

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 4, 2023 – 09:05 PM EDT

PDB ID : 3UAS

Title: Cytochrome P450 2B4 covalently bound to the mechanism-based inactivator

9-ethynylphenanthrene

Authors: Gay, S.C.; Zhang, H.; Shah, M.B.; Stout, C.D.; Halpert, J.R.; Hollenberg, P.F.

Deposited on : 2011-10-21

Resolution : 2.94 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 (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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

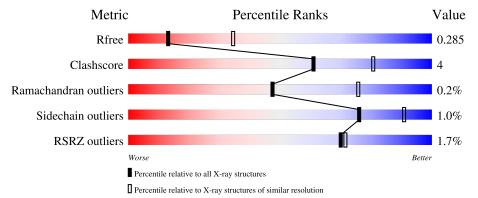
Validation Pipeline (wwPDB-VP) : 2.35

## 1 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 2.94 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
$R_{free}$	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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			
			2%			
1	A	476	86%	11%	•	



## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3892 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 Cytochrome P450 2B4.

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	A	461	Total 3704	C 2387	N 644	O 663	S 10	0	1	0	

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	GLU	engineered mutation	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	SER	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	ALA	deletion	UNP P00178
A	?	-	GLY	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	LEU	deletion	UNP P00178
A	?	-	PHE	deletion	UNP P00178
A	?	-	ARG	deletion	UNP P00178
A	22	LYS	GLY	engineered mutation	UNP P00178
A	23	LYS	HIS	engineered mutation	UNP P00178
A	24	THR	PRO	engineered mutation	UNP P00178
A	25	SER	LYS	engineered mutation	UNP P00178
A	26	SER	ALA	engineered mutation	UNP P00178
A	27	LYS	HIS	engineered mutation	UNP P00178
A	29	LYS	ARG	engineered mutation	UNP P00178

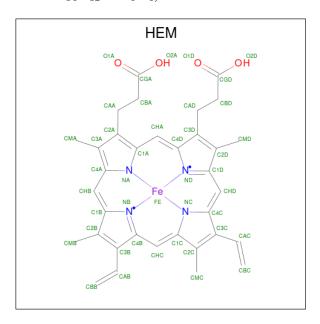
Continued on next page...



Continued from previous page...

Chain	Residue	Modelled	Actual Comment		Reference
A	221	SER	PRO	SEE REMARK 999	UNP P00178
A	226	TYR	HIS	engineered mutation	UNP P00178
A	492	HIS	-	expression tag	UNP P00178
A	493	HIS	-	expression tag	UNP P00178
A	494	HIS	-	expression tag	UNP P00178
A	495	HIS	-	expression tag	UNP P00178

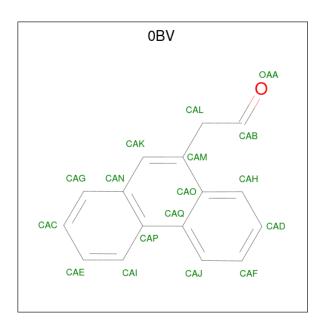
 $\bullet$  Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\rm C_{34}H_{32}FeN_4O_4).$ 



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

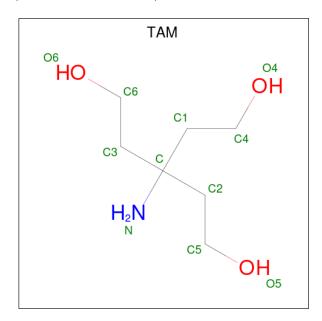
 $\bullet$  Molecule 3 is phenanthren-9-ylacetal dehyde (three-letter code: 0BV) (formula:  $\rm C_{16}H_{12}O).$ 





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 17	C 16	O 1	0	0

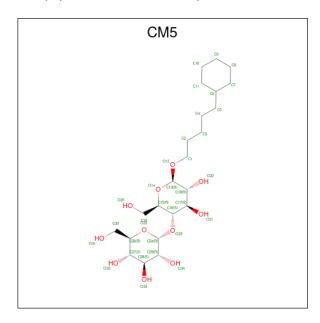
• Molecule 4 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula:  $C_7H_{17}NO_3$ ).



ľ	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	4	A	1	Total C N O 11 7 1 3	0	0
	4	A	1	Total C N O 11 7 1 3	0	0



 $\bullet$  Molecule 5 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (three-letter code: CM5) (formula: C23H42O11).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 34	C 23	O 11	0	0

• Molecule 6 is water.

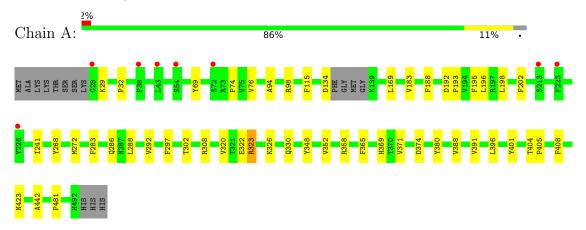
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	72	Total O 72 72	0	0



## 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: Cytochrome P450 2B4





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	90.16Å 90.16Å 148.62Å	Donositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	78.08 - 2.94	Depositor
rtesolution (A)	53.83 - 2.94	EDS
% Data completeness	99.6 (78.08-2.94)	Depositor
(in resolution range)	99.6 (53.83-2.94)	EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$< I/\sigma(I) > 1$	3.19  (at  2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
$R, R_{free}$	0.243 , $0.296$	Depositor
It, Itfree	0.236 , $0.285$	DCC
$R_{free}$ test set	765 reflections $(4.97\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.35 \; ,  20.0$	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.46, < L^2> = 0.29$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	3892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 0BV, CM5, HEM, TAM

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).

Mal	Chain	Bond	lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.36	0/3799	0.52	3/5143 (0.1%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	323[A]	ARG	CB-CA-C	-5.71	98.97	110.40
1	A	323[B]	ARG	CB-CA-C	-5.71	98.97	110.40
1	A	322	GLU	O-C-N	-5.10	114.54	122.70

There are no chirality outliers.

There are no planarity outliers.

## 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	3704	0	3711	32	0
2	A	43	0	30	3	0
3	A	17	0	11	1	0
4	A	22	0	34	1	0
5	A	34	0	42	3	0
6	A	72	0	0	0	0
All	All	3892	0	3828	34	0



The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 4.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:HG22	2:A:500:HEM:HBB2	1.64	0.78
1:A:195:PHE:HA	5:A:502:CM5:H32A	1.72	0.73
1:A:323[B]:ARG:HB3	1:A:348:TYR:CE2	2.29	0.67
1:A:442:ALA:HB1	2:A:500:HEM:HAB	1.78	0.65
1:A:98:ARG:HG2	2.A.500.HEM.HAB 1:A:115:PHE:HA	1.81	0.62
1:A:183:VAL:HG11	1:A:113.1 HE.HA 1:A:292:VAL:HG13	1.83	0.61
1:A:103:VAL:HG11 1:A:202:PHE:HD1	1:A:292: VAL:HG13 1:A:241:ILE:HD13	1.64	0.61
1:A:202:PHE:CD1	1:A:241:ILE:HD13	2.36	0.61
1:A:202:PHE:HB2	1:A:241:ILE:HD11	1.89	0.55
3:A:501:0BV:OAA	3:A:501:0BV:H12	2.08	0.53
1:A:198:LEU:HD12	5:A:502:CM5:H22A	1.91	0.52
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.46	0.51
1:A:365:PHE:HA	1:A:391:VAL:HA	1.93	0.51
1:A:169:LEU:HD11	1:A:196:LEU:HD22	1.91	0.51
1:A:272:MET:HG2	1:A:283:PHE:O	2.11	0.50
1:A:348:TYR:O	1:A:352:VAL:HG23	2.13	0.48
1:A:401:TYR:HB3	1:A:423:ASN:OD1	2.14	0.48
1:A:69:TYR:CE2	1:A:74:PRO:HB3	2.49	0.47
1:A:308:ARG:NH2	1:A:481:PRO:HD2	2.29	0.47
1:A:268:TYR:CG	1:A:288:LEU:HD13	2.51	0.45
1:A:369:HIS:HE1	2:A:500:HEM:O2A	2.00	0.44
4:A:504:TAM:H21	4:A:504:TAM:H61	1.72	0.43
1:A:32:PRO:HD3	1:A:380:TYR:CZ	2.53	0.43
1:A:202:PHE:HZ	1:A:297:PHE:HA	1.84	0.43
1:A:94:ALA:O	1:A:371:VAL:HA	2.18	0.42
1:A:188:PHE:CE2	5:A:502:CM5:H12	2.54	0.42
1:A:358:ARG:HA	1:A:396:LEU:HD22	2.03	0.41
1:A:192:ASP:HA	1:A:193:PRO:HD3	1.87	0.41
1:A:323[A]:ARG:HB2	1:A:348:TYR:CE2	2.55	0.41
1:A:76:VAL:HB	1:A:388:VAL:HG22	2.02	0.40
1:A:404:THR:HA	1:A:405:PRO:HD2	2.00	0.40
1:A:326:LYS:HE3	1:A:326:LYS:HB2	1.95	0.40
1:A:192:ASP:O	1:A:196:LEU:HG	2.22	0.40
1:A:320:VAL:HG21	1:A:408:PHE:HE2	1.85	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.

$\mathbf{M}$	ol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1		A	458/476 (96%)	443 (97%)	14 (3%)	1 (0%)	47 76

#### All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	LYS

#### 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	407/421 (97%)	403 (99%)	4 (1%)	76 91	

#### All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	ASP
1	A	286	GLN
1	A	330	GLN
1	A	374	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	A	335	HIS
1	A	369	HIS
1	A	455	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

5 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 Lin		Tiple	Link Bond lengths			Bond angles			
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CM5	A	502	-	36,36,36	0.55	0	49,49,49	1.29	6 (12%)
2	HEM	A	500	1	41,50,50	1.96	6 (14%)	45,82,82	1.56	5 (11%)
3	0BV	A	501	1	19,19,19	0.99	0	26,26,26	0.83	0
4	TAM	A	503	-	7,10,10	1.02	0	9,12,12	0.88	0
4	TAM	A	504	-	7,10,10	0.95	0	9,12,12	0.69	0

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CM5	A	502	-	-	10/17/65/65	0/3/3/3
2	HEM	A	500	1	-	2/12/54/54	-
3	0BV	A	501	1	-	0/3/3/3	0/3/3/3
4	TAM	A	503	-	-	4/12/12/12	-
4	TAM	A	504	-	-	6/12/12/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
2	A	500	HEM	C3D-C2D	8.02	1.53	1.36
2	A	500	HEM	C3C-C2C	-4.47	1.34	1.40
2	A	500	HEM	C3C-CAC	3.56	1.55	1.47
2	A	500	HEM	CAB-C3B	2.98	1.55	1.47
2	A	500	HEM	FE-ND	2.46	2.09	1.96
2	A	500	HEM	CMB-C2B	2.07	1.55	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}({}^o)$	$\operatorname{Ideal}({}^{o})$
2	A	500	HEM	C4D-ND-C1D	6.06	111.33	105.07
5	A	502	CM5	C28-C27-C26	3.33	116.18	110.24
2	A	500	HEM	C4C-CHD-C1D	3.18	126.75	122.56
5	A	502	CM5	C1-O12-C13	-3.01	108.84	113.84
5	A	502	CM5	C18-C17-C16	2.95	116.41	109.68
5	A	502	CM5	C13-C18-C17	2.73	115.68	110.00
5	A	502	CM5	C24-O23-C16	-2.63	111.46	117.96
2	A	500	HEM	C4B-CHC-C1C	2.50	125.85	122.56
2	A	500	HEM	C1B-NB-C4B	2.44	107.59	105.07
2	A	500	HEM	CAA-CBA-CGA	-2.31	107.30	113.76
5	A	502	CM5	O25-C26-C27	2.20	113.70	109.69

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	TAM	C1-C-C3-C6
4	A	503	TAM	N-C-C3-C6
4	A	503	TAM	C-C1-C4-O4
4	A	504	TAM	C1-C-C3-C6
4	A	504	TAM	C2-C-C3-C6
4	A	504	TAM	N-C-C3-C6

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	502	CM5	C18-C13-O12-C1
5	A	502	CM5	O14-C13-O12-C1
5	A	502	CM5	O14-C15-C19-O20
5	A	502	CM5	C16-C15-C19-O20
5	A	502	CM5	C3-C4-C5-C6
5	A	502	CM5	C4-C5-C6-C7
5	A	502	CM5	C1-C2-C3-C4
4	A	503	TAM	C2-C-C3-C6
5	A	502	CM5	C4-C5-C6-C11
5	A	502	CM5	C29-C24-O23-C16
5	A	502	CM5	O25-C24-O23-C16
4	A	504	TAM	C3-C-C2-C5
4	A	504	TAM	C-C3-C6-O6
2	A	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A
4	A	504	TAM	C1-C-C2-C5

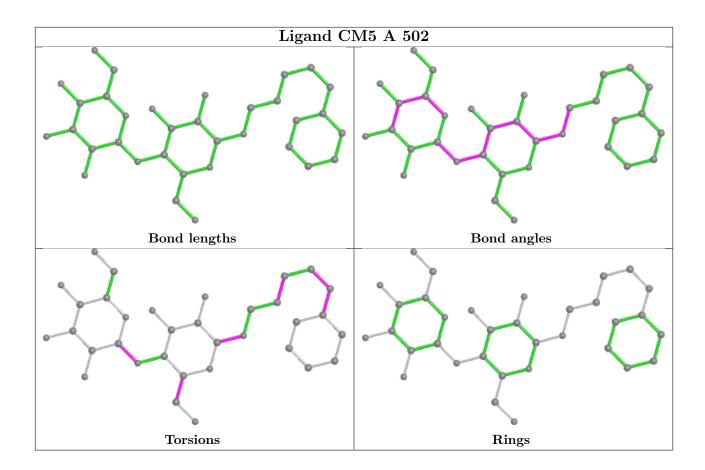
There are no ring outliers.

4 monomers are involved in 8 short contacts:

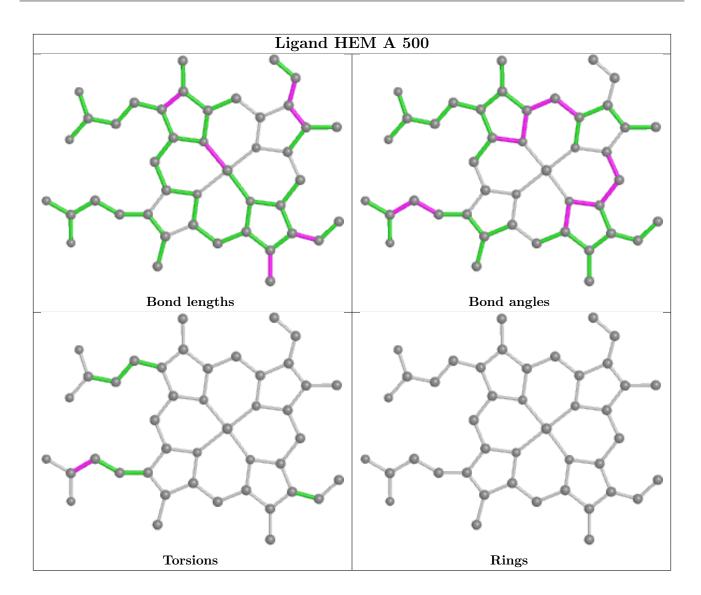
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	CM5	3	0
2	A	500	HEM	3	0
3	A	501	0BV	1	0
4	A	504	TAM	1	0

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.









## 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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>	$\#\mathrm{RSRZ}{>}2$		$OWAB(Å^2)$	Q<0.9	
1	A	461/476 (96%)	0.04	8 (1%)	70	71	20, 27, 43, 48	0

All (8) RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	A	223	PHE	3.6
1	A	226	TYR	2.9
1	A	38	PRO	2.9
1	A	72	SER	2.8
1	A	54	SER	2.8
1	A	43	LEU	2.5
1	A	28	GLY	2.4
1	A	213	SER	2.1

## 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.

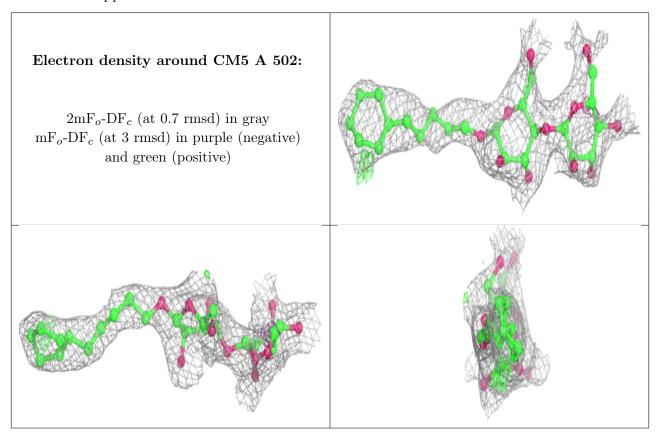
### 6.4 Ligands (i)

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.

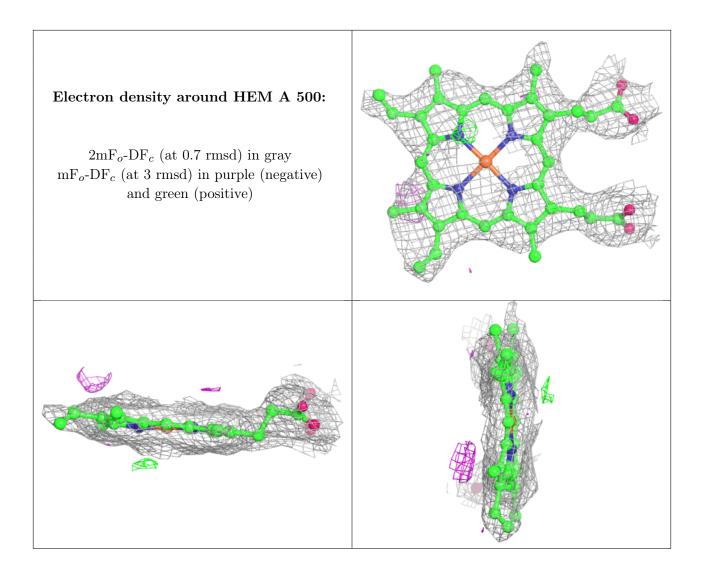


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
4	TAM	A	503	11/11	0.75	0.30	73,73,73,73	0
5	CM5	A	502	34/34	0.76	0.26	64,73,75,75	0
4	TAM	A	504	11/11	0.82	0.22	48,49,49,49	0
3	0BV	A	501	17/17	0.94	0.31	23,24,24,24	0
2	HEM	A	500	43/43	0.97	0.20	22,23,24,25	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.







## 6.5 Other polymers (i)

There are no such residues in this entry.

