Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2023 – 01:58 AM EDT

PDB ID	:	8FGU
Title	:	Structure of human endothelial nitric oxide synthase heme domain in complex with 4-(difluoromethyl)-6-(5-(2-(dimethylamino)ethyl)-2,3-difluorophenethyl) pyridin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2022-12-12
Resolution	:	2.00 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:

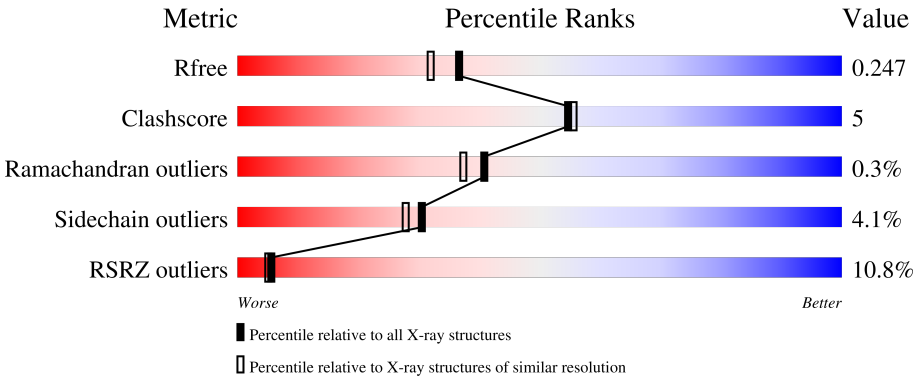
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	18% 79% 11% • 9%
1	B	440	5% 81% 9% • 9%
1	C	440	12% 78% 12% • 8%
1	D	440	5% 83% 8% • 9%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14073 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.

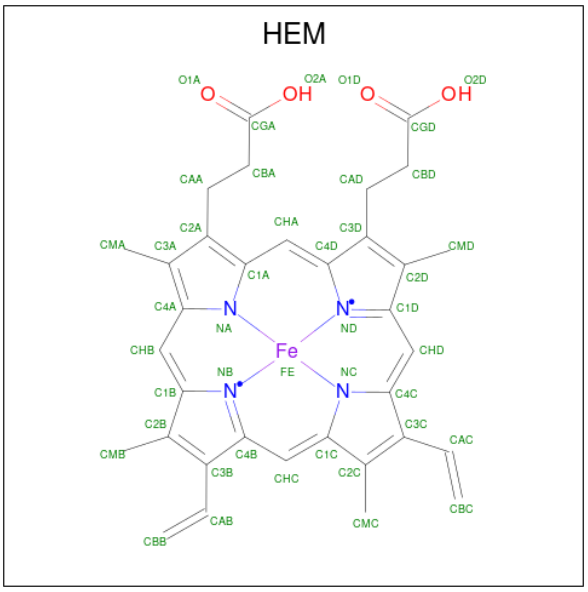
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	1	0
			3209	2043	566	584	16			
1	B	402	Total	C	N	O	S	0	3	0
			3222	2051	568	587	16			
1	C	403	Total	C	N	O	S	0	1	0
			3223	2052	569	586	16			
1	D	402	Total	C	N	O	S	0	1	0
			3214	2046	567	585	16			

There are 4 discrepancies between the modelled and reference sequences:

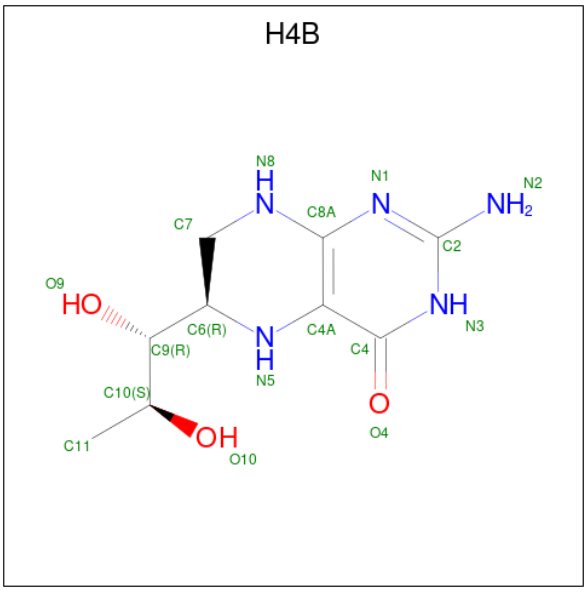
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



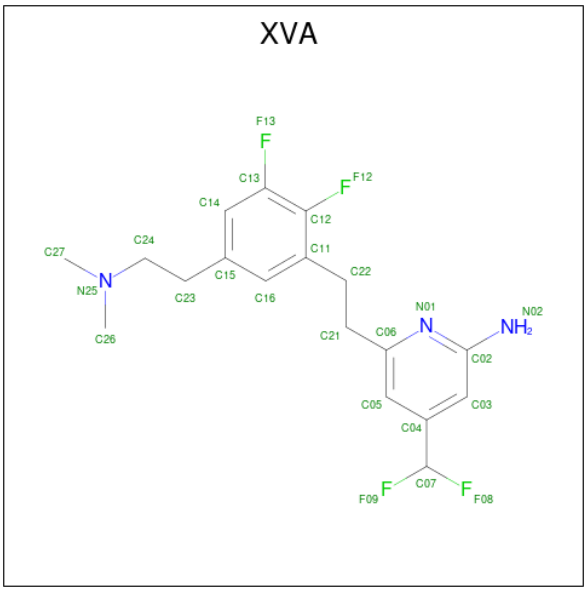
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



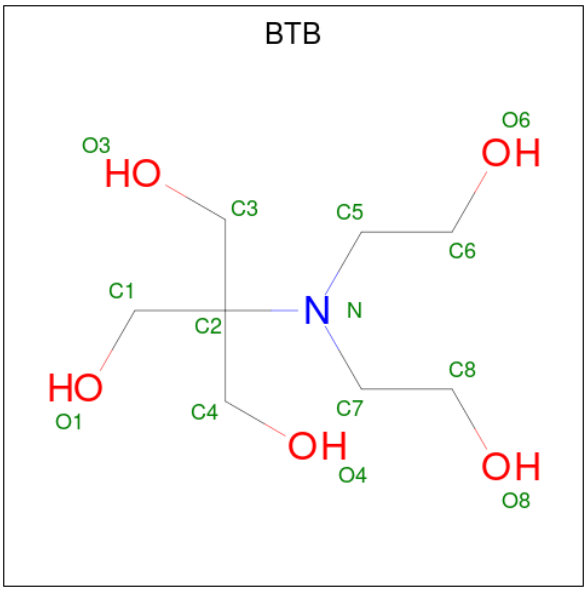
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0
3	C	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is 4-(difluoromethyl)-6-(2-{5-[2-(dimethylamino)ethyl]-2,3-difluorophenyl}ethyl)pyridin-2-amine (three-letter code: XVA) (formula: $C_{18}H_{21}F_4N_3$) (labeled as "Ligand of Interest" by depositor).



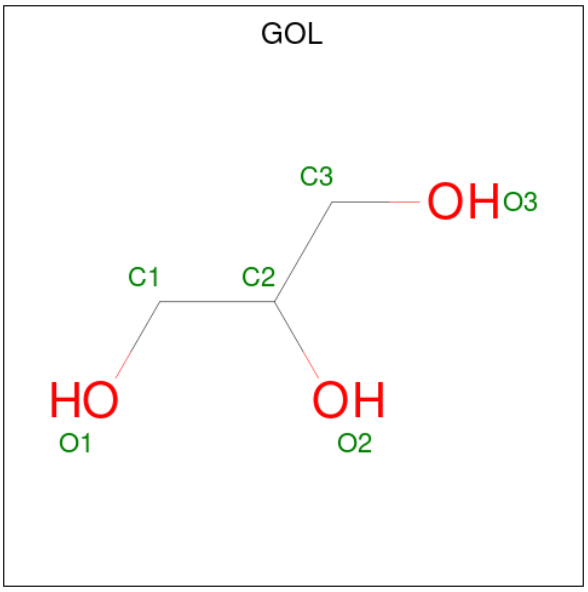
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N 25 18 4 3	0	0
4	B	1	Total C F N 25 18 4 3	0	0
4	C	1	Total C F N 25 18 4 3	0	0
4	D	1	Total C F N 25 18 4 3	0	0

- 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	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

- 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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Gd 1 1	0	0
8	C	1	Total Gd 1 1	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.

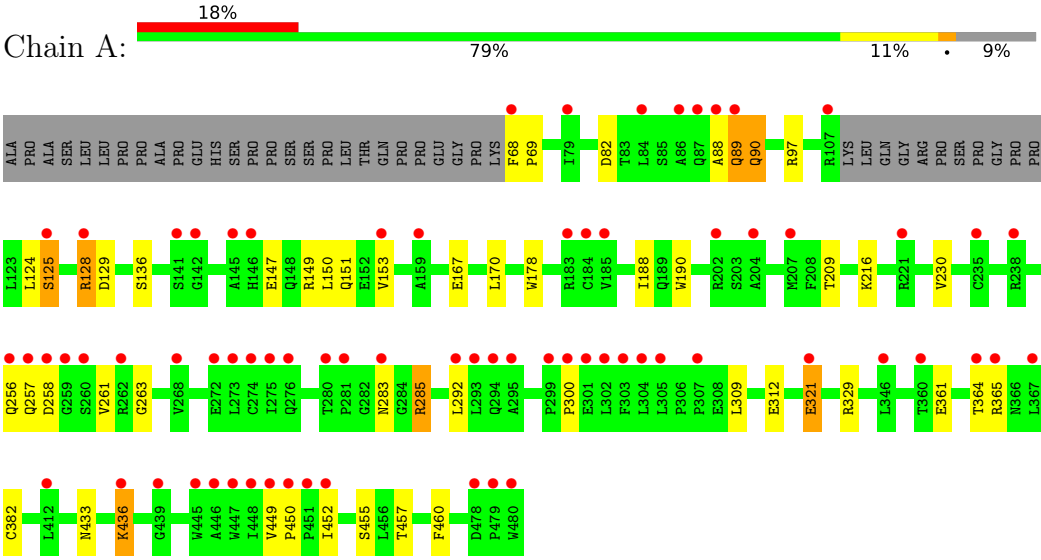
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	127	Total O 127 127	0	0
10	B	212	Total O 212 212	0	0
10	C	146	Total O 146 146	0	0
10	D	206	Total O 206 206	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

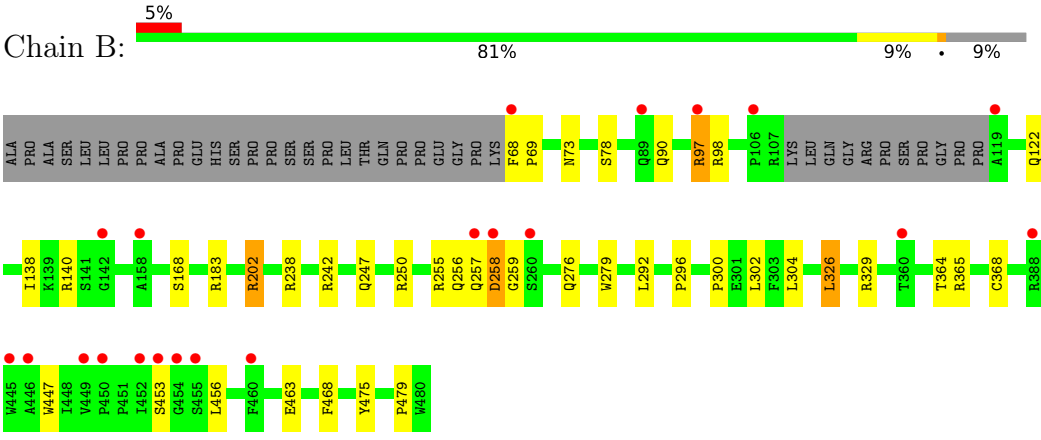
• Molecule 1: Nitric oxide synthase, endothelial

Chain A:



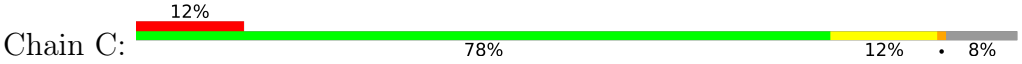
• Molecule 1: Nitric oxide synthase, endothelial

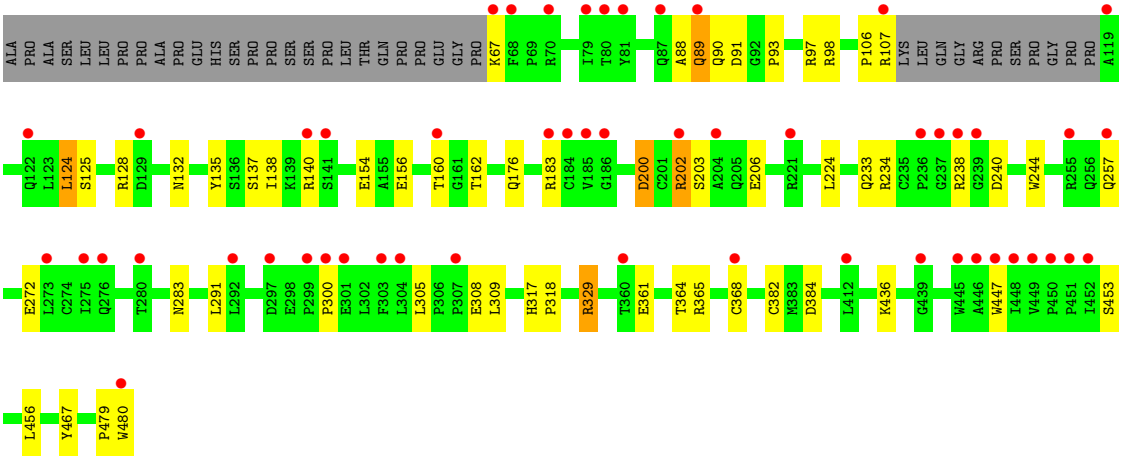
Chain B:



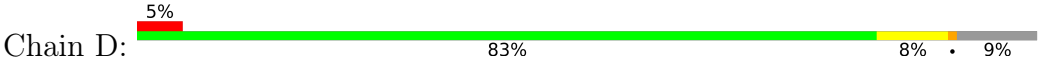
• Molecule 1: Nitric oxide synthase, endothelial

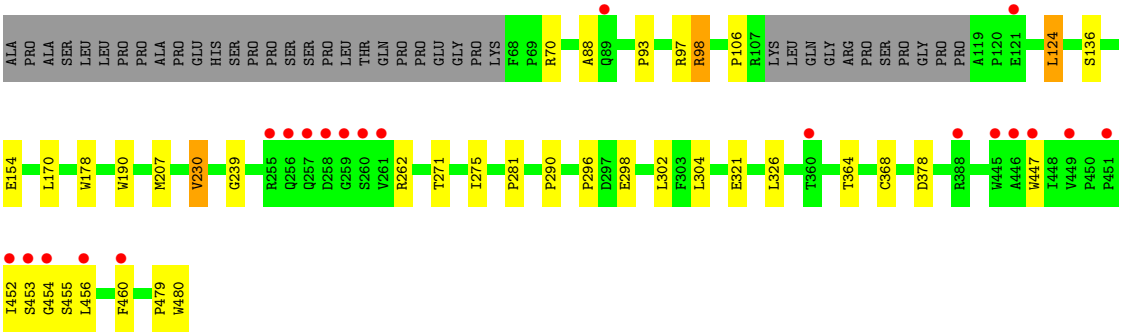
Chain C:





• Molecule 1: Nitric oxide synthase, endothelial





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.87Å 153.86Å 108.93Å 90.00° 90.65° 90.00°	Depositor
Resolution (Å)	38.95 – 2.00 39.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.5 (38.95-2.00) 95.9 (39.18-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.203 , 0.252 0.197 , 0.247	Depositor DCC
R_{free} test set	6450 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.087 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14073	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ZN, H4B, GOL, HEM, BTB, GD, XVA

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	0.36	0/3304	0.51	0/4501
1	B	0.40	0/3323	0.55	0/4528
1	C	0.35	0/3318	0.52	0/4520
1	D	0.41	0/3309	0.56	0/4509
All	All	0.38	0/13254	0.54	0/18058

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	3209	0	3112	33	0
1	B	3222	0	3127	26	0
1	C	3223	0	3129	33	0
1	D	3214	0	3116	25	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	17	0	15	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	1	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	25	0	0	1	0
4	B	25	0	0	1	0
4	C	25	0	0	2	0
4	D	25	0	0	2	0
5	A	42	0	56	7	0
5	B	42	0	55	6	0
5	C	28	0	36	5	0
5	D	28	0	36	6	0
6	A	6	0	8	1	0
6	B	6	0	8	0	0
6	C	12	0	16	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	1	0	0	0	0
8	C	1	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	127	0	0	1	0
10	B	212	0	0	1	0
10	C	146	0	0	4	0
10	D	206	0	0	1	0
All	All	14073	0	12879	136	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 (136) 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)
5:B:505:BTB:HO6	5:B:505:BTB:HO8	1.18	0.91
1:D:70:ARG:NH2	10:D:601:HOH:O	2.17	0.77
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.65	0.76
5:B:505:BTB:O8	5:B:505:BTB:O6	2.01	0.75
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ASP:OD1	1:C:200:ASP:N	2.24	0.71
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.74	0.70
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.75	0.69
1:C:329:ARG:NH1	10:C:602:HOH:O	2.25	0.68
1:C:124:LEU:O	1:C:128:ARG:HG3	1.93	0.68
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.07	0.68
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.75	0.67
1:A:82:ASP:OD2	10:A:601:HOH:O	2.14	0.66
1:B:124:LEU:HB3	1:B:128:ARG:HH22	1.62	0.65
1:C:97:ARG:HG2	1:D:88:ALA:HB3	1.80	0.64
5:A:505:BTB:O3	5:A:505:BTB:O4	2.14	0.63
1:A:312:GLU:OE2	1:A:329:ARG:NH1	2.31	0.63
1:C:382:CYS:HA	5:C:504:BTB:H11	1.81	0.62
1:A:167:GLU:OE1	6:A:507:GOL:O2	2.13	0.61
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.83	0.60
1:B:447:TRP:NE1	10:B:601:HOH:O	2.18	0.60
1:B:202:ARG:HH11	1:B:202:ARG:HB2	1.66	0.60
1:C:88:ALA:HB3	1:D:97:ARG:HD2	1.83	0.59
2:D:501:HEM:O2D	4:D:503:XVA:F13	2.11	0.59
1:A:147:GLU:O	1:A:151:GLN:NE2	2.35	0.59
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.86	0.58
1:B:258:ASP:OD2	1:B:258:ASP:N	2.35	0.58
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.17	0.58
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.86	0.58
1:A:433:ASN:O	1:A:436:LYS:HG3	2.04	0.57
1:C:91:ASP:OD1	1:D:97:ARG:NH1	2.38	0.56
5:C:504:BTB:O8	5:C:504:BTB:H62	2.06	0.56
1:C:447:TRP:NE1	10:C:604:HOH:O	2.32	0.56
1:D:93:PRO:HB3	1:D:106:PRO:HB3	1.88	0.55
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.25	0.55
1:C:202:ARG:HG2	1:C:206:GLU:CD	2.28	0.54
1:A:125:SER:HA	1:A:128:ARG:NH1	2.21	0.54
3:A:502:H4B:H113	1:B:463:GLU:HG2	1.91	0.53
1:C:160:THR:HG23	1:C:162:THR:H	1.74	0.52
5:D:505:BTB:O4	5:D:505:BTB:H52	2.09	0.52
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.48	0.52
1:A:321:GLU:H	1:A:321:GLU:CD	2.12	0.52
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.92	0.52
1:A:88:ALA:O	1:B:97:ARG:NH1	2.44	0.51
1:C:128:ARG:O	1:C:132:ASN:ND2	2.44	0.51
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:GLU:OE2	5:D:505:BTB:H41	2.11	0.50
1:C:364:THR:O	1:C:368:CYS:HB2	2.11	0.50
2:C:501:HEM:O2D	4:C:503:XVA:F13	2.20	0.49
1:A:256:GLN:C	1:A:258:ASP:H	2.15	0.49
1:A:128:ARG:HH11	1:A:128:ARG:HB2	1.78	0.49
1:D:271:THR:O	1:D:275:ILE:HG12	2.11	0.49
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.94	0.49
1:C:93:PRO:HB3	1:C:106:PRO:HB3	1.95	0.48
1:A:89:GLN:HG3	1:A:90:GLN:N	2.28	0.48
1:B:90:GLN:HB3	1:B:468:PHE:CD2	2.49	0.48
1:C:138:ILE:O	1:C:140:ARG:HG2	2.13	0.48
5:A:506:BTB:H52	5:A:506:BTB:H11	1.69	0.48
1:C:176:GLN:NE2	10:C:601:HOH:O	2.22	0.48
1:B:138:ILE:HG13	1:B:140:ARG:HB2	1.96	0.48
1:A:97:ARG:HH11	1:A:97:ARG:HB2	1.79	0.47
1:C:90:GLN:NE2	10:C:606:HOH:O	2.35	0.47
5:A:506:BTB:H41	5:A:506:BTB:H72	1.52	0.47
1:C:156:GLU:O	1:C:160:THR:HG22	2.14	0.47
5:B:505:BTB:H12	5:B:505:BTB:H51	1.52	0.47
1:D:447:TRP:HA	3:D:502:H4B:N1	2.30	0.47
1:A:364:THR:O	1:A:368:CYS:HB2	2.15	0.47
1:B:73:ASN:HB3	1:B:78:SER:HB2	1.96	0.47
1:A:258:ASP:N	1:A:258:ASP:OD1	2.48	0.47
1:A:150:LEU:HB2	1:A:151:GLN:NE2	2.30	0.46
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.96	0.46
1:A:254:TYR:O	1:A:261:VAL:HA	2.15	0.46
1:D:239:GLY:O	1:D:296:PRO:HB3	2.16	0.46
1:B:183:ARG:HD3	1:B:447:TRP:CD2	2.51	0.46
1:C:244:TRP:CZ2	1:C:300:PRO:HG3	2.51	0.46
1:A:455:SER:HA	1:A:460:PHE:CG	2.51	0.45
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.97	0.45
5:D:504:BTB:H51	5:D:504:BTB:H32	1.72	0.45
1:B:326:LEU:HD12	5:C:504:BTB:H72	1.98	0.45
1:D:97:ARG:HA	1:D:97:ARG:HD3	1.69	0.45
5:B:504:BTB:H32	5:B:504:BTB:H51	1.59	0.45
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.52	0.45
1:C:384:ASP:OD2	5:C:504:BTB:O3	2.34	0.45
5:D:505:BTB:H62	5:D:505:BTB:H71	1.75	0.45
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.52	0.44
1:D:275:ILE:CD1	1:D:281:PRO:HB3	2.48	0.44
1:A:361:GLU:OE2	4:A:503:XVA:N02	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:SER:HA	1:D:460:PHE:CG	2.52	0.44
1:A:68:PHE:HA	1:A:69:PRO:HD3	1.87	0.44
1:A:150:LEU:HB2	1:A:151:GLN:HE21	1.83	0.44
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.89	0.43
1:C:135:TYR:HA	1:C:138:ILE:HG12	2.00	0.43
1:D:479:PRO:HD2	1:D:480:TRP:CE3	2.53	0.43
1:A:125:SER:HA	1:A:128:ARG:HH12	1.82	0.43
1:C:453:SER:HA	1:D:452:ILE:HG22	2.00	0.43
5:A:505:BTB:H11	5:A:505:BTB:H51	1.64	0.43
1:C:453:SER:HB3	1:C:456:LEU:HD12	2.01	0.43
5:A:504:BTB:O6	5:A:504:BTB:H32	2.18	0.43
1:A:382:CYS:HA	5:A:504:BTB:H11	2.01	0.43
1:A:170:LEU:HD11	1:A:230:VAL:HG21	2.00	0.43
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.53	0.43
1:A:263:GLY:HA2	1:A:285:ARG:HG3	1.99	0.43
1:A:364:THR:HG21	1:A:452:ILE:HG23	2.01	0.43
1:C:234:ARG:HB3	1:C:240:ASP:OD1	2.19	0.42
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.54	0.42
1:B:292:LEU:HD22	1:B:300:PRO:HB2	2.00	0.42
2:B:501:HEM:HBA2	4:B:503:XVA:C21	2.50	0.42
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.79	0.42
1:A:376:LEU:HD12	1:A:376:LEU:HA	1.87	0.42
1:C:467:TYR:HB3	1:D:98:ARG:HB3	2.00	0.42
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.91	0.42
1:C:202:ARG:HB2	1:C:203:SER:H	1.74	0.42
1:D:364:THR:O	1:D:368:CYS:HB2	2.20	0.42
1:C:97:ARG:CG	1:D:88:ALA:HB3	2.48	0.42
5:B:505:BTB:H72	5:B:505:BTB:H42	1.28	0.41
1:B:364:THR:O	1:B:368:CYS:HB2	2.21	0.41
1:C:224:LEU:HD23	1:C:224:LEU:HA	1.79	0.41
5:A:505:BTB:H41	5:A:505:BTB:H72	1.43	0.41
1:D:124:LEU:HD11	1:D:154:GLU:HG3	2.01	0.41
2:D:501:HEM:HBA1	4:D:503:XVA:C21	2.51	0.41
5:C:505:BTB:H31	5:C:505:BTB:H72	1.92	0.41
1:D:298:GLU:CD	5:D:505:BTB:H41	2.41	0.41
1:B:68:PHE:HA	1:B:69:PRO:HD3	1.88	0.41
1:C:361:GLU:OE2	4:C:503:XVA:N02	2.53	0.41
1:A:149:ARG:O	1:A:153:VAL:HG22	2.21	0.41
1:B:238:ARG:HG2	1:B:296:PRO:HB3	2.02	0.41
1:B:256:GLN:HB3	1:B:257:GLN:H	1.55	0.41
1:C:479:PRO:HD2	1:C:480:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ARG:HE	1:B:238:ARG:HB3	1.63	0.40
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.35	0.40
1:B:365:ARG:HH12	3:B:502:H4B:C4	2.35	0.40
5:B:504:BTB:H72	5:B:504:BTB:H12	1.83	0.40
1:C:291:LEU:HD11	1:C:305:LEU:HD21	2.03	0.40
1:D:454:GLY:O	1:D:460:PHE:HB2	2.20	0.40
1:A:449:VAL:HA	1:A:450:PRO:HD3	1.95	0.40
1:D:170:LEU:HD11	1:D:230:VAL:HG21	2.03	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%)	381 (96%)	15 (4%)	2 (0%)	29	23
1	B	401/440 (91%)	391 (98%)	9 (2%)	1 (0%)	47	44
1	C	400/440 (91%)	387 (97%)	11 (3%)	2 (0%)	29	23
1	D	399/440 (91%)	393 (98%)	6 (2%)	0	100	100
All	All	1598/1760 (91%)	1552 (97%)	41 (3%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	GLN
1	C	202	ARG
1	A	89	GLN
1	B	259	GLY
1	A	257	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%)	327 (96%)	15 (4%)	28	25
1	B	344/373 (92%)	329 (96%)	15 (4%)	28	25
1	C	343/373 (92%)	325 (95%)	18 (5%)	23	19
1	D	342/373 (92%)	333 (97%)	9 (3%)	46	48
All	All	1371/1492 (92%)	1314 (96%)	57 (4%)	30	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	121	GLU
1	A	124	LEU
1	A	125	SER
1	A	128	ARG
1	A	129	ASP
1	A	136	SER
1	A	188	ILE
1	A	209	THR
1	A	216	LYS
1	A	283	ASN
1	A	285	ARG
1	A	309	LEU
1	A	321	GLU
1	A	436	LYS
1	B	97	ARG
1	B	98	ARG
1	B	122	GLN
1	B	128	ARG
1	B	168[A]	SER
1	B	168[B]	SER
1	B	202	ARG
1	B	255	ARG
1	B	258	ASP

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Mol	Chain	Res	Type
1	B	276	GLN
1	B	304	LEU
1	B	326	LEU
1	B	329	ARG
1	B	389	THR
1	B	396	ASP
1	C	67	LYS
1	C	89	GLN
1	C	98	ARG
1	C	107	ARG
1	C	124	LEU
1	C	125	SER
1	C	137	SER
1	C	154	GLU
1	C	200	ASP
1	C	233	GLN
1	C	238	ARG
1	C	257	GLN
1	C	272	GLU
1	C	283	ASN
1	C	308	GLU
1	C	309	LEU
1	C	329	ARG
1	C	436	LYS
1	D	98	ARG
1	D	124	LEU
1	D	136	SER
1	D	207	MET
1	D	230	VAL
1	D	262	ARG
1	D	302	LEU
1	D	326	LEU
1	D	378	ASP

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	90	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 36 ligands modelled in this entry, 10 are monoatomic - leaving 26 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	C	504	8	13,13,13	0.38	0	7,16,16	0.66	0
2	HEM	A	501	1	41,50,50	1.54	5 (12%)	45,82,82	1.73	8 (17%)
3	H4B	A	502	-	16,18,18	1.07	1 (6%)	11,26,26	2.75	6 (54%)
5	BTB	B	504	8	13,13,13	0.48	0	7,16,16	0.61	0
3	H4B	D	502	-	16,18,18	0.95	1 (6%)	11,26,26	2.74	6 (54%)
5	BTB	B	505	-	13,13,13	0.31	0	7,16,16	0.92	0
6	GOL	A	507	-	5,5,5	0.39	0	5,5,5	0.70	0
5	BTB	C	505	-	13,13,13	0.38	0	7,16,16	0.74	0
3	H4B	B	502	-	16,18,18	1.23	1 (6%)	11,26,26	2.90	5 (45%)
5	BTB	A	504	8	13,13,13	0.41	0	7,16,16	0.63	0
5	BTB	A	506	-	13,13,13	0.40	0	7,16,16	0.50	0
5	BTB	A	505	-	13,13,13	0.48	0	7,16,16	0.79	0
4	XVA	C	503	-	25,26,26	0.54	0	30,36,36	1.82	8 (26%)
4	XVA	D	503	-	25,26,26	0.60	0	30,36,36	1.54	5 (16%)
5	BTB	D	504	8	13,13,13	0.42	0	7,16,16	0.73	0
4	XVA	B	503	-	25,26,26	0.61	0	30,36,36	1.73	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BTB	B	509	-	13,13,13	0.74	0	7,16,16	1.19	1 (14%)
5	BTB	D	505	-	13,13,13	0.83	1 (7%)	7,16,16	1.04	1 (14%)
2	HEM	B	501	1	41,50,50	1.43	5 (12%)	45,82,82	1.88	14 (31%)
2	HEM	D	501	1	41,50,50	1.40	6 (14%)	45,82,82	1.68	11 (24%)
4	XVA	A	503	-	25,26,26	0.46	0	30,36,36	1.73	7 (23%)
6	GOL	B	506	-	5,5,5	0.38	0	5,5,5	0.29	0
3	H4B	C	502	-	16,18,18	1.16	1 (6%)	11,26,26	2.75	5 (45%)
2	HEM	C	501	1	41,50,50	1.46	7 (17%)	45,82,82	1.83	11 (24%)
6	GOL	C	507	-	5,5,5	0.39	0	5,5,5	0.25	0
6	GOL	C	506	-	5,5,5	0.29	0	5,5,5	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	C	504	8	-	7/21/21/21	-
2	HEM	A	501	1	-	5/12/54/54	-
3	H4B	A	502	-	-	4/8/17/17	0/2/2/2
5	BTB	B	504	8	-	0/21/21/21	-
3	H4B	D	502	-	-	3/8/17/17	0/2/2/2
5	BTB	B	505	-	-	12/21/21/21	-
6	GOL	A	507	-	-	2/4/4/4	-
5	BTB	C	505	-	-	4/21/21/21	-
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
5	BTB	A	504	8	-	8/21/21/21	-
5	BTB	A	506	-	-	4/21/21/21	-
5	BTB	A	505	-	-	11/21/21/21	-
4	XVA	C	503	-	-	3/14/14/14	0/2/2/2
4	XVA	D	503	-	-	4/14/14/14	0/2/2/2
5	BTB	D	504	8	-	4/21/21/21	-
4	XVA	B	503	-	-	4/14/14/14	0/2/2/2
5	BTB	B	509	-	-	11/21/21/21	-
5	BTB	D	505	-	-	3/21/21/21	-
2	HEM	B	501	1	-	4/12/54/54	-
2	HEM	D	501	1	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XVA	A	503	-	-	4/14/14/14	0/2/2/2
6	GOL	B	506	-	-	2/4/4/4	-
3	H4B	C	502	-	-	3/8/17/17	0/2/2/2
2	HEM	C	501	1	-	3/12/54/54	-
6	GOL	C	507	-	-	1/4/4/4	-
6	GOL	C	506	-	-	3/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-CAC	3.82	1.55	1.47
2	B	501	HEM	C3C-CAC	3.63	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.56	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.51	1.35	1.40
2	C	501	HEM	C3C-CAC	3.41	1.54	1.47
2	A	501	HEM	CAB-C3B	3.08	1.55	1.47
2	C	501	HEM	CAB-C3B	2.96	1.55	1.47
2	D	501	HEM	C3C-CAC	2.91	1.53	1.47
3	B	502	H4B	C4A-C4	-2.90	1.37	1.41
2	D	501	HEM	C3C-C2C	-2.83	1.36	1.40
2	A	501	HEM	FE-NB	2.79	2.10	1.96
2	B	501	HEM	CAB-C3B	2.78	1.55	1.47
2	D	501	HEM	CAB-C3B	2.77	1.55	1.47
2	D	501	HEM	FE-NB	2.71	2.10	1.96
2	B	501	HEM	C3C-C2C	-2.70	1.36	1.40
2	C	501	HEM	FE-NB	2.34	2.08	1.96
3	C	502	H4B	C4A-C4	-2.30	1.38	1.41
2	B	501	HEM	C3B-C2B	-2.29	1.32	1.37
5	D	505	BTB	C4-C2	-2.25	1.50	1.53
3	A	502	H4B	C4A-C4	-2.24	1.38	1.41
2	A	501	HEM	CAA-C2A	2.23	1.55	1.52
2	C	501	HEM	CAA-C2A	2.23	1.55	1.52
2	D	501	HEM	CMC-C2C	2.15	1.56	1.51
2	C	501	HEM	CMB-C2B	2.11	1.55	1.50
3	D	502	H4B	C4A-C4	-2.06	1.38	1.41
2	B	501	HEM	FE-ND	2.05	2.07	1.96
2	D	501	HEM	CAA-C2A	2.04	1.55	1.52
2	C	501	HEM	FE-ND	2.00	2.06	1.96

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	H4B	C8A-C4A-C4	6.66	120.49	114.57
3	C	502	H4B	C8A-C4A-C4	6.33	120.19	114.57
3	A	502	H4B	C8A-C4A-C4	6.21	120.08	114.57
4	C	503	XVA	C02-N01-C06	5.36	122.16	118.10
3	D	502	H4B	C8A-C4A-C4	5.26	119.24	114.57
4	D	503	XVA	C02-N01-C06	5.06	121.93	118.10
2	B	501	HEM	CBA-CAA-C2A	-4.82	104.39	112.62
2	C	501	HEM	C4B-CHC-C1C	4.82	128.91	122.56
4	A	503	XVA	C02-N01-C06	4.59	121.58	118.10
2	C	501	HEM	CBA-CAA-C2A	-4.43	105.06	112.62
2	A	501	HEM	C4B-CHC-C1C	4.25	128.17	122.56
4	B	503	XVA	C02-N01-C06	4.15	121.25	118.10
2	B	501	HEM	C3B-C2B-C1B	4.00	109.45	106.49
2	A	501	HEM	C1B-NB-C4B	3.97	109.17	105.07
4	A	503	XVA	C16-C11-C12	3.84	120.28	116.76
4	C	503	XVA	C16-C11-C12	3.84	120.28	116.76
3	B	502	H4B	N1-C2-N3	-3.69	119.63	125.42
3	D	502	H4B	N1-C2-N3	-3.66	119.68	125.42
2	A	501	HEM	C3B-C2B-C1B	3.62	109.17	106.49
4	B	503	XVA	F12-C12-C11	3.61	121.66	117.85
2	B	501	HEM	C4B-CHC-C1C	3.53	127.22	122.56
4	B	503	XVA	C21-C06-N01	3.52	121.20	115.95
3	C	502	H4B	N1-C2-N3	-3.51	119.92	125.42
3	D	502	H4B	C2-N3-C4	3.46	121.43	115.93
4	A	503	XVA	C22-C21-C06	-3.43	105.30	112.99
3	B	502	H4B	C2-N3-C4	3.42	121.37	115.93
2	C	501	HEM	C1B-NB-C4B	3.42	108.61	105.07
2	D	501	HEM	C4B-CHC-C1C	3.40	127.04	122.56
4	C	503	XVA	C21-C06-N01	3.31	120.88	115.95
3	A	502	H4B	N1-C2-N3	-3.27	120.29	125.42
2	B	501	HEM	C4D-ND-C1D	3.24	108.42	105.07
2	A	501	HEM	C4A-C3A-C2A	3.20	109.22	107.00
2	D	501	HEM	CMA-C3A-C4A	-3.16	123.60	128.46
3	A	502	H4B	C2-N3-C4	3.15	120.94	115.93
4	A	503	XVA	C21-C06-N01	3.09	120.55	115.95
2	C	501	HEM	C4D-ND-C1D	3.03	108.21	105.07
4	D	503	XVA	F12-C12-C11	3.02	121.04	117.85
3	C	502	H4B	C2-N3-C4	2.98	120.66	115.93
2	D	501	HEM	CMC-C2C-C3C	2.96	130.22	124.68
4	D	503	XVA	C05-C06-N01	-2.90	119.82	122.90
2	D	501	HEM	C4D-ND-C1D	2.89	108.06	105.07
3	C	502	H4B	C2-N1-C8A	2.89	121.02	114.54
3	B	502	H4B	C2-N1-C8A	2.86	120.96	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C4D-ND-C1D	2.80	107.96	105.07
4	A	503	XVA	F12-C12-C11	2.80	120.80	117.85
3	D	502	H4B	C2-N1-C8A	2.80	120.80	114.54
2	C	501	HEM	CBD-CAD-C3D	-2.77	104.93	112.63
2	C	501	HEM	C3D-C4D-ND	-2.74	107.12	110.17
2	B	501	HEM	C1B-NB-C4B	2.69	107.85	105.07
2	B	501	HEM	CAD-CBD-CGD	-2.69	107.82	113.60
3	A	502	H4B	C2-N1-C8A	2.67	120.52	114.54
4	D	503	XVA	C21-C06-N01	2.65	119.90	115.95
4	B	503	XVA	C22-C11-C12	2.65	122.86	120.73
3	D	502	H4B	C4-C4A-N5	2.64	121.34	119.12
2	D	501	HEM	C4A-C3A-C2A	2.64	108.83	107.00
2	D	501	HEM	C2C-C3C-C4C	2.61	108.72	106.90
2	B	501	HEM	C3D-C4D-ND	-2.58	107.30	110.17
2	C	501	HEM	CMA-C3A-C4A	-2.55	124.54	128.46
4	A	503	XVA	C05-C06-N01	-2.55	120.20	122.90
2	D	501	HEM	C3B-C2B-C1B	2.46	108.31	106.49
2	D	501	HEM	C1B-NB-C4B	2.45	107.61	105.07
2	A	501	HEM	C2B-C1B-NB	-2.45	106.93	109.84
4	C	503	XVA	C22-C21-C06	-2.43	107.53	112.99
2	C	501	HEM	CHA-C4D-ND	2.43	127.38	124.38
2	A	501	HEM	C4C-CHD-C1D	2.40	125.73	122.56
4	C	503	XVA	C04-C03-C02	2.37	120.28	118.09
2	C	501	HEM	CMC-C2C-C3C	2.37	129.11	124.68
4	C	503	XVA	C05-C06-N01	-2.37	120.39	122.90
4	C	503	XVA	F12-C12-C11	2.37	120.35	117.85
2	B	501	HEM	CMC-C2C-C3C	2.35	129.07	124.68
2	D	501	HEM	C3D-C4D-ND	-2.34	107.56	110.17
2	B	501	HEM	CMA-C3A-C4A	-2.31	124.92	128.46
3	A	502	H4B	N2-C2-N3	2.27	120.79	117.25
4	B	503	XVA	C21-C06-C05	-2.27	118.21	121.22
2	B	501	HEM	C2D-C1D-ND	-2.25	107.19	109.88
5	B	509	BTB	O1-C1-C2	-2.24	105.30	111.44
4	D	503	XVA	C16-C11-C12	2.22	118.80	116.76
2	B	501	HEM	CHA-C4D-ND	2.21	127.11	124.38
2	D	501	HEM	CHA-C4D-ND	2.18	127.08	124.38
4	B	503	XVA	C05-C06-N01	-2.18	120.59	122.90
3	C	502	H4B	N2-C2-N3	2.16	120.60	117.25
2	D	501	HEM	CHC-C4B-C3B	2.15	127.86	124.57
3	D	502	H4B	N2-C2-N1	2.14	120.58	117.25
4	B	503	XVA	C21-C22-C11	-2.13	109.36	112.81
2	B	501	HEM	CAB-C3B-C2B	-2.13	121.59	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CHC-C4B-C3B	2.12	127.82	124.57
2	C	501	HEM	C4A-C3A-C2A	2.11	108.46	107.00
3	A	502	H4B	C4A-N5-C6	-2.10	115.45	121.16
5	D	505	BTB	O1-C1-C2	-2.06	105.80	111.44
4	C	503	XVA	C23-C24-N25	-2.05	107.31	114.02
3	B	502	H4B	N2-C2-N1	2.05	120.44	117.25
2	A	501	HEM	CBD-CAD-C3D	-2.05	106.94	112.63
4	A	503	XVA	N02-C02-N01	2.04	119.72	116.49
2	B	501	HEM	C2B-C1B-NB	-2.02	107.44	109.84
2	C	501	HEM	O2A-CGA-CBA	2.00	120.46	114.03

There are no chirality outliers.

All (116) 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	D	501	HEM	C1A-C2A-CAA-CBA
2	D	501	HEM	C3A-C2A-CAA-CBA
3	A	502	H4B	N5-C6-C9-O9
3	A	502	H4B	C7-C6-C9-O9
3	A	502	H4B	C7-C6-C9-C10
3	D	502	H4B	C7-C6-C9-O9
3	D	502	H4B	C7-C6-C9-C10
4	A	503	XVA	C05-C04-C07-F09
4	D	503	XVA	C05-C04-C07-F09
5	A	504	BTB	O1-C1-C2-C3
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	A	504	BTB	N-C2-C3-O3
5	A	504	BTB	C3-C2-C4-O4
5	A	505	BTB	O1-C1-C2-C3
5	A	505	BTB	O1-C1-C2-C4
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
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

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Mol	Chain	Res	Type	Atoms
5	A	505	BTB	C4-C2-N-C7
5	A	506	BTB	O1-C1-C2-C3
5	A	506	BTB	O1-C1-C2-C4
5	A	506	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	C3-C2-C4-O4
5	B	509	BTB	C1-C2-C4-O4
5	B	509	BTB	C3-C2-C4-O4
5	B	509	BTB	N-C2-C4-O4
5	B	509	BTB	C1-C2-N-C5
5	B	509	BTB	C1-C2-N-C7
5	B	509	BTB	C3-C2-N-C5
5	B	509	BTB	C3-C2-N-C7
5	B	509	BTB	C4-C2-N-C5
5	B	509	BTB	C4-C2-N-C7
5	C	504	BTB	O1-C1-C2-C3
5	C	504	BTB	O1-C1-C2-C4
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	C1-C2-C3-O3
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	C6-C5-N-C7
6	C	506	GOL	O1-C1-C2-C3
5	D	505	BTB	N-C5-C6-O6
4	A	503	XVA	C23-C24-N25-C26
4	A	503	XVA	C23-C24-N25-C27
5	A	505	BTB	N-C7-C8-O8
5	A	506	BTB	N-C7-C8-O8
5	B	505	BTB	N-C7-C8-O8
4	B	503	XVA	C23-C24-N25-C26
4	B	503	XVA	C23-C24-N25-C27
4	D	503	XVA	C23-C24-N25-C27
2	C	501	HEM	C3D-CAD-CBD-CGD
5	C	504	BTB	N-C7-C8-O8
4	D	503	XVA	C23-C24-N25-C26
4	B	503	XVA	C15-C23-C24-N25
6	B	506	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	C	507	GOL	C1-C2-C3-O3
4	D	503	XVA	C15-C23-C24-N25
6	B	506	GOL	O1-C1-C2-O2
6	C	506	GOL	O1-C1-C2-O2
5	B	505	BTB	N-C5-C6-O6
3	B	502	H4B	C7-C6-C9-O9
5	C	505	BTB	N-C7-C8-O8
2	D	501	HEM	C2A-CAA-CBA-CGA
3	C	502	H4B	C7-C6-C9-O9
5	B	509	BTB	N-C5-C6-O6
4	B	503	XVA	C16-C11-C22-C21
2	A	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
5	A	504	BTB	C1-C2-C4-O4
5	C	505	BTB	C4-C2-C3-O3
5	D	504	BTB	C3-C2-C4-O4
2	C	501	HEM	C2A-CAA-CBA-CGA
5	A	504	BTB	O1-C1-C2-N
5	B	505	BTB	N-C2-C4-O4
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	C4-C2-N-C7
5	C	504	BTB	O1-C1-C2-N
5	C	505	BTB	N-C2-C3-O3
2	A	501	HEM	C3D-CAD-CBD-CGD
3	B	502	H4B	C7-C6-C9-C10
3	C	502	H4B	C7-C6-C9-C10
3	A	502	H4B	N5-C6-C9-C10
2	B	501	HEM	CAA-CBA-CGA-O2A
4	C	503	XVA	C14-C15-C23-C24
2	B	501	HEM	CAA-CBA-CGA-O1A
6	A	507	GOL	O2-C2-C3-O3
2	D	501	HEM	C3D-CAD-CBD-CGD
4	C	503	XVA	C16-C15-C23-C24
5	B	509	BTB	N-C7-C8-O8
6	C	506	GOL	O2-C2-C3-O3
2	B	501	HEM	CAD-CBD-CGD-O2D
4	A	503	XVA	C16-C11-C22-C21
2	B	501	HEM	CAD-CBD-CGD-O1D
6	A	507	GOL	C1-C2-C3-O3
3	B	502	H4B	N5-C6-C9-O9

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Mol	Chain	Res	Type	Atoms
3	C	502	H4B	N5-C6-C9-O9
3	D	502	H4B	N5-C6-C9-O9
5	B	505	BTB	C1-C2-C4-O4
5	D	505	BTB	C4-C2-C3-O3
4	C	503	XVA	C23-C24-N25-C27

There are no ring outliers.

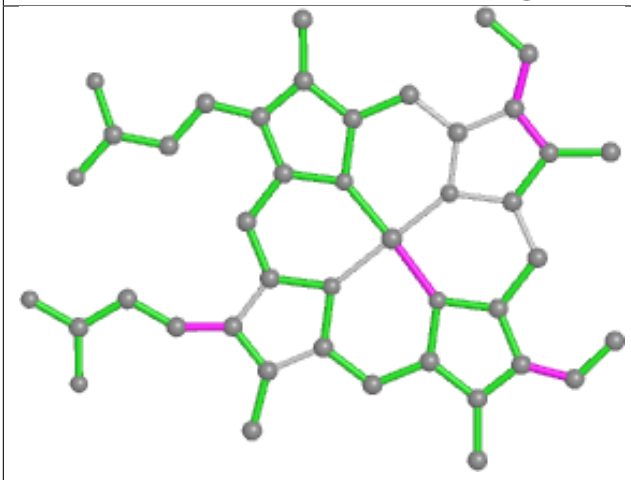
22 monomers are involved in 42 short contacts:

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

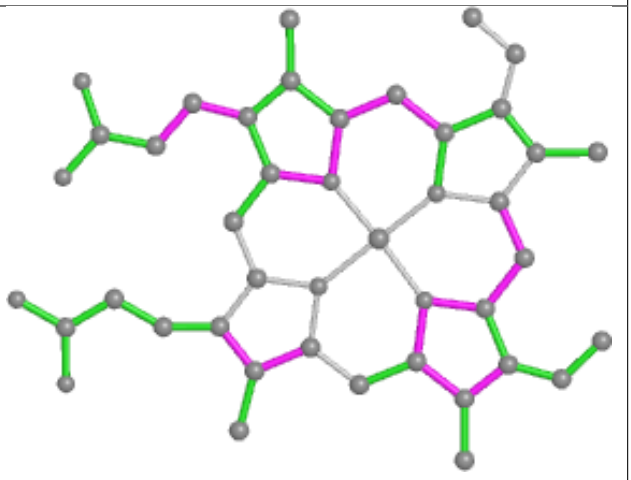
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

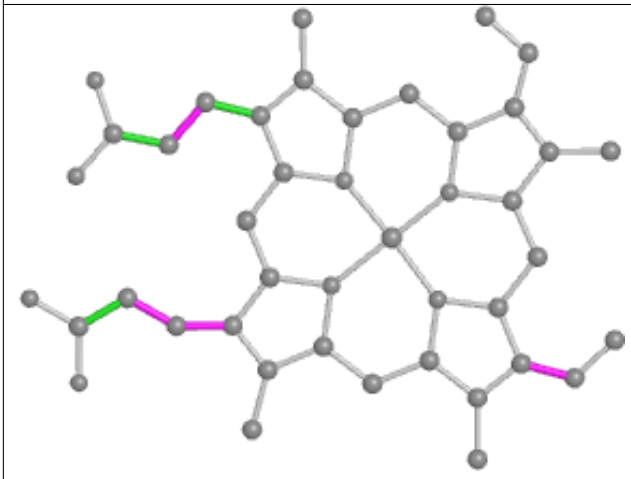
Ligand HEM A 501



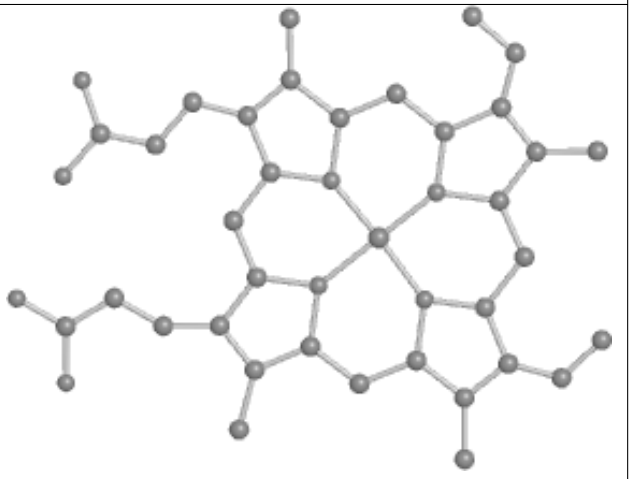
Bond lengths



Bond angles

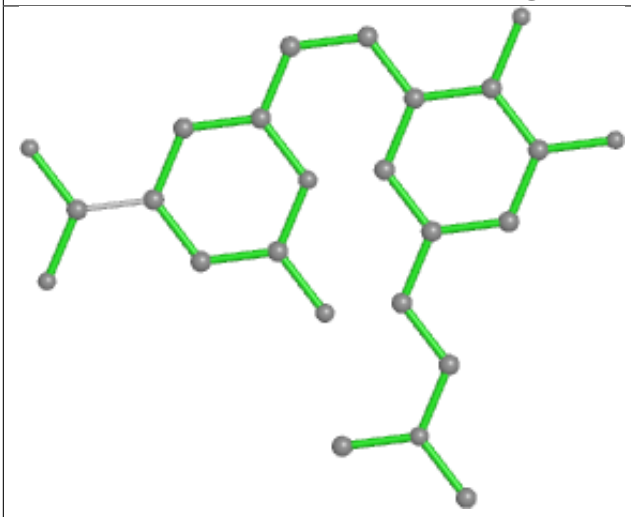


Torsions

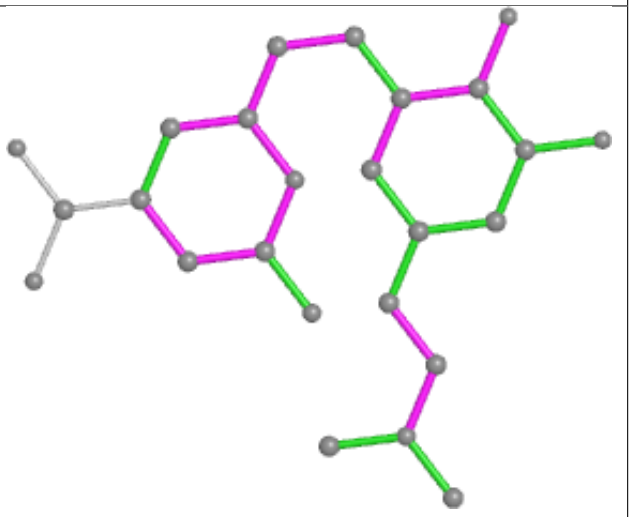


Rings

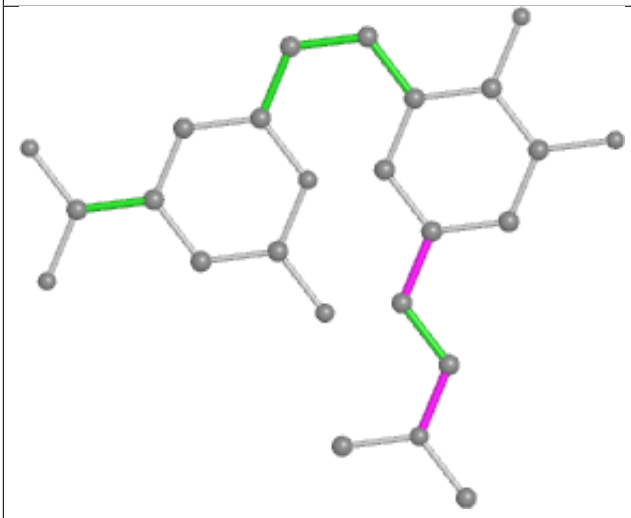
Ligand XVA C 503



Bond lengths



Bond angles



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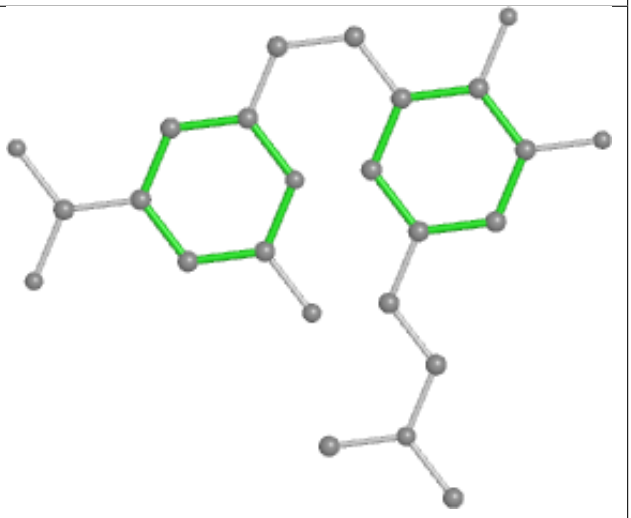
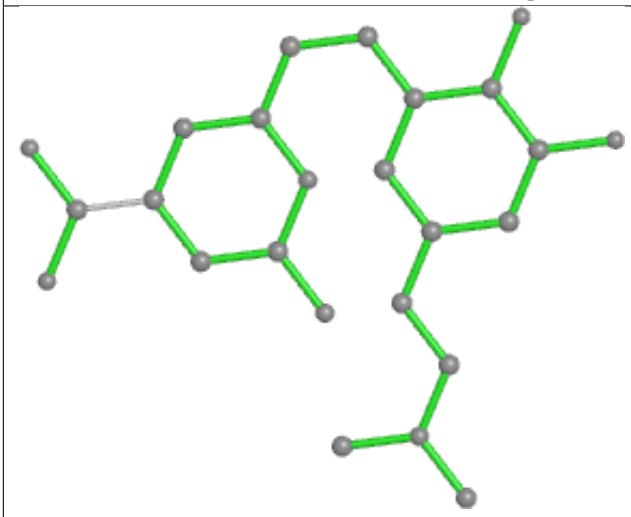
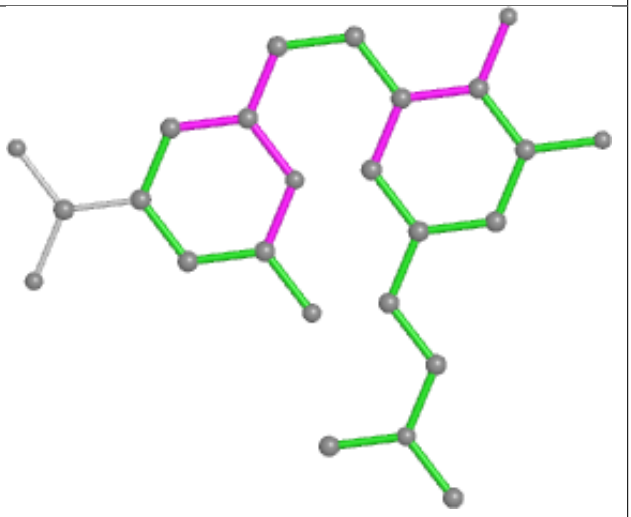


Rings

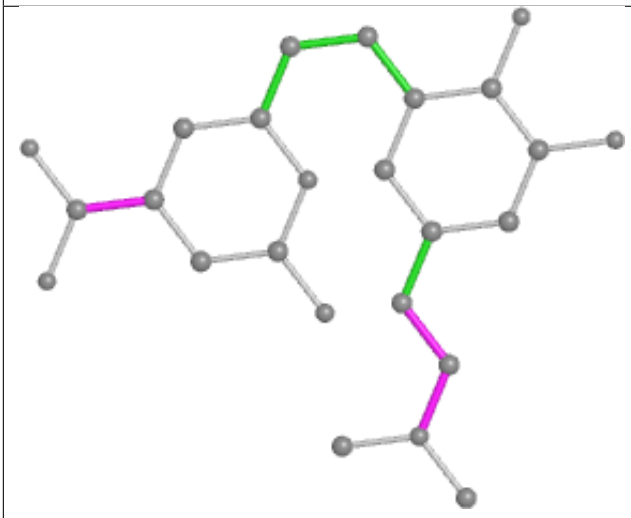
Ligand XVA D 503



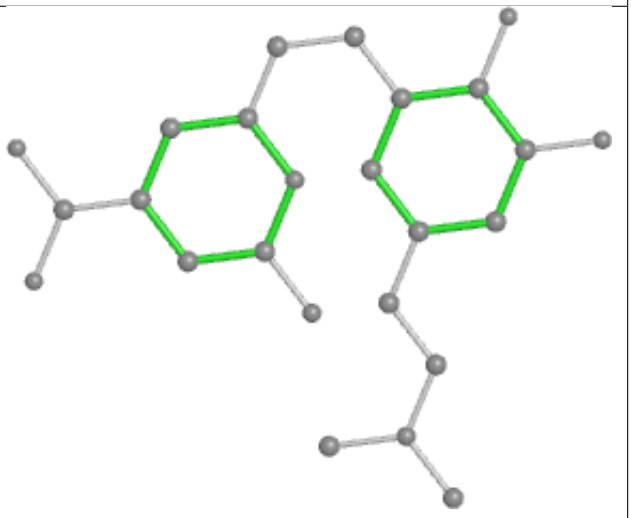
Bond lengths



Bond angles

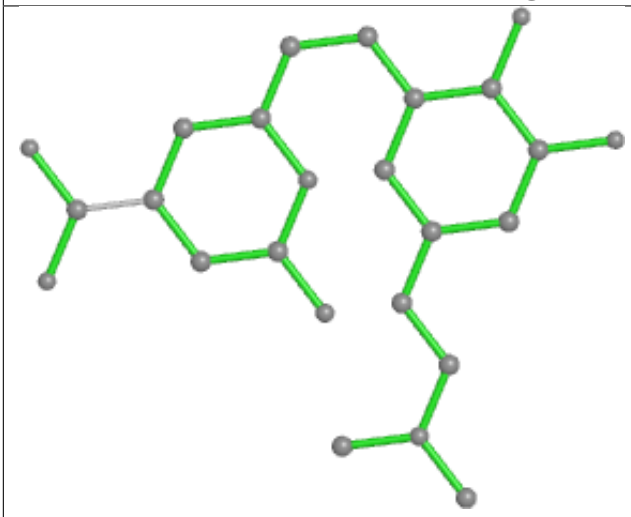


Torsions

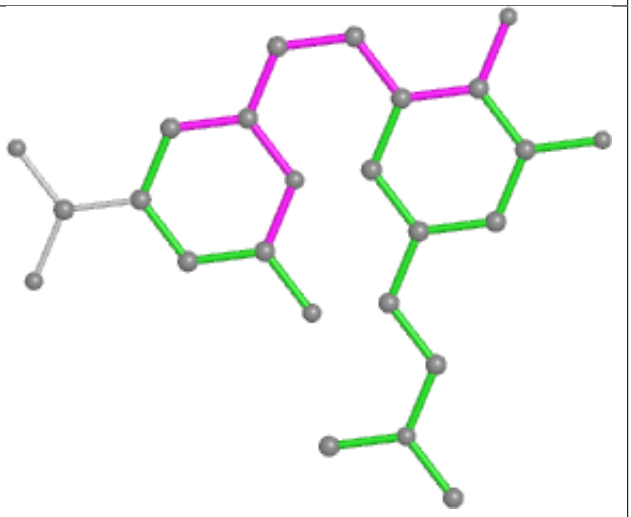


Rings

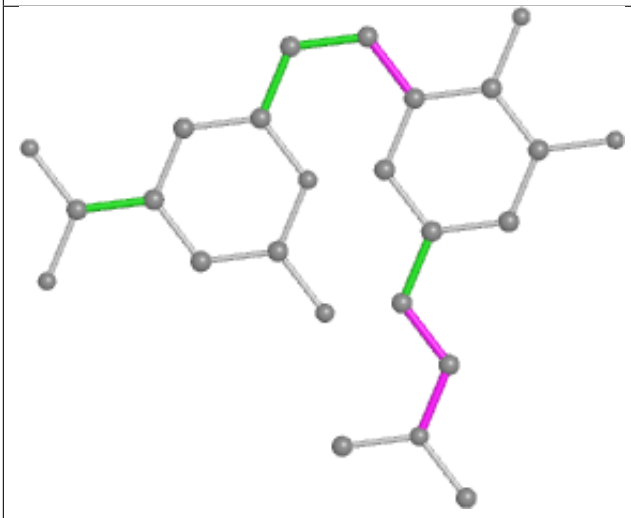
Ligand XVA B 503



Bond lengths



Bond angles



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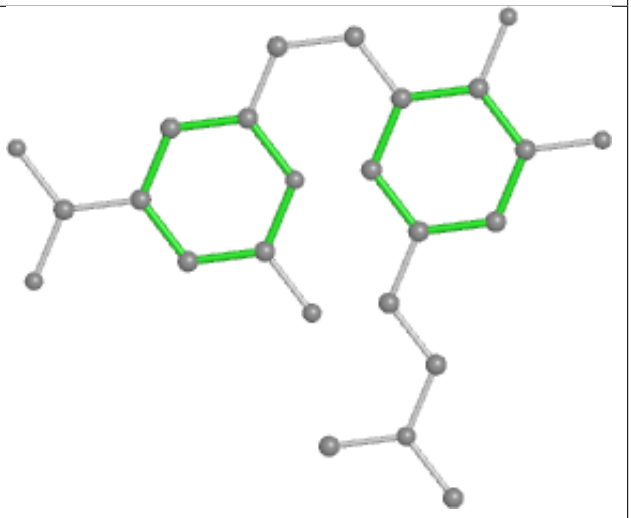
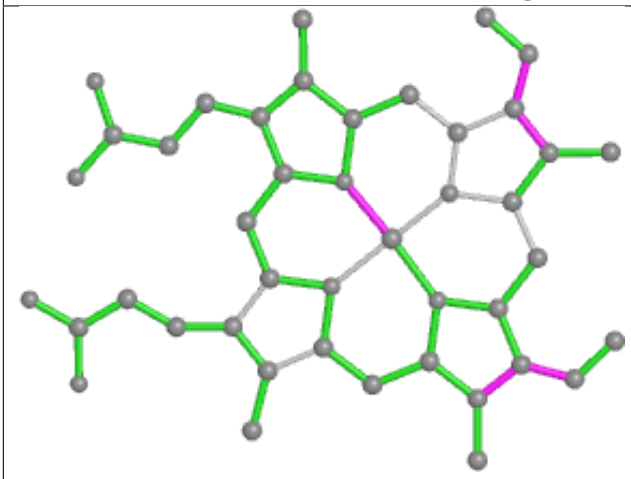
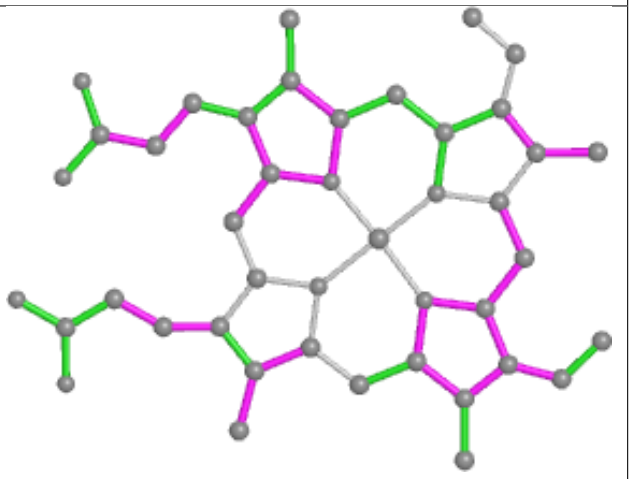


Rings

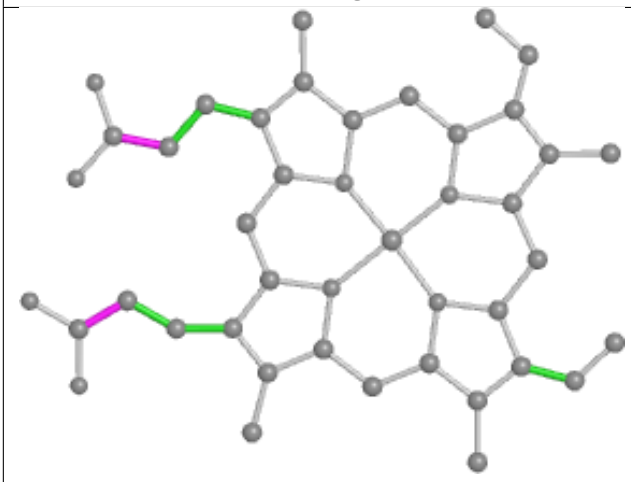
Ligand HEM B 501



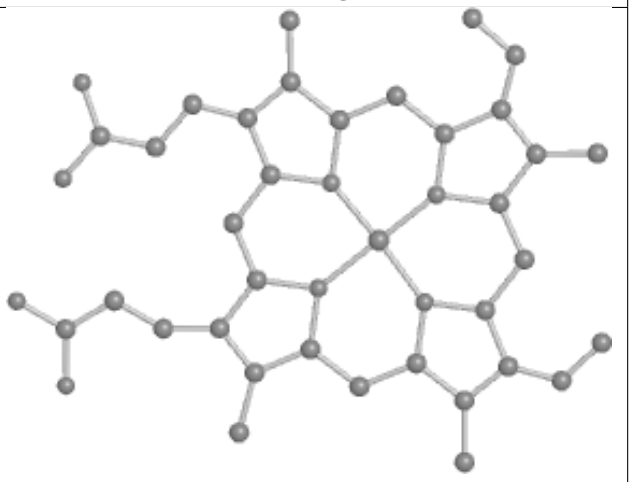
Bond lengths



Bond angles

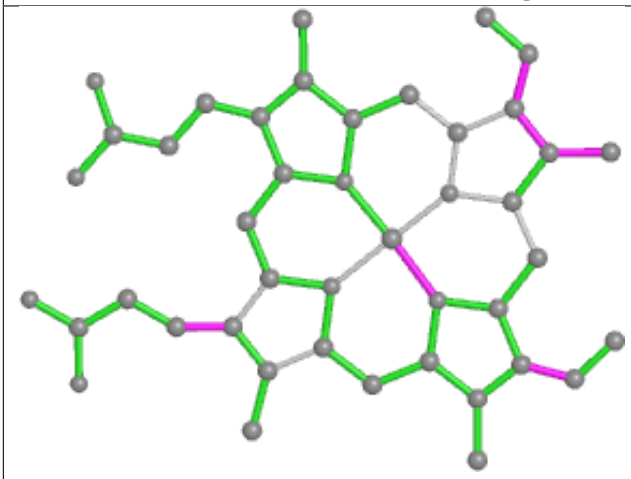


Torsions

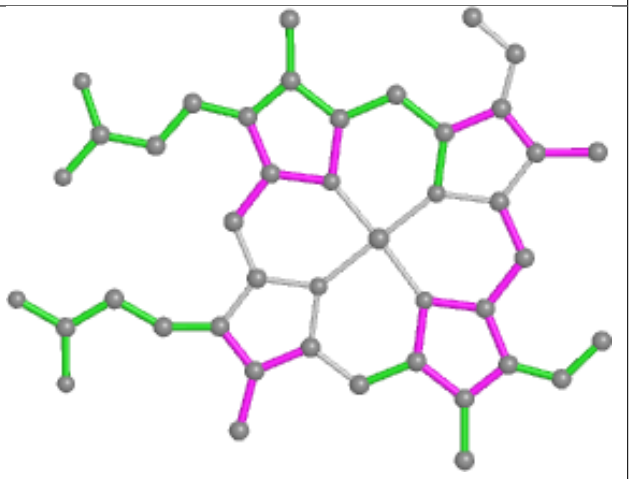


Rings

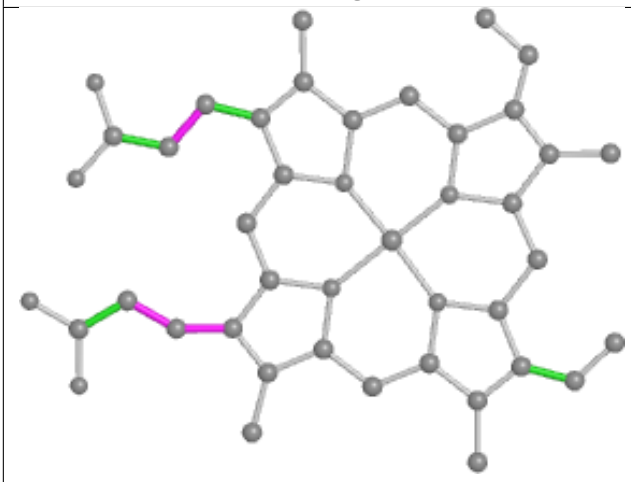
Ligand HEM D 501



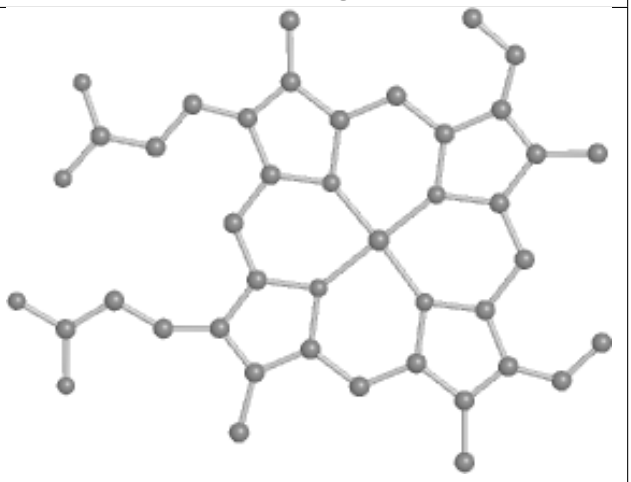
Bond lengths



Bond angles

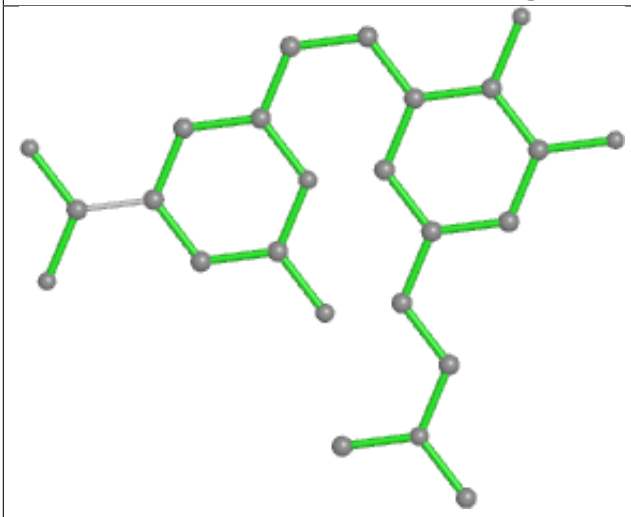


Torsions

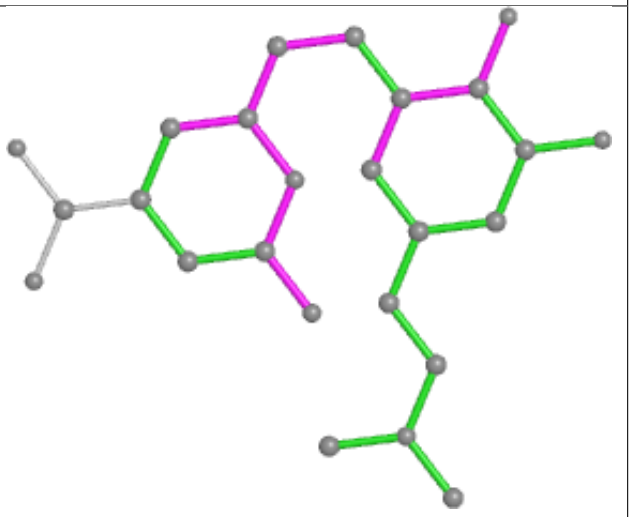


Rings

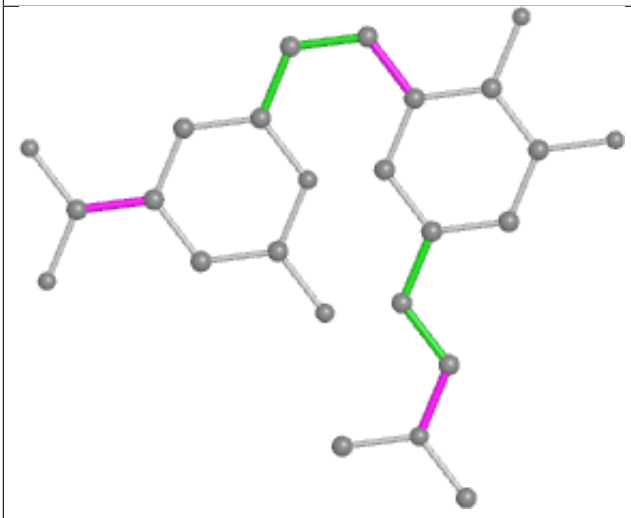
Ligand XVA A 503



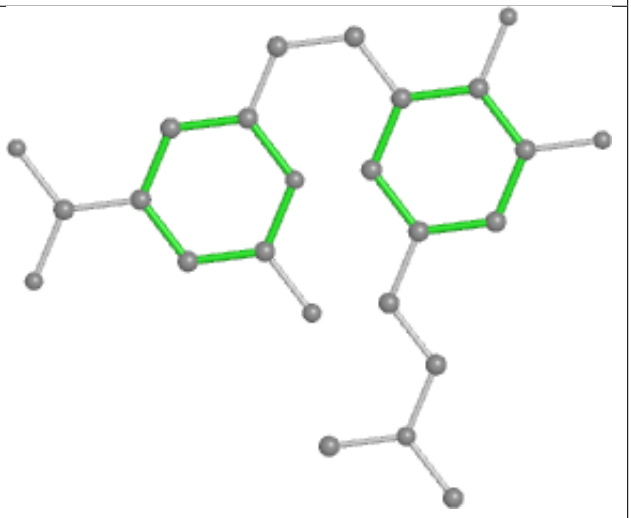
Bond lengths



Bond angles

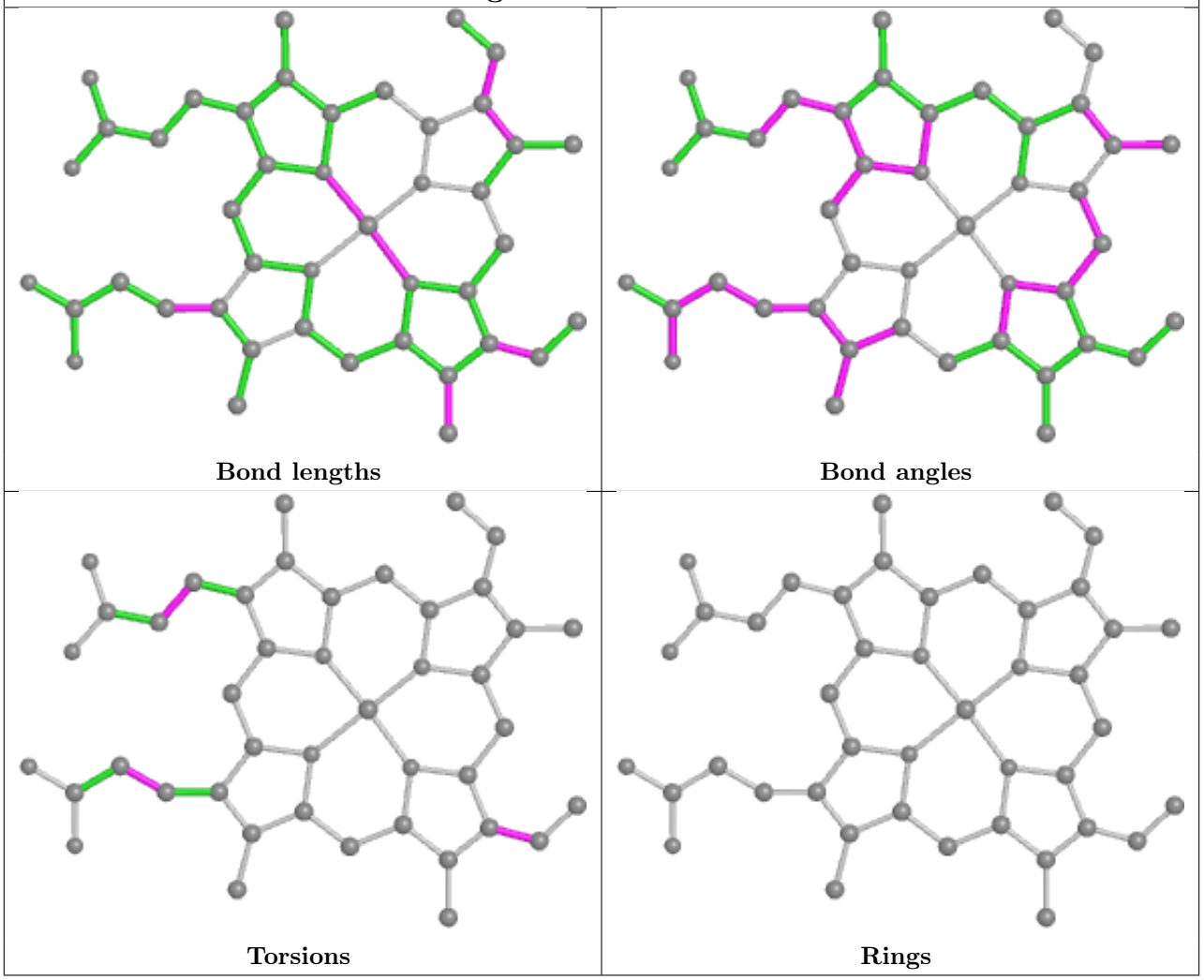


Torsions



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%)	0.88	79 (19%) 1 0	28, 62, 110, 134	0
1	B	402/440 (91%)	0.03	21 (5%) 27 26	27, 43, 77, 117	0
1	C	403/440 (91%)	0.62	53 (13%) 3 2	33, 57, 102, 148	0
1	D	402/440 (91%)	-0.05	21 (5%) 27 26	28, 43, 71, 129	0
All	All	1608/1760 (91%)	0.37	174 (10%) 5 5	27, 50, 99, 148	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	GLY	8.1
1	C	238	ARG	5.9
1	C	68	PHE	5.9
1	A	204	ALA	5.2
1	A	275	ILE	5.2
1	A	153	VAL	5.1
1	A	447	TRP	5.1
1	A	142	GLY	4.8
1	A	480	TRP	4.7
1	C	448	ILE	4.6
1	A	89	GLN	4.6
1	A	451	PRO	4.5
1	C	275	ILE	4.4
1	B	89	GLN	4.2
1	A	452	ILE	4.2
1	A	238	ARG	4.2
1	A	302	LEU	4.2
1	A	448	ILE	4.2
1	B	257	GLN	4.2
1	A	281	PRO	4.1
1	C	447	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	480	TRP	4.1
1	B	449	VAL	4.0
1	C	184	CYS	3.9
1	A	244	TRP	3.8
1	C	360	THR	3.8
1	A	120	PRO	3.8
1	C	299	PRO	3.8
1	B	158	ALA	3.8
1	D	452	ILE	3.8
1	D	257	GLN	3.8
1	B	454	GLY	3.7
1	C	257	GLN	3.7
1	A	184	CYS	3.7
1	C	439	GLY	3.6
1	C	449	VAL	3.6
1	B	460	PHE	3.6
1	A	412	LEU	3.6
1	C	202	ARG	3.6
1	C	451	PRO	3.5
1	D	449	VAL	3.5
1	D	89	GLN	3.5
1	A	295	ALA	3.4
1	A	254	TYR	3.4
1	A	122	GLN	3.4
1	A	257	GLN	3.4
1	A	255	ARG	3.4
1	B	452	ILE	3.3
1	A	304	LEU	3.3
1	A	299	PRO	3.3
1	A	346	LEU	3.2
1	A	446	ALA	3.2
1	A	256	GLN	3.2
1	A	449	VAL	3.2
1	C	79	ILE	3.2
1	C	452	ILE	3.2
1	D	258	ASP	3.1
1	C	119	ALA	3.1
1	A	479	PRO	3.1
1	C	450	PRO	3.1
1	A	268	VAL	3.1
1	A	360	THR	3.1
1	A	128	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	183	ARG	3.1
1	A	107	ARG	3.1
1	A	280	THR	3.0
1	B	453	SER	3.0
1	A	300	PRO	3.0
1	C	89	GLN	3.0
1	C	237	GLY	3.0
1	A	450	PRO	3.0
1	D	255	ARG	2.9
1	C	81	TYR	2.9
1	D	121	GLU	2.9
1	A	68	PHE	2.8
1	A	202	ARG	2.8
1	D	446	ALA	2.8
1	A	274	CYS	2.8
1	B	260	SER	2.8
1	C	239	GLY	2.8
1	C	446	ALA	2.7
1	C	221	ARG	2.7
1	D	259	GLY	2.7
1	B	455	SER	2.7
1	C	185	VAL	2.7
1	A	141	SER	2.7
1	D	454	GLY	2.6
1	A	364	THR	2.6
1	C	300	PRO	2.6
1	A	293	LEU	2.6
1	D	388	ARG	2.6
1	C	292	LEU	2.6
1	B	360	THR	2.6
1	D	451	PRO	2.6
1	C	445	TRP	2.6
1	A	303	PHE	2.6
1	A	307	PRO	2.6
1	B	119	ALA	2.5
1	A	445	TRP	2.5
1	A	305	LEU	2.5
1	A	86	ALA	2.5
1	D	460	PHE	2.5
1	C	107	ARG	2.5
1	A	478	ASP	2.5
1	C	307	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	159	ALA	2.5
1	C	204	ALA	2.5
1	A	185	VAL	2.5
1	A	84	LEU	2.4
1	B	258	ASP	2.4
1	A	145	ALA	2.4
1	D	360	THR	2.4
1	D	260	SER	2.4
1	C	304	LEU	2.4
1	C	183	ARG	2.4
1	A	272	GLU	2.4
1	A	367	LEU	2.4
1	C	141	SER	2.4
1	C	276	GLN	2.4
1	D	445	TRP	2.4
1	D	453	SER	2.3
1	C	280	THR	2.3
1	A	273	LEU	2.3
1	C	236	PRO	2.3
1	A	260	SER	2.3
1	B	388	ARG	2.3
1	C	297	ASP	2.3
1	A	294	GLN	2.3
1	C	160	THR	2.3
1	B	142	GLY	2.3
1	C	303	PHE	2.3
1	A	439	GLY	2.2
1	A	88	ALA	2.2
1	B	106	PRO	2.2
1	C	186	GLY	2.2
1	A	292	LEU	2.2
1	A	301	GLU	2.2
1	C	301	GLU	2.2
1	A	87	GLN	2.2
1	A	436	LYS	2.2
1	B	97	ARG	2.2
1	D	256	GLN	2.2
1	A	146	HIS	2.2
1	A	79	ILE	2.2
1	B	450	PRO	2.2
1	C	412	LEU	2.2
1	A	365	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	87	GLN	2.1
1	D	456	LEU	2.1
1	A	368	CYS	2.1
1	B	68	PHE	2.1
1	A	258	ASP	2.1
1	C	122	GLN	2.1
1	A	121	GLU	2.1
1	A	283	ASN	2.1
1	D	447	TRP	2.1
1	C	140	ARG	2.1
1	C	273	LEU	2.1
1	C	67	LYS	2.1
1	A	321	GLU	2.1
1	A	207	MET	2.1
1	A	276	GLN	2.0
1	B	446	ALA	2.0
1	A	125	SER	2.0
1	A	221	ARG	2.0
1	A	262	ARG	2.0
1	B	445	TRP	2.0
1	C	255	ARG	2.0
1	C	80	THR	2.0
1	C	129	ASP	2.0
1	A	235	CYS	2.0
1	C	368	CYS	2.0
1	C	70	ARG	2.0
1	D	261	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

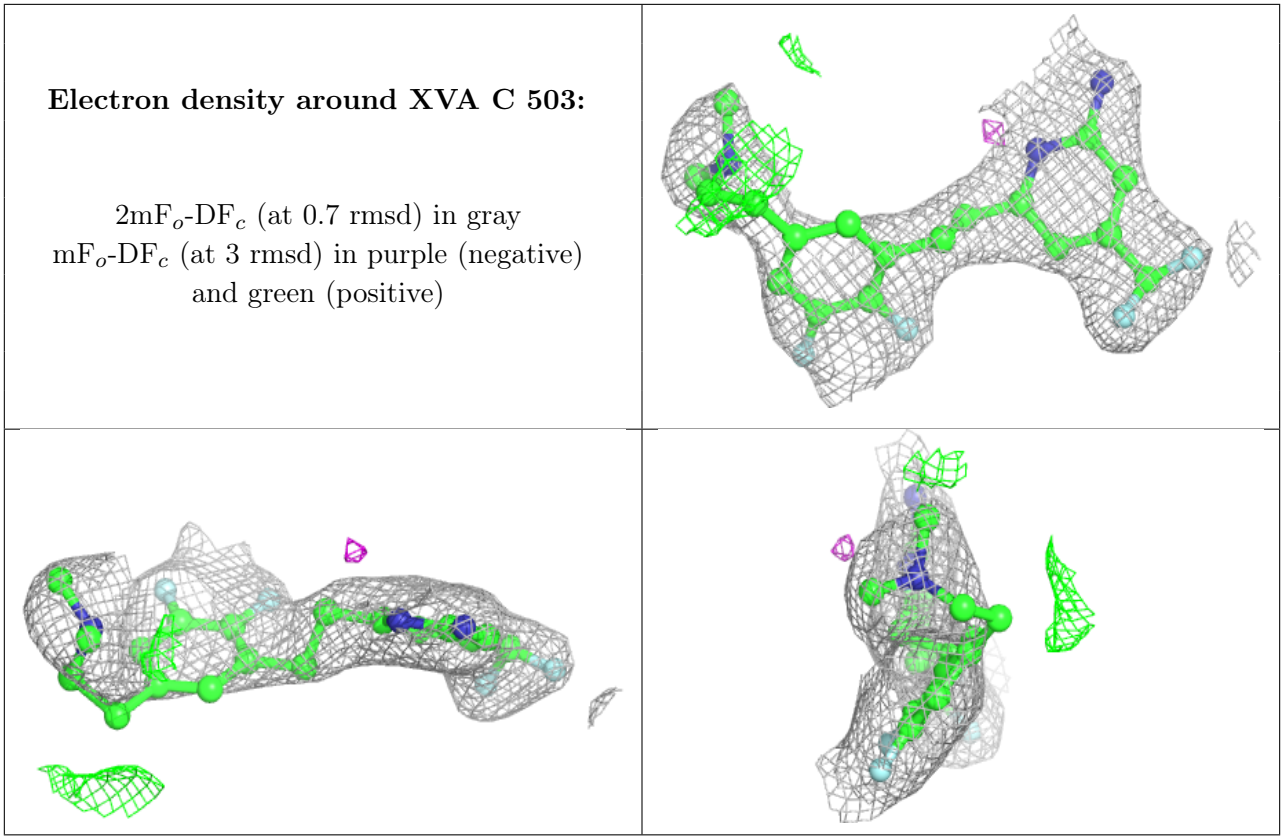
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BTB	C	505	14/14	0.75	0.20	93,100,115,117	0
3	H4B	C	502	17/17	0.77	0.35	59,78,90,95	0
5	BTB	A	506	14/14	0.78	0.22	84,100,111,113	0
3	H4B	A	502	17/17	0.78	0.32	69,81,93,95	0
5	BTB	B	504	14/14	0.82	0.13	31,52,76,78	0
3	H4B	B	502	17/17	0.86	0.21	51,66,79,86	0
6	GOL	C	507	6/6	0.86	0.12	77,80,81,83	0
5	BTB	B	505	14/14	0.87	0.19	55,73,100,101	0
8	GD	A	509	1/1	0.87	0.05	112,112,112,112	1
5	BTB	D	504	14/14	0.88	0.17	50,65,74,76	0
6	GOL	C	506	6/6	0.88	0.22	52,59,66,68	0
3	H4B	D	502	17/17	0.88	0.22	45,62,74,75	0
5	BTB	A	505	14/14	0.88	0.11	58,72,87,95	0
4	XVA	C	503	25/25	0.89	0.32	46,73,96,100	0
6	GOL	B	506	6/6	0.90	0.10	71,79,81,82	0
6	GOL	A	507	6/6	0.90	0.19	63,66,72,75	0
4	XVA	B	503	25/25	0.91	0.18	29,62,89,100	0
5	BTB	C	504	14/14	0.92	0.26	36,73,85,93	0
4	XVA	A	503	25/25	0.92	0.32	48,71,85,86	0
5	BTB	B	509	14/14	0.93	0.11	49,62,76,83	0
4	XVA	D	503	25/25	0.93	0.16	29,45,89,97	0
5	BTB	A	504	14/14	0.93	0.29	59,88,97,100	0
5	BTB	D	505	14/14	0.94	0.23	32,69,85,93	0
2	HEM	A	501	43/43	0.96	0.24	42,59,88,94	0
2	HEM	C	501	43/43	0.97	0.21	30,47,84,89	0
7	CL	A	508	1/1	0.97	0.27	54,54,54,54	0
2	HEM	B	501	43/43	0.97	0.13	22,34,76,88	0
2	HEM	D	501	43/43	0.98	0.12	24,34,76,82	0
8	GD	C	509	1/1	0.98	0.05	82,82,82,82	1
8	GD	D	507	1/1	0.98	0.14	52,52,52,52	0
7	CL	B	507	1/1	0.99	0.14	40,40,40,40	0
8	GD	B	508	1/1	0.99	0.11	45,45,45,45	0
7	CL	C	508	1/1	0.99	0.23	50,50,50,50	0
7	CL	D	506	1/1	0.99	0.11	42,42,42,42	0
9	ZN	A	510	1/1	0.99	0.11	47,47,47,47	0
9	ZN	C	510	1/1	1.00	0.09	38,38,38,38	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.

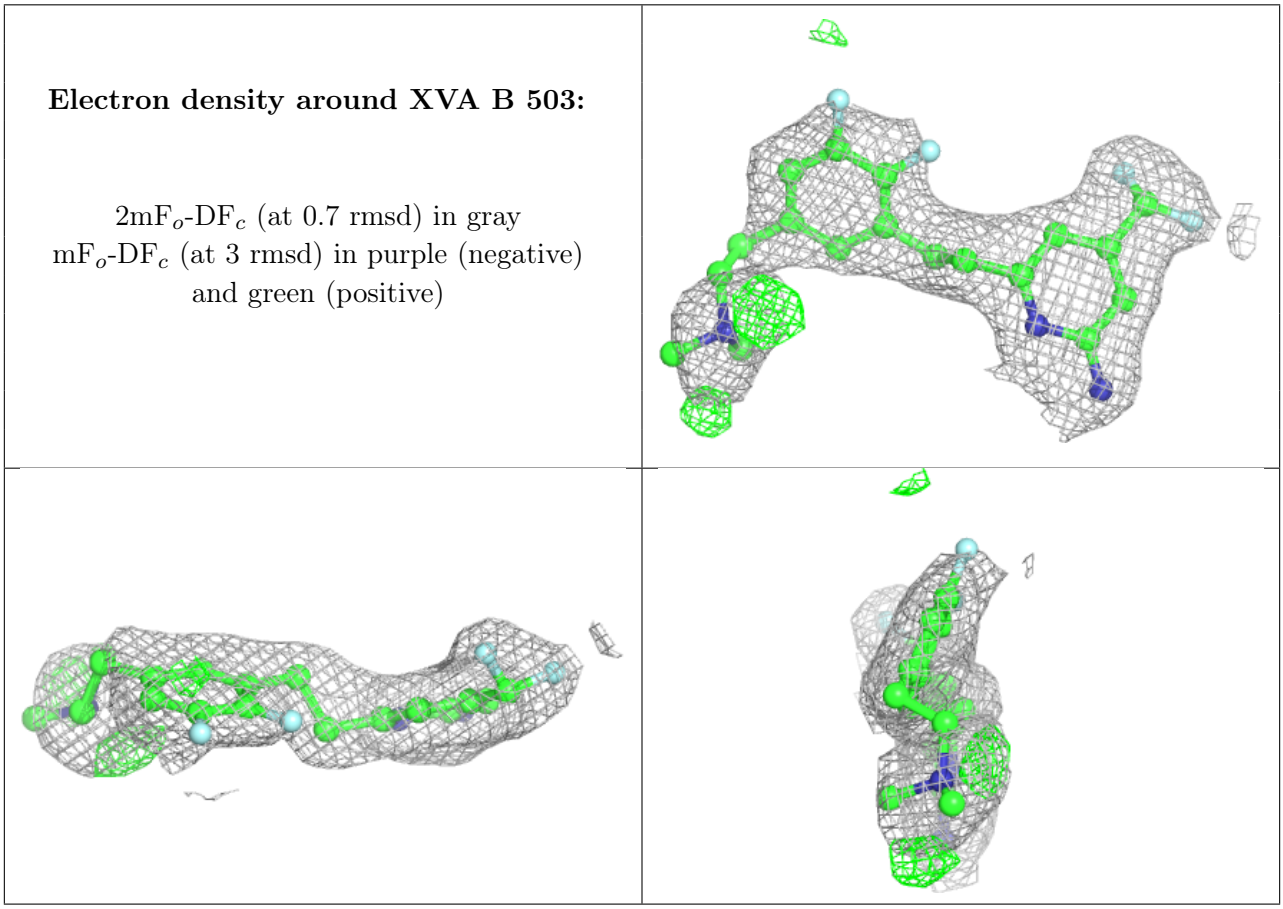
Electron density around XVA C 503:

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



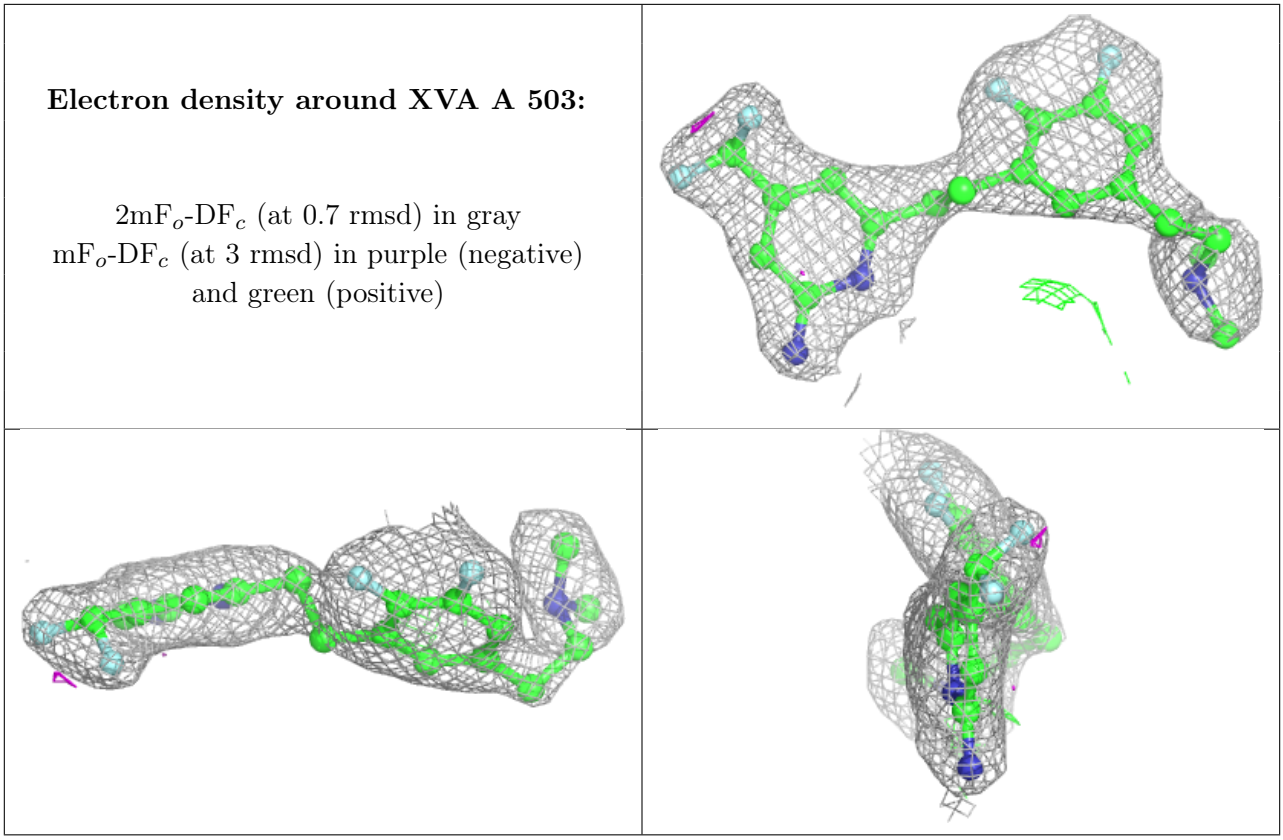
Electron density around XVA B 503:

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



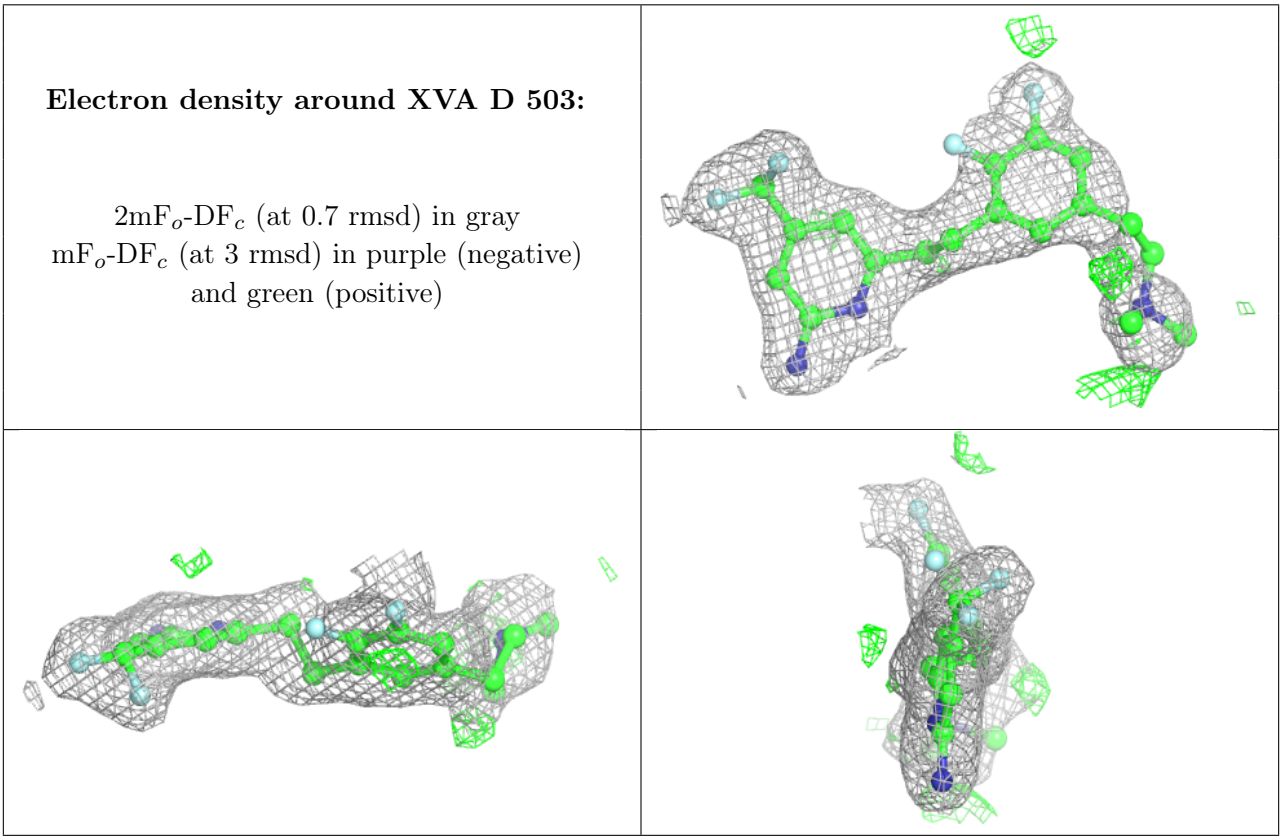
Electron density around XVA A 503:

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



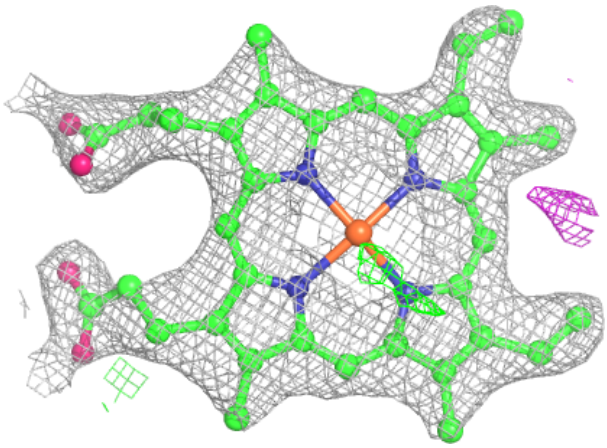
Electron density around XVA D 503:

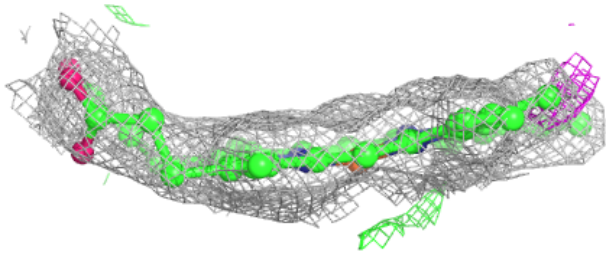
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

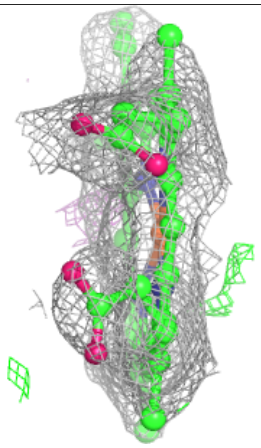


Electron density around HEM A 501:

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

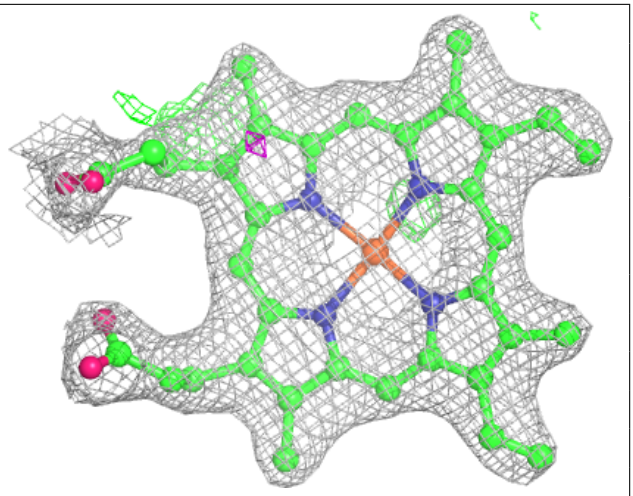


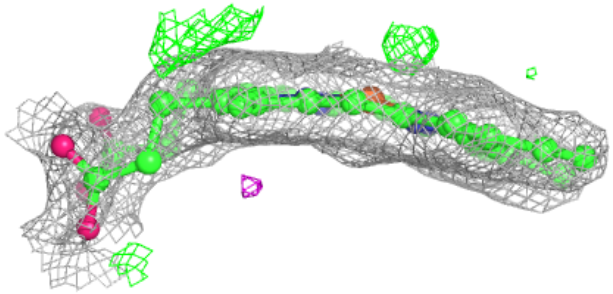


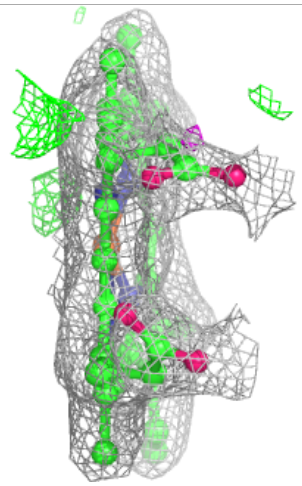


Electron density around HEM C 501:

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

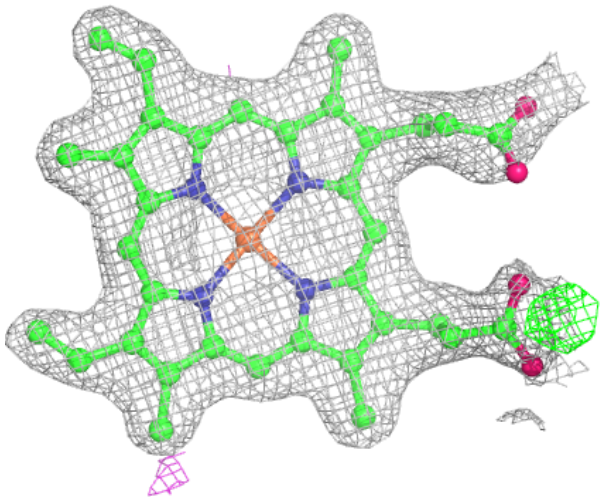


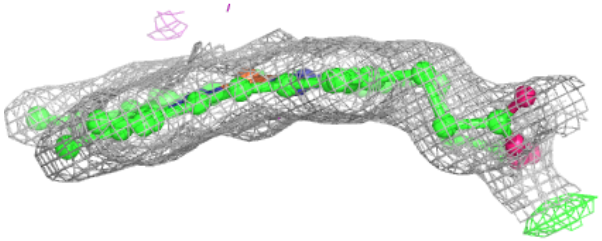


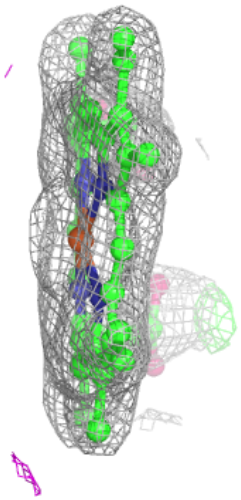


Electron density around HEM B 501:

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

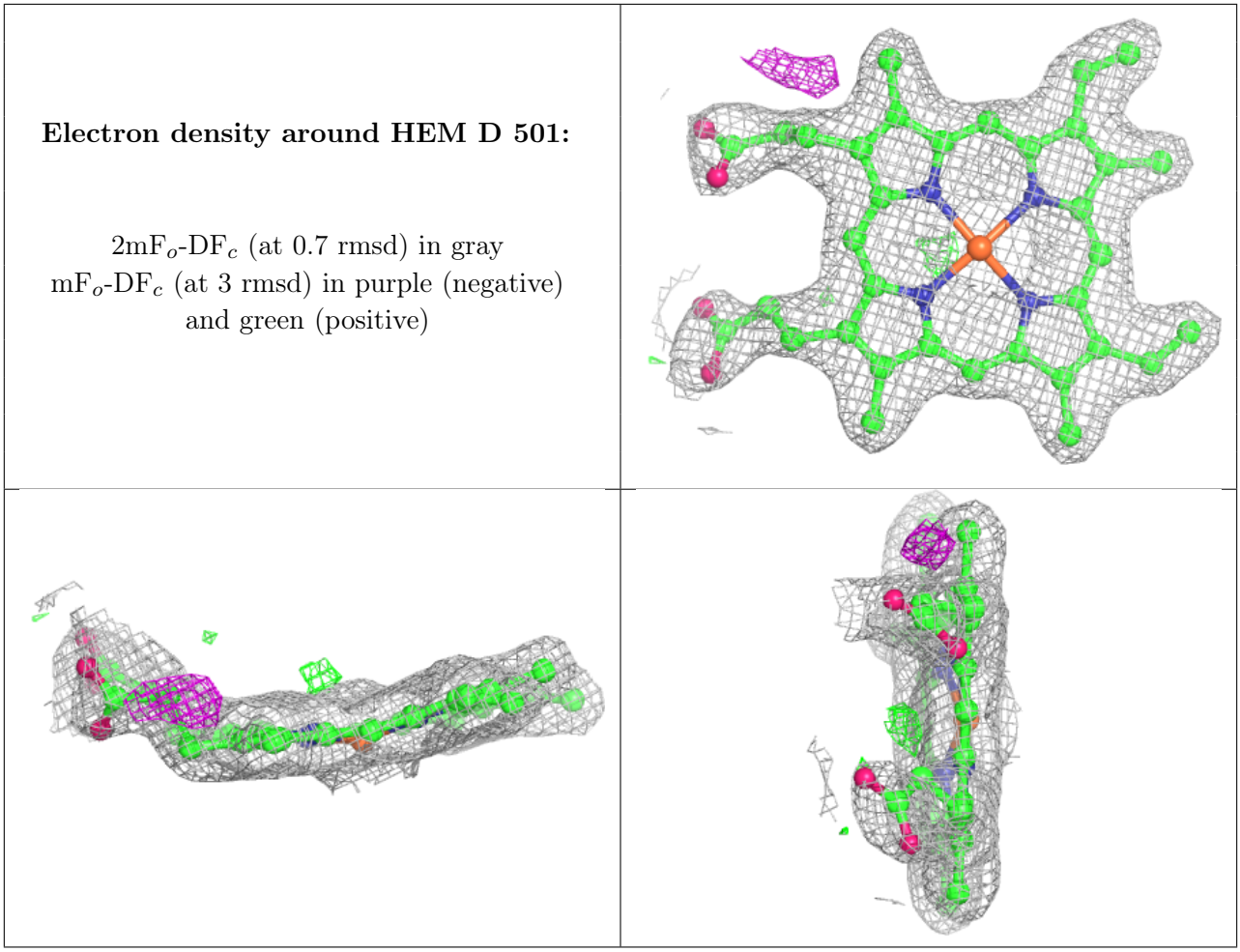






Electron density around HEM D 501:

$2mF_o$-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.