Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 03:01 AM EST

PDB ID	:	8UFU
Title	:	Structure of human endothelial nitric oxide synthase heme domain in complex with 7-(9-amino-6,7,8,9-tetrahydro-5H-benzo[7]annulen-2-yl)-4-methylquinolin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2023-10-04
Resolution	:	2.05 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:

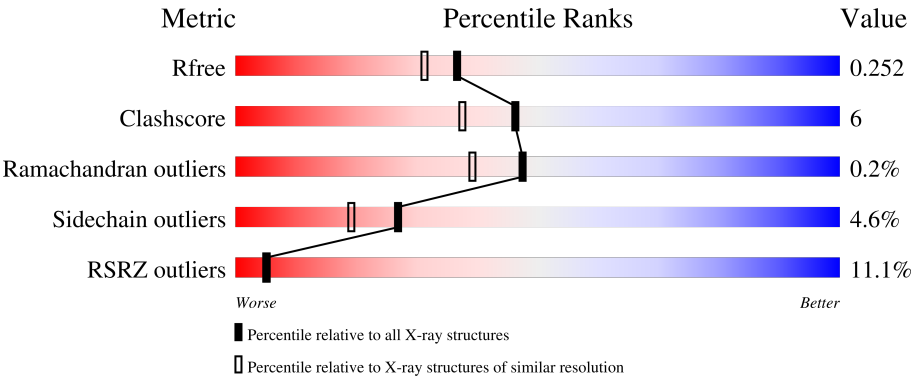
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	17% 74% 15% • 9%
1	B	440	7% 78% 12% • 9%
1	C	440	11% 73% 17% • 9%
1	D	440	6% 79% 12% • 9%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13720 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.

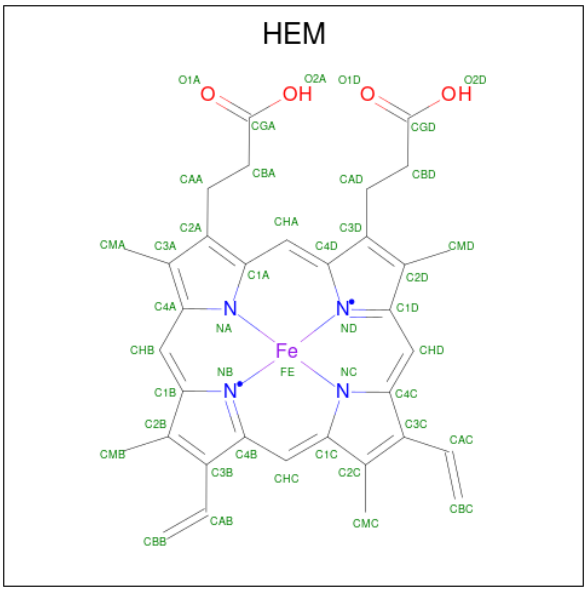
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	2	0
			3215	2047	566	586	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	2	0
			3218	2050	565	587	16			
1	D	401	Total	C	N	O	S	0	2	0
			3206	2042	563	585	16			

There are 4 discrepancies between the modelled and reference sequences:

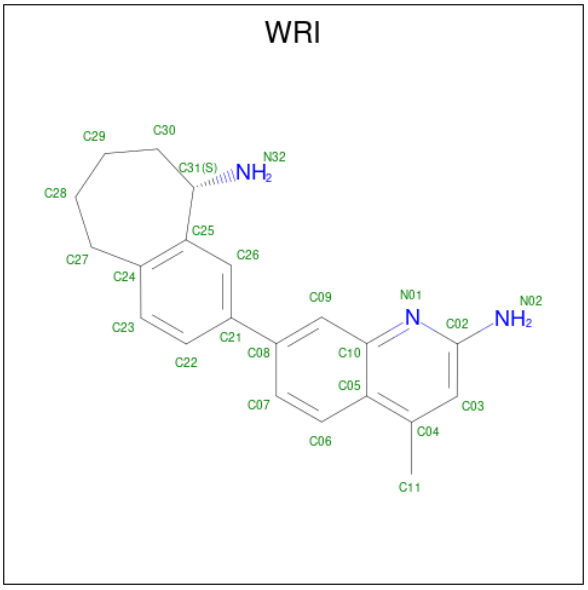
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



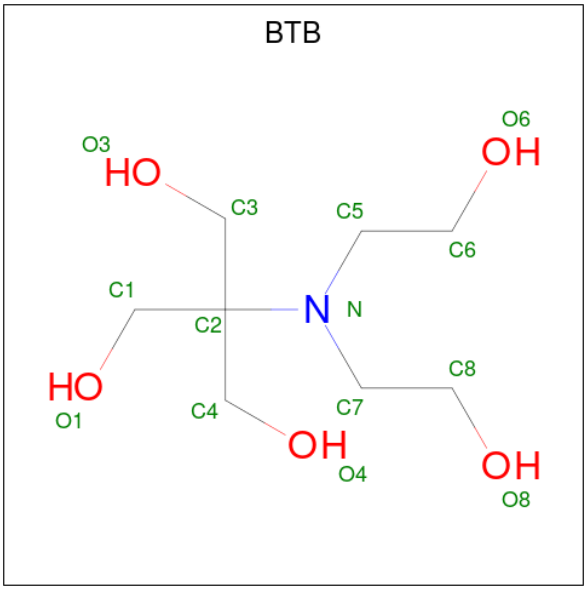
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (7M)-7-[(9S)-9-amino-6,7,8,9-tetrahydro-5H-benzo[7]annulen-2-yl]-4-methylquinolin-2-amine (three-letter code: WRI) (formula: $C_{21}H_{23}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 24 21 3	0	0
3	A	1	Total C N 24 21 3	0	0
3	B	1	Total C N 24 21 3	0	0
3	B	1	Total C N 24 21 3	0	0
3	C	1	Total C N 24 21 3	0	0
3	C	1	Total C N 24 21 3	0	0
3	C	1	Total C N 24 21 3	0	0
3	D	1	Total C N 24 21 3	0	0

- Molecule 4 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
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

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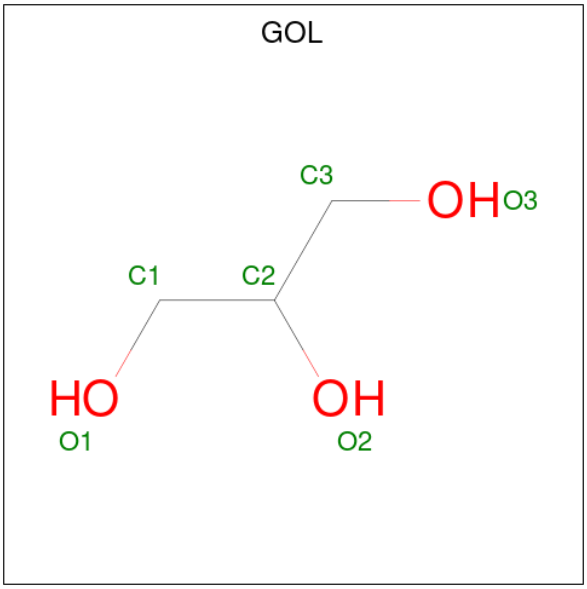
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

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



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Zn 2 2	0	0
7	B	1	Total Zn 1 1	0	0
7	C	3	Total Zn 3 3	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0
8	C	1	Total Ca 1 1	0	0

- Molecule 9 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Gd 1 1	0	0
9	D	1	Total Gd 1 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	50	Total O 50 50	0	0
10	B	118	Total O 118 118	0	0
10	C	75	Total O 75 75	0	0

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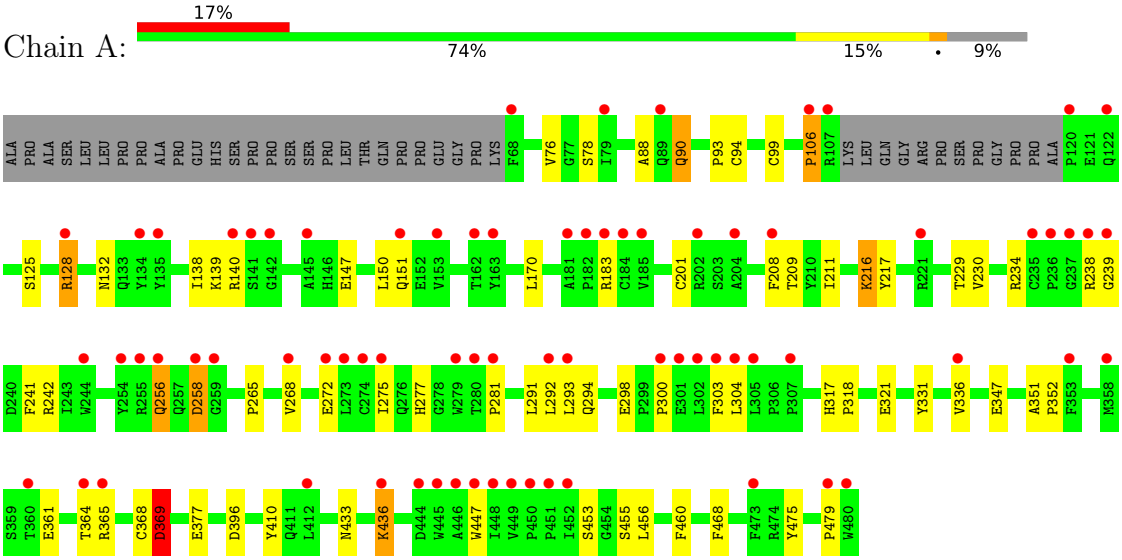
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	119	Total	O	0	0
			119	119		

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.

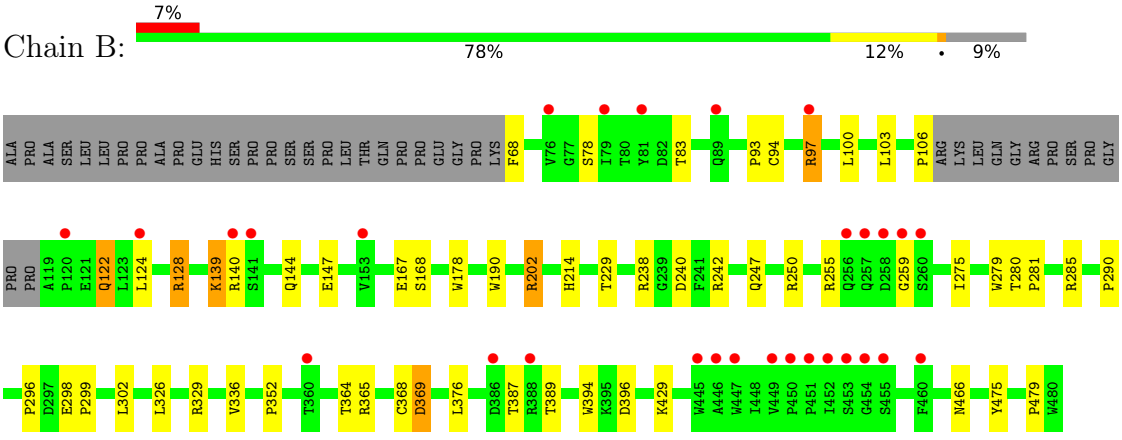
• Molecule 1: Nitric oxide synthase, endothelial

Chain A:



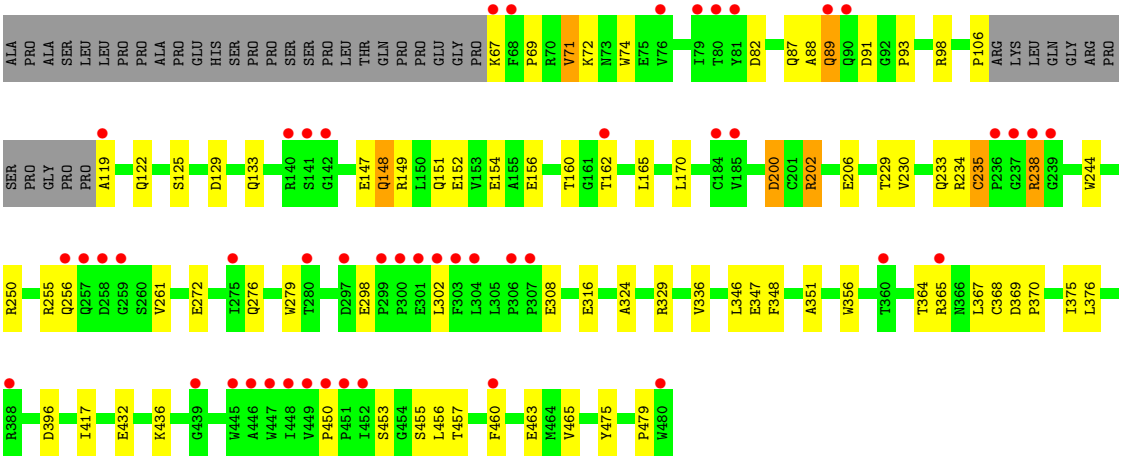
• Molecule 1: Nitric oxide synthase, endothelial

Chain B:



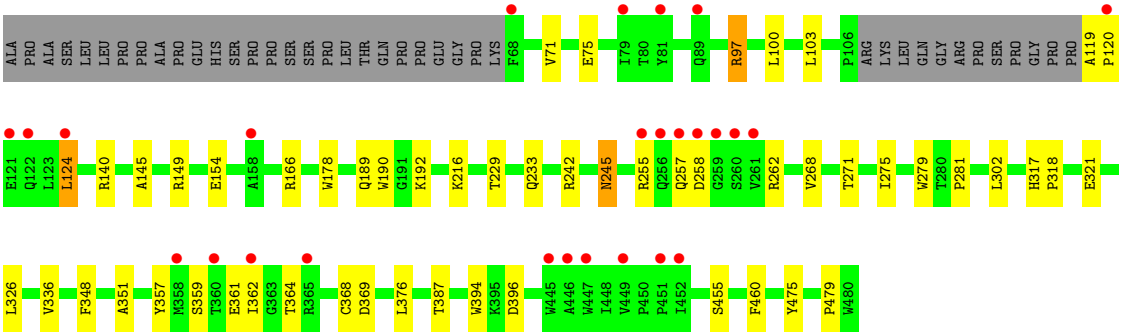
• Molecule 1: Nitric oxide synthase, endothelial

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	59.67Å 152.83Å 109.16Å 90.00° 90.82° 90.00°	Depositor
Resolution (Å)	38.74 – 2.05 38.74 – 2.05	Depositor EDS
% Data completeness (in resolution range)	94.2 (38.74-2.05) 94.7 (38.74-2.05)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.205 , 0.256 0.199 , 0.252	Depositor DCC
R_{free} test set	5867 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.108 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13720	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: ZN, WRI, GOL, BTB, CL, HEM, GD, CA

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	0/3313	0.53	1/4513 (0.0%)
1	B	0.40	0/3312	0.56	1/4514 (0.0%)
1	C	0.39	0/3316	0.55	1/4518 (0.0%)
1	D	0.43	0/3304	0.59	1/4503 (0.0%)
All	All	0.40	0/13245	0.56	4/18048 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	369	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	369	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	369	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	369	ASP	CB-CG-OD2	5.15	122.93	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	240	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3215	0	3118	42	0
1	B	3211	0	3114	33	0
1	C	3218	0	3122	43	0
1	D	3206	0	3108	29	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	48	0	0	3	0
3	B	48	0	0	1	0
3	C	72	0	0	1	0
3	D	24	0	0	2	0
4	A	28	0	38	6	0
4	B	28	0	36	5	0
4	C	28	0	38	7	0
4	D	28	0	36	5	0
5	A	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	1	0
6	D	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	A	50	0	0	1	0
10	B	118	0	0	1	0
10	C	75	0	0	2	0
10	D	119	0	0	2	0
All	All	13720	0	12754	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

All (164) 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:D:321:GLU:OE2	4:D:503:BTB:O4	2.04	0.76
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.20	0.75
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.69	0.74
1:D:475:TYR:OH	2:D:501:HEM:O2D	2.06	0.73
1:B:124:LEU:HB3	1:B:128:ARG:HH12	1.52	0.73
1:D:100:LEU:HB3	1:D:103:LEU:HD22	1.73	0.70
1:A:433:ASN:HA	1:A:436:LYS:HE3	1.74	0.68
1:C:91:ASP:OD1	10:C:601:HOH:O	2.10	0.68
1:D:154:GLU:OE2	10:D:601:HOH:O	2.11	0.68
1:B:475:TYR:OH	2:B:501:HEM:O2D	2.11	0.67
1:C:475:TYR:OH	2:C:501:HEM:O2D	2.13	0.67
1:C:453:SER:HB3	1:C:456:LEU:HD12	1.77	0.66
1:C:88:ALA:HB3	1:D:97:ARG:HD2	1.77	0.66
1:D:255:ARG:HD3	1:D:268:VAL:HG11	1.77	0.66
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.77	0.66
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.78	0.65
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.77	0.65
1:C:200:ASP:OD1	1:C:200:ASP:N	2.29	0.65
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.79	0.64
1:C:93:PRO:HG3	1:C:106:PRO:HB3	1.81	0.63
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.81	0.62
1:C:365:ARG:NH1	2:C:501:HEM:O2A	2.33	0.62
1:C:119:ALA:HB1	1:C:122:GLN:HB2	1.82	0.61
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.83	0.61
1:B:298:GLU:OE2	4:B:505:BTB:N	2.34	0.61
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.81	0.60
1:A:128:ARG:O	1:A:132:ASN:ND2	2.34	0.60
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.84	0.60
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.34	0.59
1:A:475:TYR:OH	2:A:501:HEM:O2D	2.18	0.59
1:D:140:ARG:HH12	1:D:145:ALA:HB3	1.67	0.59
4:C:504:BTB:HO3	4:C:504:BTB:HO8	1.51	0.59
1:C:147:GLU:O	1:C:151:GLN:HG2	2.04	0.58
1:A:90:GLN:HB3	1:A:468:PHE:CD2	2.38	0.58
1:C:370:PRO:HG2	1:D:75:GLU:HG2	1.86	0.58
1:D:124:LEU:HD11	1:D:154:GLU:HG3	1.87	0.57
1:B:285:ARG:NH2	10:B:601:HOH:O	2.23	0.57
1:B:93:PRO:HG3	1:B:106:PRO:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLU:OE1	4:A:504:BTB:H11	2.05	0.56
4:B:505:BTB:H81	4:B:505:BTB:O6	2.06	0.56
1:C:160:THR:HG23	1:C:162:THR:H	1.69	0.56
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.87	0.56
1:A:453:SER:HB3	1:A:456:LEU:HD12	1.89	0.55
1:A:238:ARG:HH21	1:A:241:PHE:HD1	1.56	0.53
1:B:279:TRP:CD1	1:B:290:PRO:HG3	2.43	0.53
1:A:321:GLU:H	1:A:321:GLU:CD	2.09	0.53
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.89	0.53
1:C:156:GLU:O	1:C:160:THR:HG22	2.08	0.53
1:B:229:THR:O	1:B:352:PRO:HD2	2.08	0.53
1:B:336:VAL:HG21	3:B:502:WRI:C07	2.39	0.52
1:A:331:TYR:O	1:A:410:TYR:OH	2.28	0.52
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.92	0.52
1:A:88:ALA:O	1:B:97:ARG:NH1	2.43	0.52
1:B:298:GLU:HG3	1:B:299:PRO:HD2	1.92	0.51
1:A:242:ARG:NH2	1:A:479:PRO:HD3	2.25	0.51
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.25	0.51
1:A:93:PRO:HG3	1:A:106:PRO:HB3	1.92	0.51
1:A:258:ASP:N	1:A:258:ASP:OD1	2.44	0.50
1:A:361:GLU:OE2	3:A:502:WRI:N02	2.44	0.50
1:C:87:GLN:O	1:C:89:GLN:NE2	2.44	0.50
1:D:387:THR:HA	1:D:394:TRP:CD1	2.46	0.50
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.52	0.50
1:A:256:GLN:C	1:A:258:ASP:H	2.13	0.50
1:D:455:SER:HA	1:D:460:PHE:CG	2.46	0.50
1:C:356:TRP:CZ2	2:C:501:HEM:HBB1	2.47	0.49
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.95	0.49
1:A:291:LEU:HD23	1:A:293:LEU:HD21	1.92	0.49
1:B:364:THR:O	1:B:368:CYS:HB2	2.12	0.49
1:C:336:VAL:HG21	3:C:502:WRI:C07	2.42	0.49
1:A:365:ARG:O	1:A:369:ASP:HB2	2.12	0.49
4:C:504:BTB:O8	4:C:504:BTB:O3	2.18	0.49
1:C:298:GLU:OE1	4:C:505:BTB:O1	2.31	0.48
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.48	0.48
1:D:245:ASN:N	1:D:245:ASN:OD1	2.46	0.48
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.96	0.48
1:C:364:THR:O	1:C:368:CYS:HB2	2.13	0.48
1:C:316[B]:GLU:HG2	1:C:324:ALA:HB2	1.94	0.48
1:A:76:VAL:HG12	1:A:78:SER:H	1.78	0.47
1:D:271:THR:O	1:D:275:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:VAL:HG21	1:C:465:VAL:HG23	1.96	0.47
1:A:170:LEU:HD11	1:A:230:VAL:HG11	1.96	0.47
1:C:133:GLN:NE2	10:C:605:HOH:O	2.40	0.47
4:D:504:BTB:H31	4:D:504:BTB:H71	1.36	0.47
4:A:505:BTB:H41	4:A:505:BTB:H72	1.60	0.47
1:C:202:ARG:HG2	1:C:206:GLU:OE1	2.15	0.47
1:A:183:ARG:HG2	1:A:447:TRP:CG	2.50	0.47
1:A:128:ARG:HE	1:A:128:ARG:HB3	1.53	0.46
1:A:336:VAL:HG21	3:A:502:WRI:C07	2.46	0.46
1:B:202:ARG:HB2	1:B:202:ARG:NH1	2.31	0.46
1:D:189:GLN:HB3	10:D:666:HOH:O	2.14	0.46
4:C:504:BTB:H12	4:C:504:BTB:H51	1.82	0.46
1:D:368:CYS:SG	1:D:376:LEU:HD13	2.55	0.46
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.51	0.46
4:C:505:BTB:H42	4:C:505:BTB:H51	1.48	0.46
1:B:275:ILE:HG12	1:B:281:PRO:HG3	1.97	0.45
1:A:455:SER:HA	1:A:460:PHE:CG	2.51	0.45
2:A:501:HEM:HBD1	3:A:502:WRI:C22	2.47	0.45
1:C:235:CYS:SG	1:C:238:ARG:HD3	2.56	0.45
1:A:364:THR:O	1:A:368:CYS:HB2	2.16	0.45
4:A:504:BTB:O3	4:A:504:BTB:O1	2.32	0.45
4:D:504:BTB:H52	4:D:504:BTB:H82	1.43	0.45
1:D:336:VAL:HG21	3:D:502:WRI:C07	2.47	0.45
1:C:368:CYS:SG	1:C:376:LEU:HD13	2.57	0.45
1:C:229:THR:O	1:C:351:ALA:HA	2.17	0.45
4:D:504:BTB:H51	4:D:504:BTB:H42	1.38	0.44
1:A:216:LYS:HG3	1:A:217:TYR:N	2.31	0.44
1:C:455:SER:HA	1:C:460:PHE:CG	2.52	0.44
1:A:147:GLU:O	1:A:151:GLN:HG2	2.17	0.44
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.99	0.44
4:B:505:BTB:O3	4:B:505:BTB:H51	2.17	0.44
1:A:138:ILE:HG13	1:A:140:ARG:HB2	1.99	0.44
1:C:272:GLU:O	1:C:276:GLN:HG3	2.17	0.43
1:A:208:PHE:CE1	1:A:303:PHE:HB3	2.53	0.43
4:A:504:BTB:H12	10:A:647:HOH:O	2.18	0.43
4:A:505:BTB:H11	4:A:505:BTB:H51	1.75	0.43
1:B:298:GLU:CD	4:B:505:BTB:H31	2.39	0.43
1:C:432:GLU:O	1:C:436:LYS:HE3	2.17	0.43
4:C:505:BTB:H31	4:C:505:BTB:H72	1.39	0.43
1:B:202:ARG:HB2	1:B:202:ARG:HH11	1.84	0.43
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ARG:NH2	1:D:479:PRO:HD3	2.33	0.43
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.53	0.43
1:D:361:GLU:OE2	3:D:502:WRI:N02	2.52	0.43
1:A:99:CYS:HB3	1:B:466:ASN:HB3	2.01	0.43
1:B:139:LYS:O	1:B:140:ARG:HD2	2.19	0.43
1:C:255:ARG:HG3	1:C:261:VAL:HG22	2.00	0.42
1:B:279:TRP:CG	1:B:290:PRO:HG3	2.54	0.42
4:C:504:BTB:H72	4:C:504:BTB:H41	1.57	0.42
1:C:463:GLU:HB3	1:D:103:LEU:HD12	2.02	0.42
1:A:211:ILE:HG21	1:A:291:LEU:HD21	2.01	0.42
1:A:139:LYS:HB2	1:A:139:LYS:HE3	1.82	0.42
4:A:504:BTB:H72	4:A:504:BTB:H41	1.61	0.42
1:B:280:THR:HA	1:B:281:PRO:HD3	1.89	0.42
1:C:244:TRP:CD1	1:C:479:PRO:HG2	2.54	0.42
1:A:234:ARG:HA	1:A:238:ARG:HH12	1.85	0.42
1:C:235:CYS:SG	1:C:238:ARG:NH1	2.92	0.42
1:A:242:ARG:HB2	1:A:294:GLN:NE2	2.34	0.41
1:B:122:GLN:CD	1:B:122:GLN:H	2.23	0.41
1:C:367:LEU:O	1:C:375:ILE:HG12	2.20	0.41
1:D:364:THR:O	1:D:368:CYS:HB2	2.20	0.41
1:B:68:PHE:CD1	1:B:83:THR:HG22	2.55	0.41
1:D:357:TYR:CD2	1:D:362:ILE:HD11	2.55	0.41
1:A:229:THR:O	1:A:351:ALA:HA	2.21	0.41
1:C:69:PRO:HG2	1:C:82:ASP:HB3	2.02	0.41
1:D:149:ARG:HD3	1:D:166:ARG:CZ	2.49	0.41
1:A:94:CYS:HB3	1:B:94:CYS:HB3	2.03	0.41
1:A:229:THR:O	1:A:352:PRO:HD2	2.20	0.41
1:D:229:THR:O	1:D:351:ALA:HA	2.20	0.41
1:B:365:ARG:O	1:B:369:ASP:HB2	2.20	0.41
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.86	0.41
1:C:89:GLN:H	1:C:89:GLN:HG2	1.60	0.41
4:D:503:BTB:H12	4:D:503:BTB:H72	1.74	0.41
1:B:214:HIS:CD2	1:B:214:HIS:C	2.94	0.41
1:C:170:LEU:HD11	1:C:230:VAL:HG11	2.03	0.41
1:D:119:ALA:N	1:D:120:PRO:HD3	2.36	0.41
4:B:505:BTB:H42	4:B:505:BTB:H72	1.82	0.40
1:C:148:GLN:HE21	1:C:148:GLN:C	2.25	0.40
1:D:275:ILE:HD12	1:D:281:PRO:HG3	2.03	0.40
1:C:165:LEU:HG	1:C:346:LEU:HD12	2.04	0.40
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.56	0.40
1:B:387:THR:HA	1:B:394:TRP:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.57	0.40
1:C:72:LYS:HE2	1:C:74:TRP:CE3	2.57	0.40
1:C:365:ARG:NH2	6:C:507:CL:CL	2.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/440 (91%)	381 (96%)	16 (4%)	2 (0%)	29	18
1	B	400/440 (91%)	388 (97%)	11 (3%)	1 (0%)	41	31
1	C	400/440 (91%)	392 (98%)	8 (2%)	0	100	100
1	D	399/440 (91%)	389 (98%)	10 (2%)	0	100	100
All	All	1598/1760 (91%)	1550 (97%)	45 (3%)	3 (0%)	47	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO
1	A	239	GLY
1	B	259	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	343/373 (92%)	328 (96%)	15 (4%)	28 21
1	B	343/373 (92%)	326 (95%)	17 (5%)	24 16
1	C	343/373 (92%)	323 (94%)	20 (6%)	20 11
1	D	342/373 (92%)	330 (96%)	12 (4%)	36 29
All	All	1371/1492 (92%)	1307 (95%)	64 (5%)	27 18

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	125	SER
1	A	128	ARG
1	A	201	CYS
1	A	209	THR
1	A	216	LYS
1	A	256	GLN
1	A	258	ASP
1	A	272	GLU
1	A	277	HIS
1	A	298	GLU
1	A	304	LEU
1	A	369	ASP
1	A	396	ASP
1	A	436	LYS
1	B	78	SER
1	B	97	ARG
1	B	122	GLN
1	B	128	ARG
1	B	139	LYS
1	B	144	GLN
1	B	147	GLU
1	B	167	GLU
1	B	168[A]	SER
1	B	168[B]	SER
1	B	202	ARG
1	B	255	ARG
1	B	326	LEU
1	B	329	ARG
1	B	389	THR
1	B	396	ASP
1	B	429	LYS
1	C	67	LYS

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Mol	Chain	Res	Type
1	C	71	VAL
1	C	89	GLN
1	C	98	ARG
1	C	125	SER
1	C	129	ASP
1	C	148	GLN
1	C	149	ARG
1	C	152	GLU
1	C	154	GLU
1	C	200	ASP
1	C	202	ARG
1	C	235	CYS
1	C	238	ARG
1	C	250	ARG
1	C	256	GLN
1	C	308	GLU
1	C	329	ARG
1	C	396	ASP
1	C	417	ILE
1	D	71	VAL
1	D	97	ARG
1	D	124	LEU
1	D	192	LYS
1	D	216	LYS
1	D	245	ASN
1	D	257	GLN
1	D	258	ASP
1	D	262	ARG
1	D	326	LEU
1	D	359	SER
1	D	396	ASP

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 14 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	501	1	41,50,50	1.46	5 (12%)	45,82,82	1.80	13 (28%)
4	BTB	C	505	-	13,13,13	0.37	0	7,16,16	0.67	0
4	BTB	A	505	-	13,13,13	0.37	0	7,16,16	0.45	0
2	HEM	B	501	1	41,50,50	1.55	5 (12%)	45,82,82	1.86	13 (28%)
4	BTB	D	504	-	13,13,13	0.52	0	7,16,16	0.92	0
4	BTB	D	503	9	13,13,13	0.42	0	7,16,16	0.95	0
3	WRI	B	502	-	26,27,27	1.04	3 (11%)	34,39,39	2.34	14 (41%)
4	BTB	B	504	9	13,13,13	0.55	0	7,16,16	0.60	0
4	BTB	B	505	-	13,13,13	0.52	0	7,16,16	0.94	0
4	BTB	C	504	-	13,13,13	0.68	0	7,16,16	1.53	2 (28%)
2	HEM	D	501	1	41,50,50	1.57	7 (17%)	45,82,82	1.73	14 (31%)
3	WRI	C	510	-	26,27,27	0.93	1 (3%)	34,39,39	1.58	10 (29%)
5	GOL	C	506	-	5,5,5	0.42	0	5,5,5	0.39	0
3	WRI	C	502	-	26,27,27	0.90	2 (7%)	34,39,39	1.61	8 (23%)
3	WRI	A	503	-	26,27,27	0.91	0	34,39,39	1.38	5 (14%)
3	WRI	B	503	-	26,27,27	0.89	1 (3%)	34,39,39	1.30	4 (11%)
5	GOL	A	506	-	5,5,5	0.33	0	5,5,5	0.38	0
2	HEM	C	501	1	41,50,50	1.49	6 (14%)	45,82,82	1.86	13 (28%)
3	WRI	C	503	-	26,27,27	0.95	2 (7%)	34,39,39	1.26	5 (14%)
3	WRI	D	502	-	26,27,27	0.80	0	34,39,39	1.58	7 (20%)
4	BTB	A	504	-	13,13,13	0.52	0	7,16,16	0.76	0
3	WRI	A	502	-	26,27,27	0.87	1 (3%)	34,39,39	1.87	9 (26%)
5	GOL	D	505	-	5,5,5	0.36	0	5,5,5	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	501	1	-	1/12/54/54	-
4	BTB	C	505	-	-	11/21/21/21	-
4	BTB	A	505	-	-	3/21/21/21	-
2	HEM	B	501	1	-	2/12/54/54	-
4	BTB	D	504	-	-	13/21/21/21	-
4	BTB	D	503	9	-	2/21/21/21	-
3	WRI	B	502	-	-	0/4/15/15	0/4/4/4
4	BTB	B	504	9	-	4/21/21/21	-
4	BTB	B	505	-	-	3/21/21/21	-
4	BTB	C	504	-	-	10/21/21/21	-
2	HEM	D	501	1	-	2/12/54/54	-
3	WRI	C	510	-	-	4/4/15/15	0/4/4/4
5	GOL	C	506	-	-	4/4/4/4	-
3	WRI	C	502	-	-	0/4/15/15	0/4/4/4
3	WRI	A	503	-	-	4/4/15/15	1/4/4/4
3	WRI	B	503	-	-	4/4/15/15	0/4/4/4
5	GOL	A	506	-	-	4/4/4/4	-
2	HEM	C	501	1	-	3/12/54/54	-
3	WRI	C	503	-	-	4/4/15/15	0/4/4/4
3	WRI	D	502	-	-	0/4/15/15	0/4/4/4
4	BTB	A	504	-	-	4/21/21/21	-
3	WRI	A	502	-	-	0/4/15/15	0/4/4/4
5	GOL	D	505	-	-	2/4/4/4	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3C-C2C	-4.05	1.34	1.40
2	B	501	HEM	C3C-CAC	3.69	1.55	1.47
2	A	501	HEM	C3C-CAC	3.67	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.62	1.35	1.40
2	D	501	HEM	C3C-CAC	3.56	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.47	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.38	1.35	1.40
2	C	501	HEM	C3C-CAC	3.33	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-NB	3.32	2.13	1.96
2	B	501	HEM	FE-NB	3.22	2.12	1.96
2	B	501	HEM	CAB-C3B	3.04	1.55	1.47
2	A	501	HEM	CAB-C3B	3.04	1.55	1.47
2	C	501	HEM	CAB-C3B	2.98	1.55	1.47
2	D	501	HEM	CAB-C3B	2.92	1.55	1.47
3	C	510	WRI	C02-N01	2.62	1.36	1.33
3	B	502	WRI	C05-C10	-2.52	1.38	1.42
3	B	502	WRI	C02-N01	2.45	1.36	1.33
3	C	502	WRI	C02-N01	2.40	1.36	1.33
2	A	501	HEM	FE-NB	2.35	2.08	1.96
2	C	501	HEM	FE-ND	2.32	2.08	1.96
3	B	503	WRI	C02-N01	2.08	1.36	1.33
3	C	503	WRI	C03-C04	2.08	1.40	1.37
2	D	501	HEM	CMA-C3A	2.05	1.55	1.51
3	B	502	WRI	C04-C05	-2.05	1.38	1.42
2	B	501	HEM	C3B-C2B	-2.05	1.33	1.37
2	D	501	HEM	CAA-C2A	2.04	1.55	1.52
3	C	503	WRI	C06-C07	2.04	1.40	1.36
3	A	502	WRI	C05-C10	-2.04	1.39	1.42
2	A	501	HEM	CAA-C2A	2.03	1.55	1.52
2	C	501	HEM	CMB-C2B	2.03	1.55	1.50
2	D	501	HEM	CMB-C2B	2.03	1.55	1.50
2	C	501	HEM	FE-NB	2.01	2.06	1.96
3	C	502	WRI	C05-C10	-2.00	1.39	1.42

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	WRI	C22-C21-C08	-4.98	112.73	121.36
3	B	502	WRI	N02-C02-N01	4.85	122.27	118.26
3	A	502	WRI	C04-C05-C10	4.77	120.59	118.01
2	C	501	HEM	C4B-CHC-C1C	4.51	128.51	122.56
3	B	502	WRI	C29-C28-C27	-4.46	107.06	114.23
3	B	502	WRI	C26-C21-C08	4.32	128.01	120.86
2	C	501	HEM	C3D-C4D-ND	-4.19	105.50	110.17
3	A	502	WRI	C05-C10-N01	-4.16	118.40	122.81
2	A	501	HEM	C4B-CHC-C1C	3.92	127.73	122.56
2	C	501	HEM	C4D-ND-C1D	3.91	109.11	105.07
2	B	501	HEM	C1B-NB-C4B	3.84	109.04	105.07
2	B	501	HEM	C4D-ND-C1D	3.78	108.98	105.07
2	A	501	HEM	C1B-NB-C4B	3.78	108.98	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	WRI	C04-C05-C10	3.70	120.01	118.01
2	D	501	HEM	C4D-ND-C1D	3.66	108.85	105.07
2	A	501	HEM	C3B-C2B-C1B	3.57	109.13	106.49
3	D	502	WRI	C05-C10-N01	-3.56	119.03	122.81
3	C	510	WRI	C22-C21-C08	-3.56	115.19	121.36
2	B	501	HEM	C3B-C2B-C1B	3.50	109.08	106.49
2	C	501	HEM	C1B-NB-C4B	3.50	108.68	105.07
2	D	501	HEM	C3D-C4D-ND	-3.48	106.29	110.17
3	D	502	WRI	C04-C05-C10	3.48	119.89	118.01
2	B	501	HEM	CMA-C3A-C4A	-3.42	123.21	128.46
3	A	502	WRI	C07-C08-C21	-3.39	115.48	121.36
2	C	501	HEM	CAD-CBD-CGD	-3.38	106.34	113.60
3	C	503	WRI	C22-C21-C08	-3.34	115.57	121.36
3	B	502	WRI	C05-C10-N01	-3.34	119.27	122.81
3	C	502	WRI	C28-C27-C24	-3.33	107.54	113.91
3	C	502	WRI	C05-C10-N01	-3.28	119.33	122.81
2	B	501	HEM	C4C-CHD-C1D	3.24	126.83	122.56
2	D	501	HEM	CAD-CBD-CGD	-3.22	106.67	113.60
2	A	501	HEM	C4D-ND-C1D	3.21	108.39	105.07
3	C	502	WRI	C04-C05-C10	3.20	119.74	118.01
3	B	502	WRI	C07-C08-C21	-3.20	115.82	121.36
3	D	502	WRI	C29-C30-C31	-3.15	108.15	114.21
3	A	503	WRI	C22-C21-C08	-3.15	115.89	121.36
2	D	501	HEM	C3B-C2B-C1B	3.09	108.78	106.49
3	C	510	WRI	N02-C02-N01	3.08	120.81	118.26
2	C	501	HEM	CHC-C4B-NB	3.03	127.73	124.43
2	C	501	HEM	CAD-C3D-C2D	-3.02	122.25	127.88
3	C	503	WRI	C26-C21-C08	3.00	125.82	120.86
2	D	501	HEM	CMA-C3A-C4A	-2.98	123.88	128.46
3	C	502	WRI	N02-C02-N01	2.87	120.64	118.26
3	A	502	WRI	N02-C02-N01	2.86	120.62	118.26
2	A	501	HEM	CAD-CBD-CGD	-2.85	107.46	113.60
2	D	501	HEM	C4C-CHD-C1D	2.84	126.30	122.56
2	A	501	HEM	C3D-C4D-ND	-2.83	107.01	110.17
2	B	501	HEM	C3D-C4D-ND	-2.81	107.03	110.17
3	B	502	WRI	C03-C04-C05	2.81	120.55	117.78
3	C	502	WRI	C29-C28-C27	-2.81	109.72	114.23
3	C	510	WRI	C24-C25-C31	-2.81	120.81	124.73
3	A	503	WRI	C29-C28-C27	-2.80	109.72	114.23
4	C	504	BTB	O3-C3-C2	-2.77	103.87	111.44
3	B	503	WRI	C29-C28-C27	-2.72	109.86	114.23
3	B	503	WRI	C04-C05-C10	2.71	119.48	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	WRI	C24-C25-C31	-2.69	120.98	124.73
3	A	502	WRI	C24-C25-C31	-2.67	121.00	124.73
2	B	501	HEM	CAD-CBD-CGD	-2.67	107.86	113.60
3	A	502	WRI	C08-C09-C10	-2.61	119.15	121.44
3	C	510	WRI	C26-C21-C08	2.60	125.17	120.86
2	B	501	HEM	CHD-C1D-ND	2.59	127.24	124.43
2	B	501	HEM	C2D-C1D-ND	-2.58	106.80	109.88
2	D	501	HEM	C1B-NB-C4B	2.57	107.72	105.07
3	B	502	WRI	C06-C05-C10	2.56	121.19	118.33
3	B	502	WRI	C06-C05-C04	-2.55	118.79	123.66
3	D	502	WRI	C22-C21-C08	-2.50	117.02	121.36
3	C	510	WRI	C05-C10-N01	-2.49	120.17	122.81
2	A	501	HEM	CHD-C1D-ND	2.48	127.13	124.43
2	A	501	HEM	CHB-C1B-NB	2.45	127.41	124.38
3	C	503	WRI	C29-C28-C27	-2.43	110.32	114.23
3	B	503	WRI	C05-C10-N01	-2.43	120.23	122.81
3	B	502	WRI	C21-C26-C25	-2.41	119.61	122.09
3	C	510	WRI	C29-C28-C27	-2.41	110.36	114.23
2	C	501	HEM	CMC-C2C-C3C	2.40	129.16	124.68
2	B	501	HEM	C4B-CHC-C1C	2.39	125.71	122.56
2	B	501	HEM	C2B-C1B-NB	-2.38	107.01	109.84
3	D	502	WRI	C29-C28-C27	-2.37	110.43	114.23
2	C	501	HEM	CHD-C1D-ND	2.36	127.00	124.43
2	A	501	HEM	C2B-C1B-NB	-2.34	107.06	109.84
2	D	501	HEM	CHB-C1B-NB	2.33	127.26	124.38
2	B	501	HEM	CMA-C3A-C2A	2.30	129.27	124.94
3	A	502	WRI	C06-C05-C04	-2.28	119.30	123.66
2	D	501	HEM	CMC-C2C-C3C	2.27	128.92	124.68
3	C	502	WRI	C22-C21-C08	-2.27	117.43	121.36
2	D	501	HEM	C4B-CHC-C1C	2.26	125.55	122.56
2	D	501	HEM	CHD-C1D-ND	2.26	126.89	124.43
4	C	504	BTB	O4-C4-C2	-2.24	105.31	111.44
3	C	510	WRI	C03-C04-C05	2.24	119.98	117.78
3	C	510	WRI	C28-C27-C24	-2.23	109.64	113.91
2	B	501	HEM	CHC-C4B-C3B	2.23	127.98	124.57
3	A	503	WRI	C09-C08-C21	-2.19	116.05	121.05
2	A	501	HEM	C4A-C3A-C2A	2.15	108.50	107.00
3	A	502	WRI	C22-C21-C08	-2.14	117.65	121.36
2	C	501	HEM	CHA-C4D-ND	2.12	127.01	124.38
2	A	501	HEM	CAA-CBA-CGA	-2.12	107.83	113.76
2	C	501	HEM	C4A-C3A-C2A	2.11	108.47	107.00
3	C	502	WRI	C03-C04-C05	2.10	119.85	117.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	WRI	C26-C21-C08	2.10	124.33	120.86
2	D	501	HEM	CHA-C4D-ND	2.08	126.95	124.38
3	B	503	WRI	C22-C21-C08	-2.07	117.77	121.36
3	C	510	WRI	C21-C26-C25	-2.07	119.95	122.09
2	D	501	HEM	CBD-CAD-C3D	-2.07	106.88	112.63
3	C	503	WRI	C04-C05-C10	2.07	119.13	118.01
2	A	501	HEM	CHC-C4B-C3B	2.06	127.73	124.57
3	D	502	WRI	C03-C04-C05	2.06	119.81	117.78
2	C	501	HEM	C4D-C3D-C2D	2.06	109.90	106.90
2	A	501	HEM	CMA-C3A-C4A	-2.05	125.31	128.46
3	B	502	WRI	C28-C27-C24	-2.04	110.00	113.91
3	D	502	WRI	C07-C08-C21	-2.04	117.81	121.36
3	A	502	WRI	C03-C04-C05	2.04	119.79	117.78
3	C	510	WRI	C04-C05-C10	2.04	119.11	118.01
3	B	502	WRI	C09-C10-N01	2.03	121.81	118.72
2	C	501	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
2	D	501	HEM	CAD-C3D-C2D	-2.02	124.11	127.88
3	A	503	WRI	C21-C26-C25	-2.02	120.01	122.09
3	C	502	WRI	C28-C29-C30	-2.01	109.58	115.84
3	C	503	WRI	C05-C10-N01	-2.00	120.69	122.81

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	BTB	O1-C1-C2-C3
4	A	504	BTB	O1-C1-C2-C4
4	A	504	BTB	O1-C1-C2-N
4	A	505	BTB	C1-C2-C4-O4
4	A	505	BTB	C3-C2-C4-O4
4	A	505	BTB	N-C2-C4-O4
4	B	504	BTB	O1-C1-C2-C3
4	B	504	BTB	O1-C1-C2-C4
4	B	504	BTB	O1-C1-C2-N
4	B	505	BTB	C1-C2-C4-O4
4	B	505	BTB	C3-C2-C4-O4
4	C	504	BTB	C1-C2-C3-O3
4	C	504	BTB	C4-C2-C3-O3
4	C	504	BTB	N-C2-C3-O3
4	C	504	BTB	C1-C2-N-C5
4	C	504	BTB	C1-C2-N-C7
4	C	504	BTB	C3-C2-N-C5

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Mol	Chain	Res	Type	Atoms
4	C	504	BTB	C3-C2-N-C7
4	C	504	BTB	C4-C2-N-C5
4	C	504	BTB	C4-C2-N-C7
4	C	505	BTB	O1-C1-C2-C3
4	C	505	BTB	O1-C1-C2-C4
4	C	505	BTB	O1-C1-C2-N
4	C	505	BTB	C1-C2-C4-O4
4	C	505	BTB	C3-C2-C4-O4
4	C	505	BTB	N-C2-C4-O4
4	D	504	BTB	O1-C1-C2-C3
4	D	504	BTB	C1-C2-C3-O3
4	D	504	BTB	C4-C2-C3-O3
4	D	504	BTB	N-C2-C3-O3
4	D	504	BTB	C1-C2-N-C5
4	D	504	BTB	C1-C2-N-C7
4	D	504	BTB	C3-C2-N-C5
4	D	504	BTB	C3-C2-N-C7
4	D	504	BTB	C4-C2-N-C5
4	D	504	BTB	C4-C2-N-C7
4	D	504	BTB	C8-C7-N-C5
5	A	506	GOL	O1-C1-C2-C3
5	A	506	GOL	C1-C2-C3-O3
5	C	506	GOL	C1-C2-C3-O3
5	D	505	GOL	O1-C1-C2-C3
3	B	503	WRI	C07-C08-C21-C26
3	B	503	WRI	C09-C08-C21-C22
3	C	510	WRI	C07-C08-C21-C22
3	C	510	WRI	C09-C08-C21-C22
3	C	510	WRI	C09-C08-C21-C26
3	B	503	WRI	C07-C08-C21-C22
3	B	503	WRI	C09-C08-C21-C26
3	C	510	WRI	C07-C08-C21-C26
3	A	503	WRI	C07-C08-C21-C26
3	A	503	WRI	C07-C08-C21-C22
3	A	503	WRI	C09-C08-C21-C26
3	A	503	WRI	C09-C08-C21-C22
5	C	506	GOL	O1-C1-C2-C3
5	A	506	GOL	O1-C1-C2-O2
5	A	506	GOL	O2-C2-C3-O3
5	C	506	GOL	O2-C2-C3-O3
2	B	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
3	C	503	WRI	C07-C08-C21-C26
3	C	503	WRI	C07-C08-C21-C22
5	C	506	GOL	O1-C1-C2-O2
5	D	505	GOL	O1-C1-C2-O2
4	A	504	BTB	N-C7-C8-O8
3	C	503	WRI	C09-C08-C21-C22
3	C	503	WRI	C09-C08-C21-C26
4	D	503	BTB	N-C7-C8-O8
2	A	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
4	D	504	BTB	C3-C2-C4-O4
4	B	505	BTB	N-C2-C4-O4
4	C	504	BTB	N-C2-C4-O4
4	C	505	BTB	C1-C2-N-C5
4	C	505	BTB	C3-C2-N-C7
4	C	505	BTB	C4-C2-N-C5
4	C	505	BTB	C4-C2-N-C7
2	C	501	HEM	C2B-C3B-CAB-CBB
4	C	505	BTB	N-C7-C8-O8
2	C	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C2A-CAA-CBA-CGA
4	B	504	BTB	C4-C2-C3-O3
4	D	503	BTB	C4-C2-C3-O3
4	D	504	BTB	C1-C2-C4-O4
2	D	501	HEM	C2A-CAA-CBA-CGA

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	WRI	C24-C25-C27-C28-C29-C30-C31

15 monomers are involved in 40 short contacts:

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

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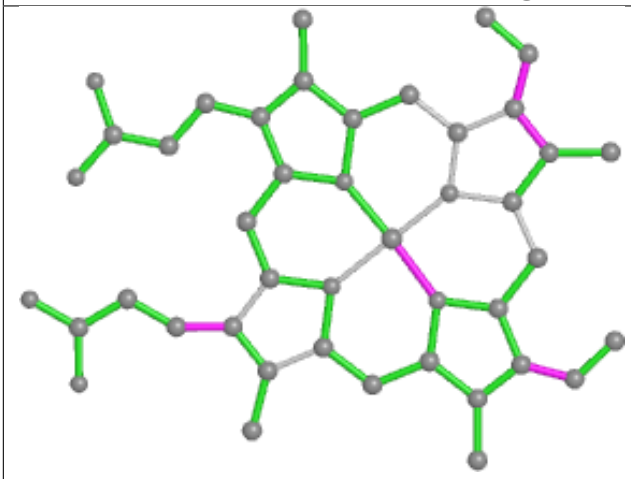
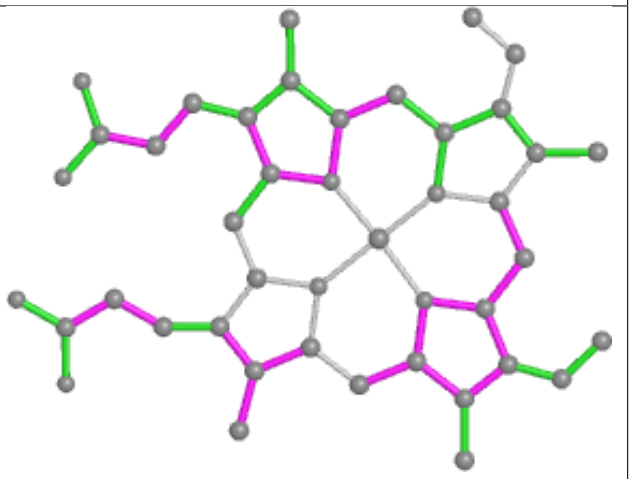
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	BTB	4	0
2	D	501	HEM	2	0
3	C	502	WRI	1	0
2	C	501	HEM	3	0
3	D	502	WRI	2	0
4	A	504	BTB	4	0
3	A	502	WRI	3	0

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

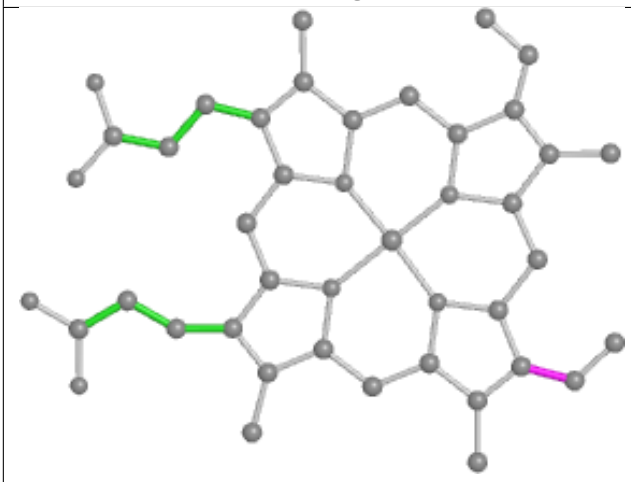
Ligand HEM A 501



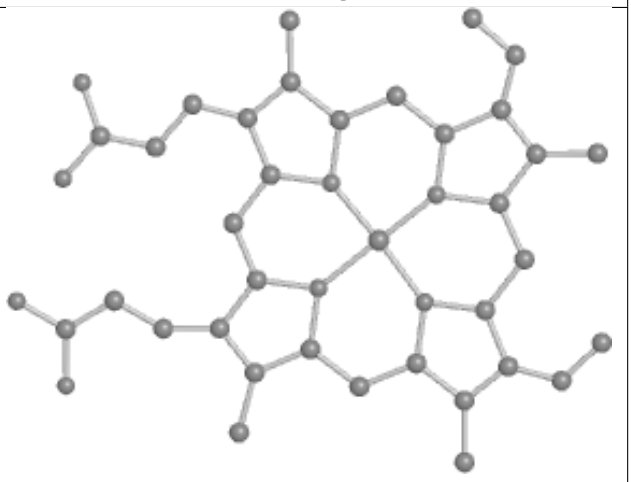
Bond lengths



Bond angles

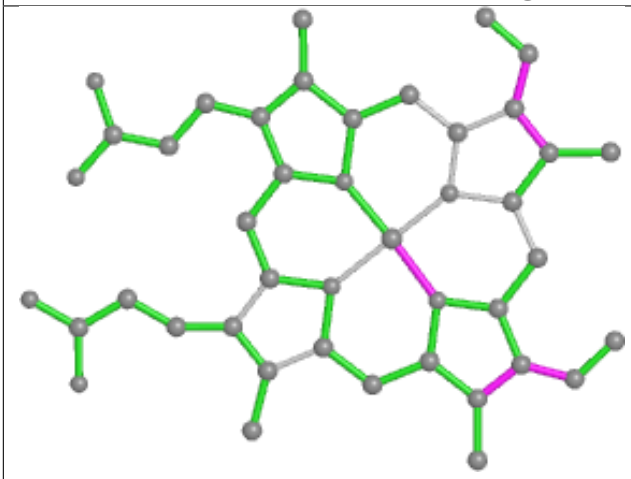


Torsions

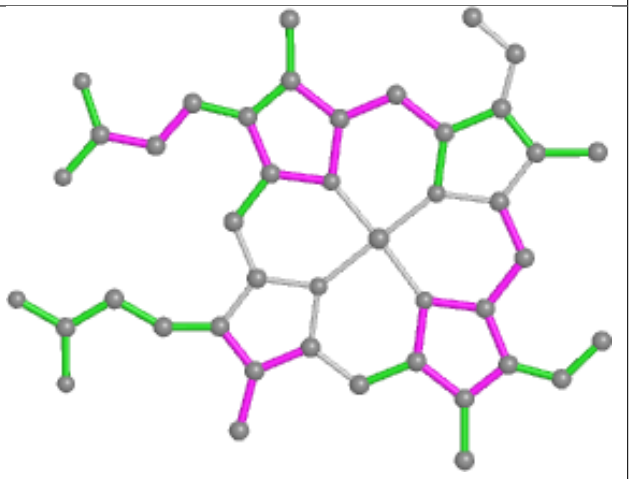


Rings

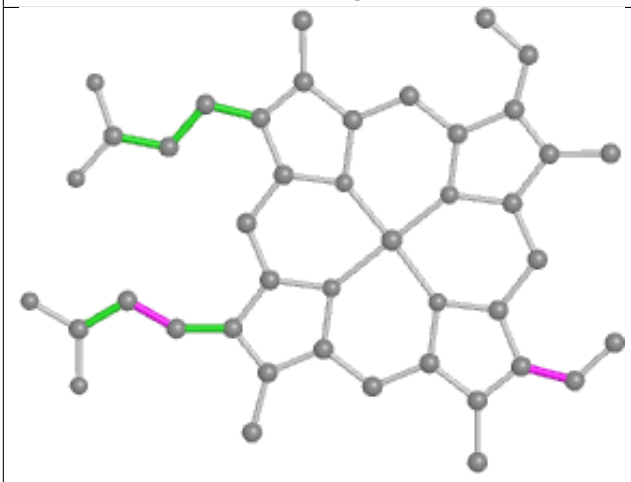
Ligand HEM B 501



Bond lengths



Bond angles



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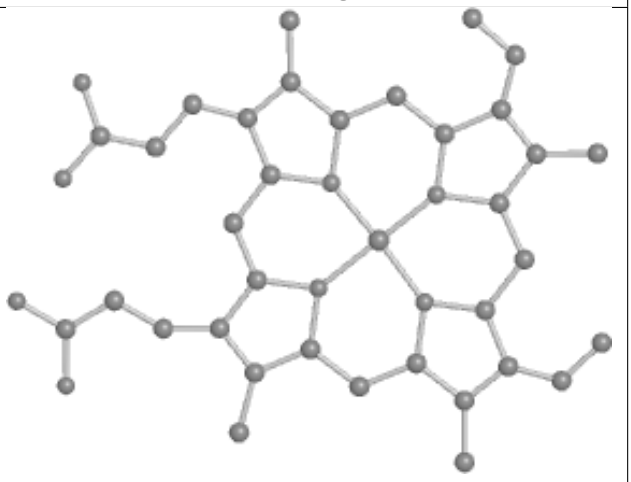
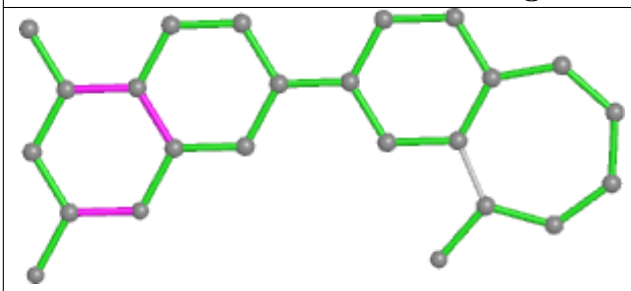
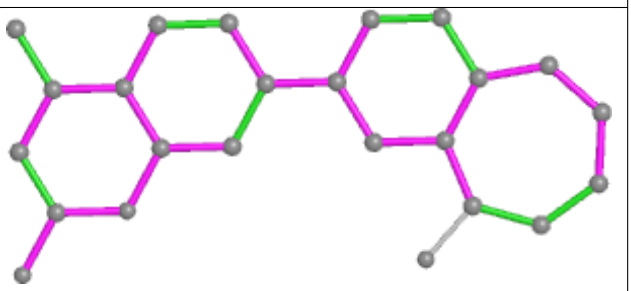


Rings

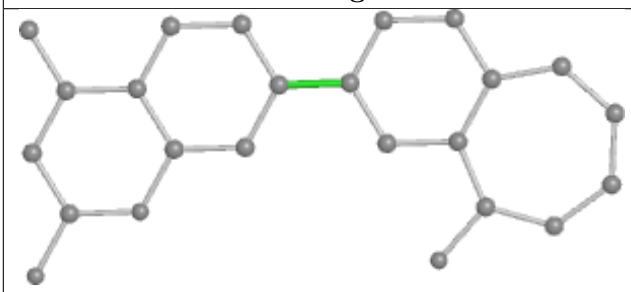
Ligand WRI B 502



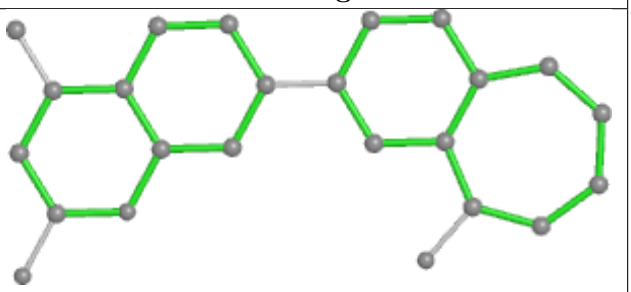
Bond lengths



Bond angles

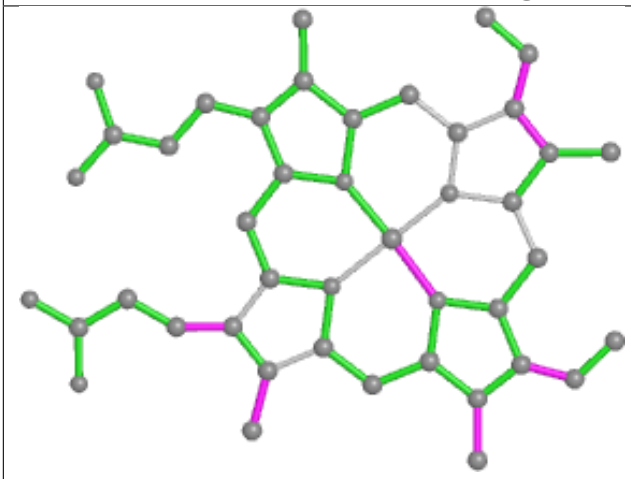


Torsions

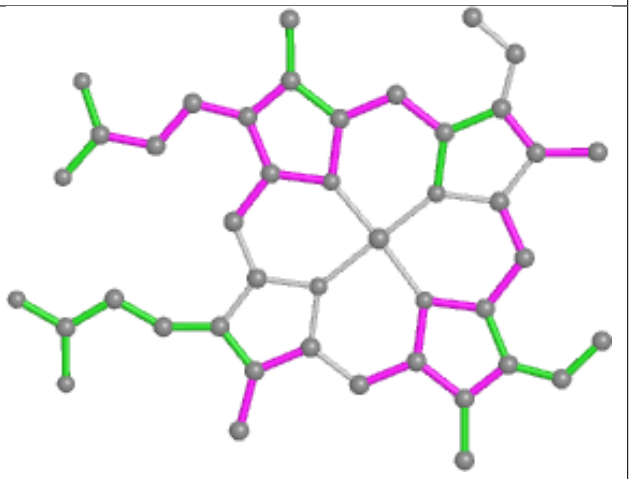


Rings

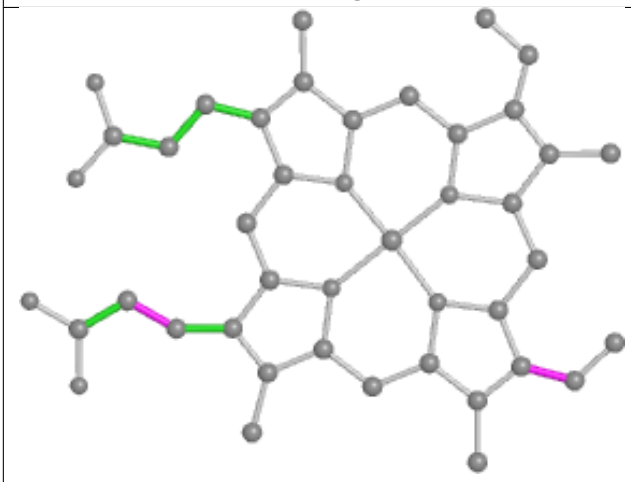
Ligand HEM D 501



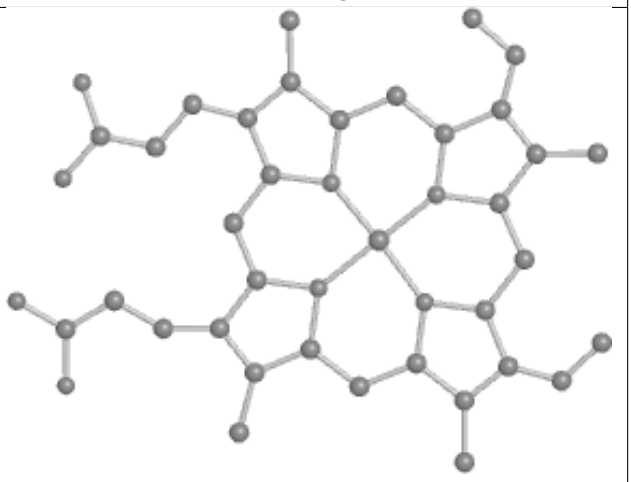
Bond lengths



Bond angles

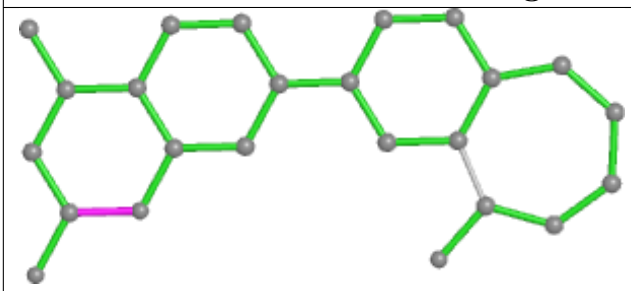


Torsions

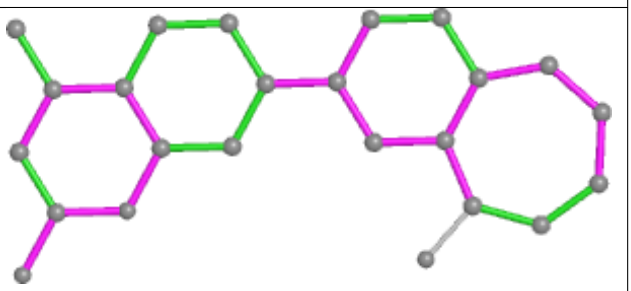


Rings

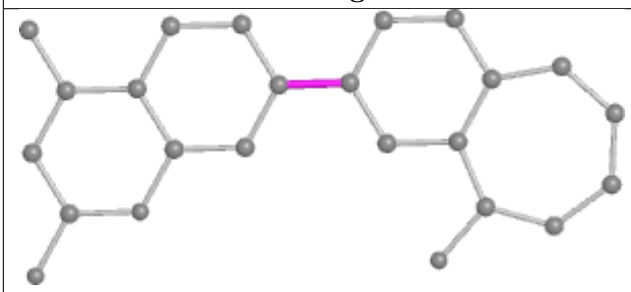
Ligand WRI C 510



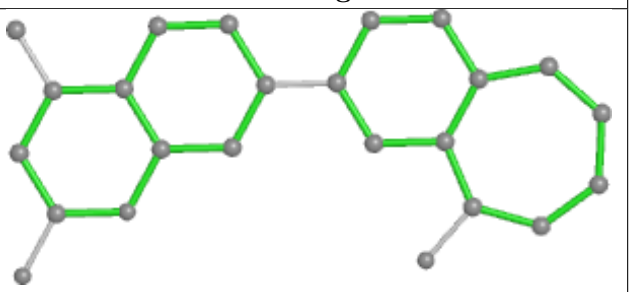
Bond lengths



Bond angles

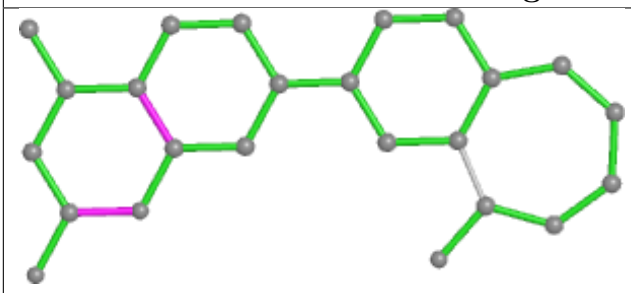


Torsions

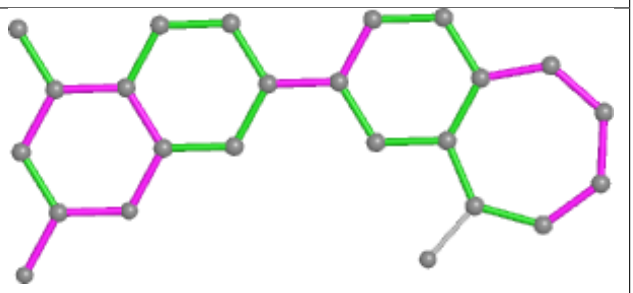


Rings

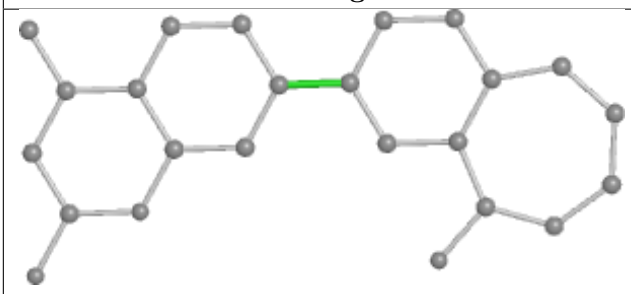
Ligand WRI C 502



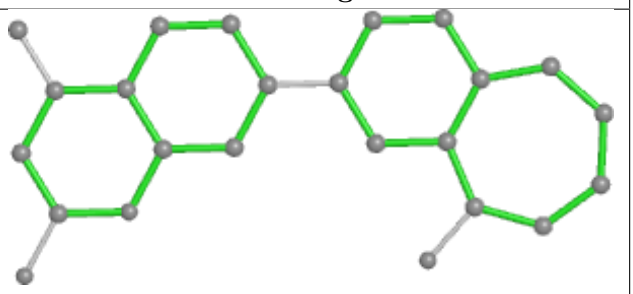
Bond lengths



Bond angles

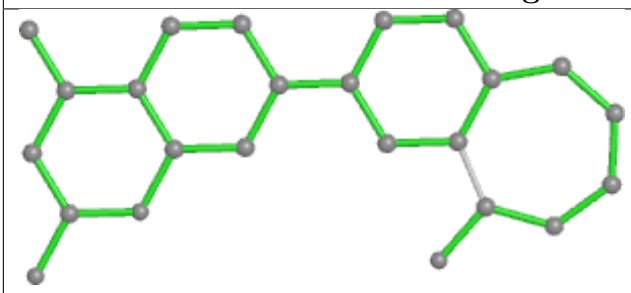


Torsions

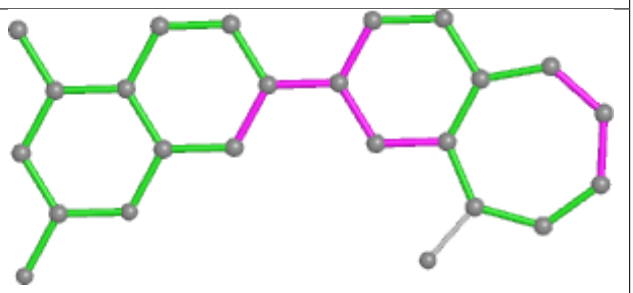


Rings

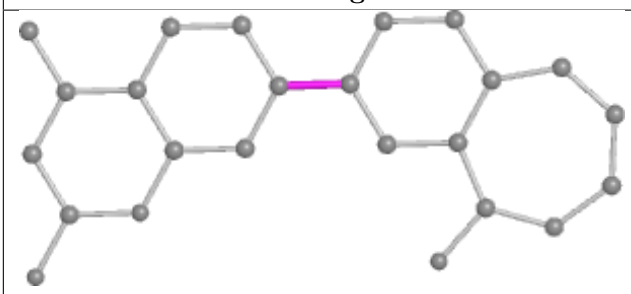
Ligand WRI A 503



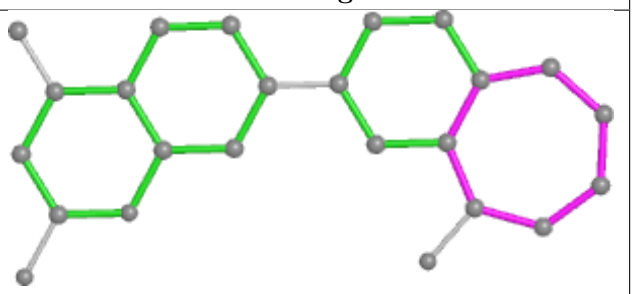
Bond lengths



Bond angles

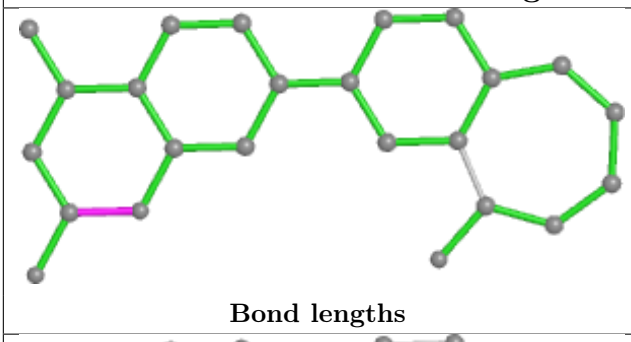


Torsions

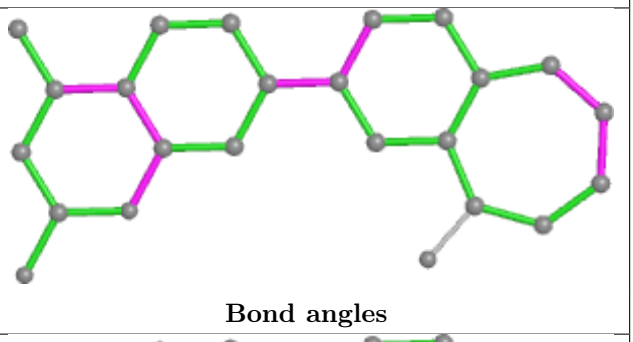


Rings

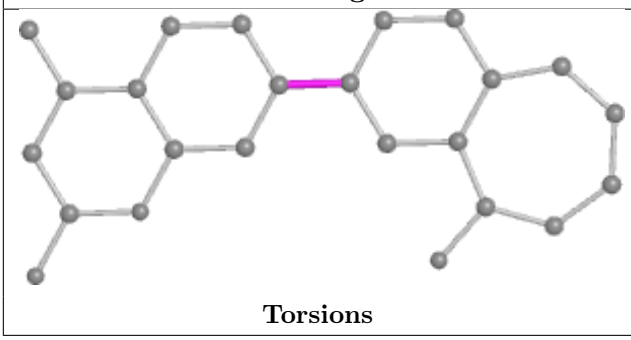
Ligand WRI B 503



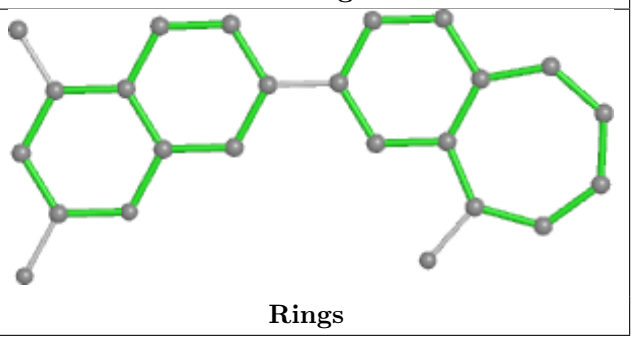
Bond lengths



Bond angles

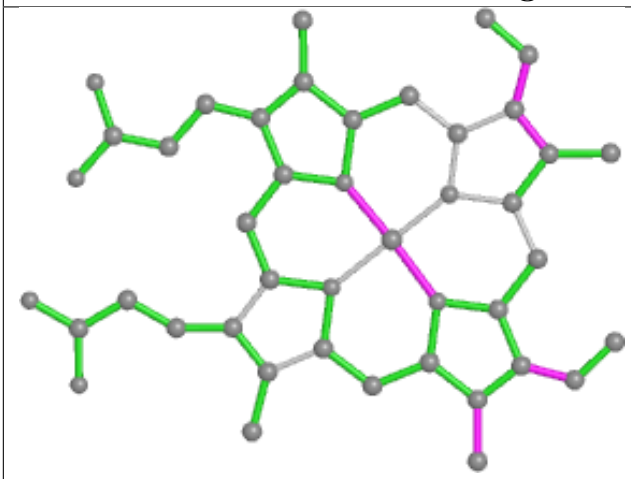


Torsions

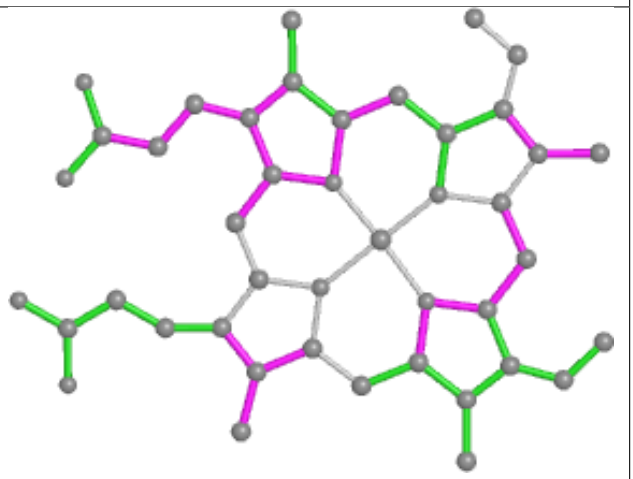


Rings

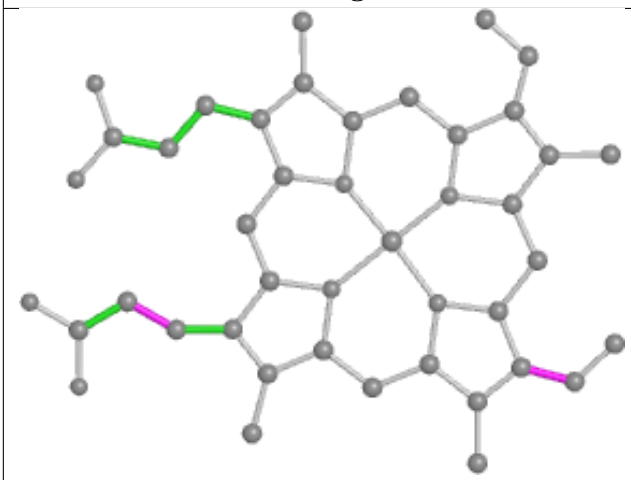
Ligand HEM C 501



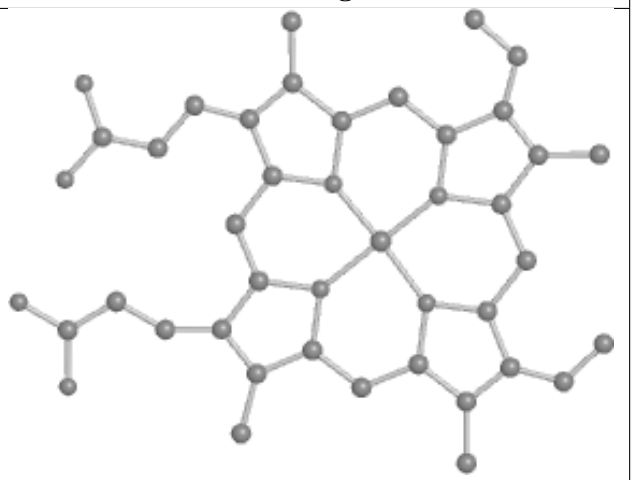
Bond lengths



Bond angles

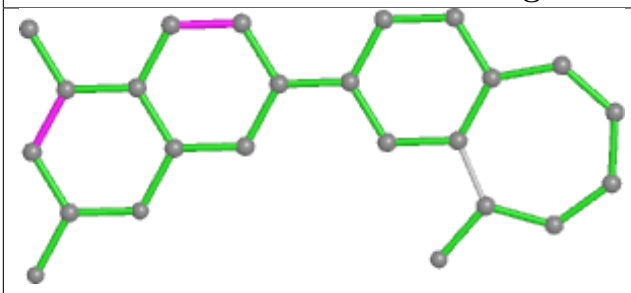


Torsions

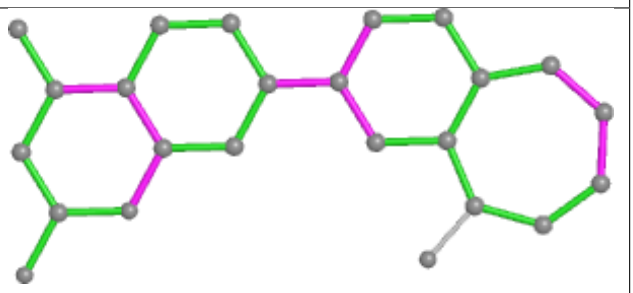


Rings

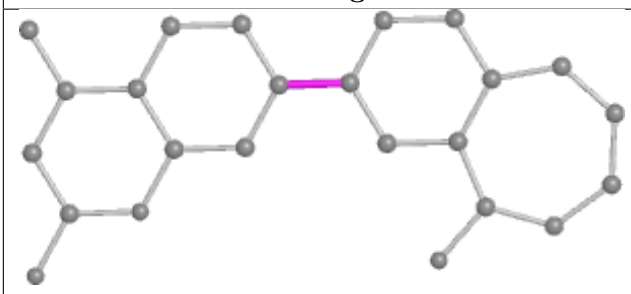
Ligand WRI C 503



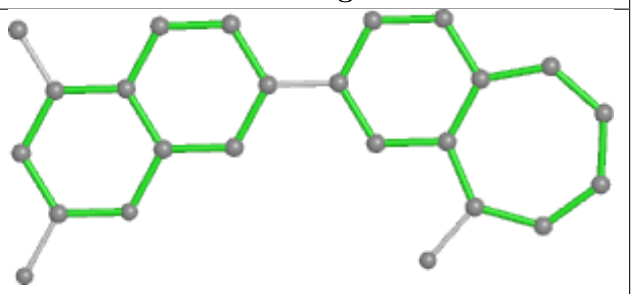
Bond lengths



Bond angles

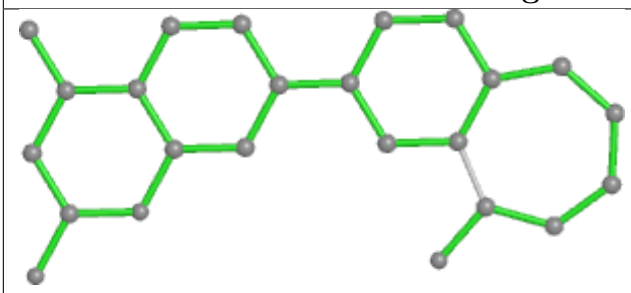


Torsions

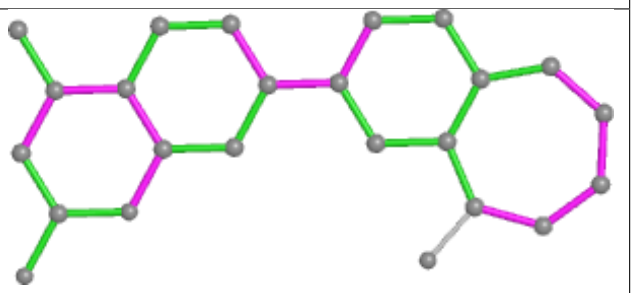


Rings

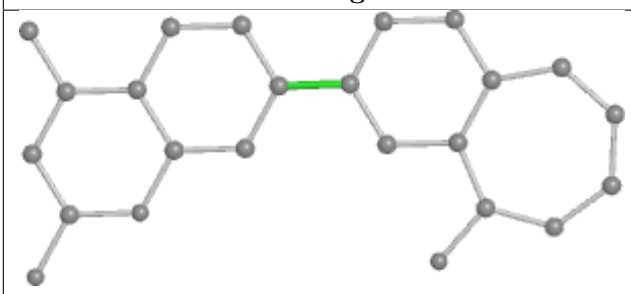
Ligand WRI D 502



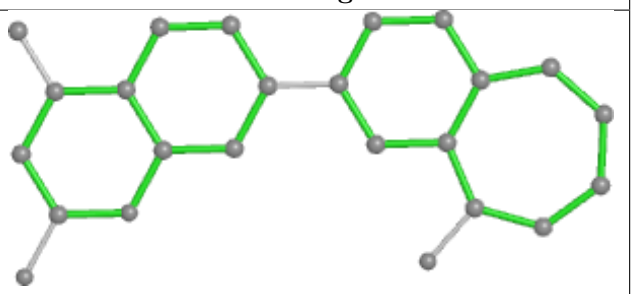
Bond lengths



Bond angles

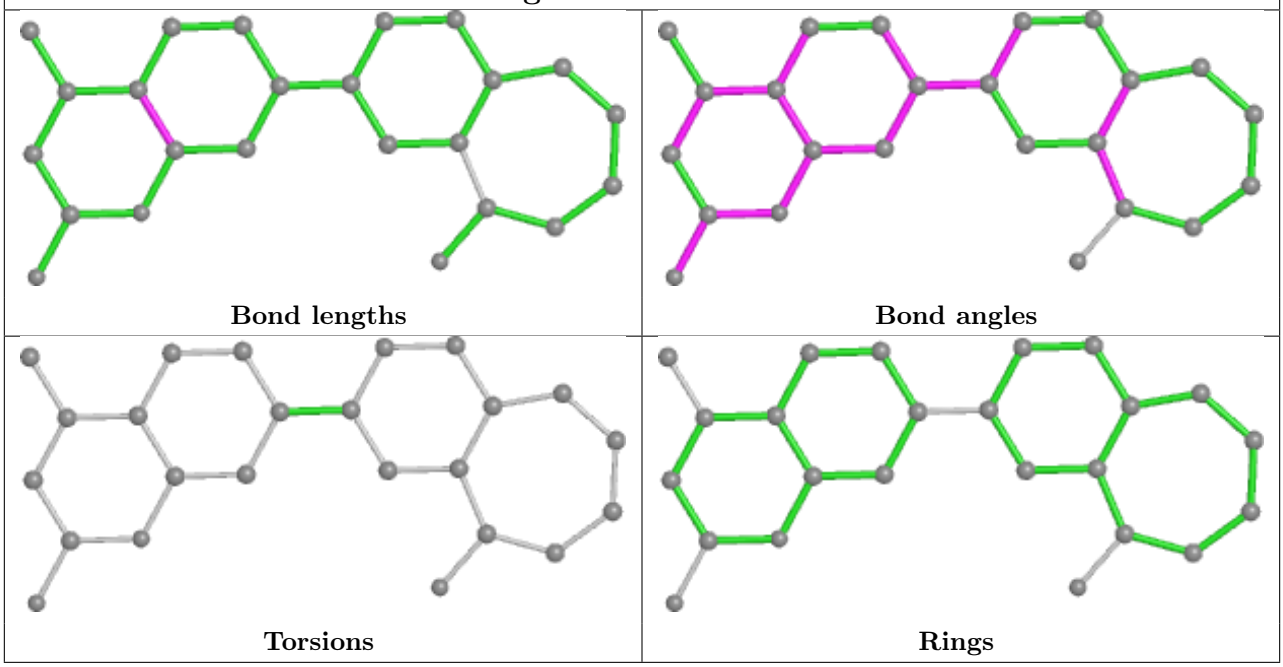


Torsions



Rings

Ligand WRI A 502



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%)	1.00	75 (18%) 1 1	38, 71, 120, 154	0
1	B	401/440 (91%)	0.36	29 (7%) 15 17	31, 50, 90, 135	0
1	C	402/440 (91%)	0.70	48 (11%) 4 4	37, 61, 101, 130	0
1	D	401/440 (91%)	0.36	26 (6%) 18 20	29, 50, 84, 141	0
All	All	1605/1760 (91%)	0.60	178 (11%) 5 5	29, 57, 106, 154	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	VAL	7.6
1	A	259	GLY	7.1
1	A	447	TRP	6.3
1	B	257	GLN	6.2
1	D	258	ASP	5.9
1	A	141	SER	5.2
1	D	257	GLN	5.2
1	A	204	ALA	4.9
1	D	259	GLY	4.8
1	D	260	SER	4.6
1	C	447	TRP	4.6
1	B	89	GLN	4.6
1	A	448	ILE	4.5
1	A	280	THR	4.5
1	A	142	GLY	4.4
1	C	280	THR	4.3
1	C	68	PHE	4.3
1	B	452	ILE	4.2
1	C	448	ILE	4.2
1	C	119	ALA	4.1
1	A	452	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	258	ASP	4.0
1	D	121	GLU	4.0
1	A	451	PRO	4.0
1	C	388	ARG	4.0
1	A	449	VAL	4.0
1	A	235	CYS	3.9
1	A	107	ARG	3.9
1	A	446	ALA	3.9
1	A	480	TRP	3.9
1	A	302	LEU	3.8
1	C	259	GLY	3.8
1	D	452	ILE	3.7
1	C	480	TRP	3.7
1	D	89	GLN	3.7
1	B	260	SER	3.6
1	C	451	PRO	3.6
1	C	256	GLN	3.6
1	C	236	PRO	3.6
1	A	275	ILE	3.6
1	A	185	VAL	3.6
1	A	237	GLY	3.6
1	B	258	ASP	3.6
1	B	259	GLY	3.6
1	B	449	VAL	3.5
1	A	140	ARG	3.5
1	B	141[A]	SER	3.5
1	C	275	ILE	3.5
1	C	445	TRP	3.5
1	C	238	ARG	3.4
1	B	446	ALA	3.4
1	C	306	PRO	3.3
1	C	257	GLN	3.3
1	C	452	ILE	3.3
1	C	299	PRO	3.3
1	A	256	GLN	3.2
1	A	244	TRP	3.2
1	A	145	ALA	3.2
1	A	162	THR	3.2
1	D	255	ARG	3.2
1	B	153	VAL	3.2
1	A	445	TRP	3.2
1	A	268	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	360	THR	3.1
1	C	449	VAL	3.1
1	A	89	GLN	3.1
1	B	454	GLY	3.1
1	C	141	SER	3.1
1	A	184	CYS	3.1
1	B	460	PHE	3.1
1	A	183	ARG	3.0
1	A	281	PRO	3.0
1	A	122	GLN	3.0
1	A	238	ARG	3.0
1	A	293	LEU	3.0
1	B	79	ILE	3.0
1	A	353	PHE	3.0
1	B	388	ARG	3.0
1	A	79	ILE	2.9
1	D	79	ILE	2.9
1	A	272	GLU	2.9
1	A	120	PRO	2.9
1	A	444	ASP	2.9
1	A	450	PRO	2.9
1	D	256	GLN	2.8
1	A	134	TYR	2.8
1	B	360	THR	2.8
1	A	300	PRO	2.8
1	D	446	ALA	2.8
1	C	79	ILE	2.8
1	C	300	PRO	2.7
1	A	365	ARG	2.7
1	B	140	ARG	2.7
1	C	185	VAL	2.7
1	D	449	VAL	2.7
1	C	450	PRO	2.7
1	C	142	GLY	2.7
1	A	68	PHE	2.7
1	A	364	THR	2.7
1	D	120	PRO	2.7
1	C	258	ASP	2.7
1	B	445	TRP	2.6
1	D	447	TRP	2.6
1	A	239	GLY	2.6
1	B	386	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	255	ARG	2.6
1	C	439	GLY	2.6
1	C	446	ALA	2.6
1	C	460	PHE	2.6
1	A	254	TYR	2.6
1	C	140	ARG	2.5
1	C	239	GLY	2.5
1	D	360	THR	2.5
1	D	445	TRP	2.5
1	A	274	CYS	2.5
1	C	360	THR	2.5
1	C	303	PHE	2.5
1	A	301	GLU	2.5
1	A	305	LEU	2.5
1	B	450	PRO	2.5
1	A	208	PHE	2.5
1	D	261	VAL	2.5
1	D	81	TYR	2.5
1	A	151	GLN	2.5
1	A	236	PRO	2.5
1	B	120	PRO	2.5
1	B	97	ARG	2.5
1	D	122	GLN	2.5
1	C	304	LEU	2.4
1	A	436	LYS	2.4
1	C	184	CYS	2.4
1	B	124	LEU	2.4
1	A	279	TRP	2.4
1	D	158	ALA	2.4
1	B	81	TYR	2.4
1	C	81	TYR	2.4
1	C	67	LYS	2.4
1	C	365	ARG	2.4
1	A	304	LEU	2.4
1	D	451	PRO	2.4
1	C	90	GLN	2.3
1	A	303	PHE	2.3
1	B	453	SER	2.3
1	D	365	ARG	2.3
1	B	256	GLN	2.3
1	A	163	TYR	2.2
1	B	76	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	135	TYR	2.2
1	A	128	ARG	2.2
1	D	68	PHE	2.2
1	C	89	GLN	2.2
1	C	307	PRO	2.2
1	B	447	TRP	2.2
1	C	297	ASP	2.2
1	D	362	ILE	2.2
1	C	302	LEU	2.2
1	B	455	SER	2.2
1	A	202	ARG	2.2
1	A	307	PRO	2.2
1	A	292	LEU	2.2
1	A	358	MET	2.2
1	C	162	THR	2.2
1	A	221	ARG	2.1
1	C	301	GLU	2.1
1	A	181	ALA	2.1
1	B	451	PRO	2.1
1	A	182	PRO	2.1
1	A	336	VAL	2.1
1	A	412	LEU	2.0
1	C	80	THR	2.0
1	A	473	PHE	2.0
1	C	76	VAL	2.0
1	C	237	GLY	2.0
1	A	106	PRO	2.0
1	A	479	PRO	2.0
1	D	358	MET	2.0
1	A	273	LEU	2.0
1	D	124	LEU	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)

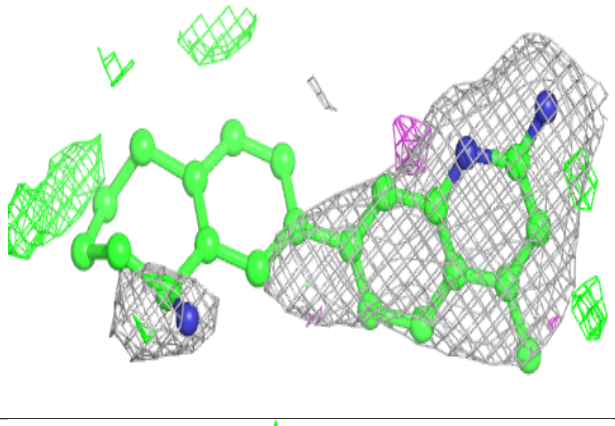
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

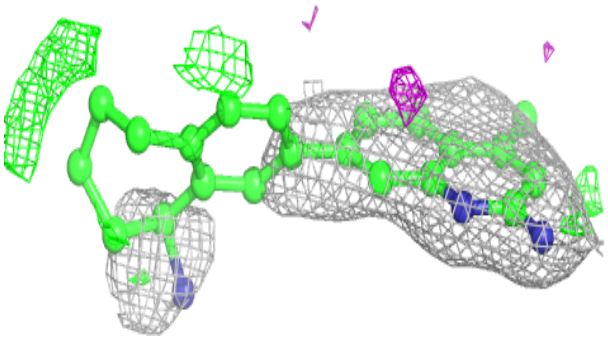
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BTB	C	505	14/14	0.72	0.21	81,111,118,119	0
3	WRI	C	503	24/24	0.79	0.35	45,94,129,131	0
3	WRI	B	503	24/24	0.80	0.30	40,85,128,133	0
4	BTB	A	505	14/14	0.81	0.20	103,119,123,125	0
3	WRI	A	503	24/24	0.84	0.35	53,96,136,139	0
4	BTB	D	504	14/14	0.86	0.20	76,83,91,93	0
5	GOL	D	505	6/6	0.86	0.10	80,81,90,92	0
3	WRI	C	510	24/24	0.87	0.32	38,78,126,126	0
6	CL	A	507	1/1	0.87	0.28	70,70,70,70	0
4	BTB	D	503	14/14	0.89	0.20	42,72,84,87	0
4	BTB	C	504	14/14	0.90	0.14	56,79,88,90	0
4	BTB	A	504	14/14	0.90	0.13	81,91,100,100	0
3	WRI	C	502	24/24	0.90	0.30	53,67,85,87	0
5	GOL	C	506	6/6	0.91	0.24	58,65,83,88	0
3	WRI	A	502	24/24	0.91	0.37	64,77,99,107	0
4	BTB	B	505	14/14	0.91	0.21	55,69,79,80	0
7	ZN	C	509	1/1	0.91	0.07	61,61,61,61	0
7	ZN	C	511	1/1	0.91	0.08	68,68,68,68	0
4	BTB	B	504	14/14	0.92	0.14	46,64,79,82	0
7	ZN	B	508	1/1	0.92	0.08	64,64,64,64	0
6	CL	C	507	1/1	0.93	0.29	60,60,60,60	0
3	WRI	B	502	24/24	0.93	0.21	41,53,97,104	0
3	WRI	D	502	24/24	0.93	0.26	36,55,93,99	0
5	GOL	A	506	6/6	0.93	0.14	64,77,80,84	0
7	ZN	A	509	1/1	0.95	0.08	65,65,65,65	0
2	HEM	A	501	43/43	0.96	0.25	44,65,86,89	0
6	CL	D	506	1/1	0.97	0.13	53,53,53,53	0
2	HEM	B	501	43/43	0.97	0.14	24,41,70,74	0
2	HEM	C	501	43/43	0.97	0.20	36,49,86,98	0
6	CL	B	506	1/1	0.97	0.18	55,55,55,55	0
2	HEM	D	501	43/43	0.97	0.16	26,39,77,90	0
7	ZN	A	508	1/1	0.98	0.08	52,52,52,52	0
8	CA	A	510	1/1	0.98	0.18	48,48,48,48	0
8	CA	C	512	1/1	0.98	0.08	56,56,56,56	0
9	GD	D	507	1/1	0.98	0.10	54,54,54,54	0
9	GD	B	507	1/1	0.99	0.12	55,55,55,55	0
7	ZN	C	508	1/1	0.99	0.10	45,45,45,45	0

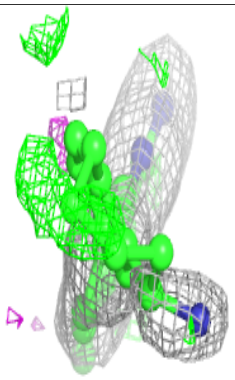
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WRI 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)

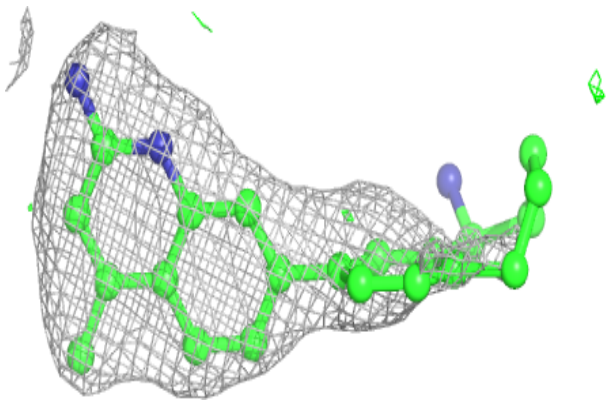


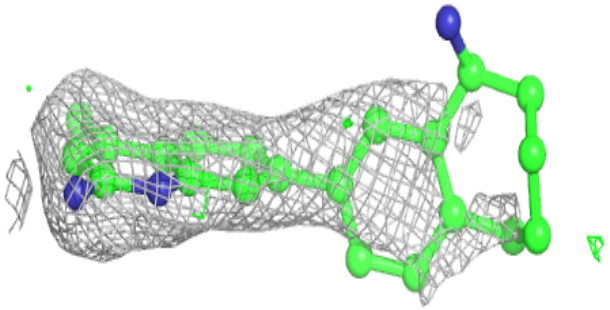


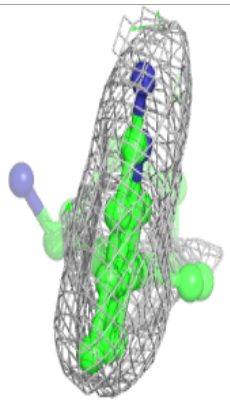


Electron density around WRI B 503:

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

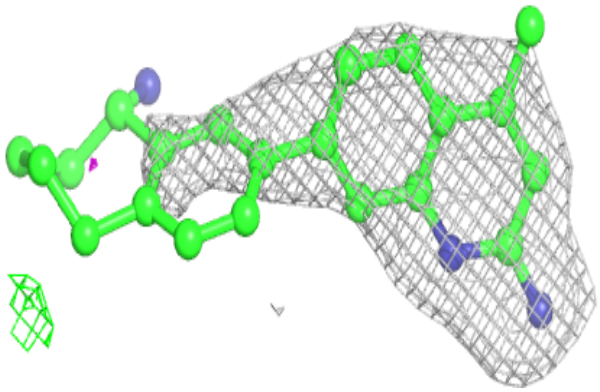


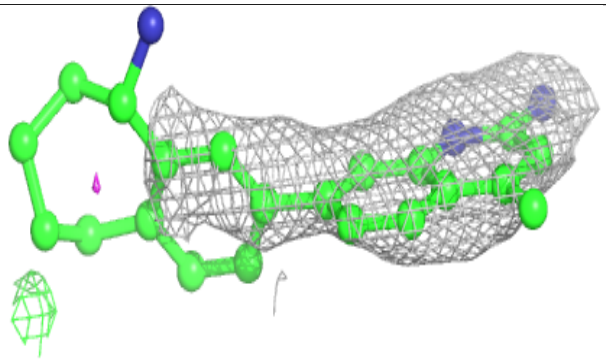


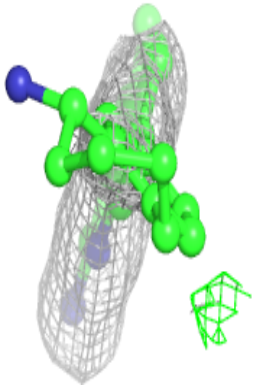


Electron density around WRI A 503:

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

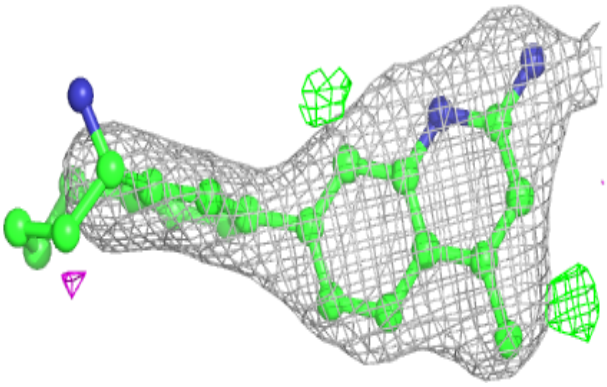


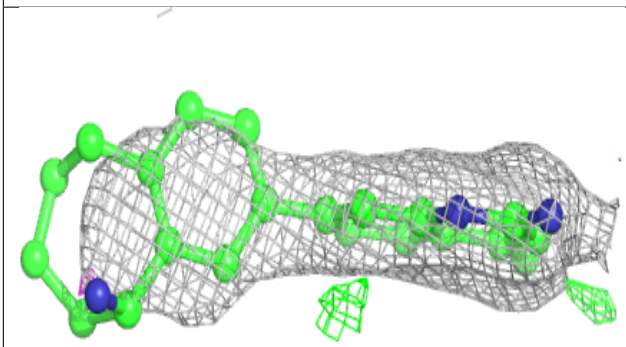


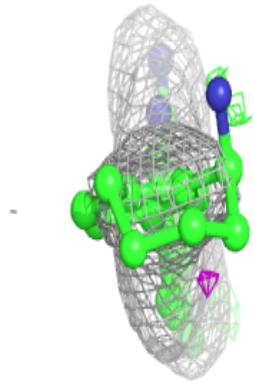


Electron density around WRI C 510:

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

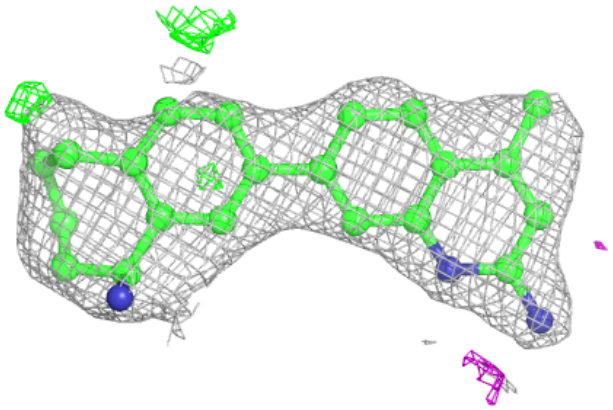


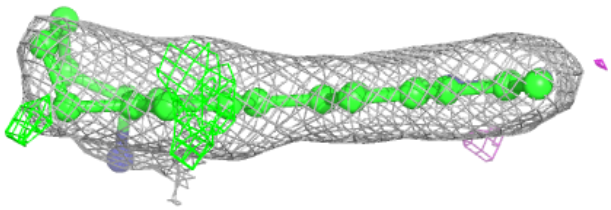


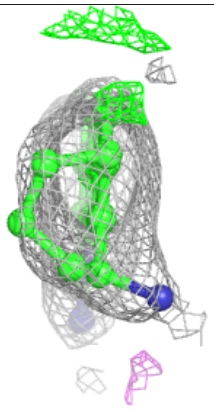


Electron density around WRI C 502:

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

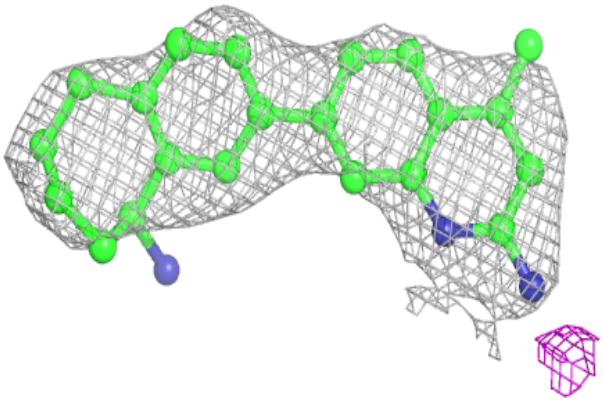


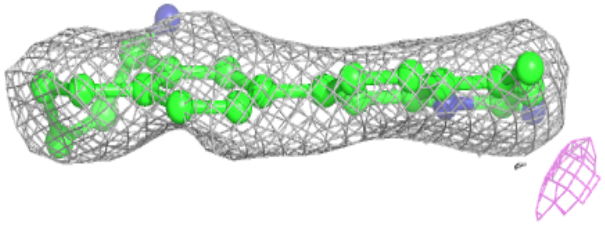


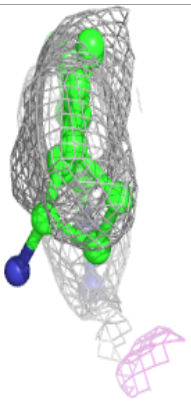


Electron density around WRI A 502:

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

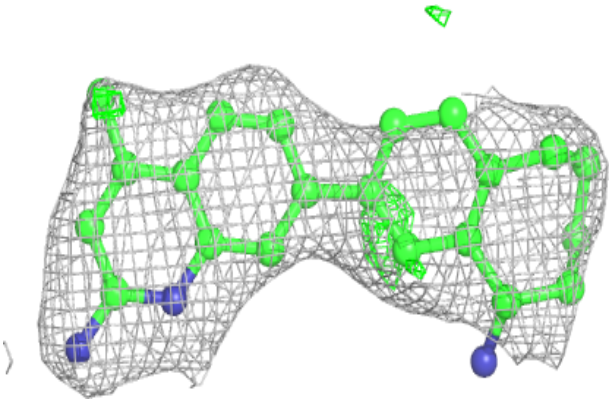


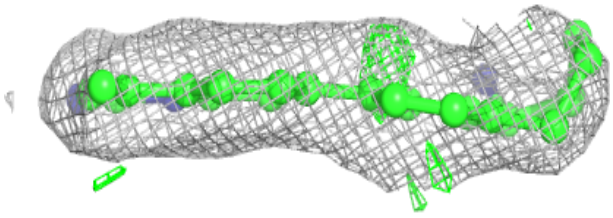


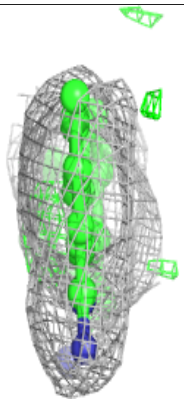


Electron density around WRI B 502:

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

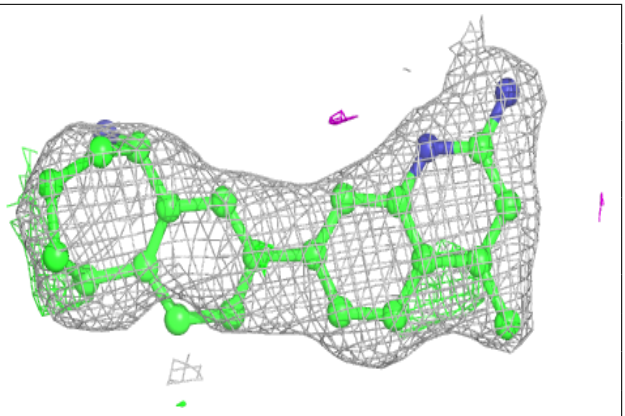


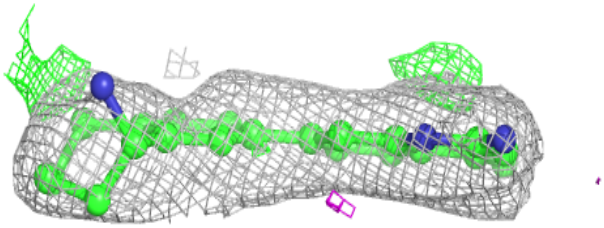


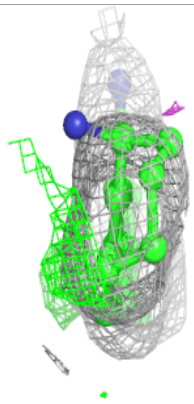


Electron density around WRI D 502:

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

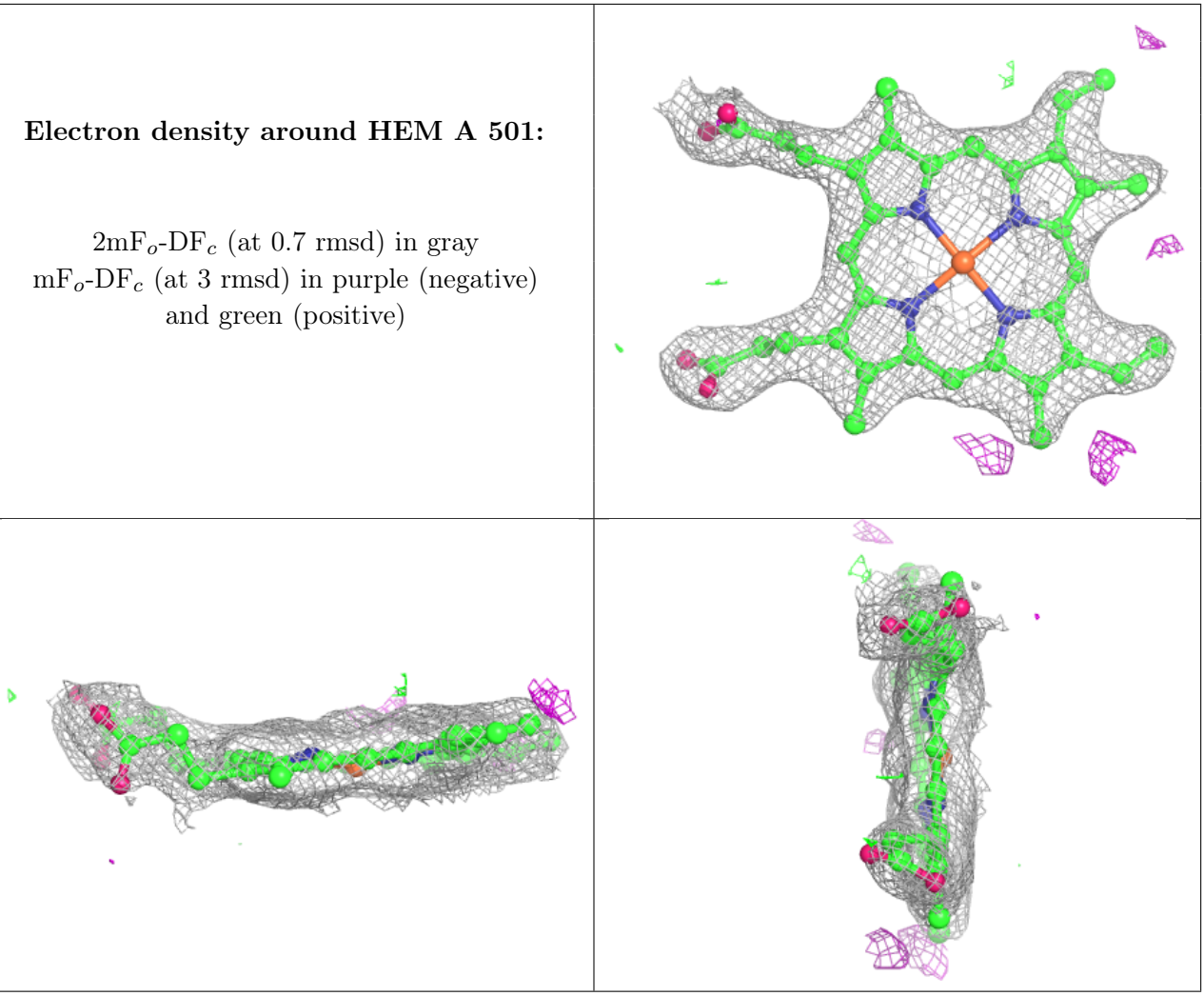






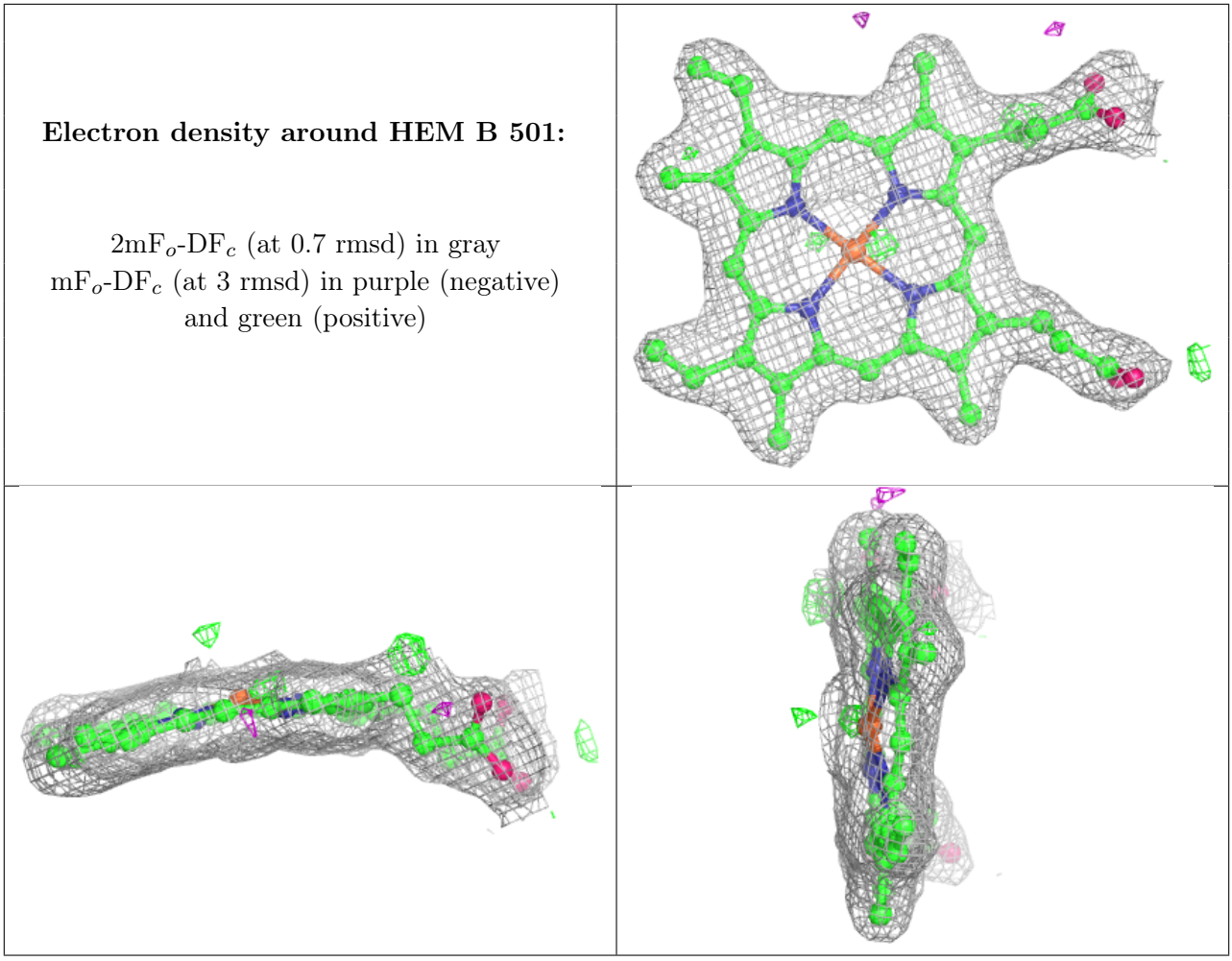
Electron density around HEM A 501:

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



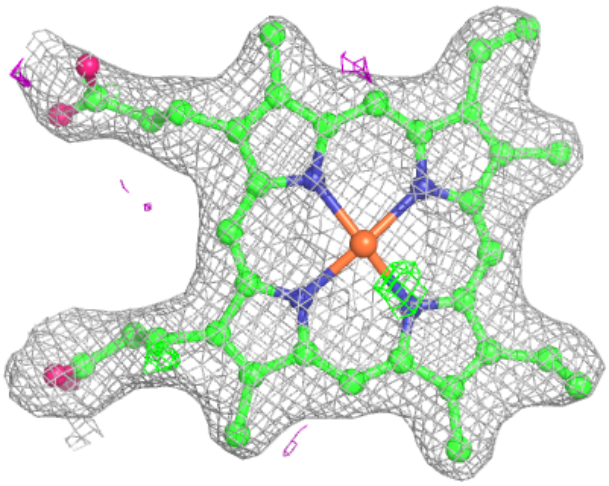
Electron density around HEM B 501:

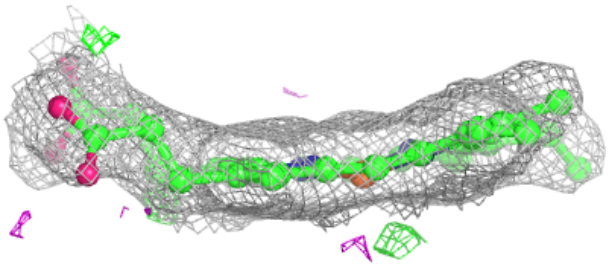
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

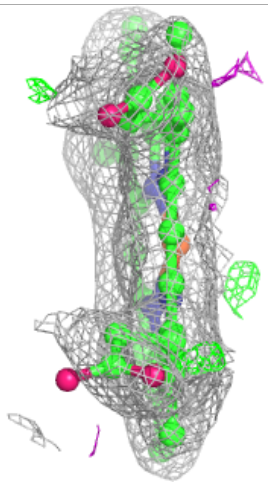


Electron density around HEM C 501:

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

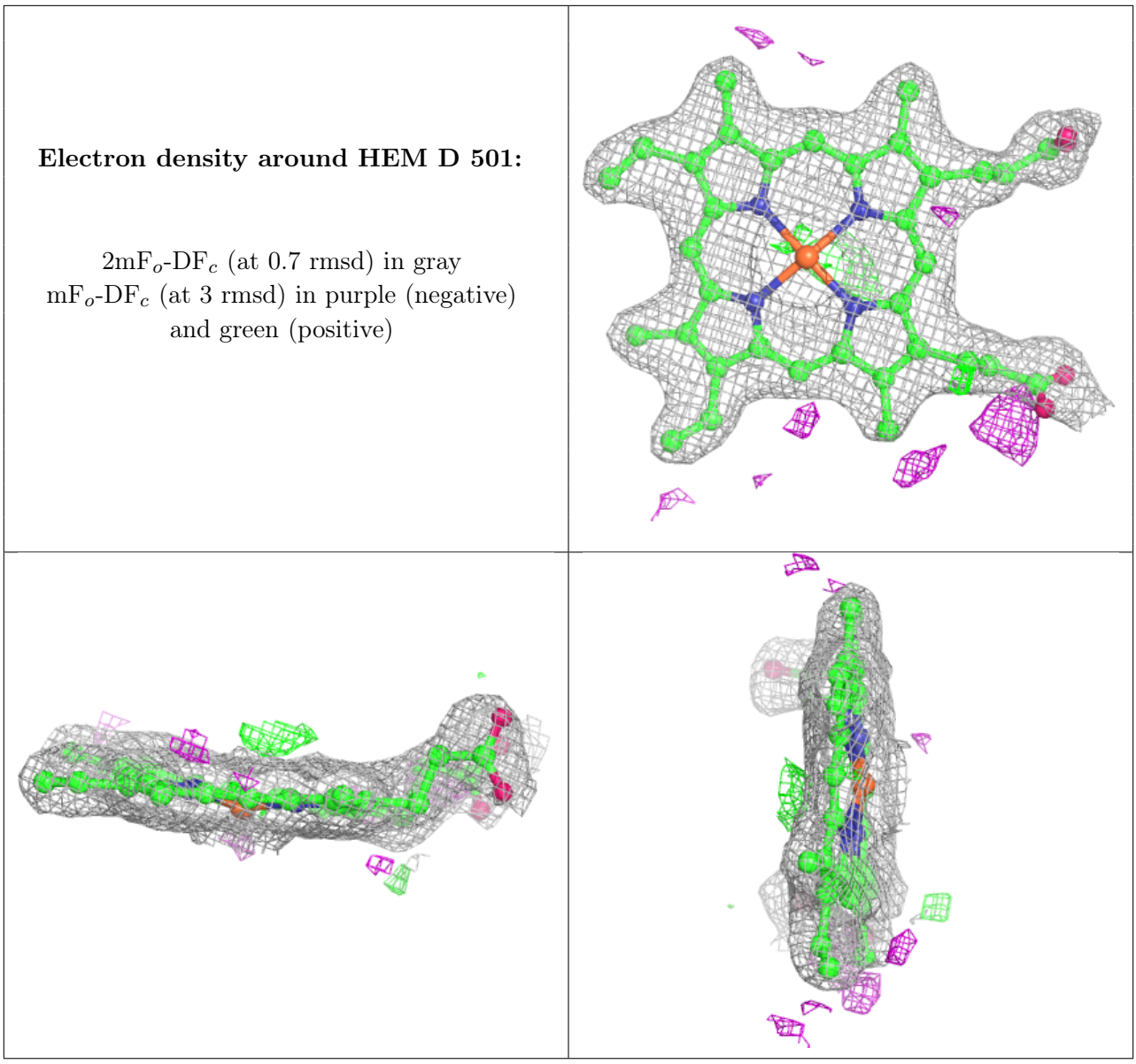






Electron density around HEM D 501:

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



6.5 Other polymers

There are no such residues in this entry.