Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2023 – 01:39 AM EDT

PDB ID	:	8FGS
Title	:	Structure of human endothelial nitric oxide synthase heme domain in complex with 6-(5-(2-(diethylamino)ethyl)-2,3-difluorophenethyl)-4-methylpyridin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2022-12-12
Resolution	:	1.84 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:

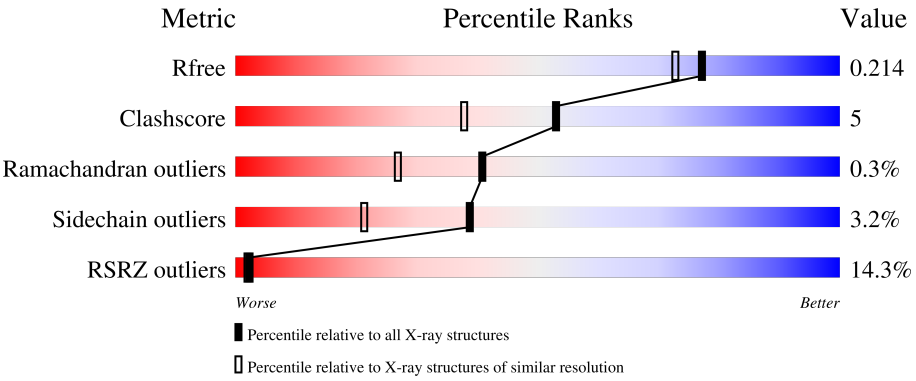
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	20% 78% 11% • 9%
1	B	440	8% 82% 8% 9%
1	C	440	18% 79% 11% • 9%
1	D	440	6% 84% 7% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	C	508	-	X	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14229 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.

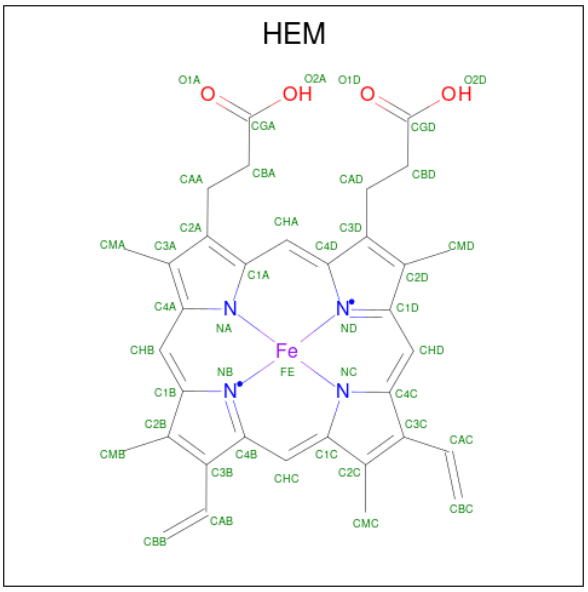
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	1	0
			3207	2043	564	584	16			
1	B	401	Total	C	N	O	S	0	3	0
			3211	2045	564	586	16			
1	C	402	Total	C	N	O	S	0	1	0
			3212	2046	565	585	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:

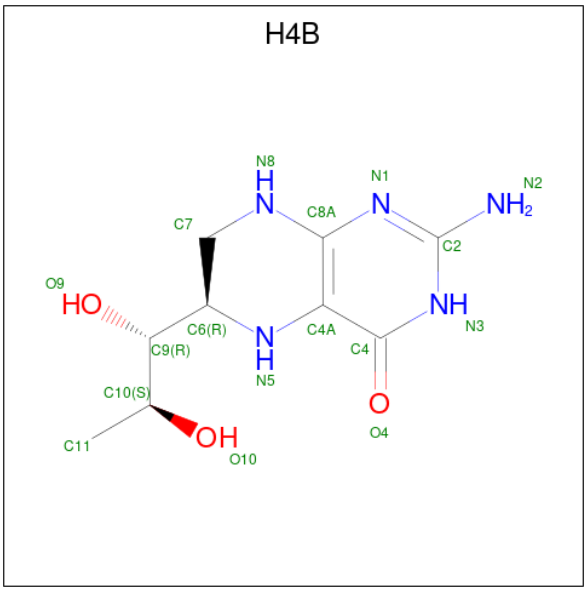
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



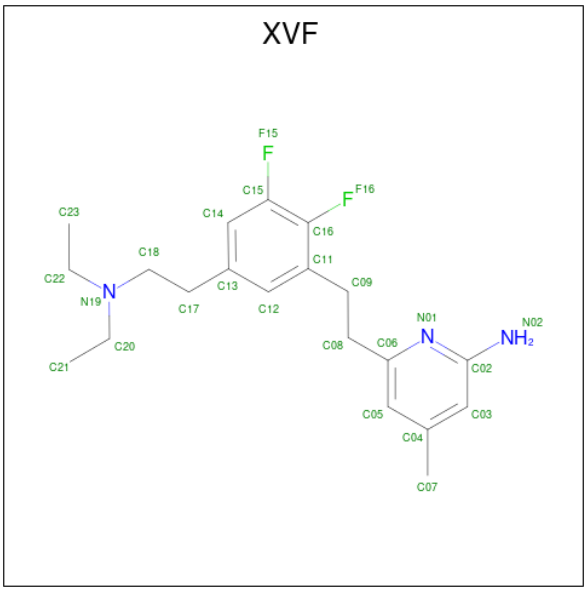
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



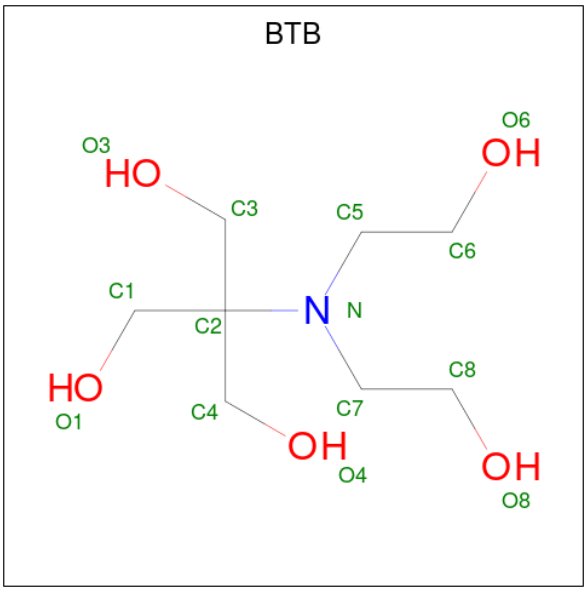
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0
3	C	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is 6-(2-{5-[2-(diethylamino)ethyl]-2,3-difluorophenyl}ethyl)-4-methylpyridin-2-amine (three-letter code: XVF) (formula: $C_{20}H_{27}F_2N_3$) (labeled as "Ligand of Interest" by depositor).



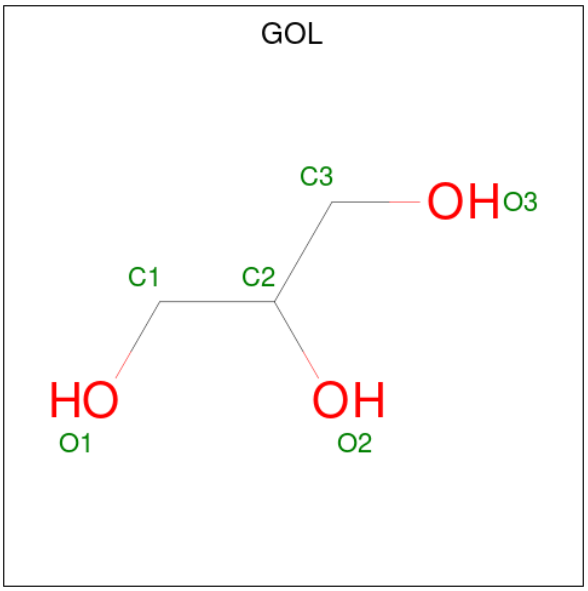
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N 25 20 2 3	0	0
4	B	1	Total C F N 25 20 2 3	0	0
4	C	1	Total C F N 25 20 2 3	0	0
4	D	1	Total C F N 25 20 2 3	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: 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	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	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 (three-letter code: 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	B	1	Total C O 6 3 3	0	0
6	B	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	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 (three-letter code: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 (three-letter code: 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 (three-letter code: 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.

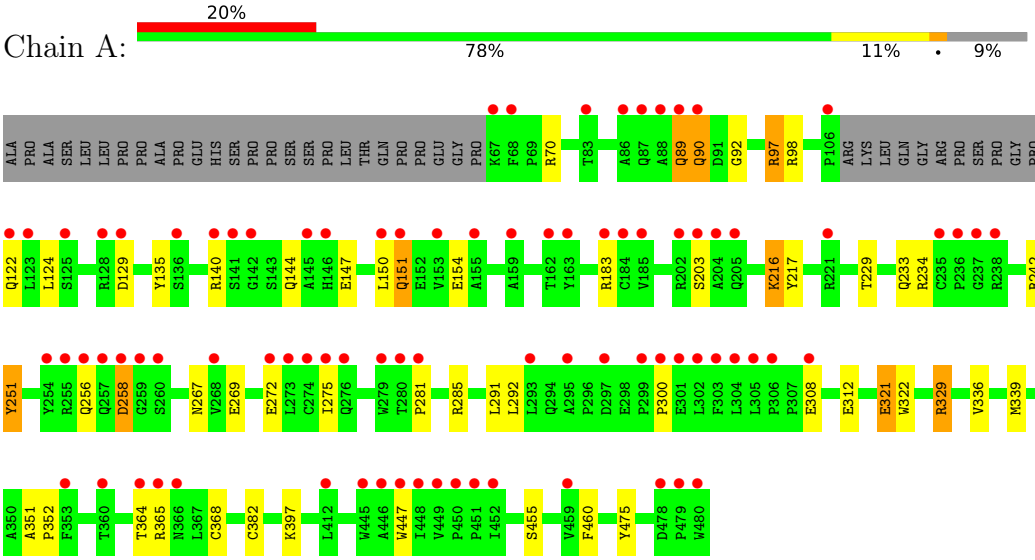
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	156	Total O 156 156	0	0
10	B	231	Total O 231 231	0	0
10	C	174	Total O 174 174	0	0
10	D	271	Total O 271 271	0	0

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.

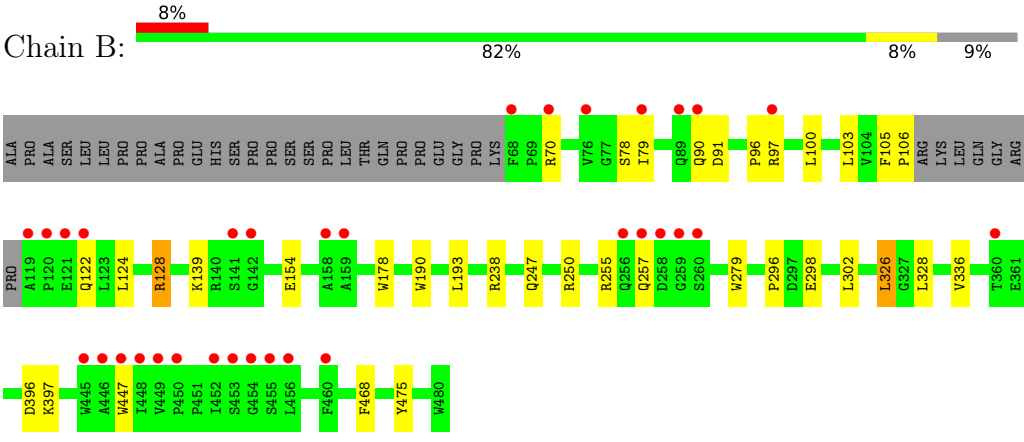
• Molecule 1: Nitric oxide synthase, endothelial

Chain A:



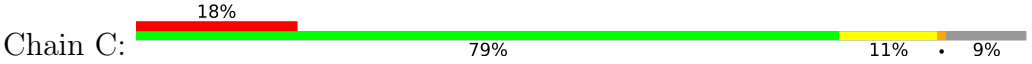
• Molecule 1: Nitric oxide synthase, endothelial

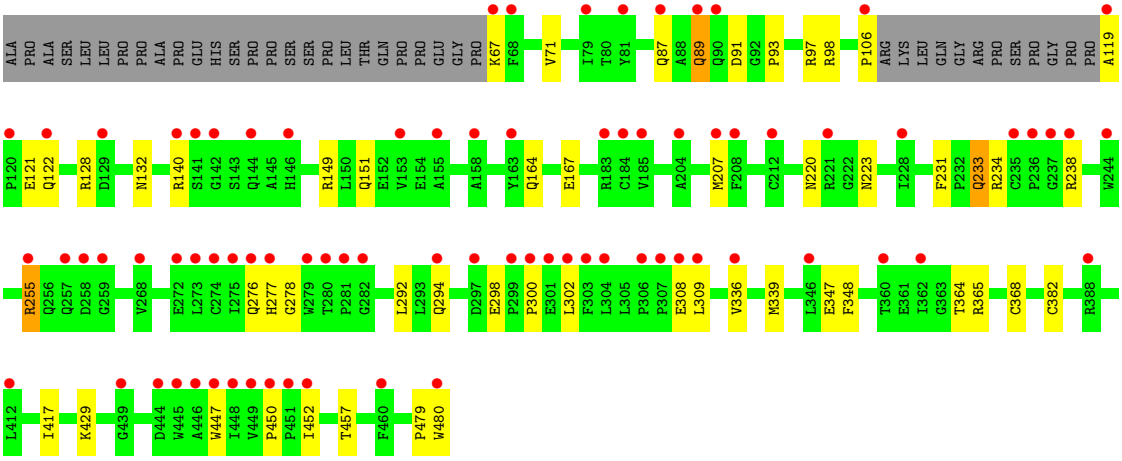
Chain B:



• Molecule 1: Nitric oxide synthase, endothelial

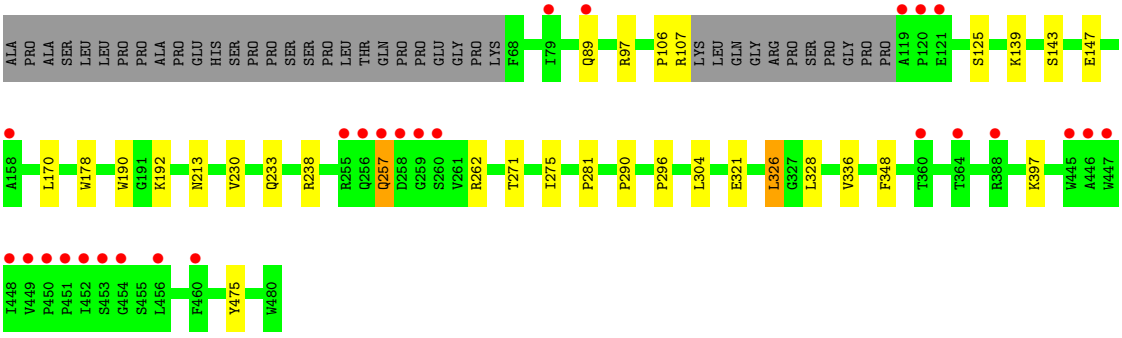
Chain C:





• Molecule 1: Nitric oxide synthase, endothelial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.52Å 153.10Å 108.75Å 90.00° 90.70° 90.00°	Depositor
Resolution (Å)	38.75 – 1.84 39.05 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.75-1.84) 99.4 (39.05-1.84)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.184 , 0.218 0.180 , 0.214	Depositor DCC
R_{free} test set	8364 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.058 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14229	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: BTB, H4B, HEM, GD, CL, XVF, ZN, GOL

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	0.34	0/3302	0.50	0/4498
1	B	0.38	0/3312	0.53	0/4514
1	C	0.34	0/3307	0.50	0/4506
1	D	0.41	0/3303	0.53	0/4501
All	All	0.37	0/13224	0.51	0/18019

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	3207	0	3112	39	0
1	B	3211	0	3114	26	0
1	C	3212	0	3116	27	0
1	D	3211	0	3111	22	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
2	C	43	0	30	3	0
2	D	43	0	30	5	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	3	0
3	D	17	0	15	0	0
4	A	25	0	0	3	0
4	B	25	0	0	3	0
4	C	25	0	0	2	0
4	D	25	0	0	3	0
5	A	42	0	56	8	0
5	B	28	0	36	7	0
5	C	42	0	56	7	0
5	D	28	0	36	3	0
6	A	12	0	16	0	0
6	B	24	0	32	1	0
6	C	24	0	32	1	0
6	D	6	0	8	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	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	156	0	0	4	0
10	B	231	0	0	6	0
10	C	174	0	0	1	0
10	D	271	0	0	4	0
All	All	14229	0	12905	142	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 5.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:O	10:A:601:HOH:O	1.95	0.85
1:A:233:GLN:NE2	10:A:602:HOH:O	2.14	0.80
5:D:504:BTB:O6	5:D:504:BTB:O8	1.99	0.80
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.74	0.69
5:B:505:BTB:O1	10:B:601:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.75	0.67
1:C:276:GLN:O	1:C:278:GLY:N	2.28	0.66
2:B:501:HEM:HBD1	4:B:503:XVF:C15	2.27	0.65
1:C:382:CYS:HA	5:C:504:BTB:H12	1.77	0.65
1:B:397:LYS:NZ	10:B:605:HOH:O	2.32	0.63
1:A:312:GLU:OE2	1:A:329:ARG:NH1	2.31	0.63
1:A:147:GLU:O	1:A:151:GLN:NE2	2.29	0.63
1:D:397:LYS:NZ	10:D:603:HOH:O	2.29	0.63
1:D:213:ASN:ND2	10:D:602:HOH:O	2.27	0.63
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.32	0.63
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.09	0.62
1:A:70:ARG:NH2	10:A:603:HOH:O	2.32	0.62
1:C:128:ARG:O	1:C:132:ASN:ND2	2.32	0.61
5:A:505:BTB:O3	5:A:505:BTB:O4	2.20	0.60
1:C:234:ARG:HA	1:C:238:ARG:HH21	1.67	0.60
1:B:91:ASP:OD1	10:B:602:HOH:O	2.16	0.59
1:A:321:GLU:H	1:A:321:GLU:CD	2.06	0.58
1:A:336:VAL:HG21	4:A:503:XVF:C16	2.34	0.58
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.86	0.57
5:D:505:BTB:O4	5:D:505:BTB:O1	2.19	0.57
2:D:501:HEM:HBD1	4:D:503:XVF:C15	2.35	0.56
1:C:91:ASP:OD1	1:D:97:ARG:NH1	2.39	0.56
1:D:271:THR:O	1:D:275:ILE:HG12	2.06	0.56
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.87	0.56
1:A:256:GLN:C	1:A:258:ASP:H	2.10	0.56
2:D:501:HEM:HBD1	4:D:503:XVF:F15	1.95	0.56
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.88	0.55
1:A:382:CYS:HA	5:A:504:BTB:H11	1.89	0.55
1:C:336:VAL:HG21	4:C:503:XVF:C16	2.36	0.55
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.24	0.55
1:A:339:MET:SD	4:A:503:XVF:F15	2.56	0.54
2:B:501:HEM:HBD1	4:B:503:XVF:F15	1.98	0.54
1:B:238:ARG:NH2	10:B:609:HOH:O	2.40	0.54
1:D:170:LEU:HD11	1:D:230:VAL:HG11	1.90	0.53
2:A:501:HEM:HBD2	4:A:503:XVF:C16	2.38	0.53
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.90	0.53
1:A:242:ARG:HD2	1:A:349:PRO:HB2	1.91	0.53
1:C:97:ARG:NH2	10:C:609:HOH:O	2.41	0.53
1:B:298:GLU:OE2	5:B:505:BTB:H42	2.08	0.53
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.26	0.53
1:D:336:VAL:HG21	4:D:503:XVF:C15	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.23	0.52
1:B:336:VAL:HG21	4:B:503:XVF:C15	2.40	0.51
1:A:92:GLY:N	1:B:96:PRO:O	2.42	0.51
1:C:167:GLU:OE2	6:C:507:GOL:O2	2.27	0.51
1:D:257:GLN:OE1	10:D:601:HOH:O	2.19	0.50
1:C:364:THR:O	1:C:368:CYS:HB2	2.12	0.50
1:C:87:GLN:O	1:C:89:GLN:NE2	2.44	0.50
1:C:339:MET:SD	4:C:503:XVF:F15	2.60	0.49
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.93	0.49
1:A:250:ARG:O	1:A:267:ASN:ND2	2.46	0.49
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.94	0.49
1:C:149:ARG:NH2	1:C:164:GLN:O	2.40	0.49
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.94	0.49
1:A:364:THR:O	1:A:368:CYS:HB2	2.13	0.49
1:A:216:LYS:HG3	1:A:217:TYR:N	2.28	0.48
1:C:119:ALA:HB1	1:C:122:GLN:HG3	1.94	0.48
1:B:397:LYS:NZ	10:B:613:HOH:O	2.43	0.48
1:C:294:GLN:HB2	1:C:300:PRO:HB3	1.95	0.48
1:C:479:PRO:HD2	1:C:480:TRP:CZ3	2.48	0.48
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.95	0.48
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.95	0.48
1:B:70:ARG:HD2	1:B:79:ILE:HD13	1.94	0.48
1:A:135:TYR:HD1	1:A:140:ARG:HB3	1.78	0.48
1:B:364:THR:O	1:B:368:CYS:HB2	2.13	0.47
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.96	0.47
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.96	0.47
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.97	0.47
1:A:121:GLU:H	1:A:121:GLU:CD	2.18	0.47
1:A:147:GLU:OE1	1:A:147:GLU:N	2.40	0.47
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.49	0.47
5:A:506:BTB:H72	5:A:506:BTB:O4	2.15	0.47
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.50	0.47
1:B:298:GLU:CD	5:B:505:BTB:H42	2.35	0.47
1:B:326:LEU:HB3	1:B:328:LEU:HG	1.96	0.47
5:A:504:BTB:H51	5:A:504:BTB:H32	1.64	0.46
1:B:447:TRP:HA	3:B:502:H4B:N1	2.30	0.46
1:D:107:ARG:HD2	1:D:107:ARG:H	1.81	0.46
1:D:89:GLN:NE2	10:D:605:HOH:O	2.37	0.46
1:A:250:ARG:O	1:A:251:TYR:HB2	2.15	0.46
5:A:504:BTB:H72	5:A:504:BTB:H41	1.69	0.46
1:B:298:GLU:OE2	5:B:505:BTB:H72	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.51	0.46
2:C:501:HEM:O1A	3:C:502:H4B:N3	2.45	0.46
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.34	0.45
1:A:229:THR:O	1:A:351:ALA:HA	2.17	0.45
5:C:506:BTB:O4	5:C:506:BTB:O1	2.31	0.45
1:A:150:LEU:HB2	1:A:151:GLN:HE21	1.81	0.45
1:D:143:SER:O	1:D:147:GLU:HG2	2.16	0.45
1:B:106:PRO:HB3	10:B:660:HOH:O	2.17	0.45
1:B:250:ARG:HD2	1:B:250:ARG:HA	1.72	0.45
1:D:257:GLN:H	1:D:257:GLN:HG2	1.51	0.45
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.98	0.44
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.99	0.44
5:A:505:BTB:H11	5:A:505:BTB:H51	1.59	0.44
1:A:89:GLN:HG3	1:A:90:GLN:N	2.31	0.44
5:C:505:BTB:H51	5:C:505:BTB:H42	1.36	0.44
1:B:193:LEU:O	6:B:506:GOL:H12	2.17	0.44
5:B:505:BTB:H11	5:B:505:BTB:H51	1.48	0.44
1:C:220:ASN:HB3	1:C:223:ASN:O	2.17	0.44
1:B:90:GLN:HB2	1:B:468:PHE:CD2	2.53	0.43
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.54	0.43
1:C:447:TRP:HA	3:C:502:H4B:N1	2.33	0.43
1:A:269:GLU:O	1:A:272:GLU:HG2	2.19	0.43
1:B:238:ARG:HE	1:B:238:ARG:HB3	1.68	0.43
1:D:106:PRO:HB2	1:D:107:ARG:HD2	2.00	0.42
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.54	0.42
1:A:308:GLU:H	1:A:308:GLU:CD	2.23	0.42
5:C:506:BTB:H72	5:C:506:BTB:H31	1.62	0.42
1:A:229:THR:O	1:A:352:PRO:HD2	2.20	0.42
1:B:124:LEU:HB3	1:B:128:ARG:HH22	1.83	0.42
5:C:505:BTB:H72	5:C:505:BTB:H31	1.38	0.42
5:A:505:BTB:H41	5:A:505:BTB:H72	1.51	0.42
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.55	0.42
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.55	0.42
1:C:364:THR:HG21	1:C:452:ILE:HG23	2.02	0.42
5:C:506:BTB:H62	5:C:506:BTB:H71	1.90	0.42
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.52	0.42
1:D:326:LEU:HB3	1:D:328:LEU:HG	2.02	0.41
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.33	0.41
1:B:105:PHE:HA	1:B:106:PRO:HD3	1.86	0.41
1:C:93:PRO:HG3	1:C:106:PRO:HB3	2.02	0.41
1:D:238:ARG:HG3	1:D:296:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:TYR:HH	2:D:501:HEM:CGD	2.33	0.41
1:B:238:ARG:HG2	1:B:296:PRO:HB3	2.01	0.41
1:A:150:LEU:O	1:A:154:GLU:HG3	2.21	0.41
1:C:298:GLU:OE2	5:C:506:BTB:O8	2.34	0.41
1:A:89:GLN:HG3	1:A:90:GLN:H	1.85	0.41
1:C:292:LEU:HD23	1:C:292:LEU:HA	1.89	0.41
1:A:322:TRP:CD1	5:A:504:BTB:H61	2.56	0.40
1:D:107:ARG:HD2	1:D:107:ARG:N	2.36	0.40
1:A:455:SER:HA	1:A:460:PHE:CG	2.55	0.40
2:A:501:HEM:HBD1	2:A:501:HEM:HHA	2.03	0.40
1:C:255:ARG:HB2	1:C:255:ARG:NH1	2.37	0.40
5:B:505:BTB:O8	5:B:505:BTB:O3	2.38	0.40
1:A:397:LYS:NZ	10:A:619:HOH:O	2.52	0.40
5:B:504:BTB:H51	5:B:504:BTB:H32	1.76	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	398/440 (90%)	380 (96%)	15 (4%)	3 (1%)	19 7
1	B	400/440 (91%)	394 (98%)	6 (2%)	0	100 100
1	C	399/440 (91%)	386 (97%)	12 (3%)	1 (0%)	41 27
1	D	398/440 (90%)	388 (98%)	10 (2%)	0	100 100
All	All	1595/1760 (91%)	1548 (97%)	43 (3%)	4 (0%)	41 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLN

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Mol	Chain	Res	Type
1	C	277	HIS
1	A	203	SER
1	A	251	TYR

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/373 (92%)	328 (96%)	14 (4%)	30	13
1	B	343/373 (92%)	333 (97%)	10 (3%)	42	25
1	C	342/373 (92%)	328 (96%)	14 (4%)	30	13
1	D	341/373 (91%)	335 (98%)	6 (2%)	59	44
All	All	1368/1492 (92%)	1324 (97%)	44 (3%)	39	21

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

Mol	Chain	Res	Type
1	A	89	GLN
1	A	90	GLN
1	A	97	ARG
1	A	121	GLU
1	A	122	GLN
1	A	124	LEU
1	A	129	ASP
1	A	151	GLN
1	A	216	LYS
1	A	258	ASP
1	A	285	ARG
1	A	291	LEU
1	A	321	GLU
1	A	329	ARG
1	B	78	SER
1	B	97	ARG
1	B	122	GLN
1	B	128	ARG

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Mol	Chain	Res	Type
1	B	139	LYS
1	B	154	GLU
1	B	255	ARG
1	B	257	GLN
1	B	326	LEU
1	B	396	ASP
1	C	67	LYS
1	C	71	VAL
1	C	89	GLN
1	C	98	ARG
1	C	121	GLU
1	C	140	ARG
1	C	151	GLN
1	C	233	GLN
1	C	255	ARG
1	C	302	LEU
1	C	308	GLU
1	C	309	LEU
1	C	417	ILE
1	C	429	LYS
1	D	125	SER
1	D	139	LYS
1	D	192	LYS
1	D	257	GLN
1	D	262	ARG
1	D	326	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	GLN
1	A	277	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 10 are monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	C	501	1	41,50,50	1.47	7 (17%)	45,82,82	1.77	10 (22%)
5	BTB	C	505	-	13,13,13	0.67	0	7,16,16	1.13	0
6	GOL	C	510	-	5,5,5	0.34	0	5,5,5	0.33	0
3	H4B	C	502	-	16,18,18	0.93	1 (6%)	11,26,26	2.81	5 (45%)
5	BTB	A	504	8	13,13,13	0.41	0	7,16,16	1.01	1 (14%)
5	BTB	C	504	8	13,13,13	0.40	0	7,16,16	0.89	0
6	GOL	D	506	-	5,5,5	0.34	0	5,5,5	0.44	0
3	H4B	B	502	-	16,18,18	1.03	0	11,26,26	2.77	6 (54%)
4	XVF	B	503	-	26,26,26	1.81	1 (3%)	34,35,35	1.85	8 (23%)
6	GOL	C	508	-	5,5,5	0.67	0	5,5,5	2.01	2 (40%)
5	BTB	B	504	8	13,13,13	0.37	0	7,16,16	0.33	0
2	HEM	D	501	1	41,50,50	1.46	5 (12%)	45,82,82	1.41	3 (6%)
5	BTB	C	506	-	13,13,13	0.42	0	7,16,16	0.43	0
3	H4B	D	502	-	16,18,18	0.84	0	11,26,26	2.64	5 (45%)
6	GOL	B	509	-	5,5,5	0.32	0	5,5,5	0.39	0
6	GOL	B	507	-	5,5,5	0.39	0	5,5,5	0.37	0
2	HEM	A	501	1	41,50,50	1.54	6 (14%)	45,82,82	1.60	6 (13%)
6	GOL	C	507	-	5,5,5	0.33	0	5,5,5	0.61	0
5	BTB	A	506	-	13,13,13	0.54	0	7,16,16	0.44	0
3	H4B	A	502	-	16,18,18	0.88	0	11,26,26	2.65	6 (54%)
4	XVF	D	503	-	26,26,26	1.90	1 (3%)	34,35,35	1.88	6 (17%)
5	BTB	D	504	8	13,13,13	0.42	0	7,16,16	0.78	0
4	XVF	A	503	-	26,26,26	1.77	1 (3%)	34,35,35	1.74	8 (23%)
2	HEM	B	501	1	41,50,50	1.49	6 (14%)	45,82,82	1.64	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	A	508	-	5,5,5	0.38	0	5,5,5	0.20	0
5	BTB	A	505	-	13,13,13	0.47	0	7,16,16	0.91	0
5	BTB	B	505	-	13,13,13	0.66	0	7,16,16	0.90	0
6	GOL	B	508	-	5,5,5	0.38	0	5,5,5	0.30	0
4	XVF	C	503	-	26,26,26	1.92	1 (3%)	34,35,35	1.67	5 (14%)
6	GOL	A	507	-	5,5,5	0.37	0	5,5,5	0.41	0
6	GOL	B	506	-	5,5,5	0.49	0	5,5,5	0.62	0
5	BTB	D	505	-	13,13,13	0.56	0	7,16,16	1.43	1 (14%)
6	GOL	C	509	-	5,5,5	0.36	0	5,5,5	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	501	1	-	4/12/54/54	-
5	BTB	C	505	-	-	15/21/21/21	-
6	GOL	C	510	-	-	3/4/4/4	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
5	BTB	A	504	8	-	6/21/21/21	-
5	BTB	C	504	8	-	3/21/21/21	-
6	GOL	D	506	-	-	4/4/4/4	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
4	XVF	B	503	-	-	4/14/14/14	0/2/2/2
6	GOL	C	508	-	-	4/4/4/4	-
5	BTB	B	504	8	-	3/21/21/21	-
2	HEM	D	501	1	-	1/12/54/54	-
5	BTB	C	506	-	-	9/21/21/21	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
6	GOL	B	509	-	-	2/4/4/4	-
6	GOL	B	507	-	-	4/4/4/4	-
2	HEM	A	501	1	-	5/12/54/54	-
6	GOL	C	507	-	-	2/4/4/4	-
5	BTB	A	506	-	-	6/21/21/21	-
3	H4B	A	502	-	-	2/8/17/17	0/2/2/2
4	XVF	D	503	-	-	2/14/14/14	0/2/2/2
5	BTB	D	504	8	-	4/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XVF	A	503	-	-	3/14/14/14	0/2/2/2
2	HEM	B	501	1	-	5/12/54/54	-
6	GOL	A	508	-	-	2/4/4/4	-
5	BTB	A	505	-	-	12/21/21/21	-
5	BTB	B	505	-	-	12/21/21/21	-
6	GOL	B	508	-	-	2/4/4/4	-
4	XVF	C	503	-	-	3/14/14/14	0/2/2/2
6	GOL	A	507	-	-	2/4/4/4	-
6	GOL	B	506	-	-	2/4/4/4	-
5	BTB	D	505	-	-	9/21/21/21	-
6	GOL	C	509	-	-	2/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	XVF	C11-C16	9.53	1.48	1.38
4	D	503	XVF	C11-C16	9.22	1.48	1.38
4	A	503	XVF	C11-C16	8.92	1.48	1.38
4	B	503	XVF	C11-C16	8.79	1.48	1.38
2	D	501	HEM	C3C-C2C	-4.24	1.34	1.40
2	C	501	HEM	C3C-CAC	3.75	1.55	1.47
2	B	501	HEM	C3C-CAC	3.71	1.55	1.47
2	A	501	HEM	C3C-CAC	3.68	1.55	1.47
2	D	501	HEM	C3C-CAC	3.37	1.54	1.47
2	A	501	HEM	C3C-C2C	-3.34	1.35	1.40
2	B	501	HEM	C3C-C2C	-3.32	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.28	1.35	1.40
2	A	501	HEM	FE-NB	3.09	2.12	1.96
2	A	501	HEM	CAB-C3B	3.09	1.55	1.47
2	B	501	HEM	CAB-C3B	3.04	1.55	1.47
2	C	501	HEM	CAB-C3B	3.01	1.55	1.47
2	B	501	HEM	FE-NB	2.89	2.11	1.96
2	D	501	HEM	FE-NB	2.85	2.10	1.96
2	D	501	HEM	CAB-C3B	2.63	1.54	1.47
2	A	501	HEM	CAA-C2A	2.42	1.55	1.52
2	C	501	HEM	CMB-C2B	2.31	1.55	1.50
2	C	501	HEM	FE-NB	2.20	2.07	1.96
2	C	501	HEM	CAA-C2A	2.19	1.55	1.52
3	C	502	H4B	C4A-C4	-2.18	1.38	1.41
2	B	501	HEM	CMB-C2B	2.14	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CMA-C3A	2.10	1.56	1.51
2	D	501	HEM	CMD-C2D	2.10	1.55	1.50
2	A	501	HEM	FE-ND	2.04	2.07	1.96
2	C	501	HEM	FE-ND	2.00	2.06	1.96

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	503	XVF	C08-C09-C11	-6.07	102.98	112.81
4	C	503	XVF	C02-N01-C06	5.77	122.47	118.10
3	B	502	H4B	C8A-C4A-C4	5.33	119.31	114.57
4	A	503	XVF	C02-N01-C06	5.22	122.06	118.10
4	B	503	XVF	C08-C09-C11	-5.09	104.58	112.81
3	A	502	H4B	C8A-C4A-C4	4.97	118.98	114.57
3	C	502	H4B	C8A-C4A-C4	4.94	118.95	114.57
2	B	501	HEM	CBA-CAA-C2A	-4.88	104.29	112.62
2	C	501	HEM	C4B-CHC-C1C	4.81	128.91	122.56
3	D	502	H4B	C8A-C4A-C4	4.74	118.78	114.57
2	D	501	HEM	CBA-CAA-C2A	-4.68	104.64	112.62
2	A	501	HEM	C4B-CHC-C1C	4.45	128.43	122.56
2	C	501	HEM	CBA-CAA-C2A	-4.45	105.03	112.62
3	C	502	H4B	C2-N3-C4	4.40	122.92	115.93
4	B	503	XVF	C02-N01-C06	4.00	121.13	118.10
3	C	502	H4B	N1-C2-N3	-3.96	119.21	125.42
2	B	501	HEM	C4B-CHC-C1C	3.94	127.75	122.56
3	B	502	H4B	N1-C2-N3	-3.90	119.31	125.42
4	B	503	XVF	C09-C11-C16	-3.79	117.68	120.73
4	D	503	XVF	F16-C16-C11	3.70	121.76	117.85
3	D	502	H4B	C2-N3-C4	3.65	121.74	115.93
4	D	503	XVF	C12-C11-C16	3.62	120.08	116.76
4	C	503	XVF	C05-C06-N01	-3.60	119.08	122.90
2	D	501	HEM	C4B-CHC-C1C	3.55	127.24	122.56
3	B	502	H4B	C2-N3-C4	3.52	121.52	115.93
6	C	508	GOL	O2-C2-C1	-3.47	93.85	109.12
3	D	502	H4B	N1-C2-N3	-3.45	120.00	125.42
4	B	503	XVF	C12-C11-C16	3.42	119.89	116.76
3	A	502	H4B	C4-C4A-N5	3.42	121.99	119.12
5	D	505	BTB	C6-C5-N	3.38	124.79	111.59
3	A	502	H4B	N1-C2-N3	-3.38	120.12	125.42
2	A	501	HEM	C1B-NB-C4B	3.34	108.52	105.07
4	D	503	XVF	C02-N01-C06	3.33	120.62	118.10
4	C	503	XVF	C08-C06-N01	3.20	120.71	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	CMA-C3A-C4A	-3.18	123.58	128.46
3	D	502	H4B	C4-C4A-N5	3.15	121.77	119.12
3	A	502	H4B	C2-N3-C4	3.13	120.90	115.93
2	A	501	HEM	C3B-C2B-C1B	3.01	108.72	106.49
4	D	503	XVF	C09-C11-C16	-3.00	118.32	120.73
4	A	503	XVF	C09-C11-C16	-2.98	118.34	120.73
3	B	502	H4B	C2-N1-C8A	2.97	121.20	114.54
2	C	501	HEM	C1B-NB-C4B	2.96	108.13	105.07
2	D	501	HEM	CMA-C3A-C4A	-2.93	123.95	128.46
3	C	502	H4B	N2-C2-N1	2.93	121.81	117.25
4	B	503	XVF	C13-C14-C15	2.88	121.24	119.37
2	A	501	HEM	C4A-C3A-C2A	2.88	109.00	107.00
2	C	501	HEM	C4D-ND-C1D	2.85	108.02	105.07
4	A	503	XVF	C13-C14-C15	2.80	121.19	119.37
3	A	502	H4B	C2-N1-C8A	2.77	120.74	114.54
4	D	503	XVF	C13-C14-C15	2.74	121.14	119.37
6	C	508	GOL	O1-C1-C2	-2.73	97.10	110.20
4	A	503	XVF	C09-C08-C06	-2.64	107.07	112.99
2	A	501	HEM	C4D-ND-C1D	2.64	107.80	105.07
4	B	503	XVF	F16-C16-C11	2.63	120.63	117.85
4	B	503	XVF	C08-C06-N01	2.62	119.86	115.95
4	A	503	XVF	C05-C06-N01	-2.60	120.14	122.90
4	A	503	XVF	C12-C11-C16	2.59	119.14	116.76
4	B	503	XVF	C05-C06-N01	-2.58	120.17	122.90
3	D	502	H4B	C2-N1-C8A	2.56	120.27	114.54
2	C	501	HEM	C3D-C4D-ND	-2.56	107.32	110.17
2	B	501	HEM	CMC-C2C-C3C	2.48	129.32	124.68
3	C	502	H4B	C2-N1-C8A	2.47	120.07	114.54
2	B	501	HEM	CHC-C4B-C3B	2.47	128.35	124.57
2	B	501	HEM	C4D-ND-C1D	2.44	107.59	105.07
4	C	503	XVF	C13-C14-C15	2.42	120.94	119.37
3	B	502	H4B	N2-C2-N1	2.41	121.00	117.25
2	A	501	HEM	CMA-C3A-C4A	-2.38	124.80	128.46
4	A	503	XVF	C08-C06-N01	2.32	119.40	115.95
4	C	503	XVF	F16-C16-C11	2.28	120.25	117.85
5	A	504	BTB	O3-C3-C2	2.27	117.66	111.44
2	C	501	HEM	O2A-CGA-CBA	2.26	121.30	114.03
2	C	501	HEM	C3B-C2B-C1B	2.26	108.16	106.49
3	A	502	H4B	N2-C2-N3	2.22	120.70	117.25
4	A	503	XVF	C18-C17-C13	-2.17	105.95	112.16
2	B	501	HEM	C4C-CHD-C1D	2.17	125.42	122.56
2	C	501	HEM	CAD-CBD-CGD	-2.13	109.01	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	O1A-CGA-CBA	-2.12	116.26	123.08
2	B	501	HEM	C1B-NB-C4B	2.11	107.25	105.07
2	B	501	HEM	CMB-C2B-C1B	2.10	128.24	125.04
2	B	501	HEM	CMA-C3A-C4A	-2.10	125.24	128.46
2	B	501	HEM	C3B-C2B-C1B	2.07	108.02	106.49
3	B	502	H4B	O9-C9-C6	2.02	113.82	108.98

There are no chirality outliers.

All (137) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	C2A-CAA-CBA-CGA
2	C	501	HEM	C3D-CAD-CBD-CGD
4	B	503	XVF	C06-C08-C09-C11
4	B	503	XVF	C17-C18-N19-C22
4	C	503	XVF	C06-C08-C09-C11
4	D	503	XVF	C06-C08-C09-C11
5	A	504	BTB	O1-C1-C2-C3
5	A	504	BTB	O1-C1-C2-C4
5	A	504	BTB	O1-C1-C2-N
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	O1-C1-C2-C3
5	A	505	BTB	O1-C1-C2-C4
5	A	505	BTB	O1-C1-C2-N
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C3-C2-N-C7
5	A	505	BTB	C4-C2-N-C5
5	A	505	BTB	C4-C2-N-C7
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

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

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Mol	Chain	Res	Type	Atoms
6	C	508	GOL	O1-C1-C2-C3
6	C	508	GOL	C1-C2-C3-O3
6	C	508	GOL	O2-C2-C3-O3
6	C	509	GOL	O1-C1-C2-C3
6	C	510	GOL	O1-C1-C2-C3
4	D	503	XVF	C17-C18-N19-C22
5	B	505	BTB	N-C7-C8-O8
5	A	505	BTB	N-C7-C8-O8
5	C	505	BTB	N-C5-C6-O6
4	C	503	XVF	C17-C18-N19-C22
6	A	508	GOL	O1-C1-C2-C3
6	B	509	GOL	O1-C1-C2-C3
6	D	506	GOL	O1-C1-C2-C3
6	A	507	GOL	O1-C1-C2-O2
6	B	506	GOL	O2-C2-C3-O3
6	C	507	GOL	O1-C1-C2-O2
6	C	508	GOL	O1-C1-C2-O2
6	C	509	GOL	O1-C1-C2-O2
6	C	510	GOL	O1-C1-C2-O2
6	D	506	GOL	O1-C1-C2-O2
5	D	505	BTB	N-C5-C6-O6
4	A	503	XVF	C21-C20-N19-C18
5	B	505	BTB	N-C5-C6-O6
2	C	501	HEM	C2A-CAA-CBA-CGA
6	B	508	GOL	O2-C2-C3-O3
6	B	509	GOL	O1-C1-C2-O2
4	A	503	XVF	C21-C20-N19-C22
4	B	503	XVF	C23-C22-N19-C20
5	C	505	BTB	N-C7-C8-O8
6	B	507	GOL	O1-C1-C2-O2
6	B	507	GOL	O2-C2-C3-O3
4	C	503	XVF	C13-C17-C18-N19
5	A	505	BTB	C1-C2-C4-O4
2	C	501	HEM	C1A-C2A-CAA-CBA
2	C	501	HEM	C3A-C2A-CAA-CBA
5	B	505	BTB	O1-C1-C2-N
5	C	505	BTB	C1-C2-N-C5
5	C	505	BTB	C3-C2-N-C7
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
5	C	506	BTB	C1-C2-N-C5
5	C	506	BTB	C1-C2-N-C7

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Mol	Chain	Res	Type	Atoms
5	C	506	BTB	C3-C2-N-C5
5	C	506	BTB	C3-C2-N-C7
2	B	501	HEM	C3D-CAD-CBD-CGD
4	B	503	XVF	C17-C18-N19-C20
2	A	501	HEM	C4D-C3D-CAD-CBD
6	C	510	GOL	C1-C2-C3-O3
2	D	501	HEM	C3D-CAD-CBD-CGD
5	C	506	BTB	N-C7-C8-O8
6	D	506	GOL	O2-C2-C3-O3
2	A	501	HEM	C2D-C3D-CAD-CBD
6	B	507	GOL	O1-C1-C2-C3
2	B	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAA-CBA-CGA-O1A
3	A	502	H4B	C7-C6-C9-C10
6	A	508	GOL	O1-C1-C2-O2
6	D	506	GOL	C1-C2-C3-O3
3	A	502	H4B	N5-C6-C9-O9
4	A	503	XVF	C06-C08-C09-C11
5	A	505	BTB	C3-C2-C4-O4
5	D	504	BTB	C3-C2-C4-O4

There are no ring outliers.

23 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	3	0
5	C	505	BTB	2	0
3	C	502	H4B	3	0
5	A	504	BTB	4	0
5	C	504	BTB	1	0
3	B	502	H4B	1	0
4	B	503	XVF	3	0
5	B	504	BTB	1	0
2	D	501	HEM	5	0
5	C	506	BTB	4	0
2	A	501	HEM	4	0
6	C	507	GOL	1	0
5	A	506	BTB	1	0
3	A	502	H4B	1	0
4	D	503	XVF	3	0

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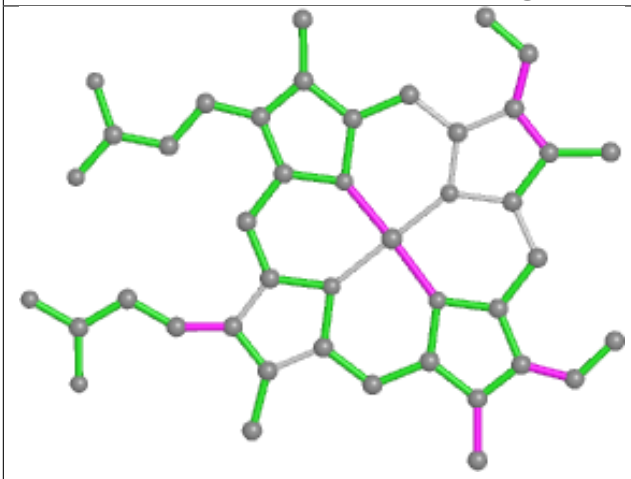
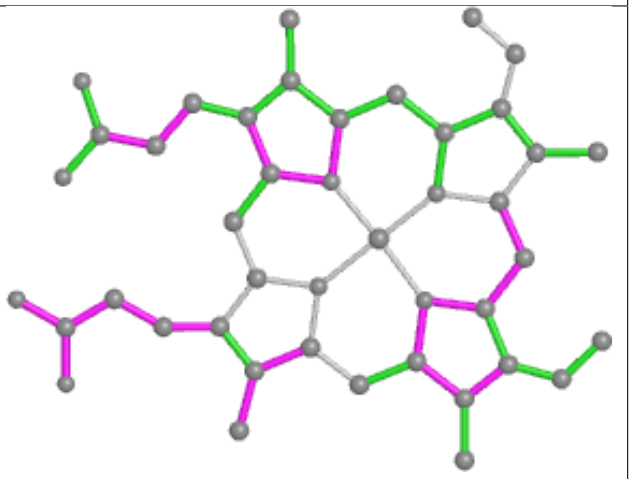
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	504	BTB	2	0
4	A	503	XVF	3	0
2	B	501	HEM	5	0
5	A	505	BTB	3	0
5	B	505	BTB	6	0
4	C	503	XVF	2	0
6	B	506	GOL	1	0
5	D	505	BTB	1	0

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.

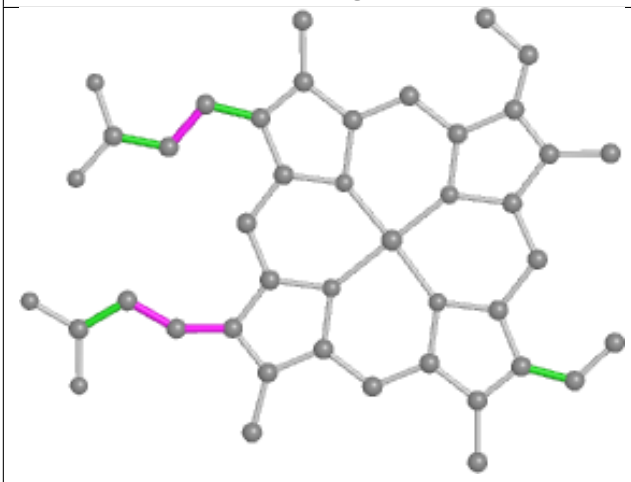
Ligand HEM C 501



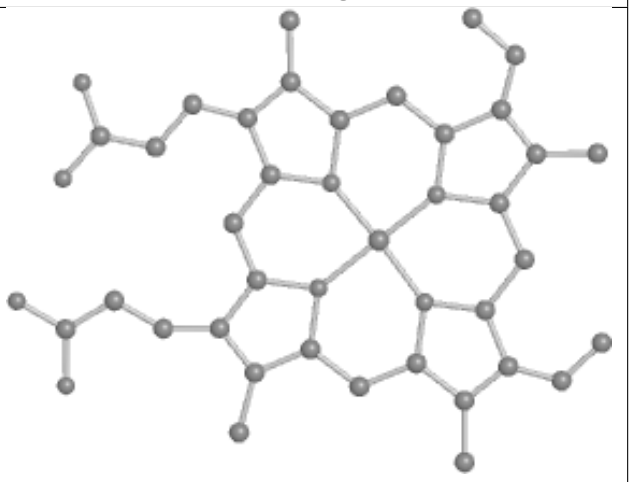
Bond lengths



Bond angles

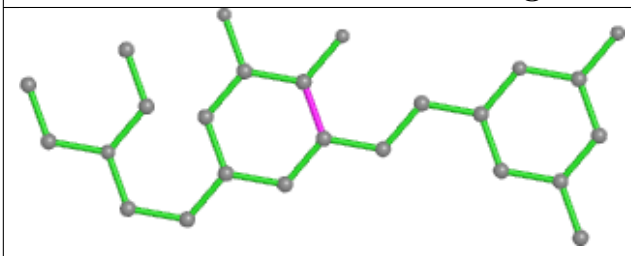


Torsions

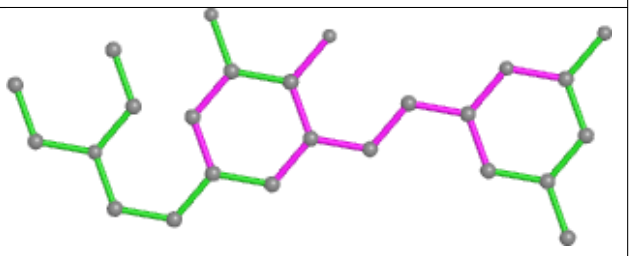


Rings

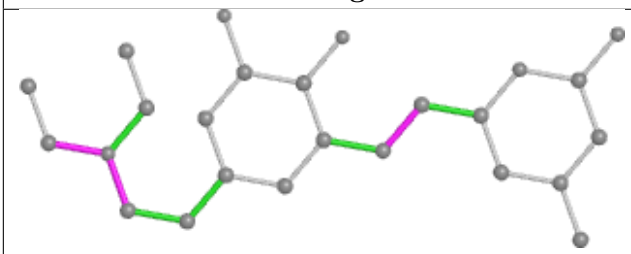
Ligand XVF B 503



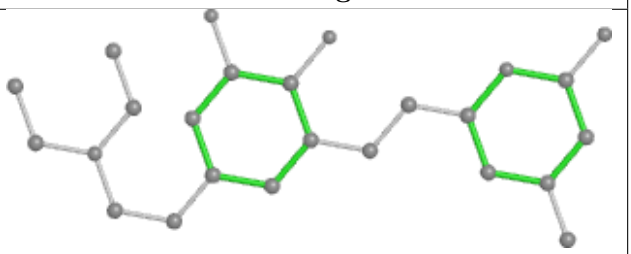
Bond lengths



Bond angles

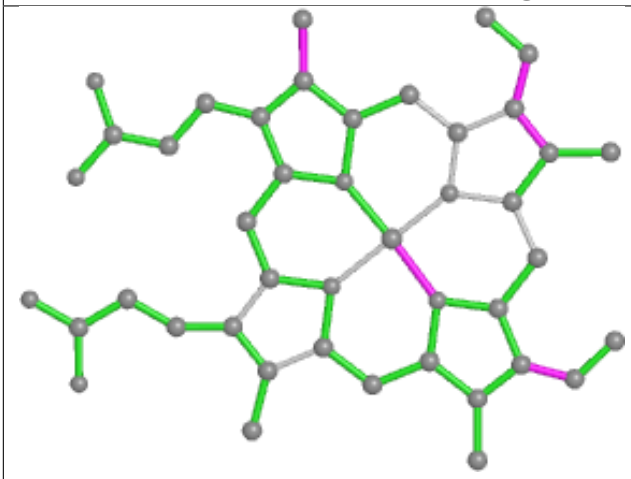


Torsions

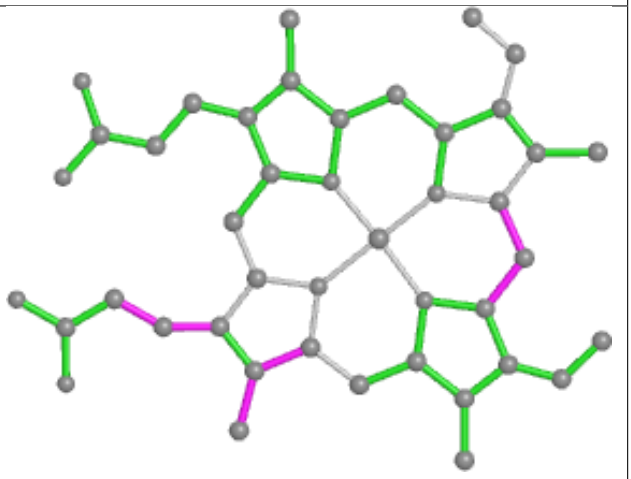


Rings

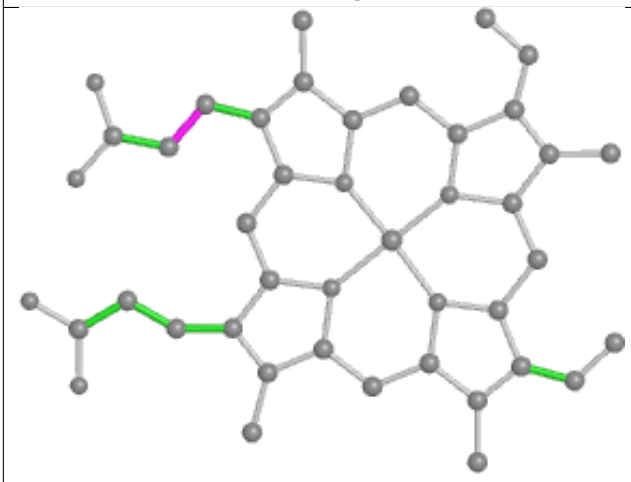
Ligand HEM D 501



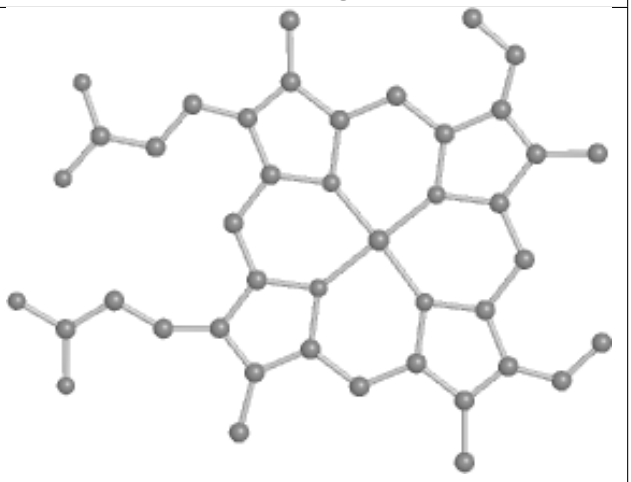
Bond lengths



Bond angles

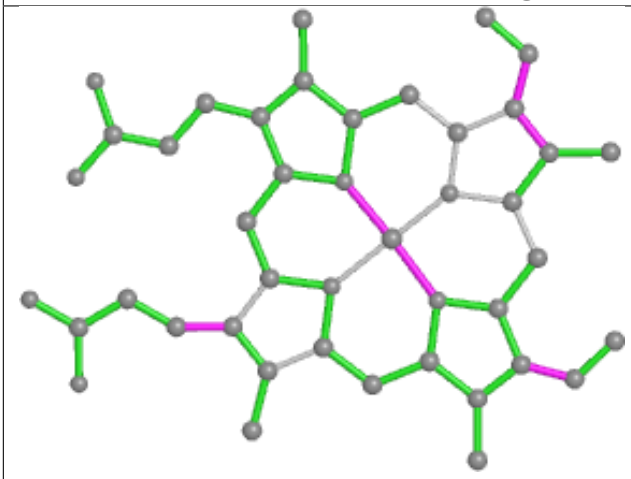


Torsions

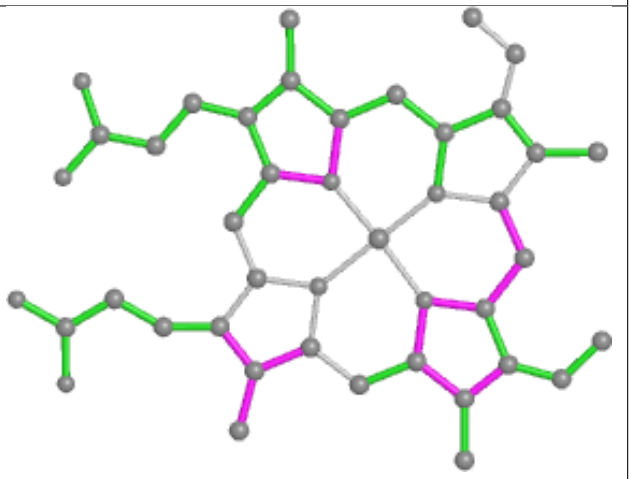


Rings

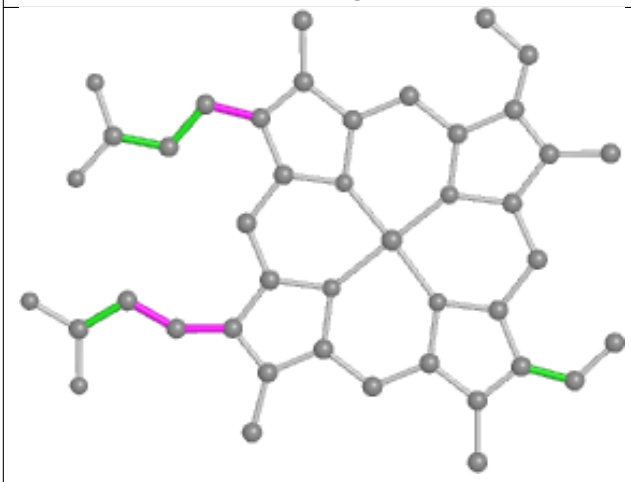
Ligand HEM A 501



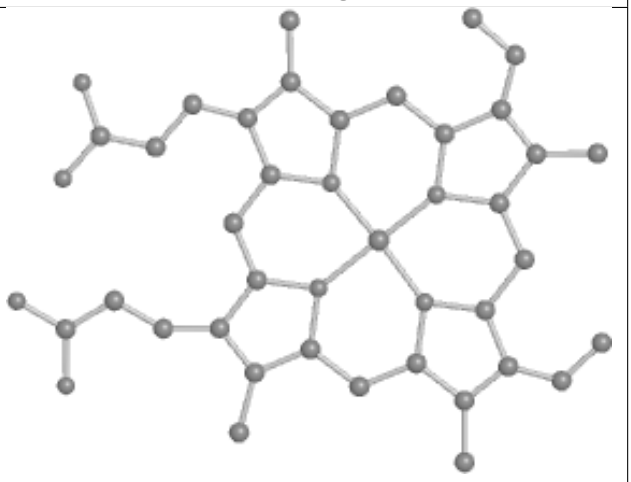
Bond lengths



Bond angles

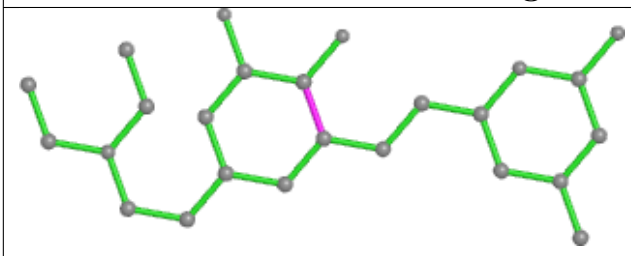


Torsions

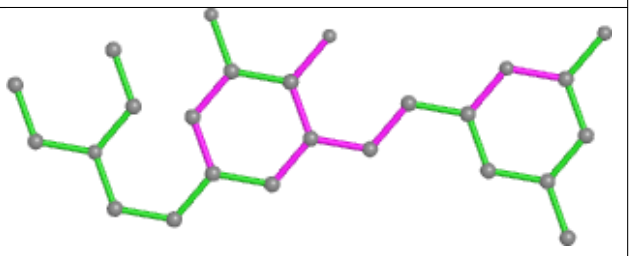


Rings

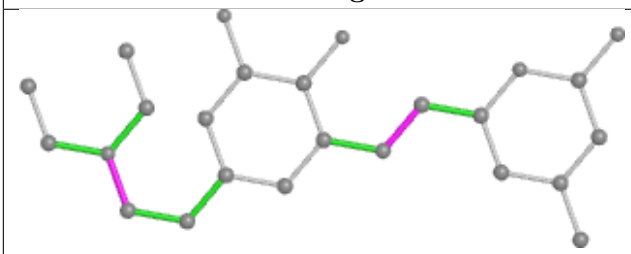
Ligand XVF D 503



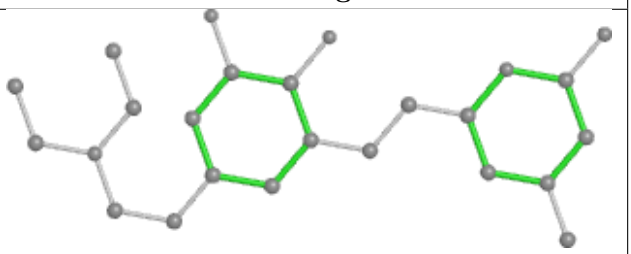
Bond lengths



Bond angles

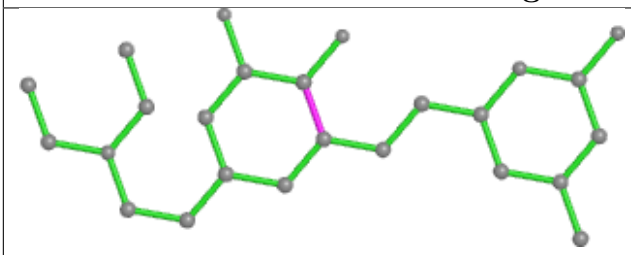


Torsions

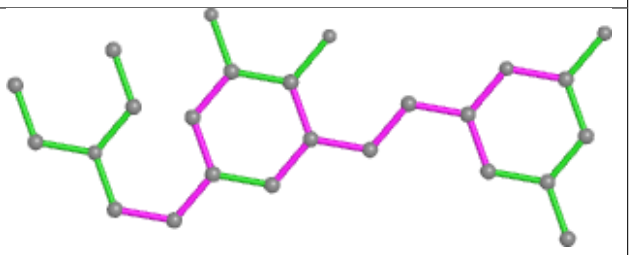


Rings

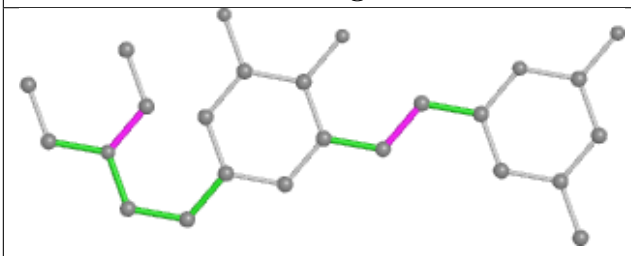
Ligand XVF A 503



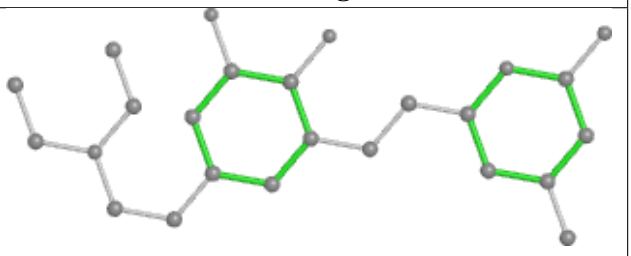
Bond lengths



Bond angles

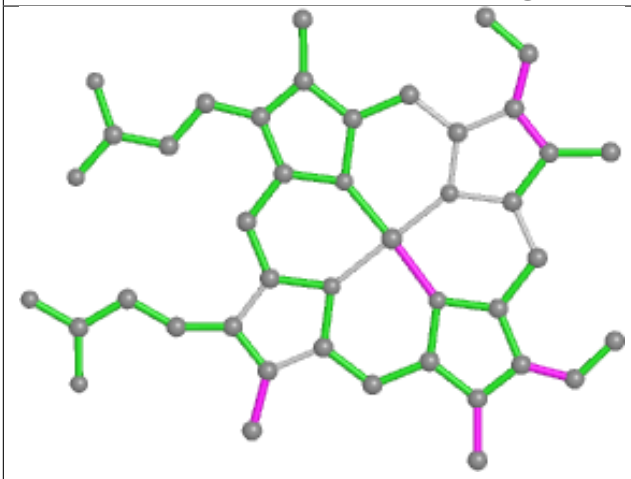


Torsions

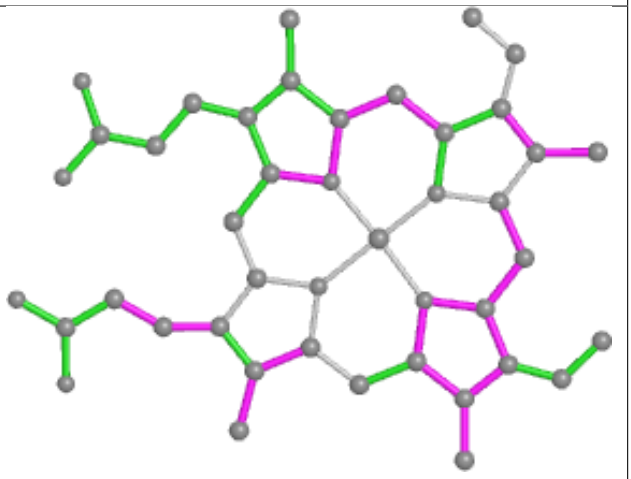


Rings

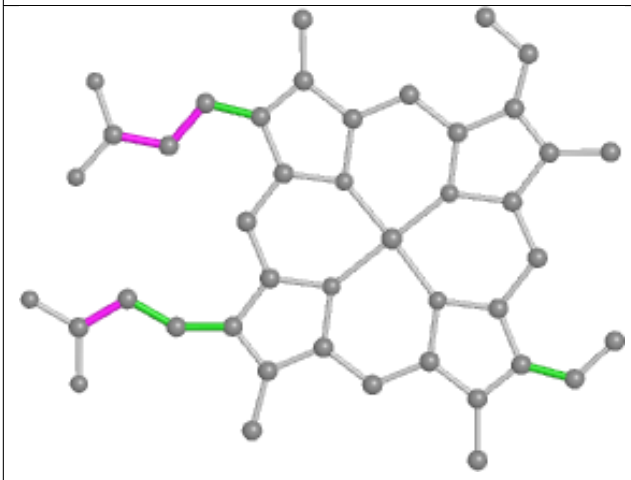
Ligand HEM B 501



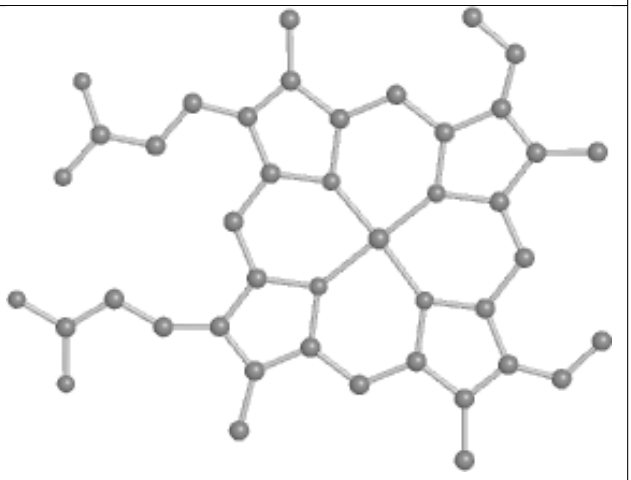
Bond lengths



Bond angles

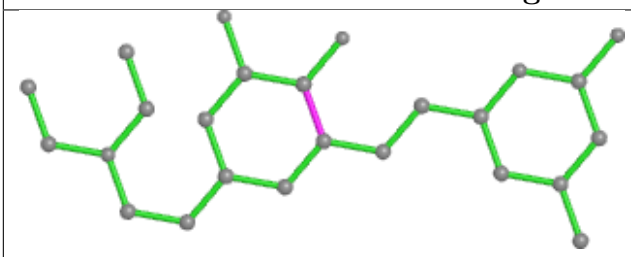


Torsions

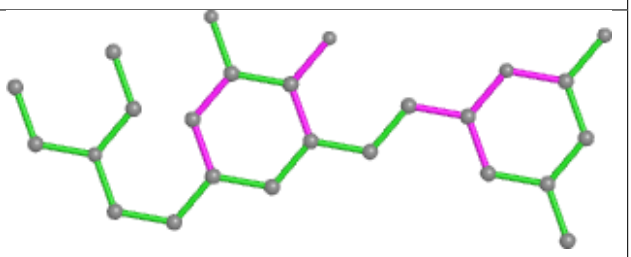


Rings

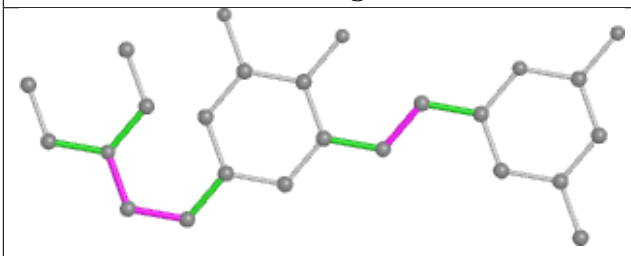
Ligand XVF C 503



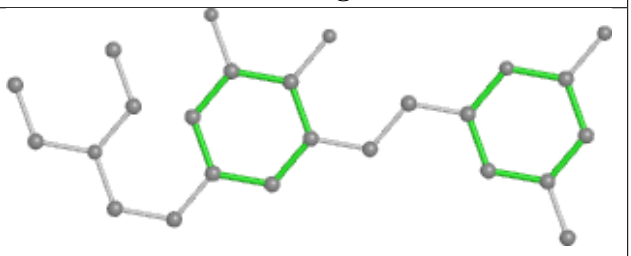
Bond lengths



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	401/440 (91%)	1.20	89 (22%) 0 0	28, 59, 109, 142	0
1	B	401/440 (91%)	0.27	34 (8%) 10 9	25, 40, 76, 115	0
1	C	402/440 (91%)	0.97	80 (19%) 1 0	28, 54, 99, 129	0
1	D	402/440 (91%)	0.18	27 (6%) 17 15	24, 39, 71, 126	0
All	All	1606/1760 (91%)	0.66	230 (14%) 2 2	24, 47, 95, 142	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	GLY	13.1
1	A	480	TRP	7.1
1	A	275	ILE	6.6
1	A	204	ALA	6.5
1	A	280	THR	6.0
1	D	257	GLN	5.6
1	C	236	PRO	5.4
1	C	448	ILE	5.4
1	C	275	ILE	5.3
1	A	447	TRP	5.3
1	A	237	GLY	5.3
1	A	281	PRO	5.2
1	C	447	TRP	5.1
1	C	235	CYS	5.1
1	A	448	ILE	5.1
1	A	304	LEU	5.1
1	C	142	GLY	5.0
1	B	89	GLN	4.9
1	A	153	VAL	4.8
1	B	257	GLN	4.8
1	C	257	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	302	LEU	4.7
1	A	268	VAL	4.7
1	C	303	PHE	4.7
1	A	244	TRP	4.6
1	C	480	TRP	4.5
1	D	89	GLN	4.5
1	C	68	PHE	4.5
1	C	452	ILE	4.5
1	C	204	ALA	4.5
1	C	238	ARG	4.4
1	C	304	LEU	4.4
1	A	120	PRO	4.3
1	A	257	GLN	4.2
1	A	452	ILE	4.2
1	A	235	CYS	4.2
1	C	299	PRO	4.2
1	C	119	ALA	4.1
1	A	122	GLN	4.1
1	A	89	GLN	4.0
1	C	445	TRP	4.0
1	D	255	ARG	4.0
1	B	452	ILE	4.0
1	A	256	GLN	4.0
1	B	460	PHE	3.9
1	C	450	PRO	3.9
1	A	446	ALA	3.9
1	B	449	VAL	3.9
1	C	302	LEU	3.8
1	A	142	GLY	3.8
1	A	68	PHE	3.8
1	A	303	PHE	3.8
1	D	449	VAL	3.8
1	A	128	ARG	3.8
1	B	119	ALA	3.8
1	C	244	TRP	3.8
1	B	158	ALA	3.7
1	A	449	VAL	3.7
1	A	67	LYS	3.7
1	C	308	GLU	3.7
1	A	295	ALA	3.7
1	C	185	VAL	3.7
1	D	452	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	254	TYR	3.6
1	C	255	ARG	3.6
1	A	141	SER	3.6
1	D	259	GLY	3.6
1	C	307	PRO	3.6
1	A	185	VAL	3.6
1	C	449	VAL	3.6
1	A	151	GLN	3.5
1	C	297	ASP	3.5
1	C	141	SER	3.5
1	A	150	LEU	3.5
1	A	412	LEU	3.5
1	C	451	PRO	3.5
1	B	259	GLY	3.5
1	A	300	PRO	3.5
1	A	451	PRO	3.5
1	C	258	ASP	3.4
1	A	445	TRP	3.4
1	C	446	ALA	3.4
1	D	121	GLU	3.4
1	C	184	CYS	3.4
1	A	360	THR	3.4
1	A	308	GLU	3.4
1	C	140	ARG	3.4
1	C	89	GLN	3.4
1	C	144	GLN	3.4
1	A	86	ALA	3.3
1	A	202	ARG	3.3
1	A	279	TRP	3.3
1	C	122	GLN	3.3
1	D	460	PHE	3.3
1	B	120	PRO	3.3
1	A	301	GLU	3.3
1	B	454	GLY	3.3
1	A	159	ALA	3.3
1	C	309	LEU	3.3
1	A	238	ARG	3.3
1	A	478	ASP	3.2
1	A	479	PRO	3.2
1	A	299	PRO	3.2
1	A	90	GLN	3.2
1	A	184	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	280	THR	3.2
1	B	258	ASP	3.2
1	B	142	GLY	3.1
1	C	439	GLY	3.1
1	C	300	PRO	3.1
1	D	258	ASP	3.1
1	D	454	GLY	3.1
1	A	364	THR	3.1
1	C	360	THR	3.1
1	A	293	LEU	3.1
1	C	301	GLU	3.1
1	A	255	ARG	3.1
1	B	446	ALA	3.1
1	C	158	ALA	3.1
1	C	259	GLY	3.1
1	D	456	LEU	3.0
1	A	155	ALA	3.0
1	A	272	GLU	3.0
1	C	412	LEU	3.0
1	A	88	ALA	3.0
1	C	87	GLN	3.0
1	A	258	ASP	3.0
1	B	453	SER	3.0
1	D	446	ALA	3.0
1	A	106	PRO	3.0
1	A	276	GLN	2.9
1	D	256	GLN	2.9
1	C	79	ILE	2.9
1	A	145	ALA	2.9
1	A	274	CYS	2.9
1	A	346	LEU	2.9
1	A	260	SER	2.9
1	A	450	PRO	2.9
1	C	221	ARG	2.9
1	C	81	TYR	2.8
1	D	260	SER	2.8
1	C	306	PRO	2.8
1	B	360	THR	2.8
1	D	445	TRP	2.8
1	A	353	PHE	2.8
1	C	277	HIS	2.7
1	B	68	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	273	LEU	2.7
1	C	90	GLN	2.7
1	B	260	SER	2.7
1	C	67	LYS	2.7
1	C	388	ARG	2.7
1	C	237	GLY	2.7
1	C	281	PRO	2.7
1	A	136	SER	2.7
1	A	163	TYR	2.7
1	A	306	PRO	2.7
1	B	141[A]	SER	2.7
1	B	447	TRP	2.7
1	A	146	HIS	2.7
1	C	163	TYR	2.6
1	C	106	PRO	2.6
1	C	120	PRO	2.6
1	B	450	PRO	2.6
1	A	236	PRO	2.6
1	C	129	ASP	2.6
1	B	79	ILE	2.5
1	B	76	VAL	2.5
1	D	450	PRO	2.5
1	A	162	THR	2.5
1	D	360	THR	2.5
1	A	305	LEU	2.5
1	B	456	LEU	2.5
1	B	122	GLN	2.5
1	B	445	TRP	2.5
1	D	447	TRP	2.5
1	A	221	ARG	2.5
1	A	123	LEU	2.5
1	A	87	GLN	2.5
1	C	268	VAL	2.5
1	C	274	CYS	2.5
1	D	451	PRO	2.4
1	A	365	ARG	2.4
1	A	121	GLU	2.4
1	A	83	THR	2.4
1	C	212	CYS	2.4
1	D	120	PRO	2.3
1	A	183	ARG	2.3
1	C	362	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	208	PHE	2.3
1	D	448	ILE	2.3
1	D	158	ALA	2.3
1	D	388	ARG	2.3
1	C	294	GLN	2.3
1	C	146	HIS	2.3
1	C	183	ARG	2.3
1	C	276	GLN	2.3
1	A	297	ASP	2.3
1	B	70	ARG	2.3
1	B	256	GLN	2.2
1	C	272	GLU	2.2
1	A	125	SER	2.2
1	C	282	GLY	2.2
1	C	207	MET	2.2
1	C	155	ALA	2.2
1	D	119	ALA	2.2
1	D	79	ILE	2.2
1	C	346	LEU	2.2
1	C	336	VAL	2.2
1	A	366	ASN	2.2
1	C	460	PHE	2.2
1	B	448	ILE	2.1
1	B	121	GLU	2.1
1	A	140	ARG	2.1
1	B	97	ARG	2.1
1	A	203	SER	2.1
1	B	362	ILE	2.1
1	C	273	LEU	2.1
1	D	453	SER	2.1
1	A	129	ASP	2.1
1	D	364	THR	2.1
1	B	455	SER	2.1
1	C	444	ASP	2.1
1	C	228	ILE	2.1
1	A	205	GLN	2.0
1	B	159	ALA	2.0
1	B	90	GLN	2.0
1	A	459	VAL	2.0
1	C	153	VAL	2.0
1	C	279	TRP	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
6	GOL	C	509	6/6	0.41	0.23	70,79,82,83	0
6	GOL	C	510	6/6	0.53	0.15	69,76,78,82	0
5	BTB	A	506	14/14	0.54	0.27	87,91,94,95	0
5	BTB	C	506	14/14	0.63	0.21	82,95,103,105	0
5	BTB	D	504	14/14	0.71	0.17	41,65,84,89	0
6	GOL	A	508	6/6	0.72	0.27	50,81,82,93	0
6	GOL	B	506	6/6	0.73	0.20	69,81,87,91	0
6	GOL	B	509	6/6	0.75	0.15	75,81,83,85	0
6	GOL	D	506	6/6	0.76	0.34	66,79,80,80	0
5	BTB	A	505	14/14	0.80	0.17	52,73,80,81	0
5	BTB	B	504	14/14	0.80	0.16	44,58,76,81	0
5	BTB	D	505	14/14	0.82	0.18	62,71,80,81	0
6	GOL	B	508	6/6	0.83	0.11	78,82,87,89	0
4	XVF	A	503	25/25	0.84	0.38	38,92,112,127	0
4	XVF	C	503	25/25	0.85	0.35	36,87,104,126	0
3	H4B	A	502	17/17	0.87	0.24	45,64,72,72	0
5	BTB	B	505	14/14	0.87	0.16	43,70,77,82	0
3	H4B	C	502	17/17	0.88	0.24	52,56,61,65	0
6	GOL	B	507	6/6	0.89	0.31	72,80,87,91	0
3	H4B	D	502	17/17	0.90	0.20	37,47,54,54	0
6	GOL	C	508	6/6	0.91	0.20	26,40,69,75	0
5	BTB	A	504	14/14	0.91	0.30	47,79,88,89	0
5	BTB	C	504	14/14	0.92	0.26	22,75,86,87	0
5	BTB	C	505	14/14	0.92	0.14	25,67,73,77	0
6	GOL	A	507	6/6	0.92	0.24	70,78,79,83	0
4	XVF	B	503	25/25	0.92	0.20	24,56,84,98	0
3	H4B	B	502	17/17	0.93	0.14	33,41,49,50	0

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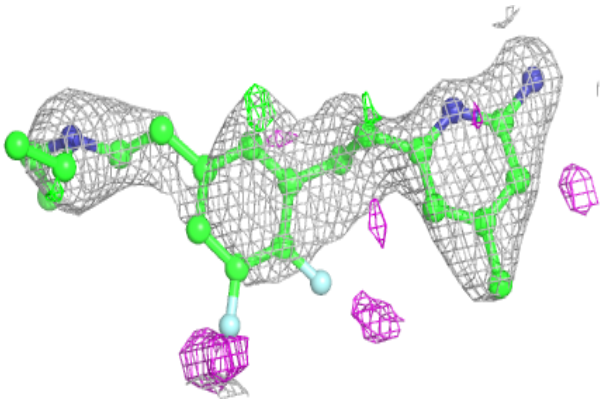
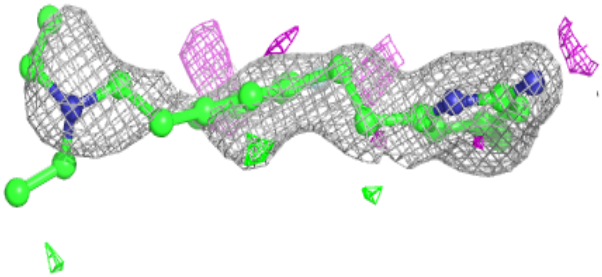
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	XVF	D	503	25/25	0.94	0.18	24,58,85,89	0
6	GOL	C	507	6/6	0.94	0.12	46,56,67,67	0
7	CL	A	509	1/1	0.94	0.20	51,51,51,51	0
2	HEM	A	501	43/43	0.95	0.21	38,49,77,79	0
2	HEM	C	501	43/43	0.96	0.20	32,41,73,96	0
2	HEM	B	501	43/43	0.97	0.13	23,31,67,83	0
2	HEM	D	501	43/43	0.97	0.13	24,28,70,80	0
8	GD	A	510	1/1	0.97	0.05	68,68,68,68	1
8	GD	D	508	1/1	0.97	0.06	42,42,42,42	0
7	CL	B	510	1/1	0.98	0.14	38,38,38,38	0
8	GD	B	511	1/1	0.98	0.06	38,38,38,38	0
8	GD	B	512	1/1	0.98	0.06	67,67,67,67	1
7	CL	C	511	1/1	0.98	0.20	48,48,48,48	0
7	CL	D	507	1/1	0.99	0.08	39,39,39,39	0
9	ZN	A	511	1/1	0.99	0.05	37,37,37,37	0
9	ZN	C	512	1/1	1.00	0.05	28,28,28,28	0

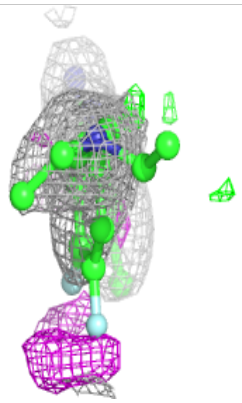
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XVF 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)

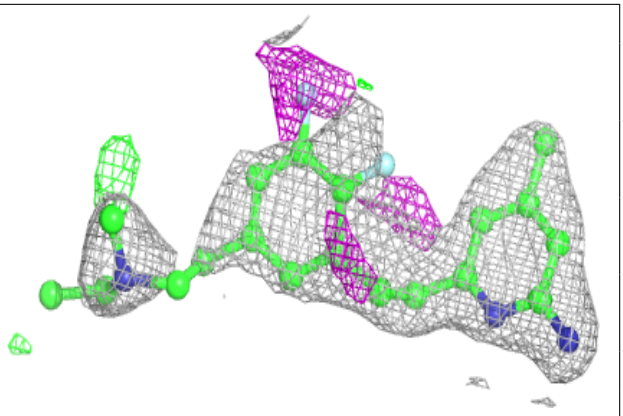


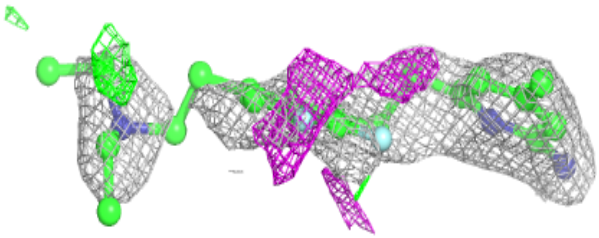


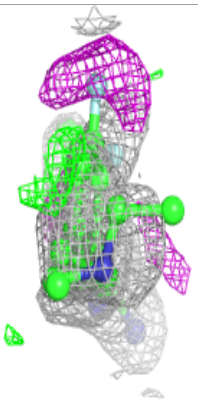


Electron density around XVF C 503:

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

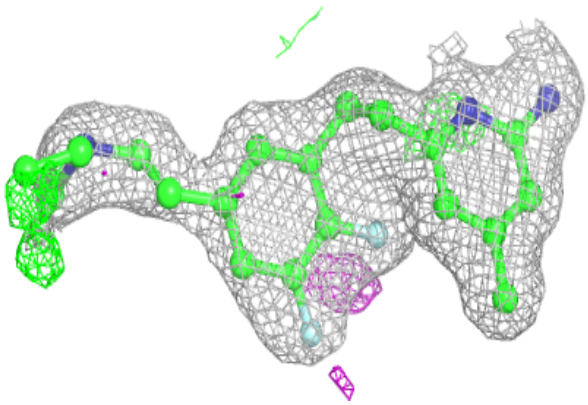


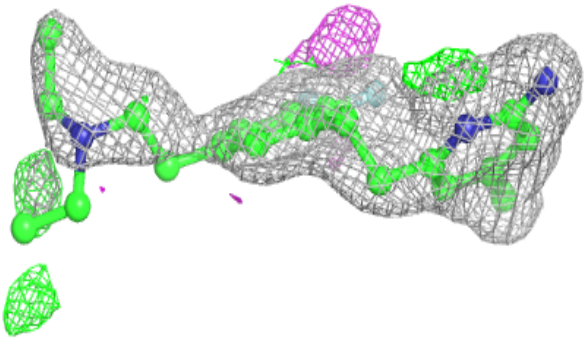


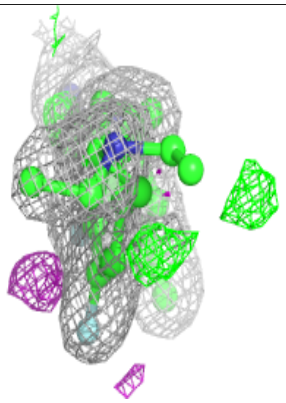


Electron density around XVF B 503:

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

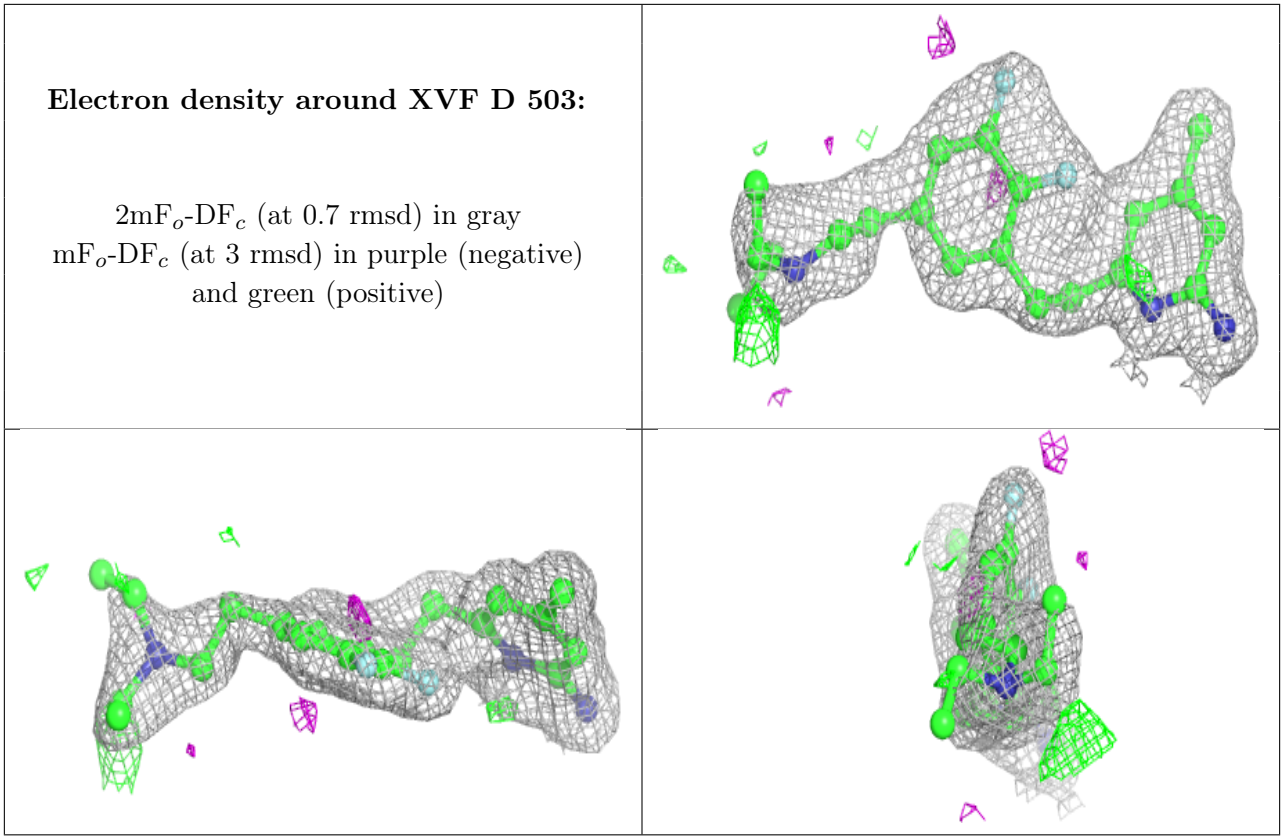






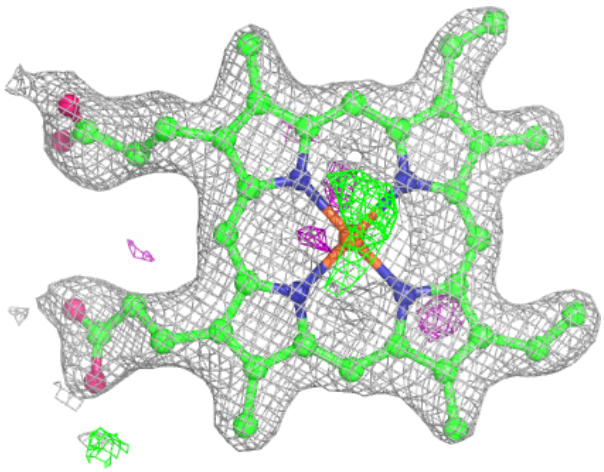
Electron density around XVF D 503:

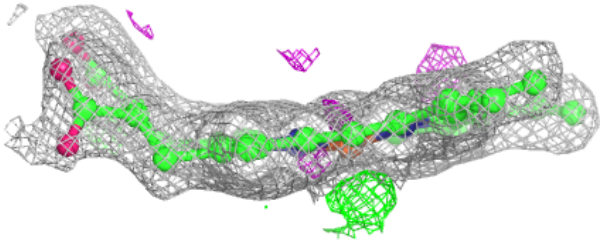
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

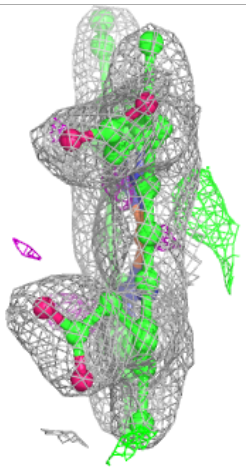


Electron density around HEM A 501:

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

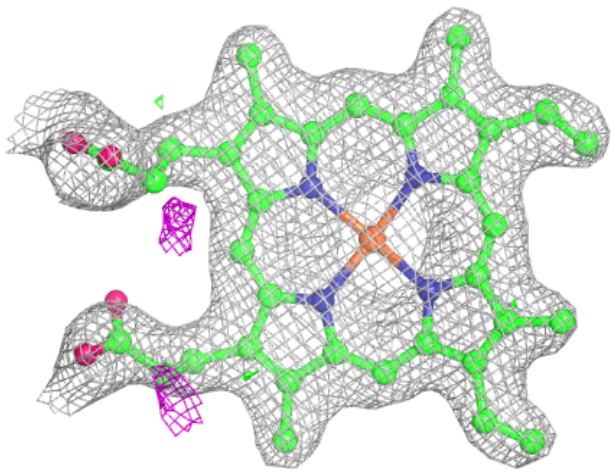


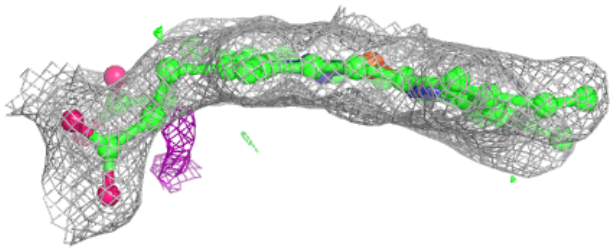


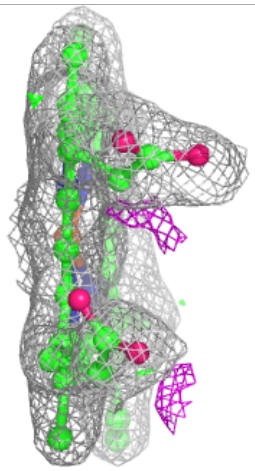


Electron density around HEM C 501:

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

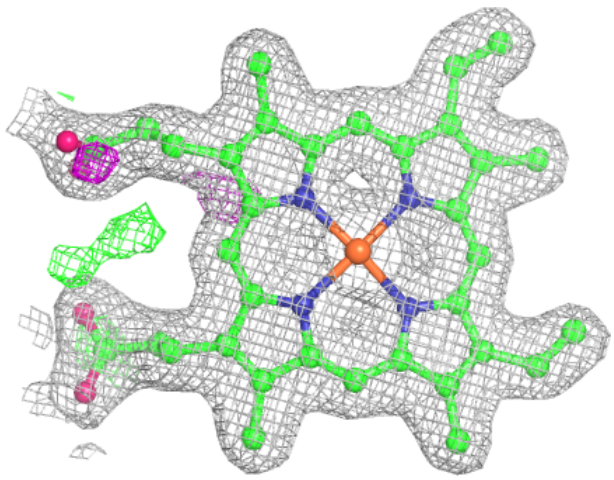


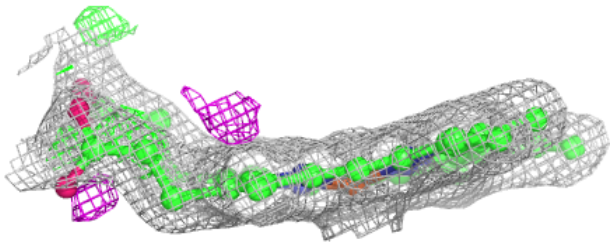


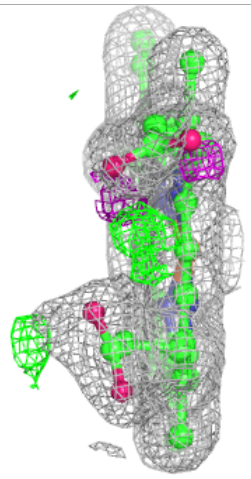


Electron density around HEM B 501:

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

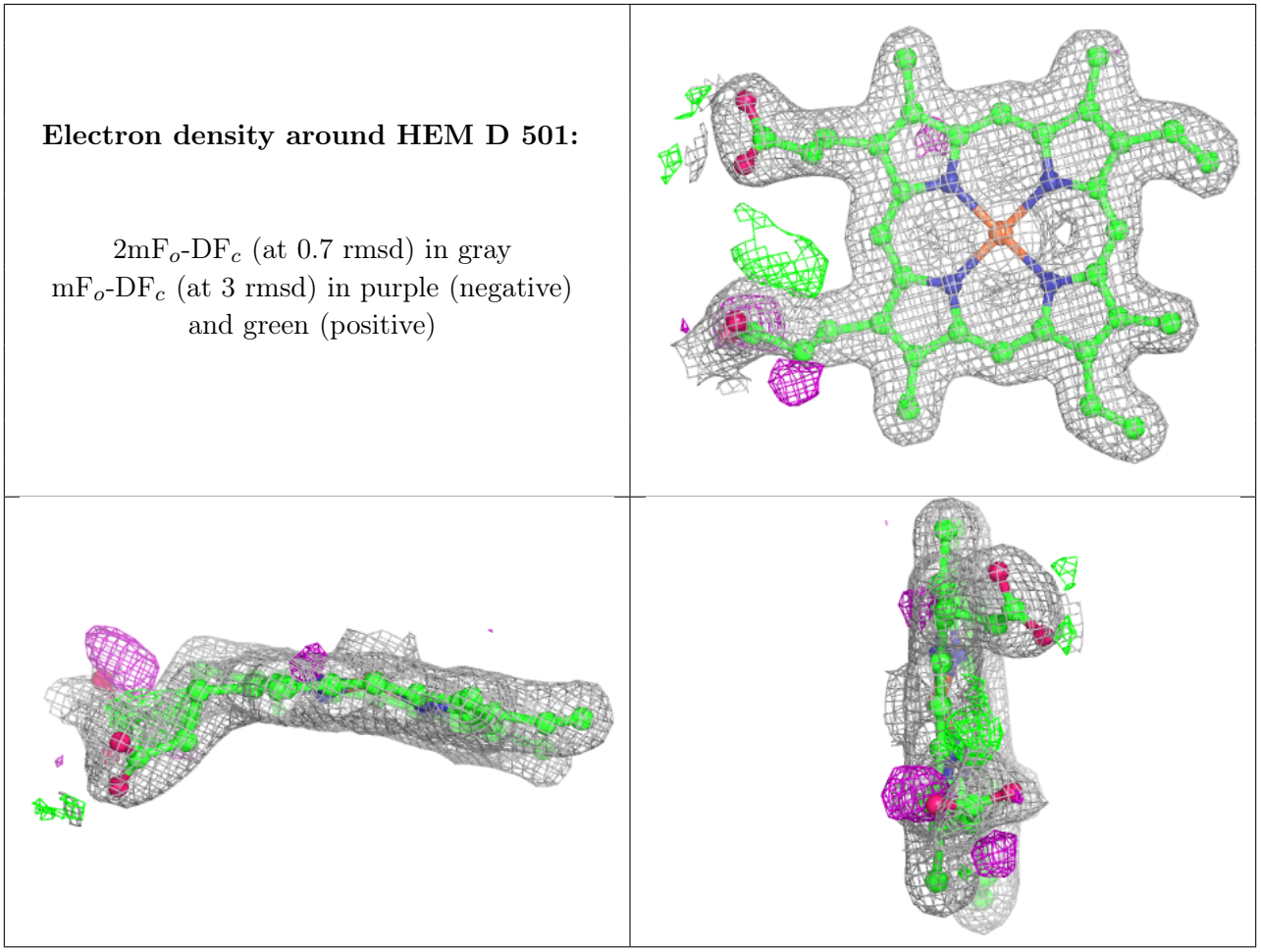






Electron density around HEM D 501:

$2mF_o$-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.