wwPDB X-ray Structure Validation Summary Report (i)

Apr 23, 2025 – 06:57 PM EDT

PDB ID	:	9CW7 / pdb_00009cw7
Title	:	Structure of human endothelial nitric oxide synthase heme domain bound with 4-methyl-5'-((methylamino)methyl)-[2,3'-bipyridin]-6-amine dihydrochloride
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2024-07-29
Resolution	:	1.83 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

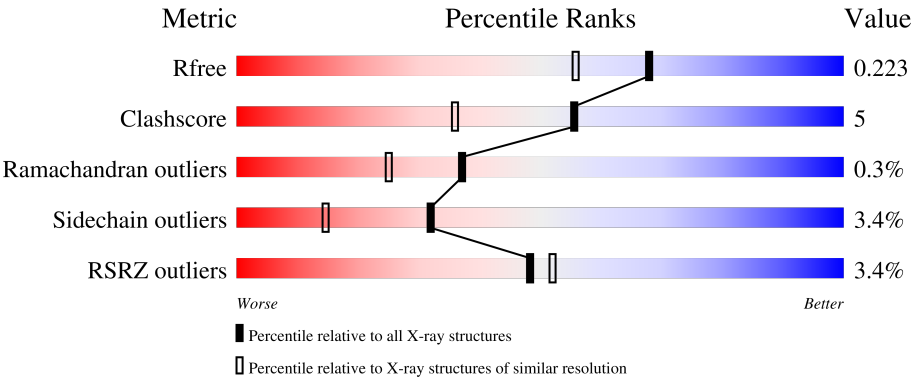
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.83 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	9% 75% 13% • 9%
1	B	440	86% 5% • 9%
1	C	440	2% 80% 10% • 9%
1	D	440	% 84% 7% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	512	-	X	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 14314 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.

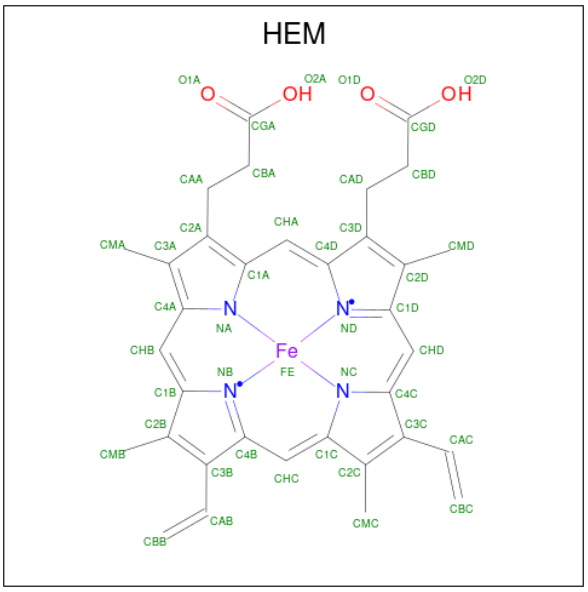
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	1	0
			3200	2038	563	583	16			
1	B	401	Total	C	N	O	S	0	2	0
			3206	2042	563	585	16			
1	C	402	Total	C	N	O	S	0	1	0
			3212	2046	565	585	16			
1	D	402	Total	C	N	O	S	0	0	0
			3211	2044	567	584	16			

There are 4 discrepancies between the modelled and reference sequences:

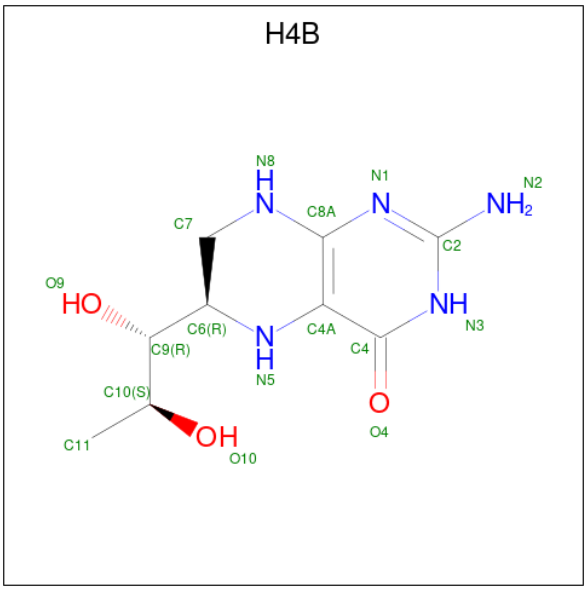
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



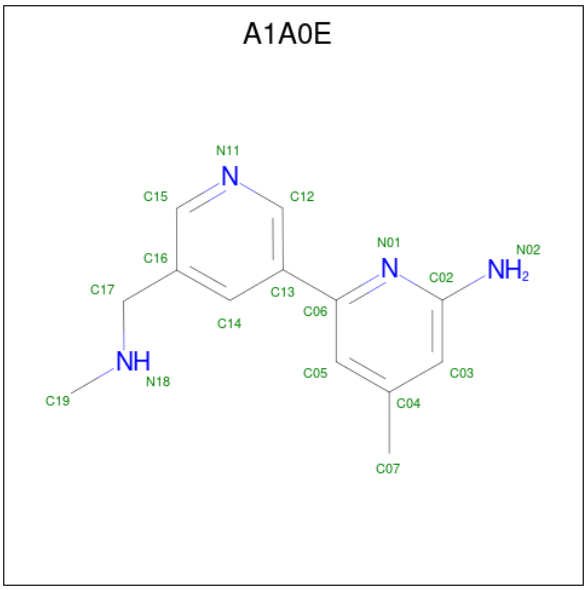
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



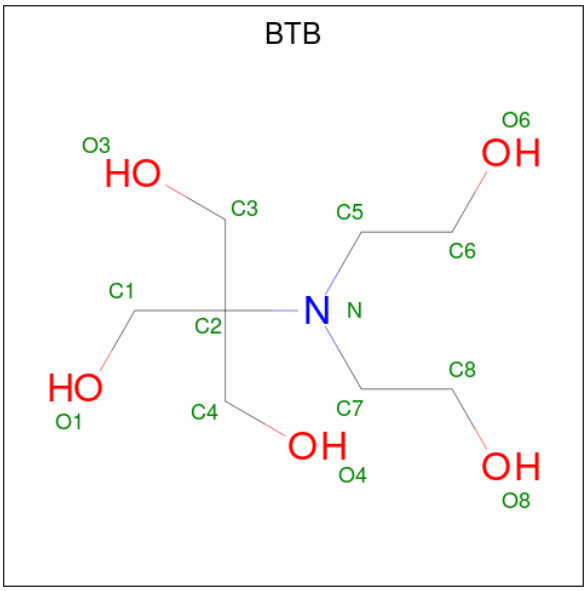
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0
3	C	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is (2M)-4-methyl-5'-[(methylamino)methyl][2,3'-bipyridin]-6-amine (CCD ID: A1A0E) (formula: $C_{13}H_{16}N_4$) (labeled as "Ligand of Interest" by depositor).



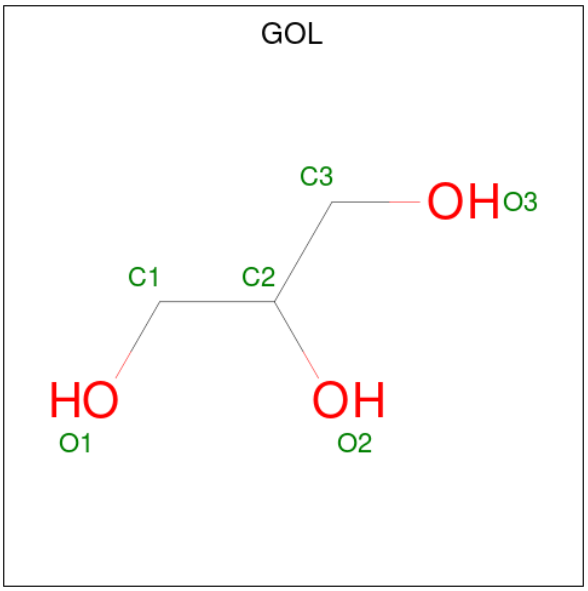
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 17 13 4	0	0
4	B	1	Total C N 17 13 4	0	0
4	C	1	Total C N 17 13 4	0	0
4	D	1	Total C N 17 13 4	0	0

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



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

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



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

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

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

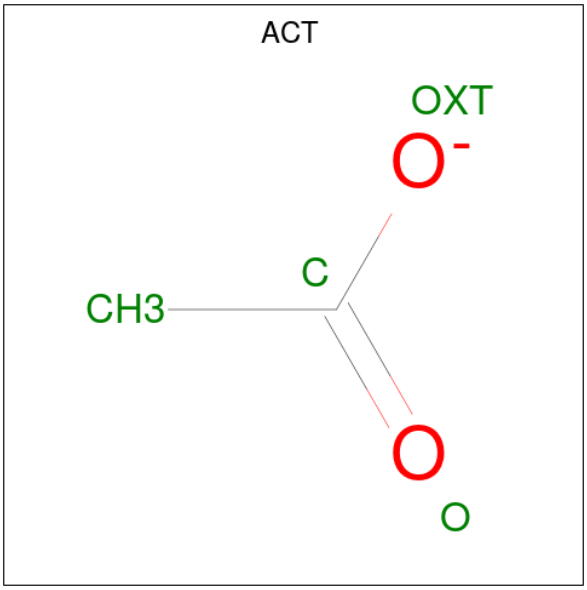
- Molecule 8 is GADOLINIUM ION (CCD ID: GD3) (formula: Gd).

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

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

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

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 4 2 2	0	0
10	C	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0

- Molecule 11 is water.

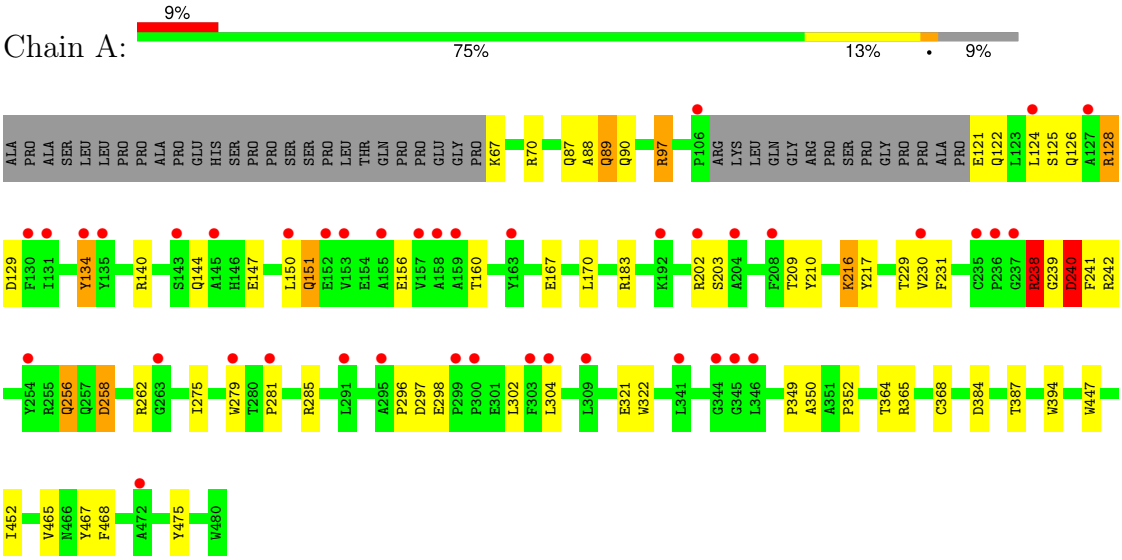
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	148	Total O 148 148	0	0
11	B	293	Total O 293 293	0	0
11	C	223	Total O 223 223	0	0
11	D	317	Total O 317 317	0	0

3 Residue-property plots (i)

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

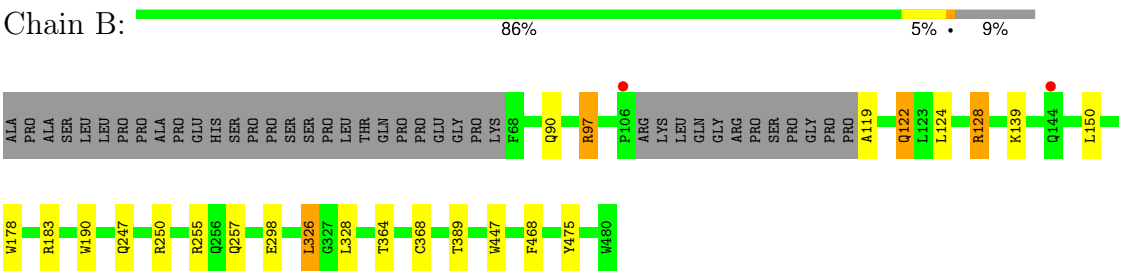
• Molecule 1: Nitric oxide synthase, endothelial

Chain A:



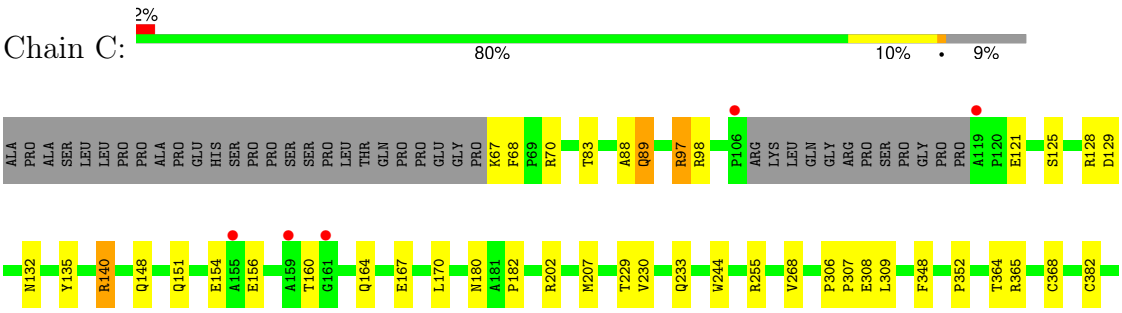
• Molecule 1: Nitric oxide synthase, endothelial

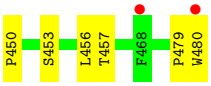
Chain B:



• Molecule 1: Nitric oxide synthase, endothelial

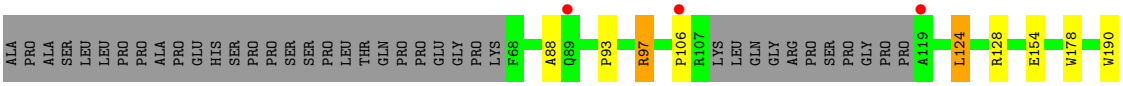
Chain C:

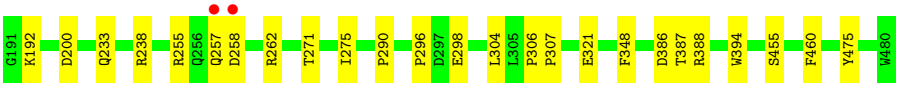




• Molecule 1: Nitric oxide synthase, endothelial

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.95Å 152.42Å 108.69Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	49.37 – 1.83 49.37 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.37-1.83) 98.5 (49.37-1.83)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.189 , 0.228 0.183 , 0.223	Depositor DCC
R_{free} test set	8617 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14314	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: HEM, ZN, CL, A1A0E, BTB, GOL, H4B, ACT, GD3

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	0.32	0/3294	0.51	1/4487 (0.0%)
1	B	0.39	0/3304	0.53	0/4503
1	C	0.35	0/3307	0.51	0/4506
1	D	0.42	0/3303	0.53	0/4501
All	All	0.37	0/13208	0.52	1/17997 (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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	ASP	CB-CG-OD1	5.62	123.36	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	ARG	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	3200	0	3104	44	0
1	B	3206	0	3108	16	0
1	C	3212	0	3116	26	0
1	D	3211	0	3111	19	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	1	0
3	B	17	0	15	1	0
3	C	17	0	15	1	0
3	D	17	0	15	0	0
4	A	17	0	0	0	0
4	B	17	0	0	0	0
4	C	17	0	0	0	0
4	D	17	0	0	0	0
5	A	42	0	56	10	0
5	B	42	0	55	3	0
5	C	14	0	18	3	0
5	D	28	0	36	4	0
6	A	18	0	24	1	0
6	B	6	0	8	0	0
6	C	18	0	24	1	0
6	D	6	0	8	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	4	0	3	1	0
10	C	4	0	3	0	0
10	D	4	0	3	0	0
11	A	148	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	293	0	0	0	0
11	C	223	0	0	3	0
11	D	317	0	0	0	0
All	All	14314	0	12857	121	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.

The worst 5 of 121 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:475:TYR:OH	2:D:501:HEM:O1D	2.08	0.72
1:D:386:ASP:OD1	1:D:388:ARG:NH1	2.24	0.70
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.72	0.70
1:A:242:ARG:HD2	1:A:349:PRO:HB2	1.76	0.68
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.76	0.68

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	397/440 (90%)	374 (94%)	19 (5%)	4 (1%)	13 4
1	B	399/440 (91%)	389 (98%)	10 (2%)	0	100 100
1	C	399/440 (91%)	391 (98%)	7 (2%)	1 (0%)	37 25
1	D	398/440 (90%)	392 (98%)	6 (2%)	0	100 100
All	All	1593/1760 (90%)	1546 (97%)	42 (3%)	5 (0%)	37 25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	240	ASP
1	A	88	ALA
1	A	203	SER
1	C	89	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	341/373 (91%)	323 (95%)	18 (5%)	19 4
1	B	342/373 (92%)	335 (98%)	7 (2%)	50 35
1	C	342/373 (92%)	329 (96%)	13 (4%)	28 11
1	D	341/373 (91%)	333 (98%)	8 (2%)	45 29
All	All	1366/1492 (92%)	1320 (97%)	46 (3%)	32 15

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	98	ARG
1	C	207	MET
1	C	121	GLU
1	C	148	GLN
1	C	309	LEU

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

Mol	Chain	Res	Type
1	A	151	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 10 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
6	GOL	A	512	-	5,5,5	0.69	0	5,5,5	2.44	2 (40%)
5	BTB	B	506	-	13,13,13	0.61	0	7,16,16	1.17	0
5	BTB	D	506	-	13,13,13	0.63	0	7,16,16	1.13	1 (14%)
10	ACT	B	504	-	3,3,3	0.94	0	3,3,3	0.75	0
6	GOL	C	507	-	5,5,5	0.38	0	5,5,5	0.27	0
3	H4B	B	502	-	16,18,18	0.88	0	14,26,26	2.40	5 (35%)
4	A1A0E	A	503	-	18,18,18	0.33	0	23,24,24	1.86	7 (30%)
5	BTB	B	510	-	13,13,13	0.48	0	7,16,16	0.68	0
3	H4B	C	502	-	16,18,18	0.90	0	14,26,26	2.55	5 (35%)
5	BTB	D	505	8	13,13,13	0.35	0	7,16,16	0.70	0
3	H4B	A	502	-	16,18,18	0.82	0	14,26,26	2.29	5 (35%)
6	GOL	A	507	-	5,5,5	0.37	0	5,5,5	0.30	0
6	GOL	C	506	-	5,5,5	0.32	0	5,5,5	0.29	0
4	A1A0E	B	503	-	18,18,18	0.40	0	23,24,24	1.89	8 (34%)
5	BTB	A	506	-	13,13,13	0.32	0	7,16,16	0.74	0
5	BTB	C	505	8	13,13,13	0.37	0	7,16,16	1.07	1 (14%)
2	HEM	D	501	1	42,50,50	1.52	7 (16%)	46,82,82	1.50	7 (15%)
6	GOL	C	508	-	5,5,5	0.37	0	5,5,5	0.20	0
2	HEM	B	501	1	42,50,50	1.49	5 (11%)	46,82,82	1.69	9 (19%)
6	GOL	B	507	-	5,5,5	0.31	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	ACT	D	504	-	3,3,3	1.03	0	3,3,3	0.79	0
2	HEM	A	501	1	42,50,50	1.53	6 (14%)	46,82,82	1.62	9 (19%)
4	A1A0E	C	503	-	18,18,18	0.32	0	23,24,24	2.31	8 (34%)
2	HEM	C	501	1	42,50,50	1.48	5 (11%)	46,82,82	1.83	14 (30%)
5	BTB	A	504	8	13,13,13	0.39	0	7,16,16	0.62	0
10	ACT	C	504	-	3,3,3	1.01	0	3,3,3	0.91	0
6	GOL	A	508	-	5,5,5	0.56	0	5,5,5	0.44	0
6	GOL	D	507	-	5,5,5	0.34	0	5,5,5	0.34	0
3	H4B	D	502	-	16,18,18	0.79	0	14,26,26	2.34	5 (35%)
5	BTB	B	505	8	13,13,13	0.43	0	7,16,16	0.38	0
4	A1A0E	D	503	-	18,18,18	0.53	0	23,24,24	2.31	7 (30%)
5	BTB	A	505	-	13,13,13	0.46	0	7,16,16	0.94	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
6	GOL	A	512	-	-	4/4/4/4	-
5	BTB	B	506	-	-	9/21/21/21	-
5	BTB	D	506	-	-	9/21/21/21	-
6	GOL	C	507	-	-	4/4/4/4	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
4	A1A0E	A	503	-	-	5/7/7/7	0/2/2/2
5	BTB	B	510	-	-	15/21/21/21	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
5	BTB	D	505	8	-	6/21/21/21	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
6	GOL	A	507	-	-	0/4/4/4	-
6	GOL	C	506	-	-	2/4/4/4	-
4	A1A0E	B	503	-	-	5/7/7/7	0/2/2/2
5	BTB	A	506	-	-	10/21/21/21	-
5	BTB	C	505	8	-	4/21/21/21	-
2	HEM	D	501	1	-	0/12/54/54	-
6	GOL	C	508	-	-	2/4/4/4	-
2	HEM	B	501	1	-	1/12/54/54	-
6	GOL	B	507	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	501	1	-	0/12/54/54	-
4	A1A0E	C	503	-	-	4/7/7/7	0/2/2/2
2	HEM	C	501	1	-	2/12/54/54	-
5	BTB	A	504	8	-	4/21/21/21	-
6	GOL	A	508	-	-	2/4/4/4	-
6	GOL	D	507	-	-	2/4/4/4	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
5	BTB	B	505	8	-	3/21/21/21	-
4	A1A0E	D	503	-	-	5/7/7/7	0/2/2/2
5	BTB	A	505	-	-	5/21/21/21	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-C2C	-3.64	1.35	1.40
2	B	501	HEM	C3C-CAC	3.60	1.55	1.47
2	A	501	HEM	C3C-CAC	3.42	1.55	1.47
2	D	501	HEM	C3C-C4C	3.35	1.46	1.41
2	C	501	HEM	C3C-CAC	3.31	1.55	1.47

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	H4B	C8A-C4A-C4	5.97	119.94	114.50
3	B	502	H4B	C8A-C4A-C4	5.63	119.62	114.50
3	A	502	H4B	C8A-C4A-C4	5.62	119.61	114.50
4	D	503	A1A0E	C06-N01-C02	5.51	121.94	118.52
4	C	503	A1A0E	C06-N01-C02	4.99	121.62	118.52

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	A1A0E	C16-C17-N18-C19
4	B	503	A1A0E	C16-C17-N18-C19
4	D	503	A1A0E	C16-C17-N18-C19
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4

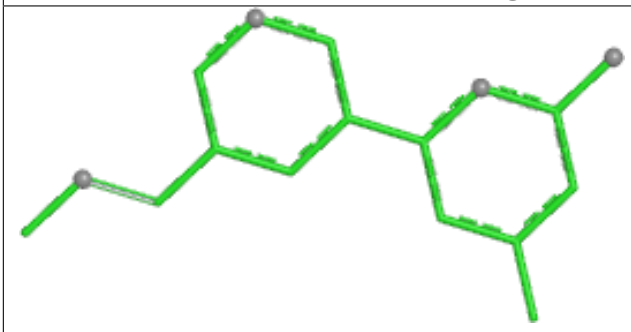
There are no ring outliers.

19 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	506	BTB	1	0
5	D	506	BTB	3	0
10	B	504	ACT	1	0
3	B	502	H4B	1	0
5	B	510	BTB	1	0
3	C	502	H4B	1	0
5	D	505	BTB	1	0
3	A	502	H4B	1	0
6	A	507	GOL	1	0
6	C	506	GOL	1	0
5	A	506	BTB	3	0
5	C	505	BTB	3	0
2	D	501	HEM	3	0
2	B	501	HEM	3	0
2	A	501	HEM	2	0
2	C	501	HEM	2	0
5	A	504	BTB	6	0
5	B	505	BTB	1	0
5	A	505	BTB	1	0

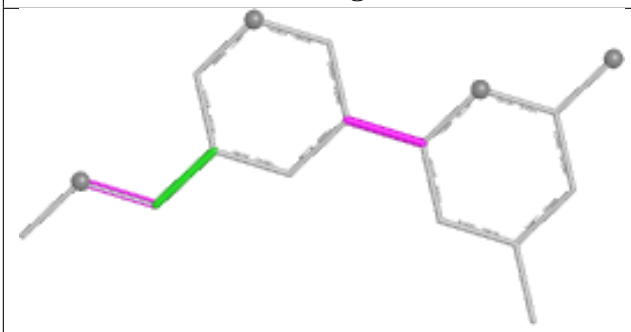
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand A1A0E A 503

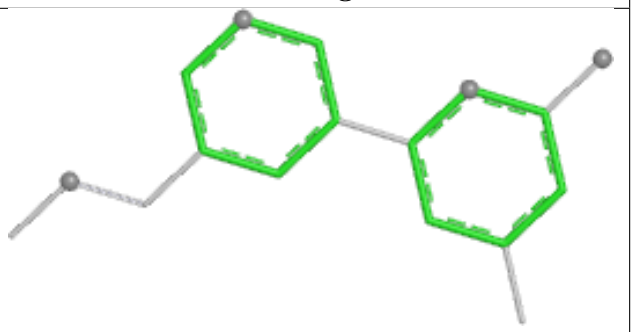


Bond lengths

Bond angles

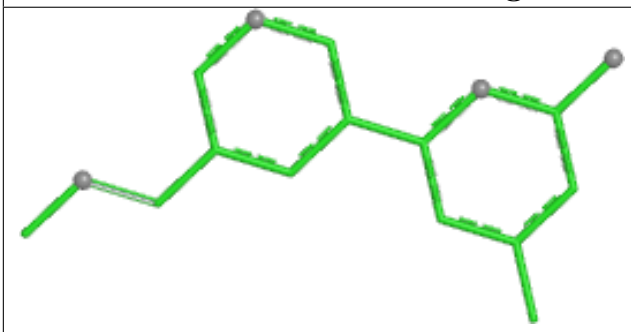


Torsions



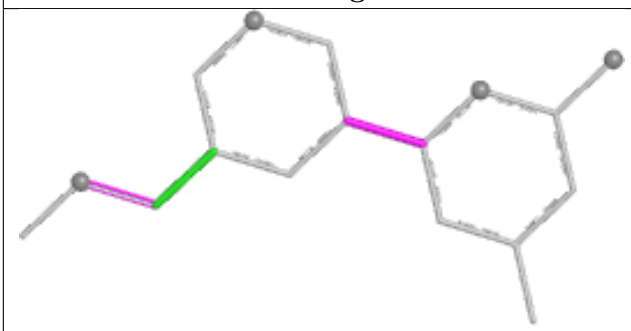
Rings

Ligand A1A0E B 503

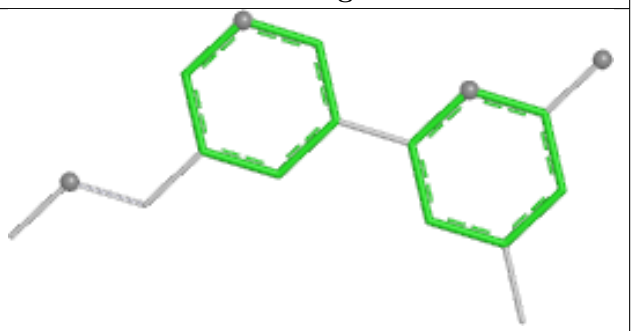


Bond lengths

Bond angles

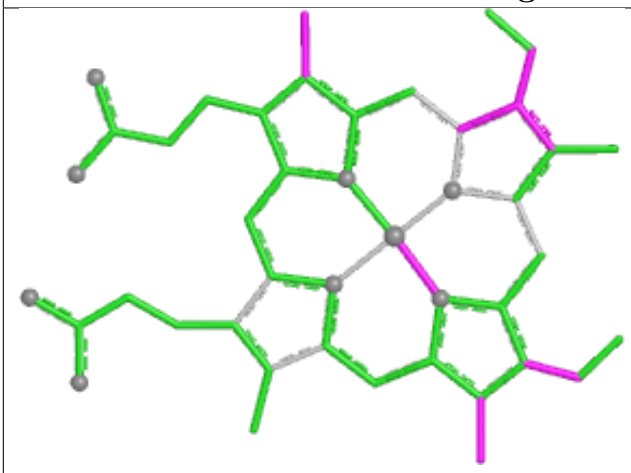


Torsions

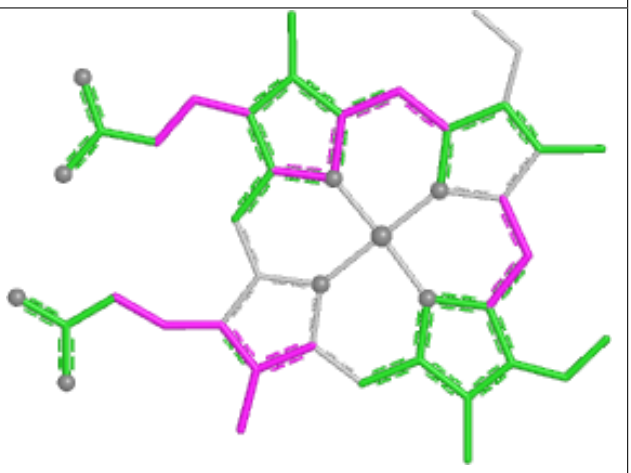


Rings

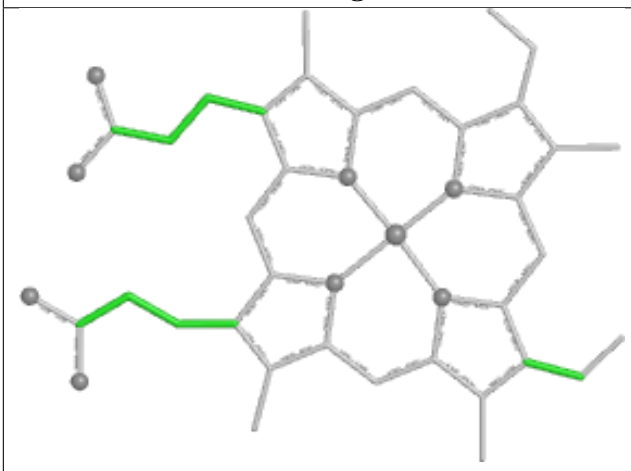
Ligand HEM D 501



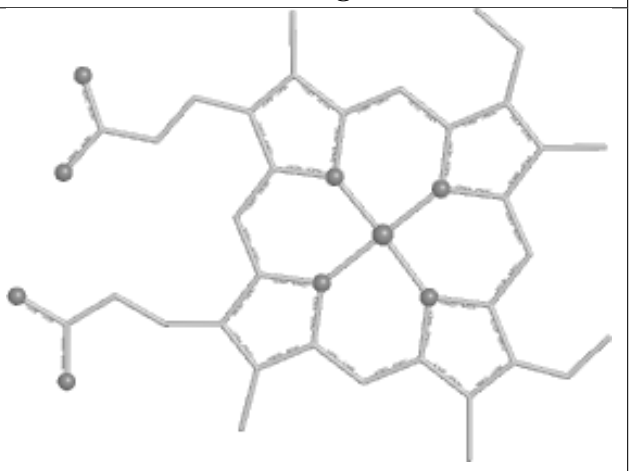
Bond lengths



Bond angles

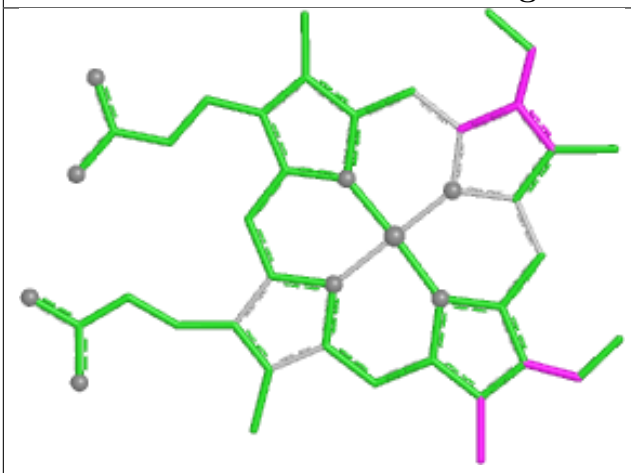


Torsions

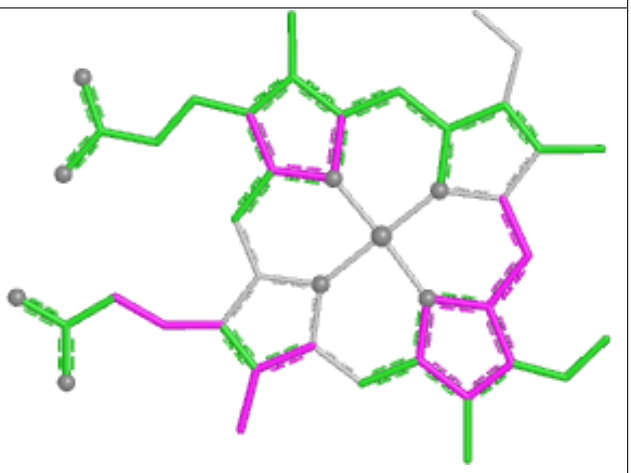


Rings

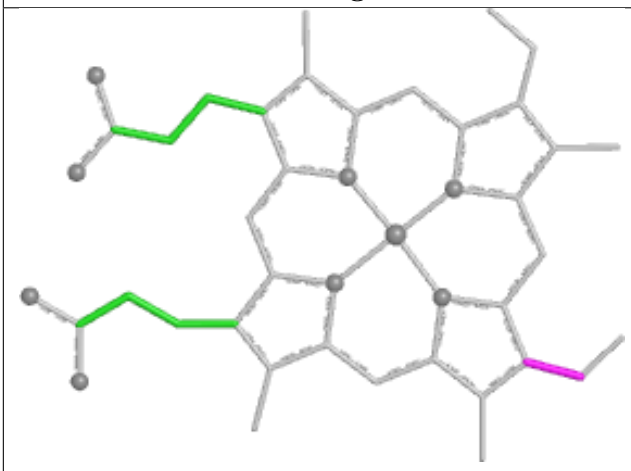
Ligand HEM B 501



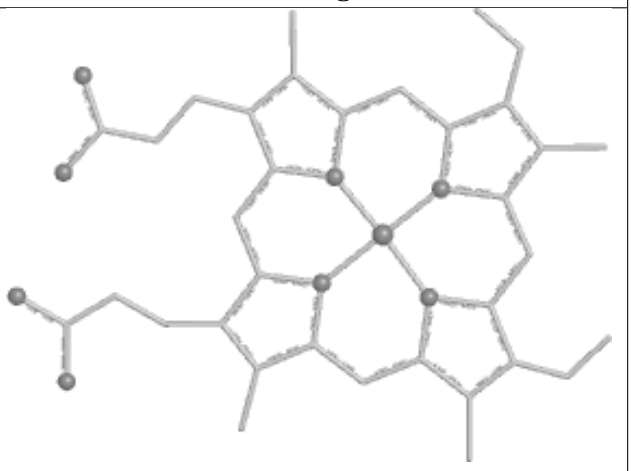
Bond lengths



Bond angles

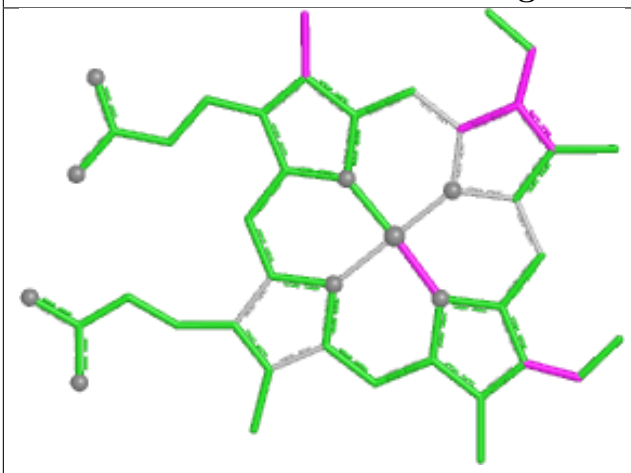


Torsions

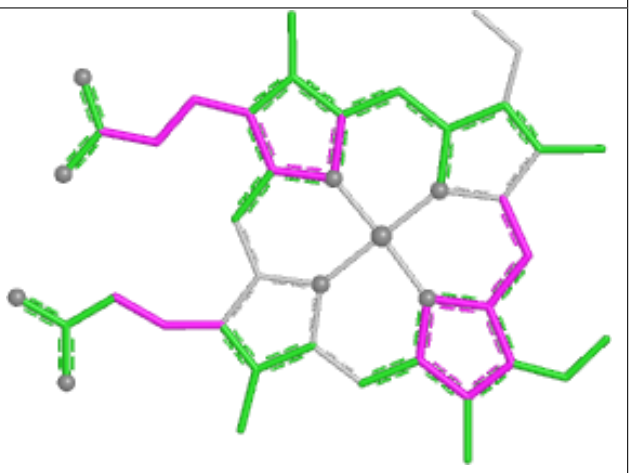


Rings

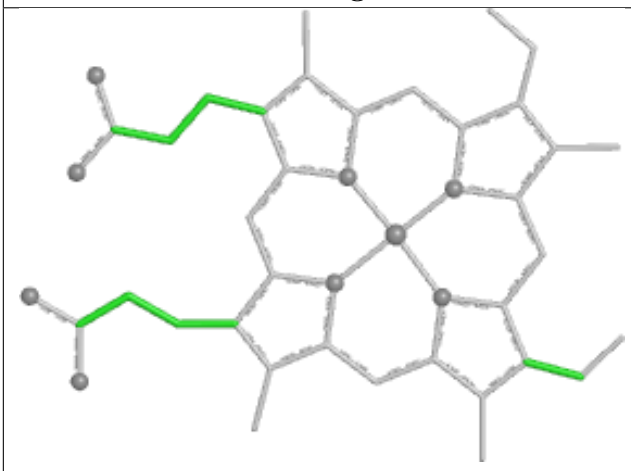
Ligand HEM A 501



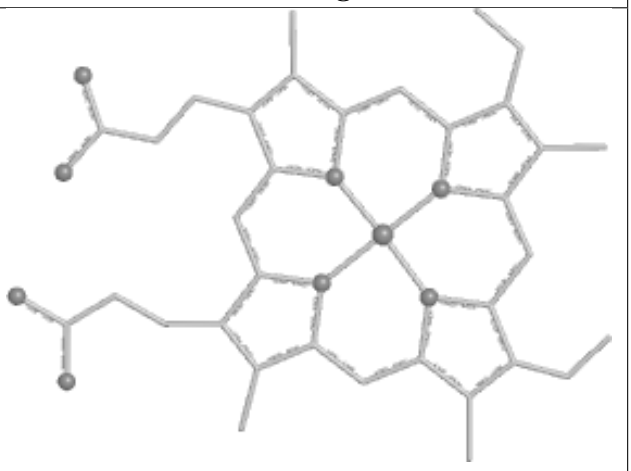
Bond lengths



Bond angles

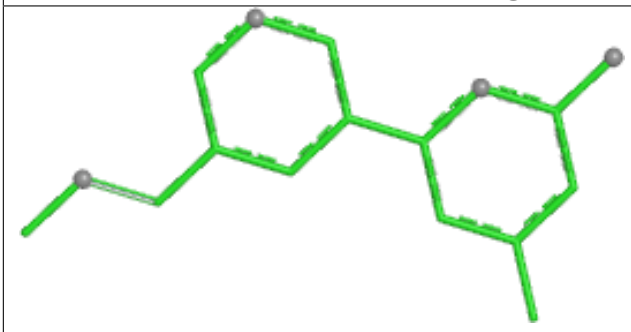


Torsions

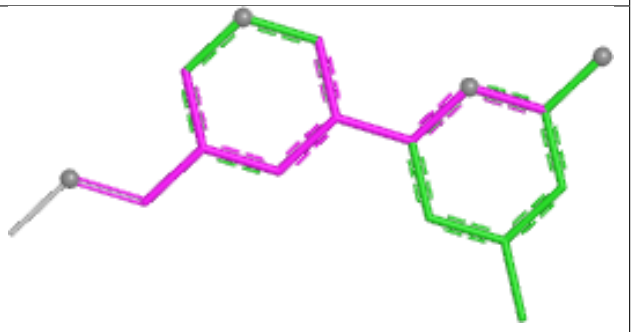


Rings

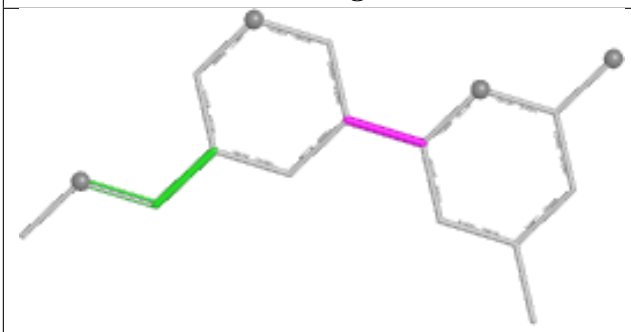
Ligand A1A0E C 503



Bond lengths



Bond angles



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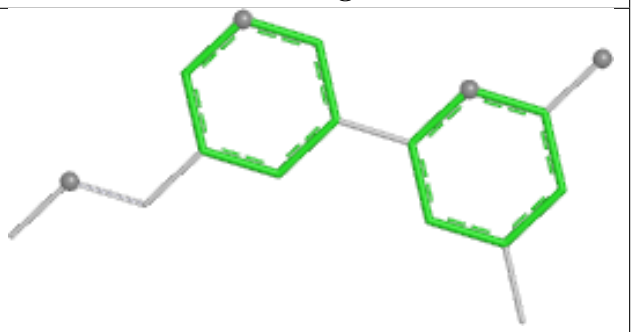
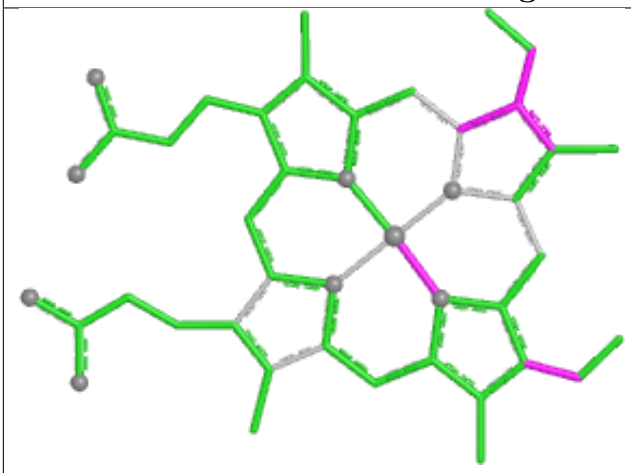
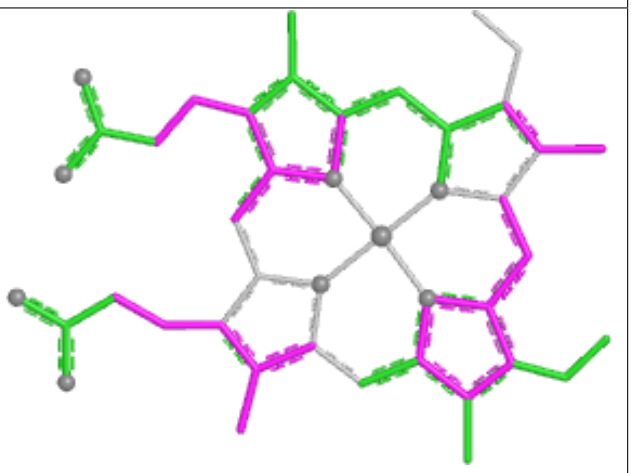


Rings

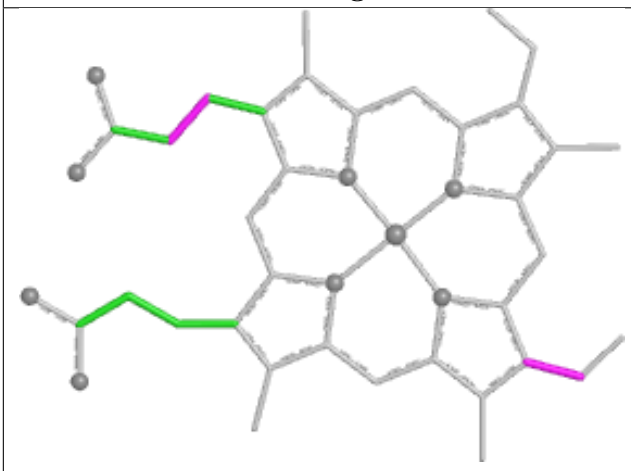
Ligand HEM C 501



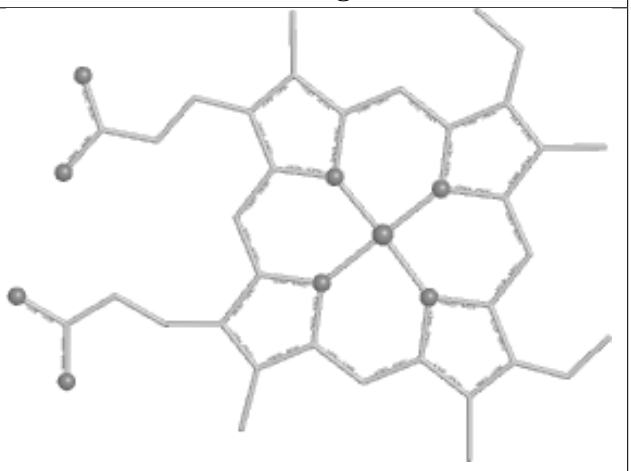
Bond lengths



Bond angles

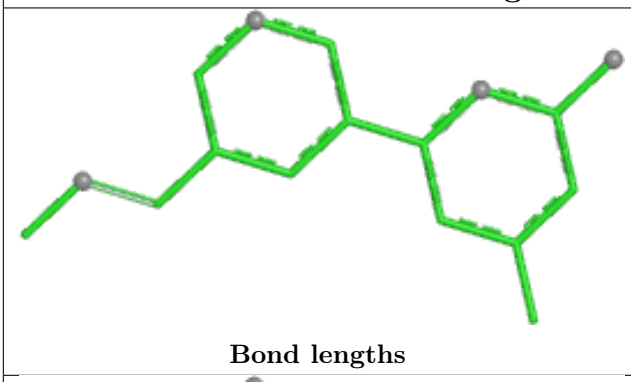


Torsions

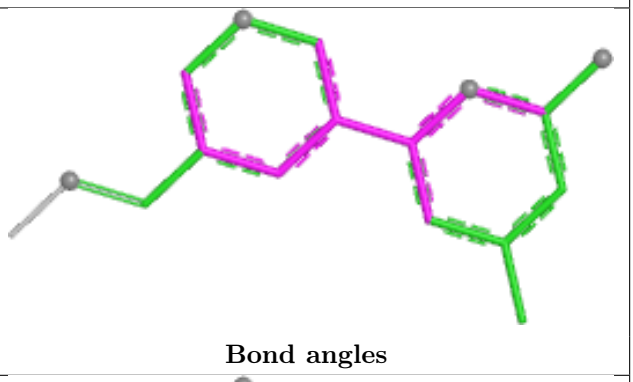


Rings

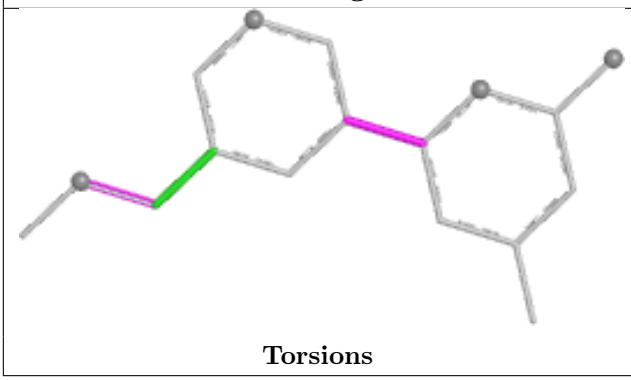
Ligand A1A0E D 503



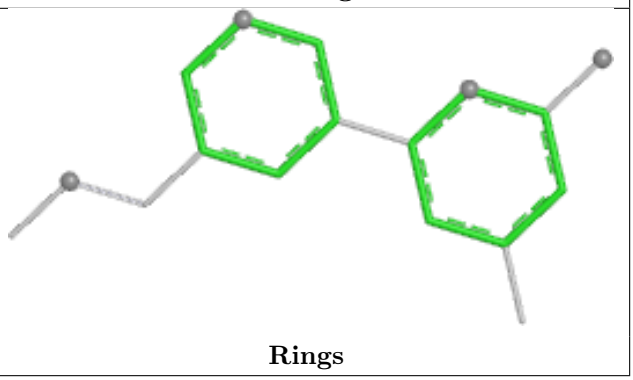
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	400/440 (90%)	0.62	41 (10%) 13 13	23, 59, 116, 147	1 (0%)
1	B	401/440 (91%)	-0.23	2 (0%) 87 92	23, 37, 71, 109	2 (0%)
1	C	402/440 (91%)	0.09	7 (1%) 69 75	23, 48, 86, 107	1 (0%)
1	D	402/440 (91%)	-0.31	5 (1%) 76 82	21, 35, 61, 126	0
All	All	1605/1760 (91%)	0.04	55 (3%) 48 52	21, 43, 94, 147	4 (0%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	PRO	5.6
1	A	106	PRO	4.8
1	A	153	VAL	4.4
1	A	204	ALA	4.2
1	A	163	TYR	3.7

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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.

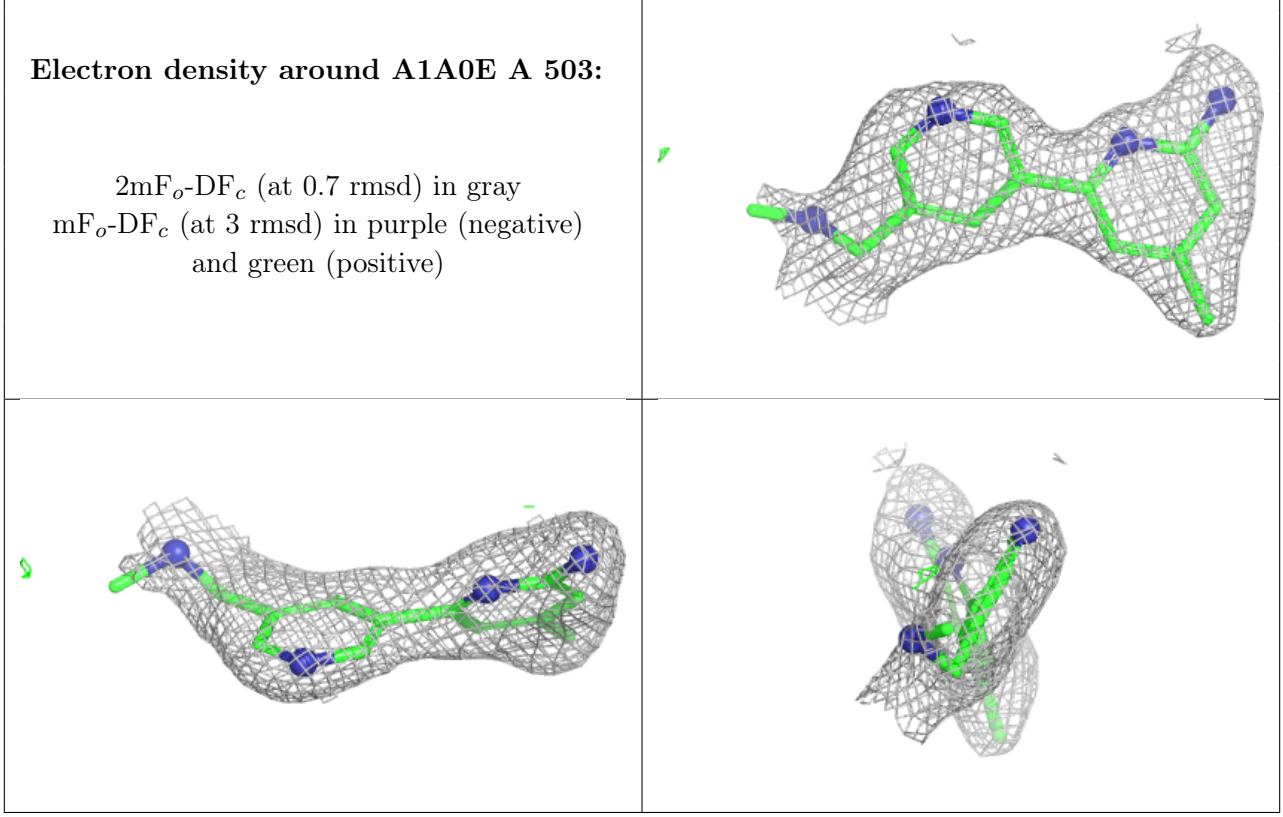
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BTB	D	506	14/14	0.69	0.19	51,69,75,77	0
6	GOL	C	508	6/6	0.71	0.11	73,78,84,89	0
5	BTB	A	506	14/14	0.72	0.15	89,96,100,102	0
5	BTB	B	506	14/14	0.73	0.18	48,71,80,80	0
6	GOL	C	507	6/6	0.74	0.14	75,76,79,81	0
6	GOL	A	507	6/6	0.75	0.13	63,73,78,82	0
10	ACT	C	504	4/4	0.80	0.21	61,74,77,82	0
5	BTB	A	505	14/14	0.84	0.14	60,71,82,83	0
5	BTB	B	510	14/14	0.85	0.16	22,62,72,73	0
6	GOL	D	507	6/6	0.86	0.17	54,63,64,66	0
5	BTB	D	505	14/14	0.87	0.15	41,66,82,87	0
6	GOL	A	508	6/6	0.88	0.18	26,56,66,70	0
10	ACT	D	504	4/4	0.88	0.20	55,65,68,79	0
4	A1A0E	A	503	17/17	0.89	0.13	33,54,76,78	0
5	BTB	B	505	14/14	0.90	0.14	39,52,72,76	0
5	BTB	A	504	14/14	0.90	0.15	45,83,95,101	0
6	GOL	C	506	6/6	0.91	0.09	48,61,64,67	0
10	ACT	B	504	4/4	0.91	0.13	31,48,51,59	0
4	A1A0E	C	503	17/17	0.92	0.12	33,46,80,81	0
3	H4B	C	502	17/17	0.93	0.08	33,41,47,51	0
3	H4B	A	502	17/17	0.93	0.09	42,48,58,60	0
5	BTB	C	505	14/14	0.94	0.12	20,67,75,78	0
3	H4B	B	502	17/17	0.94	0.08	27,35,41,42	0
4	A1A0E	D	503	17/17	0.94	0.10	20,30,68,68	0
6	GOL	B	507	6/6	0.95	0.14	53,56,62,63	0
7	CL	A	509	1/1	0.95	0.11	51,51,51,51	0
4	A1A0E	B	503	17/17	0.95	0.09	22,30,65,72	0
3	H4B	D	502	17/17	0.95	0.07	26,35,41,42	0
6	GOL	A	512	6/6	0.95	0.12	14,37,55,56	0
2	HEM	A	501	43/43	0.96	0.10	35,52,67,74	0
8	GD3	A	510	1/1	0.96	0.06	91,91,91,91	1
8	GD3	D	509	1/1	0.96	0.05	43,43,43,43	0
8	GD3	B	511	1/1	0.97	0.05	63,63,63,63	1
2	HEM	C	501	43/43	0.97	0.07	28,37,63,88	0
9	ZN	A	511	1/1	0.97	0.05	40,40,40,40	0
2	HEM	D	501	43/43	0.98	0.06	19,23,43,64	0
7	CL	C	509	1/1	0.99	0.09	44,44,44,44	0
7	CL	D	508	1/1	0.99	0.11	40,40,40,40	0
2	HEM	B	501	43/43	0.99	0.06	18,27,49,70	0
8	GD3	B	509	1/1	0.99	0.03	38,38,38,38	0
7	CL	B	508	1/1	0.99	0.11	37,37,37,37	0
9	ZN	C	510	1/1	1.00	0.03	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

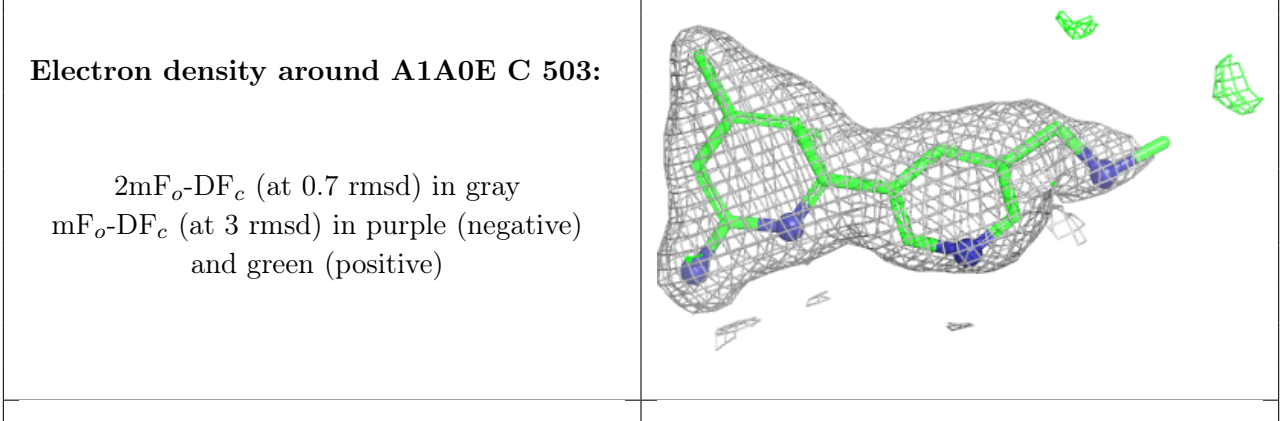
Electron density around A1A0E A 503:

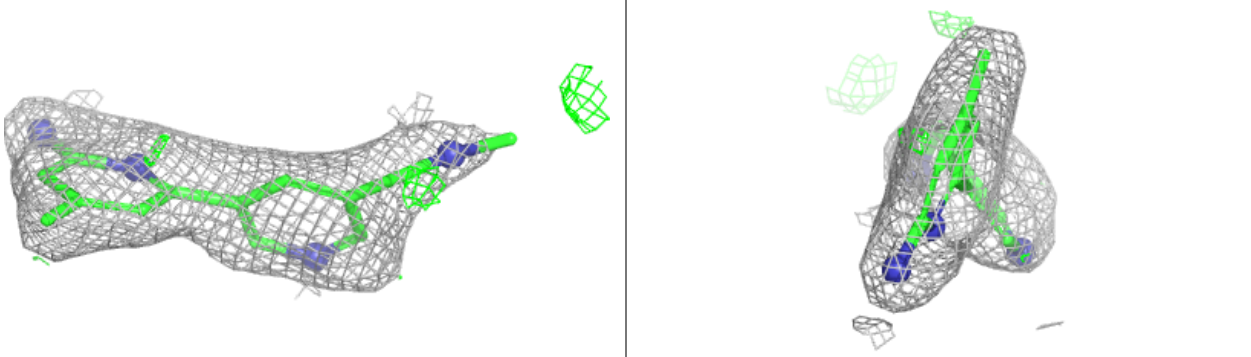
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around A1A0E C 503:

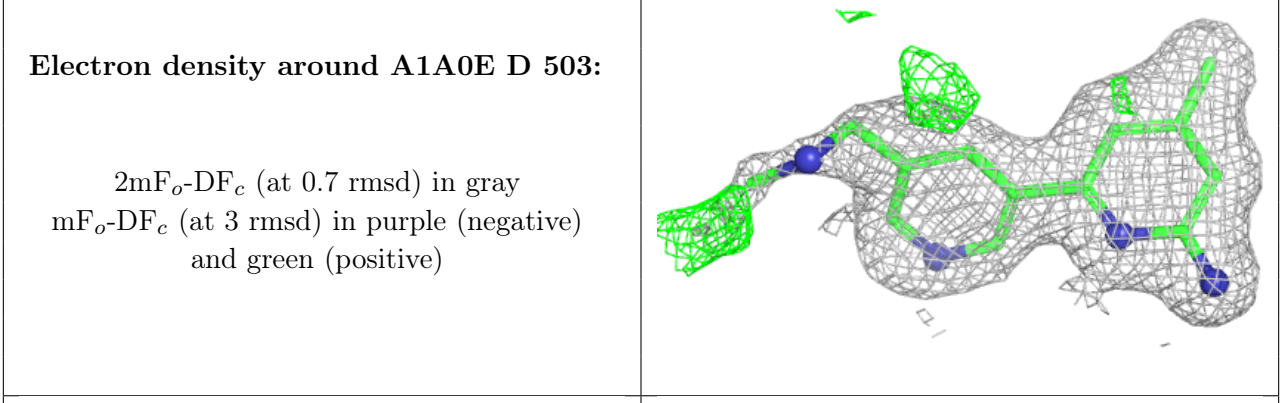
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

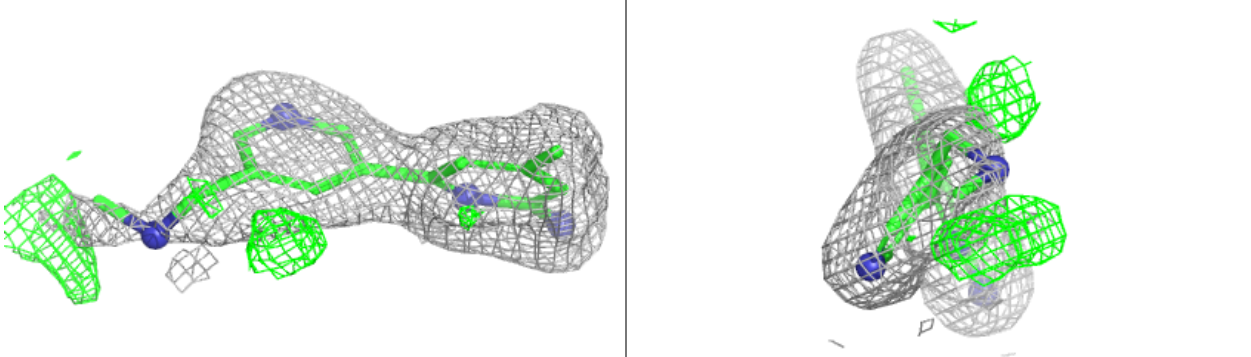




Electron density around A1A0E D 503:

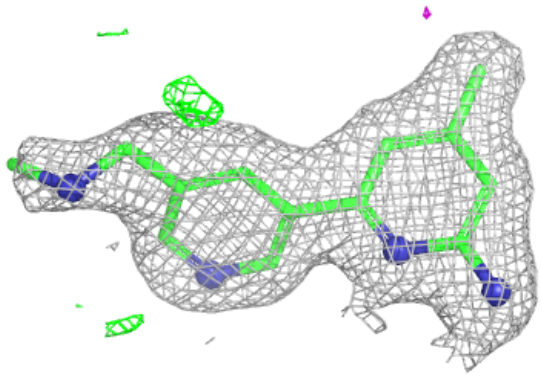
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

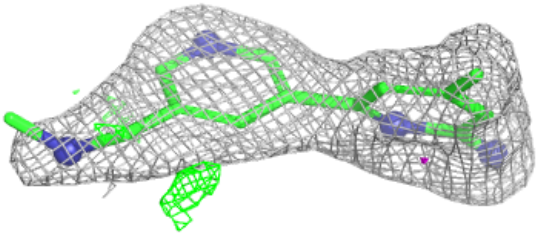


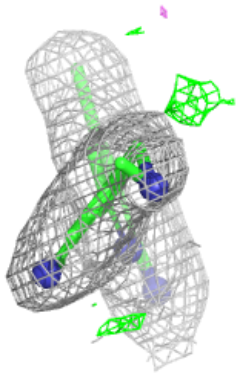


Electron density around A1A0E B 503:

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

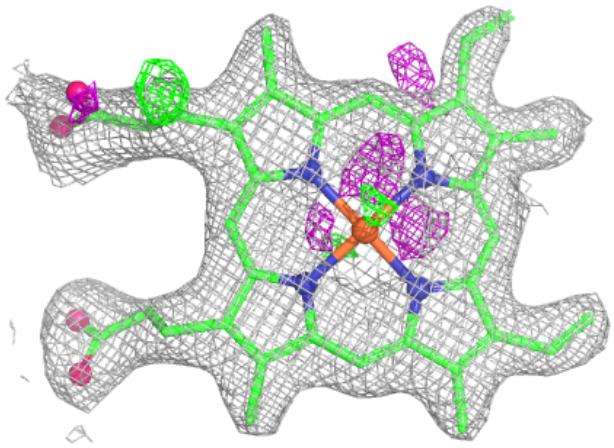


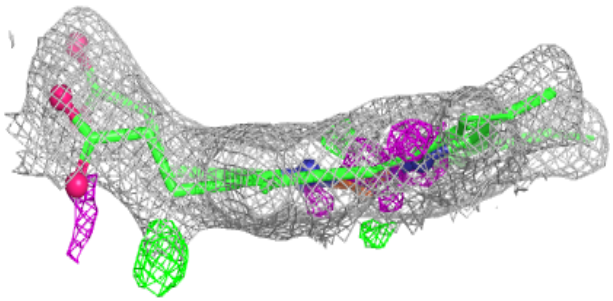


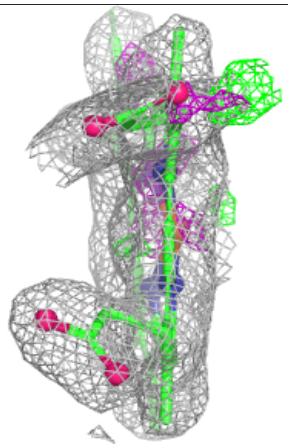


Electron density around HEM A 501:

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

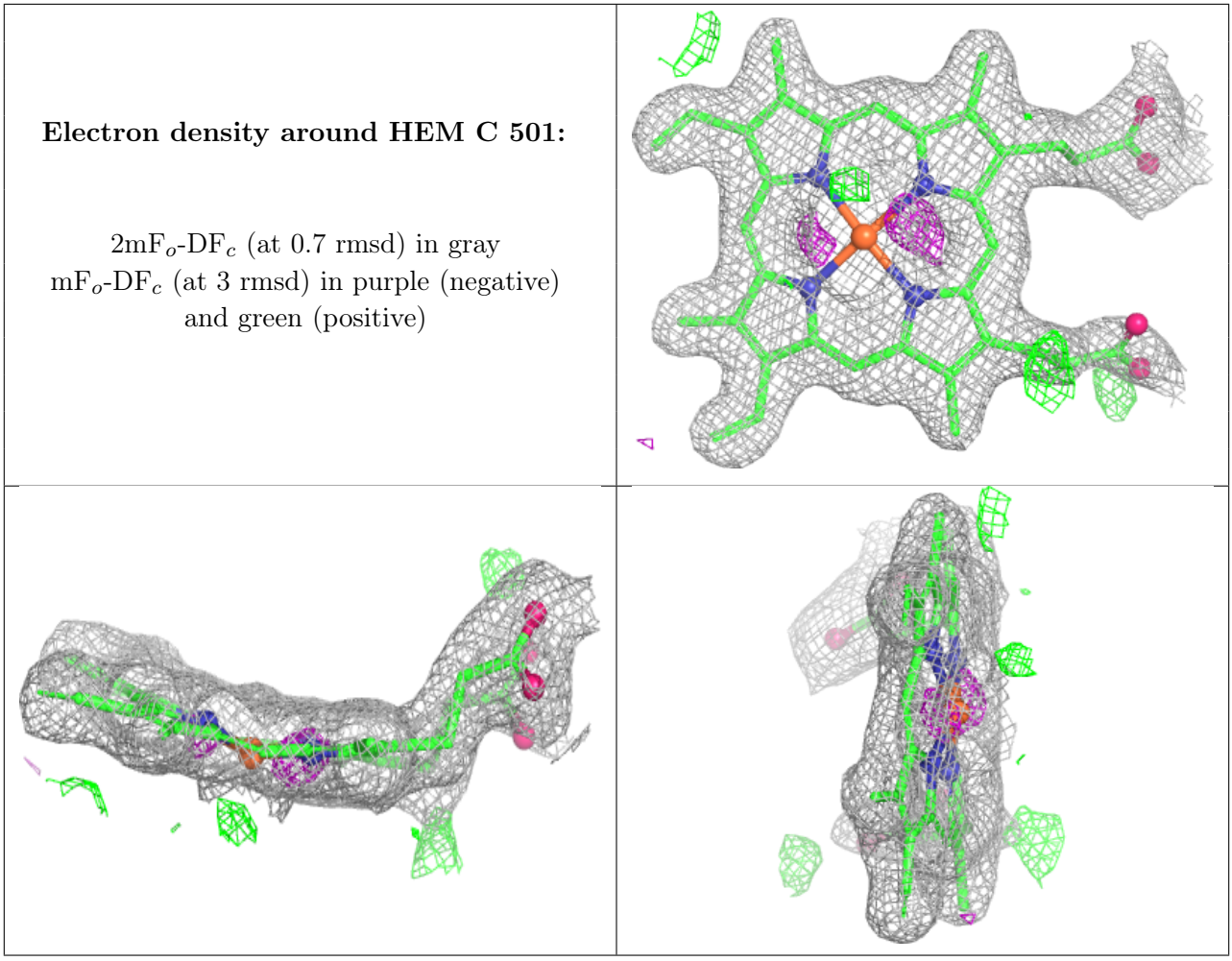






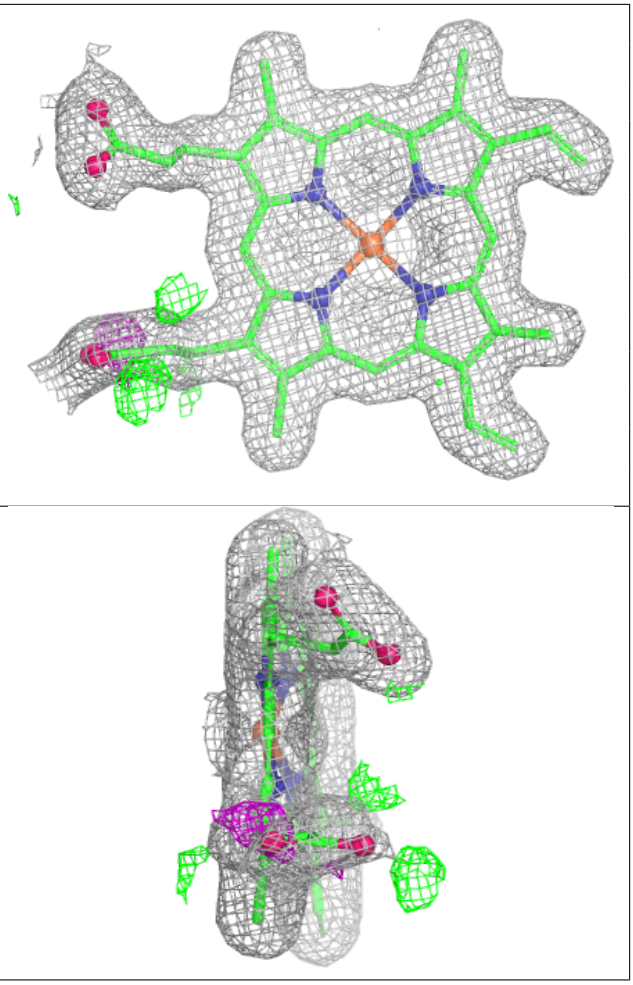
Electron density around HEM C 501:

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



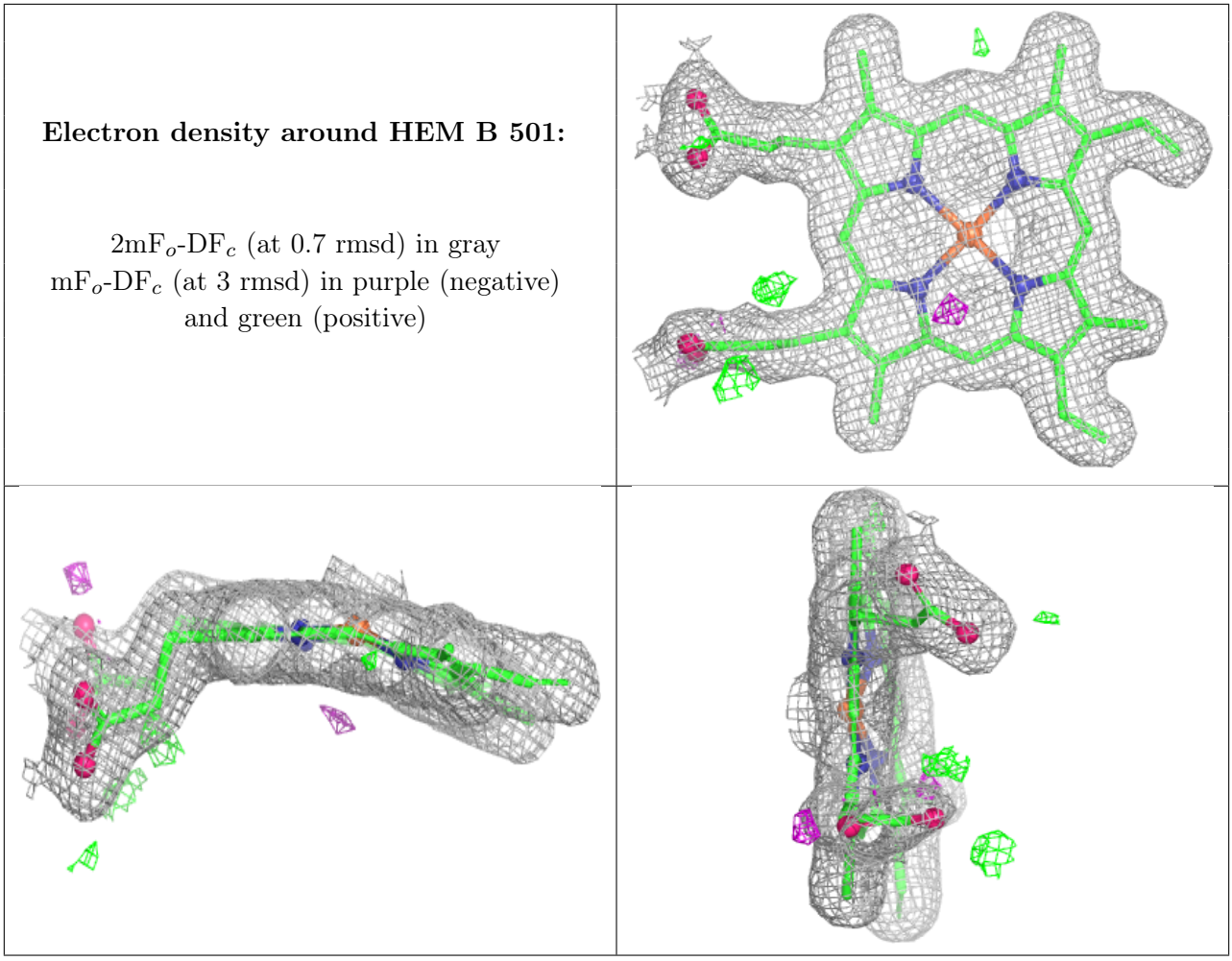
Electron density around HEM D 501:

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



Electron density around HEM B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.