

Electronic Supplementary Information for

Influence of key amino acid mutation on active site structure and on folding in Acetyl-CoA synthase: a theoretical perspective

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1. Bioinformatics analysis of the conservation of the 503-599 region of *M. thermoacetica* ACS enzyme

Results of a search for homologues in the SwissProt protein sequences database, using the 503-599 region of sequence of *Moorella thermoacetica* ACS enzyme, provided the results reported in Table S1. In total, 11 homologues were retrieved, with amino acid sequence conservation between 48% and 41%. Such high values of sequence identity is indicative of the conservation of the protein fold in the surroundings of the A-cluster.

Table S1. Results of a search for homologs in the SwissProt protein sequences database, using the 503-599 region of sequence of *M. thermoacetica* ACS enzyme.

Entry	Entry name	Protein names	Organism	Identity	E-value	Gene names
P27988	DCMA_MO OTH	Carbon monoxide dehydrogenase/ acetyl-CoA synthase	<i>Moorella thermoacetica</i> (<i>Clostridium thermoaceticum</i>)	100.0%	8.0×10^{-63}	
O29868	ACDB_ARC FU	Acetyl-CoA decarbonylase/ synthase complex	<i>Archaeoglobus fulgidus</i> (strain ATCC 49558 / VC- 16 / DSM 4304 / JCM 9628 / NBRC 100126)	48.0%	2.0×10^{-26}	cdhC AF_0379
Q8TXF4	ACDB_MET KA	Acetyl-CoA decarbonylase/ synthase complex	<i>Methanopyrus kandleri</i> (strain AV19 / DSM 6324 / JCM 9639 / NBRC 100938)	48.0%	9.0×10^{-26}	cdhC MK0720
Q57620	ACDB2_ME TJA	Acetyl-CoA decarbonylase/ synthase complex	<i>Methanocaldococc us jannaschii</i> (strain ATCC 43067 / DSM 2661 / JAL-1 / JCM 10045 / NBRC 100440)	48.0%	3.0×10^{-25}	cdhC2 MJ0156
Q57616	ACDB1_ME TJA	Acetyl-CoA decarbonylase/ synthase complex	<i>Methanocaldococc us jannaschii</i> (strain ATCC 43067 / DSM 2661 / JAL-1 / JCM 10045 / NBRC 100440)	48.0%	2.0×10^{-24}	cdhC1 MJ0152
O27745	ACDB_MET TH	Acetyl-CoA decarbonylase/ synthase complex	<i>Methanothermobac ter thermautotrophicus</i> (strain ATCC 29096 / DSM 1053	46.0%	2.0×10^{-23}	cdhC MTH_1710

			/ JCM 10044 / NBRC 100330 / Delta H) (<i>Methanobacterium thermoautotrophicu m</i>) <i>Methanosarcina acetivorans</i> (strain ATCC 35395 / DSM 2834 / JCM 12185 / C2A)			
Q8TJC4	ACDB2_ME TAC	Acetyl-CoA decarbonylase/ synthase complex		45.0% 1.0×10 ⁻²²	cdhC2 MA_3862	
P72021	ACDB1_ME TTE	Acetyl-CoA decarbonylase/ synthase complex	<i>Methanosarcina thermophila</i>	41.0% 2.0×10 ⁻²²	cdhC1	
Q8PZ11	ACDB1_ME TMA	Acetyl-CoA decarbonylase/ synthase complex	<i>Methanosarcina mazei</i> (strain ATCC BAA-159 / DSM 3647 / Goe1 / Go1 / JCM 11833 / OCM 88) (<i>Methanosarcina frisida</i>) <i>Methanosarcina mazei</i> (strain ATCC BAA-159 / DSM 3647 / Goe1 / Go1 / JCM 11833 / OCM 88) (<i>Methanosarcina frisida</i>)	41.0% 2.0×10 ⁻²²	cdhC1 MM_0686	
Q8PV85	ACDB2_ME TMA	Acetyl-CoA decarbonylase/ synthase complex	<i>Methanosarcina frisida</i> <i>Methanosarcina acetivorans</i> (strain ATCC 35395 / DSM 2834 / JCM 12185 / C2A)	42.0% 3.0×10 ⁻²²	cdhC2 MM_2087	
Q8TRZ6	ACDB1_ME TAC	Acetyl-CoA decarbonylase/ synthase complex	<i>Methanosarcina acetivorans</i> (strain ATCC 35395 / DSM 2834 / JCM 12185 / C2A)	43.0% 6.0×10 ⁻²²	cdhC1 MA_1014	
Q9V2Z4	ACDB2_ME TTE	Acetyl-CoA decarbonylase/ synthase complex	<i>Methanosarcina thermophila</i>	42.0% 2.0×10 ⁻²¹	cdhC2	

Pairwise sequence alignments between the *M. thermoacetica* sequence region of interest (tagged as “Query” in the following) and the corresponding regions in the homolog proteins listed in Table S1 are reported below:

```

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269	EYSGVNEFAKQESGGEYERIKLHSFFEYPHTSCGCFE	305 O29868
1	FYSCVLCQSFAPNHVCIVTPERVGLCGAVSWLDAKASYEINHAGPNQPIPKGEIDPIKG	60 Query
	FY C++CQSFAP HVC++TP+R LCG+++W DAKA+Y+I+ GP PI K +DP G	
190	FYVCLMCQSFAPTHVCVITPDRPSLCGSITWHDAKAAKIDPEGPIFFIEKGECLDPEAG	249 Q8TXF4
61	IWKSVNDYLYTASNRLNQVCLYTLMENPMTSCGCFE	97 Query
	++ VN+ + S +E+V L++ +E P TSCGCF+	
250	EYEGVNEAVKEHSQGTVERVYLHSCLEYPHTSCGCFQ	286 Q8TXF4
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	FY CV+CQSFAP HVC++TP+R LCG +++LDA+A+ +I+ GP IPK +D G	
184	FYGCVMCQSFAPTHVCVITPDRPALCGGINYLDAKAAKIDPNGPIFEIPKGECLDEKLG	243 Q57620
61	IWKSVNDYLYTASNRLNQVCLYTLMENPMTSCGCFE	97 Query
	I+ VN+ + S +E+V L++ +E P TSCGCFE	
244	IYSGVNEVVRERSQGTVEEVTLHSALEKPCTSCGCFE	280 Q57620
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	FY CV+CQSFAP HVC+TP+R LCG++++LDA+A+ +I+ GP IPK +D G	
477	FYGCVMCQSFAPTHVCIITPDRPSLCGSINYLDARAAKIDPNGPIFEIPKGECLDEKLG	536 Q57616

61	IWKSVNDYLYTASNRLNQVCLYTLMENPMTSCGCFE	97 Query
	I+ VN+ + S ++E++ L++ + NP TSCGCFE	
537	IYTGVEVVRERSQGSVEEMALHSALTNPCTSCGCFE	573 Q57616
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	FY C++CQSFAP HVCIVTP+R LCGA++W D +A+Y+++ GP I K +DP +G	
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61	IWKSVNDYLYTASNRLNQVCLYTLMENPMTSCGCFE	97 Query
	+ +VN + S ++V L+++ P TSCGCFE	
245	EYANVNAAVEENSQGTDRVYLHSVFGYPHTSCGCFE	281 O27745
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	FY C LCQSFAP +VC+V+P+RV LCGA++W D +A+ +++ GP I K ID KG	
186	FYGCTLCQSFAPTNVCVVPDRVSLCGAINWFDG R A A A K V D P E G P Q F E I T K G D L I D A E K G	245 Q8TJC4
61	IWKSVNDYLYTASNRLNQVCLYTLMENPMTSCGCFE	97 Query
	+ VND S +++ L++ + P TSCGCFE	
246	EYTGVN DIAKKLSAGEFDKIKLHSFFDAPHTSCGCFE	282 Q8TJC4
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	FY C LCQSFAP +VC+V+P+R+ LCGA++W D +A+ +++ GP I K +D + G	
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	FY C LCQSFAP +VC+V+P+R+ LCGA++W D +A+ +++ GP I K ID + G	
187	FYGCTLCQSFAPTNVCVVPDRISLCGAINWFDGRAAAKVDPEGPQFEIAKGDLLIDAVTG	246 Q8PV85
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	+ VN+ S+ +++ L++ + P TSCGCFE	
247	EYTGvNEIakKLSSGEFDKIKLHSFFDCPHTSCGCFE	283 Q8PV85
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	FY C LCQSFAP +VC+V+P+RV LCGA++W D +A+ +++ GP I K +D G	
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      FY C LCQSFAP +VC+V+P+RV LCGA++W D +A+ +++  GP   I K   +D   G

186    FYGCTLCQSFAPTNCVVPDRVSLCGAINWFDGRAAAKVDPEGPQFAIEKGELLDAKTG      245 Q9V2Z4


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246    EYSGVNEVAKKLSSGEFDKIKLHSFFDAPHTSCGCFE      282 Q9V2Z4

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2. Amino acid sequence of the wild-type and mutant DFT models considered in the present study

As reported in the main text of the paper, the size of the DFT model was reduced by neglecting the region 537-572, and by mutating selected amino acid sidechains towards glycine. The sequence alignment reported below illustrates the glycine mutations we introduced, highlighted in yellow. Figure S1 also shows the spatial disposition of the sidechains that underwent mutation, based on crystallographic data (PDB code of the reference structure: 1MJG).

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1MJG      FYSCVLCQSFAPNHVCIVTPERVGLCGAVSWLDAKASYEINHAGPNQPIPKE      554

DFT Model  GGSCVGCQGGAPGHVCIVTPGRGGLCGAVGGGGA-----


1MJG      GEIDPIKGIWKSVNDYLYTASNRNLEQVCLYTLMENPMTSCGCFE      599

DFT Model  -----GASGGGLGGVGLYGGGGPMTSCGCFG

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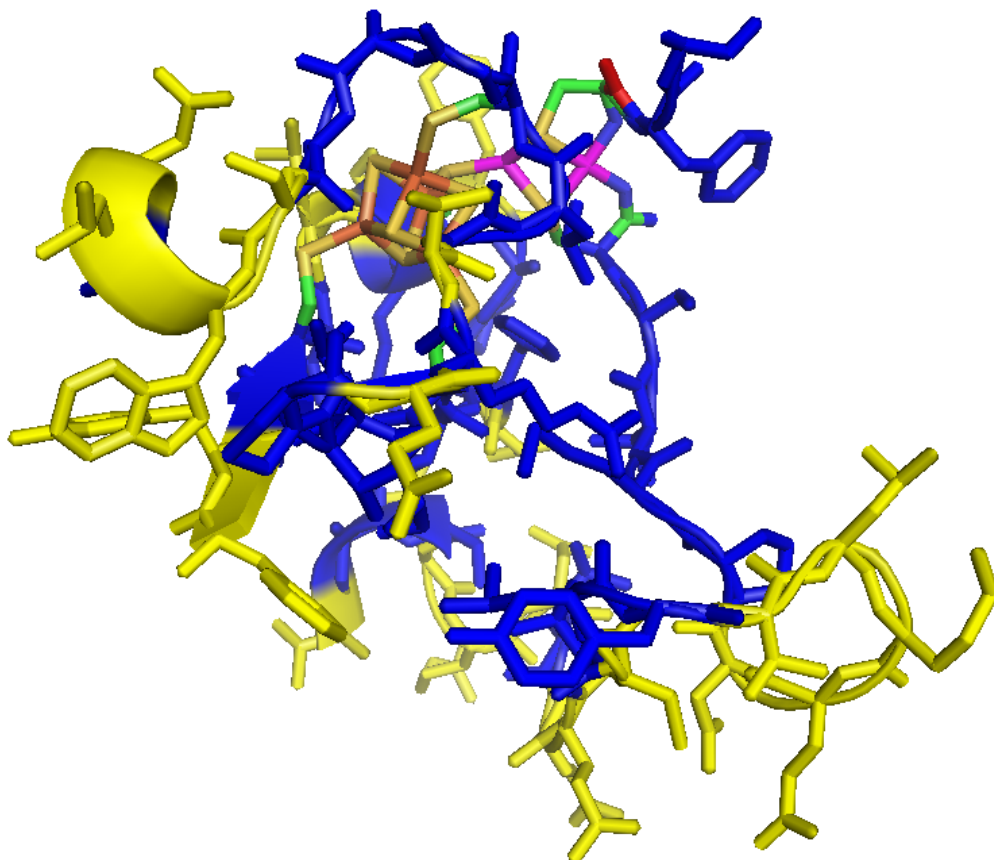


Figure S1: In yellow, residues that were mutated to glycine in order to obtain the big-size DFT model used for the present study.

3. Methodological details of quantum chemical calculations, and additional results

All the quantum chemical calculations described in the following were carried out in the framework of Density Functional Theory, employing the TURBOMOLE package¹ and the resolution of identity (RI) technique.² Geometry optimizations were carried out *in vacuo* in all cases, on models in which the Ni_p center was not bound to substrates. The level of theory used for the various kind of calculations will be specified in the following subsections; Subsections 3.1 and 3.2 deal with the detailed description of results obtained as a result of geometry optimization of small-size models of the isolated A-cluster, and relevant methodological details will be provided. Subsection 3.3 regards the methodological details of the calculations carried out on the large-size protein model, including description of the approach here followed for the evaluation of strain imposed by the protein matrix on the mutant A-cluster; finally, the following subsections provide additional results on large-size models.

It has to be noticed that all the models here considered, independently of their size, feature the presence of a Fe_4S_4 cluster. As anticipated in the paper main text, the antiferromagnetic (AF) coupling that characterizes the latter was modelled using the broken symmetry (BS) approach. The latter is based on the presence of spin excess with opposite signs at the level of two different Fe_2S_2 layers composing the Fe_4S_4 cubane, within a monodeterminantal representation of the electronic structure of the models. Figures 2 and 4 in the paper main text schematically illustrate the three

possible BS couplings in the models here considered, which invariably feature an equal number of spin up and spin down electrons. If not explicitly stated otherwise, the total energy differences reported below and in the paper main text are computed between species modelled by means of the same BS coupling scheme.

3.1 Comparison of B3LYP and BP86 energies on small size models of the isolated A-cluster: ΔE of protonation at selected sulphur atoms

In literature, key structural and electronic properties of the wild-type A-cluster, as well as its reactivity, were modelled successfully by applying the BP86 functional^{3,4} as well as the B3LYP functional^{5,6} (see e.g. ref. ⁷ for B3LYP calculations, and ref. ⁸ for an application of the BP86 functional). As a first preparatory step before proceeding with optimization of large size models, we performed geometry optimization on small size models of the A-cluster, with the aim of comparing BP86 and B3LYP relative energies. More specifically, we considered the energy differences associated with proton transfer between two sulphur sites within the model represented in Figure S2.

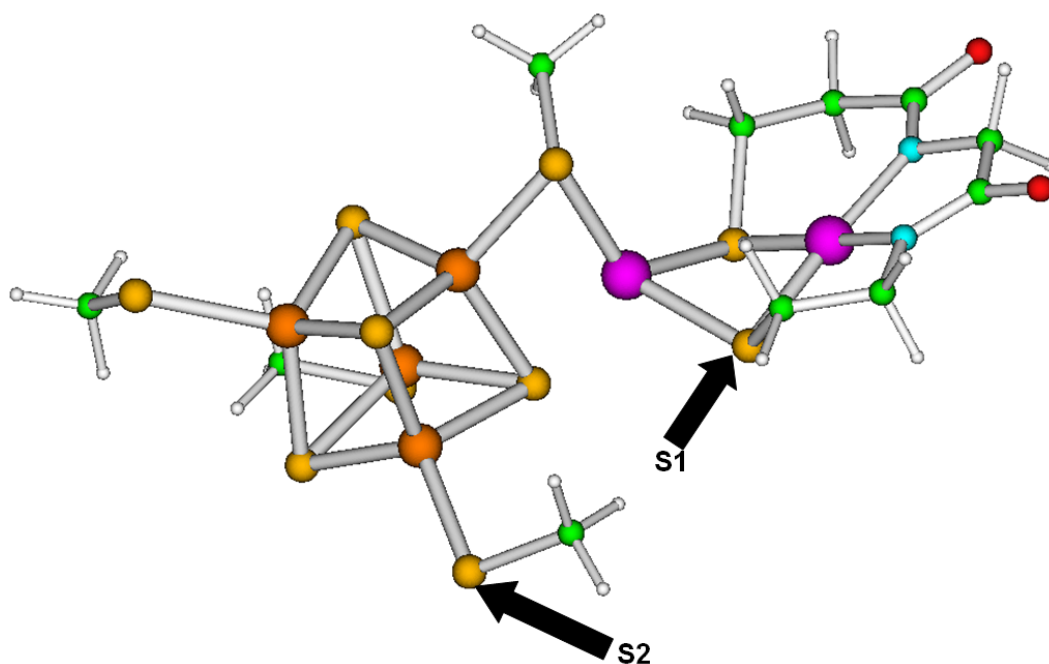


Figure S2: Small-size model of the wild-type A-cluster used for calculation of protonation energies at site S1 and S2, both indicated by an arrow. The overall charge of the protonated models was -1 in all cases. The colour code of the atoms is the same as in Fig. 3 of the paper main text.

Such sites were previously considered by A. Chmielowska *et al.*⁸ in the above cited paper, which deals with calculation of pK_a and redox potential of the enzyme active site. In that investigation, the authors adopted the BP86/TZVP level theory (basis set described in ref. ⁹), and the environmental effects were modelled by means of a continuum solvent model, with dielectric constant $\epsilon = 20$. In the present study, we performed geometry optimization of models of the fully oxidized A-cluster, protonated either at the S1 or at the S2 sites (see Figure S2), using four different levels of theory: BP86/TZVP, BP86/SVP, B3LYP/TZVP and B3LYP/SVP (the SVP basis set is described in ref. ¹⁰). All such protonated model featured overall -1 charge and, as already mentioned, their geometry optimizations were carried out *in vacuo*. The obtained minimum structures – the atomic coordinates of which are all reported at the end of this document – were used for single point calculations using

the COSMO continuum solvent model,¹¹ at dielectric constant $\epsilon = 20$. The differences in total energies thus obtained were the following: for the B3LYP optimization, $\Delta E_{S1-S2} = 6.7$ kcal/mol when the TZVP basis is used (while in the case of B3LYP/SVP calculations, the energy gap amounts to 8.4 kcal/mol). As for BP86 calculations, the energy gap between the two protonation states are 5.1 and 7.6 kcal/mol in case of usage of TZVP and SVP bases, respectively. In other words, the variation in computed ΔE values as a function of the applied density functional does not exceed 1.6 kcal/mol in the test case here considered, a satisfactory result in terms of consistence of the theoretical picture.

3.2 Comparison of structures of small-size models of the A-cluster with and without C509H mutation

Figure S3 and S4 present the geometries of the small-size models ^{wt}**a** and ^{mut}**a**, respectively (see the paper main text) optimized *in vacuo* at the BP86/TZVP level; both models feature -2 charge; notice that, differently from the species investigated in section 3.1, they present no protonation of cysteinyl sulphur atoms. Each of the two models were re-optimized also at the BP86/SVP and B3LYP/SVP levels, which provided consistent results (see the caption of figure S3 and S4).

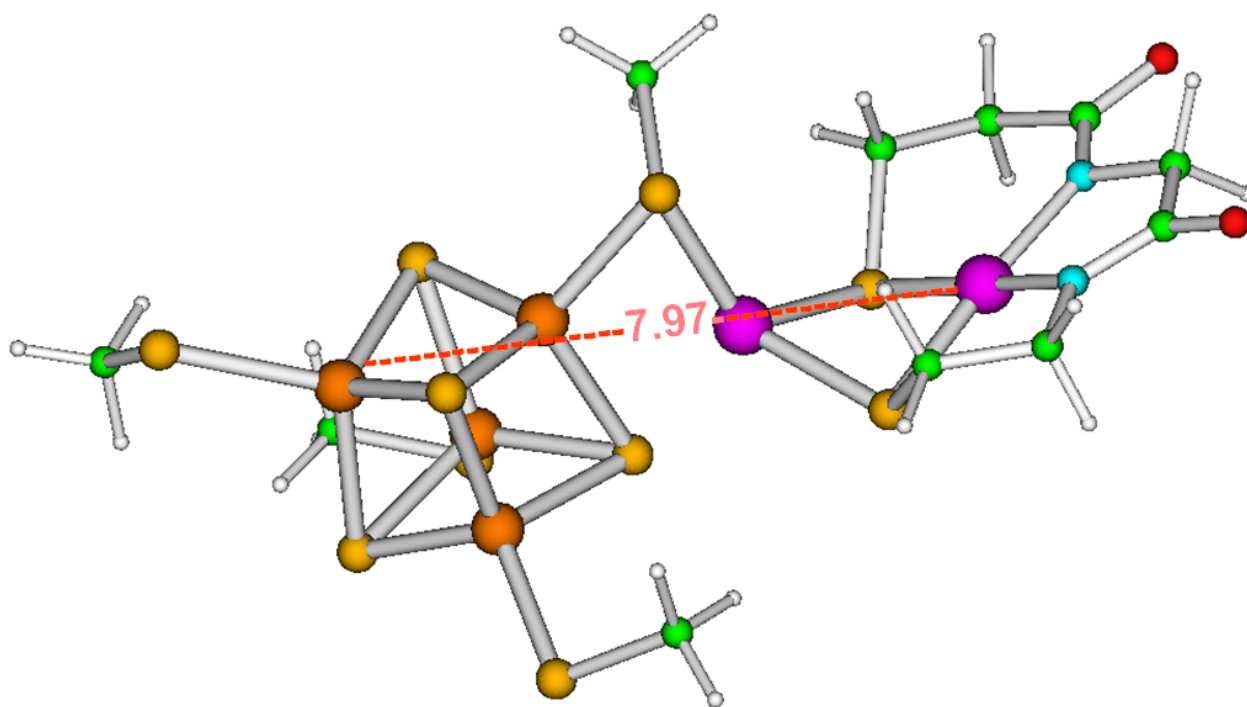


Figure S3: Small-size model of the wild-type A-cluster (^{wt}**a**), optimized at the BP86/TZVP level. The Ni-Fe distance of larger value is reported in Å. The corresponding interatomic distance in the BP86/SVP and B3LYP/SVP optimized models (structures not shown) is 8.01 Å and 8.33 Å, respectively. The colour code of the atoms is the same as in Fig. 3 of the paper main text.

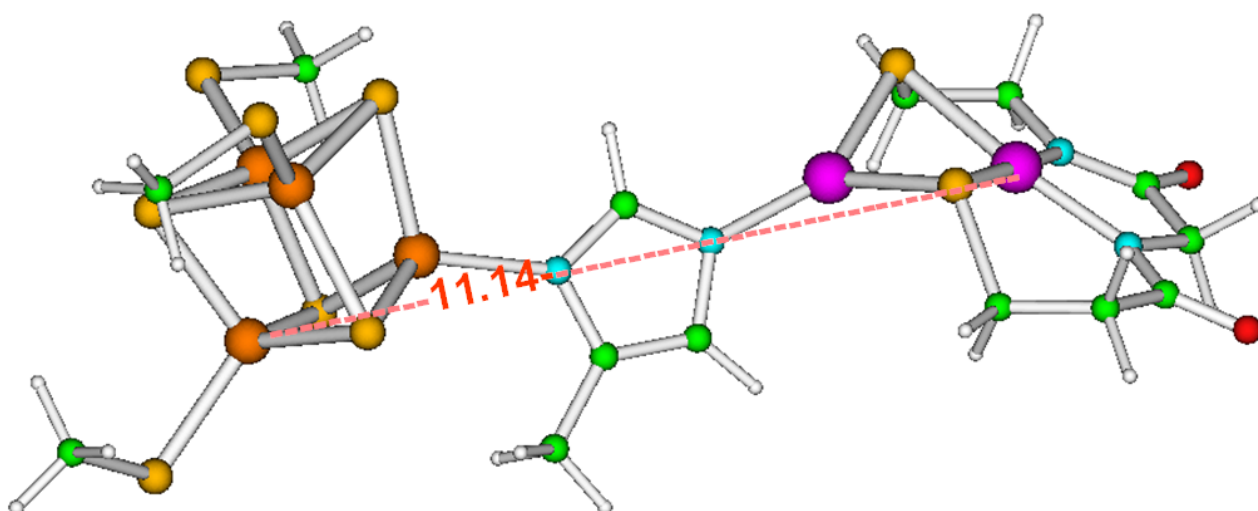


Figure S4: Small-size model of the C509H mutant A-cluster (^{mut}a), optimized at the BP86/TZVP level. The Ni-Fe distance of larger value is reported in Å. The corresponding interatomic distance in the BP86/SVP and B3LYP/SVP optimized models (structures not shown) is 11.31 Å and 11.36 Å. The colour code of the atoms is the same as in Fig. 3 of the paper main text.

3.3 Methodological details on large-size models (including calculation of strain and assignment of redox states to the dinickel and Fe_4S_4 sites)

Geometry optimizations on large-size models were carried *in vacuo* at the level of theory reported in the main text of the paper, *i.e.* using the BP86 functional and a combination of SV and TZVP basis (see Figure S5 for specification of the atoms that were assigned TZVP basis). The choice of BP86 functional is supported by the above comparison with B3LYP results on smaller models and by previous successful modelling of the A-cluster embedded in explicit (constrained) representation of the surrounding protein matrix.⁸ Notably, combination of the pure functional with the RI approach (*vide infra*) allows for an efficient evaluation of Coulomb integrals, thus providing a positive effect on the CPU time required for calculations on the large-size models here described. Apart from the case of model $^{mut}A4-red_{His}$, we considered the fully oxidized form of the A-cluster; this means that the overall charge of $^{wt}A1_{Cys-}$, $^{mut}A2_{His-}$, $^{mut}A3_{His-}$, $^{mut}A4_{His}$ and $^{mut}A5_{His-}$ – which feature a protonated arginine residue – ranges from -1 to 0, with the latter value attained only by $^{mut}A4_{His}$ (the latter species is characterized by a neutral His509 residue, whereas $^{mut}A2_{His-}$, $^{mut}A3_{His-}$ and $^{mut}A5_{His-}$ feature a formally anionic histidinate). As far as the $^{mut}A4-red_{His}$ is concerned, it is two electrons more reduced than $^{mut}A4_{His}$, therefore it features an overall charge of -2.

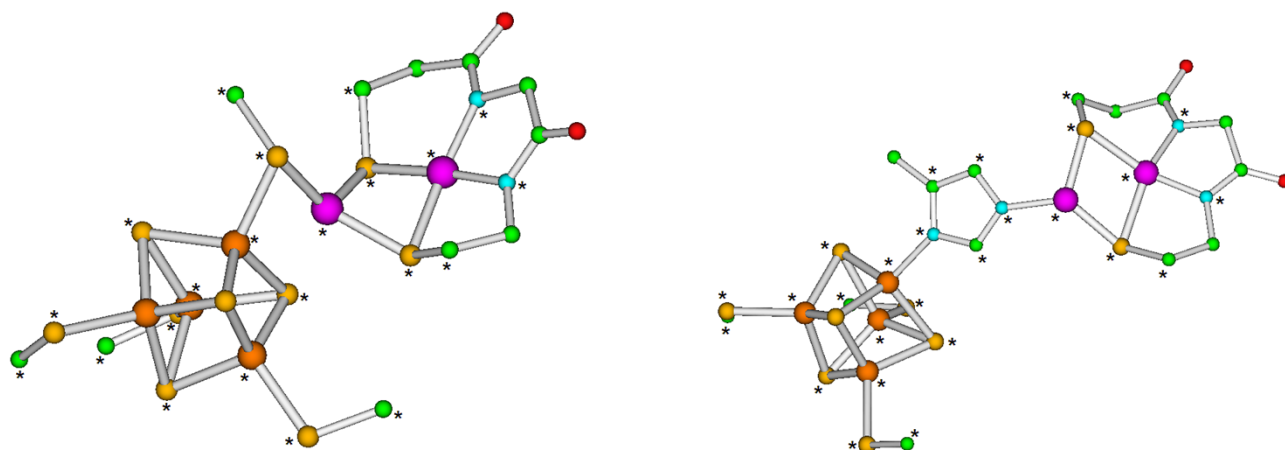


Figure S5. Specification of the atoms in the large-size protein model that were assigned the TZVP basis: atoms that feature an asterisk are the ones that were assigned the TZVP basis as far as wild-type (on the left) and mutant (on the right) ACS forms are concerned. The atoms without an asterisk, together with all the other atoms in the large-size enzyme representation (see Fig. 2C in the paper main text) were assigned the SV basis. The colour code of the atoms is the same as in Fig. 3 of the paper main text.

To estimate the energy associated with the strain induced by the protein matrix on the mutated A-cluster in $\text{mutA2}_{\text{His-}}$, we applied the following approach: the atoms belonging to the A-cluster were extracted from $\text{mutA2}_{\text{His-}}$: atomic composition of the extracted subsystem is identical to the one of model muta , see Figure S3 (when needed, C atoms were saturated by means of the addition of H atoms along the original C-C bond, and their positions were optimized by means of geometry optimizations in which all the other atoms were kept fixed in space; see section 4 below, and in particular the note marked with an asterisk * at the end of the present document). Subsequently, an unconstrained geometry optimization at the BP86/TZVP level was carried out on the resulting model. A single point SCF calculation, again at BP86/TZVP level, was then performed on both geometries using the COSMO continuum solvent model at $\epsilon = 20$ (see above), in order to take into account the effect of the environment. The total energy values thus obtained were used for strain calculation, giving place to the 14.1 kcal/mol energy difference reported in the main text of the paper. The SCF calculations with COSMO at $\epsilon = 20$ were performed also at B3LYP/TZVP level on the same geometries, to test the effects of the chosen functional on the estimate of the strain.

Attribution of redox states to the dinickel and Fe_4S_4 subsites was based on extraction of the A-cluster atoms from $\text{mutA4-red}_{\text{His}}$ and substitution of selected C atoms with H atoms, applying a procedure identical to the one above reported for calculation of strain. A single-point B3LYP calculation at the BP86 geometry was then carried out to compute atomic spin populations, as well as the overall charge of the two fragments composing the A-cluster (also in this case, the TZVP basis was employed, as well as the COSMO continuum solvent model, see above). As shown previously,¹² this approach gives a reliable picture as far as the calculation of the overall Mulliken population of protein-embedded clusters is concerned.

3.4 Charges and spin populations in $^{mut}A2-red_{His-}$, A-cluster geometry in $^{mut}A5_{His-}$ and analysis of protein backbone position and orientation in model $^{mut}A3_{His-}$

As mentioned in the paper main text, we considered not only $^{mut}A4-red_{His}$ as a model of the reductively activated form of the enzyme, but also $^{mut}A2-red_{His-}$. The latter, the optimized coordinates of which are reported below in section 4, is the two-electron reduced version of $^{mut}A2_{His-}$. In $^{mut}A2-red_{His-}$, the $Fe_4S_4(Cys)_3(His)$ fragment – which features a formally anionic histidine sidechain, as opposed to the formally neutral histidine in $^{mut}A4-red_{His}$ – has an overall charge of $-2.66 e$, whereas the dinickel site (i.e. the $Ni_2(RNR')(R''NR''')(\mu-Cys)_2$ bisamidate/bisthiolate fragment) has an overall charge of $-1.34 e$. Such charge values are respectively compatible with the $3Fe(II)Fe(III)$ and the $Ni(I)Ni(II)$ states, a result analogous to the one already found for $^{mut}A4-red_{His}$ (even though comparison between the above results and those reported in the paper main text for $^{mut}A4-red_{His}$ indicate that $^{mut}A2_{His-}$ presents a higher degree of delocalization). Notably, atomic spin population of Ni_d is zero, whereas the one of Ni_p is 0.80: this indicates that the site which attains the monovalent state is the latter.

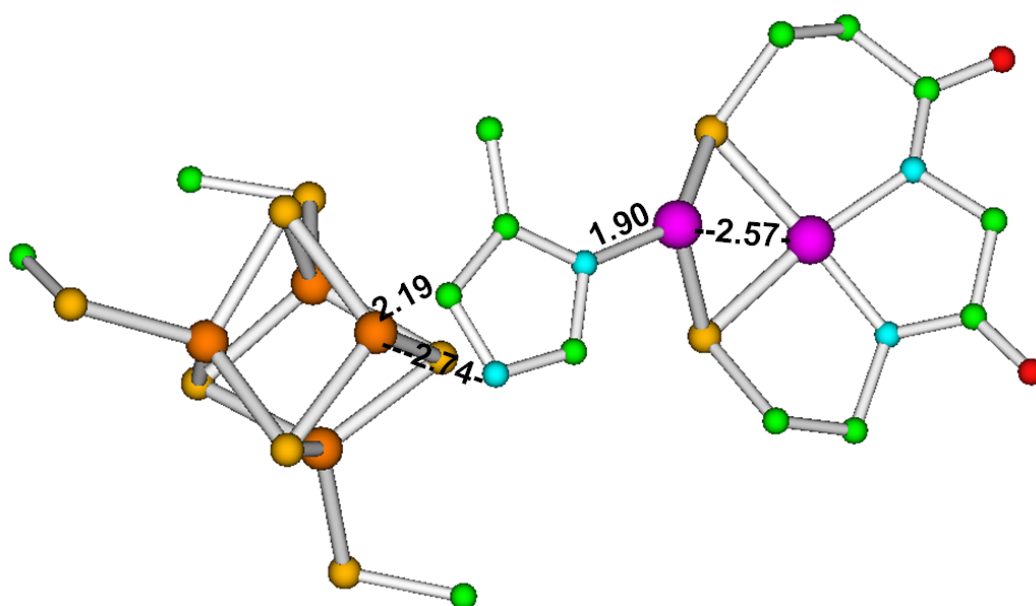


Figure S6. Optimized geometry of the A-cluster in $^{mut}A5_{His-}$.

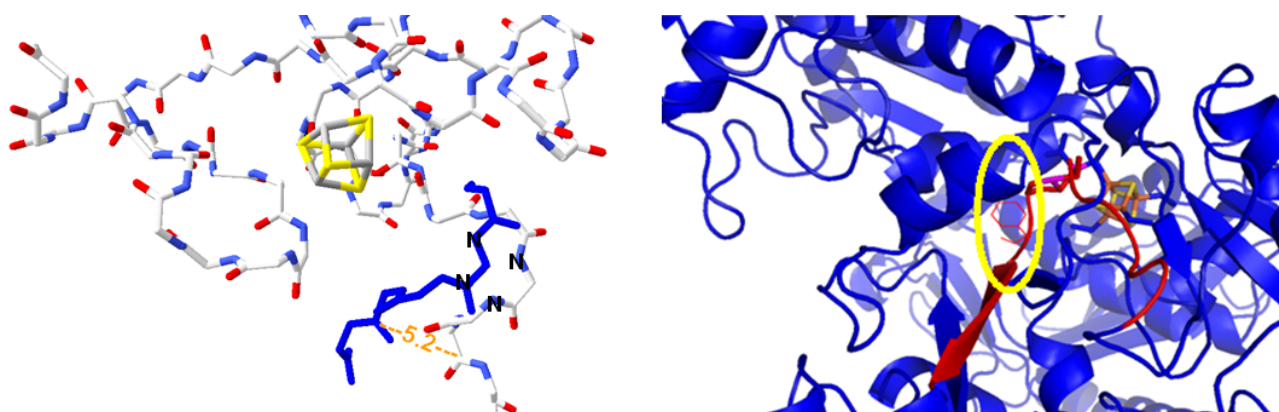
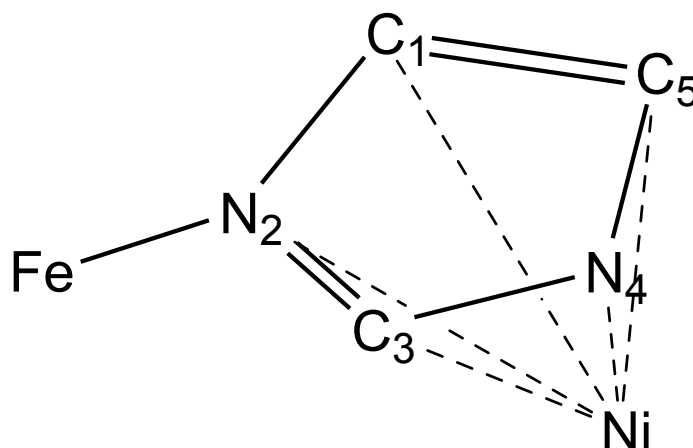


Figure S7. Positioning of Phe598 residue in the optimized model as compared to its crystallographic position (on the left), and disposition of this residue in the context of secondary and tertiary structure of the ACS enzyme (on the right). In the left half of the figure, the crystallographic structure of the protein backbone (completely blue, sticks representation) is superimposed with the backbone of the DFT model $^{mut}A3_{His-}$ (which is also represented with sticks, but coloured using the following code: C, green; N, blue, O, red). The dotted line in yellow shows that the C atom of the peptidic bond at the level of Phe598 is displaced by 5.2 Å with respect to the crystallographic structure; the Fe_4S_4 cluster as found in the X-ray structure is also shown in yellow-grey, to highlight the position of the A-cluster in the representation (notice that Ni atoms are not shown, however the N atoms coordinated to the Ni_d atom in the X-ray structure or in the model are highlighted by addition of an “N” tag). In the right half of the figure, the position of Phe598 (highlighted with a yellow elliptic line, and represented with red sticks) in the context of secondary and tertiary structure of the ACS enzyme is shown. The β strand downhill in the protein sequence with respect to Phe598 is also represented in red.

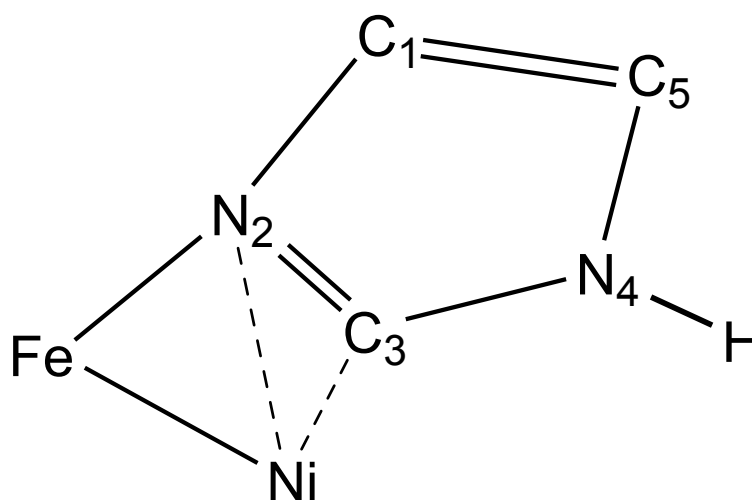
3.5 Results in Natural Bond Orbital calculations on models ^{mut}A2_{His}- and ^{mut}A4_{His}

Table S1. π and π^* NBO orbital population of the histidine ring of the ^{mut}a model in the optimized geometry of ^{mut}A2_{His}- calculated using the BP86/TZVP computational scheme. In parenthesis are the orbital populations calculated for the $[(\text{CH}_3\text{S})_3\text{Fe}_4\text{S}_4(\text{CH}_3\text{ImidN})]^{-2}$ (CH_3ImidN = methyl-imidazolate) fragment obtained by removing the dinickel subcomponent of the cluster. The scheme below shows the atom numbering used in the table and the bonding scheme which has been manually defined using the ‘choose’ option in the NBO analysis. Population analysis clearly shows the interaction between the π system of the imidazolate ring and Ni as the π orbital population significantly decreases after removing the dinickel subcomponent of the cluster. Interestingly, π^* orbital population is not affected by the removal of the dinickel subcomponent, indicating that the interaction can be represented by a π -donation from the imidazolate ring to Ni, with a negligible back-donation from Ni to π^* orbitals of imidazolate. For the sake of clarity, notice that N ^{δ 1}, N ^{ϵ 2} and C ^{ϵ 1} cited in the main text of the paper correspond respectively to N₂, C₃ and N₄ in the table and in the sketch below.



	α occupation	β occupation	Sum ($\alpha + \beta$)
q(Ni)	0.06 (0.20)	0.07 (0.20)	0.13 (0.40)
$p_{\pi}(\text{N4})$	0.61 (0.63)	0.61 (0.63)	
$\pi(\text{C1-C5})$	0.80 (0.91)	0.80 (0.91)	
$\pi(\text{N2-C3})$	0.86 (0.91)	0.86 (0.93)	
Sum $\pi(\text{Imid})$	2.27 (2.45)	2.27 (2.47)	4.54 (4.92)
$\pi^*(\text{C1-C5})$	0.22 (0.19)	0.23 (0.21)	
$\pi^*(\text{N2-C3})$	0.31 (0.31)	0.30 (0.31)	
Sum $\pi^*(\text{Imid})$	0.53 (0.50)	0.53 (0.52)	1.06 (1.02)
Sum $\pi(\text{Imid}) + \pi^*(\text{Imid})$	2.80 (2.95)	2.80 (2.99)	5.60 (5.94)

Table S2. π and π^* NBO orbital population of the histidine ring of the **muta** model in the optimized geometry of **mutA4_{His}** calculated using the BP86/TZVP computational scheme. In parenthesis are the orbital populations calculated for the $[(\text{CH}_3\text{S})_3\text{Fe}_4\text{S}_4(\text{CH}_3\text{ImidNH})]^{2-}$ (CH_3ImidN = methyl-imidazole) fragment obtained by removing the dinickel subcomponent of the cluster. The scheme below shows the atom numbering used in the table and the bonding scheme which has been manually defined using the ‘choose’ option in the NBO analysis. Results shows the interaction between π^* orbitals of the imidazole ring and Ni as the π^* orbital population significantly decreases after removing the dinickel subcomponent of the cluster. Interestingly, the π orbital population is not affected by the removal of the di-nickel subcomponent, indicating that in this case the interaction can be represented by a back-donation from Ni to π^* orbitals of imidazole. For the sake of clarity, notice that $\text{N}^{\delta 1}$, $\text{N}^{\epsilon 2}$ and $\text{C}^{\epsilon 1}$ cited in the main text of the paper correspond respectively to N_2 , C_3 and N_4 in the table and in the sketch below.



	α occupation	β occupation	Sum ($\alpha + \beta$)
q(Ni)	0.13 (0.48)	-0.17 (0.01)	-0.04 (0.49)
$p_{\pi}(\text{N4})$	0.79 (0.77)	0.77 (0.78)	
$\pi(\text{C1-C5})$	0.91 (0.90)	0.91 (0.90)	
$\pi(\text{N2-C3})$	0.87 (0.93)	0.91 (0.93)	
Sum $\pi(\text{Imid})$	2.57 (2.60)	2.59 (2.61)	5.16 (5.21)
$\pi^*(\text{C1-C5})$	0.15 (0.16)	0.15 (0.16)	
$\pi^*(\text{N2-C3})$	0.34 (0.24)	0.35 (0.25)	
Sum $\pi^*(\text{Imid})$	0.49 (0.40)	0.48 (0.41)	0.97 (0.81)
Sum $\pi(\text{Imid}) + \pi^*(\text{Imid})$	3.06 (3.00)	3.07 (3.02)	6.13 (6.02)

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4. Cartesian coordinates of DFT-optimized models, and their computed total energies *in vacuo* (in hartree).

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H	-44.8919507	122.7717820	57.9521281
H	-60.7815632	119.1996451	79.1656938
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Model ^{Mut}A2_{His}- (with BS1 broken symmetry coupling)

Energy = -29133.62664703

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C	-69.5921303	133.2919938	61.8610274
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Ni	-65.1267245	131.6173939	64.3843503
C	-63.0654718	131.0912486	61.6176557
C	-63.0873787	131.4844649	60.1228717
C	-64.3931047	131.1105030	59.3786452
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N	-68.3246785	137.1998191	63.9007206
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Model $\text{mutA2}_{\text{His-}}$ (with BS2 broken symmetry coupling)

Energy = -29133.65011247

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Model ^{mut}A2_{His-} (with BS3 broken symmetry coupling)
Energy = -29133.64202324

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Model **mutA3_{His}**-

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Model **mutA4_{His}**
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Model mutA4-red_{His}

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Model **mutA2-red_{His}-**

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H	-56.3827521	134.2163210	58.0740483
H	-60.7080303	138.1158078	58.8469558
H	-59.9001929	135.0372569	58.5438138
H	-61.7514083	135.7280860	60.7318932
H	-63.3353096	136.7841048	59.0877916
H	-62.1588946	136.4989695	57.7465124
H	-62.3804360	131.4463008	61.4696745
H	-63.4892240	134.0970024	60.6222203
H	-62.7116459	131.7051897	59.0394372
H	-63.8834735	130.5272924	61.0677992
H	-67.2457908	132.6047025	57.9913608
H	-67.1150174	130.8650737	58.2872019
H	-68.3782076	130.7503702	63.4448245
H	-69.9724282	131.2468539	61.6840743
H	-69.3527106	132.1062425	64.1574469
H	-75.0358573	131.3381776	56.5137434
H	-70.6790333	132.8882620	60.0490291
H	-70.8331306	135.7009496	60.8280654
H	-70.9272110	135.0926688	58.5116539
H	-74.6615354	134.9642031	58.8967447
H	-71.1016947	132.7214652	57.7568789
H	-76.0926624	133.3001727	57.6991350
H	-72.5217317	131.0728258	56.5555988
H	-72.3773482	136.0371153	58.9680819
H	-71.6921359	136.4534227	62.6026935
H	-73.9536609	135.1543953	63.9247206
H	-74.7662471	137.2696466	61.8922878
H	-47.8175770	138.2857130	70.7605499
H	-69.0512193	147.5190777	73.8630263
N	-65.4298547	130.5324660	65.6818435
C	-64.0622625	130.2963321	65.5438695
C	-65.4565674	131.7583573	66.2901685
N	-64.2207389	132.2291141	66.6830468
Fe	-63.6866000	136.0087927	69.1484308
C	-63.3277051	131.3040449	66.1889370
C	-61.8491217	131.2833987	66.4654104

Model **vt_a**, optimized with SVP basis set and BP86 functional:

Energy = -12745.81832144

C	159.8009332	88.5991568	-3.5586760
S	159.6755955	86.7847764	-3.8302176
C	164.9158917	84.3386207	-0.4340174
S	164.7276502	83.3925092	-2.0116254
C	163.7799453	90.3871910	-3.7242987
S	165.1604851	89.2979266	-4.2563763
C	164.3839282	82.5526540	-7.5455760
S	163.7915052	84.2431979	-7.9621806
C	170.0911090	84.8964690	-1.0746723
C	170.1602414	83.4326234	-0.6151509
O	170.9361802	83.1575959	0.3281143
C	168.7522595	85.3840435	-1.6138378
S	168.4447626	84.6859350	-3.2890346
N	169.3874881	82.4992132	-1.2361728
C	169.5333581	81.1637686	-0.6579243
C	168.7514401	80.1195043	-1.4435994
O	168.7310677	78.9117966	-1.1344861
N	168.1073306	80.6729481	-2.5027201
C	167.3340711	79.8141770	-3.3889418
C	166.2505068	80.6644116	-4.0383616
S	167.0557561	82.2169242	-4.6559236
Fe	161.8023591	86.2011157	-4.2633147
Fe	163.5274959	85.2373795	-5.9904189
Fe	164.1929505	87.2904330	-4.4703905
Fe	163.9217624	84.8966117	-3.5173363
S	165.5864988	85.5480974	-4.9984163
S	163.1965531	86.7325193	-2.4937870
S	162.1515439	84.0146588	-4.6520142
S	162.6393491	87.2535483	-6.1572468
Ni	166.2783058	84.0320647	-3.5161630
Ni	168.2917223	82.5114656	-2.8113619
H	158.7943702	89.0055817	-3.3220107
H	160.4834058	88.8275006	-2.7145418
H	160.1855268	89.1106785	-4.4649137
H	164.1631741	91.4200682	-3.5818989
H	162.9741398	90.4107675	-4.4864806
H	163.3450021	90.0323112	-2.7674524
H	164.5904790	82.0031956	-8.4880333
H	165.3129182	82.5921286	-6.9413083
H	163.6133397	82.0016766	-6.9689406
H	165.6776938	83.8229125	0.1845084
H	165.2310248	85.3780521	-0.6368588
H	163.9461787	84.3533441	0.1017477
H	167.9183522	85.0994470	-0.9433511
H	168.7386579	86.4893030	-1.7240885
H	170.3948218	85.4888240	-0.1846593
H	170.8793266	85.0643634	-1.8436888
H	167.9840465	79.3632396	-4.1799721
H	166.9084275	78.9633514	-2.8091910
H	165.7582898	80.1584180	-4.8951683
H	165.4810573	80.9587527	-3.2969061
H	170.6036618	80.8565200	-0.6176897
H	169.2052241	81.1398130	0.4077162

Model ^{wt}a, optimized with TZVP basis set and BP86 functional:

Energy = -12749.02272117

C	159.6726898	88.8798050	-3.6677159
S	159.5129688	87.0359157	-3.6931166
C	164.7426350	84.3531346	-0.3373766
S	164.5798000	83.4348860	-1.9455271
C	163.9883814	90.5060666	-4.1419815
S	165.2462028	89.2170505	-4.5646232
C	164.1521883	82.4594888	-7.4186696
S	163.3919525	84.0910549	-7.8469447
C	169.9619504	84.8212360	-0.7422524
C	170.2315271	83.3341183	-0.4815175
O	171.0719690	83.0501021	0.4098747
C	168.5734220	85.2088306	-1.2308228
S	168.3522921	84.6945836	-2.9950077
N	169.5744945	82.4019076	-1.2090265
C	169.9035085	81.0198049	-0.8363700
C	169.1506123	80.0168320	-1.6991765
O	169.2663055	78.7795894	-1.5418972
N	168.3806666	80.6249151	-2.6238140
C	167.6146818	79.8249447	-3.5751000
C	166.4572046	80.6772088	-4.0716616
S	167.1679686	82.3383253	-4.5444014
Fe	161.6022023	86.3227551	-4.1293432
Fe	163.2154109	85.1800705	-5.9062141
Fe	164.1071293	87.2882546	-4.5384912
Fe	163.7161960	84.9450762	-3.4103602
S	165.3269063	85.4218790	-4.9789896
S	163.1445454	86.8878977	-2.5174399
S	161.8610359	84.1208835	-4.4127846
S	162.4270977	87.2220173	-6.0890556
Ni	166.1823916	84.0819053	-3.4104449
Ni	168.4595108	82.4945769	-2.7669389
H	158.6819638	89.3189301	-3.4785599

H	160.3622197	89.1978241	-2.8744935
H	160.0489159	89.2445397	-4.6324796
H	164.4840353	91.4876777	-4.1175374
H	163.1885997	90.5273360	-4.8942227
H	163.5456260	90.3034375	-3.1576591
H	164.2799780	81.8819797	-8.3455671
H	165.1319677	82.6034771	-6.9454539
H	163.5013080	81.9015807	-6.7331500
H	165.4431313	83.7940868	0.2972748
H	165.1161350	85.3673510	-0.5068671
H	163.7587345	84.4035024	0.1459766
H	167.7928737	84.7341686	-0.6219408
H	168.4289635	86.2995260	-1.1945030
H	170.1782747	85.3247342	0.2141913
H	170.7170918	85.1817530	-1.4633314
H	168.2503704	79.5195417	-4.4302862
H	167.2604664	78.8992812	-3.0886367
H	165.9583727	80.2468129	-4.9524302
H	165.7197693	80.8451843	-3.2759652
H	170.9862831	80.8307469	-0.9430104
H	169.6782364	80.8249974	0.2265313

Model **muta**, optimized with SVP basis set and BP86 functional:
Energy = -12572.57700763

N	166.8256409	83.3365745	-1.8970251
C	166.0456787	83.6388049	-0.7887099
C	164.9946419	84.4541506	-1.1851990
N	165.1258718	84.6595095	-2.5544536
C	166.2300309	83.9733352	-2.9305733
C	163.8752691	85.0517838	-0.3920983
Fe	163.9190732	85.7946541	-3.6989984
Ni	168.4039630	82.2531713	-1.9529731
Ni	170.1383085	80.7609369	-0.9090591
S	169.5901949	80.7620405	-3.1106697
C	168.6971245	79.1292717	-3.0200248
C	169.5239071	78.1932497	-2.1502863
N	169.9066092	78.9061921	-0.9404543
C	170.2709122	78.1902590	0.1558913
O	170.2540643	76.9481466	0.2417015
C	170.7283654	79.0985948	1.2910496
N	170.6796316	80.5074336	0.9034266
C	171.1397612	81.3494929	1.8693823
O	171.5970502	80.9456023	2.9608917
C	171.0982134	82.8691310	1.6346429
C	169.9707975	83.4100944	0.7623810
S	170.2766374	82.9663513	-0.9991603
Fe	161.6415396	87.0254567	-4.0200977
S	161.6545309	87.5326690	-6.2706561
Fe	163.7487921	87.8086774	-5.3501538
S	163.5293366	87.9205058	-3.0601935
S	159.7959478	87.8683458	-3.0768585
C	159.8982282	89.6591184	-3.4744981
Fe	162.5914847	85.5259712	-5.9590386
S	161.8220130	84.8188092	-3.8769221
S	162.1274957	83.9838861	-7.5165569
C	162.9205700	82.4654597	-6.8468095
S	164.8773033	85.9518149	-5.8030326
S	164.6408723	89.6863842	-6.1722287
C	163.3886275	90.9647383	-5.7570732
H	159.0122950	90.1769419	-3.0497152
H	160.8151081	90.1100077	-3.0429260
H	159.9132435	89.8161437	-4.5722589
H	163.7318273	91.9474315	-6.1441020
H	162.4096043	90.7187670	-6.2168459
H	163.2500446	91.0432790	-4.6593755
H	162.7217857	81.6192886	-7.5374731
H	164.0174842	82.5971027	-6.7537169
H	162.5113725	82.2149792	-5.8471019
H	168.9885495	83.0020328	1.0707549
H	169.9144711	84.5182508	0.8139455
H	171.0442369	83.3103696	2.6524313
H	172.0770907	83.1893051	1.2108572
H	170.4268061	77.8583420	-2.7195250
H	168.9625497	77.2677806	-1.8848394
H	168.5716559	78.7501849	-4.0557572
H	167.6940188	79.3036401	-2.5826764
H	171.7569273	78.7985173	1.5962860
H	170.1060671	78.9001561	2.1944710
H	163.8693168	86.1594574	-0.4780979
H	163.9631809	84.7811488	0.6784816
H	162.8873011	84.7056410	-0.7633118
H	166.2854062	83.2529771	0.2090237
H	166.5980604	83.9525948	-3.9633498

Model ^{mut}a, optimized with TZVP basis set and BP86 functional:

Energy = -12575.88393008

N	166.7888205	83.3824613	-1.8811413
C	165.9770398	83.6291625	-0.7809836
C	164.9435249	84.4587700	-1.1600863
N	165.1076097	84.7369828	-2.5143429
C	166.2215202	84.0714416	-2.8946239
C	163.8068293	85.0086898	-0.3638116
Fe	163.9112620	85.8667442	-3.6671719
Ni	168.2886974	82.1973950	-2.0217472
Ni	170.1646116	80.6631812	-0.9111372
S	169.4338026	80.5794018	-3.0348535
C	168.5708481	78.9313350	-2.8117057
C	169.4984140	78.0394297	-2.0058843
N	169.9684495	78.7991377	-0.8512361
C	170.4320264	78.1408274	0.2338092
O	170.4592375	76.8985263	0.3734596
C	170.9476002	79.0926375	1.3030480
N	170.7876032	80.4925847	0.8929078
C	171.2498110	81.3859300	1.7968082
O	171.8016640	81.0530802	2.8752719
C	171.1038123	82.8892746	1.5192149
C	169.9162676	83.3399389	0.6776966
S	170.1867497	82.8434256	-1.0865791
Fe	161.5952144	87.0600609	-4.0486215
S	161.6811613	87.5960295	-6.2794410
Fe	163.7551145	87.9061798	-5.3441733
S	163.4514654	87.9744933	-3.0702362
S	159.7173670	87.8601850	-3.1224327
C	159.7669716	89.6733677	-3.4788807
Fe	162.6046482	85.5916235	-6.0124551
S	161.8515861	84.8695588	-3.9475803
S	162.1924005	84.0798206	-7.6170300
C	163.0216010	82.5419066	-7.0073983
S	164.8674411	86.0462836	-5.7644027
S	164.6566773	89.7933277	-6.1450912
C	163.4107981	91.0985223	-5.7437020
H	158.8577720	90.1372324	-3.0694905
H	160.6469699	90.1337424	-3.0107998
H	159.8058223	89.8485405	-4.5618360
H	163.7812124	92.0638372	-6.1180895
H	162.4499826	90.8698136	-6.2233787
H	163.2603550	91.1680150	-4.6583877
H	162.8286714	81.7326971	-7.7260862
H	164.1049366	82.6951541	-6.9225510
H	162.6236556	82.2540480	-6.0259818
H	168.9832021	82.8849806	1.0326121
H	169.8039396	84.4345202	0.6941180
H	171.0542834	83.3606609	2.5134681
H	172.0409447	83.2429405	1.0540416
H	170.3534016	77.7233203	-2.6362712
H	168.9879741	77.1201457	-1.6689230
H	168.3563789	78.5247019	-3.8109915
H	167.6263643	79.1029292	-2.2794611
H	172.0076202	78.8558493	1.5013076
H	170.4215942	78.8905373	2.2523189
H	163.7884317	86.1094182	-0.4000289
H	163.8900305	84.6967817	0.6867194
H	162.8367350	84.6616899	-0.7528267
H	166.1926734	83.1969939	0.1910658
H	166.6152927	84.1046902	-3.9052739

Model ^{vt}a, optimized with SVP basis set and B3LYP functional:

Energy = -12742.44694455

C	159.6641735	89.1211084	-3.8071356
S	159.3679828	87.3220705	-4.0475574
C	165.0579730	83.4935139	-0.7468268
S	164.5410700	82.8661115	-2.4041831
C	163.8585622	90.5540831	-3.2704556
S	165.2563555	89.4822777	-3.7989723
C	164.1159738	82.7180407	-7.7705013
S	163.6461551	84.4462647	-8.1940927
C	170.0219441	85.0312816	-1.3731063
C	170.0884381	83.6833979	-0.6345942
O	170.7721561	83.6432617	0.4010724
C	168.7414684	85.3804913	-2.1224249
S	168.5883495	84.3725561	-3.6531165
N	169.4323181	82.6192159	-1.1386569
C	169.5806280	81.4022065	-0.3463601
C	168.9013228	80.2121130	-1.0111278
O	168.9220112	79.0780877	-0.5183922
N	168.3072881	80.5592597	-2.1706648
C	167.6560566	79.5475662	-2.9793381
C	166.5762989	80.2136044	-3.8223572
S	167.2961741	81.7300762	-4.6008895

Fe	161.5076948	86.5506517	-4.3065708
Fe	163.3556326	85.3614861	-6.1298721
Fe	164.2061134	87.4900166	-4.2168425
Fe	163.5396394	84.7602897	-3.4457038
S	165.3877017	85.4825407	-4.8660084
S	162.8676276	86.6889873	-2.3779119
S	161.6950093	84.2901844	-4.8651482
S	162.6662363	87.5553086	-6.0872858
Ni	166.3928091	83.6643904	-3.6348770
Ni	168.5108865	82.3091213	-2.7826490
H	158.6923077	89.6207066	-3.6607335
H	160.2902812	89.3080400	-2.9208167
H	160.1573482	89.5634408	-4.6866449
H	164.2507642	91.5543510	-3.0221692
H	163.1124605	90.6655859	-4.0736746
H	163.3558107	90.1456758	-2.3793721
H	164.3127740	82.1723918	-8.7075443
H	165.0250220	82.6876320	-7.1509224
H	163.3012427	82.2098323	-7.2318064
H	166.0032621	83.0069224	-0.4661586
H	165.1885288	84.5845663	-0.7527181
H	164.2775192	83.2369267	-0.0155213
H	167.8596257	85.2221968	-1.4836445
H	168.7409449	86.4384547	-2.4304786
H	170.2149402	85.7878438	-0.5948094
H	170.8782612	85.0824725	-2.0714874
H	168.3853982	79.0398222	-3.6470504
H	167.2276058	78.7601778	-2.3315334
H	166.2090287	79.5561222	-4.6274507
H	165.7259014	80.5270394	-3.2003858
H	170.6463381	81.1504564	-0.1872712
H	169.1717484	81.5233629	0.6754333

Model **muta**, optimized with SVP basis set and B3LYP functional:

Energy = -12569.16272101

N	166.8448198	83.2985300	-1.7995002
C	166.0425455	83.5725796	-0.7027274
C	165.0046400	84.3815418	-1.1096903
N	165.1648083	84.6110828	-2.4649403
C	166.2689219	83.9525520	-2.8280180
C	163.8627096	84.9581650	-0.3354477
Fe	163.9317650	85.7950635	-3.6501340
Ni	168.4476106	82.2306046	-1.7811370
Ni	170.2493903	80.7314832	-0.9000230
S	169.6339658	80.7786265	-3.0957775
C	168.7186726	79.1682927	-3.0151936
C	169.5307401	78.2102895	-2.1569602
N	169.9331330	78.8984305	-0.9444635
C	170.2140438	78.1730083	0.1640432
O	170.1158087	76.9484698	0.2575375
C	170.6820882	79.0517818	1.3100566
N	170.7293221	80.4569859	0.9201801
C	171.1988940	81.2713330	1.8942407
O	171.5851414	80.8553504	2.9942244
C	171.2688670	82.7858492	1.6545521
C	170.1779181	83.4069876	0.7938195
S	170.4322029	82.9697243	-0.9705584
Fe	161.4231408	87.1344201	-4.0740270
S	161.5720002	87.4525737	-6.4242725
Fe	163.7014278	87.9734722	-5.5034053
S	163.4341213	87.9996998	-3.1323607
S	159.5255676	88.0246608	-3.1154725
C	159.7515503	89.8165300	-3.4616252
Fe	162.5567503	85.3940063	-6.0633118
S	161.7570031	84.8149346	-3.9199492
S	162.1307259	83.7983399	-7.6555155
C	162.9620222	82.3388584	-6.9063656
S	164.8434045	85.9465823	-5.8593324
S	164.6047164	89.9183337	-6.3436618
C	163.3327728	91.1506210	-5.8491018
H	158.9024296	90.3741274	-3.0313239
H	160.6823025	90.1960966	-3.0108772
H	159.7832176	90.0135308	-4.5450679
H	163.6510266	92.1500326	-6.1909090
H	162.3558656	90.9214307	-6.3040822
H	163.2091612	91.1804143	-4.7547388
H	162.8136416	81.4688872	-7.5673622
H	164.0441448	82.5112172	-6.7941255
H	162.5381039	82.1051476	-5.9172044
H	169.1797978	83.0765706	1.1160606
H	170.2042962	84.5066890	0.8550685
H	171.2487561	83.2312789	2.6621399
H	172.2586905	83.0296977	1.2268552
H	170.4146483	77.8640728	-2.7320724
H	168.9484689	77.3060320	-1.9029413
H	168.5879858	78.8022060	-4.0455729
H	167.7231258	79.3446336	-2.5807644

H	171.6716459	78.6922062	1.6468235
H	170.0179613	78.8913400	2.1802558
H	163.8482570	86.0583841	-0.4120329
H	163.9305159	84.6803892	0.7273981
H	162.8961444	84.6041533	-0.7314569
H	166.2574938	83.1736040	0.2878058
H	166.6559989	83.9530503	-3.8468166

Model discussed in section 3.1, protonated in S1, B3LYP/SVP
Energy = -12742.98737437

C	160.1798170	89.2095907	-3.2696189
S	159.6422810	87.4954082	-3.6667547
C	164.6659867	82.4706906	-1.4006607
S	164.5962542	82.3901204	-3.2421405
C	165.0440442	89.5285864	-2.0458004
S	165.8832977	88.7407781	-3.4802807
C	163.4294905	82.9005879	-8.3146403
S	163.2159463	84.7170366	-8.5037019
C	169.6411145	85.6241657	-2.0325637
C	169.2528586	84.6684590	-0.9032166
O	169.4938537	85.0090294	0.2565055
C	168.6125106	85.8434622	-3.1301475
S	168.4579801	84.3622479	-4.2080232
N	168.7026100	83.4568103	-1.2014877
C	168.4906248	82.6009962	-0.0356749
C	168.2981343	81.1553340	-0.4493015
O	168.2333197	80.2213334	0.3448289
N	168.1987161	81.0354748	-1.8019850
C	168.0707545	79.7082226	-2.3678273
C	167.3787699	79.8096135	-3.7160025
S	168.1065497	81.2123933	-4.6691375
Fe	161.6039672	86.5208089	-4.2229486
Fe	163.1156227	85.3947271	-6.3543161
Fe	164.4241981	87.1684716	-4.2308035
Fe	163.4532952	84.4169051	-3.8469717
S	165.3030109	85.1466968	-5.2971256
S	163.1240892	86.1860246	-2.4439223
S	161.4555730	84.3470629	-5.1045656
S	162.7745239	87.6121891	-5.9466594
Ni	166.3495540	83.6901550	-3.9177095
Ni	168.3943612	82.5844069	-2.8292770
H	159.2879962	89.7906860	-2.9881646
H	160.8854210	89.2186611	-2.4249069
H	160.6534387	89.6865068	-4.1408099
H	165.7660635	90.1916293	-1.5443092
H	164.1853508	90.1356952	-2.3722117
H	164.6939885	88.7737429	-1.3266831
H	163.4864682	82.4540287	-9.3193993
H	164.3596642	82.6678029	-7.7734659
H	162.5786922	82.4563825	-7.7763551
H	165.6095044	82.0197993	-1.0679268
H	164.5997657	83.5094225	-1.0511355
H	163.8167790	81.8989796	-1.0007428
H	167.6265155	86.1185297	-2.7296021
H	168.9176862	86.6647241	-3.7955800
H	169.8503477	86.5836565	-1.5357126
H	170.5921336	85.2789613	-2.4771572
H	169.0608769	79.2189070	-2.4951720
H	167.4959111	79.0570192	-1.6854417
H	167.4441198	78.8967488	-4.3261908
H	166.3240749	80.1075313	-3.6140348
H	169.3444673	82.6657683	0.6584632
H	167.6146720	82.9216226	0.5608444
H	169.3755018	80.7242979	-4.7563260

Model discussed in section 3.1, protonated in S1, B3LYP/TZVP
Energy = -12746.16982679

C	159.0650878	89.2204590	-4.2767830
S	159.0118260	87.4027719	-3.9398426
C	164.8555270	85.8023042	0.1858077
S	164.5131245	84.4864095	-1.0729362
C	163.5105172	91.1110297	-4.7449172
S	164.8582437	89.8572383	-4.9238317
C	163.6174788	82.1912875	-6.6896228
S	163.1321934	83.7691971	-7.5248151
C	169.8547422	84.0262613	-0.1731948

C	170.1550955	82.5273817	-0.1343312
O	170.8831988	82.1227768	0.7870272
C	168.4290937	84.4267154	-0.5078715
S	168.0810798	84.1673749	-2.2953484
N	169.6558281	81.7166731	-1.0875207
C	170.1048545	80.3263231	-0.9609081
C	169.8315559	79.5429183	-2.2243949
O	170.2310887	78.3855171	-2.3874831
N	169.1201915	80.2579417	-3.1200561
C	168.8433596	79.6694144	-4.4149086
C	167.5108024	80.1910697	-4.9127479
S	167.4321604	82.0218182	-4.6204012
Fe	161.1708421	86.7828400	-4.1442532
Fe	162.9575517	85.2094229	-5.8116202
Fe	163.8461074	87.8615058	-4.6087981
Fe	163.3817142	85.5523634	-2.7784020
S	164.9813153	85.7444888	-4.5892499
S	162.6255422	87.6589560	-2.5202282
S	161.6388359	84.5070264	-3.9598141
S	162.1320712	87.2691400	-6.2250948
Ni	165.9881081	84.8213459	-2.7694745
Ni	168.6477660	82.0213640	-2.6764419
H	158.0446754	89.5975941	-4.2124089
H	159.6795063	89.7317415	-3.5372627
H	159.4538000	89.4153805	-5.2750961
H	163.9581596	92.0995635	-4.8476960
H	162.7575062	90.9842547	-5.5220738
H	163.0392999	91.0383348	-3.7653364
H	163.7971870	81.4495010	-7.4671328
H	164.5266770	82.3260658	-6.1060625
H	162.8140874	81.8445552	-6.0419823
H	165.7651161	85.5307555	0.7178453
H	164.9734053	86.7762906	-0.2803515
H	164.0187809	85.8279574	0.8813180
H	167.7131123	83.8430254	0.0707480
H	168.2681115	85.4860869	-0.3031114
H	170.1064173	84.3928246	0.8241681
H	170.5454062	84.5066138	-0.8742306
H	169.6277045	79.9183475	-5.1462417
H	168.8212404	78.5781760	-4.3317222
H	167.3210070	79.9958028	-5.9682377
H	166.6851199	79.7989183	-4.3187812
H	171.1760750	80.2816094	-0.7490037
H	169.6170926	79.8206555	-0.1190480
H	168.3861573	82.3735017	-5.5197939

Model discussed in section 3.1, protonated in S1, BP86/SVP
Energy = -12746.37263664

C	159.7941380	88.6335584	-3.3859568
S	159.7708047	86.8170505	-3.6620414
C	165.1109971	83.4016100	-0.8012689
S	164.7598057	82.9819933	-2.5690126
C	163.8124195	90.3781877	-3.1114162
S	165.1790881	89.3252703	-3.7405354
C	164.3625244	83.0066697	-7.7702495
S	163.8188853	84.7456303	-8.0090320
C	170.1150108	85.0614022	-1.7750259
C	169.8328529	83.8939904	-0.8218206
O	170.3844169	83.8967172	0.2949896
C	168.9308150	85.5746237	-2.5824519
S	168.5051875	84.3768051	-3.9173509
N	169.0095137	82.8753628	-1.2190905
C	168.8860795	81.8042877	-0.2268448
C	168.2774149	80.5538832	-0.8400327
O	168.1194335	79.4861414	-0.2306180
N	167.9379157	80.7570909	-2.1474975
C	167.3959513	79.6339832	-2.8988531
C	166.5403955	80.1747015	-4.0321761
S	167.4447030	81.5824170	-4.8276866
Fe	161.8777067	86.3000364	-4.1073891
Fe	163.5694140	85.5327139	-5.9591549
Fe	164.2306123	87.3769567	-4.1701071
Fe	163.9641819	84.8682993	-3.5816898
S	165.6423867	85.7445953	-4.9278105
S	163.2877288	86.5247037	-2.3024413
S	162.1764673	84.1922482	-4.7805257
S	162.7130239	87.5727655	-5.8312578
Ni	166.3355470	84.0934378	-3.6588417
Ni	168.2295486	82.4457286	-2.8918789
H	158.7604960	88.9700953	-3.1662230
H	160.4433001	88.8977621	-2.5272300
H	160.1600843	89.1632100	-4.2881995
H	164.2190622	91.3828099	-2.8769306
H	163.0148331	90.4842085	-3.8735284
H	163.3742126	89.9444005	-2.1904117
H	164.5233316	82.5492325	-8.7677188
H	165.3107032	82.9587924	-7.1985516

H	163.5888838	82.4268612	-7.2281058
H	166.1514945	83.1061312	-0.5707943
H	164.9714131	84.4844685	-0.6335876
H	164.4021922	82.8322303	-0.1696350
H	168.0416535	85.7424604	-1.9442804
H	169.1653447	86.5313160	-3.0932922
H	170.5116086	85.8712170	-1.1291737
H	170.9404962	84.7736061	-2.4641514
H	168.2110653	78.9871852	-3.3123679
H	166.7992862	78.9808667	-2.2234123
H	166.2817005	79.4297500	-4.8103698
H	165.6182534	80.6576541	-3.6500615
H	169.8780010	81.5498985	0.2056003
H	168.2699272	82.1179534	0.6477109
H	168.5102351	80.8139209	-5.2641684

Model discussed in section 3.1, protonated in S1, BP86/TZVP

Energy = -12749.56712867

C	159.2968172	89.0115149	-4.2169585
S	159.3713811	87.1968155	-3.8836302
C	164.7900202	85.8009675	0.2431191
S	164.4355484	84.5165732	-1.0566563
C	163.5534330	90.8445044	-4.9084092
S	164.8726938	89.5542765	-4.8467395
C	163.7125217	82.2456485	-6.4949908
S	163.2845099	83.8746766	-7.2608009
C	169.8030948	84.0891578	-0.2858405
C	170.0481815	82.5831557	-0.2015418
O	170.7807618	82.1567448	0.7195427
C	168.3603171	84.4930240	-0.5463187
S	167.9276573	84.1932905	-2.3154357
N	169.4671303	81.7644140	-1.1153970
C	169.8495991	80.3530654	-0.9748450
C	169.6358897	79.6002316	-2.2721861
O	169.9782149	78.4170228	-2.4419122
N	169.0254236	80.3797420	-3.2059867
C	168.7980626	79.8371537	-4.5387728
C	167.4678170	80.3564603	-5.0464419
S	167.3533835	82.1731604	-4.6392508
Fe	161.4972924	86.6371385	-4.0439408
Fe	163.1239375	85.2709846	-5.5444705
Fe	163.8424001	87.6394929	-4.4684477
Fe	163.5125068	85.6040439	-2.8084918
S	165.1531103	85.8265051	-4.4727659
S	162.7615749	87.6680738	-2.4932686
S	161.8532361	84.4705258	-3.8431571
S	162.2939425	87.2723424	-6.0615474
Ni	165.8643318	84.7842570	-2.6893818
Ni	168.5115222	82.1155989	-2.7288644
H	158.2444092	89.3233409	-4.1756412
H	159.8680889	89.5647366	-3.4612697
H	159.7012223	89.2326944	-5.2127768
H	164.0334647	91.8131342	-5.1026497
H	162.8412206	90.6251742	-5.7133326
H	163.0191012	90.8911604	-3.9514697
H	163.8995755	81.5275110	-7.3048559
H	164.6124184	82.3330733	-5.8733825
H	162.8800153	81.8851484	-5.8778181
H	165.6281827	85.4492199	0.8576585
H	165.0339187	86.7643747	-0.2129808
H	163.8933478	85.9032673	0.8668246
H	167.6648592	83.9165188	0.0776669
H	168.2017464	85.5652776	-0.3651901
H	170.1325117	84.4954210	0.6816897
H	170.4568847	84.5252717	-1.0601779
H	169.6050342	80.1420391	-5.2338877
H	168.8056046	78.7351056	-4.4901837
H	167.3099708	80.2287116	-6.1255638
H	166.6263307	79.9142559	-4.4974624
H	170.9052919	80.2645046	-0.6759416
H	169.2689580	79.8563369	-0.1771453
H	168.3040777	82.5820512	-5.5422726

Model discussed in section 3.1, protonated in S2, B3LYP/SVP

Energy = -12743.00023360

C	159.1608115	88.3722987	-3.8924136
S	159.2728627	86.5748924	-4.2649317
C	165.3393358	84.6867957	-0.6813487
S	164.9248895	83.4805326	-2.0084204
C	163.2595595	90.6094147	-3.0703670
S	164.7670720	89.7304315	-3.6511776
C	165.6255736	83.3932310	-7.8879980
S	164.7404767	84.9163464	-8.3947500
C	170.5556812	84.4142633	-1.9470891

C	170.2964215	83.1912572	-1.0628779
O	170.9811965	83.0480917	-0.0460551
C	169.3362530	85.0859804	-2.5615094
S	168.6259403	84.0864384	-3.9268903
N	169.3416606	82.2985736	-1.4244930
C	169.2227304	81.1536140	-0.5322948
C	168.2804572	80.1094361	-1.0965124
O	168.0177534	79.0565196	-0.5345377
N	167.7553750	80.4843095	-2.3136424
C	166.8287881	79.6005992	-3.0089433
C	165.8202243	80.4531061	-3.7637491
S	166.7417560	81.7797156	-4.6672011
Fe	161.5137738	86.2679517	-4.4819008
Fe	163.5635707	85.6500270	-6.3115327
Fe	163.9587402	87.6876644	-4.2438287
Fe	163.8158862	84.8490076	-3.6120209
S	165.5701128	85.9973082	-4.9035661
S	162.7780288	86.5963297	-2.5104236
S	162.2413244	84.0774707	-5.1506591
S	162.5068899	87.6523080	-6.1532218
Ni	166.2324383	84.0128702	-3.8364300
Ni	168.2278984	82.1222143	-2.9740241
H	158.0974489	88.6379796	-3.7833567
H	159.6798332	88.6165294	-2.9526865
H	159.5924298	88.9745470	-4.7065241
H	163.5546496	91.6102928	-2.7176970
H	162.5288927	90.7294847	-3.8854623
H	162.7805163	90.0705332	-2.2386420
H	164.9410491	82.6925507	-7.3942613
H	166.1100415	82.9334237	-8.7595758
H	166.3816022	83.7162358	-7.1617423
H	166.1778906	84.2774224	-0.0992014
H	165.6157422	85.6634641	-1.1003913
H	164.4618760	84.8156130	-0.0330706
H	168.5540679	85.2688756	-1.8107074
H	169.6028034	86.0566054	-3.0091189
H	171.0873937	85.1289413	-1.2994406
H	171.2623255	84.1277843	-2.7468721
H	167.3878551	78.9563855	-3.7153260
H	166.3373994	78.9331762	-2.2806398
H	165.2556190	79.8668102	-4.5050156
H	165.1133937	80.9298061	-3.0698803
H	170.2033677	80.6781932	-0.3474404
H	168.8596908	81.4445717	0.4712872
H	163.7344980	84.3279072	-9.0890994

Model discussed in section 3.1, protonated in S2, B3LYP/TZVP
 Energy = -12746.17941832

C	159.2852375	88.7749740	-3.8389776
S	159.2429631	86.9654700	-4.2209692
C	165.0416876	83.7992261	-0.6318521
S	164.5878210	83.0866290	-2.2816859
C	163.6491728	90.6807122	-2.9128438
S	165.0773357	89.6204863	-3.4213073
C	164.4944275	82.5611863	-7.5034012
S	164.1711646	84.2737866	-8.1117237
C	170.3869743	84.8081040	-1.9515647
C	170.2250618	83.6000400	-1.0246088
O	170.9003909	83.5897302	0.0159679
C	169.1359384	85.3276912	-2.6439759
S	168.6219290	84.1824368	-3.9979145
N	169.3868621	82.6015980	-1.3675627
C	169.3476975	81.4946740	-0.4097850
C	168.5650686	80.3198799	-0.9615001
O	168.4560228	79.2534672	-0.3506592
N	168.0306619	80.5846190	-2.1736042
C	167.2998997	79.5457193	-2.8863105
C	166.2477373	80.2002786	-3.7635209
S	167.0291468	81.6285648	-4.6596999
Fe	161.4344000	86.4358654	-4.3606178
Fe	163.5425680	85.5707346	-6.0499197
Fe	164.1460689	87.6446603	-4.0172280
Fe	163.5908718	84.8398722	-3.4369586
S	165.4640550	85.7158860	-4.6299337
S	162.6888674	86.6153510	-2.3763431
S	161.9323696	84.2212125	-4.9568016
S	162.6668371	87.6471187	-5.9615503
Ni	166.4127908	83.7108847	-3.6433850
Ni	168.3615894	82.2462810	-2.9370239
H	158.2544439	89.1202749	-3.7606644
H	159.7925248	88.9580646	-2.8927585
H	159.7854799	89.3245737	-4.6347899
H	164.0438889	91.6517175	-2.6134454
H	162.9560637	90.8246413	-3.7410843
H	163.1205540	90.2401564	-2.0683492
H	164.9074956	81.9691094	-8.3163830
H	165.1671889	82.5734233	-6.6494158
H	163.5264037	82.1662845	-7.2045351
H	165.8555299	83.2032933	-0.2243906

H	165.3544905	84.8362669	-0.7227925
H	164.1715159	83.7373848	0.0183839
H	168.3164748	85.4458800	-1.9365711
H	169.3232787	86.2960829	-3.1103698
H	170.8021991	85.5973108	-1.3209051
H	171.1489271	84.5682242	-2.7006889
H	167.9879457	78.9580164	-3.5085733
H	166.8413760	78.8568987	-2.1698851
H	165.8576594	79.5093245	-4.5130757
H	165.4238522	80.5840710	-3.1642071
H	170.3567961	81.1540944	-0.1614935
H	168.9007919	81.8030777	0.5422998
H	165.4566132	84.6822710	-8.2086123

Model discussed in section 3.1, protonated in S2, BP86/SVP
 Energy = -12746.38362068

C	159.7699455	88.4965663	-3.6039097
S	159.7551605	86.7745965	-4.2448019
C	165.2065214	83.7904366	-0.7641966
S	164.6627362	83.1338733	-2.4029183
C	163.7760813	90.2924526	-2.9194814
S	165.1565472	89.3268842	-3.6480573
C	164.6510244	82.6847241	-7.5964951
S	164.5633238	84.4606452	-8.0633348
C	170.1067060	84.9779640	-1.7597982
C	169.9268288	83.7547125	-0.8464310
O	170.5485161	83.7345538	0.2341079
C	168.8878286	85.4521846	-2.5462095
S	168.5285380	84.2675738	-3.9109890
N	169.1150455	82.7318633	-1.2431205
C	169.0621065	81.6171713	-0.2975294
C	168.3196920	80.4262075	-0.8903326
O	168.1852701	79.3390792	-0.3096324
N	167.8420662	80.7071784	-2.1400821
C	167.1584908	79.6677898	-2.9016823
C	166.1492892	80.3317825	-3.8283255
S	166.9884549	81.7580686	-4.6664351
Fe	161.8991589	86.2771550	-4.5069375
Fe	163.8389459	85.5479536	-6.0330858
Fe	164.2641400	87.4065258	-4.2852239
Fe	163.9530299	84.9195538	-3.5949903
S	165.7918521	85.7824118	-4.7848263
S	163.0576629	86.6154762	-2.5159365
S	162.3044510	84.1532644	-5.0745237
S	162.9388318	87.5588236	-6.1389828
Ni	166.3202809	83.8278772	-3.8037997
Ni	168.1836301	82.3742125	-2.8639886
H	158.7234267	88.8127616	-3.4172347
H	160.3387570	88.5565129	-2.6548560
H	160.2258881	89.1895394	-4.3389509
H	164.1786429	91.2562460	-2.5469032
H	162.9947546	90.5012255	-3.6768877
H	163.3185912	89.7396805	-2.0747919
H	164.8281592	82.0699958	-8.4986556
H	165.5036759	82.5882235	-6.8950271
H	163.7234412	82.3929457	-7.0711336
H	166.1835982	83.3342787	-0.5149002
H	165.2926587	84.8917024	-0.7885756
H	164.4469639	83.4978986	-0.0130053
H	167.9932883	85.5459360	-1.9012948
H	169.0679787	86.4390312	-3.0209402
H	170.4550525	85.7883908	-1.0867246
H	170.9457833	84.7744723	-2.4626563
H	167.8925241	79.0782130	-3.5027061
H	166.6707696	78.9539033	-2.2006370
H	165.7769049	79.6441989	-4.6153844
H	165.2906858	80.7406228	-3.2576724
H	170.0835626	81.2929449	0.0013210
H	168.5730650	81.9117144	0.6598841
H	163.3547839	84.4175823	-8.6998856

Model discussed in section 3.1, protonated in S2, BP86/TZVP
 Energy = -12749.57526777

C	159.5816091	88.5627378	-3.4128340
S	159.5552979	86.7972250	-3.9581276
C	165.1132148	83.8901806	-0.6449828
S	164.5773500	83.1857896	-2.2771550
C	163.8240306	90.4398222	-3.3502657
S	165.1304217	89.2992751	-3.9848658
C	164.6295380	82.6651582	-7.5969273
S	163.9334114	84.3148167	-8.0582306
C	170.1494303	84.9424793	-1.7250992
C	170.1003753	83.6386016	-0.9211813
O	170.8485901	83.5461093	0.0766870
C	168.8456896	85.4194601	-2.3535234
S	168.4383129	84.3400743	-3.7998038

N	169.2599257	82.6395915	-1.3029524
C	169.3170744	81.4538930	-0.4398783
C	168.5173640	80.3055969	-1.0312171
O	168.4555344	79.1792486	-0.5058059
N	167.9040309	80.6576213	-2.1909568
C	167.1699854	79.6456404	-2.9493866
C	166.1220256	80.3494834	-3.7936015
S	166.9343283	81.8065528	-4.6207107
Fe	161.6763217	86.2750037	-4.3408469
Fe	163.4906681	85.4301287	-5.9949554
Fe	164.1270454	87.3637228	-4.3623943
Fe	163.7856304	84.9139808	-3.4866199
S	165.5091421	85.6389692	-4.8670601
S	163.0035122	86.7108908	-2.4998708
S	162.0409017	84.1387567	-4.8162779
S	162.6432124	87.4561121	-6.0653297
Ni	166.2326688	83.8367960	-3.7293469
Ni	168.1910572	82.3715883	-2.8627350
H	158.5520924	88.8632230	-3.1752221
H	160.2066495	88.6785959	-2.5186668
H	159.9682303	89.2078762	-4.2119170
H	164.2935810	91.4053536	-3.1181855
H	163.0442088	90.5918366	-4.1068748
H	163.3706544	90.0296807	-2.4391606
H	165.0521198	82.1858138	-8.4869819
H	165.3752706	82.7651975	-6.7998906
H	163.7789116	82.0836024	-7.2255904
H	165.9748075	83.3135236	-0.2884967
H	165.3824799	84.9456277	-0.7483637
H	164.2754110	83.7930866	0.0568441
H	168.0191315	85.3864239	-1.6339626
H	168.9352564	86.4463572	-2.7360738
H	170.5168736	85.7021306	-1.0180865
H	170.9223549	84.8397532	-2.5062494
H	167.8636697	79.0797932	-3.5995100
H	166.7107512	78.9221614	-2.2546458
H	165.7104694	79.6988917	-4.5787842
H	165.3062684	80.7373721	-3.1689198
H	170.3580856	81.1227436	-0.2938701
H	168.9371601	81.6772323	0.5722886
H	165.1129749	84.9159987	-8.3829925

Fully optimized A-cluster model used for calculation of strain (see section 3.3)

E = -12575.86308219

C	-62.2735542	130.2357183	60.7354511
C	-63.6028121	130.3286298	60.2270076
N	-63.5786834	130.2174405	58.8351410
C	-62.2635796	129.9580805	58.5813638
N	-61.4245005	130.0637751	59.6748578
Ni	-63.5097555	128.3418895	59.6288110
S	-64.1765188	126.9616144	61.2202142
C	-65.5834958	127.6871798	62.1917681
C	-66.4756268	126.5563090	62.6938772
C	-67.3886418	125.8605248	61.6704513
N	-66.9619803	125.7286976	60.3978808
Ni	-65.2805192	126.0635710	59.5639845
S	-63.4725981	126.5006149	58.3922823
C	-64.4076580	126.7483791	56.7836588
C	-65.4323034	125.6253504	56.7072540
N	-66.1358636	125.5666803	57.9853132
C	-67.3883409	125.0670939	58.0604236
C	-67.9185612	125.0852397	59.4904368
Fe	-57.3241538	131.8124203	59.2417906
Fe	-59.3964925	130.1828157	59.5841811
S	-55.5784063	130.4182770	59.8380734
Fe	-57.2758363	129.9803464	61.1953703
S	-58.6564891	131.8567800	61.0275501
C	-61.7971970	130.3268456	62.1401192
O	-68.4971200	125.4349308	62.0831041
O	-68.0565721	124.6291969	57.0987480
Fe	-57.1392369	129.1764838	58.6525110
S	-55.9796086	127.8578315	57.2387078
C	-57.3153607	126.7791131	56.5411976
S	-58.4061687	128.2032194	60.2069169
S	-58.5298704	130.7019933	57.6056392
S	-56.7498328	129.4275903	63.3292150
C	-55.2288220	130.4289957	63.6661181
S	-56.6226650	133.7964907	58.4136895
C	-56.0199090	134.6487420	59.9441805
H	-68.1229665	124.0447160	59.8012170
H	-68.8963705	125.5948527	59.5084844
H	-65.1505399	128.2575125	63.0281122
H	-67.1551396	126.9406715	63.4708737
H	-66.1420553	128.3722220	61.5413085
H	-64.8921970	127.7318644	56.8240445
H	-66.1520212	125.7907829	55.8868832
H	-63.6858309	126.7217932	55.9545206
H	-61.8723891	129.8107991	57.5783369
H	-64.4993971	130.6387163	60.7576409

H	-61.2075698	129.4385409	62.4107701
H	-62.6405563	130.4239528	62.8360584
H	-57.8130058	126.2103805	57.3369982
H	-58.0642934	127.3826963	56.0123500
H	-55.4465794	131.5037612	63.6124244
H	-54.4426582	130.1902662	62.9385694
H	-55.2309019	134.0605506	60.4304676
H	-55.6075078	135.6280585	59.6585565
H	-56.8424932	134.7970410	60.6559484 *
H	-56.8582201	126.0771138	55.8284422 *
H	-54.8728529	130.1901404	64.6793240 *
H	-61.1227586	131.1915556	62.2532170 *
H	-65.8529447	125.7838648	63.1801759 *
H	-64.9187725	124.6648264	56.5007662 *

* these correspond to the H atoms which were used to saturate cysteine C atoms after extraction of the A-cluster atoms from the large size model. The second model used for calculation of strain was optimized only at the level of such added H atoms, while all the other A-cluster atoms were kept fixed at the coordinates found in the parent model **mutA2_{His}**- (see section 3.3)