

Supporting Information

# **Quantum Refinement Does Not Support Dinuclear Copper Sites in Crystal Structures of Particulate Methane Monooxygenase**

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# Methods

#### Quantum refinement

Quantum refinement is standard crystallographic refinement supplemented by QM calculations for a small, but interesting part of the protein.<sup>[1,2]</sup> Crystallographic refinement software change the protein model (coordinates, occupancies, B factors, etc.) to improve the fit of the observed and calculated structure-factor amplitudes (usually estimated as the residual disagreement, the *R* factor). Owing to the limited resolution normally obtained for biomolecules, the experimental data are supplemented by some chemical information, usually in the form of a MM force field.<sup>[3]</sup> Then, the refinement takes the form of a minimization or simulated annealing calculation by molecular dynamics using an energy function of the form

$$E_{\rm cryst} = w_{\rm A} \, E_{\rm Xray} + E_{\rm MM} \tag{1}$$

where  $E_{Xray}$  is a penalty function that describes how well the model agrees with the experimental data (we have used a maximum-likelihood refinement target using amplitudes,  $MLF^{[4,5]}$ ).  $E_{MM}$  is an empirical (molecular mechanics, MM) energy function with bond, angle, dihedral and non-bonded terms, and  $w_A$  is a weight factor, which is necessary because  $E_{MM}$  is in energy units whereas  $E_{Xray}$  is unit-less. It determines the relative importance of the crystallographic raw data and the MM force field for the final structure.

Quantum chemistry can be introduced in this function by replacing the MM potential for a small region of the protein (system 1) by QM calculations, yielding a QM energy for system 1,  $E_{QM1}$ . To avoid double counting, we must then subtract the MM energy of system 1,  $E_{MM1}$ ,

$$E_{\rm cqx} = w_{\rm A} E_{\rm Xray} + E_{\rm MM12} + w_{\rm QM} E_{\rm QM1} - E_{\rm MM1}$$
(2)

Thereby, we introduce an accurate energy function for the system of interest. Such an energy function is implemented in the software ComQum-X,<sup>[1]</sup> which is a combination of the QM software Turbomole<sup>[6]</sup> and the crystallography and NMR system (CNS), <sup>[7,8]</sup> version 1.3. The factor  $w_{QM}$  in Eq. 5 is another weight, which is needed because the CNS MM force field is based on a statistical analysis of crystal structures.<sup>[9]</sup> Therefore, the force constants are not energy-derived, as is the QM term, but they are in arbitrary statistical units. Experience has shown that the CNS force constants are typically three times larger than energy-based force constants,<sup>[9]</sup> and  $w_{QM} = 3$  has therefore been used throughout this work.<sup>[1]</sup> Crystallographic refinement is traditionally performed without any electrostatic interactions, because hydrogen atoms are not discerned in the structure. We have followed this custom and excluded electrostatics and hydrogen atoms from all crystallography and MM calculations (but they are of course included in the QM calculations).

Two crystal structures were studied in this investigation, viz. the revised pMMO structure from *M. capsulatus* (Bath) (3RGB) at 2.8 Å resolution<sup>[10]</sup> and the 2.68-Å structure of pMMO from *Methylocystis sp.* strain M (3RFR).<sup>[10]</sup> Coordinates, occupancies, B factors and structure factors were obtained from the protein databank files. From these files, we also obtained the space group, unit-cell parameters, resolution limits, *R* factors and the test set used for the evaluation of the  $R_{\text{free}}$  factor.

The full protein was used in all calculations, including all crystal water molecules. In each cycle of the geometry optimization, the surrounding protein was allowed to relax by one cycle of crystallographic minimization and one cycle of individual B-factor refinement. However, the new coordinates and B factors were accepted only if the *R* factor was reduced. The  $w_A$  factor was determined by CNS in the first iteration of the refinement and then kept fixed. It was 4.91 for 3RGB and 4.93 for 3RFR. Electron-density maps were generated using

# phenix.maps.<sup>[11]</sup>

We used the standard CNS MM force field for all atoms (protein\_rep.param, water\_rep.param, and ion.param). For the junctions, where a bond is broken between the QM and MM regions, we employed the hydrogen link-atom approach i.e. the QM systems were truncated by H atoms (called HL below), replacing a C atom in the protein (called CL). The force field for the QM system was constructed automatically from that of the protein. For the HL atoms, we employed the same angle and dihedral parameters as for the CL atoms. For the XL–HL bond (where XL is the atom in the QM system bound to HL), we used as the equilibrium bond length ( $r_{XL-HL}^0$ ) that obtained by geometry optimisation with the TPSS-D3/def2-SV(P) approach for a model of the isolated ligand (e.g. imidazole). The force constant ( $k_{XL-HL}$ ) was obtained from the corresponding force constant and equilibrium bond length of the XL–CL bond according to:

$$k_{\rm XL-HL} = k_{\rm XL-CL} \left(\frac{r_{\rm XL-HL}^0}{r_{\rm XL-CL}^0}\right)^2$$
(3)

Van der Waals parameters of 0.0188 kJ/mol and 2.2272 Å were used for all junction atoms (taken from the HA atom type).

The quality of the models was compared using the real-space difference density Zscore<sup>[12]</sup> (RSZD), calculated by EDSTATS in the CCP4 suite,<sup>[13]</sup> which measures the local accuracy of the model. The maximum of the absolute values of the positive and negative RSZD (combined RSZD) for the Cu ion and all the first-sphere ligands was taken as the quality metric (individual values for each of the groups are given in the supplementary material). It is called RSZD in the main text and RSZD<sub>max</sub> in this supplementary material (to differ it from RSZD for the individual residues and atoms, which also will be discussed). RSZD is typically < 3.0 for a good model. In addition, the strain energy of the active site ( $\Delta E_{str}$ ) was calculated, i.e. the difference in the QM energy of the QM region when optimised in the crystal or freely in vacuum.<sup>[14]</sup>

#### QM calculations

All QM calculations were performed with the Turbomole software, version 7.1.<sup>[6]</sup> We employed the density-functional theory (DFT) method TPSS<sup>[15]</sup> and the def2-SV(P)<sup>[16]</sup> basis set. The calculations were sped up by expanding the Coulomb interactions in an auxiliary basis set, the resolution-of-identity (RI) approximation.<sup>[17,18]</sup> Empirical dispersion corrections were included with the DFT-D3 approach<sup>[19]</sup> and Becke–Johnson damping,<sup>[20]</sup> as implemented in Turbomole.

The QM system consisted of one or two Cu ions, two imidazole groups modelling the sidechains of His-137 and 139, and  $H_2N-(CH_2)_2$ -imidazole, as a model of His-33 (sidechain and backbone). Sometimes, one or two water molecules were added or models of Glu-35, Asp-79C (modelled by an acetate groups), Tyr-374 (modelled by phenol) or His-137 was extended to imidazole–(CH<sub>2</sub>)<sub>2</sub>–CO–NH–CH<sub>3</sub>, including the backbone towards the next residue. The Cu ions were always modelled in both the Cu<sup>+</sup> and Cu<sup>2+</sup> states, in the latter case with unrestricted formalism. For dimeric Cu sites, we employed three oxidation states: fully reduced, fully oxidised and the mixed-valence Cu<sup>+</sup>–Cu<sup>2+</sup> state. After some test calculations, we decided to use the ferromagnetically coupled triplet state for the fully oxidised state, which was lower in energy than the antiferromagnetically coupled open-shell singlet state (obtained with the broken-symmetry approach), owing to the lack of any strong bridging ligand.

For the study of the reaction mechanism (Figure 6 in the main article), structures with the same QM model (plus a methane molecule) were optimised in gas phase with the TPSS-D3/def2-SV(P) approach. Then, more accurate single-point energies were calculated with the def2-TZVPD<sup>[21,22]</sup> basis set and both the TPSS-D3 and B3LYP-D3<sup>[23-25]</sup> methods. These calculations were run in a COSMO continuum solvent.<sup>[26,27]</sup> The default optimised COSMO radii (and a water solvent radius of 1.3 Å),<sup>[28]</sup> whereas a radius of 2 Å was used for the metals.<sup>[29]</sup> The dielectric constant was 4, whereas we used default values for all other parameters. Frequency calculations were performed at the TPSS-D3/def2-SV(P) level of theory and from these, zero-point energies were calculations and it was confirmed that transition states had one and minima had no imaginary frequencies.

# Details of quantum refined structures of protomer 1 of the 3RGB structure

We started by performing quantum refinement of site A in the first protomer of the 3RGB structure using a dinuclear Cu site (called C2W0 in the tables to indicate that it contains two Cu ions and no extra water molecules). This gave structures quite similar to the starting crystal geometry as can be seen in Figures S1a and S1b: The two Cu ions are on top of each other, but in variance to the starting structure (Figure 1a in the main article), all three imidazole groups are directed towards the Cu ions with the ND1 (His-33 and His-137; called N<sub>A</sub> and N<sub>B</sub> in the following and in the Tables) or NE2 (His-139; N<sub>C</sub>) atoms binding. One of the Cu ions (Cu<sub>A</sub>) coordinates to all four N atoms, whereas the other (Cu<sub>B</sub>) coordinates to only one or two of them (N<sub>A</sub> and possibly also N<sub>C</sub>). The distance to the His-33 backbone amide group (N<sub>D</sub>) is typically longer than that to the imidazole groups. The detailed distances depend on the oxidation states of the two Cu ions and are listed in Table S1. In the (fully) reduced state, the two Cu<sub>B</sub>–N distances (to N<sub>A</sub> and N<sub>C</sub>) are short (2.02–2.03 Å), whereas the four Cu<sub>A</sub>–N distances are longer and much more varying (2.07–2.63 Å). This reflects the preference of Cu<sup>+</sup> for low coordination numbers. However, in the mixed-valence (MV) and (fully) oxidised states, the Cu<sub>A</sub>-N distances to the imidazole groups are short, 2.05–2.15 Å, that to  $N_D$  is somewhat longer, 2.24–2.30 Å, whereas only the Cu<sub>B</sub>–N<sub>A</sub> distance is short (2.08–2.13 Å) and the Cu<sub>B</sub>–N<sub>C</sub> bond is essentially broken, 2.89–2.93 Å. The Cu–Cu distance is 2.21–2.25 Å. The spin densities show that  $Cu_B$  is actually in the reduced state also in the fully oxidised structure. Instead, the spin is spread over  $Cu_A$  (0.34 e) and the ligands. Also in the MV state, there is no spin on  $Cu_B$  and only 0.41 *e* spin on  $Cu_A$ .

If we set  $w_A = 0$  in Eqn. 2, i.e. turn off the restraint towards the experimental data, thereby obtaining a QM/MM calculation with the CNS MM force field, the MV and especially the oxidised structures reorganise significantly, as can be seen in Table S1 (method Q). However, the reduced structure remains more intact, with both Cu ions two-coordinate with Cu–N distances of 1.89–2.08 Å and a Cu–Cu distance of 2.46 Å. This reflects the intrinsic preferences of the metals and the ligands in the protein.

Further information about the preferences of the metal can be obtained by freely optimising the metals and the four ligands in vacuum, i.e. ignoring the covalent and steric influence of the protein (besides the covalent link between  $N_A$  and  $N_D$ ). For the reduced site, this gave little changes from the QM/MM structure (cf. Table S1, method V). For the MV and oxidised states, the differences were larger, but mainly related to  $Cu_B$ , which bound with side-on interactions with the imidazole rings, because all N atoms were occupied in a square-planar coordination to  $Cu_A$ .

To obtain structures that better fitted the experimental data, we attempted to model the site in other ways. First, we tried to use the model suggested by Yoshizawa and coworkers in their QM/MM studies of the reaction mechanism,<sup>[30–32]</sup> i.e. a dimeric model with the two Cu ions and the four N ligands in the same plane (Figure S2a). We could successfully obtain such a structure by model building and then refining the structure with  $w_A = 0$ . The structures are

described in Table S1 (called Y2W0a). Cu<sub>A</sub> binds to His-33 (both sidechain and backbone amide) and His-137 with Cu<sub>A</sub>–N = 1.97–2.09 Å. The latter group bridges to Cu<sub>B</sub>, which also binds to His-139 with distances of 1.86–1.99 Å. The Cu–Cu distance is 2.35–2.45 Å, actually increasing with the oxidation state of the Cu ions. However, if we turned on the restraint towards the experimental data, the site went back to something similar to the original QM-refined structures, i.e. with the four N atoms mainly coordinating to Cu<sub>A</sub>.

A prime problem with site A, especially in the higher oxidation states, is that it contains too few ligands for two metal ions. Therefore, we tried to enhance the site with two water molecules. After many attempts, we were able to obtain some reasonable structures and the best (in terms of RSZD<sub>max</sub>) are shown in Tables S1 and S2 (called Y2W2), and in Figure 2b. In the MV and oxidised structures, Cu<sub>A</sub> is still coordinated by all four N atoms in a square plane (Cu–N distances of 1.98–2.13 Å) and also by one of the water molecules in an axial position (2.52–2.53 Å). N<sub>B</sub> and N<sub>C</sub> bridges to Cu<sub>B</sub> but with a quite poor geometry (2.07–2.19 Å). Cu<sub>B</sub> also binds to the other water molecule (2.02–2.04 Å). The RSZD<sub>max</sub> scores are higher for the reduced structure, but appreciably better for the MV and oxidised states (1.5) than the structures started from the original crystal structure. The strain energies are also appreciably better, 149–159 kJ/mol. However, the  $2F_o - F_c$  electron-density maps in Figure 3a in the main article show that there is no electron density around the water molecules.

Consequently, we also optimised the corresponding structures without the water molecules (Y2W0 in Tables S1 and S2). They are more similar for all three oxidation states (except that  $N_C$  does not bind to  $Cu_A$  in the reduced state) with  $Cu_A$ –N distances of 1.91–2.19 Å and  $Cu_B$ –N distances of 1.90–2.28 Å to  $N_B$  and  $N_C$ . They gave slightly better RSZD<sub>max</sub> scores (1.3 for the MV and oxidised states), but somewhat higher strain energies (170–220 kJ/mol).

Yoshizawa and coworkers have also sometimes suggested structures in which nearby residues coordinate to site A.<sup>[30–32]</sup> Therefore, we tried to enhance the QM system with models of the sidechains Glu-35, Asp-79C or Tyr-374 and then repeated the QM refinement. However, it turned out that these residues were too far away in the crystal structure to coordinate to any of the Cu ions and therefore the structures were closely similar to those obtained without any added residues (Table S1). However, if the QM region was extended with the carbonyl group of His-137, this group was found to coordinate to Cu<sub>B</sub> with Cu–O distances of 2.30–2.52 Å in all three oxidation states as can be seen in Figure S2c. This led to a shortening of the Cu<sub>A</sub>–N<sub>D</sub> bond (2.16–2.19 Å) and a slight elongation of the Cu<sub>A</sub>–N<sub>B</sub> bond (2.11–2.23 Å), but otherwise the structures were similar to the original QM-refined structures. Yet, these structures reproduced the crystallographic data quite poorly, with RSZD<sub>max</sub> scores of 2.6–2.7 (Table S2). The strain energies were also nearly as high as for the original C2W0 structures, 178–226 kJ/mol.

Finally, we instead tried to model site A with a single Cu ion (C1W0 in Tables S1 and S2). This gave structures that were similar to that of Cu<sub>A</sub> in the dinuclear sites. The geometry was distorted square planar with a rather small N<sub>B</sub>–Cu–N<sub>D</sub> angle of 117° (reduced state) to 133° (oxidised state), as can be seen in Figure S3a and S3b. Otherwise, the geometry was quite regular. In the oxidised state, the Cu–N distances were 1.85–2.22 Å, with the longest bond to N<sub>D</sub>. In the reduced state, the three bonds to the sidechains were similar (1.84–2.23 Å), but the bond to N<sub>D</sub> increased to 2.62 Å. If the same structures were optimised with  $w_A = 0$ , the structures became more square-planar with N<sub>B</sub>–Cu–N<sub>D</sub> angles of 139° and 165°. The Cu–N distances become more similar, 1.97–2.10 Å for the oxidised state and 1.96–2.12 (N<sub>A</sub>–N<sub>C</sub>) and 2.33 Å (N<sub>D</sub>) for the reduced state. If the structures were instead optimised in vacuum, the reduced state became tetrahedral with all four Cu–N distances of 1.99–2.05 (N<sub>A</sub>–N<sub>C</sub>) and 2.14 Å (N<sub>D</sub>), whereas the oxidised state became almost perfectly square planar (N<sub>B</sub>–Cu–N<sub>D</sub> angle of 1.99–2.02 (N<sub>A</sub>–N<sub>C</sub>) and 2.07 Å (N<sub>D</sub>). In all three oxidised

structures, the spin of the Cu ion was  $\sim 0.5 e$ .

There remains some positive difference density on top of the Cu ion in this structure, which was interpreted as an additional Cu ion in the original crystal structure. Yet, it is too close to the Cu ion and with a too low density to be another metal. Therefore, we tried to model it as a water molecule instead (C1W1 in Tables S1 and S2). In the reduced state, the water molecule did not coordinate to Cu (as could be expected from the preference of Cu<sup>+</sup> for low coordination numbers). Therefore, the structure did not change significantly from that obtained without the water molecule. However, for the oxidised state, the water molecule coordinate of 2.20 Å as can be seen in Figure S4. As a consequence of the increased coordination number, the distance to the other ligands increased by 0.03-0.07 Å. If optimised with QM/MM or in vacuum, the Cu–O distance increased somewhat (2.25–2.31 Å) and the Cu–N distances became more similar.

#### The other protomers of the 3RGB structure

Next, we studied site A in the other two protomers of the 3RGB structure. As mentioned in the main text, the structure of these two sites is different from that in the first protomer. This was also reflected in the quantum-refined structures of this site, started from the crystal structure with two Cu ions (C2W0): For all three oxidation states, strongly distorted structures were obtained with Cu<sub>A</sub> coordinating to His-137 and bidentately to His-33 as can be seen in Figure S5a. His-137 bridges to Cu<sub>B</sub>, which also interacts with the sidechain of His-139, but with a far-from-ideal, side-on geometry. The corresponding distances are listed in Table S1. The RSZD<sub>max</sub> scores were worse than in protomer 1, 2.8–2.9, whereas the strain energies were similar, 178–247 kJ/mol (Table S2). Protomer 3 gave similar structures (also described in Tables S1 and S2). However, the RSZD<sub>max</sub> scores were somewhat smaller, 2.0–2.8, as was the strain energies (160–224 kJ/mol).

To check whether this striking difference in the metal-site geometry is really dictated by the crystallographic data, we used the trifold non-crystallographic symmetry to copy the structure of protomer 1 to site A in protomer 2 and 3 also. However, the structures converged back to the original structures again.

Next, we also optimised Yoshizawa-type dinuclear structures in the other two protomers (Y2W2). They are also presented in Tables S1, S2 and Figure S5b, and it can be seen that the structures are rather similar to those in protomer 1, but with some variation. For protomer 2, these structures fitted the crystallographic data better than the other dinuclear structures with RSZD<sub>max</sub> scores of 1.9–2.2 and strain energies of 110–144 kJ/mol. However, for protomer 3, they were much worse in terms of RSZD<sub>max</sub> (2.9–3.2), but the strain energies were still lower (104–160 kJ/mol).

We also optimised the corresponding structures without water molecules (Y2W0). From the results in Tables S1 and S2, it can be seen that they were similar to the corresponding structures with water, except that for  $Cu_B$  in protomer 3,  $N_D$  was replaced by  $N_A$ . In protomer 3, these structures gave lower RSZD<sub>max</sub> scores than the structures with water, but higher strain energies, whereas both measures were worse for protomer 2.

Next, we tried to model a single Cu ion in both protomers. This gave structures that were similar to the corresponding structures in protomer 1 (Figure S5c). The Cu–N distances (shown in Table S1) were also rather similar. The electron-density maps were also better than those of the dinuclear Cu model, with  $RSZD_{max}$  of 1.1–1.7 for protomer 2 and 1.5–2.0 for protomer 3. The strain energies were also much lower than for the dinuclear structures, 37–76 kJ/mol.

Finally, we also tried a single Cu ion with an additional water molecule. It gave results similar to that of protomer 1, with the difference that the water molecule did not coordinate to

Cu in protomer 3. However, in both protomers, the structures without the axial water molecule gave lower  $RSZD_{max}$  scores and strain energies (Table S2).

## The 3RFR crystal structure

Finally, we considered the 3RFR crystal structure. As mentioned in the introduction, it contains a dinuclear site A only in protomer 1, whereas this site is mononuclear in the other two protomers. Therefore, we performed quantum-refinement also of that site, using the 3RFR crystallographic data. With two Cu ions in the oxidised state (C2W0), the dinuclear site gave a structure similar to that of the first protomer in the 3RGB crystal (Table S1). However, for the reduced state, the structure was distorted and less similar. The side chains of His-137 and 139 coordinate primarily to Cu<sub>A</sub>, whereas both N<sub>A</sub> and N<sub>D</sub> coordinate primarily to Cu<sub>B</sub>, although all atoms except N<sub>B</sub> are within 3 Å also of the other Cu ion. The Cu–Cu distance is 2.24 Å. These structures fitted the crystallographic raw data quite poorly with RSZD<sub>max</sub> scores of 1.6–1.9 and very high strain energies, 292–357 kJ/mol.

However, much more reasonable structures were obtained with a single Cu ion in this site. Both the reduced and oxidised states gave almost perfectly square-planar structures with N<sub>B</sub>-Cu-N<sub>D</sub> angles of 171–177°. The Cu-N distances were similar to those of the 3RGB structure, 1.94–2.40 Å for the reduced state and 1.96–2.15 Å for the oxidised state (Table S1). These structures also fitted the experimental data better, with RSZD<sub>max</sub> = 1.3–1.4 and strain energies of 32 (oxidised state) or 88 kJ/mol (reduced state). Structures with a coordinated water molecule could also be obtained for both oxidation states (Cu–O distances of 2.43–2.50 Å). However, they gave larger RSZD<sub>max</sub> scores of 2.3 and 2.6.

For the other two protomers, the original crystal structure contained mononuclear sites. This was confirmed by the quantum-refinement, which gave structures similar to the other mononuclear sites in the 3RGB or 3RFR structures (Tables S1 and S2). However, no structures were obtained with a bound water molecule, not even for the oxidised state. The structures fitted the experimental data appreciably better than for protomer 1, with RSZD<sub>max</sub> = 0.4-0.9 without the water molecule. On the other hand, the strain energies were similar, 37–47 kJ/mol for the oxidised state and 89–101 kJ/mol for the reduced state.

## **Discussion of different RSZD scores**

In this study, we have used quantum refinement to re-refine the putative dinuclear Cu site A in two crystal structures of pMMO. We have tried several different dinuclear structures, as well as a mononuclear structure in all three protomers in both enzymes and also tried to add one or two extra water molecules. We have observed some variation among the two crystal structures and the three protomers.

In terms of the strain energies, our results are quite conclusive (Table 1 in the main article): The mononuclear models always give lower strain energies than the dinuclear models (37–85 kJ/mol, compared to 104–300 kJ/mol). For the same crystal and protomer, the best mononuclear structure always give a 63–85 kJ/mol lower strain energy than the best dinuclear structure. This confirms the impression that the dinuclear structures are not reasonable, even after the quantum refinement.

The  $RSZD_{max}$  results are slightly less conclusive (Tables 1 and S2). For the 3RFR structure and protomers 2 and 3 of the 3RGB structure, the mononuclear sites still give the lowest scores (1.3 compared to 1.6 in 3RFR, 1.1 compared to 1.9 in protomer 2 and 1.5 compared to 1.8 for protomer 3 of 3RGB). However, for protomer 1 in 3RGB, the lowest scores are actually obtained for the Y2W0 structure (1.3, compared to 1.5 for the best mononuclear site). On the other hand, it is not entirely clear how to compare RSZD scores

between sites of different composition. The RSZD scores are calculated for individual residues (viz. for His-33, 137 and 139, as well as for the Cu ions and water molecules; the individual RSZD result are shown in Table S2). These are not the same for all systems and they do not cover the same space in the various structures. Moreover, it is unclear how to combine 4–7 RSZD results to a single score in and unambiguous manner: We have used the maximum value (RSZD<sub>max</sub>, called simply RSZD in the main article), but other measures are also conceivable. Table S2 show two additional scores, obtained from the sum or the average. In fact, the mononuclear site gives the lowest RSZD score if the sum is considered (3.1, compared to 3.4), whereas the Y2W2 structure gives the best results if the average is considered (0.5 compared to 0.7).

A third argument against a dinuclear site is the large variation of the dinuclear structures in the various protomers and crystals: The geometries vary extensively (cf. Table S1) and the best one also varies between the crystals and protomers (the Y2W0 structure is best in protomer 1, the Y2W2 in protomer 2, whereas C2W0 is best in protomer 3 of the 3RGB structures.

Taken all results together, we find no conclusive evidence that the crystal structures of pMMO show a dinuclear Cu site. Instead, a mononuclear site fits the experimental data at least as well and it also gives chemically much more reasonable structures that are similar in both crystals and all protomers. Such a site is more similar to the mononuclear Cu site in the lytic polysaccharide monooxygenases, although it contains an additional histidine residue and lacks the nearby tyrosine residue.<sup>[33]</sup> The main evidence for a dinuclear site comes from EXAFS investigations, showing a striking reproducibility of the Cu–Cu interaction in pMMOs from four different methanotrophs.<sup>[10,34–36]</sup> One possibility is that the dicopper site detected by EXAFS is disrupted upon crystallization. On the other hand, EXAFS fits are known to give multiple local minima, so that different structures can give equally good fits.<sup>[37,38]</sup> This will be examined in future studies by a similar combination of computational and EXAFS methods.<sup>[39]</sup>

## **Reaction mechanism**

To provide a further check of the suggested mononuclear Cu site, we studied the reaction of the suggested mononuclear active site with a molecule of methane. Yoshizawa and Shiota have already studied with QM method putative reaction mechanisms of mono- and dinuclear Cu sites in pMMO.<sup>[30]</sup> However, their mononuclear model came from site B in the protein and therefore contained two His side chains and an acetate group and no His brace or amino group. Therefore, we repeated their study using our preferred mononuclear site in Figure 4 in the main article, i.e. with three His side chains, one of which is connected to a terminal amino group, as is shown in Figure 6 in the main article. Geometries were optimised at the TPSS-D3/def2-SV(P) level of theory in gas phase. Then, more accurate energies were calculated with the def2-TZVDP basis set with both the TPSS-D3 and B3LYP-D3 methods in a COSMO continuum solvent with a dielectric constant of 4. All energies are given in Table S3. Reported energies in Figure 6 and in the text are B3LYP-D3/def2-SV(P) level of theory.

Following the previous study, we started with a Cu(III) ion with an oxo ligand (or equivalently Cu(II)–O<sup>•-</sup>; net charge +1; called RS in Figure 6). All structures were studied in both the singlet and triplet states. In both cases, there was 0.5 spin on the Cu ion, 0.05–0.06 spins on each His ligand and the remainder on O (0.7 for the singlet and 1.3 for the triplet). In the singlet, the O spin was opposite to that of the other atoms and groups. Unlike the study by Yoshizawa and Shiota,<sup>[30]</sup> the two states were not degenerate; instead the triplet was 85 kJ/mol more stable than the singlet. Next, a methane molecule was added to the complex, forming a weak hydrogen bond to the oxo group (2.58 Å CH–O distance; R). It had nearly the

same energy as the RS structure (plus a free methane molecule).

A transition state (TS1) for the transfer of one of the hydrogen atoms of the methane molecule could be located. It had a CH–O distance of 1.17 Å and was 22 kJ/mol higher in energy than RS for the triplet. It is characterised by a single imaginary frequency of 1475*i* cm<sup>-1</sup>, similar to that found by Yoshizawa and Shiota (1445*i* cm<sup>-1</sup>).<sup>[30]</sup> This transition state leads to an intermediate with Cu–OH interacting with a methyl radical (Im1). It had a O–H distance of 0.99 Å and a OH–C distance of 2.18 Å and it was 16 kJ/mol more stable than RS. The Cu ion still had 0.5 spin, whereas 0.3 spin resided on OH and there was 0.95 spin on the methyl radical.

This intermediate could rearrange essentially barrierless to a second intermediate (Im2) in which the methyl radical also binds to the Cu ion. In this intermediate, the spins on Cu and OH have increased slightly, whereas that on the methyl radical has decreased strongly to 0.6. For the triplet state, Im2 is 10 kJ/mol less stable than Im1. However, for the singlet-state structures (which up to Im1 has been 75–150 kJ/mol less stable than the triplet states), Im2 is strongly stabilised and actually becomes 46 kJ/mol more stable than the triplet state (and 52 kJ/mol more stable than  ${}^{3}RS$ ). Therefore, we suggest, in accordance with the study of Yoshizawa and Shiota,  ${}^{[30]}$  that the spin state changes from triplet to singlet at this point.  ${}^{1}Im2$  is a closed-shell singlet, indicating a Cu(III)–OH–CH $_{3}^{-}$  complex.

Finally, the methanol product (P) can form by a recombination of OH and the methyl group. The corresponding transition state (TS2) has a rather complicated structure because both groups are still bound to Cu. The C–O distance is 1.91 Å and the imaginary frequency is  $396i \text{ cm}^{-1}$ , slightly smaller than that obtained by Yoshizawa and Shiota ( $473i \text{ cm}^{-1}$ ).<sup>[30]</sup> It is still a closed-shell species and it is 53 kJ/mol higher in energy than <sup>1</sup>Im2. In the product, methanol has dissociated from the Cu(I) ion and is 217 kJ/mol more stable than the starting point (<sup>3</sup>RS).

From the energy components in Table S3, it can be seen that the effect of an increase in the basis set from def2-SV(P) to def2-TZVPD (for the TPSS-D3 method) is quite small for the triplet state (up to 17 kJ/mol, in general reducing the relative energies), whereas it is larger for the R, TS1, and Im1 states (up to 67 kJ/mol), increasing the energies. Likewise, the effect of changing the DFT functional from TPSS to B3LYP has a relatively small effect on the triplet energies (up to 24 kJ/mol, increasing the energies), but a much larger effect on the singlet energies (again up to 67 kJ/mol), although it is mainly an effect of decreasing the relative energy of all open-shell singlet states by 50–67 kJ/mol. Thus, the singlet and triplet states are much closer in energy at the TPSS level of theory. The zero-point energy has a rather small effect on all energies, up to 17 kJ/mol with a varying sign (but nearly the same energy for the singlet and triplet states).

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**Table S1.** Cu–ligand distances (Å) in the various complexes. The results for different crystal structures and protomers are presented in separated sections of the table. The structures are described with a four-letter code, giving the number of Cu ions (C2 and C1; Y2 represent Yoshizawa-like structures with two Cu ions, such as those in Figure S2) and the number of water molecules, W2, W1 or W0 (the Glu35, Asp79, Tyr374 and His137 structures of 3RGB, subunit A all represent C2W0 structures, but with enhanced QM regions). The methods are quantum refinement (R), QM/MM (Q; i.e. quantum refinement with  $w_A = 0$ ) and vacuum optimisations (V). State is the oxidation state of the Cu ion(s), reduced (Red; one or two Cu<sup>I</sup>), oxidised (Ox; one or two Cu<sup>II</sup>) or mixed valence (MV; Cu<sup>I</sup>+Cu<sup>II</sup>). Cu–ligand distances are reported only if they were shorter than 3.0 Å. N<sub>A</sub>, N<sub>B</sub> and N<sub>C</sub> are the coordinating sidechain atoms of His-33, His-137 and His-139, respectively. N<sub>D</sub> is the backbone (amino-terminal) N atom or His-33. O<sub>1</sub> and O<sub>2</sub> are the O atoms of the water molecules that are present in some structures. In the structure with the QM region enhanced with the backbone of His137, O<sub>1</sub> represents the carbonyl oxygen.

Structure	Method	State			Dista	nce to	o Cu <sub>A</sub>				Di	istanc	e to C	u <sub>B</sub>	
			$Cu_B$	N <sub>A</sub>	$N_B$	N <sub>C</sub>	N <sub>D</sub>	$O_1$	O <sub>2</sub>	N <sub>A</sub>	$N_B$	N <sub>C</sub>	N <sub>D</sub>	$O_1$	$O_2$
3RGB, pr	otomer 1														
C2W0	R	Red	2.21	2.34	2.07	2.63	2.25			2.02		2.03			
		MV	2.25	2.07	2.10	2.06	2.24			2.08		2.89			
		Ox	2.25	2.05	2.15	2.06	2.30			2.13		2.93			
	Q	Red	2.46	2.76	2.01		2.08			1.89		1.89			
		MV	2.69	2.15	2.03	2.00	2.09			1.94					
		Ox	5.49	2.05	2.13	2.05	2.09								
	V	Red	2.54	2.72	1.91		1.96			1.90		1.89			
		MV	3.63	2.05	2.06	2.00	2.07			2.67	2.64				
		Ox	5.67	2.09	2.06	2.09	2.07								
Y2W0a	Q	Red	2.35	1.97	2.07		2.09				1.97	1.87			
		MV	2.43	1.97	2.08		2.07				1.99	1.86			
		Ox	2.45	2.01	2.07		2.08				1.99	1.87			
	R	Red	2.27	2.01	2.01	1.93				2.09			1.98		
		MV	2.59	1.91	2.17	2.09	2.02				2.15	2.11			
		Ox	3.54	1.98	2.03	2.03	2.02								
	V	Red	2.41	2.00	2.02		2.01				1.97	1.90			
Y2W2	R	Red	2.51	2.01	2.06	1.99	2.99	2.23		2.17			2.02	2.08	2.07
		MV	2.51	1.94	2.07	2.12	1.98	2.53			2.19	2.09			2.04
		Ox	2.51		2.19	2.09		2.04		1.94	2.07	2.12	1.98		2.53
		Ox,alt	2.60	1.98	2.06	2.13	1.98	2.52			2.19	2.07			2.02
	V	Red	2.56	1.98	2.08	1.96				2.50			1.95		1.94
		MV	2.46		2.15	1.96		2.06	2.18	1.98	2.01		2.00		2.89
		Ox	3.66			2.08		2.00	2.09	2.06	2.00	2.39	2.02		
Y2W0	R	Red	2.18	1.94	2.19		1.95				1.90	1.83			
		MV	2.42	1.91	2.08	2.13	2.00				2.21	2.11			
		Ox	2.47	1.98	2.05	2.13	2.00				2.28	2.11			
	V	Red	2.41	2.00	2.02		2.01				1.97	1.90			
		MV	3.93	1.98	2.10	2.10	2.06				2.85	2.83			
		Ox	3.89	2.12	2.07	2.08	2.06				2.89	2.83			
Glu35	R	Red	2.21	2.45	2.09	2.61	2.15			2.01		2.01	2.94		
		MV	2.21	2.34	2.07	2.62	2.17			2.03		2.03	2.94		
		Ox	2.20	2.26	2.07	2.57	2.16			2.05		2.08	2.95		
Asp79	R	Red	2.21	2.34	2.07	2.64	2.25			2.01		2.02			
-		MV	2.21	2.34	2.07	2.64	2.25			2.01		2.02			
		Ox	2.25	2.09	2.10	2.09	2.25			2.06		2.79			

Tyr374	R	Red	2.21 2.35 2.06	2.64 2.24		2.01	2.02	
		MV	2.21 2.35 2.06	2.64 2.24		2.01	2.02	
		Ox	2.21 2.27 2.06	2.62 2.24		2.03	2.04	
His137	R	Red	2.25 2.23 2.11	2.49 2.19		2.09	2.19	2.52
		MV	2.30 2.01 2.21	2.03 2.16		2.14	2.97	2.30
		Ox	2.28 2.01 2.23	2.05 2.18		2.15	2.94	2.39
	V	Red	2.49 2.90 1.92	1.98		1.93	1.93	2.13
		MV	2.42 1.97	2.02 2.03	2.52	1.88	2.91	1.89
		Ox	2.55 1.99	2.07 2.05	2.31	1.91	2.90	1.90
C1W0	R	Red	1.84 2.23	1.90 2.62				
		Ox	1.85 2.13	1.94 2.22				
	0	Red	1.96 2.12	2.02 2.33				
		Ox	1.97 2.06	2.01 2.10				
	V	Red	2.01 1.99	2.05 2.14				
		Ox	1.99 2.02	2.02 2.07				
C1W1	R	Red	1.87 2.25	1.93 2.55	3.09			
		Ox	1 89 2 16	1 99 2 29	2.20			
	0	Ox	2.00 2.08	2.03 2.09	2.25			
	Ň	Red	2 28 2 01	2 02 2 06	2.20			
	•	Ox	2.02 2.01	2.02 2.00	2 31			
3RGB	nrotomer	2	2.02 2.03	2.01 2.00	2.51			
C2W0	R	Red	2 29 1 85	2 12 2 18		1 97	2 27	
02110	K	MV	2.29 1.05	2.12 2.10		1.97	2.27	
		Ov	2.30 1.84	2.12 2.13		1.95	2.25	
	$\mathbf{V}$	Red	2.40 1.00	2.13 2.13		1.90	1.07	
	v	MV	2.42 1.93	2.01 2.09		1.90	1.97	
		$O_{\mathbf{Y}}$	2.55 1.94	2.04 2.07		1.94	2.02	
vowo	p	Red	$3.02 \ 2.00$	2.10 2.07	2 83	2.88	2.02	1 05 1 04
1 2 99 2	K	MV	2.51 1.52 2.00	2.05 2.34	2.05	2.00	2.47	1.03
		Ov	2.90 1.09 2.07	2.03 2.18	2.20	2.31	2.14	1.95
	V	Red	$3.00 \ 1.92 \ 2.07$ $2.50 \ 2.34 \ 1.03$	2.07 2.19	2.30	2.20	2.14	2 16 1 05
	v	MV	2.39 2.34 1.93	1.77	2.90	1.02	2.40	2.10 1.93
		$O_{\mathbf{Y}}$	2.47 1.93	1.97 2.08	2.85	1.95	2.49	2.12 2.03
VOWO	D	Dad	2.90 2.07 2.10	2.24 2.07		2.21	2.07	2.04 2.03
12W0	К	MV	2.43 1.67 2.20	1.90 2.30		2.39	2.09	
			2.92 1.07 2.07	2.01 2.13		2.43	2.24	
	V	Dad	3.12 1.93 2.03 2.41 1.02	2.01 2.13		2.39	2.30	
	v	Keu MV	2.41 1.92	2.01 2.10		2.73	2.02	
			3.69 1.96 2.10	2.10 2.07		2.04	2.02	
C1W0	D	Dad	3.90 2.12 2.07	2.09 2.00		2.90	2.85	
CIWU	ĸ	Red Ou	1.00 2.13	1.95 2.49				
	<b>V</b>	D x J	1.89 2.04	2.01 2.20				
	v	Red Or	2.01 1.98	2.03 2.14				
C1W1	р	Ox	1.99 2.02	2.02 2.07	2.27			
CIWI	K	Ox	1.91 2.02	2.02 2.21	2.37			
anon	V	Ox	2.02 2.03	2.04 2.08	2.34			
3RGB,	protomer	· 3	2 20 1 00	2 2 4 2 0 2		1.05	2 0 4	
C2W0	R	Red	2.29 1.98	2.24 2.03		1.95	2.04	
		MV	2.30 1.95	2.1/ 2.00		1.93	2.06	
	* *	Ox	2.33 1.98	2.15 2.00		1.93	2.08	
	V	Red	2.41 1.93	2.01 2.09		1.90	1.97	
		MV	2.56 1.94	2.03 2.07		1.89	1.95	
		Ox	3.62 2.00	2.10 2.07	• • • •	1.94	2.02	1.0.1.1.25
Y2W2	ĸ	Red	2.47 2.21 2.04	2.01 2.21	2.89	2.93	2.65	1.94 1.92
		MV	3.94 2.00 2.02	2.01 2.11			2.72	1.89
		Ox	3.93 2.07 2.01	2.01 2.11			2.74	1.92

	V	Red	2.59	2.32	1.93		1.99	2.95				1.91		2.17	1.95
		MV	4.76	1.99	2.02	2.10	2.04							1.93	
		Ox	4.93	2.08	2.05	2.10	2.04							1.92	
Y2W0	R	Red	2.45	2.04	2.35	1.95	2.19			2	.38	2.06			
		MV	2.77	2.01	2.08	2.00	2.11			2	.36	2.23			
		Ox	2.86	2.09	2.06	1.99	2.11			2	.47	2.29			
	V	Red	2.42	1.93		2.01	2.09			1	.90	1.97			
		MV	3.90	1.98	2.11	2.10	2.07			2	.84	2.82			
		Ox	3.90	2.12	2.07	2.08	2.06			2	.90	2.83			
C1W0	R	Red		2.03	2.19	1.92	2.27								
		Ox		2.00	2.02	1.97	2.12								
	V	Red		2.01	1.99	2.05	2.14								
		Ox		1.99	2.02	2.02	2.07								
C1W1	R	Ox		2.02	2.01	1.98	2.12	3.05							
	V	Ox		2.02	2.03	2.04	2.08	2.34							
3RFR, pr	otomer 1														
C2W0	R	Red	2.24	2.73	2.06	1.92	2.93		2.0	)9		2.79	2.34		
		MV	2.34	2.23	2.07	1.92	2.54		2.3	36		3.00	2.46		
		Ox	2.32	2.34	2.11	1.93	2.70		2.3	32		2.94	2.17		
C1W0	R	Red		2.12	2.26	1.94	2.39								
		Ox		2.05	2.09	1.96	2.15								
C1W1	R	Red		2.06	2.19	1.92	2.76	2.43							
		Ox		2.04	2.08	1.96	2.14	2.50							
3RFR, pro	otomer 2														
C1W0	R	Red		2.12	2.08	2.06	2.56								
		Ox		2.01	2.01	2.03	2.30								
C1W1	R	Ox		2.02	2.01	2.03	2.28								
3RFR, pr	otomer 3														
C1W0	R	Red		2.00	2.31	1.96	2.34								
		Ox		2.00	2.10	1.96	2.16								
C1W1	R	Ox		2.01	2.08	1.96	2.15								

**Table S2.** RSZD scores for each ligand in the active site, together with the maximum, sum and average. The last two columns give  $R_{\text{free}}$  and R of the structures. PM, Struct and State are the protomer, the structure and the oxidation state of site A.

PM	Struct	State					RSZ	ZD					R <sub>free</sub>	R
			H33	H137	H139	Cu <sub>A</sub>	Cu <sub>B</sub>	Wat <sub>1</sub>	Wat <sub>2</sub>	Max	Sum	Av		
3RG	B crystal s	structure					D	•						
1	start		1.0	2.0	0.8	4.7				4.7	8.5	2.1		
	C2W2	Red	0.2	2.0	0.8	2.1	1.5			2.1	6.6	1.3	0.2831	0.2627
		MV	0.4	1.8	0.8	0.9	1.9			1.9	5.8	1.2	0.2832	0.2627
		Ox	0.5	1.9	0.9	0.8	2.1			2.1	6.2	1.2	0.2832	0.2627
	Y2W2	Red	1.3	1.6	0.4	0.0	0.8	0.4	3.2	3.2	7.7	1.1	0.2879	0.2437
		MV	1.0	1.5	0.5	0.1	0.6	0.2	0.3	1.5	4.2	0.6	0.2878	0.2437
		Ox	0.6	1.5	0.4	0.1	0.4	0.1	0.3	1.5	3.4	0.5	0.2878	0.2437
		Ox,alt	3.0	2.5	4.3	1.4	4.2	0.7	2.0	4.3	18.1	2.6	0.2879	0.2439
	Y2W0	Red	1.8	1.5	1.8	2.7	0.9			2.7	8.7	1.7	0.2881	0.2439
		MV	0.7	1.3	0.4	1.2	0.9			1.3	4.5	0.9	0.2879	0.2438
		Ox	0.8	1.3	0.6	1.1	0.6			1.3	4.4	0.9	0.2879	0.2438
	His137	Red	0.3	2.7	1.4	2.5	1.4			2.7	8.3	1.7	0.2831	0.2627
		MV	1.5	2.7	0.8	1.9	2.6			2.7	9.5	1.9	0.2831	0.2627
		Ox	0.4	2.3	0.7	1.5	2.6			2.6	7.5	1.5	0.2832	0.2627
	C1W0	Red	0.2	1.7	0.3	0.9				1.7	3.1	0.8	0.2824	0.2627
		Ox	0.3	1.6	0.4	1.2				1.6	3.5	0.9	0.2823	0.2626
	C1W1	Red	0.3	1.7	0.2	0.7		0.6		1.7	3.5	0.7	0.2827	0.2626
		Ox	0.3	1.5	0.3	0.7		0.5		1.5	3.3	0.7	0.2822	0.2626
2	C2W2	Red	1.3	1.5	1.4	2.0	2.8			2.8	9.0	1.8	0.2832	0.2626
		MV	1.3	1.5	1.6	2.1	2.9			2.9	9.4	1.9	0.2832	0.2626
		Ox	1.3	1.5	1.6	2.1	2.9			2.9	9.4	1.9	0.2832	0.2626
	Y2W2	Red	1.7	0.3	1.6	0.7	0.5	0.8	2.2	2.2	7.8	1.1	0.2832	0.2626
		MV	1.2	0.7	1.3	1.6	0.4	0.5	1.9	1.9	7.6	1.1	0.2822	0.2626
		Ox	1.2	0.6	1.5	1.5	0.3	0.5	2.1	2.1	7.7	1.1	0.2823	0.2626
	Y2W0	Red	1.7	0.4	0.8	2.5	0.4			2.5	5.8	1.2	0.2823	0.2625
		MV	1.2	0.6	0.6	2.7	0.8			2.7	5.9	1.2	0.2823	0.2625
		Ox	1.4	0.7	0.7	2.8	1.0			2.8	6.6	1.3	0.2823	0.2625
	C1W0	Red	1.1	0.5	0.4	0.7				1.1	2.7	0.7	0.2823	0.2625
		Ox	1.7	0.5	0.4	0.3				1.7	2.9	0.7	0.2823	0.2625
	C1W1	Ox	1.1	0.4	1.1	0.4		2.4		2.4	5.4	1.1	0.2822	0.2625
3	C2W2	Red	0.3	2.0	1.4	0.1	1.9			2.0	5.7	1.1	0.2830	0.2627
		MV	0.5	1.9	1.5	0.5	2.6			2.6	7.0	1.4	0.2830	0.2627
		Ox	0.5	1.8	1.6	0.5	2.8			2.8	7.2	1.4	0.2830	0.2627
	Y2W2	Red	0.3	1.5	0.0	0.1	1.4	0.2	3.0	3.0	6.5	0.9	0.2828	0.2627
		MV	0.3	1.5	0.2	0.9	1.6	0.0	3.2	3.2	7.7	1.1	0.2821	0.2627
		Ox	0.5	1.5	0.2	0.9	1.6	0.0	2.9	2.9	7.6	1.1	0.2821	0.2627
	Y2W0	Red	0.3	1.5	0.3	1.0	1.8			1.8	4.9	1.0	0.2827	0.2627
		MV	0.2	1.5	0.4	0.9	2.1			2.1	5.1	1.0	0.2819	0.2627
		Ox	0.2	1.6	0.5	0.9	2.2			2.2	5.4	1.1	0.2819	0.2627
	C1W0	Red	0.1	1.5	0.3	1.0				1.5	2.9	0.7	0.2822	0.2626
	~~~~	Ox	0.4	1.6	0.0	1.3				1.6	3.3	0.8	0.2829	0.2627
	CIWI	Ox	0.4	1.6	0.0	2.0		1.6		2.0	5.6	1.1	0.2829	0.2627
3RFI	crystal s	tructure	0.0	0.1	0.1	0.7	0.7			<u> </u>	2.5	0.7	0.07/2	0.0402
1	C2W2	Red	0.0	0.1	0.1	0.6	2.7			2.7	3.5	0.7	0.2763	0.2483
		MV	0.0	0.0	0.3	0.5	1.6			1.6	2.4	0.5	0.2763	0.2483
	~	Ox	0.0	0.4	0.4	0.6	1.9			1.9	3.3	0.7	0.2763	0.2483
	CIW0	Red	0.4	0.0	0.1	1.4				1.4	1.9	0.5	0.2765	0.2483
	01774	Ux	0.1	0.0	0.1	1.3				1.3	1.5	0.4	0.2765	0.2483
	CIWI	Red	0.6	0.0	0.1	1.3		2.6		2.6	4.6	0.9	0.2767	0.2484
	CINC	Dx 1	0.0	0.0	0.1	0.9		2.5		2.5	5.5	0.7	0.2764	0.2483
2	CIWO	Ked	0.2	0.0	0.4	0.1				0.4	0.7	0.2	0.2765	0.2485
	CIWI	Ox Or	0.4	0.1	0.4	0.2		1.2		0.4	1.1	0.5	0.2765	0.2485
	CIWI	Dx 1	0.3	0.1	0.4	0.5		1.5		1.5	2.6	0.5	0.2764	0.2484
3	CIW0	кеd	0.0	0.3	0.2	0.9				0.9	1.4	0.4	0.2762	0.2484
	01324	Ox	0.0	0.3	0.2	0.9		0.5		0.9	1.4	0.4	0.2762	0.2484
	CIWI	UX	0.0	0.2	0.2	1.0		0.5		1.0	1.9	0.4	0.2760	0.2483

**Table S3.** Energy components of the various reactant states in the reaction with methanol. Five energies are given for each reactant in both the triplet (S = 1) and singlet state (S = 0): TPSS-D3/def2-SV(P) optimised geometries, TPSS-D3/def2-TZVPD and B3LYP-D3/def2-TZVPD single point energies, obtained in a COSMO continuum solvent with a dielectric constant of 4, zero-point energies (ZPE) from TPSS-D3/def2-SV(P) frequencies and the total energies, which are the sum of the ZPE and the B3LYP-D3/def2-TZVPD energies. The reference energy is always the triplet RS state.

Energy	Q	QM		QM+COSMO		COSMO	ZI	PE	To	Total		
Method	TPS	TPSS-D3		TPSS-D3		YP-D3	TPS	S-D3	B3LYP-D3			
Basis	def2-	SV(P)	def2-7	TZVPD	def2-7	def2-TZVPD		SV(P)	def2-7	<b>ZVPD</b>		
S	1	0	1	0	1	0	1	0	1	0		
RS	0.0	19.4	0.0	33.0	0.0	85.2	0.0	-0.3	0.0	84.8		
R	-21.0	-2.5	-11.7	24.6	-1.2	74.2	2.9	2.9	1.7	77.1		
TS1	24.0	28.1	20.7	61.1	35.1	124.4	-13.2	-12.6	21.9	111.8		
Im1	6.9	6.8	-10.0	74.2	-8.8	141.2	-6.8	-7.0	-15.6	134.2		
Im2	-20.1	-87.0	-32.2	-100.0	-8.1	-60.8	1.9	9.0	-6.2	-51.8		
TS2	125.6	-30.9	113.2	-34.7	132.4	-5.5	-8.3	6.2	124.2	0.7		
Р	-32.9	-237.1	-16.5	-226.9	9.0	-233.6	13.7	16.9	22.6	-216.7		

**Figure S1.** QM-refined structures of site A in the first protomer of the 3RGB structure, modelled by two Cu ions in the (a) fully reduced and (b) fully oxidised states.



**Figure S2.** (a) The Yoshizawa-type structure of pMMO (first protomer of the 3RGB structure, Y2W0a) obtained by QM/MM (i.e. QM-refinement with  $w_A = 0$ ) for the reduced state. (b) A quantum-refined structure with two extra water molecules for the MV state (Y2W2). (c) The quantum-refined structure of site A with the backbone carbonyl group coordinating to Cu<sub>B</sub> (reduced state).



**Figure S3.** QM-refined structures of site A, modelled with a single Cu ion (C1W0) in the (a) reduced and (b) oxidised states.



**Figure S4.** QM-refined structures of site A, modelled with a single Cu ion and the water molecule in the (a) oxidised state (C1W1). Part (b) shows the electron-density maps of the oxidised state. The  $2mF_{o}-DF_{c}$  maps are contoured at 1.0  $\sigma$  and the  $mF_{o}-DF_{c}$  maps are contoured at +3.0  $\sigma$  (green) and -3.0  $\sigma$  (red).



**Figure S5.** QM-refined structures of site A in the second protomer of the 3RGB structure, modelled (a) with a two Cu ions (C2W0) in the reduced state, (b) the Yoshizawa-type structure (Y2W2) or (c) with a single Cu ion (still in the reduced state).



Table S4. Coordinates of the QM system for the mononuclear site in all optimised structures.

REMARK PDB files of the mononuclear copper site in pMMO obtained by quantum refinement REMARK L. Cao, O. Caldararu, A. C. Rosenzweig, U. Ryde REMARK Quantum refinement does not support dinuclear copper sites in crystal structures REMARK of particulate methane monooxygenase REMARK Angew. Chemie 2017 REMARK Supplementary material REMARK 18 structures are given: REMARK 2 Crystal structures: 3RGB or 3RFR REMARK 3 subunits REMARK Reduced, Cu(I), oxidised, Cu(II), or oxidised state with an extra water molecule REMARK Only heavy atoms in the QM system are included; other atoms are not moved REMARK REMARK 3RGB, Subunit 1, Reduced state REMARK DATE:04-Nov-2016 15:59:39 created by user: lili REMARK CNS VERSION:1.3 1.00 73.31 ATOM 1 CB HIS 33 39.558 130.222 81.449 C 0 Α АТОМ 2 CG 39.536 130.282 C 0 HIS 33 82.943 1.00 72.87 Α CD2 HTS 40.433 130.882 1.00 72.68 C 0 АТОМ 3 33 83.811 Α ATOM 4 ND1 HIS 33 38.383 129.977 83.651 1.00 72.38 А N 0 ATOM 5 CE1 HIS 33 38.558 130.382 84.908 1.00 72.38 А C 0 N 0 ATOM 6 NE2 HIS 33 39.798 130.929 85.043 1.00 72.37 А 39.582 131.594 79.449 1.00 73.42 ATOM 7 С HIS 33 А С 0 АТОМ 8 Ν HIS 33 37.660 131.761 81.212 1.00 73.34 N 0 Α 39.101 131.627 АТОМ 9 80,915 1.00 73.37 C 0 CA HIS 33 А 10 35.988 128.077 85.420 1.00 43.65 ATOM CB HIS 137 А С 0 ATOM 11 CG HIS 137 35.055 129.223 85.194 1.00 43.97 А C 0 ATOM 12 CD2 HIS 137 33.793 129.437 85.714 1.00 43.67 А С 0 ND1 HIS 35.445 130.309 84.427 1.00 44.90 ATOM 13 137 А Ν 0 34.440 131.182 АТОМ 14 CE1 HIS 137 84.497 1.00 44.62 А С 0 33.425 130.694 ATOM 15 NE2 HIS 137 85.267 1.00 43.95 N 0 А 33.507 127.696 78.902 1.00 49.60 ATOM 16 CB HIS 139 C 0 А 34.226 128.599 79.774 АТОМ 17 CG HTS 139 1.00 50.45 А C 0 CD2 HIS ATOM 18 139 35.368 128.398 80.520 1.00 51.09 А C 0 ATOM 19 ND1 HIS 139 33.792 129.883 80.036 1.00 50.61 А N 0 20 CE1 HIS 139 34.668 130.428 80.938 1.00 51.73 C 0 ATOM А 35.625 129.541 АТОМ 21 NE2 HIS 139 81.267 1.00 51.75 А N 0 ATOM 22 CU+1 CU1 416 36.806 129.802 82.728 1.00 64.05 А CU 1 END REMARK 3RGB, Subunit 1, Oxidised state REMARK DATE:04-Nov-2016 15:59:39 created by user: lili REMARK CNS VERSION:1.3 ATOM 1 CB HIS 33 39.911 130.476 81.572 1.00 74.85 А C 0 ATOM 2 CG HIS 33 39.672 130.484 83.055 1.00 74.33 C 0 А C 0 АТОМ 3 CD2 HIS 33 40.522 130.877 84.072 1.00 74.26 Α ATOM 38.438 130.187 83.638 1.00 73.84 4 ND1 HIS 33 Α N 0 38.532 130.410 84.955 1.00 73.92 ATOM 5 CE1 HIS 33 А C 0 ATOM 6 NE2 HIS 33 39.789 130.817 85.246 1.00 74.06 N 0 А ATOM 7 С HIS 33 39.578 131.593 79.450 1.00 75.04 А С 0 ATOM 8 Ν HIS 33 37.650 131.186 81.051 1.00 75.22 Ν 0 А 39.071 131.617 АТОМ 9 CA HIS 33 80.906 1.00 75.00 0 А С 10 36.012 128.058 85.421 1.00 43.37 С ATOM СВ HIS 137 А 0 1.00 43.47 АТОМ CG HIS 137 35.116 129.201 85.158 C 0 11 А ATOM 12 CD2 HIS 137 33.902 129.524 85.725 1.00 42.88 A С 0 ATOM 13 ND1 HIS 137 35.514 130.203 84.285 1.00 44.35 N 0 А ATOM 14 CE1 HIS 137 34.554 131.143 84.346 1.00 44.08 А С 0 33.575 130.760 ATOM 15 NE2 HIS 137 85.205 1.00 43.00 А Ν 0 АТОМ 16 СВ HIS 139 33.513 127.691 78.906 1.00 47.68 А С 0 34.225 128.591 79.782 ATOM 17 CG HIS 139 1.00 48.49 C 0 Α CD2 HTS 1.00 49.04 АТОМ 18 139 35.316 128.377 80.597 Α C 0 33.795 129.881 ATOM 19 ND1 HTS 139 80.000 1.00 48.66 А N O ATOM 20 CE1 HIS 139 34.602 130.431 80.945 1.00 49.68 C 0 А АТОМ NE2 HIS 35.525 129.530 N 0 21 139 81.346 1.00 49.68 А 22 CU+1 CU1 36.881 129.891 ATOM 416 82.686 1.00 64.20 А CU 1 END REMARK 3RGB, Subunit 1, Oxidised state with an extra water molecule REMARK DATE:08-Nov-2016 15:55:59 created by user: lili REMARK CNS VERSION:1.3 ATOM 1 CB HIS A 33 39.883 130.479 81.582 1.00 71.86 А C 0 39.690 130.528 ATOM 2 CG HIS A 33 83.075 1.00 71.34 А C 0 CD2 HIS A 33 C 0 ATOM 3 40.598 130.819 84.076 1.00 71.43 Α АТОМ 4 ND1 HIS A 33 38.442 130.380 83.686 1.00 70.70 N 0 А 38.584 130.569 CE1 HIS A 33 1.00 70.88 C 0 ATOM 5 84.998 А NE2 HIS A 39.886 130.832 85.265 1.00 71.25 АТОМ 6 33 А N 0 ATOM 7 С HIS A 33 39.579 131.595 79.450 1.00 72.08 А C 0 8 Ν HIS A 33 37.642 131.281 81.056 1.00 72.17 N 0 ATOM А 9 CA HIS A 33 39.079 131.634 80.904 1.00 72.04 C 0 ATOM А

ATOM	10	CB	HIS	А	137	36.006	128.065	85.426	1.00	42.08	А	C 0
ATOM	11	CG	HIS	А	137	35.102	129.208	85.170	1.00	42.46	А	C 0
АТОМ	12	CD2	HTS	A	137	33.873	129.505	85.718	1.00	41.85	A	C 0
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АТОМ	14	CE1	HTS	Δ	137	34.532	131.157	84.383	1.00	43.48	A	
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ATOM	17	CB	пто	A	120	24 206	127.092	70.904	1.00	40.10	A	
ATOM	1/	CG	HIS HIC	A	139	34.200	128.017	/9.//3	1.00	47.19	A	
ATOM	18	CD2	HIS	A	139	35.312	128.435	80.569	1.00	4/./4	A	0 0
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ATOM	20	CE1	HIS	Α	139	34.555	130.464	80.937	1.00	48.85	A	C 0
ATOM	21	NE2	HIS	А	139	35.502	129.588	81.320	1.00	48.45	A	N 0
ATOM	22	0	HOH	А	416	37.843	127.924	82.467	1.00	52.69	A	00
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ATOM	5	CE1	HIS	Е	33	34.133	160.860	31.154	1.00	61.46	E	C 0
ATOM	6	NE2	HIS	Е	33	35.362	161.058	30.613	1.00	63.11	E	N 0
ATOM	7	С	HIS	Е	33	35.696	155.460	32.461	1.00	61.00	E	C 0
ATOM	8	N	HIS	Е	33	33.609	156.748	32.014	1.00	62.27	E	N 0
ATOM	9	CA	HIS	Е	33	35.054	156.648	31.755	1.00	61.93	E	C 0
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АТОМ	13	ND1	HTS	Е	137	31.184	160.218	31.909	1.00	42.05	E	N O
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ATOM	10	CB	HIS	E	139	30.178	156.685	37.123	1.00	45.17	E	0
ATOM	1/	CG	HIS	E	139	30.622	157.008	35.//9	1.00	44.56	E	C 0
ATOM	18	CD2	HIS	Ε	139	31.601	157.862	35.329	1.00	45.27	E	C 0
ATOM	19	ND1	HIS	Е	139	30.063	156.436	34.661	1.00	44.86	E	N 0
ATOM	20	CE1	HIS	Е	139	30.674	156.975	33.565	1.00	45.65	E	C 0
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ATOM	10	СВ	HIS	Е	137	31.848	162.241	33.292	1.00	39.65	Е	C 0
ATOM	11	CG	HIS	Е	137	30.869	161.386	32.558	1.00	39.95	E	C 0
ATOM	12	CD2	HIS	E	137	29.577	161.680	32.189	1.00	39.80	E	C 0
ATOM	13	NDI	HIS	E	137	31.1/1	160.110	32.113	1.00	40.08	E	
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АТОМ	16	CB	HIS	E	139	30.186	156.696	37.125	1.00	41.73	E	C 0
ATOM	17	CG	HIS	E	139	30.582	157.002	35.765	1.00	40.91	E	C 0
ATOM	18	CD2	HIS	Е	139	31.427	157.943	35.234	1.00	41.13	Е	C 0
ATOM	19	ND1	HIS	Е	139	30.090	156.276	34.711	1.00	41.47	Е	N 0
ATOM	20	CE1	HIS	Е	139	30.600	156.792	33.563	1.00	42.20	Е	C 0
АТОМ	21	NE2	HIS	Е	139	31.427	157.802	33.856	1.00	41.45	E	N 0
ATOM	22	0	HOH	E	416	33.826	159.548	34.573	1.00	48.02	E	0 0
ATOM	23	CU+1	CUI	E	417	32.656	158.842	32.632	1.00	62.64	Е	CU 1
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АТОМ	1	CB	HIS	Ι	33	34.208	101.593	33.639	1.00	65.19	I	C 0
АТОМ	2	CG	HIS	Ι	33	33.709	100.358	32.950	1.00	63.32	I	C 0
ATOM	3	CD2	HIS	Ι	33	34.393	99.184	32.704	1.00	62.66	I	C 0
ATOM	4	ND1	HIS	Ι	33	32.362	100.165	32.640	1.00	62.85	I	N 0
АТОМ	5	CE1	HIS	Ι	33	32.236	98.899	32.241	1.00	61.69	I	C 0
ATOM	6	NE2	HIS	I	33	33.443	98.278	32.260	1.00	61.82	I	N O
ATOM	7	C	HIS	I	33	34.334	102.858	35.741	1.00	67.59	I	C 0
ATOM	8		HIS	Т Т	33	32.195	102.113	34.8/8	1.00	66.92	L T	
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АТОМ	11	CG	HTS	Ť	137	28.741	99.823	31.519	1.00	56.37	т	
ATOM	12	CD2	HIS	ī	137	27.384	99.728	31.741	1.00	56.56	I	C 0
ATOM	13	ND1	HIS	Ι	137	29.413	99.669	32.729	1.00	55.16	I	N 0
АТОМ	14	CE1	HIS	Ι	137	28.481	99.502	33.657	1.00	55.62	I	C 0
АТОМ	15	NE2	HIS	Ι	137	27.235	99.536	33.102	1.00	55.52	I	N 0
ATOM	16	СВ	HIS	Ι	139	28.174	106.072	33.340	1.00	48.56	I	C 0
ATOM	17	CG	HIS	I	139	28.627	104.733	33.712	1.00	48.95	I	C 0
ATOM	18	CD2	HIS	I	139	29.466	103.864	33.053	1.00	49.86	I	C 0
ATOM	19	NDI CE1	HIS	T T	139	28.25/	104.090	34.8/5	1.00	49.19	1	
	20	NE2	нтс	T	139	20.039	102.655	34.000	1 00	49.72	T T	N O
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ATOM	10	СВ	HIS	А	133	55.147	36.089	48.320	1.00	49.64	A	C 0
ATOM	11	CG	HIS	Α	133	54.624	36.076	49.695	1.00	53.16	A	C 0
ATOM	12	CD2	HIS	A	133	55.244	36.654	50.785	1.00	52.66	A	
АТОМ	13	CE1	HIS	A A	133	53.328	35.493	50.085	1.00	55.22	A A	
ATOM	15	NE2	HIS	A	133	54.400	36.430	51.852	1.00	54.43	A	N O
ATOM	16	СВ	HIS	А	135	55.203	29.470	50.334	1.00	53.71	А	C 0
ATOM	17	CG	HIS	А	135	54.332	30.604	50.095	1.00	53.64	A	C 0
ATOM	18	CD2	HIS	Α	135	54.265	31.598	49.142	1.00	53.89	A	C 0
ATOM	19	NDI CE1	HIS	A	135	53.299	30.83/	50.978	1.00	55.3/	A A	
ATOM	20	NE2	HIS	A	135	53.217	32.453	49.466	1.00	55.01	A A	N O
ATOM	22	CU+2	CU2	A	419	52.513	34.050	48.621	1.00	79.73	A	CU 2
END												
REMARK	3RFR	, Subi	unit	1,	, Oxidise	ed state						
REMARK	DATE	:11-Aj	pr-20	017	7 17:59:	:04	created	by user	: lili	Ĺ		
REMARK	CNS	/ERSI		• 3	20	E0 200	21 202	45 070	1 0 0	70 02	7	C 0
ATOM	2	CG	HTS	A	29	50.621	35.625	46.705	1.00	78.80	A	
ATOM	3	CD2	HIS	A	29	50.048	36.876	46.632	1.00	78.59	A	C 0
АТОМ	4	ND1	HIS	A	29	51.581	35.637	47.721	1.00	78.91	А	N 0
ATOM	5	CE1	HIS	А	29	51.585	36.876	48.235	1.00	78.27	A	C 0
ATOM	6	NE2	HIS	A	29	50.669	37.636	47.602	1.00	79.12	A	N O
ATOM	7	C	HIS	A	29	49.122	32.198	46.333	1.00	79.01	A	
	0 9		нте	A	29	50 050	32.750	47.297	1 00	00.40 79 19	A A	
ATOM	10	CB	HIS	A	133	55.148	36.089	48.284	1.00	49.30	A	
ATOM	11	CG	HIS	A	133	54.589	36.034	49.630	1.00	52.69	A	C 0
ATOM	12	CD2	HIS	А	133	55.082	36.685	50.738	1.00	51.36	A	C 0
ATOM	13	ND1	HIS	А	133	53.475	35.302	49.989	1.00	55.17	A	N 0
ATOM	14	CE1	HIS	А	133	53.275	35.525	51.296	1.00	54.77	A	C 0
ATOM	15	NE2	HIS	Α	133	54.231	36.362	51.770	1.00	53.16	A	N 0
ATOM	16	СВ	HIS	A	135	55.205	29.470	50.334	1.00	53.53	A	C 0
ATOM	19	CG CD2	HIS	A	135	54.334	30.603	50.099 19 163	1.00	53.54	A A	
ATOM	19	ND1	HIS	A	135	53.285	30.818	50.965	1.00	53.36	A	N 0
ATOM	20	CE1	HIS	A	135	52.627	31.931	50.572	1.00	55.24	A	C 0
ATOM	21	NE2	HIS	А	135	53.234	32.452	49.495	1.00	54.11	А	N 0
	22	C111-2	C112	Α	410	F0 400	24 050	18 630	1 00	81 / 8	Δ	CII 2
ATOM	22	CUTZ	C02		419	52.498	34.050	40.030	1.00	01.40	11	C0 2
END	22	012	02		419	52.498	34.050	40.050	1.00		11	0 2
END REMARK REMARK REMARK	3RFR DATE CNS	, Sub 11-Aj	unit pr-20	1, 017	419 Oxidise 7 17 <b>:</b> 45:	52.498 ed state :49	with an o	extra wa by user	ter mo	olecule		02
END REMARK REMARK REMARK ATOM	3RFR DATE CNS 1	, Sub 11-Aj VERSIO	unit pr-20 DN:1 HIS	1, 017 .3 A	419 Oxidise 7 17:45: 29	52.498 ed state :49 50.553	with an ocreated 34.233	extra wa by user 45.910	ter mo : lili 1.00	olecule	A	C 0
END REMARK REMARK REMARK ATOM ATOM	3RFR DATE CNS 1 2	, Subi 11-Aj VERSIO CB CG	unit pr-20 DN:1 HIS HIS	1, 017 .3 A A	419 Oxidise 7 17:45: 29 29	52.498 ed state :49 50.553 50.819	34.030 with an o created 34.233 35.534	45.930 extra wa by user 45.910 46.606	ter mc : lili 1.00 1.00	75.20 75.45	AAA	C 0 C 0
END REMARK REMARK REMARK ATOM ATOM	3RFR DATE CNS 1 2 3	, Subi 11-Aj VERSIO CB CG CD2	unit pr-20 DN:1 HIS HIS HIS	1, 017 .3 A A A	419 Oxidise 7 17:45: 29 29 29 29	52.498 ed state :49 50.553 50.819 50.157	with an o created 34.233 35.534 36.737	extra wa by user 45.910 46.606 46.466	ter mc : lili 1.00 1.00 1.00	75.20 75.65	A A A	C 0 C 0 C 0
END REMARK REMARK REMARK ATOM ATOM ATOM	3RFR DATE CNS 1 2 3 4	, Subi 11-Aj VERSIC CB CG CD2 ND1	unit pr-20 DN:1 HIS HIS HIS HIS	1, 017 .3 A A A A	419 , Oxidise 7 17:45: 29 29 29 29	52.498 ed state :49 50.553 50.819 50.157 51.642	with an or created 34.233 35.534 36.737 35.620	extra wa by user 45.910 46.606 46.466 47.728	ter mc : lili 1.00 1.00 1.00	75.20 75.45 75.65 75.53	A A A A	C 0 C 0 C 0 N 0
END REMARK REMARK REMARK ATOM ATOM ATOM ATOM	3RFR DATE CNS 1 2 3 4 5	, Subi 11-Aj VERSIO CB CG CD2 ND1 CE1	unit pr-20 DN:1 HIS HIS HIS HIS HIS	1, 017 .3 A A A A A	419 Oxidise 7 17:45: 29 29 29 29 29 29 29 29	52.498 ed state 49 50.553 50.819 50.157 51.642 51.484	with an ocreated 34.233 35.534 36.737 35.620 36.847	45.050 extra wa by user 45.910 46.606 46.466 47.728 48.242	ter mc : lili 1.00 1.00 1.00 1.00	75.20 75.45 75.65 75.53 75.15	A A A A A	C 0 C 0 C 0 N 0 C 0
ATOM END REMARK REMARK ATOM ATOM ATOM ATOM ATOM	3RFR DATE CNS 1 2 3 4 5 6 7	, Subu :11-Aj VERSIC CB CG CD2 ND1 CE1 NE2 C	unit pr-20 DN:1 HIS HIS HIS HIS HIS	1, 017 .3 A A A A A A A A	419 , Oxidise 7 17:45: 29 29 29 29 29 29 29 29 29 29	52.498 ed state :49 50.553 50.819 50.157 51.642 51.484 50.588	with an ocreated 34.233 35.534 36.737 35.620 36.847 37.537 32.206	extra wa by user 45.910 46.606 46.466 47.728 48.242 47.505 46.325	ter mc : lili 1.00 1.00 1.00 1.00 1.00	75.20 75.45 75.65 75.53 75.15 75.75 75.75	A A A A A A	C 0 C 0 C 0 N 0 C 0 N 0 C 0
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ATOM END REMARK REMARK ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3RFR DATE CNS 7 1 2 3 4 5 6 7 8 9	, Subi :11-Aj VERSIC CB CG CD2 ND1 CE1 NE2 C N CA	unit pr-20 DN:1 HIS HIS HIS HIS HIS HIS HIS HIS	1, 017 .3 A A A A A A A A A A A A A	419 , Oxidise 7 17:45: 29 29 29 29 29 29 29 29 29 29	52.498 ed state :49 50.553 50.819 50.157 51.642 51.484 50.588 49.116 51.127 50.006	with an ocreated 34.233 35.534 36.737 35.620 36.847 37.537 32.206 32.728 33.265	45.050 extra wa by user 45.910 46.606 46.466 47.728 48.242 47.505 46.325 47.746 46.969	ter mcc : lili 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0	75.20 75.45 75.65 75.53 75.15 75.75 75.32 76.22 75.23	A A A A A A A A A	C 0 C 0 C 0 N 0 C 0 N 0 C 0 N 0 C 0
ATOM END REMARK REMARK ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3RFR DATE CNS 1 2 3 4 5 6 7 8 9 10	, Subi 111-A JERSIC CB CG CD2 ND1 CE1 NE2 C N CA CB	unit pr-20 DN:1 HIS HIS HIS HIS HIS HIS HIS HIS HIS	1, 017.3 A A A A A A A A A A A A A A A A A A	419 , Oxidise 7 17:45: 29 29 29 29 29 29 29 29 29 29	52.498 ed state :49 50.553 50.819 50.157 51.642 51.484 50.588 49.116 51.127 50.006 55.148	with an ocreated 34.233 35.534 36.737 35.620 36.847 37.537 32.206 32.728 33.265 36.084	45.050 extra wa by user 45.910 46.606 46.466 47.728 48.242 47.505 46.325 47.746 46.969 48.289	ter mcc : lili 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0	75.20 75.45 75.65 75.53 75.15 75.75 75.75 75.32 76.22 75.23 50.55	A A A A A A A A A A	C 0 C 0 C 0 N 0 C 0 N 0 C 0 N 0 C 0 C 0 C 0
ATOM END REMARK REMARK ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3RFR DATE CNS 1 2 3 4 5 6 7 8 9 10 11	, Subi 111-Aj JERSIC CB CG CD2 ND1 CE1 NE2 C N CA CB CG	unit pr-20 DN:1 HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS	1, D17 .3 A A A A A A A A A A A A A A A A A A	419 , Oxidise 7 17:45: 29 29 29 29 29 29 29 29 29 29	52.498 ed state :49 50.553 50.819 50.157 51.642 51.484 50.588 49.116 51.127 50.006 55.148 54.598	with an ocreated 34.233 35.534 36.737 35.620 36.847 37.537 32.206 32.728 33.265 36.084 36.053	45.050 extra wa by user 45.910 46.606 46.466 47.728 48.242 47.505 46.325 47.746 46.325 47.746 969 48.289 49.642	ter mc : lili 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0	75.20 75.45 75.65 75.53 75.15 75.75 75.32 76.22 75.23 50.55 53.60	A A A A A A A A A A	C 0 C 0 C 0 C 0 N 0 C 0 N 0 C 0 N 0 C 0 C 0 C 0 C 0 C 0 C 0
ATOM END REMARK REMARK ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3RFR DATE CNS 1 2 3 4 5 6 7 7 8 9 10 11 12	, Subi ;11-Aj VERSIC CB CG CD2 ND1 CE1 NE2 C N CA CB CG CD2 CD2 ND2 CD2 ND1 CE1 NE2 CA CB CG CD2 CD2 CD2 CD2 CD2 CD2 CD2 CD2	unit or-20 N:1 HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS	1, D17 A A A A A A A A A A A A A A A A A A A	419 , Oxidise 7 17:45: 29 29 29 29 29 29 29 29 29 29	52.498 ed state :49 50.553 50.819 50.157 51.642 51.484 50.588 49.116 51.127 50.006 55.148 54.598 55.109	with an ocreated 34.233 35.534 36.737 35.620 36.847 37.537 32.206 32.728 33.265 36.084 36.053 36.707	45.050 extra wa by user 45.910 46.606 46.466 47.728 48.242 47.505 46.325 47.746 46.325 47.746 969 48.289 49.642 50.741	ter mc : lili 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0	75.20 75.45 75.65 75.53 75.15 75.75 75.32 76.22 75.23 50.55 53.60 52.24	A A A A A A A A A A A A	C 0 C 0 C 0 C 0 N 0 C 0 N 0 C 0 N 0 C 0 C 0 C 0 C 0 C 0 C 0
ATOM END REMARK REMARK ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3RFR DATE CNS 1 2 3 4 5 6 7 7 8 9 10 11 12 13	, Subi ;11-Aj VERSIC CB CG CD2 ND1 CE1 NE2 C N CA CB CG CD2 ND1 CA CB CG CD2 ND1	unit or-20 N:1 HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS	1,017 · 3 · A · A · A · A · A · A · A · A · A · A	419 , Oxidise 7 17:45: 29 29 29 29 29 29 29 29 29 133 133 133 133	52.498 ed state :49 50.553 50.819 50.157 51.642 51.484 50.588 49.116 51.127 50.006 55.148 54.598 55.109 53.488	<pre>with an original created 34.233 35.534 36.737 35.620 36.847 37.537 32.206 32.728 33.265 36.084 36.053 36.707 35.330 </pre>	45.050 extra wa by user 45.910 46.606 46.466 47.728 48.242 47.505 46.325 47.746 46.969 48.289 49.642 50.741 50.018	ter mc : lili 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0	75.20 75.45 75.65 75.53 75.75 75.75 75.23 76.22 75.23 50.55 53.60 52.24 56.05	A A A A A A A A A A A A A A	C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0
ATOM END REMARK REMARK ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3RFR DATE CNS 1 2 3 4 5 6 7 8 9 10 11 12 13 14	, Subi ;11-Aj /ERSIC CB CG CD2 ND1 CE1 NE2 C N CA CB CG CD2 ND1 CE1 NE1 NE2 CA CB CA CB CB CB CD2 ND1 CE1 NE2 CA CB CB CB CB CD2 ND1 CE1 NE2 CA CB CB CB CD2 ND1 CE1 NE2 CB CB CD2 ND1 CE1 NE2 CB CB CB CD2 ND1 CE1 NE2 CB CB CD2 ND1 CE1 NE2 CB CB CB CD2 ND1 CE1 NE2 CB CB CD2 ND1 CE1 NE2 CB CB CD2 CD2 ND1 CE1 NE2 CB CD2 CD2 CD2 CD2 CD2 CD2 CD2 CD2	unit pr-20 DN:1 HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS	1, 017 A A A A A A A A A A A A A A A A A A A	419 , Oxidise 7 17:45: 29 29 29 29 29 29 29 29 29 133 133 133 133 133	52.498 ed state :49 50.553 50.819 50.157 51.642 51.484 50.588 49.116 51.127 50.006 55.148 54.598 55.109 53.488 53.304	<pre>with an original systems of the system system</pre>	45.050 extra wa by user 45.910 46.606 46.466 47.728 48.242 47.505 46.325 47.746 46.969 48.289 49.642 50.741 50.018 51.325	ter mc : lili 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0	75.20 75.45 75.65 75.53 75.75 75.32 75.23 50.55 53.60 52.24 56.05 55.02	A A A A A A A A A A A A A A A A A A A	C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0
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ATOM END REMARK REMARK ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3RFR DATE CNS 1 2 3 4 4 5 6 7 8 9 10 11 12 13 14 15 16 17	, Subi :11-Aj VERSIC CB CG CD2 ND1 CE1 NE2 CA CB CG CD2 ND1 CE1 NE2 CB CG CD2	unit pr-22 NN:1 HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS	1,01 · A A A A A A A A A A A A A A A A A A A	419 , Oxidise 7 17:45: 29 29 29 29 29 29 29 29 29 29	52.498 ed state :49 50.553 50.819 50.157 51.642 51.484 50.588 49.116 51.127 50.006 55.148 54.598 55.109 53.488 53.304 54.270 55.210 55.210	<pre>with an original systems of the system system</pre>	45.050 extra wa by user 45.910 46.606 46.466 47.728 48.242 47.505 46.325 47.746 46.969 48.289 49.642 50.741 50.018 51.325 51.785 50.331 50.113	ter mc : lili 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0	75.20 75.45 75.65 75.53 75.15 75.75 75.23 76.22 75.23 50.55 53.60 52.24 56.05 55.02 53.81 52.38 52.71	А А А А А А А А А А А А А А А А А А А	C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0
ATOM END REMARK REMARK ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3RFR DATE CNS 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	, Subi :11-Aj VERSIC CB CG CD2 ND1 CE1 NE2 CA CB CG CD2 ND1 CE1 NE2 CB CG CD2 CD2	unit pr-22DN:1 HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS	1,017 • A A A A A A A A A A A A A A A A A A A	419 , Oxidise 7 17:45: 29 29 29 29 29 29 29 29 29 29	22.498 ed state 49 50.553 50.819 50.157 51.642 51.484 50.588 49.116 51.127 50.006 55.148 54.598 55.109 53.488 53.304 54.270 55.210 54.333 54.285	<pre>with an original created 34.233 35.534 36.737 35.620 36.847 37.537 32.206 32.728 33.265 36.084 36.053 36.707 35.330 35.559 36.392 29.462 30.586 31.610</pre>	45.050 extra wa by user 45.910 46.606 46.466 47.728 48.242 47.505 46.325 47.746 46.969 48.289 49.642 50.741 50.018 51.325 51.785 50.331 50.113 49.191	ter mc : lili 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0	75.20 75.45 75.65 75.53 75.75 75.75 75.23 75.23 76.22 75.23 50.55 53.60 52.24 56.05 55.02 53.81 52.38 52.71 52.23	A A A A A A A A A A A A A A A A A A A	C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0
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ATOM	10	CB	HIS	E	133	14.307	-10.420	60.056	1.00	64.38	E	C 0
АТОМ	11	CG	HIS	Е	133	15.150	-11.339	60.881	1.00	66.46	E	C 0
ATOM	12	CD2	HIS	Ε	133	15.146	-11.545	62.247	1.00	67.43	E	C 0
АТОМ	13	ND1	HIS	Е	133	16.102	-12.150	60.303	1.00	66.98	E	N 0
АТОМ	14	CE1	HIS	Е	133	16.676	-12.835	61.284	1.00	65.96	E	C 0
АТОМ	15	NE2	HIS	Е	133	16.124	-12.498	62.481	1.00	66.39	E	N 0
ATOM	16	CB	HIS	Е	135	20.623	-7.700	60.115	1.00	47.31	E	C 0
АТОМ	17	CG	HIS	Е	135	19.864	-8.938	59.747	1.00	48.28	E	C 0
АТОМ	18	CD2	HIS	Е	135	18.658	-9.176	59.124	1.00	48.99	Е	C 0
АТОМ	19	ND1	HIS	Е	135	20.391	-10.189	59.998	1.00	48.89	Е	N 0
АТОМ	20	CE1	HIS	Е	135	19.512	-11.126	59.553	1.00	49.05	Е	C 0
АТОМ	21	NE2	HTS	Е	135	18,449	-10.538	59.021	1.00	48.87	E	N O
ΔΤΟΜ	22	CII+2	CII2	Е	420	16 767	_11 565	58 421	1 00	82 94	E	
FND	22	0012	002	Ц	420	10.707	-11.505	50.421	1.00	02.94	-	C0 2
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REMARK	DALL			4 <b>,</b>				1				
REMARK	DATE	28-NG	$\nabla \nabla - 20$	116	) IZ:	00:25	created	by user	: 1111	L		
REMARK	CNS	/ERSI	)N:1	.3						~~ ~-	_	~ ^
ATOM	T	СВ	HIS	Е	29	16.481	-12.623	54.981	1.00	80.85	Е	C 0
АТОМ	2	CG	HIS	Е	29	15.406	-12.855	56.012	1.00	80.62	E	C 0
ATOM	3	CD2	HIS	Ε	29	14.133	-13.330	55.797	1.00	81.09	E	C 0
АТОМ	4	ND1	HIS	Е	29	15.595	-12.757	57.396	1.00	79.64	E	N 0
АТОМ	5	CE1	HIS	Е	29	14.478	-13.195	57.985	1.00	80.54	E	C 0
АТОМ	6	NE2	HIS	Е	29	13.577	-13.540	57.043	1.00	81.64	E	N 0
АТОМ	7	С	HIS	Е	29	18.765	-12.495	54.379	1.00	81.43	E	C 0
АТОМ	8	N	HIS	Е	29	17.839	-11.183	56.363	1.00	82.06	Е	N 0
АТОМ	9	CA	HIS	Е	29	17.879	-12.461	55.607	1.00	81.34	Е	C 0
АТОМ	10	CB	HTS	Е	133	14.298	-10.410	60.035	1.00	64.90	E	C 0
атом	11	CC	нтс	F	133	15 154	_11 333	60 826	1 00	66 17	F	
	12	CD2	пте	Ē	122	15 095	11 667	62 161	1 00	67 06		
ATOM	12	CDZ ND1	пто	E E	122	16 212	-11.00/	62.101	1.00	67.00		
ATOM	13		пто	E E	122	16.213	-12.014	60.257	1.00	00.00		
ATOM	14	CEI	HIS	E T	133	16./89	-12.742	01.218	1.00	00.30	E	
ATOM	15	NE2	HIS	Е	133	16.125	-12.555	62.381	1.00	66.13	Е	N O
АТОМ	16	CB	HIS	Е	135	20.627	-7.695	60.116	1.00	47.65	E	C 0
АТОМ	17	CG	HIS	Е	135	19.882	-8.934	59.755	1.00	48.47	E	C 0
АТОМ	18	CD2	HIS	Е	135	18.636	-9.171	59.224	1.00	48.90	E	C 0
АТОМ	19	ND1	HIS	Е	135	20.453	-10.177	59.929	1.00	48.82	E	N 0
АТОМ	20	CE1	HIS	Е	135	19.573	-11.126	59.543	1.00	49.03	E	C 0
АТОМ	21	NE2	HIS	Е	135	18.456	-10.538	59.117	1.00	48.70	E	N 0
АТОМ	22	CU+2	CU2	Е	420	16.855	-11.559	58.403	1.00	86.08	Е	CU 2
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END REMARK REMARK REMARK	3RFR DATE CNS	, Subi 12-Aj VERSIO	unit pr-20 DN:1	2, 017 .3	Oxid 0 14:	lised state 20:10	with an created	extra wa by user	ter mo : lili	olecule	r T	C 0
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END REMARK REMARK ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3RFR, DATE: CNS V 1 2 3 4 5 6 7 8	, Subi 12-Aj VERSIC CB CG CD2 ND1 CE1 NE2 C N	nit pr-20 N:1 HIS HIS HIS HIS HIS HIS HIS HIS	2, 017 .3 E E E E E E E E	Oxid 7 14: 29 29 29 29 29 29 29 29 29 29 29	lised state 20:10 16.503 15.410 14.109 15.605 14.461 13.540 18.771 17.794	<pre>with an created -12.684 -12.873 -13.263 -12.809 -13.186 -13.459 -12.496 -11.169</pre>	extra wa by user 54.985 55.005 57.779 57.390 57.970 57.022 54.383 56.352	ter mo : lil: 1.00 1.00 1.00 1.00 1.00 1.00 1.00	81.59 81.34 81.73 80.25 81.19 82.26 82.28 82.90	E E E E E E E E	C 0 C 0 C 0 N 0 C 0 N 0 C 0 N 0
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END REMARK REMARK REMARK ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3RFR DATE: CNS 1 2 3 4 5 6 7 7 8 9 10 11 12 13 14 15 16 17	, Suby :12-Aj VERSIC CB CG CD2 ND1 CE1 NE2 C N CA CB CG CD2 ND1 CE1 NE2 C ND1 CE1 NE2 CB CG CD2 ND1 CE1 NE2 CB CG CD2 CD2 ND1 CE1 NE2 CB CG CD2 CD2 CD2 CD2 CD2 CD2 CD2 CD2	unit pr-2()N:1 HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS	2,7	29 29 29 29 29 29 29 29 29 29 29 29 29 2	lised state 20:10 16.503 15.410 14.109 15.605 14.461 13.540 18.771 17.794 17.887 14.300 15.159 15.113 16.202 16.792 16.150 20.624 19.873	<pre>with an created -12.684 -12.873 -13.263 -13.186 -13.459 -12.496 -11.169 -12.464 -10.410 -11.324 -11.656 -12.017 -12.747 -12.551 -7.703 -8.929</pre>	extra wa by user 54.985 56.005 55.779 57.390 57.970 57.022 54.383 56.352 55.627 60.034 60.816 62.154 60.231 61.181 62.356 60.117 59.759	ter md : lil: 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0	81.59 81.34 81.73 80.25 81.19 82.26 82.28 82.90 82.16 64.98 66.53 67.00 66.38 66.09 47.70 48.53		C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0 C 0
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<li>Oxid</li> <li>14:</li> <li>29</li> <li>133</li> <li>133</li> <li>133</li> <li>133</li> <li>135</li> <li>135</li></ul>	lised state 20:10 16.503 15.410 14.109 15.605 14.461 13.540 18.771 17.794 17.887 14.300 15.159 15.113 16.202 16.792 16.150 20.624 19.873 18.628 20.431 19.547 18.438 18.763 16.863 16.863 16.863	<pre>with an created -12.684 -12.873 -13.263 -13.2809 -13.186 -13.459 -12.496 -11.169 -12.464 -10.410 -11.324 -11.656 -12.017 -12.747 -12.551 -7.703 -8.929 -9.156 -10.180 -11.123 -10.522 -14.119 -11.579 created -19.302 -20.295 -20.827 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 -2.551 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ND1 CB3 ND1 CB3 ND1 CB3 ND1 CB3 ND1 CB3 ND1 CB3 ND1	unit pr-22DN:1 HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS	213 EEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEE	<ul> <li>Oxid</li> <li>Oxid</li> <li>14:</li> <li>29</li> <li>133</li> <li>133</li> <li>133</li> <li>133</li> <li>135</li> <li>29</li> <li>2</li></ul>	lised state 20:10 16.503 15.410 14.109 15.605 14.461 13.540 18.771 17.794 17.887 14.300 15.159 15.113 16.202 16.792 16.150 20.624 19.873 18.628 20.431 19.547 18.438 18.763 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 16.863 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59.759 59.220 59.932 59.537 59.106 58.597 58.389 by user 34.919 35.141 34.204 36.406 36.216 34.891 35.655 37.154	ter mo : lil: 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	81.59 81.34 81.73 80.25 81.19 82.26 82.28 82.90 82.16 64.98 66.53 67.04 67.00 66.38 66.09 47.70 48.53 67.04 82.5 67.04 84.98 48.78 76.39 84.92 76.64 76.90 76.91 77.04 76.21 78.29 78.47		СССNО0000000000000000000000000000000000

απом	10	CB	HIC	т	133	72 019	-23 668	38 116	1 00	68 19	т	C
	11	CC	ите	Ť	122	72.015	22.000	20 205	1 00	60.13		
ATOM	10	CG	1115	+ +	122	73.110	-23.008	39.295	1.00	09.03		
ATOM	12	CD2	HIS	Т	133	/4.1/9	-23.625	39.951	1.00	69.37	1	C
ATOM	13	ND1	HIS	Ι	133	73.222	-21.629	39.434	1.00	68.64	I	N (
ATOM	14	CE1	HIS	Ι	133	74.313	-21.403	40.158	1.00	68.41	I	C
ATOM	15	NE2	HIS	Ι	133	74.932	-22.579	40.489	1.00	69.35	I	N (
АТОМ	16	CB	HIS	т	135	68.328	-19,987	42.685	1.00	43.79	т	C (
	17	CC	ите	Ŧ	125	60 3/1	10 060	11 612	1 00	13 01	- T	C
ATOM	10	CG	UTC		125	60 620	20 706	41.042	1 00	12 76		
ATOM	10		п15 ита	1 -	135	09.039	-20.790	40.577	1.00	43.70	1	
ATOM	19	NDI	HIS	T	135	70.149	-18.862	41.521	1.00	43.89	T	N
ATOM	20	CE1	HIS	Ι	135	70.893	-19.016	40.385	1.00	44.83	I	C
ATOM	21	NE2	HIS	Ι	135	70.614	-20.184	39.803	1.00	43.38	I	N (
ATOM	22	CU+2	CU2	Ι	420	71.598	-20.589	38.156	1.00	82.47	I	CU 2
END												
REMARK	3RFR	Sub	uni+	3	Oxi	dised state						
DEMADK	DATE	28_N	-17 - 2(	116	5 12	•00•25	created	by user	• 111			
REMARK	DAIL		0v - 20	210	5 12	.00.25	Cleated	by user	• 111.	L		
REMARK	CNS	/ERS10	JN:1.	. 3								_
ATOM	1	СВ	HIS	Ι	29	71.003	-19.318	34.918	1.00	75.89	I	C (
ATOM	2	CG	HIS	Ι	29	72.119	-20.308	35.143	1.00	76.17	I	C
ATOM	3	CD2	HIS	Ι	29	73.003	-20.823	34.220	1.00	76.17	I	C
АТОМ	4	ND1	HIS	Ι	29	72,531	-20.771	36.411	1.00	77.04	I	N
АТОМ	5	CF1	нтс	т	29	73 635	_21 520	36 230	1 00	75 75	т	C
ATOM	5	NEO	UTC		20	73.033	21.520	24 015	1 00	75.75		
ATOM	0	NEZ	HIS	1	29	/3.932	-21.5/9	34.915	1.00	/5.55	1	N
ATOM	1	C	HIS	I	29	70.058	-17.102	35.657	1.00	77.52	I	C
ATOM	8	N	HIS	Ι	29	70.266	-19.125	37.215	1.00	77.77	I	N (
ATOM	9	CA	HIS	Ι	29	70.880	-18.337	36.116	1.00	76.79	I	C
ATOM	10	CB	HIS	Ι	133	71.993	-23.684	38.411	1.00	69.80	I	C
АТОМ	11	CG	HIS	т	133	73.028	-22,960	39,244	1.00	70.43	т	C (
АТОМ	12	CD2	нтс	т	133	74 103	-23 117	30 072	1 00	70 29	т	C I
ATOM	12	ND1	UTC		122	72 042	21 567	20 201	1 00	70.20		
ATOM	13		п15 ито		122	73.043	-21.307	39.204	1.00	70.50	1	
ATOM	14	CEI	HIS	T	133	/4.09/	-21.207	40.035	1.00	/0.14	T	C
ATOM	15	NE2	HIS	Ι	133	74.761	-22.317	40.452	1.00	69.87	I	N (
ATOM	16	CB	HIS	Ι	135	68.323	-19.992	42.681	1.00	43.95	I	C
ATOM	17	CG	HIS	Ι	135	69.341	-19.971	41.639	1.00	44.15	I	C
АТОМ	18	CD2	HIS	Ι	135	69.649	-20.779	40.562	1.00	43.82	I	C
АТОМ	19	ND1	HTS	т	135	70.143	-18.857	41.551	1.00	44.25	Т	N
	20	CE1	ите	Ť	125	70 997	10.057	10 131	1 00	15 10	т т	C 1
ATOM	20	CE1	1115	1 T	105	70.097	-10.904	40.451	1.00	43.19	1	
ATOM	21	NE2	HIS	Т	135	/0.622	-20.123	39.816	1.00	43.42	T	N
ATOM	22	CU+2	CU2	Ι	420	71.602	-20.533	38.166	1.00	83.83	I	CU 2
END												
REMARK	3RFR	, Sub	unit	3	, Oxi	dised state	with an	extra wa	ter mo	olecule	2	
REMARK	DATE	:12-A	or-20	)17	7 14	:54:54	created	bv user	: 1i1:	i		
REMARK	CNS	ZERST	ON•1	3								
	1	CP	ите	. Э т	20	70 997	10 210	31 020	1 00	77 06	т	C I
ATOM	1		1115	+ +	29	70.997	-19.319	34.920	1.00	77.00	1	
ATOM	2	CG	HIS	T	29	/2.114	-20.311	35.138	1.00	//.31	T	CI
ATOM	3	CD2	HIS	T	29	72.969	-20.855	34.203	1.00	77.29	1	C
ATOM	4	ND1	HIS	Ι	29	72.552	-20.752	36.405	1.00	78.09	I	N (
ATOM	5	CE1	HIS	Ι	29	73.641	-21.518	36.213	1.00	76.86	I	C
ATOM	6	NE2	HIS	Ι	29	73.908	-21.606	34.891	1.00	76.67	I	N (
АТОМ	7	С	HIS	т	29	70.060	-17.099	35,661	1.00	78.66	т	C (
	, o	N	ите	Ŧ	20	70 296	10 111	37 236	1 00	70 07	- T	N
ATOM	0		1115		29	70.200	-19.111	37.230	1 00	70.07		
ATOM	9	CA	HIS	T	29	/0.893	-18.334	30.127	1.00	11.91	T	CI
ATOM	10	СВ	HIS	Ι	133	71.995	-23.681	38.415	1.00	70.54	1	C
ATOM	11	CG	HIS	Ι	133	73.017	-22.958	39.248	1.00	71.12	I	C
ATOM	12	CD2	HIS	Ι	133	74.087	-23.432	39.993	1.00	70.93	I	C
ATOM	13	ND1	HIS	Ι	133	73.038	-21.564	39.263	1.00	71.41	I	N
АТОМ	14	CE1	HTS	т	133	74.088	-21,189	40,012	1.00	70,91	т	C
ΔΟM	1 5	NEJ	цте	Ŧ	132	71 715	-22 205	10 157	1 00	70 55	- -	N
	10		1110	+ +	125	(4./4)	10 001	40.407	1 00	10.00	-	
ATOM	10	CB	HIS	T	132	68.328	-19.991	42.6/8	1.00	43.89	1	C
Allou	17	CG	HIS	Ι	135	69.339	-19.974	41.642	1.00	44.04	I	C
ATOM	18	CD2	HIS	Ι	135	69.644	-20.780	40.561	1.00	43.68	I	C
ATOM	19	ND1	HIS	Ι	135	70.146	-18.862	41.551	1.00	44.25	I	N (
ATOM	20	CE1	HIS	Ι	135	70.902	-18.969	40.429	1.00	44.79	I	C
АТОМ	21	NE2	HIS	Ţ	135	70.619	-20.126	39.816	1.00	43.21	T	N
	22	0	нон	Ŧ	419	73 621	_17 017	38 610	1 00	60 97	т Т	0.0
	22	CULT	0112	- -	420	71 601	20 507	20 120	1 00	02 12	1 T	
AIOM	23	CU+2	CUZ	т	420	/1.021	-20.50/	20.109	T.00	03.12	T	
END												