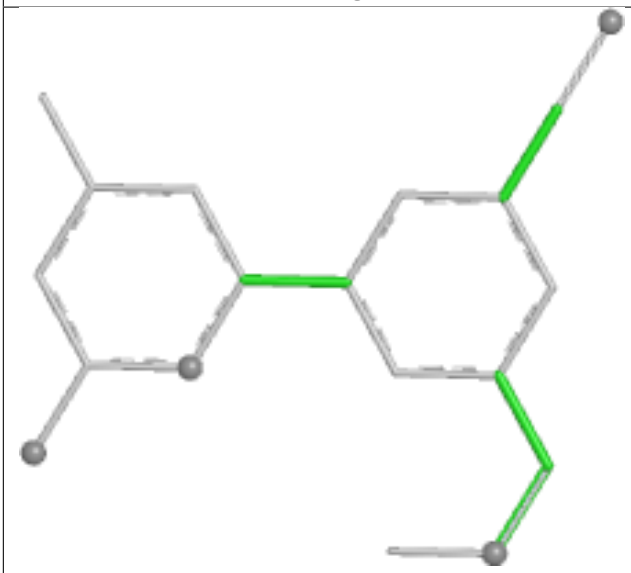
Ligand A1A3F C 503



Bond lengths



Bond angles



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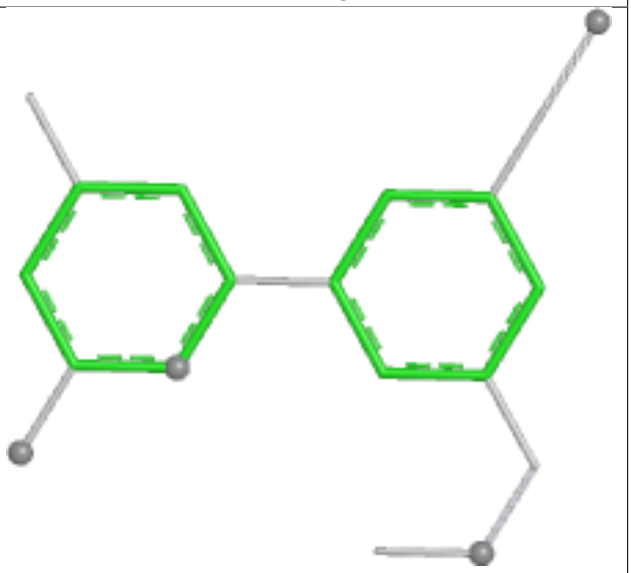
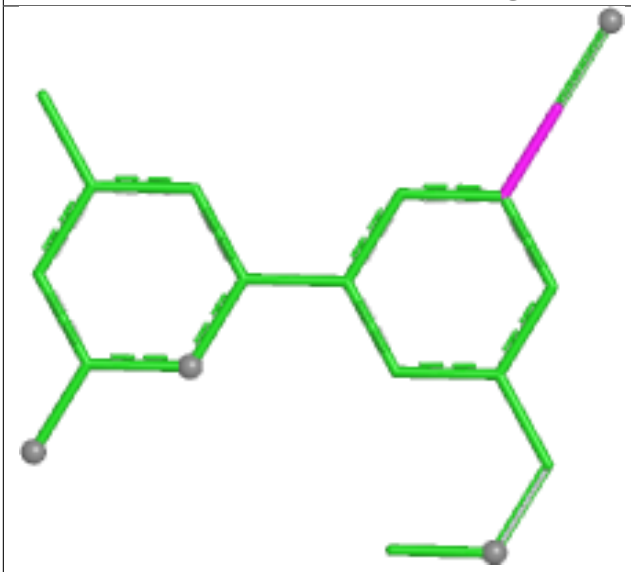
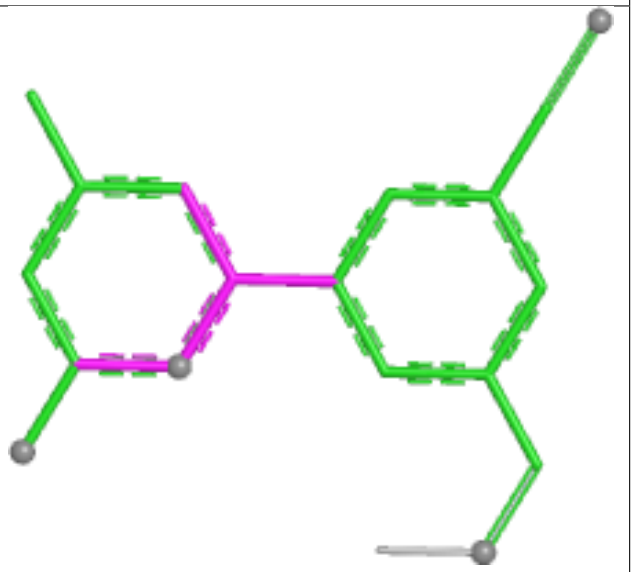


Rings

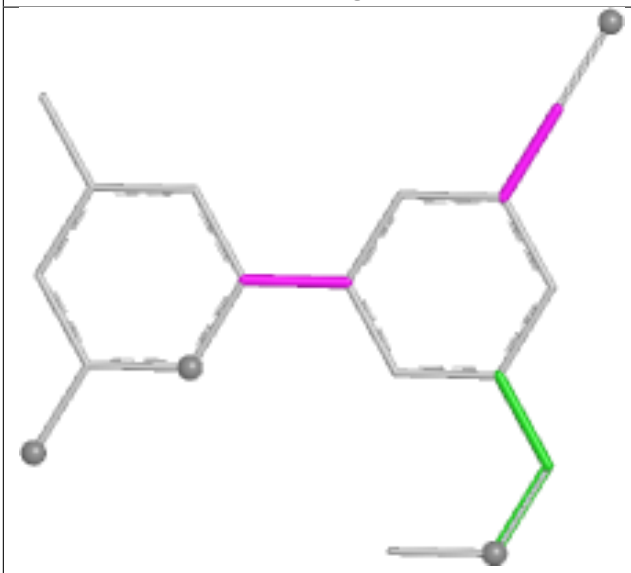
Ligand A1A3F D 503



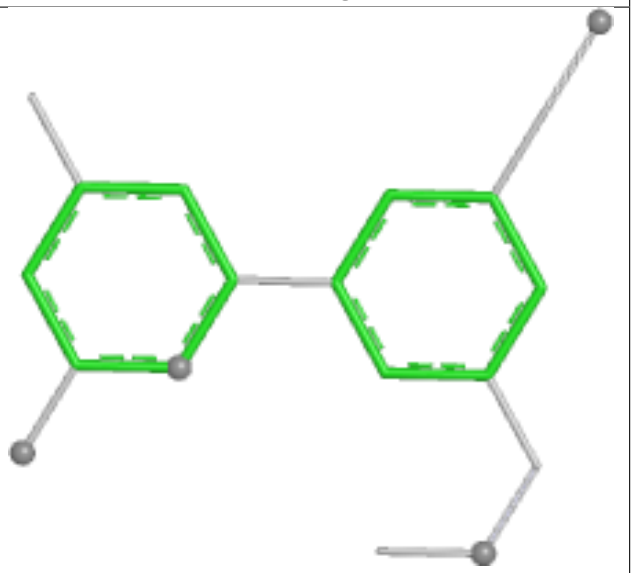
Bond lengths



Bond angles

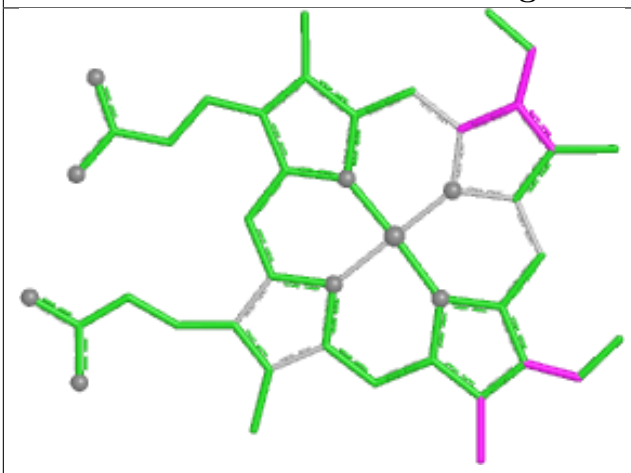


Torsions

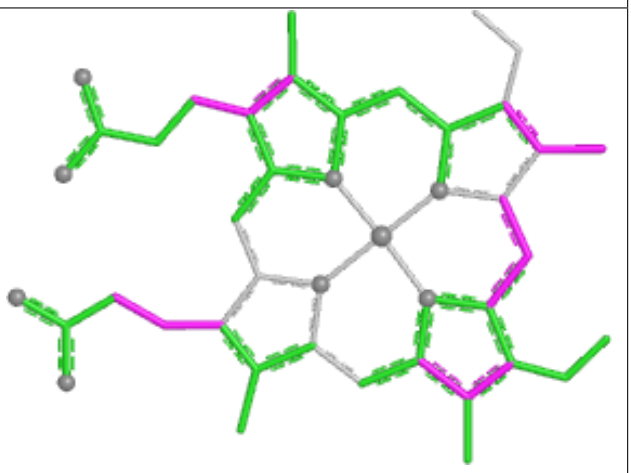


Rings

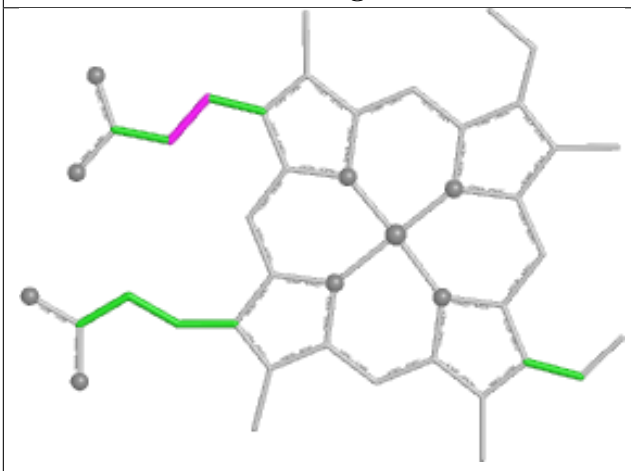
Ligand HEM B 501



Bond lengths



Bond angles



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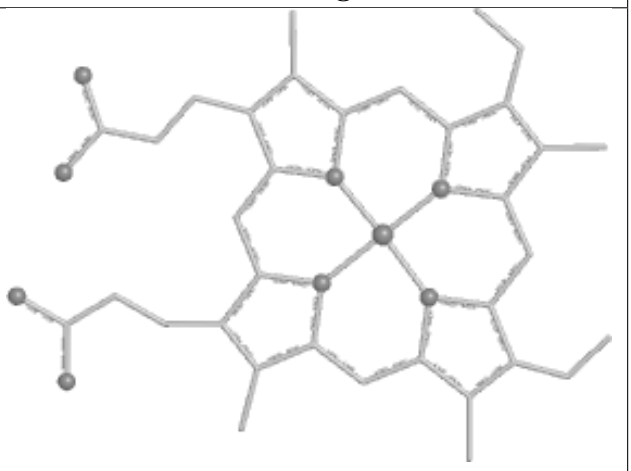
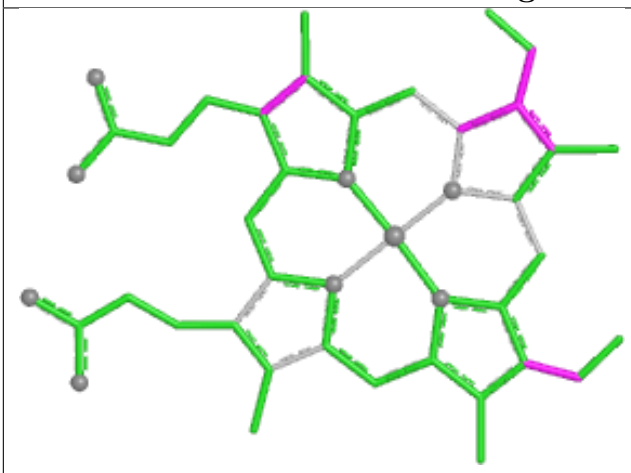
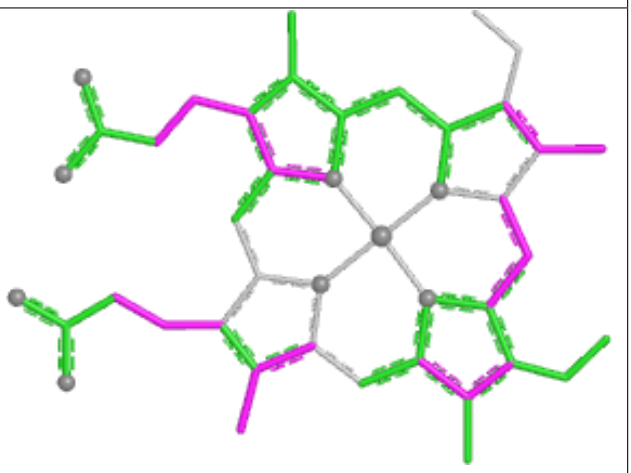


Rings

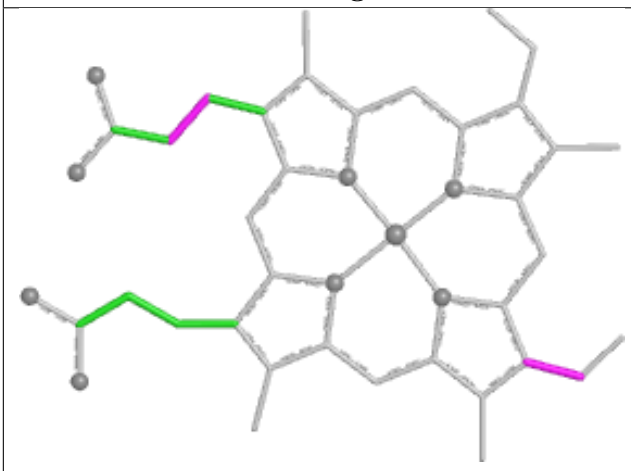
Ligand HEM D 501



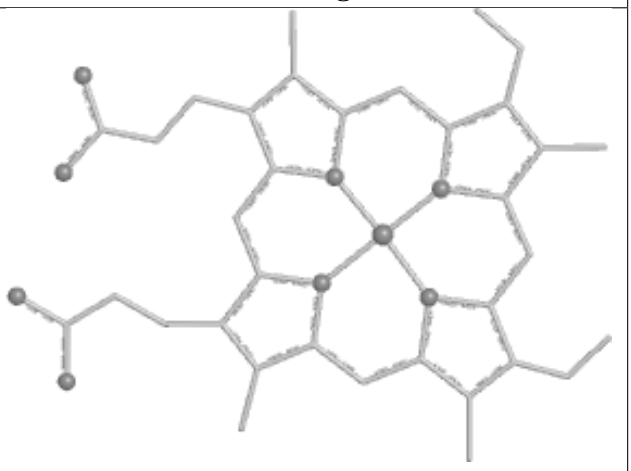
Bond lengths



Bond angles

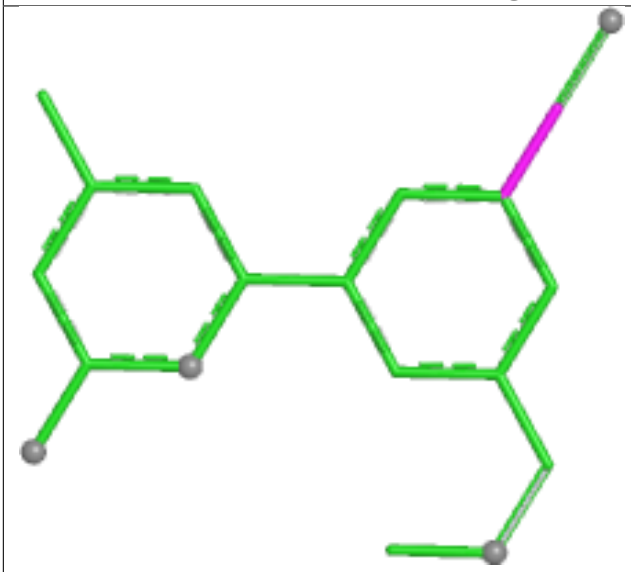


Torsions

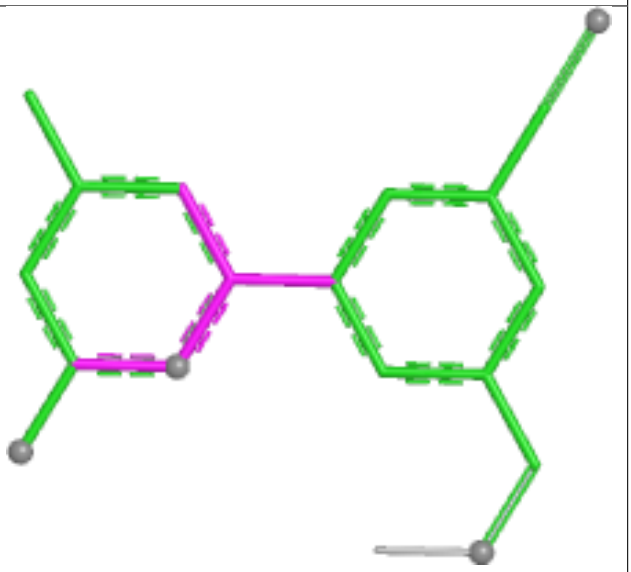


Rings

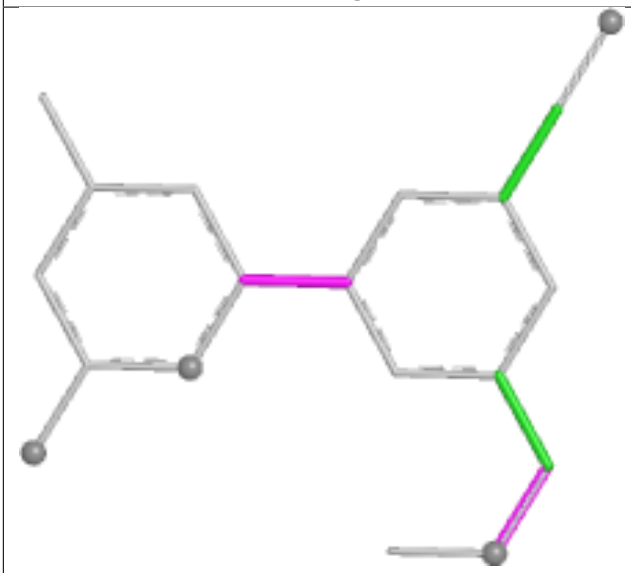
Ligand A1A3F B 503



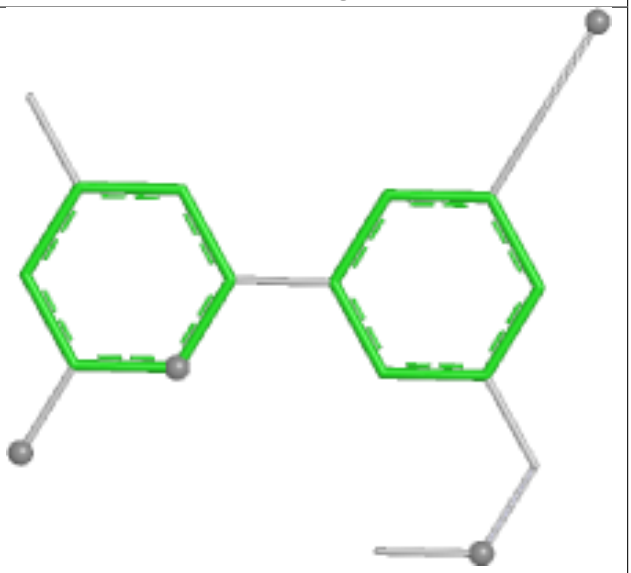
Bond lengths



Bond angles

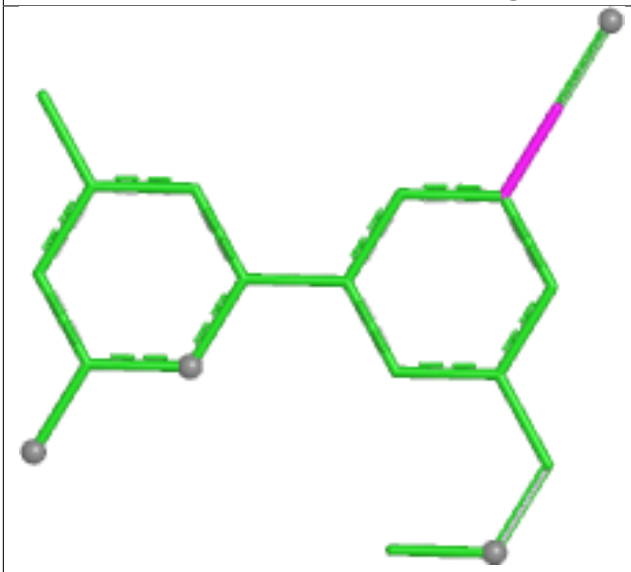


Torsions

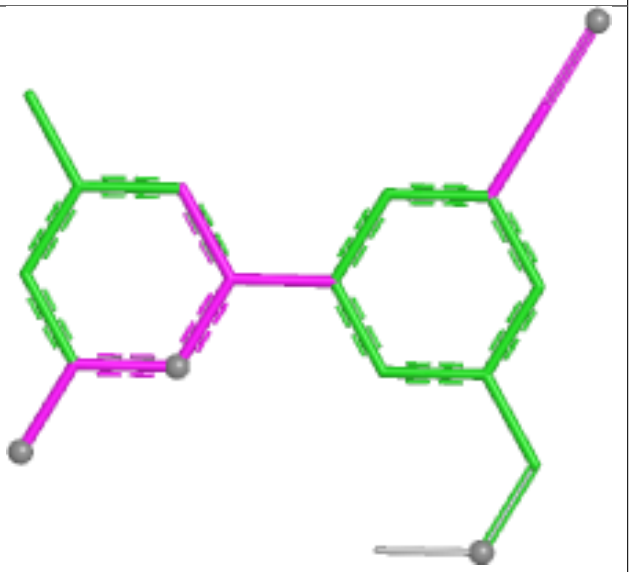


Rings

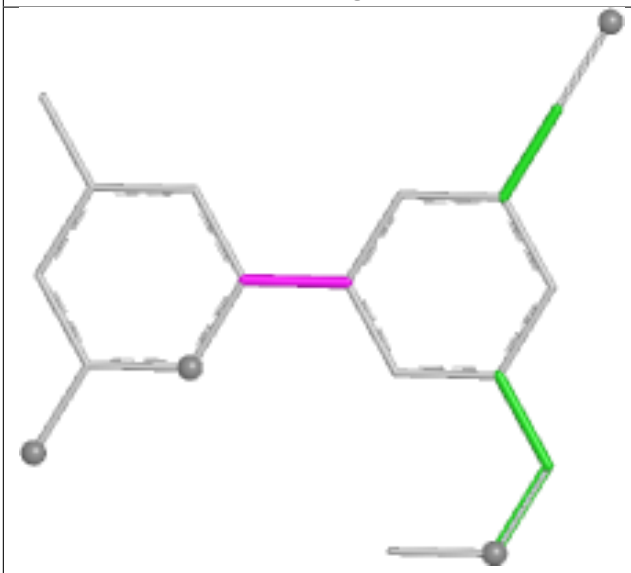
Ligand A1A3F A 503



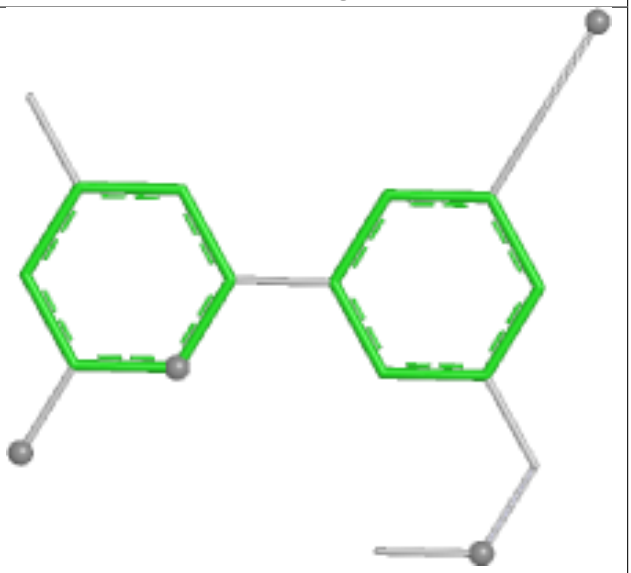
Bond lengths



Bond angles

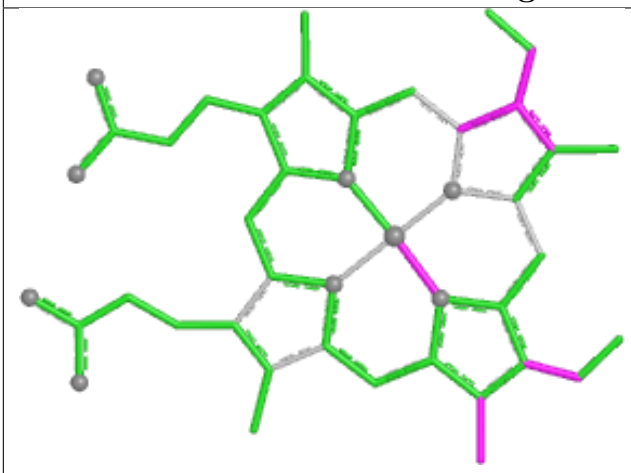


Torsions

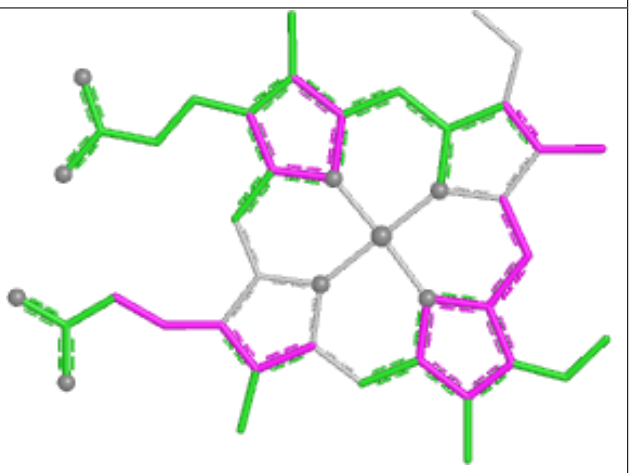


Rings

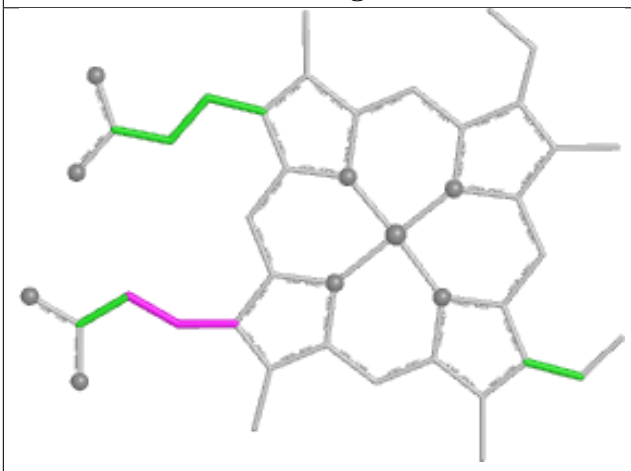
Ligand HEM A 501



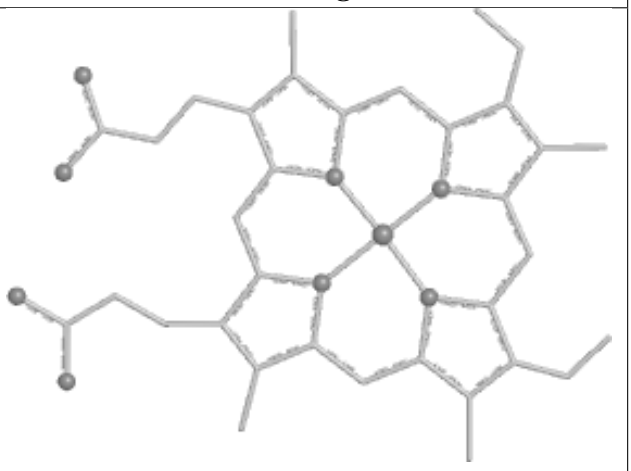
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	402/440 (91%)	0.54	26 (6%) 26 31	24, 57, 104, 129	1 (0%)
1	B	401/440 (91%)	-0.05	7 (1%) 69 74	21, 39, 69, 116	3 (0%)
1	C	403/440 (91%)	0.27	10 (2%) 58 64	28, 53, 94, 111	1 (0%)
1	D	402/440 (91%)	-0.11	3 (0%) 84 88	25, 39, 59, 120	0
All	All	1608/1760 (91%)	0.16	46 (2%) 54 59	21, 46, 92, 129	5 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	119	ALA	4.2
1	A	120	PRO	4.1
1	A	204	ALA	3.4
1	A	159	ALA	3.2
1	D	257	GLN	3.2
1	A	106	PRO	2.9
1	A	145	ALA	2.9
1	B	145	ALA	2.9
1	A	158	ALA	2.8
1	C	155	ALA	2.8
1	A	345	GLY	2.8
1	C	106	PRO	2.7
1	A	348	PHE	2.6
1	C	468	PHE	2.6
1	A	150	LEU	2.6
1	A	309	LEU	2.5
1	B	142	GLY	2.5
1	C	119	ALA	2.5
1	C	158	ALA	2.5
1	C	120	PRO	2.5
1	D	89	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	160	THR	2.5
1	A	124	LEU	2.4
1	A	304	LEU	2.4
1	A	275	ILE	2.3
1	B	119	ALA	2.3
1	C	159	ALA	2.3
1	A	299	PRO	2.3
1	A	472	ALA	2.3
1	A	160	THR	2.3
1	C	107	ARG	2.3
1	A	257	GLN	2.2
1	A	153	VAL	2.2
1	A	237	GLY	2.2
1	A	259	GLY	2.2
1	A	303	PHE	2.2
1	C	238	ARG	2.2
1	A	171	VAL	2.1
1	A	468	PHE	2.1
1	A	346	LEU	2.1
1	A	131	ILE	2.1
1	A	155	ALA	2.1
1	B	89	GLN	2.1
1	B	106	PRO	2.1
1	B	468	PHE	2.1
1	B	141[A]	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

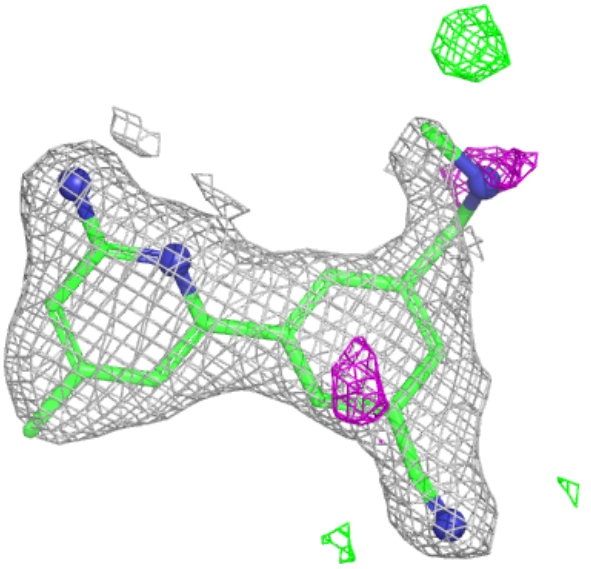
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

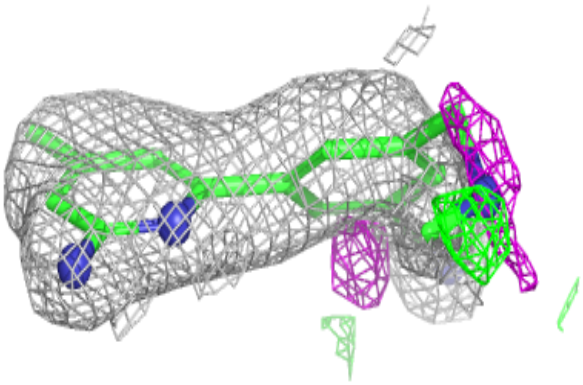
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BTB	C	505	14/14	0.63	0.14	90,101,105,105	0
5	BTB	A	506	14/14	0.64	0.17	87,101,104,104	0
6	GOL	C	507	6/6	0.69	0.14	64,75,78,78	0
6	GOL	C	508	6/6	0.72	0.11	82,85,86,90	0
6	GOL	D	506	6/6	0.73	0.20	49,59,64,68	0
5	BTB	D	505	14/14	0.75	0.17	63,70,82,82	0
6	GOL	A	507	6/6	0.78	0.11	68,75,77,79	0
5	BTB	A	505	14/14	0.81	0.16	67,74,79,79	0
5	BTB	B	505	14/14	0.83	0.13	52,71,76,77	0
5	BTB	B	509	14/14	0.83	0.15	60,68,73,74	0
5	BTB	D	504	14/14	0.85	0.14	52,62,72,81	0
5	BTB	A	504	14/14	0.87	0.13	63,72,76,78	0
3	H4B	A	502	17/17	0.87	0.11	46,49,55,58	0
4	A1A3F	C	503	19/19	0.87	0.14	39,51,78,80	0
5	BTB	C	504	14/14	0.88	0.12	42,54,64,65	0
6	GOL	B	506	6/6	0.88	0.15	51,52,58,65	0
6	GOL	C	506	6/6	0.88	0.10	63,65,70,70	0
6	GOL	A	511	6/6	0.89	0.13	45,52,57,62	0
4	A1A3F	A	503	19/19	0.89	0.13	40,53,65,65	0
3	H4B	C	502	17/17	0.89	0.10	40,43,51,52	0
5	BTB	B	504	14/14	0.90	0.13	43,52,57,60	0
4	A1A3F	B	503	19/19	0.90	0.12	26,37,58,61	0
4	A1A3F	D	503	19/19	0.92	0.11	24,38,58,60	0
3	H4B	D	502	17/17	0.92	0.08	34,40,41,42	0
3	H4B	B	502	17/17	0.94	0.08	33,38,41,42	0
2	HEM	A	501	43/43	0.96	0.10	40,47,57,67	0
7	CL	A	508	1/1	0.96	0.09	53,53,53,53	0
8	GD	B	510	1/1	0.97	0.05	60,60,60,60	1
2	HEM	B	501	43/43	0.98	0.07	25,29,42,67	0
2	HEM	C	501	43/43	0.98	0.08	36,42,52,61	0
8	GD	A	509	1/1	0.98	0.04	78,78,78,78	1
2	HEM	D	501	43/43	0.98	0.07	22,27,42,65	0
8	GD	D	508	1/1	0.98	0.04	47,47,47,47	0
7	CL	B	507	1/1	0.99	0.09	38,38,38,38	0
8	GD	B	508	1/1	0.99	0.04	44,44,44,44	0
7	CL	C	509	1/1	0.99	0.05	46,46,46,46	0
7	CL	D	507	1/1	0.99	0.05	38,38,38,38	0
9	ZN	A	510	1/1	0.99	0.03	39,39,39,39	0
9	ZN	C	510	1/1	1.00	0.02	35,35,35,35	0

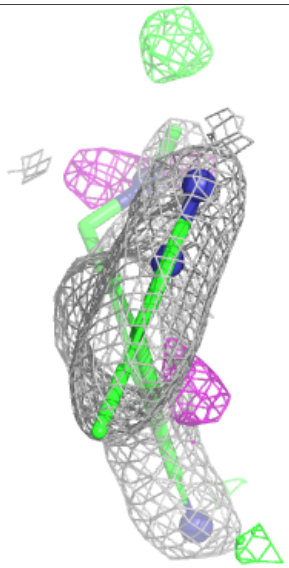
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1A3F C 503:

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

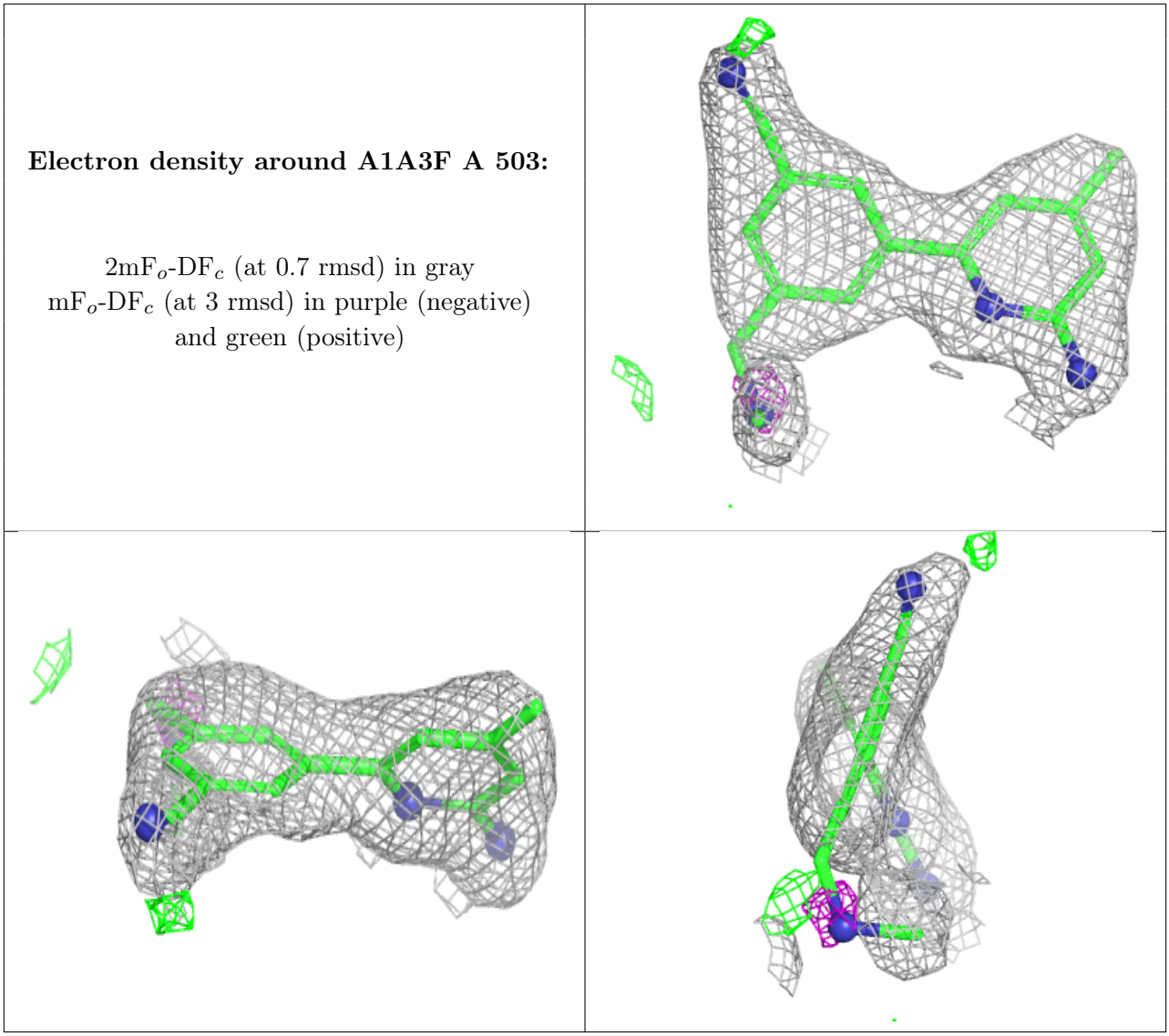






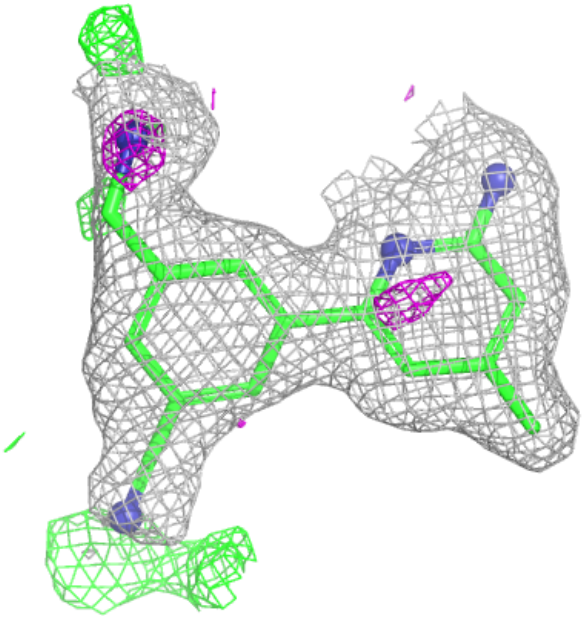
Electron density around A1A3F A 503:

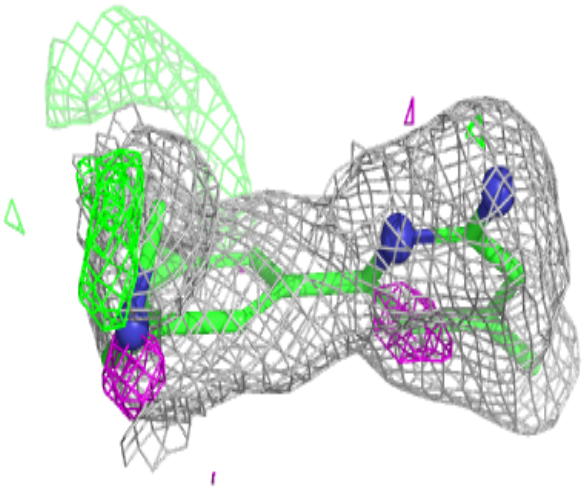
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

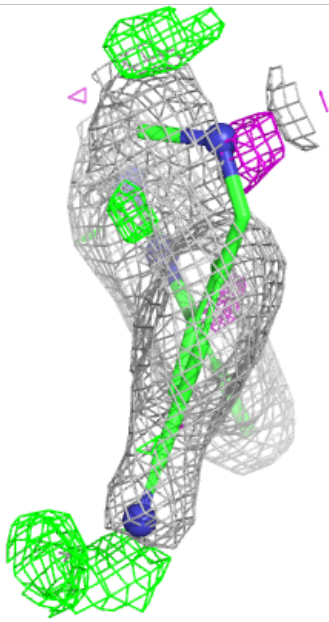


Electron density around A1A3F B 503:

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

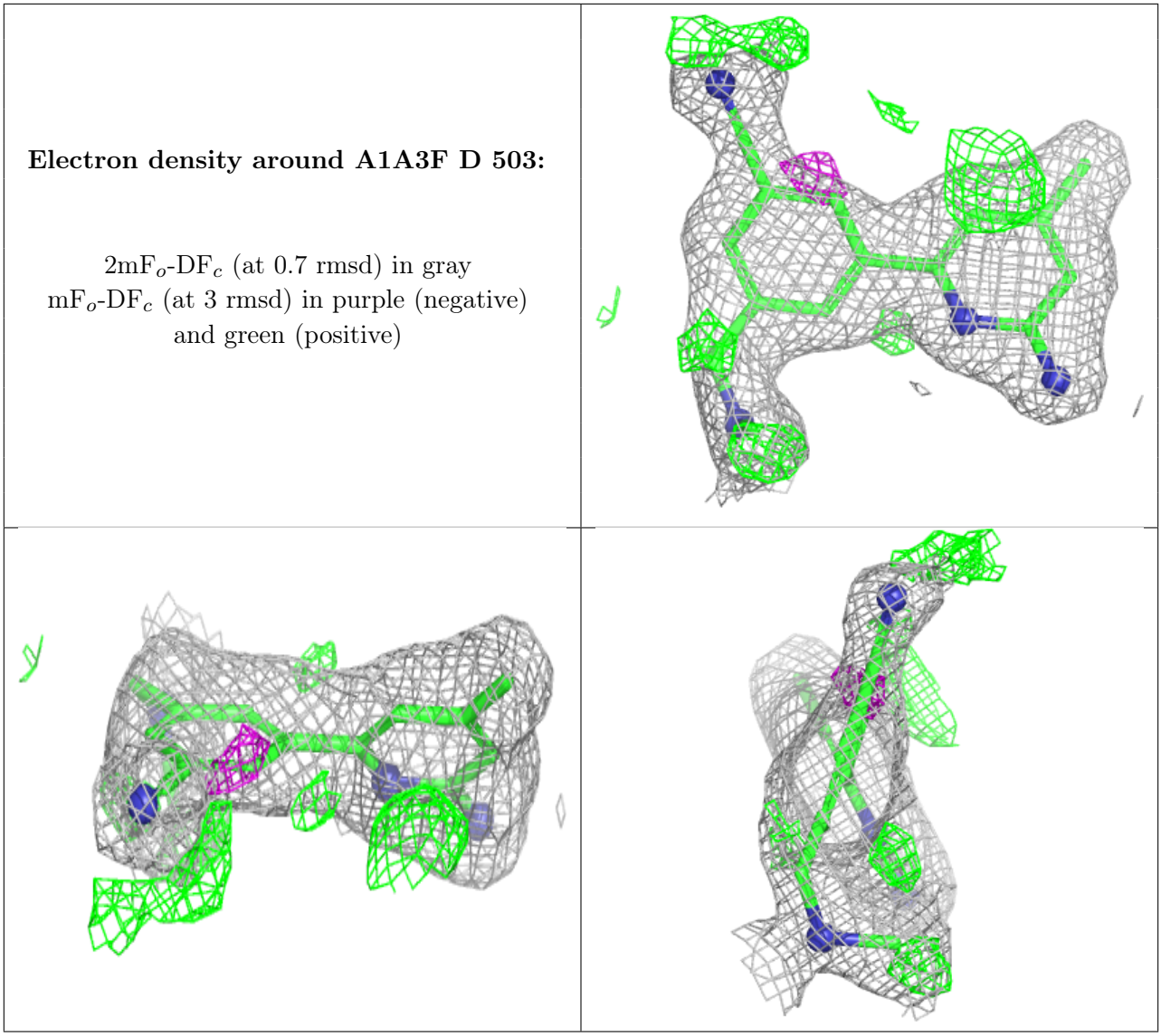






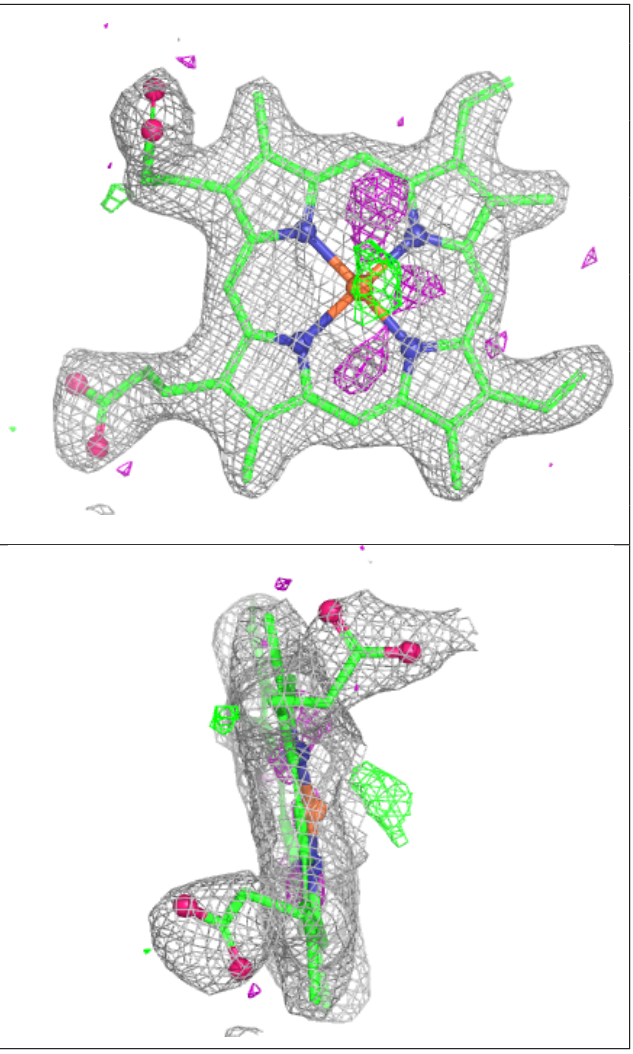
Electron density around A1A3F D 503:

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



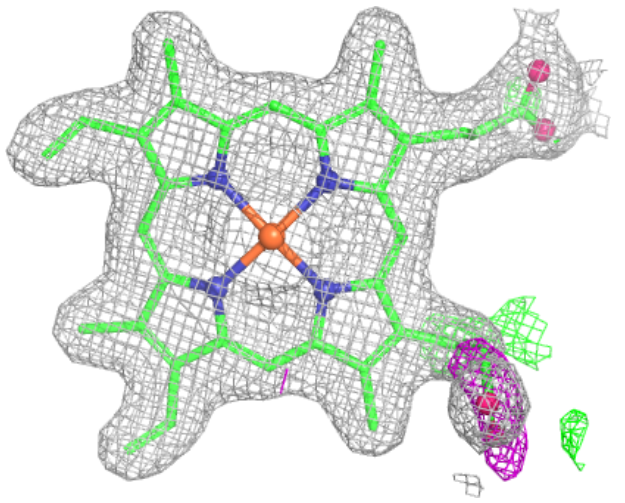
Electron density around HEM A 501:

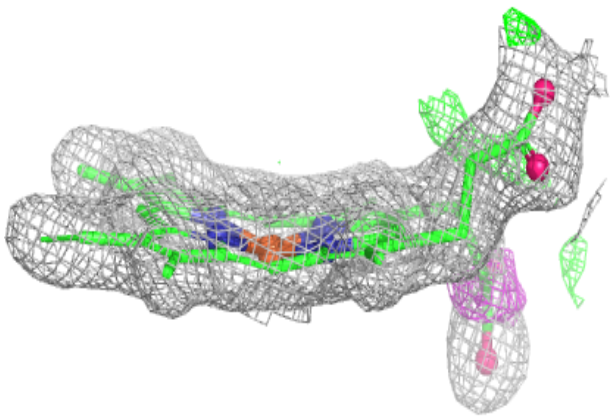
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

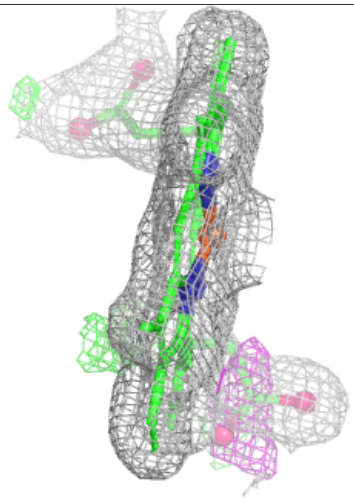


Electron density around HEM B 501:

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

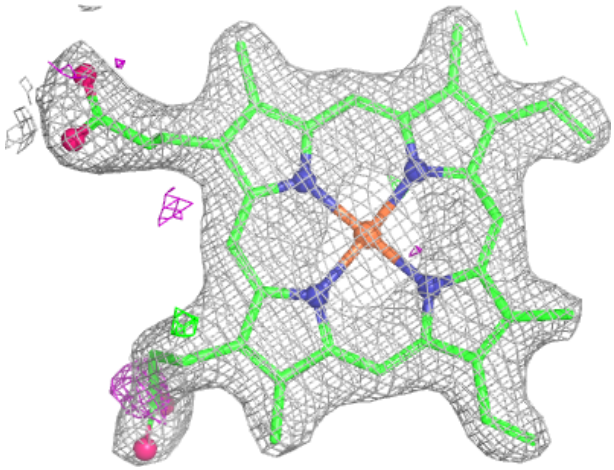


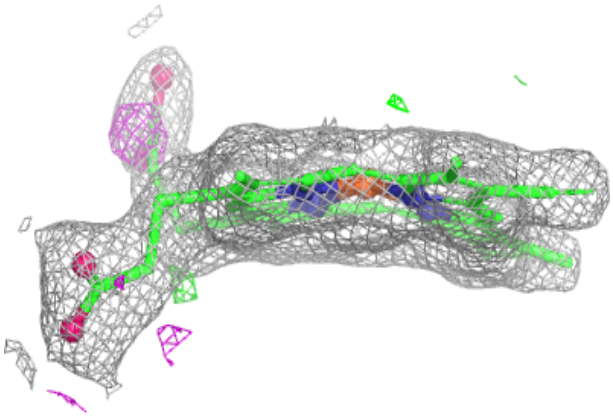


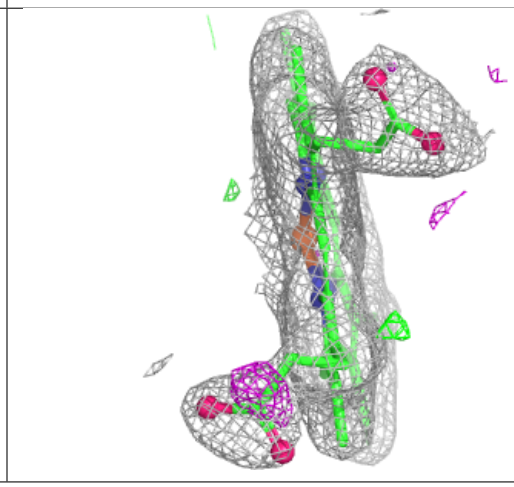


Electron density around HEM C 501:

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

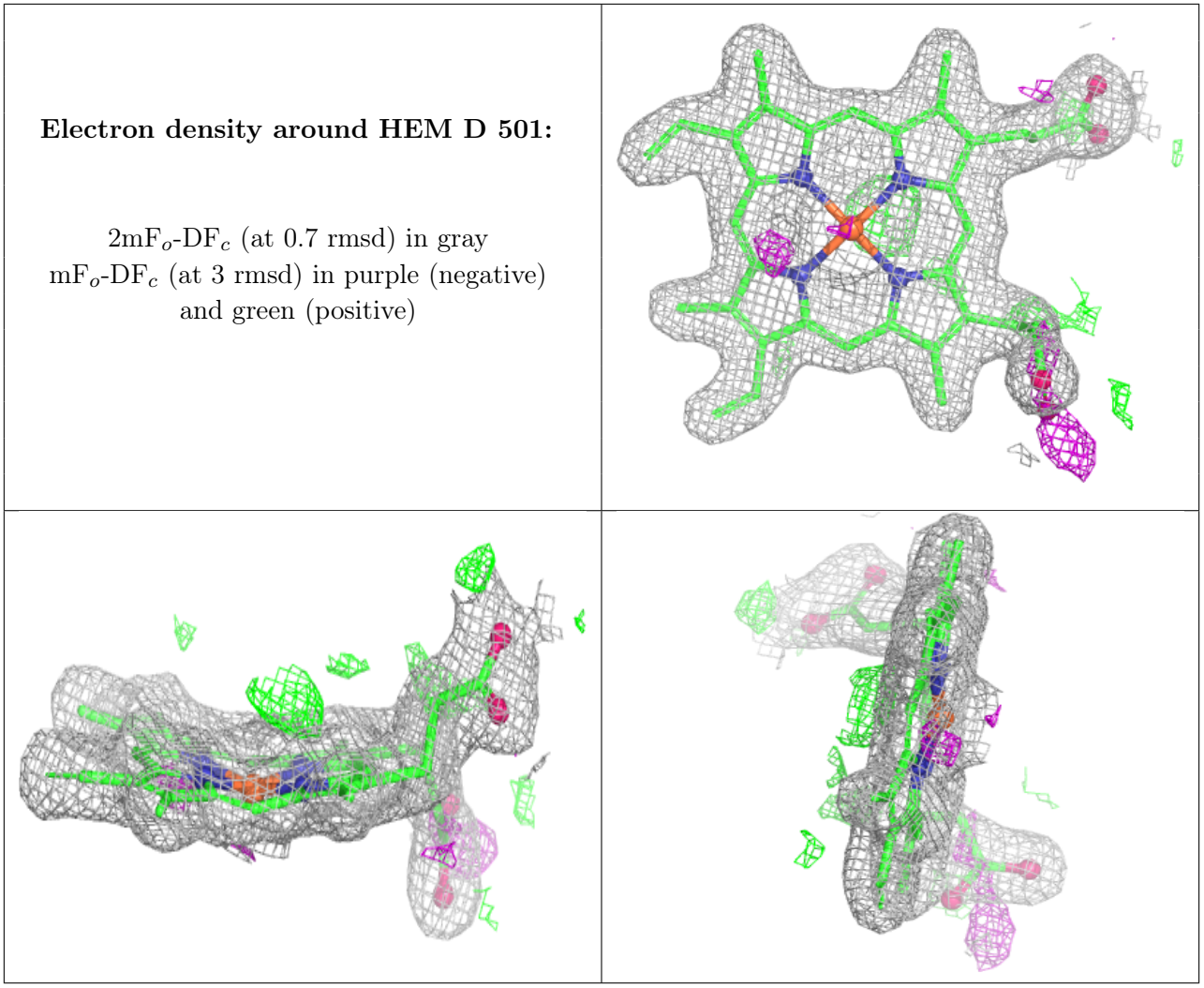






Electron density around HEM D 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.