Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2023 – 02:00 AM EDT

PDB ID	:	8FGO
Title	:	Structure of human endothelial nitric oxide synthase heme domain in complex with 6-(5-(2-(dimethylamino)ethyl)-2,3-difluorophenethyl)-4-methylpyridin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2022-12-12
Resolution	:	1.80 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:

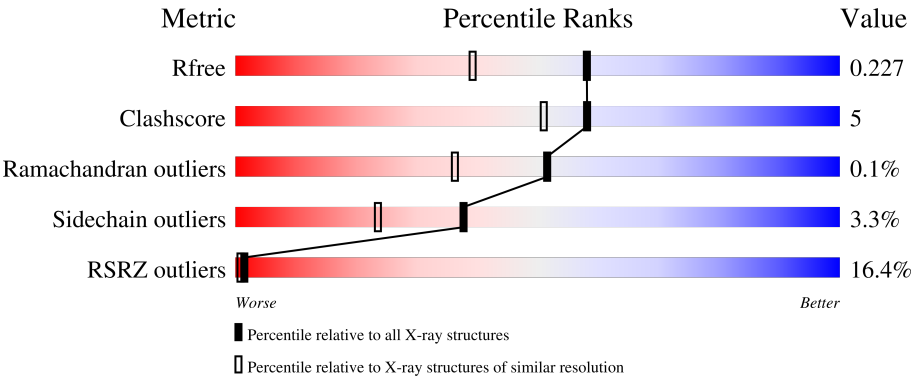
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	25% 77% 12% • 9%
1	B	440	7% 84% 6% • 9%
1	C	440	20% 80% 10% 9%
1	D	440	7% 84% 8% 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
4	XVU	A	503	-	-	-	X
6	GOL	A	512	-	X	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14344 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.

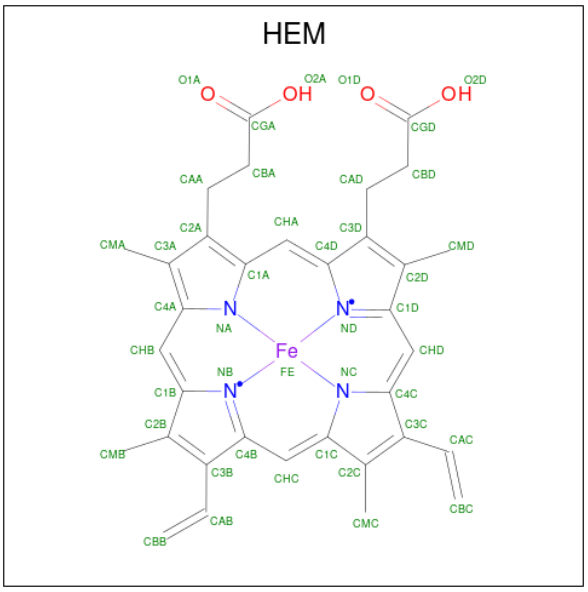
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

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	1	0
			3214	2046	567	585	16			

There are 4 discrepancies between the modelled and reference sequences:

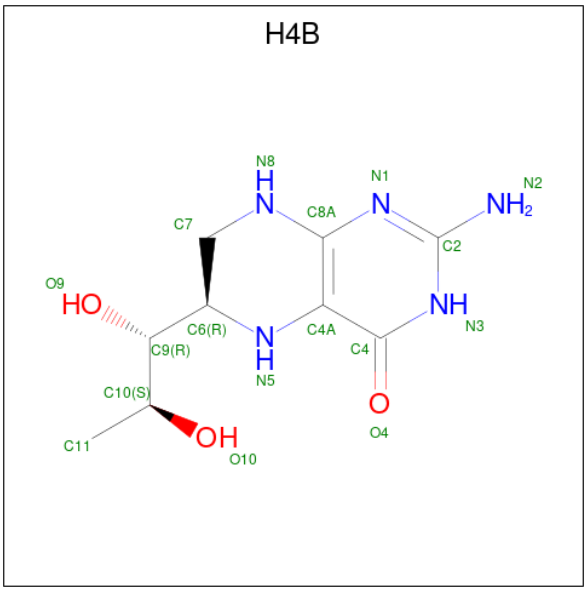
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



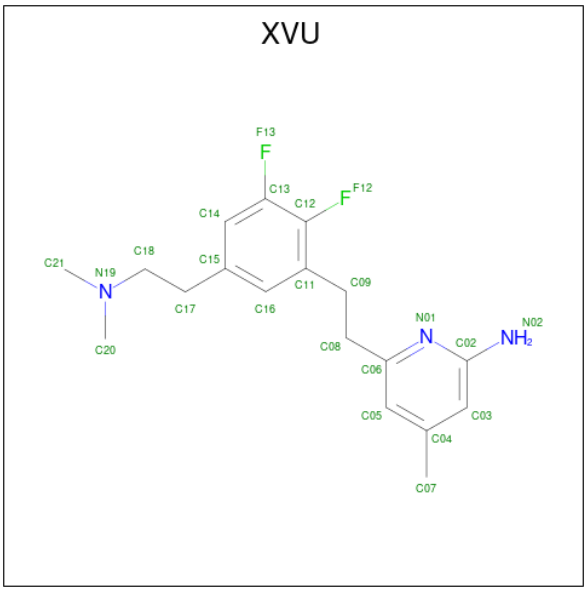
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



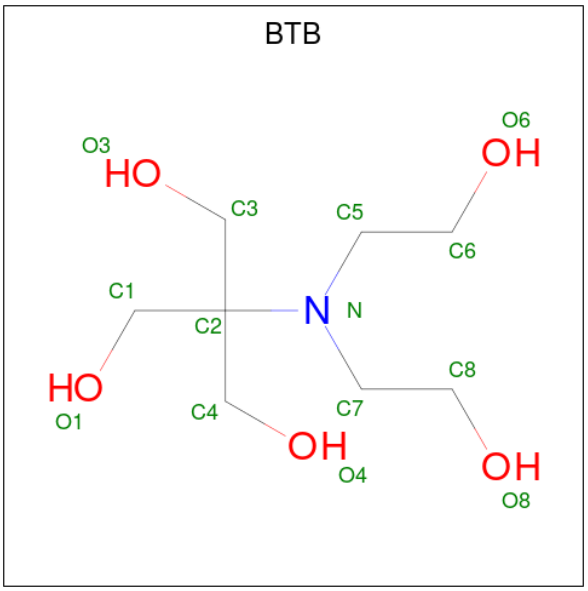
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0
3	C	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is 6-(2-{5-[2-(dimethylamino)ethyl]-2,3-difluorophenyl}ethyl)-4-methylpyridin-2-amine (three-letter code: XVU) (formula: $C_{18}H_{23}F_2N_3$) (labeled as "Ligand of Interest" by depositor).



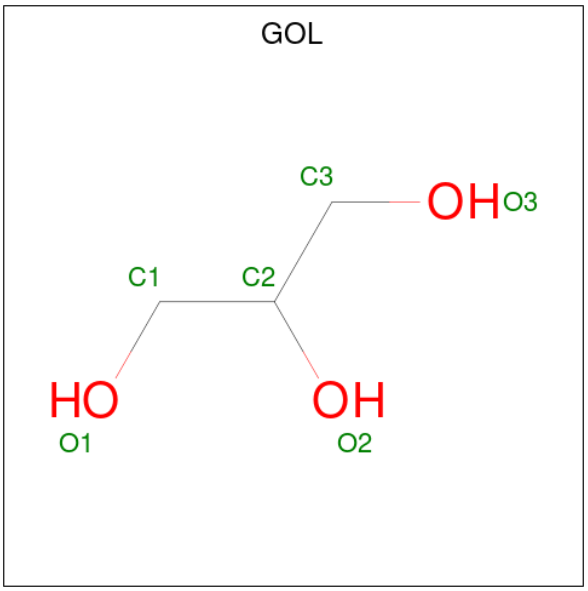
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N 23 18 2 3	0	0
4	B	1	Total C F N 23 18 2 3	0	0
4	C	1	Total C F N 23 18 2 3	0	0
4	D	1	Total C F N 23 18 2 3	0	0

- 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	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 (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	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 (three-letter code: 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 (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.

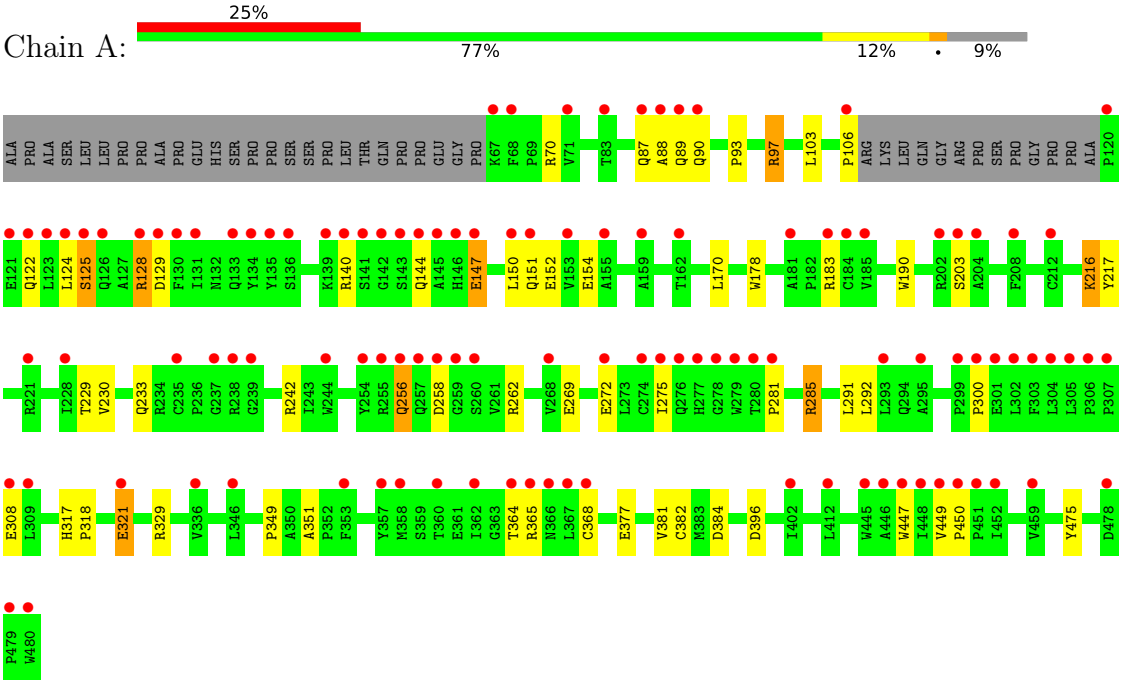
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	170	Total O 170 170	0	0
10	B	307	Total O 307 307	0	0
10	C	185	Total O 185 185	0	0
10	D	308	Total O 308 308	0	0

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.

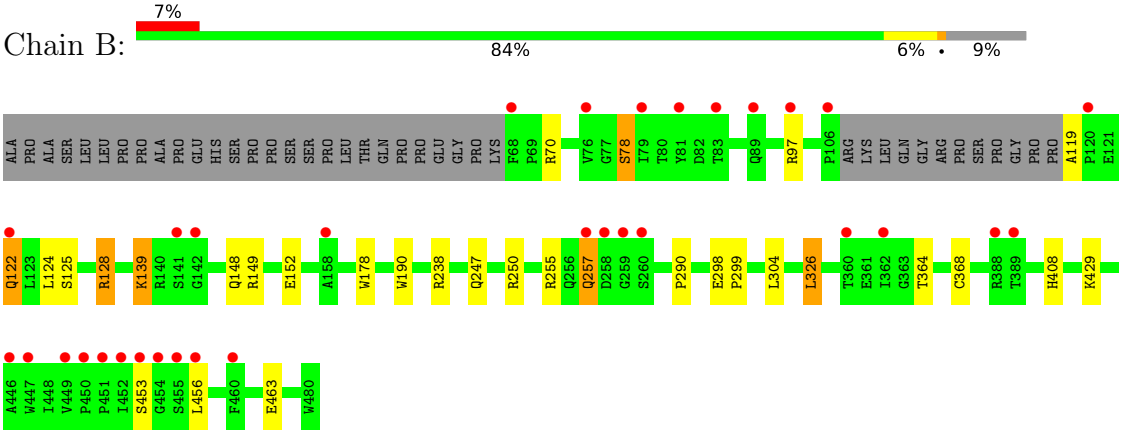
• Molecule 1: Nitric oxide synthase, endothelial

Chain A:



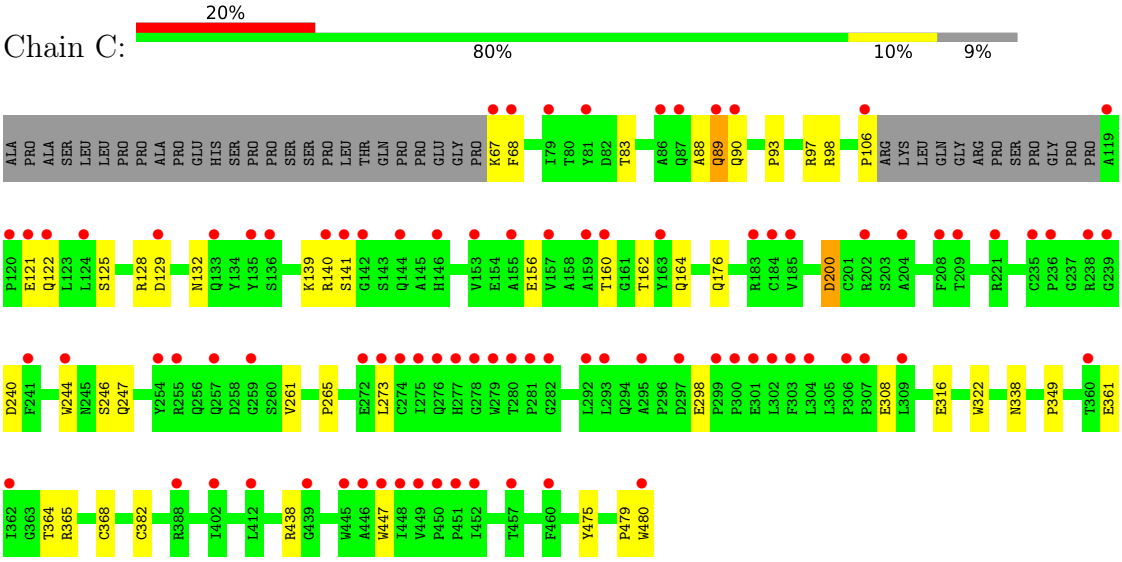
• Molecule 1: Nitric oxide synthase, endothelial

Chain B:



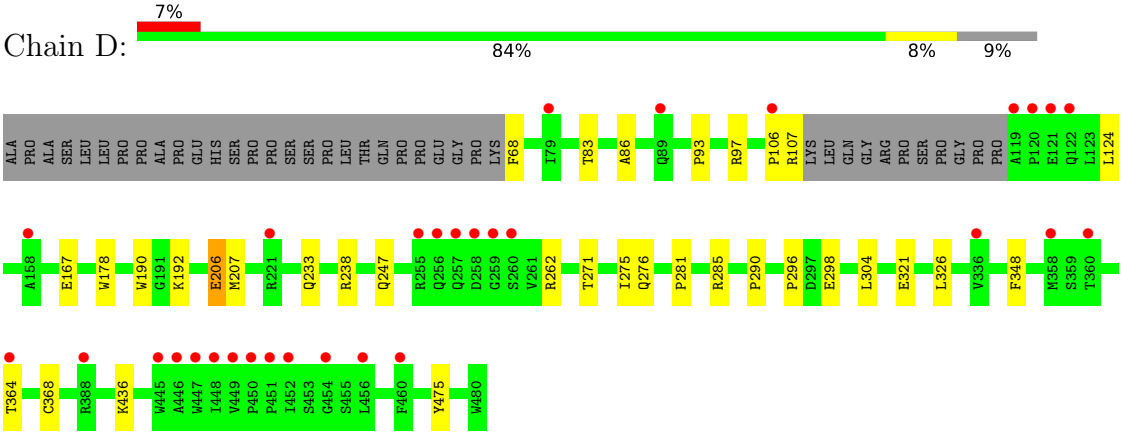
• Molecule 1: Nitric oxide synthase, endothelial

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	59.89Å 153.49Å 109.04Å 90.00° 90.79° 90.00°	Depositor
Resolution (Å)	40.05 – 1.80 40.04 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.05-1.80) 97.4 (40.04-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.188 , 0.227 0.189 , 0.227	Depositor DCC
R_{free} test set	8940 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14344	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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, GOL, CL, XVU, H4B, HEM, ZN, GD

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	0.40	0/3312	0.52	0/4514
1	C	0.33	0/3307	0.50	0/4506
1	D	0.41	0/3309	0.54	0/4509
All	All	0.37	0/13230	0.52	0/18027

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	37	1
1	B	3211	0	3114	26	0
1	C	3212	0	3116	29	0
1	D	3214	0	3116	20	1
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	4	0
2	D	43	0	30	2	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	0	0
3	C	17	0	15	2	0
3	D	17	0	15	0	0
4	A	23	0	0	0	0
4	B	23	0	0	1	0
4	C	23	0	0	2	0
4	D	23	0	0	1	0
5	A	42	0	56	7	0
5	B	42	0	55	5	1
5	C	28	0	36	8	0
5	D	28	0	35	5	1
6	A	18	0	24	0	0
6	B	6	0	8	0	0
6	C	18	0	24	0	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	170	0	0	5	0
10	B	307	0	0	4	0
10	C	185	0	0	4	0
10	D	308	0	0	3	0
All	All	14344	0	12884	126	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (126) 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:233:GLN:NE2	10:A:601:HOH:O	2.19	0.74
1:A:262:ARG:NH2	10:A:602:HOH:O	2.23	0.68
1:D:247:GLN:NE2	4:D:503:XVU:F12	2.18	0.67
1:B:70:ARG:NH1	10:B:601:HOH:O	2.27	0.66
1:C:90:GLN:NE2	10:C:602:HOH:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.15	0.65
1:B:247:GLN:NE2	4:B:503:XVU:F12	2.20	0.65
1:C:316:GLU:OE1	10:C:601:HOH:O	2.15	0.64
1:A:88:ALA:O	1:B:97:ARG:NH2	2.29	0.64
1:C:128:ARG:O	1:C:132:ASN:ND2	2.31	0.63
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.80	0.63
1:B:124:LEU:HB3	1:B:128:ARG:HH12	1.63	0.63
1:C:247:GLN:NE2	4:C:503:XVU:F12	2.24	0.61
5:D:505:BTB:H32	5:D:505:BTB:H62	1.83	0.60
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.84	0.59
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.84	0.59
1:A:321:GLU:H	1:A:321:GLU:CD	2.05	0.59
1:A:147:GLU:O	1:A:151:GLN:NE2	2.21	0.58
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.85	0.58
1:D:285:ARG:NH2	10:D:604:HOH:O	2.30	0.56
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.15	0.56
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.86	0.56
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.88	0.55
1:C:382:CYS:HA	5:C:504:BTB:H12	1.87	0.55
1:C:129:ASP:HA	1:C:132:ASN:HD22	1.71	0.54
1:C:97:ARG:NH2	1:D:86:ALA:HA	2.23	0.53
1:D:93:PRO:HB3	1:D:106:PRO:HB2	1.91	0.53
1:A:97:ARG:HH11	1:A:97:ARG:HB2	1.74	0.52
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.92	0.52
1:B:326:LEU:CD1	5:C:504:BTB:H41	2.39	0.52
1:A:150:LEU:HB2	1:A:151:GLN:NE2	2.24	0.52
1:A:384:ASP:OD1	5:A:504:BTB:O3	2.28	0.51
1:D:206:GLU:OE2	10:D:601:HOH:O	2.18	0.51
5:B:505:BTB:O8	5:B:505:BTB:O6	2.19	0.50
1:B:298:GLU:OE1	5:B:505:BTB:H42	2.12	0.50
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.94	0.50
1:C:240:ASP:HB3	1:C:349:PRO:HG2	1.94	0.50
1:C:160:THR:HG23	1:C:162:THR:H	1.77	0.49
1:A:285:ARG:HD2	10:A:669:HOH:O	2.13	0.49
1:B:298:GLU:CD	5:B:505:BTB:H42	2.32	0.49
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.18	0.49
5:A:504:BTB:H32	5:A:504:BTB:H51	1.47	0.48
1:A:269:GLU:O	1:A:272:GLU:HG2	2.13	0.48
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.95	0.48
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.95	0.48
1:D:298:GLU:OE2	5:D:505:BTB:H41	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:SER:HA	1:C:338:ASN:HB3	1.96	0.47
1:A:170:LEU:HD11	1:A:230:VAL:HG21	1.96	0.47
1:A:216:LYS:HG3	1:A:217:TYR:N	2.29	0.47
1:C:88:ALA:HB3	1:D:97:ARG:HD2	1.97	0.47
1:B:119:ALA:HB1	1:B:122:GLN:HG2	1.96	0.47
5:C:505:BTB:O4	5:C:505:BTB:O1	2.30	0.47
1:B:149:ARG:NH1	1:B:152:GLU:OE1	2.48	0.47
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.97	0.47
1:B:408:HIS:ND1	10:B:602:HOH:O	2.35	0.47
1:A:140:ARG:HG3	10:A:685:HOH:O	2.14	0.47
1:C:97:ARG:HE	1:C:97:ARG:HB3	1.61	0.46
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.50	0.46
1:C:68:PHE:CD1	1:C:83:THR:HG22	2.50	0.46
1:C:176:GLN:NE2	10:C:610:HOH:O	2.42	0.46
5:A:505:BTB:H11	5:A:505:BTB:H51	1.59	0.46
1:A:128:ARG:HH11	1:A:128:ARG:HB2	1.80	0.46
1:B:238:ARG:HE	1:B:238:ARG:HB3	1.57	0.46
5:D:505:BTB:O4	5:D:505:BTB:H52	2.15	0.46
1:A:242:ARG:HD2	1:A:349:PRO:HB2	1.98	0.45
1:C:156:GLU:OE2	1:C:164:GLN:HG2	2.16	0.45
1:D:167:GLU:OE1	10:D:602:HOH:O	2.20	0.45
1:C:200:ASP:HB2	10:C:673:HOH:O	2.16	0.45
1:D:106:PRO:HG2	1:D:107:ARG:HG3	1.98	0.45
1:D:271:THR:O	1:D:275:ILE:HG12	2.16	0.45
1:A:308:GLU:H	1:A:308:GLU:CD	2.20	0.45
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.30	0.45
1:B:257:GLN:H	1:B:257:GLN:HG3	1.39	0.45
5:C:505:BTB:H72	5:C:505:BTB:H31	1.33	0.45
1:B:298:GLU:HG3	1:B:299:PRO:HD2	1.99	0.44
5:B:509:BTB:H32	5:B:509:BTB:H72	1.69	0.44
1:C:364:THR:O	1:C:368:CYS:HB2	2.17	0.44
5:A:506:BTB:H41	5:A:506:BTB:H72	1.60	0.43
1:C:93:PRO:HB3	1:C:106:PRO:HB3	1.99	0.43
1:D:238:ARG:HG3	1:D:296:PRO:HB3	2.00	0.43
1:C:261:VAL:HG11	1:C:265:PRO:HA	2.00	0.43
5:A:505:BTB:H41	5:A:505:BTB:H72	1.48	0.43
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	2.00	0.43
5:A:504:BTB:H72	5:A:504:BTB:H12	1.43	0.43
1:C:156:GLU:O	1:C:160:THR:HG22	2.19	0.43
1:C:479:PRO:HD2	1:C:480:TRP:CZ3	2.52	0.43
1:C:298:GLU:OE2	5:C:505:BTB:O8	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:THR:O	1:A:351:ALA:HA	2.19	0.43
1:C:322:TRP:CD1	5:C:504:BTB:H61	2.53	0.42
1:D:275:ILE:HD11	1:D:281:PRO:HB3	2.01	0.42
1:A:125:SER:HA	1:A:128:ARG:NH1	2.33	0.42
1:D:298:GLU:OE1	5:D:505:BTB:H52	2.20	0.42
1:B:326:LEU:HD12	5:C:504:BTB:H41	2.00	0.42
1:C:447:TRP:HA	3:C:502:H4B:N1	2.35	0.42
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.54	0.42
1:B:326:LEU:HD11	5:C:504:BTB:H41	2.00	0.42
5:B:505:BTB:H51	5:B:505:BTB:H11	1.61	0.42
1:A:377:GLU:O	1:A:381:VAL:HG23	2.19	0.42
1:B:97:ARG:HG3	10:B:862:HOH:O	2.20	0.42
1:C:361:GLU:OE2	4:C:503:XVU:N02	2.53	0.42
1:A:70:ARG:NH2	10:A:617:HOH:O	2.52	0.42
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.55	0.42
1:A:150:LEU:O	1:A:154:GLU:HG3	2.20	0.42
1:A:364:THR:O	1:A:368:CYS:HB2	2.20	0.42
1:A:103:LEU:HD12	1:B:463:GLU:HB3	2.02	0.41
1:A:256:GLN:C	1:A:258:ASP:H	2.23	0.41
1:D:68:PHE:CD2	1:D:83:THR:HA	2.56	0.41
1:A:89:GLN:HG3	1:A:90:GLN:N	2.35	0.41
1:A:382:CYS:HA	5:A:504:BTB:H11	2.02	0.41
1:C:244:TRP:CD1	1:C:479:PRO:HG2	2.56	0.41
1:B:364:THR:O	1:B:368:CYS:HB2	2.21	0.41
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.34	0.41
1:B:139:LYS:N	1:B:139:LYS:HD2	2.36	0.41
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.26	0.41
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.56	0.41
1:A:449:VAL:HA	1:A:450:PRO:HD3	1.98	0.41
1:D:364:THR:O	1:D:368:CYS:HB2	2.21	0.41
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.56	0.40
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.55	0.40
2:C:501:HEM:HBB2	2:C:501:HEM:CHC	2.50	0.40
1:A:93:PRO:HB3	1:A:106:PRO:HB3	2.03	0.40
1:A:258:ASP:OD1	1:A:258:ASP:N	2.54	0.40
1:B:78:SER:HB2	10:B:861:HOH:O	2.22	0.40
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.87	0.40
1:B:429:LYS:HA	1:B:429:LYS:HD2	1.95	0.40
1:C:273:LEU:HA	1:C:273:LEU:HD23	1.90	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:GLU:OE1	5:B:505:BTB:O1[1_554]	2.05	0.15
1:A:152:GLU:OE2	5:D:505:BTB:O4[2_851]	2.12	0.08

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%)	381 (96%)	16 (4%)	1 (0%)	41 27
1	B	400/440 (91%)	390 (98%)	10 (2%)	0	100 100
1	C	399/440 (91%)	386 (97%)	12 (3%)	1 (0%)	41 27
1	D	399/440 (91%)	391 (98%)	8 (2%)	0	100 100
All	All	1596/1760 (91%)	1548 (97%)	46 (3%)	2 (0%)	51 36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	SER
1	C	89	GLN

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	342/373 (92%)	326 (95%)	16 (5%)	26 12
1	B	343/373 (92%)	334 (97%)	9 (3%)	46 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	342/373 (92%)	330 (96%)	12 (4%)	36 21
1	D	342/373 (92%)	334 (98%)	8 (2%)	50 37
All	All	1369/1492 (92%)	1324 (97%)	45 (3%)	38 23

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	97	ARG
1	A	122	GLN
1	A	124	LEU
1	A	125	SER
1	A	128	ARG
1	A	129	ASP
1	A	144	GLN
1	A	147	GLU
1	A	216	LYS
1	A	256	GLN
1	A	285	ARG
1	A	291	LEU
1	A	321	GLU
1	A	329	ARG
1	A	396	ASP
1	B	78	SER
1	B	122	GLN
1	B	125	SER
1	B	128	ARG
1	B	139	LYS
1	B	148	GLN
1	B	255	ARG
1	B	257	GLN
1	B	326	LEU
1	C	67	LYS
1	C	89	GLN
1	C	98	ARG
1	C	121	GLU
1	C	122	GLN
1	C	125	SER
1	C	139	LYS
1	C	140	ARG
1	C	141	SER

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Mol	Chain	Res	Type
1	C	200	ASP
1	C	308	GLU
1	C	438	ARG
1	D	124	LEU
1	D	192	LYS
1	D	206	GLU
1	D	207	MET
1	D	262	ARG
1	D	276	GLN
1	D	326	LEU
1	D	436	LYS

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	164	GLN
1	C	132	ASN

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 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 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	D	505	-	13,13,13	0.67	0	7,16,16	1.09	0
5	BTB	B	505	-	13,13,13	0.47	0	7,16,16	1.15	0
6	GOL	A	508	-	5,5,5	0.38	0	5,5,5	0.23	0
6	GOL	A	507	-	5,5,5	0.35	0	5,5,5	0.51	0
2	HEM	D	501	1	41,50,50	1.65	8 (19%)	45,82,82	1.83	12 (26%)
2	HEM	B	501	1	41,50,50	1.56	8 (19%)	45,82,82	1.76	10 (22%)
4	XVU	D	503	-	24,24,24	0.57	0	32,33,33	2.00	6 (18%)
6	GOL	D	506	-	5,5,5	0.37	0	5,5,5	0.27	0
6	GOL	A	512	-	5,5,5	0.87	0	5,5,5	2.01	2 (40%)
6	GOL	C	508	-	5,5,5	0.36	0	5,5,5	0.18	0
5	BTB	B	509	-	13,13,13	1.11	2 (15%)	7,16,16	1.25	0
5	BTB	C	505	-	13,13,13	0.33	0	7,16,16	0.49	0
3	H4B	B	502	-	16,18,18	0.94	0	11,26,26	2.54	7 (63%)
2	HEM	A	501	1	41,50,50	1.51	4 (9%)	45,82,82	1.67	11 (24%)
6	GOL	C	507	-	5,5,5	0.35	0	5,5,5	0.24	0
4	XVU	C	503	-	24,24,24	0.54	0	32,33,33	2.02	7 (21%)
5	BTB	A	505	-	13,13,13	0.69	0	7,16,16	0.93	0
6	GOL	B	506	-	5,5,5	0.36	0	5,5,5	0.50	0
5	BTB	D	504	8	13,13,13	0.38	0	7,16,16	0.60	0
5	BTB	B	504	8	13,13,13	0.38	0	7,16,16	0.40	0
4	XVU	A	503	-	24,24,24	0.50	0	32,33,33	1.81	5 (15%)
4	XVU	B	503	-	24,24,24	0.51	0	32,33,33	1.97	7 (21%)
3	H4B	C	502	-	16,18,18	0.95	0	11,26,26	2.58	4 (36%)
6	GOL	C	506	-	5,5,5	0.38	0	5,5,5	0.59	0
5	BTB	A	506	-	13,13,13	0.33	0	7,16,16	0.35	0
5	BTB	A	504	8	13,13,13	0.48	0	7,16,16	1.26	1 (14%)
3	H4B	D	502	-	16,18,18	0.94	1 (6%)	11,26,26	2.47	4 (36%)
5	BTB	C	504	8	13,13,13	0.40	0	7,16,16	0.75	0
3	H4B	A	502	-	16,18,18	0.85	0	11,26,26	2.56	5 (45%)
2	HEM	C	501	1	41,50,50	1.47	6 (14%)	45,82,82	1.77	8 (17%)

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	D	505	-	-	5/21/21/21	-
5	BTB	B	505	-	-	11/21/21/21	-
6	GOL	A	508	-	-	2/4/4/4	-
6	GOL	A	507	-	-	4/4/4/4	-
2	HEM	D	501	1	-	0/12/54/54	-
2	HEM	B	501	1	-	0/12/54/54	-
4	XVU	D	503	-	-	8/10/10/10	0/2/2/2
6	GOL	D	506	-	-	2/4/4/4	-
6	GOL	A	512	-	-	4/4/4/4	-
6	GOL	C	508	-	-	4/4/4/4	-
5	BTB	B	509	-	-	3/21/21/21	-
5	BTB	C	505	-	-	14/21/21/21	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
2	HEM	A	501	1	-	2/12/54/54	-
6	GOL	C	507	-	-	4/4/4/4	-
4	XVU	C	503	-	-	5/10/10/10	0/2/2/2
5	BTB	A	505	-	-	6/21/21/21	-
6	GOL	B	506	-	-	0/4/4/4	-
5	BTB	D	504	8	-	6/21/21/21	-
5	BTB	B	504	8	-	3/21/21/21	-
4	XVU	A	503	-	-	3/10/10/10	0/2/2/2
4	XVU	B	503	-	-	6/10/10/10	0/2/2/2
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
6	GOL	C	506	-	-	2/4/4/4	-
5	BTB	A	506	-	-	0/21/21/21	-
5	BTB	A	504	8	-	9/21/21/21	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
5	BTB	C	504	8	-	1/21/21/21	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
2	HEM	C	501	1	-	1/12/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-NB	4.47	2.19	1.96
2	A	501	HEM	C3C-CAC	3.79	1.55	1.47
2	B	501	HEM	C3C-CAC	3.77	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.72	1.35	1.40
2	D	501	HEM	C3C-CAC	3.55	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3C-CAC	3.49	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.33	1.35	1.40
2	D	501	HEM	CAB-C3B	3.26	1.56	1.47
2	D	501	HEM	C3C-C2C	-3.22	1.35	1.40
2	A	501	HEM	CAB-C3B	3.17	1.56	1.47
2	B	501	HEM	C3C-C2C	-3.13	1.36	1.40
2	B	501	HEM	CAB-C3B	3.07	1.55	1.47
2	C	501	HEM	CAB-C3B	3.07	1.55	1.47
2	B	501	HEM	FE-NB	2.91	2.11	1.96
2	A	501	HEM	FE-NB	2.87	2.11	1.96
5	B	509	BTB	C3-C2	-2.69	1.49	1.53
2	D	501	HEM	CMD-C2D	2.62	1.56	1.50
5	B	509	BTB	C7-N	-2.52	1.44	1.48
2	B	501	HEM	CMB-C2B	2.43	1.55	1.50
2	B	501	HEM	CMD-C2D	2.31	1.55	1.50
2	B	501	HEM	FE-ND	2.24	2.08	1.96
3	D	502	H4B	C4A-C4	-2.21	1.38	1.41
2	D	501	HEM	CMB-C2B	2.16	1.55	1.50
2	D	501	HEM	FE-ND	2.15	2.07	1.96
2	B	501	HEM	CAA-C2A	2.12	1.55	1.52
2	D	501	HEM	CMC-C2C	2.05	1.56	1.51
2	C	501	HEM	CAA-C2A	2.04	1.55	1.52
2	C	501	HEM	FE-NB	2.03	2.06	1.96
2	C	501	HEM	CMC-C2C	2.02	1.56	1.51

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	503	XVU	C02-N01-C06	7.51	123.80	118.10
4	C	503	XVU	C02-N01-C06	7.29	123.62	118.10
4	A	503	XVU	C02-N01-C06	6.58	123.09	118.10
4	B	503	XVU	C02-N01-C06	6.11	122.73	118.10
3	A	502	H4B	C8A-C4A-C4	5.34	119.32	114.57
3	D	502	H4B	C8A-C4A-C4	5.28	119.26	114.57
3	B	502	H4B	C8A-C4A-C4	5.08	119.08	114.57
3	C	502	H4B	C8A-C4A-C4	5.06	119.07	114.57
2	D	501	HEM	C4B-CHC-C1C	4.94	129.08	122.56
4	D	503	XVU	C05-C06-N01	-4.83	117.78	122.90
2	B	501	HEM	CBA-CAA-C2A	-4.74	104.53	112.62
2	D	501	HEM	CBA-CAA-C2A	-4.63	104.72	112.62
2	C	501	HEM	CBA-CAA-C2A	-4.59	104.79	112.62
4	B	503	XVU	C05-C06-N01	-4.21	118.44	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	HEM	C4D-ND-C1D	4.18	109.39	105.07
4	C	503	XVU	C05-C06-N01	-4.02	118.63	122.90
2	C	501	HEM	C4B-CHC-C1C	3.88	127.68	122.56
2	B	501	HEM	C4B-CHC-C1C	3.81	127.59	122.56
2	D	501	HEM	C1B-NB-C4B	3.66	108.86	105.07
4	A	503	XVU	C05-C06-N01	-3.64	119.04	122.90
2	A	501	HEM	C4B-CHC-C1C	3.60	127.31	122.56
4	C	503	XVU	F12-C12-C11	3.59	121.64	117.85
6	A	512	GOL	O2-C2-C1	-3.58	93.34	109.12
4	B	503	XVU	F12-C12-C11	3.55	121.59	117.85
2	B	501	HEM	C1B-NB-C4B	3.49	108.68	105.07
3	C	502	H4B	C2-N3-C4	3.43	121.38	115.93
4	B	503	XVU	C09-C11-C12	3.43	123.48	120.73
3	C	502	H4B	N1-C2-N3	-3.42	120.06	125.42
2	B	501	HEM	C4D-ND-C1D	3.33	108.51	105.07
2	A	501	HEM	C4D-ND-C1D	3.32	108.50	105.07
2	A	501	HEM	C3B-C2B-C1B	3.31	108.94	106.49
2	A	501	HEM	C1B-NB-C4B	3.29	108.47	105.07
3	D	502	H4B	C2-N3-C4	3.27	121.12	115.93
5	A	504	BTB	O3-C3-C2	3.19	120.17	111.44
2	C	501	HEM	CBD-CAD-C3D	-3.18	103.78	112.63
2	C	501	HEM	C1B-NB-C4B	3.17	108.35	105.07
3	B	502	H4B	N1-C2-N3	-3.15	120.48	125.42
3	B	502	H4B	C2-N3-C4	3.08	120.83	115.93
3	A	502	H4B	C2-N3-C4	3.06	120.80	115.93
4	A	503	XVU	F12-C12-C11	3.06	121.08	117.85
3	A	502	H4B	N1-C2-N3	-3.05	120.64	125.42
3	D	502	H4B	N1-C2-N3	-3.03	120.66	125.42
2	C	501	HEM	C4D-ND-C1D	2.98	108.15	105.07
2	D	501	HEM	C3D-C4D-ND	-2.89	106.95	110.17
2	B	501	HEM	C3B-C2B-C1B	2.82	108.58	106.49
2	B	501	HEM	CMC-C2C-C3C	2.79	129.90	124.68
4	C	503	XVU	C18-C17-C15	-2.78	104.21	112.16
4	D	503	XVU	C09-C11-C12	2.72	122.92	120.73
2	C	501	HEM	C3B-C2B-C1B	2.71	108.50	106.49
3	B	502	H4B	C2-N1-C8A	2.71	120.60	114.54
3	A	502	H4B	C4-C4A-N5	2.70	121.39	119.12
2	A	501	HEM	CBD-CAD-C3D	-2.70	105.13	112.63
2	B	501	HEM	CBD-CAD-C3D	-2.69	105.14	112.63
4	A	503	XVU	C16-C11-C12	2.69	119.22	116.76
3	C	502	H4B	C2-N1-C8A	2.67	120.51	114.54
2	D	501	HEM	CBD-CAD-C3D	-2.65	105.26	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	C3D-C4D-ND	-2.64	107.23	110.17
3	A	502	H4B	C2-N1-C8A	2.63	120.44	114.54
6	A	512	GOL	O1-C1-C2	-2.61	97.69	110.20
2	D	501	HEM	CMA-C3A-C4A	-2.58	124.50	128.46
2	B	501	HEM	C3D-C4D-ND	-2.56	107.31	110.17
3	D	502	H4B	C2-N1-C8A	2.54	120.22	114.54
4	D	503	XVU	F12-C12-C11	2.45	120.43	117.85
4	D	503	XVU	C05-C04-C03	2.40	120.95	118.09
4	C	503	XVU	C17-C15-C14	-2.40	116.61	120.54
4	A	503	XVU	C08-C06-C05	2.39	124.38	121.22
2	A	501	HEM	C3D-C4D-ND	-2.36	107.54	110.17
2	B	501	HEM	CHC-C4B-C3B	2.34	128.15	124.57
4	C	503	XVU	C16-C11-C12	2.34	118.90	116.76
2	D	501	HEM	C3C-C4C-NC	-2.33	106.55	110.94
2	D	501	HEM	C2C-C3C-C4C	2.31	108.51	106.90
2	D	501	HEM	C3B-C2B-C1B	2.29	108.19	106.49
3	B	502	H4B	O9-C9-C6	2.28	114.43	108.98
2	A	501	HEM	C4A-C3A-C2A	2.28	108.58	107.00
2	A	501	HEM	CBA-CAA-C2A	-2.27	108.74	112.62
3	B	502	H4B	N2-C2-N1	2.27	120.79	117.25
4	B	503	XVU	C16-C11-C12	2.26	118.83	116.76
4	B	503	XVU	C17-C18-N19	-2.24	106.71	114.02
3	B	502	H4B	C4-C4A-N5	2.14	120.92	119.12
2	A	501	HEM	CMA-C3A-C4A	-2.12	125.20	128.46
2	A	501	HEM	C2B-C1B-NB	-2.11	107.34	109.84
4	D	503	XVU	C08-C06-C05	2.11	124.00	121.22
4	B	503	XVU	C16-C15-C14	2.08	121.84	118.98
2	D	501	HEM	C2D-C1D-ND	-2.07	107.40	109.88
2	D	501	HEM	C4C-CHD-C1D	2.06	125.28	122.56
2	A	501	HEM	CMC-C2C-C3C	2.06	128.54	124.68
4	C	503	XVU	C09-C11-C12	2.05	122.38	120.73
2	B	501	HEM	C2B-C1B-NB	-2.02	107.44	109.84
2	C	501	HEM	CMC-C2C-C3C	2.02	128.45	124.68

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	BTB	O1-C1-C2-C3
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
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
5	B	505	BTB	C1-C2-N-C7
5	B	505	BTB	C3-C2-N-C7
5	B	505	BTB	C4-C2-N-C7
5	B	509	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	C4-C2-C3-O3
5	C	505	BTB	C3-C2-N-C7
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	504	BTB	C3-C2-C4-O4
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
6	A	507	GOL	O1-C1-C2-C3
6	A	508	GOL	O1-C1-C2-C3
6	A	512	GOL	O1-C1-C2-C3
6	A	512	GOL	C1-C2-C3-O3
6	C	506	GOL	O1-C1-C2-O2
6	C	506	GOL	O1-C1-C2-C3
6	C	507	GOL	O1-C1-C2-O2
6	C	507	GOL	O1-C1-C2-C3
6	C	507	GOL	C1-C2-C3-O3
6	C	507	GOL	O2-C2-C3-O3
6	C	508	GOL	O1-C1-C2-C3
6	D	506	GOL	O1-C1-C2-O2
6	D	506	GOL	O1-C1-C2-C3
5	B	509	BTB	N-C5-C6-O6
4	B	503	XVU	C08-C09-C11-C16
4	D	503	XVU	C17-C18-N19-C21
6	A	508	GOL	O1-C1-C2-O2
4	A	503	XVU	C17-C18-N19-C21

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Mol	Chain	Res	Type	Atoms
4	C	503	XVU	C08-C09-C11-C16
5	A	505	BTB	N-C7-C8-O8
4	D	503	XVU	C17-C18-N19-C20
5	A	504	BTB	N-C7-C8-O8
4	A	503	XVU	C15-C17-C18-N19
6	A	507	GOL	C1-C2-C3-O3
6	C	508	GOL	C1-C2-C3-O3
5	B	505	BTB	N-C7-C8-O8
5	D	505	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
4	D	503	XVU	C15-C17-C18-N19
6	A	507	GOL	O1-C1-C2-O2
6	A	512	GOL	O2-C2-C3-O3
6	C	508	GOL	O1-C1-C2-O2
5	D	505	BTB	C6-C5-N-C7
2	C	501	HEM	C4B-C3B-CAB-CBB
5	C	505	BTB	N-C5-C6-O6
4	C	503	XVU	N01-C06-C08-C09
6	A	512	GOL	O1-C1-C2-O2
6	C	508	GOL	O2-C2-C3-O3
4	D	503	XVU	C14-C15-C17-C18
4	B	503	XVU	C14-C15-C17-C18
4	B	503	XVU	C16-C15-C17-C18
4	D	503	XVU	C16-C15-C17-C18
4	C	503	XVU	C05-C06-C08-C09
4	A	503	XVU	C08-C09-C11-C16
4	D	503	XVU	N01-C06-C08-C09
5	B	505	BTB	N-C5-C6-O6
4	D	503	XVU	C05-C06-C08-C09
4	B	503	XVU	C08-C09-C11-C12
5	B	509	BTB	C3-C2-C4-O4
5	D	504	BTB	C1-C2-C4-O4
5	A	504	BTB	O1-C1-C2-N
5	A	505	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C4-C2-N-C5
5	B	505	BTB	C1-C2-N-C5
5	B	505	BTB	C3-C2-N-C5
5	C	505	BTB	N-C2-C3-O3
5	C	505	BTB	C1-C2-N-C5
5	C	505	BTB	C1-C2-N-C7
5	C	505	BTB	C3-C2-N-C5

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Mol	Chain	Res	Type	Atoms
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
5	D	504	BTB	N-C2-C4-O4
4	B	503	XVU	C05-C06-C08-C09
4	C	503	XVU	C14-C15-C17-C18
5	C	504	BTB	N-C7-C8-O8
4	B	503	XVU	N01-C06-C08-C09
6	A	507	GOL	O2-C2-C3-O3
4	D	503	XVU	C08-C09-C11-C16
4	C	503	XVU	C16-C15-C17-C18
5	C	505	BTB	N-C7-C8-O8
2	A	501	HEM	C4B-C3B-CAB-CBB
5	A	504	BTB	O1-C1-C2-C4
5	A	504	BTB	C1-C2-C3-O3
5	A	504	BTB	C4-C2-C3-O3
5	B	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C1-C2-C3-O3

There are no ring outliers.

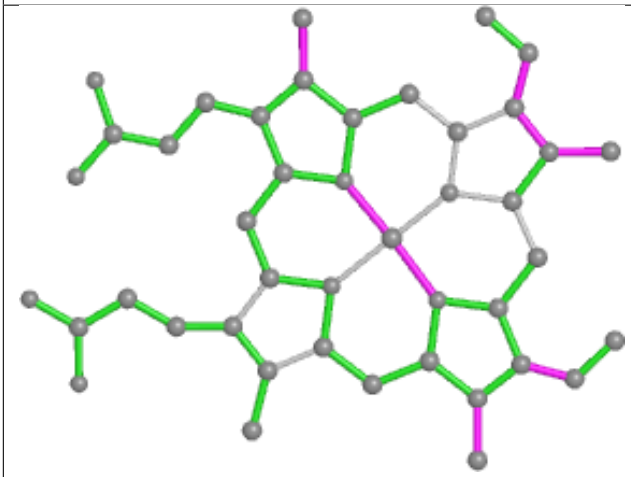
18 monomers are involved in 43 short contacts:

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

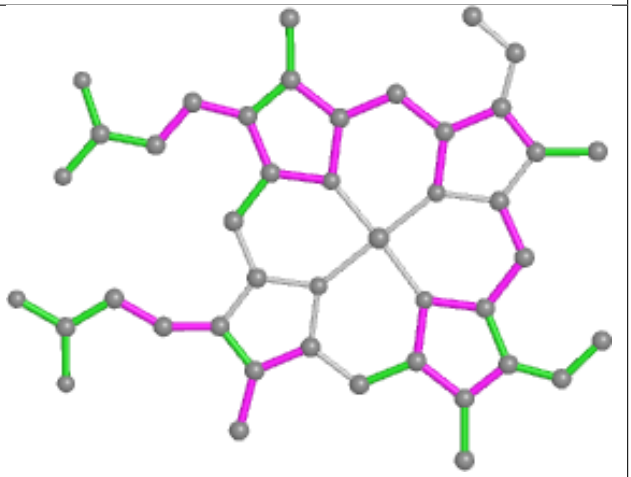
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

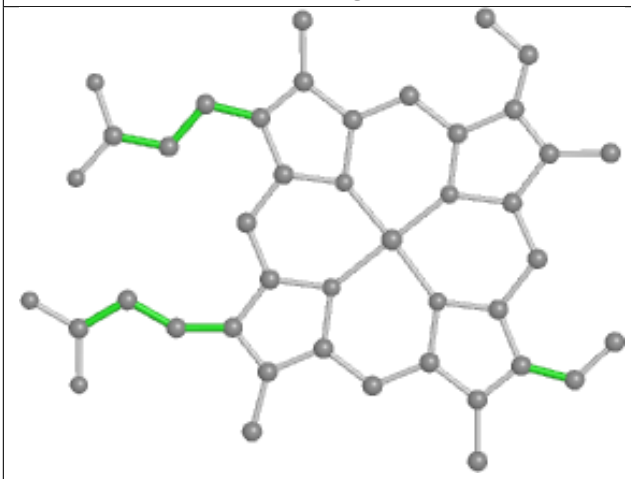
Ligand HEM D 501



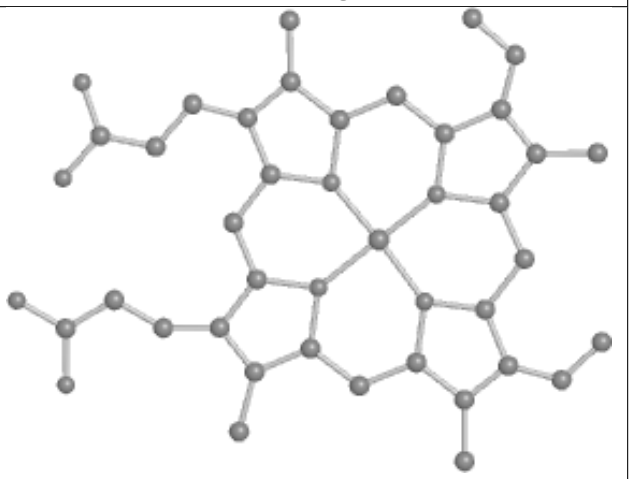
Bond lengths



Bond angles

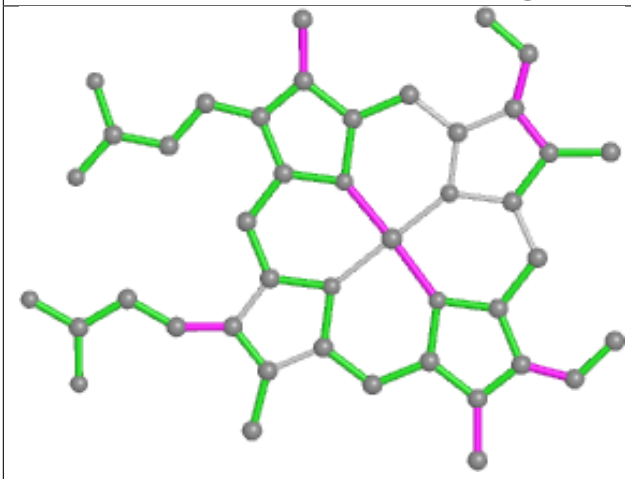


Torsions

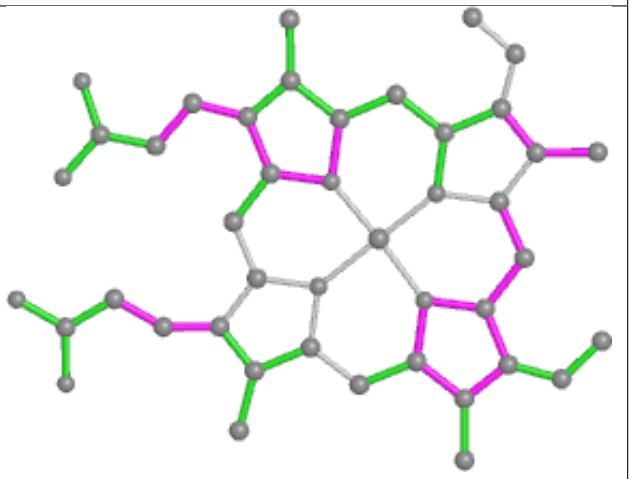


Rings

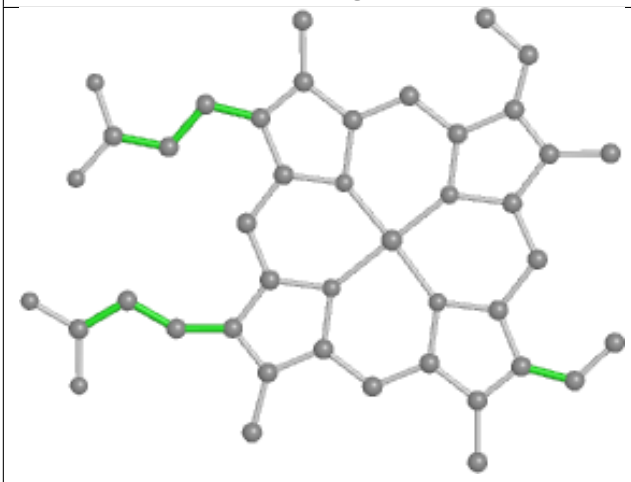
Ligand HEM B 501



Bond lengths



Bond angles



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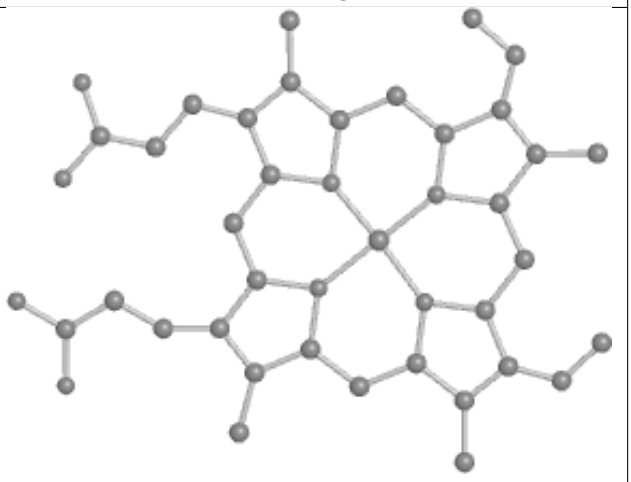
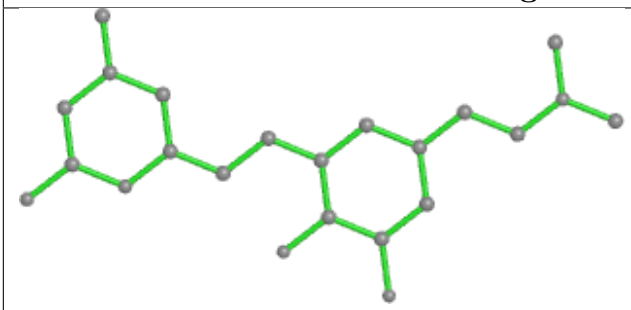


Rings

Ligand XVU D 503



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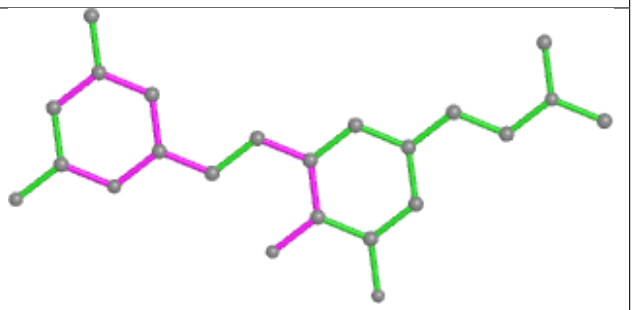
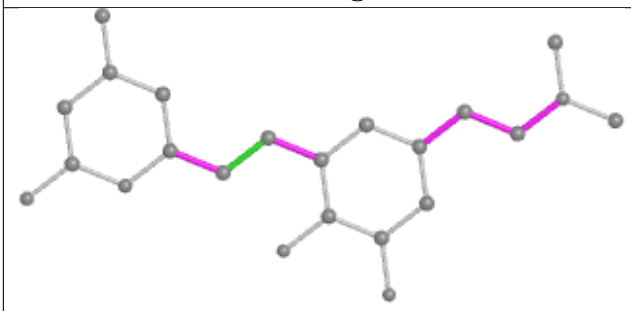


Bond angles



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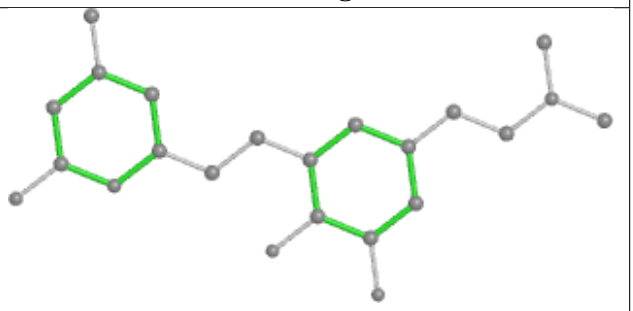
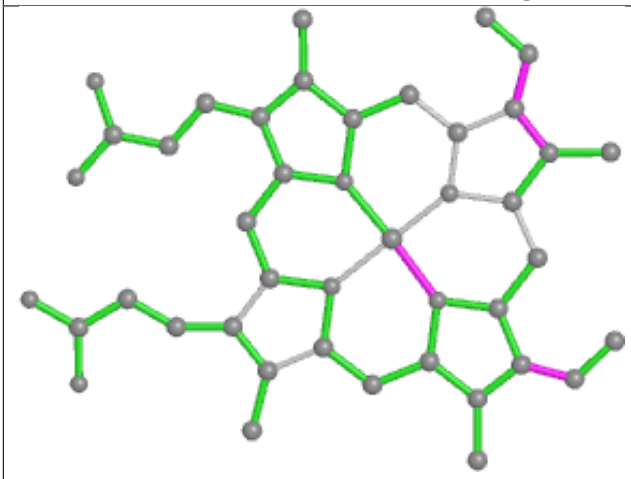
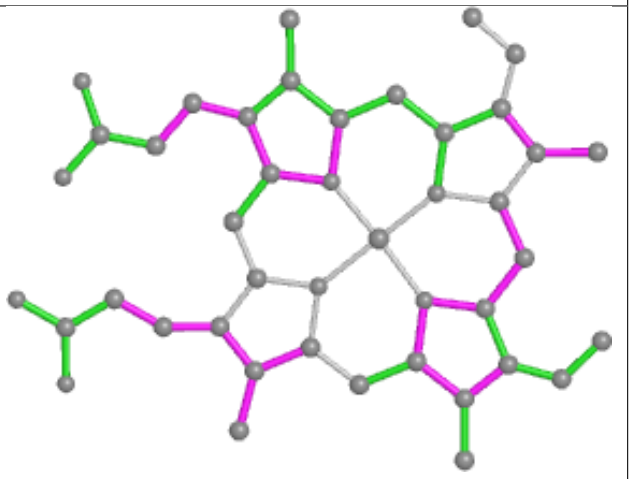


Rings

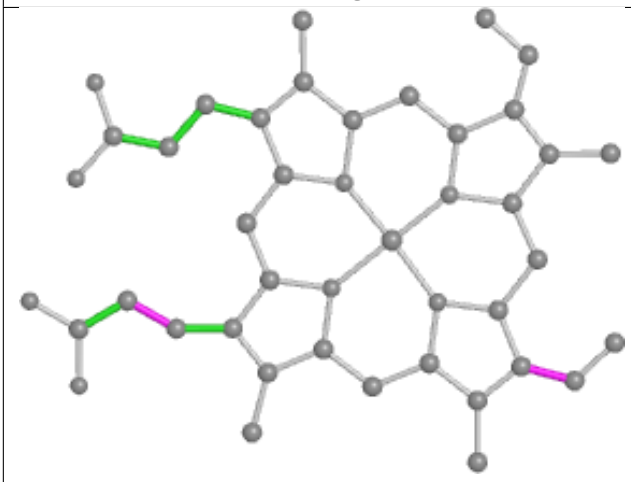
Ligand HEM A 501



Bond lengths



Bond angles



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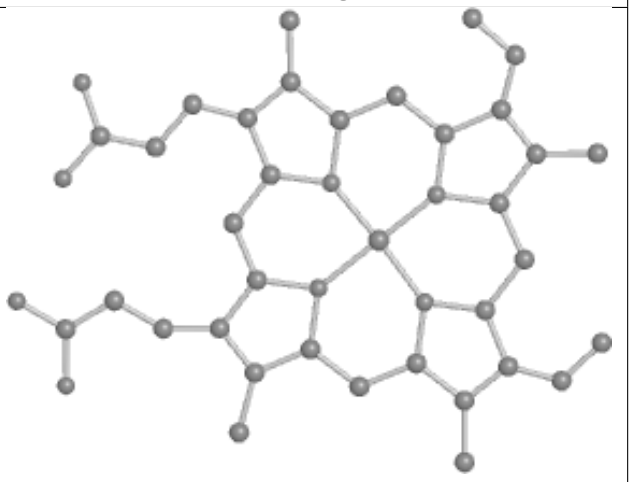
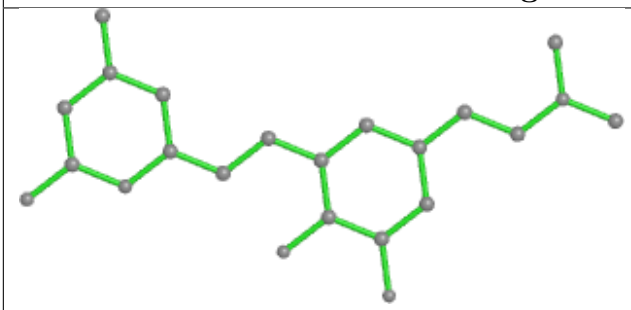


Rings

Ligand XVU C 503



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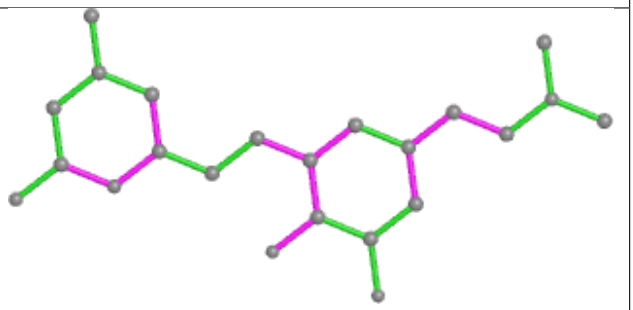

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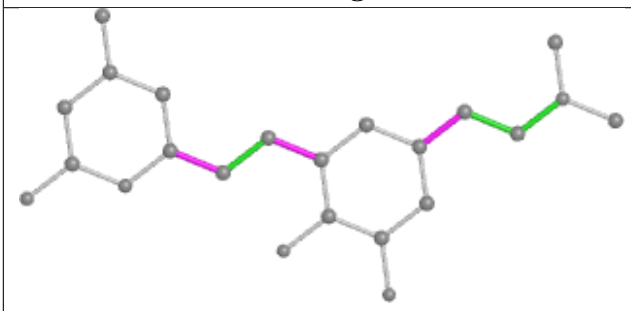

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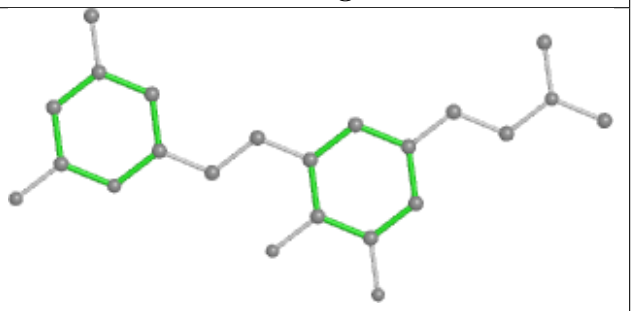
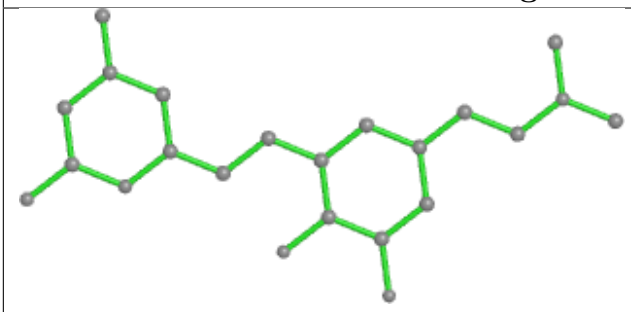


Rings

Ligand XVU A 503



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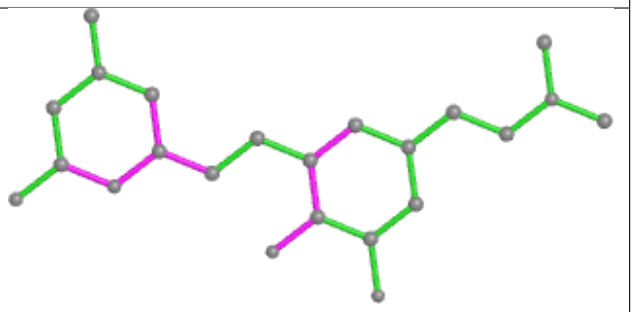
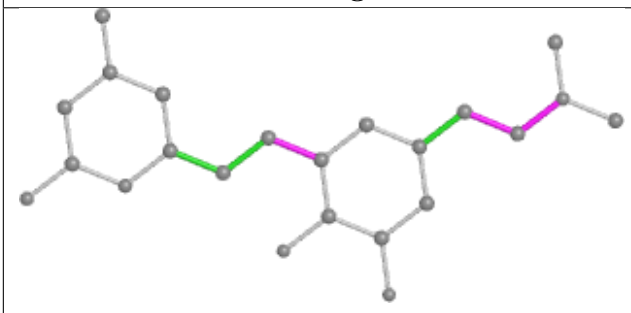


Bond angles



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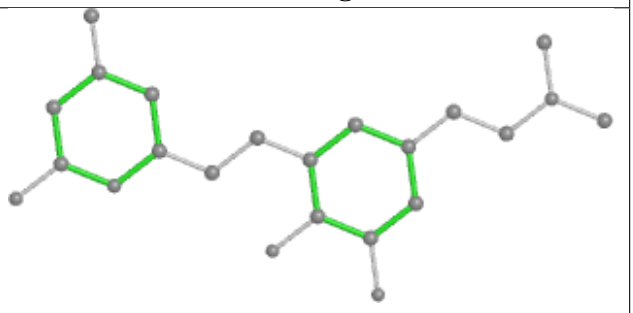
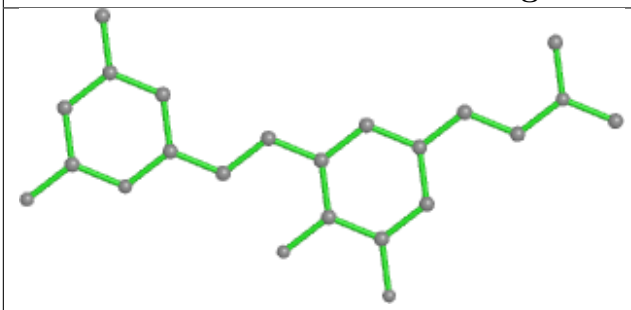
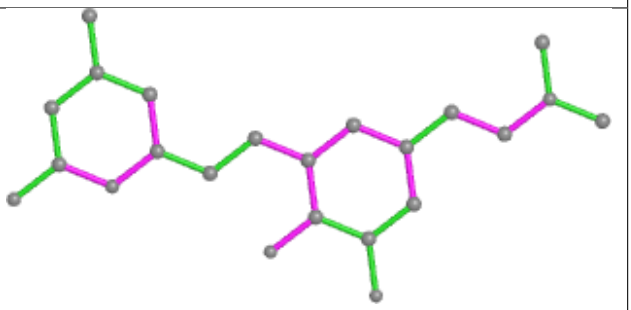


Rings

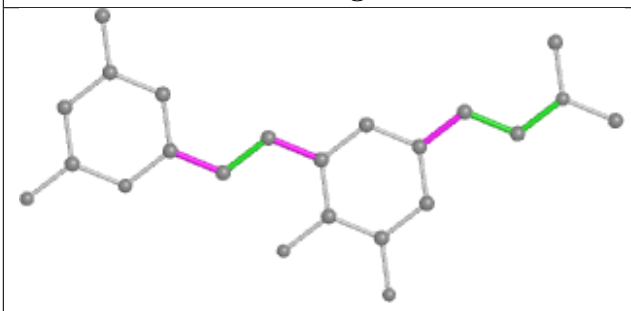
Ligand XVU B 503



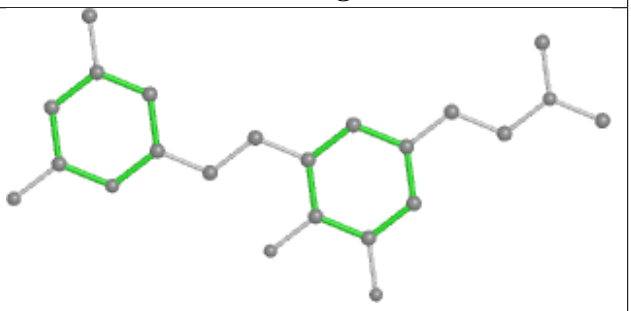
Bond lengths



Bond angles

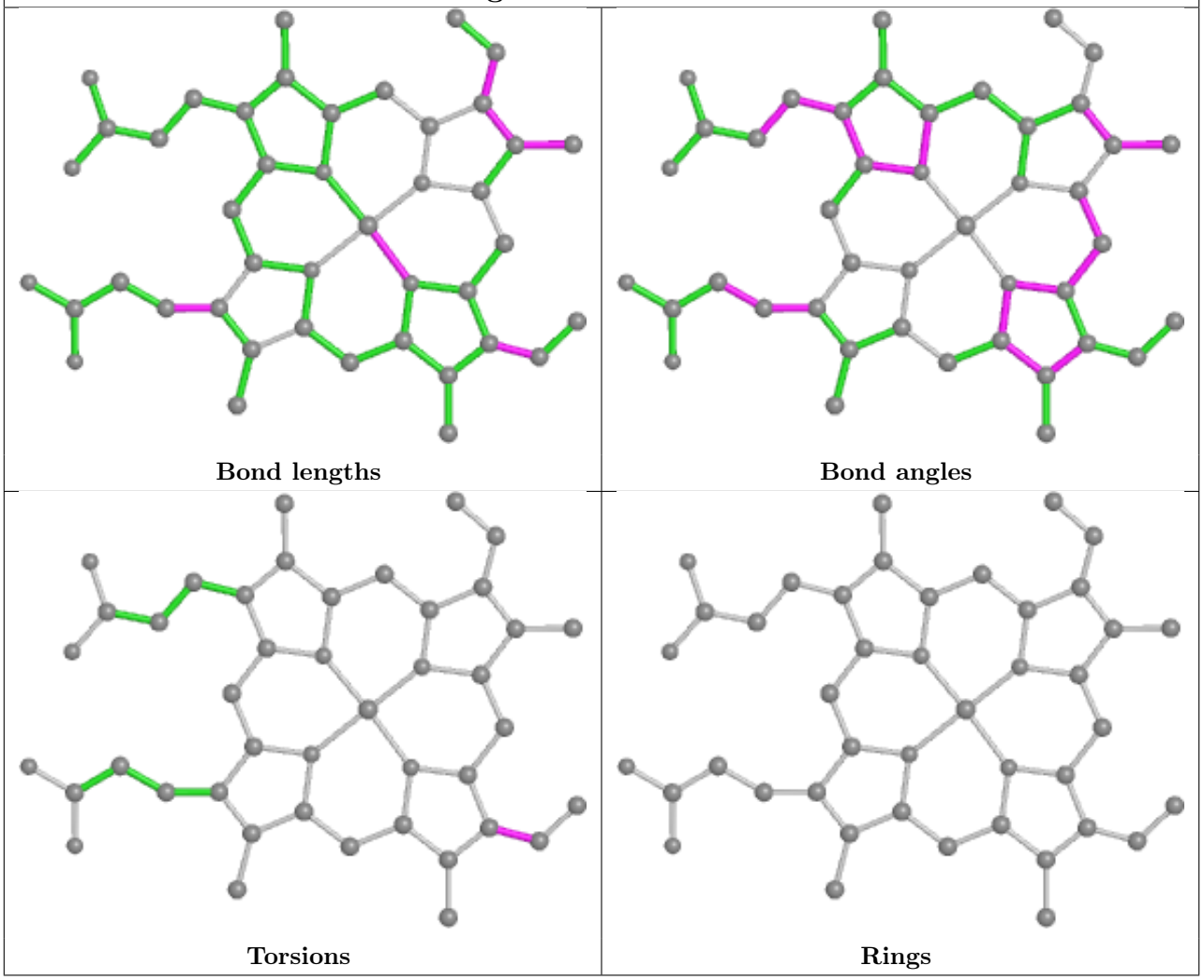


Torsions



Rings

Ligand HEM C 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	401/440 (91%)	1.46	112 (27%) 0 0	25, 56, 106, 135	0
1	B	401/440 (91%)	0.35	32 (7%) 12 9	23, 36, 71, 119	0
1	C	402/440 (91%)	1.03	88 (21%) 0 0	24, 50, 92, 115	0
1	D	402/440 (91%)	0.30	31 (7%) 13 10	22, 35, 62, 122	0
All	All	1606/1760 (91%)	0.79	263 (16%) 1 1	22, 43, 93, 135	0

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	GLY	10.6
1	A	142	GLY	8.4
1	A	204	ALA	7.8
1	A	480	TRP	7.6
1	A	304	LEU	7.2
1	A	302	LEU	7.1
1	A	275	ILE	6.9
1	A	89	GLN	6.8
1	C	447	TRP	6.1
1	A	244	TRP	6.0
1	A	447	TRP	6.0
1	A	68	PHE	5.8
1	C	68	PHE	5.8
1	A	295	ALA	5.6
1	A	280	THR	5.5
1	C	302	LEU	5.5
1	C	480	TRP	5.4
1	A	452	ILE	5.3
1	D	257	GLN	5.2
1	C	304	LEU	5.2
1	A	279	TRP	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	89	GLN	5.1
1	D	89	GLN	5.1
1	C	448	ILE	5.0
1	A	153	VAL	5.0
1	A	448	ILE	5.0
1	A	141	SER	4.9
1	A	281	PRO	4.8
1	D	449	VAL	4.7
1	A	299	PRO	4.7
1	B	460	PHE	4.6
1	A	257	GLN	4.5
1	C	300	PRO	4.5
1	A	88	ALA	4.5
1	A	122	GLN	4.5
1	A	146	HIS	4.5
1	D	255	ARG	4.4
1	C	303	PHE	4.4
1	A	300	PRO	4.4
1	C	275	ILE	4.4
1	C	153	VAL	4.3
1	C	184	CYS	4.3
1	C	299	PRO	4.3
1	A	134	TYR	4.3
1	A	479	PRO	4.3
1	C	106	PRO	4.3
1	A	305	LEU	4.3
1	A	412	LEU	4.3
1	A	184	CYS	4.2
1	C	202	ARG	4.1
1	B	68	PHE	4.1
1	A	237	GLY	4.1
1	A	150	LEU	4.1
1	A	185	VAL	4.1
1	C	452	ILE	4.1
1	A	123	LEU	4.0
1	A	128	ARG	4.0
1	A	254	TYR	4.0
1	C	439	GLY	4.0
1	A	120	PRO	4.0
1	A	90	GLN	4.0
1	A	293	LEU	4.0
1	C	119	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	449	VAL	3.9
1	A	276	GLN	3.9
1	A	67	LYS	3.8
1	D	256	GLN	3.8
1	A	478	ASP	3.8
1	B	454	GLY	3.8
1	C	236	PRO	3.8
1	D	121	GLU	3.8
1	A	255	ARG	3.8
1	A	124	LEU	3.8
1	C	124	LEU	3.8
1	A	303	PHE	3.7
1	C	360	THR	3.7
1	A	451	PRO	3.7
1	D	446	ALA	3.7
1	A	202	ARG	3.7
1	A	274	CYS	3.7
1	D	445	TRP	3.7
1	B	388	ARG	3.7
1	C	277	HIS	3.7
1	C	445	TRP	3.6
1	A	346	LEU	3.6
1	A	106	PRO	3.6
1	C	244	TRP	3.6
1	A	360	THR	3.5
1	C	160	THR	3.5
1	C	292	LEU	3.5
1	C	144	GLN	3.5
1	A	307	PRO	3.5
1	C	238	ARG	3.5
1	A	235	CYS	3.5
1	A	256	GLN	3.4
1	A	336	VAL	3.4
1	B	452	ILE	3.4
1	A	208	PHE	3.4
1	A	155	ALA	3.4
1	C	204	ALA	3.4
1	C	140	ARG	3.4
1	B	257	GLN	3.3
1	D	452	ILE	3.3
1	A	365	ARG	3.3
1	A	446	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	460	PHE	3.3
1	A	449	VAL	3.3
1	A	364	THR	3.3
1	A	367	LEU	3.3
1	C	79	ILE	3.3
1	A	301	GLU	3.3
1	C	257	GLN	3.3
1	C	67	LYS	3.3
1	C	307	PRO	3.2
1	C	309	LEU	3.2
1	D	454	GLY	3.2
1	A	445	TRP	3.2
1	A	221	ARG	3.2
1	B	142	GLY	3.2
1	C	208	PHE	3.2
1	C	255	ARG	3.2
1	D	258	ASP	3.2
1	C	142	GLY	3.2
1	C	280	THR	3.1
1	C	185	VAL	3.1
1	A	144	GLN	3.1
1	A	309	LEU	3.1
1	C	122	GLN	3.1
1	B	158	ALA	3.1
1	C	163	TYR	3.1
1	B	259	GLY	3.1
1	B	79	ILE	3.1
1	B	106	PRO	3.1
1	C	120	PRO	3.1
1	C	306	PRO	3.1
1	A	268	VAL	3.1
1	A	260	SER	3.0
1	D	119	ALA	3.0
1	D	447	TRP	3.0
1	A	238	ARG	3.0
1	C	155	ALA	3.0
1	C	259	GLY	3.0
1	D	120	PRO	3.0
1	C	449	VAL	3.0
1	A	353	PHE	3.0
1	C	221	ARG	2.9
1	A	145	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	130	PHE	2.9
1	A	239	GLY	2.9
1	A	306	PRO	2.9
1	A	258	ASP	2.9
1	D	388	ARG	2.9
1	C	450	PRO	2.9
1	D	456	LEU	2.9
1	C	141	SER	2.9
1	C	90	GLN	2.9
1	D	360	THR	2.9
1	A	277	HIS	2.8
1	C	87	GLN	2.8
1	A	83	THR	2.8
1	C	412	LEU	2.8
1	C	239	GLY	2.8
1	C	272	GLU	2.8
1	C	235	CYS	2.8
1	A	121	GLU	2.7
1	A	308	GLU	2.7
1	B	120	PRO	2.7
1	C	281	PRO	2.7
1	C	451	PRO	2.7
1	B	362	ILE	2.7
1	B	450	PRO	2.7
1	C	446	ALA	2.7
1	A	402	ILE	2.7
1	D	259	GLY	2.7
1	C	129	ASP	2.7
1	B	453	SER	2.7
1	B	446	ALA	2.6
1	D	158	ALA	2.6
1	D	448	ILE	2.6
1	A	272	GLU	2.6
1	B	260	SER	2.6
1	C	295	ALA	2.6
1	B	258	ASP	2.6
1	C	297	ASP	2.6
1	C	282	GLY	2.6
1	C	301	GLU	2.6
1	B	97	ARG	2.6
1	A	139	LYS	2.6
1	C	388	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	159	ALA	2.6
1	C	460	PHE	2.5
1	C	135	TYR	2.5
1	C	89	GLN	2.5
1	A	126	GLN	2.5
1	A	278	GLY	2.5
1	A	87	GLN	2.5
1	A	136	SER	2.5
1	C	276	GLN	2.5
1	B	360	THR	2.5
1	C	279	TRP	2.5
1	C	293	LEU	2.5
1	C	81	TYR	2.4
1	A	143	SER	2.4
1	A	147	GLU	2.4
1	C	457	THR	2.4
1	D	358	MET	2.4
1	A	131	ILE	2.4
1	A	321	GLU	2.4
1	A	140	ARG	2.4
1	B	122	GLN	2.4
1	A	228	ILE	2.4
1	C	273	LEU	2.3
1	C	402	ILE	2.3
1	C	121	GLU	2.3
1	A	183	ARG	2.3
1	A	125	SER	2.3
1	A	358	MET	2.3
1	A	151	GLN	2.3
1	A	357	TYR	2.3
1	B	81	TYR	2.3
1	B	456	LEU	2.3
1	C	183	ARG	2.2
1	A	159	ALA	2.2
1	A	362	ILE	2.2
1	A	450	PRO	2.2
1	A	366	ASN	2.2
1	A	459	VAL	2.2
1	C	136	SER	2.2
1	B	447	TRP	2.2
1	D	122	GLN	2.2
1	A	212	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	71	VAL	2.2
1	A	203	SER	2.1
1	D	221	ARG	2.1
1	C	133	GLN	2.1
1	C	86	ALA	2.1
1	A	162	THR	2.1
1	A	368	CYS	2.1
1	D	260	SER	2.1
1	C	241	PHE	2.1
1	B	389	THR	2.1
1	D	364	THR	2.1
1	B	76	VAL	2.1
1	D	336	VAL	2.1
1	D	450	PRO	2.1
1	D	451	PRO	2.1
1	C	278	GLY	2.1
1	C	274	CYS	2.1
1	B	455	SER	2.1
1	C	362	ILE	2.1
1	A	133	GLN	2.0
1	C	209	THR	2.0
1	D	106	PRO	2.0
1	A	181	ALA	2.0
1	C	254	TYR	2.0
1	C	146	HIS	2.0
1	D	79	ILE	2.0
1	A	129	ASP	2.0
1	B	451	PRO	2.0
1	B	141[A]	SER	2.0
1	A	135	TYR	2.0
1	C	157	VAL	2.0
1	B	83	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BTB	A	506	14/14	0.64	0.22	83,88,92,92	0
6	GOL	C	507	6/6	0.65	0.17	58,70,72,76	0
5	BTB	B	504	14/14	0.66	0.17	42,50,72,76	0
5	BTB	C	505	14/14	0.71	0.22	78,94,103,109	0
5	BTB	D	504	14/14	0.72	0.18	41,58,73,76	0
6	GOL	C	508	6/6	0.75	0.11	73,77,79,80	0
4	XVU	A	503	23/23	0.76	0.50	52,95,116,125	0
4	XVU	C	503	23/23	0.76	0.36	41,92,117,125	0
4	XVU	B	503	23/23	0.80	0.29	35,92,120,135	0
4	XVU	D	503	23/23	0.80	0.26	30,84,106,118	0
5	BTB	B	505	14/14	0.83	0.15	33,65,75,76	0
6	GOL	A	508	6/6	0.85	0.26	66,77,81,82	0
6	GOL	D	506	6/6	0.85	0.26	59,75,76,76	0
6	GOL	B	506	6/6	0.86	0.30	50,70,81,85	0
5	BTB	A	505	14/14	0.86	0.14	36,65,70,70	0
5	BTB	B	509	14/14	0.87	0.18	32,63,71,76	0
6	GOL	A	507	6/6	0.88	0.23	57,58,66,67	0
3	H4B	A	502	17/17	0.90	0.20	38,47,54,56	0
5	BTB	D	505	14/14	0.90	0.16	38,64,82,90	0
3	H4B	C	502	17/17	0.91	0.19	31,40,45,45	0
5	BTB	A	504	14/14	0.91	0.21	29,73,84,86	0
7	CL	A	509	1/1	0.92	0.29	62,62,62,62	0
6	GOL	A	512	6/6	0.93	0.19	25,49,59,60	0
6	GOL	C	506	6/6	0.93	0.12	42,48,57,58	0
2	HEM	A	501	43/43	0.94	0.22	36,51,61,64	0
5	BTB	C	504	14/14	0.94	0.22	14,63,68,78	0
7	CL	B	507	1/1	0.94	0.12	44,44,44,44	0
7	CL	D	507	1/1	0.95	0.12	43,43,43,43	0
2	HEM	C	501	43/43	0.96	0.18	29,37,51,66	0
3	H4B	D	502	17/17	0.96	0.14	27,32,36,39	0
3	H4B	B	502	17/17	0.96	0.14	24,32,37,38	0
2	HEM	D	501	43/43	0.97	0.12	20,24,41,45	0
7	CL	C	509	1/1	0.97	0.20	49,49,49,49	0
2	HEM	B	501	43/43	0.97	0.11	19,26,51,61	0
8	GD	A	510	1/1	0.97	0.05	69,69,69,69	1
8	GD	B	510	1/1	0.97	0.05	52,52,52,52	1
8	GD	D	508	1/1	0.97	0.09	41,41,41,41	0

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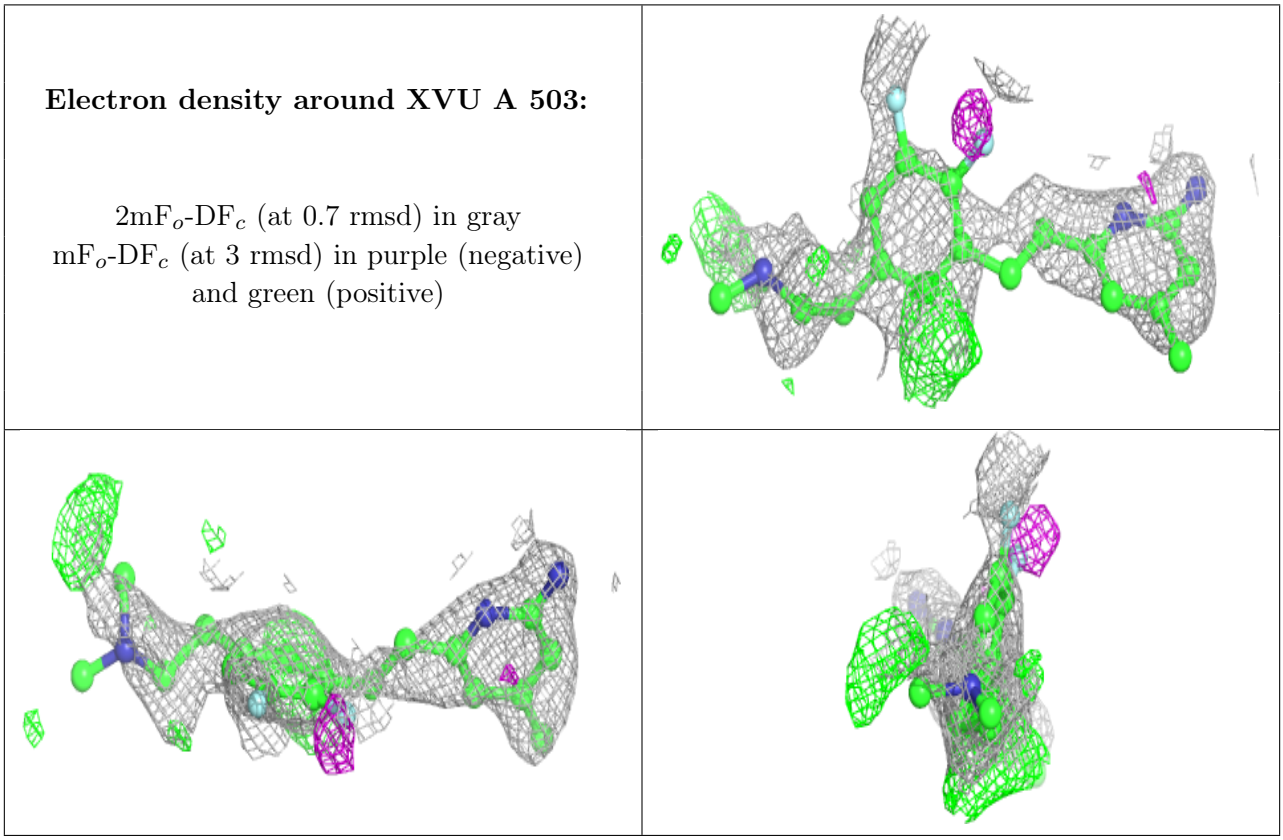
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	ZN	A	511	1/1	0.97	0.06	35,35,35,35	0
8	GD	B	508	1/1	0.99	0.10	37,37,37,37	0
9	ZN	C	510	1/1	0.99	0.07	29,29,29,29	0

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.

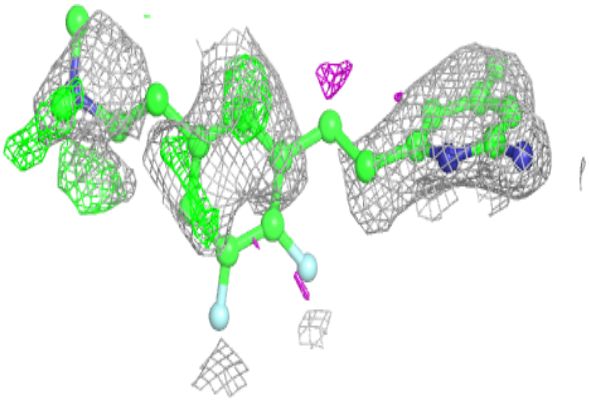
Electron density around XVU A 503:

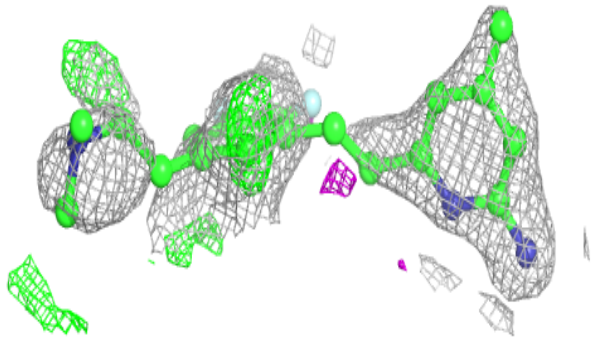
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

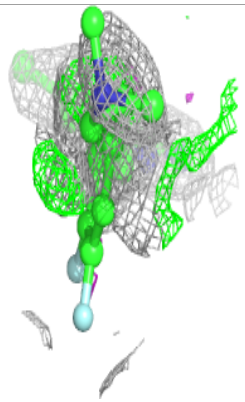


Electron density around XVU C 503:

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

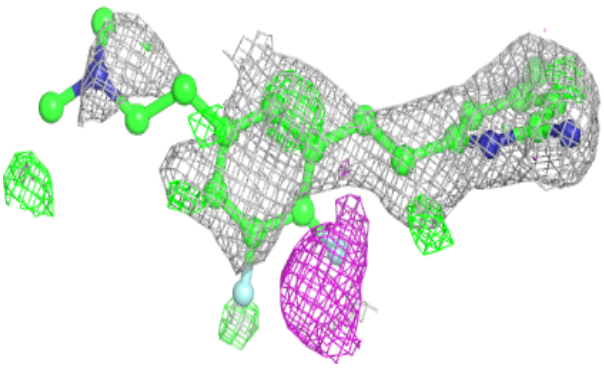


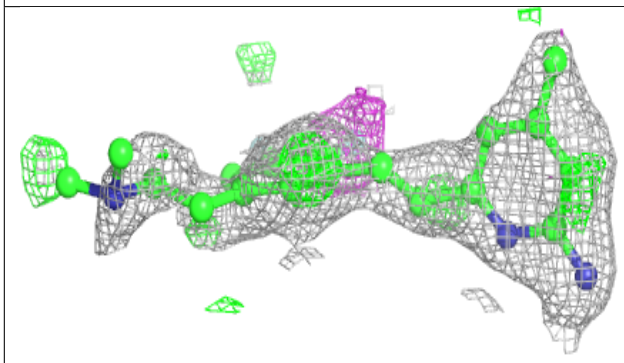


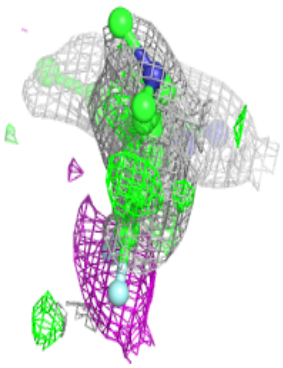


Electron density around XVU B 503:

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

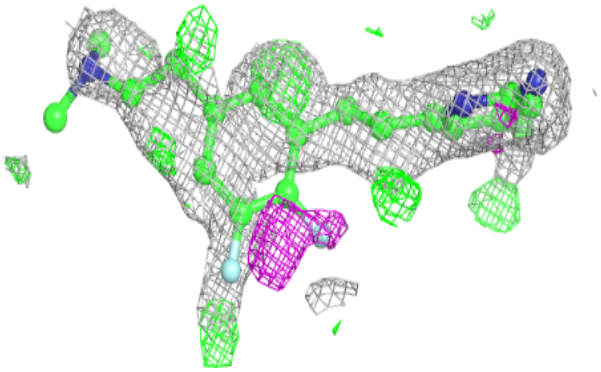


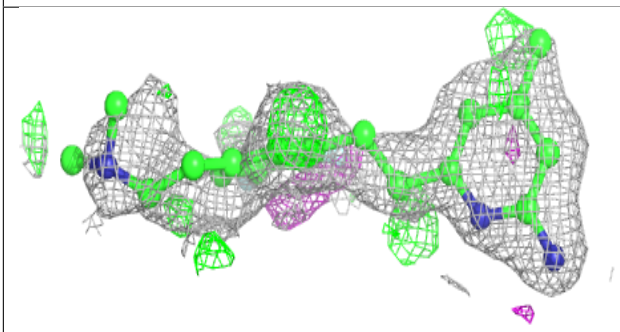


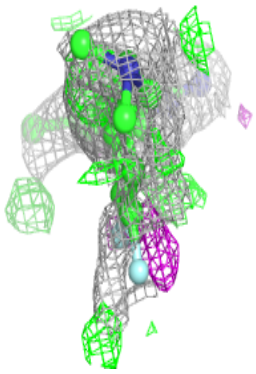


Electron density around XVU D 503:

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

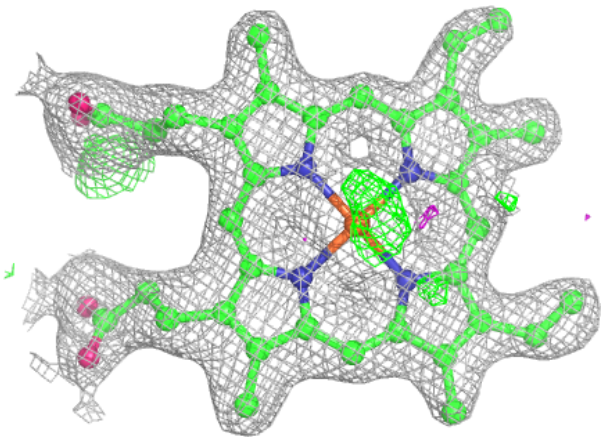


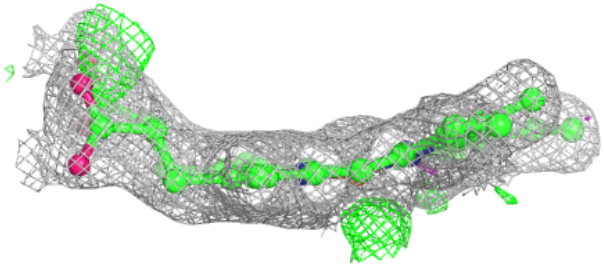


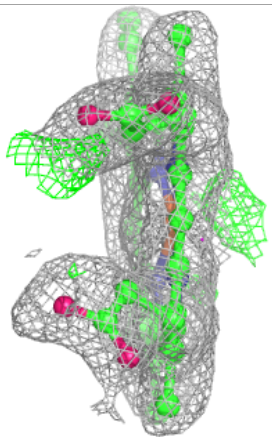


Electron density around HEM A 501:

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

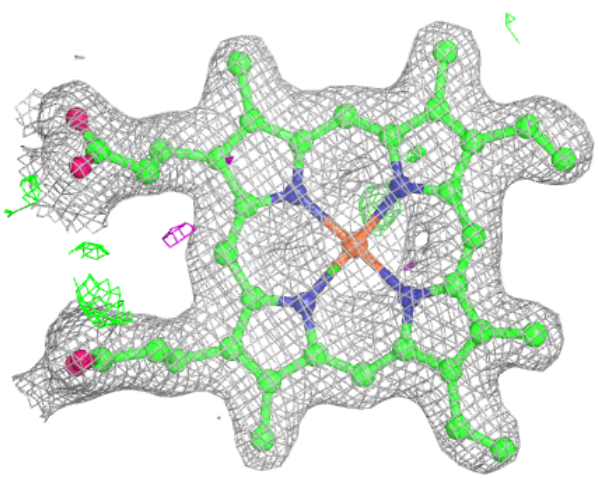


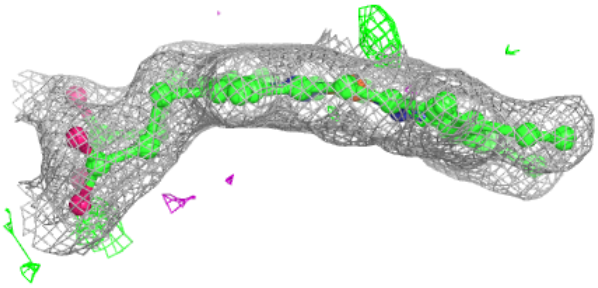


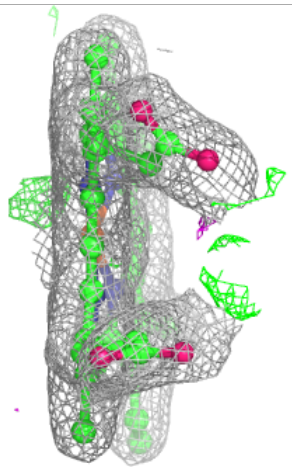


Electron density around HEM C 501:

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

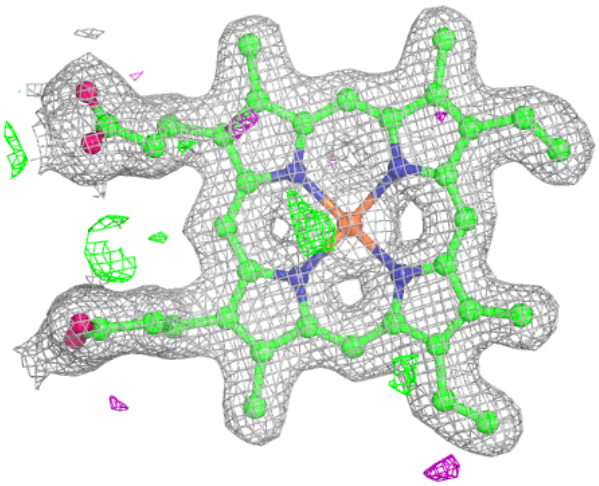


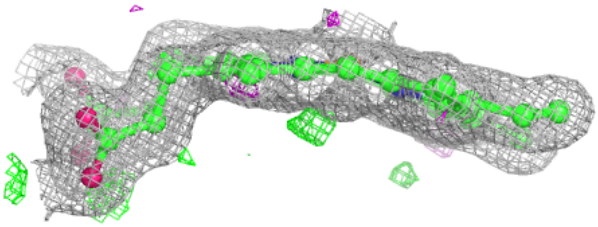


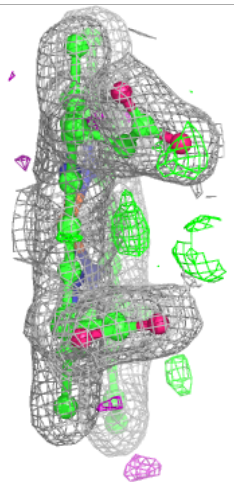


Electron density around HEM D 501:

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

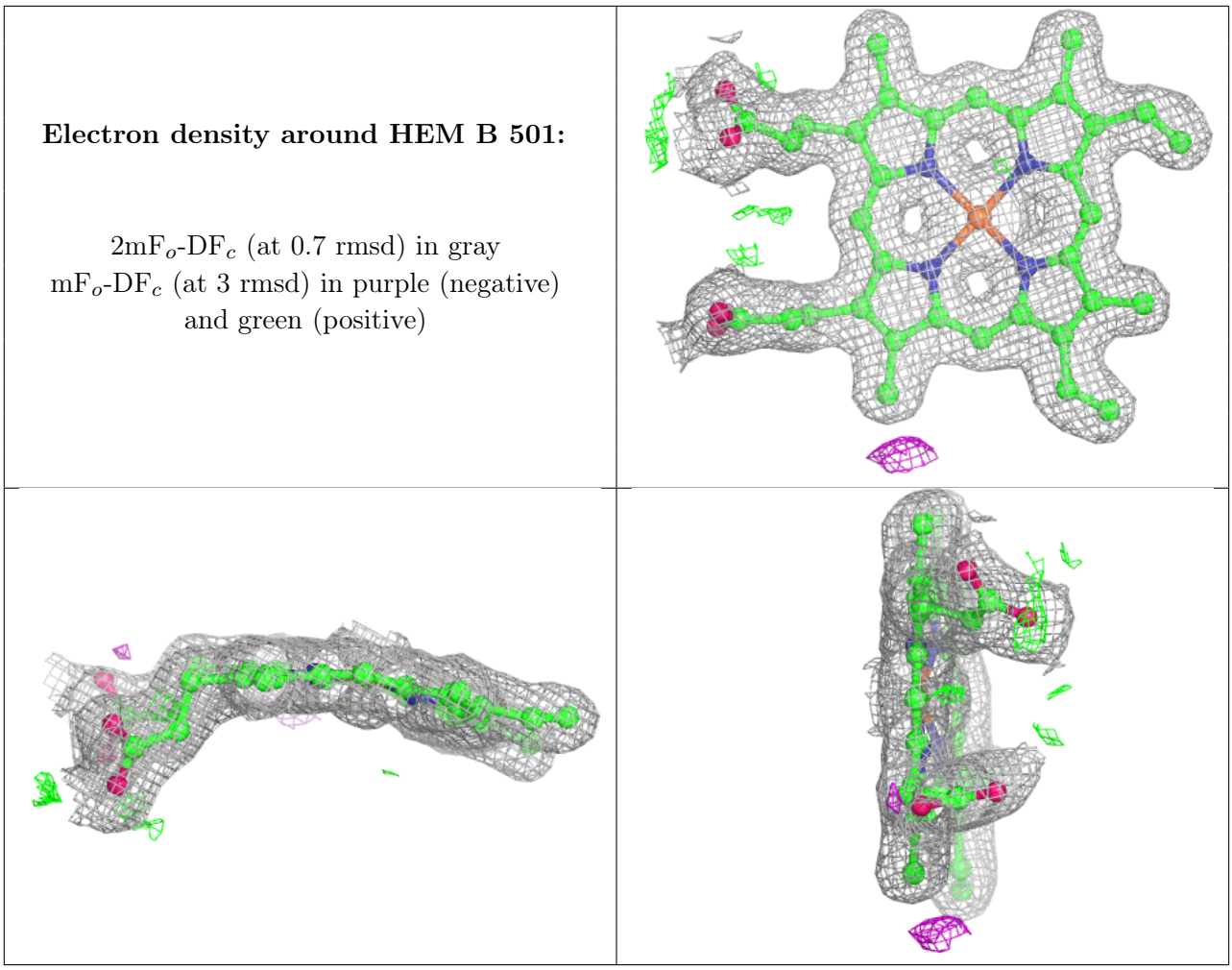






Electron density around HEM B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.