Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:30 AM JST

PDB ID	:	5XA3 / pdb_00005xa3
Title	:	Crystal Structure of P450BM3 with Benzyloxycarbonyl-L-prolyl-L-phenylalanine
Authors	:	Shoji, O.; Yanagisawa, S.; Stanfield, J.K.; Suzuki, K.; Kasai, C.; Cong, Z.; Sugimoto, H.; Shiro, Y.; Watanabe, Y.
Deposited on	:	2017-03-10
Resolution	:	2.20 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:

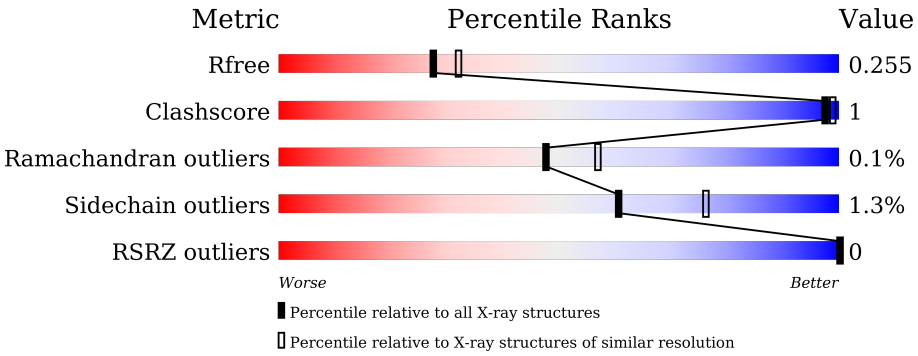
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	456	97%
1	B	456	96%
1	C	456	96%
1	D	456	96%

2 Entry composition

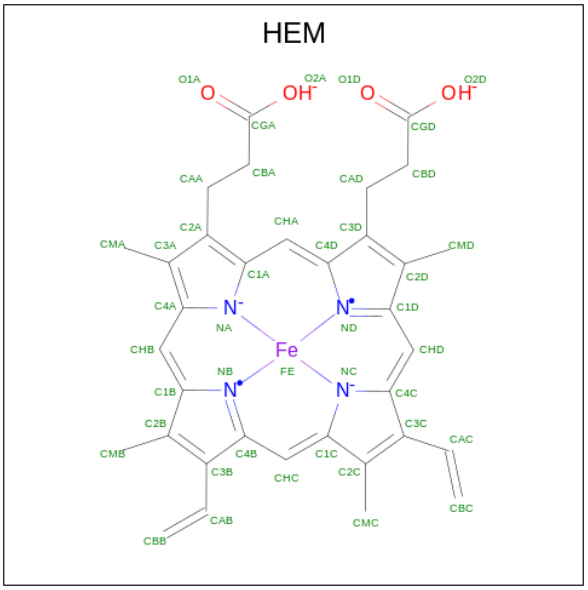
There are 7 unique types of molecules in this entry. The entry contains 15645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	2	0
			3674	2349	623	684	18			
1	B	453	Total	C	N	O	S	0	2	0
			3674	2349	623	684	18			
1	C	453	Total	C	N	O	S	0	2	0
			3674	2349	623	684	18			
1	D	453	Total	C	N	O	S	0	3	0
			3682	2354	624	685	19			

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



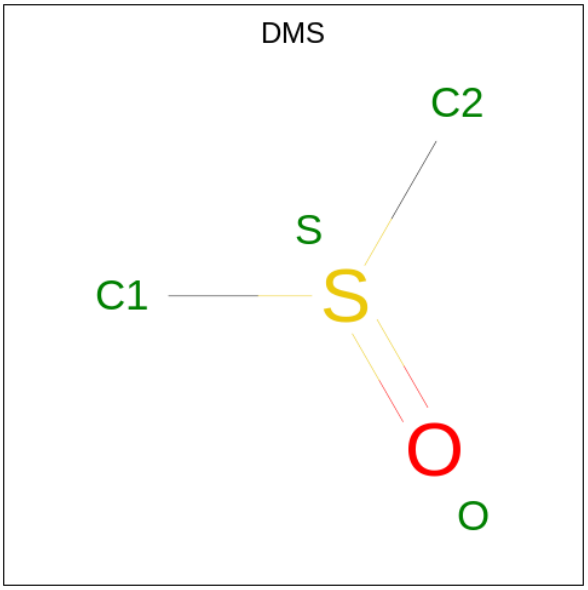
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

Continued from previous page...

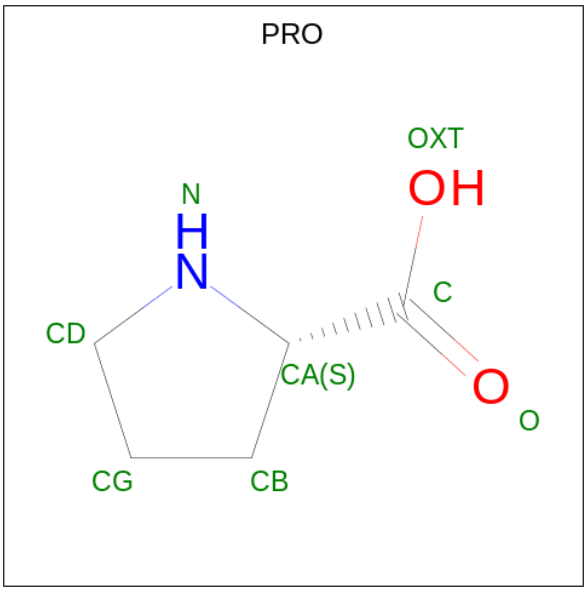
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



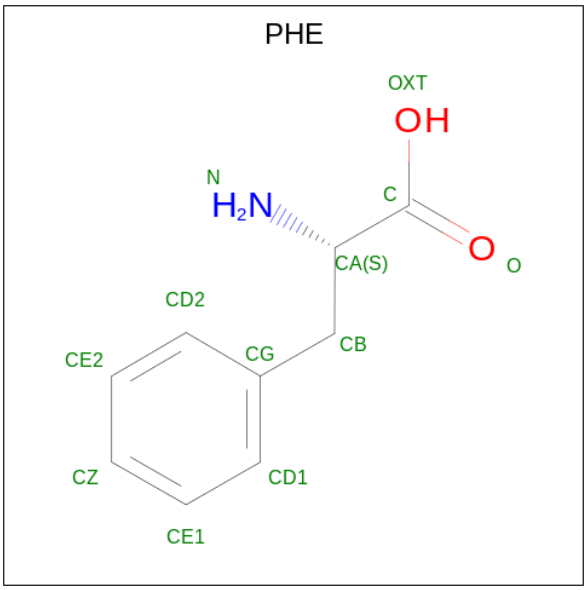
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



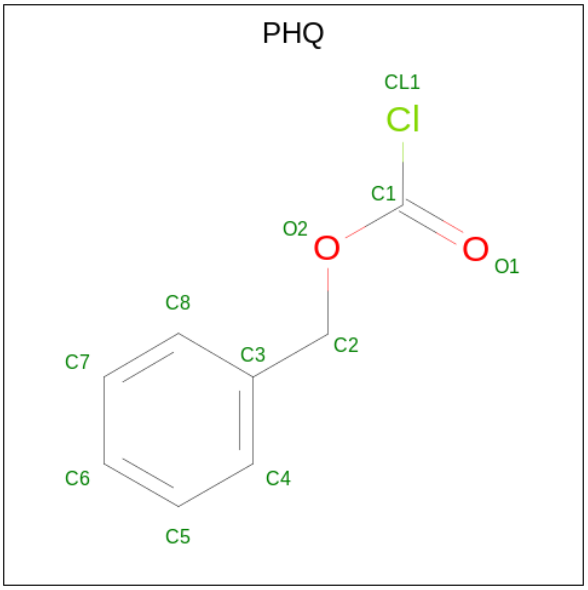
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 7 5 1 1	0	0
4	B	1	Total C N O 7 5 1 1	0	0
4	C	1	Total C N O 7 5 1 1	0	0
4	D	1	Total C N O 7 5 1 1	0	0

- Molecule 5 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 12 9 1 2	0	0
5	B	1	Total C N O 12 9 1 2	0	0
5	C	1	Total C N O 12 9 1 2	0	0
5	D	1	Total C N O 12 9 1 2	0	0

- Molecule 6 is benzyl chlorocarbonate (CCD ID: PHQ) (formula: $C_8H_7ClO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 8 2	0	0
6	B	1	Total C O 10 8 2	0	0
6	C	1	Total C O 10 8 2	0	0
6	D	1	Total C O 10 8 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	161	Total O 161 161	0	0
7	B	162	Total O 162 162	0	0

Continued on next page...

Continued from previous page...

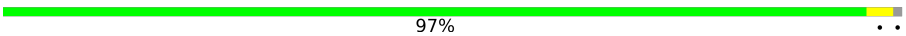
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	160	Total O 160 160	0	0
7	D	154	Total O 154 154	0	0

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: Bifunctional cytochrome P450/NADPH-P450 reductase

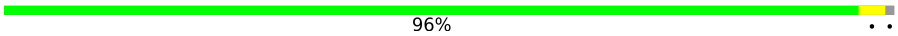
Chain A:





• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

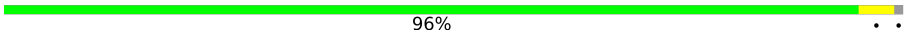
Chain B:





• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

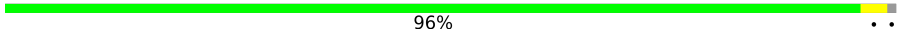
Chain C:





• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

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	126.23Å 58.52Å 145.95Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-2.20) 97.1 (50.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.221 , 0.253 0.225 , 0.255	Depositor DCC
R_{free} test set	5243 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 0.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15645	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8995e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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, DMS, PHQ

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	0.53	0/3760	0.78	0/5082
1	B	0.53	0/3760	0.80	0/5082
1	C	0.53	0/3760	0.81	1/5082 (0.0%)
1	D	0.53	0/3768	0.78	1/5092 (0.0%)
All	All	0.53	0/15048	0.79	2/20338 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	436	THR	N-CA-C	-5.21	103.75	108.75
1	D	436	THR	N-CA-C	-5.19	103.77	108.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3674	0	3640	3	0
1	B	3674	0	3640	5	0
1	C	3674	0	3640	5	0
1	D	3682	0	3648	5	0
2	A	43	0	30	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	7	0	7	0	0
4	B	7	0	7	0	0
4	C	7	0	7	0	0
4	D	7	0	7	0	0
5	A	12	0	9	0	0
5	B	12	0	9	0	0
5	C	12	0	9	0	0
5	D	12	0	9	0	0
6	A	10	0	7	0	0
6	B	10	0	7	0	0
6	C	10	0	7	0	0
6	D	10	0	7	0	0
7	A	161	0	0	0	0
7	B	162	0	0	0	0
7	C	160	0	0	0	0
7	D	154	0	0	0	0
All	All	15645	0	14804	25	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 1.

All (25) 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:B:134:ASN:HD21	1:D:161:ARG:H	1.43	0.66
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.84	0.60
2:A:501:HEM:HMB1	2:A:501:HEM:HBB2	1.85	0.59
2:C:501:HEM:HMC1	2:C:501:HEM:HBC2	1.86	0.57
1:D:148:LEU:HD21	1:D:413:VAL:HG21	1.86	0.57
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	1.87	0.56
1:B:126:LEU:HD21	1:B:145:MET:HE1	1.88	0.56
1:C:126:LEU:HD21	1:C:145:MET:HE1	1.88	0.55
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.87	0.55
1:A:220:ILE:HD11	1:A:258:ILE:HD12	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.89	0.54
1:C:220:ILE:HD11	1:C:258:ILE:HD12	1.89	0.54
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.90	0.54
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.90	0.53
1:C:148:LEU:HD21	1:C:413:VAL:HG21	1.91	0.53
1:B:150:LEU:HD11	1:B:174:ILE:HD11	1.93	0.51
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.92	0.51
1:B:220:ILE:HD11	1:B:258:ILE:HD12	1.92	0.51
2:C:501:HEM:HMB2	2:C:501:HEM:HBB2	1.92	0.51
1:A:16:ASN:HD22	1:A:43:GLU:H	1.59	0.49
1:C:118[B]:MET:HE3	1:C:155:LEU:HD21	1.97	0.47
1:C:150:LEU:HD11	1:C:174:ILE:HD11	1.97	0.45
1:D:149:THR:HA	1:D:409:GLU:OE2	2.19	0.42
1:D:267:GLU:HB3	1:D:438:THR:OG1	2.20	0.42
1:D:141:VAL:HB	1:D:142:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/456 (99%)	437 (96%)	15 (3%)	1 (0%)	43	51
1	B	453/456 (99%)	437 (96%)	16 (4%)	0	100	100
1	C	453/456 (99%)	439 (97%)	14 (3%)	0	100	100
1	D	454/456 (100%)	440 (97%)	13 (3%)	1 (0%)	43	51
All	All	1813/1824 (99%)	1753 (97%)	58 (3%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	193	PRO
1	A	193	PRO

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	399/400 (100%)	393 (98%)	6 (2%)	57	73
1	B	399/400 (100%)	393 (98%)	6 (2%)	57	73
1	C	399/400 (100%)	392 (98%)	7 (2%)	51	68
1	D	400/400 (100%)	395 (99%)	5 (1%)	61	76
All	All	1597/1600 (100%)	1573 (98%)	24 (2%)	61	73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158[A]	PHE
1	A	158[B]	PHE
1	A	228	GLU
1	A	229	GLN
1	A	233	LEU
1	A	437	LEU
1	B	148	LEU
1	B	158[A]	PHE
1	B	158[B]	PHE
1	B	233	LEU
1	B	306	LYS
1	B	440	LYS
1	C	158[A]	PHE
1	C	158[B]	PHE
1	C	200	GLU
1	C	233	LEU
1	C	310	GLN
1	C	437	LEU
1	C	440	LYS
1	D	158[A]	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	158[B]	PHE
1	D	200	GLU
1	D	218	LYS
1	D	233	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	16	ASN
1	A	101	ASN
1	A	109	GLN
1	A	110	GLN
1	A	186	ASN
1	A	239	ASN
1	A	310	GLN
1	A	381	ASN
1	A	387	GLN
1	B	7	GLN
1	B	70	ASN
1	B	95	ASN
1	B	110	GLN
1	B	134	ASN
1	B	186	ASN
1	B	189	GLN
1	B	229	GLN
1	B	239	ASN
1	B	283	ASN
1	B	288	GLN
1	B	359	GLN
1	B	395	ASN
1	B	428	ASN
1	C	7	GLN
1	C	70	ASN
1	C	95	ASN
1	C	110	GLN
1	C	186	ASN
1	C	283	ASN
1	C	310	GLN
1	C	395	ASN
1	C	420	HIS
1	D	7	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	101	ASN
1	D	110	GLN
1	D	186	ASN
1	D	285	HIS
1	D	359	GLN
1	D	395	ASN

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

20 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
4	PRO	D	504	6,5	5,7,8	0.47	0	7,8,10	1.56	2 (28%)
6	PHQ	B	503	4	9,10,11	1.52	1 (11%)	10,11,13	0.56	0
6	PHQ	A	503	4	9,10,11	1.49	1 (11%)	10,11,13	0.46	0
2	HEM	B	501	1,3	50,50,50	1.54	6 (12%)	66,82,82	1.60	13 (19%)
3	DMS	A	502	-	3,3,3	0.60	0	3,3,3	0.45	0
5	PHE	C	505	4	11,12,12	1.70	1 (9%)	14,15,15	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	A	501	1	50,50,50	1.56	6 (12%)	66,82,82	1.59	12 (18%)
5	PHE	B	505	4	11,12,12	1.73	1 (9%)	14,15,15	0.75	0
6	PHQ	C	503	4	9,10,11	1.54	1 (11%)	10,11,13	0.60	0
4	PRO	B	504	6,5	5,7,8	0.45	0	7,8,10	1.61	2 (28%)
5	PHE	A	505	4	11,12,12	1.77	1 (9%)	14,15,15	0.73	0
3	DMS	C	502	-	3,3,3	0.59	0	3,3,3	0.47	0
4	PRO	A	504	6,5	5,7,8	0.46	0	7,8,10	1.50	2 (28%)
4	PRO	C	504	6,5	5,7,8	0.44	0	7,8,10	1.57	2 (28%)
2	HEM	C	501	1	50,50,50	1.54	6 (12%)	66,82,82	1.58	13 (19%)
3	DMS	D	502	-	3,3,3	0.59	0	3,3,3	0.43	0
6	PHQ	D	503	4	9,10,11	1.53	1 (11%)	10,11,13	0.56	0
2	HEM	D	501	1	50,50,50	1.55	6 (12%)	66,82,82	1.59	12 (18%)
5	PHE	D	505	4	11,12,12	1.77	1 (9%)	14,15,15	0.76	0
3	DMS	B	502	2	3,3,3	0.54	0	3,3,3	0.48	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	PHQ	A	503	4	-	2/4/4/5	0/1/1/1
4	PRO	C	504	6,5	-	0/0/9/11	0/1/1/1
2	HEM	B	501	1,3	-	3/14/54/54	-
4	PRO	D	504	6,5	-	0/0/9/11	0/1/1/1
6	PHQ	C	503	4	-	2/4/4/5	0/1/1/1
4	PRO	B	504	6,5	-	0/0/9/11	0/1/1/1
6	PHQ	B	503	4	-	2/4/4/5	0/1/1/1
5	PHE	A	505	4	-	1/8/8/8	0/1/1/1
2	HEM	C	501	1	-	2/14/54/54	-
6	PHQ	D	503	4	-	2/4/4/5	0/1/1/1
2	HEM	D	501	1	-	2/14/54/54	-
5	PHE	C	505	4	-	0/8/8/8	0/1/1/1
5	PHE	D	505	4	-	0/8/8/8	0/1/1/1
4	PRO	A	504	6,5	-	0/0/9/11	0/1/1/1
2	HEM	A	501	1	-	2/14/54/54	-
5	PHE	B	505	4	-	0/8/8/8	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	505	PHE	CB-CG	-5.31	1.38	1.51
5	A	505	PHE	CB-CG	-5.30	1.38	1.51
5	B	505	PHE	CB-CG	-5.17	1.38	1.51
2	D	501	HEM	FE-NB	5.17	2.10	1.94
2	A	501	HEM	FE-NB	5.13	2.10	1.94
2	C	501	HEM	FE-NB	5.12	2.10	1.94
2	B	501	HEM	FE-NB	5.11	2.10	1.94
5	C	505	PHE	CB-CG	-5.02	1.39	1.51
2	D	501	HEM	FE-NC	4.36	2.09	1.95
2	B	501	HEM	FE-NC	4.36	2.09	1.95
2	C	501	HEM	FE-NC	4.35	2.09	1.95
2	A	501	HEM	FE-NC	4.32	2.09	1.95
6	D	503	PHQ	C2-C3	-4.04	1.41	1.50
6	C	503	PHQ	C2-C3	-4.03	1.41	1.50
6	B	503	PHQ	C2-C3	-4.01	1.41	1.50
6	A	503	PHQ	C2-C3	-3.89	1.41	1.50
2	A	501	HEM	C1B-NB	-3.64	1.34	1.40
2	B	501	HEM	C1B-NB	-3.62	1.34	1.40
2	D	501	HEM	C1B-NB	-3.57	1.34	1.40
2	C	501	HEM	C1B-NB	-3.56	1.34	1.40
2	D	501	HEM	C4D-ND	-2.65	1.35	1.40
2	B	501	HEM	C4D-ND	-2.59	1.35	1.40
2	C	501	HEM	C4D-ND	-2.57	1.35	1.40
2	A	501	HEM	C4D-ND	-2.52	1.36	1.40
2	B	501	HEM	C3B-C4B	2.42	1.49	1.44
2	C	501	HEM	C3B-C4B	2.42	1.49	1.44
2	A	501	HEM	C3B-C4B	2.39	1.49	1.44
2	D	501	HEM	C3B-C4B	2.34	1.49	1.44
2	A	501	HEM	C4B-NB	-2.29	1.34	1.38
2	D	501	HEM	C4B-NB	-2.23	1.34	1.38
2	C	501	HEM	C4B-NB	-2.17	1.34	1.38
2	B	501	HEM	C4B-NB	-2.10	1.34	1.38

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	HEM	C1B-NB-C4B	5.04	110.27	105.07
2	B	501	HEM	C1B-NB-C4B	5.00	110.24	105.07
2	A	501	HEM	C1B-NB-C4B	5.00	110.24	105.07
2	C	501	HEM	C1B-NB-C4B	4.89	110.12	105.07
2	B	501	HEM	CHC-C4B-NB	3.94	128.70	124.42
2	D	501	HEM	CHD-C1D-ND	3.86	128.61	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	HEM	CHC-C4B-NB	3.85	128.60	124.42
2	A	501	HEM	CHC-C4B-NB	3.80	128.54	124.42
2	B	501	HEM	CHD-C1D-ND	3.78	128.53	124.42
2	C	501	HEM	CHC-C4B-NB	3.76	128.50	124.42
2	C	501	HEM	CHD-C1D-ND	3.74	128.48	124.42
2	A	501	HEM	CHD-C1D-ND	3.71	128.44	124.42
2	A	501	HEM	CHA-C4D-ND	3.35	128.51	124.37
2	A	501	HEM	C4C-NC-C1C	3.31	108.59	105.35
2	C	501	HEM	CHA-C4D-ND	3.28	128.42	124.37
2	D	501	HEM	CHA-C4D-ND	3.28	128.41	124.37
2	B	501	HEM	CHA-C4D-ND	3.20	128.32	124.37
2	C	501	HEM	C4C-NC-C1C	3.19	108.47	105.35
2	B	501	HEM	CHD-C1D-C2D	-3.16	120.03	124.98
2	D	501	HEM	CHD-C1D-C2D	-3.15	120.06	124.98
2	D	501	HEM	C4C-NC-C1C	3.10	108.39	105.35
2	B	501	HEM	C4C-NC-C1C	3.08	108.37	105.35
2	C	501	HEM	CHD-C1D-C2D	-3.07	120.18	124.98
2	D	501	HEM	CMD-C2D-C1D	3.03	129.65	125.04
2	A	501	HEM	CHD-C1D-C2D	-3.02	120.27	124.98
4	B	504	PRO	CB-CA-C	-2.97	108.62	112.70
2	C	501	HEM	CMD-C2D-C1D	2.92	129.49	125.04
2	A	501	HEM	CMD-C2D-C1D	2.91	129.47	125.04
2	B	501	HEM	CMD-C2D-C1D	2.88	129.43	125.04
4	D	504	PRO	CB-CA-C	-2.84	108.79	112.70
2	A	501	HEM	O2A-CGA-CBA	2.83	123.12	114.03
2	B	501	HEM	O2A-CGA-CBA	2.80	123.02	114.03
4	C	504	PRO	CB-CA-C	-2.79	108.87	112.70
2	D	501	HEM	O2A-CGA-CBA	2.75	122.87	114.03
4	A	504	PRO	CB-CA-C	-2.71	108.97	112.70
2	A	501	HEM	CHA-C4D-C3D	-2.69	120.28	125.33
2	C	501	HEM	O2A-CGA-CBA	2.66	122.58	114.03
4	B	504	PRO	O-C-CA	-2.60	117.97	124.78
4	C	504	PRO	O-C-CA	-2.57	118.04	124.78
2	C	501	HEM	CHA-C4D-C3D	-2.56	120.53	125.33
2	B	501	HEM	CHA-C4D-C3D	-2.55	120.55	125.33
2	D	501	HEM	CHA-C4D-C3D	-2.52	120.61	125.33
2	B	501	HEM	CAD-C3D-C4D	2.49	129.01	124.66
4	D	504	PRO	O-C-CA	-2.44	118.38	124.78
2	D	501	HEM	C4B-C3B-C2B	-2.43	105.19	107.11
2	A	501	HEM	C4B-C3B-C2B	-2.41	105.20	107.11
2	C	501	HEM	CAD-C3D-C4D	2.38	128.82	124.66
4	A	504	PRO	O-C-CA	-2.35	118.62	124.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	C4B-C3B-C2B	-2.33	105.27	107.11
2	B	501	HEM	C4B-C3B-C2B	-2.30	105.29	107.11
2	A	501	HEM	CAD-C3D-C4D	2.28	128.63	124.66
2	D	501	HEM	CAD-C3D-C4D	2.18	128.47	124.66
2	C	501	HEM	O2D-CGD-CBD	2.08	120.72	114.03
2	D	501	HEM	CBD-CAD-C3D	-2.06	106.89	112.63
2	B	501	HEM	O2D-CGD-CBD	2.04	120.59	114.03
2	A	501	HEM	O2D-CGD-CBD	2.02	120.53	114.03
2	C	501	HEM	C1A-CHA-C4D	-2.02	121.54	126.34
2	B	501	HEM	C1A-CHA-C4D	-2.01	121.58	126.34

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	503	PHQ	C3-C2-O2-C1
6	B	503	PHQ	C3-C2-O2-C1
6	D	503	PHQ	C3-C2-O2-C1
6	C	503	PHQ	C3-C2-O2-C1
6	A	503	PHQ	O1-C1-O2-C2
6	B	503	PHQ	O1-C1-O2-C2
6	C	503	PHQ	O1-C1-O2-C2
6	D	503	PHQ	O1-C1-O2-C2
2	C	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAA-CBA-CGA-O2A
5	A	505	PHE	OXT-C-CA-N

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	2	0
2	A	501	HEM	2	0
2	C	501	HEM	2	0

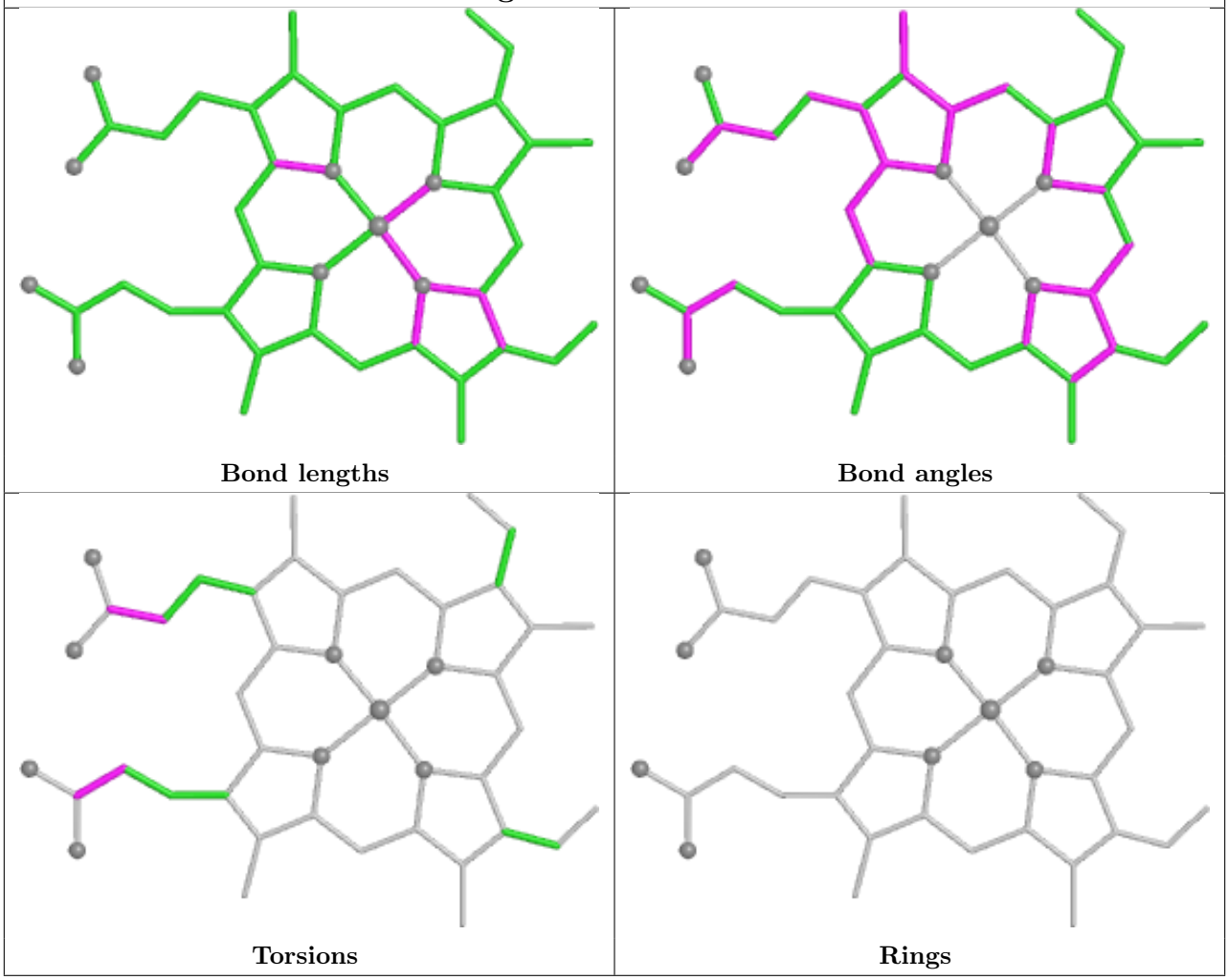
Continued on next page...

Continued from previous page...

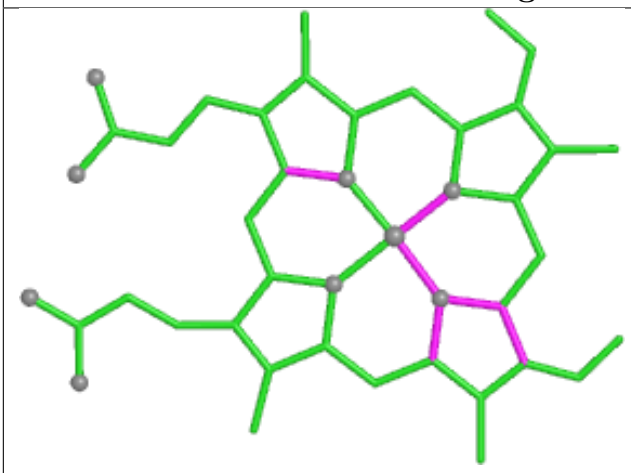
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	HEM	2	0

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

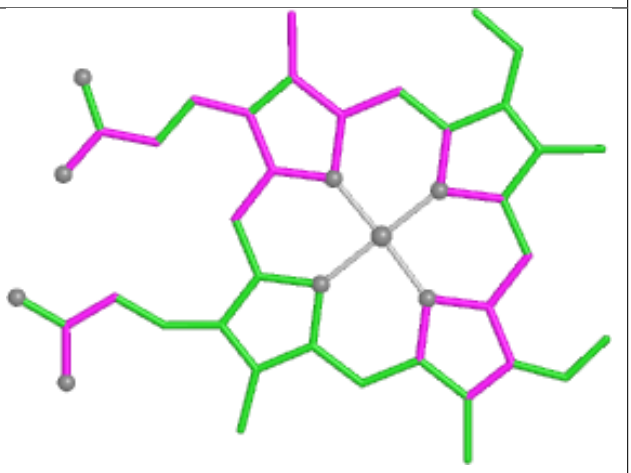
Ligand HEM B 501



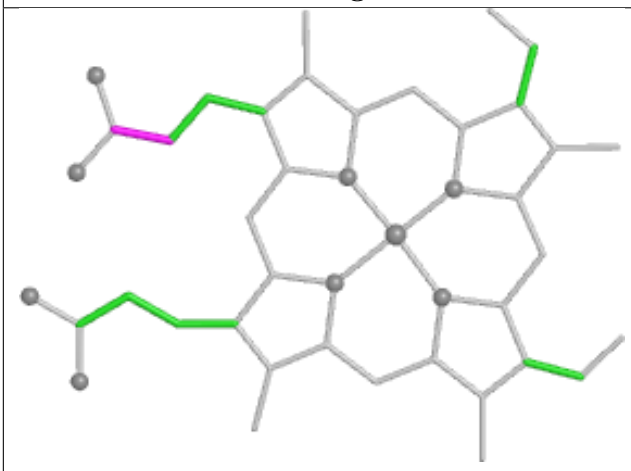
Ligand HEM A 501



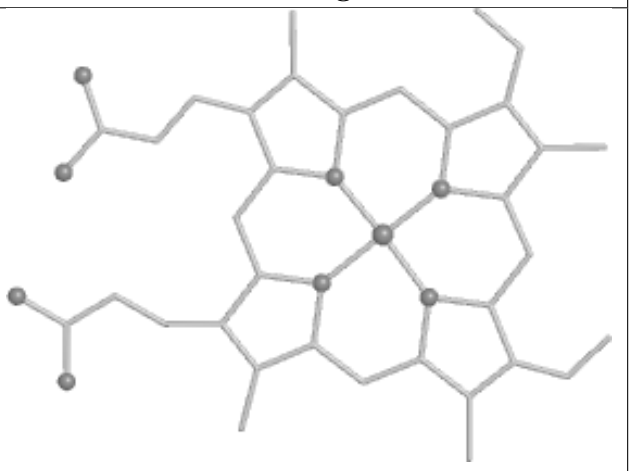
Bond lengths



Bond angles

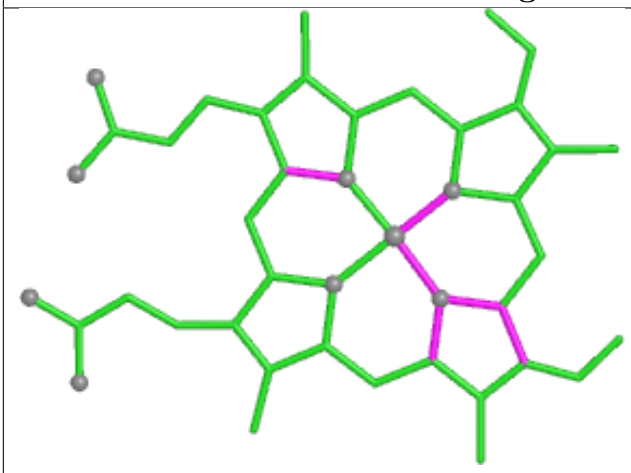


Torsions

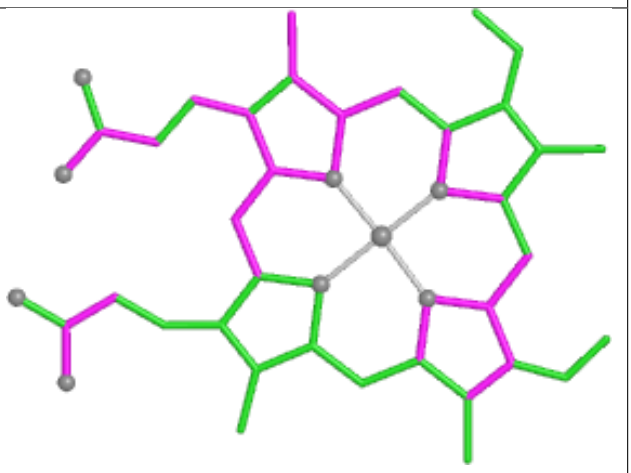


Rings

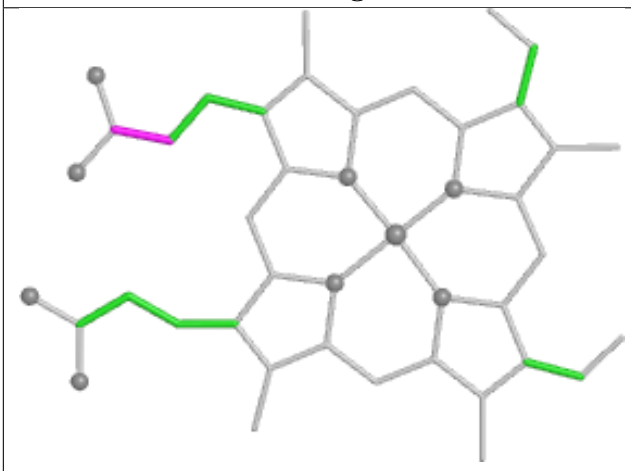
Ligand HEM C 501



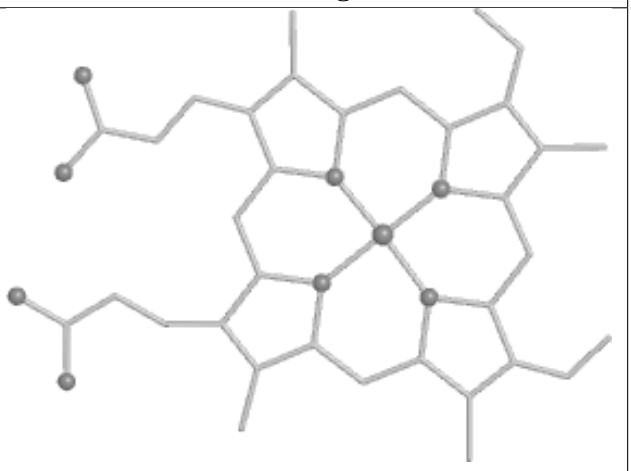
Bond lengths



Bond angles

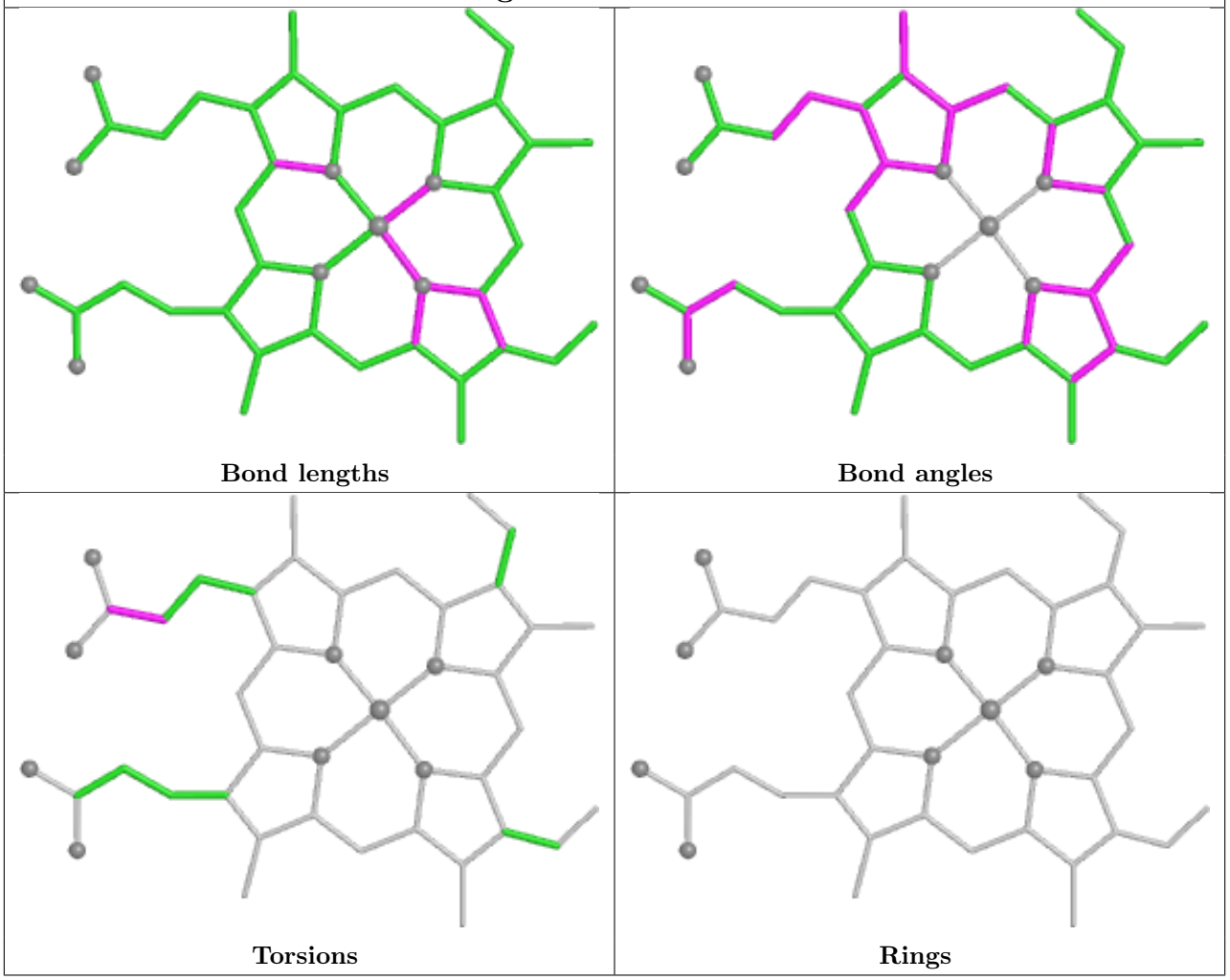


Torsions



Rings

Ligand HEM D 501



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	453/456 (99%)	-1.44	0	100	100	7, 18, 50, 82	2 (0%)
1	B	453/456 (99%)	-1.48	0	100	100	8, 17, 45, 70	2 (0%)
1	C	453/456 (99%)	-1.47	0	100	100	8, 17, 45, 69	2 (0%)
1	D	453/456 (99%)	-1.44	0	100	100	7, 18, 50, 84	3 (0%)
All	All	1812/1824 (99%)	-1.46	0	100	100	7, 17, 48, 84	9 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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
6	PHQ	A	503	10/11	0.98	0.06	33,37,38,38	0
3	DMS	C	502	4/4	0.99	0.07	30,31,31,32	0
4	PRO	A	504	7/8	0.99	0.03	28,30,31,32	0
4	PRO	B	504	7/8	0.99	0.03	24,25,26,26	0

Continued on next page...

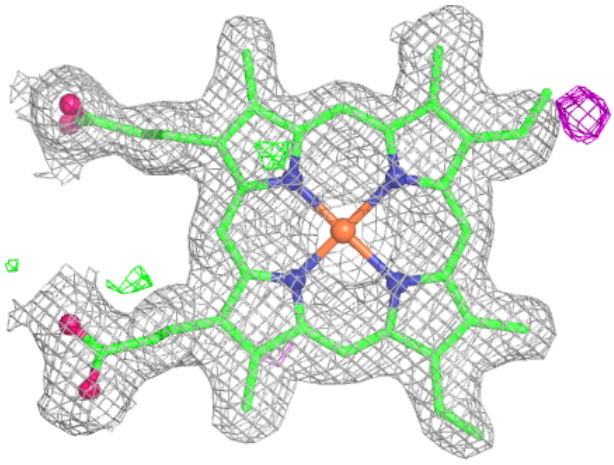
Continued from previous page...

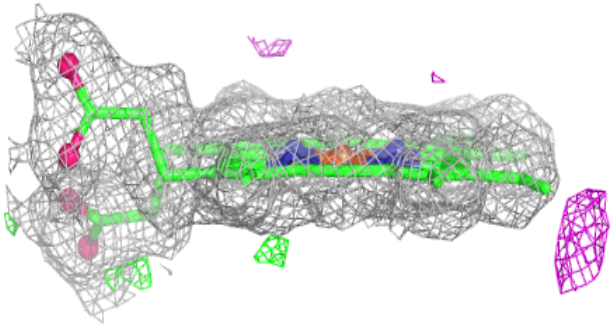
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PRO	C	504	7/8	0.99	0.03	25,26,27,27	0
4	PRO	D	504	7/8	0.99	0.03	30,32,33,33	0
5	PHE	A	505	12/12	0.99	0.03	26,27,27,28	0
5	PHE	B	505	12/12	0.99	0.03	23,24,24,24	0
5	PHE	C	505	12/12	0.99	0.03	24,25,25,25	0
5	PHE	D	505	12/12	0.99	0.03	28,29,29,30	0
3	DMS	A	502	4/4	0.99	0.06	36,36,36,38	0
6	PHQ	B	503	10/11	0.99	0.06	27,29,30,30	0
6	PHQ	C	503	10/11	0.99	0.07	28,30,31,31	0
6	PHQ	D	503	10/11	0.99	0.06	35,39,41,41	0
2	HEM	C	501	43/43	1.00	0.02	9,9,9,10	0
2	HEM	D	501	43/43	1.00	0.03	10,10,10,10	0
2	HEM	A	501	43/43	1.00	0.03	9,9,10,10	0
3	DMS	B	502	4/4	1.00	0.04	26,26,26,26	0
2	HEM	B	501	43/43	1.00	0.03	8,8,8,9	0
3	DMS	D	502	4/4	1.00	0.04	32,33,33,33	0

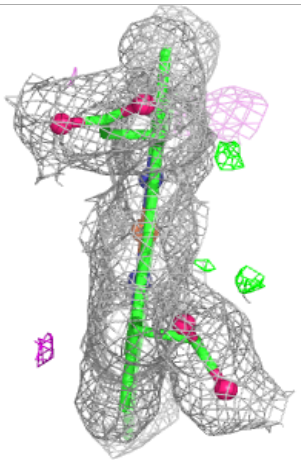
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

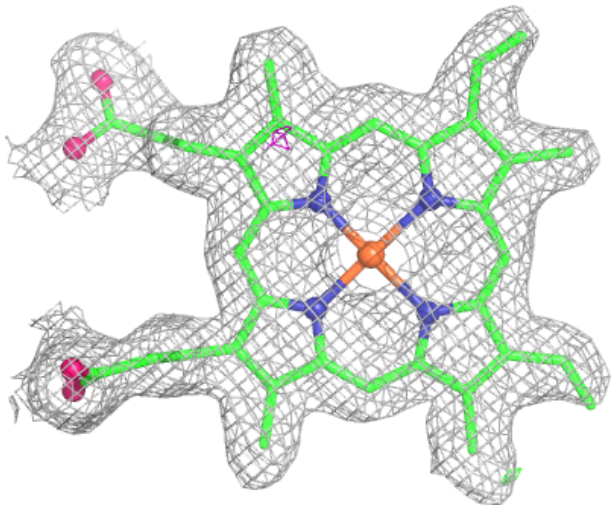


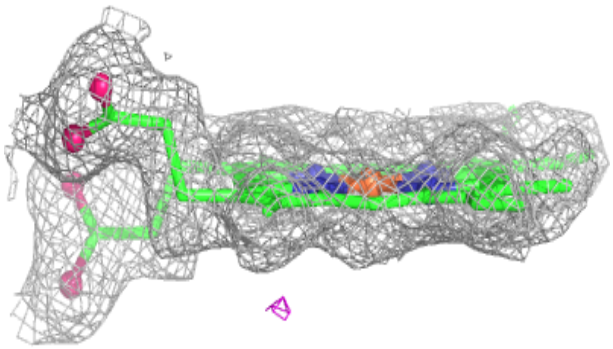


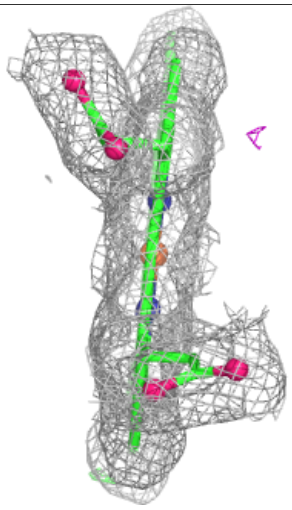


Electron density around HEM D 501:

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

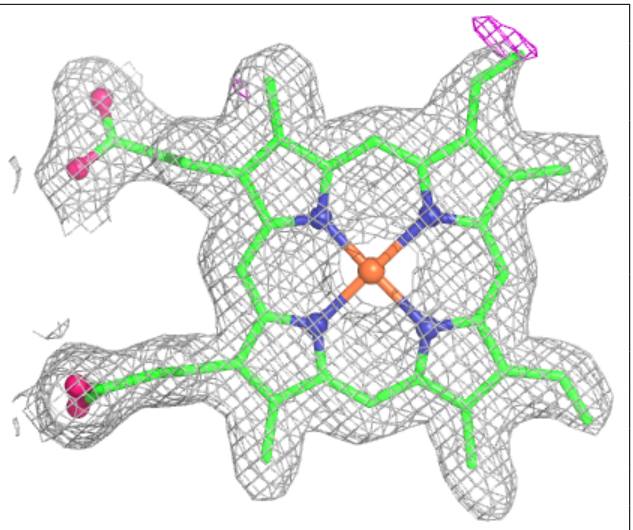


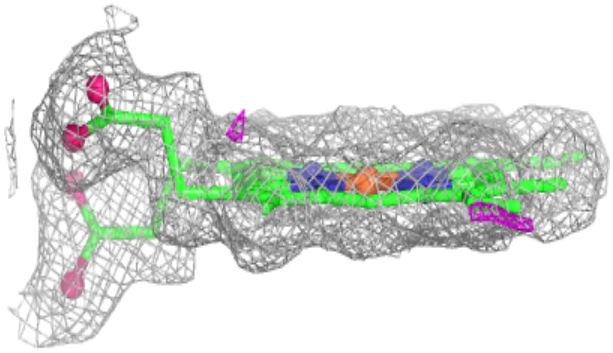


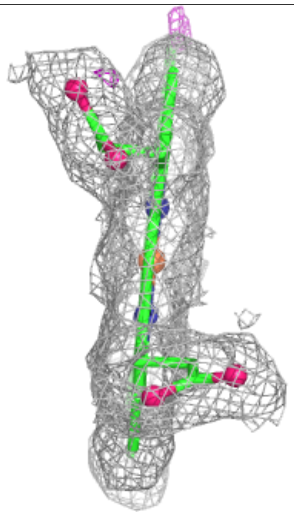


Electron density around HEM A 501:

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

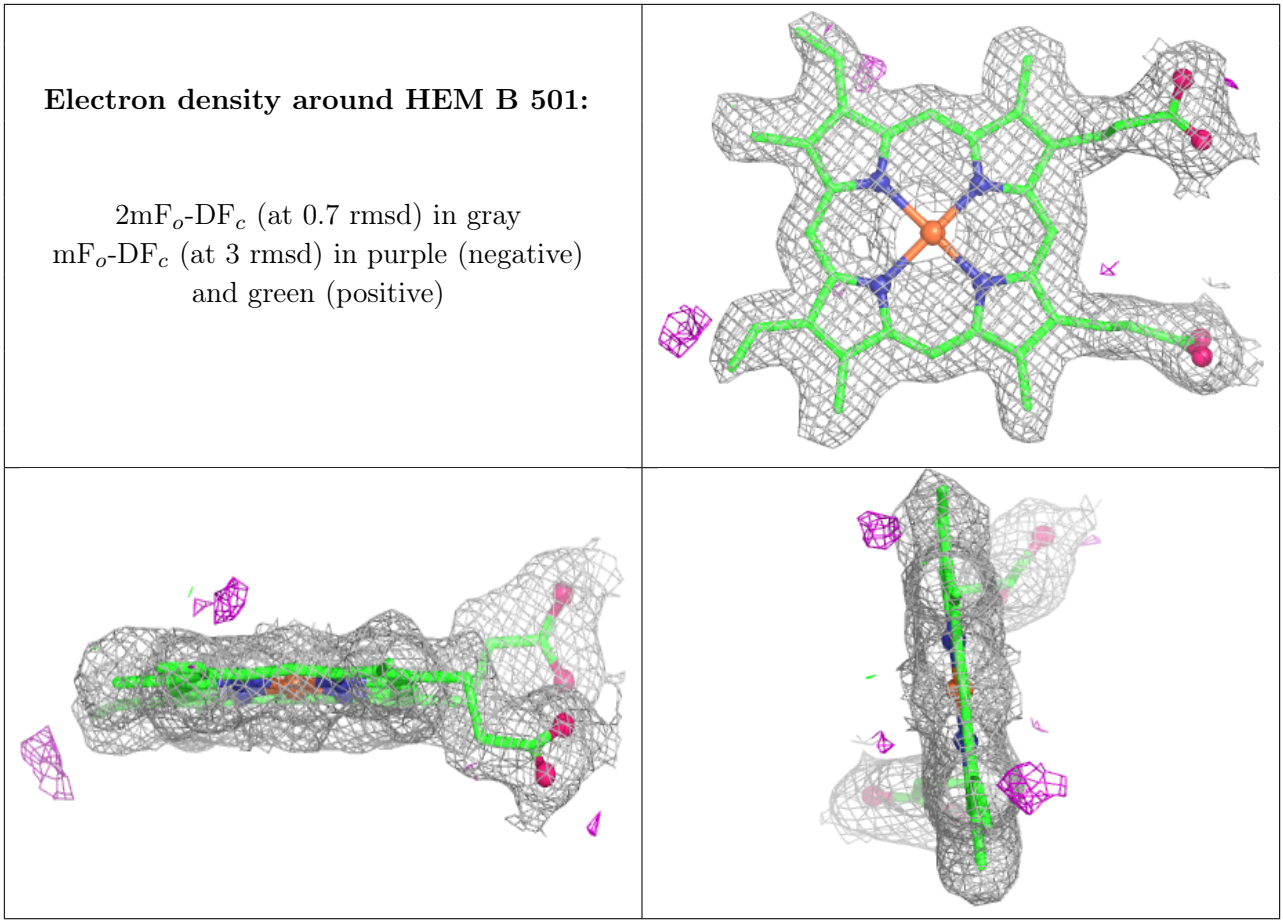






Electron density around HEM B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.