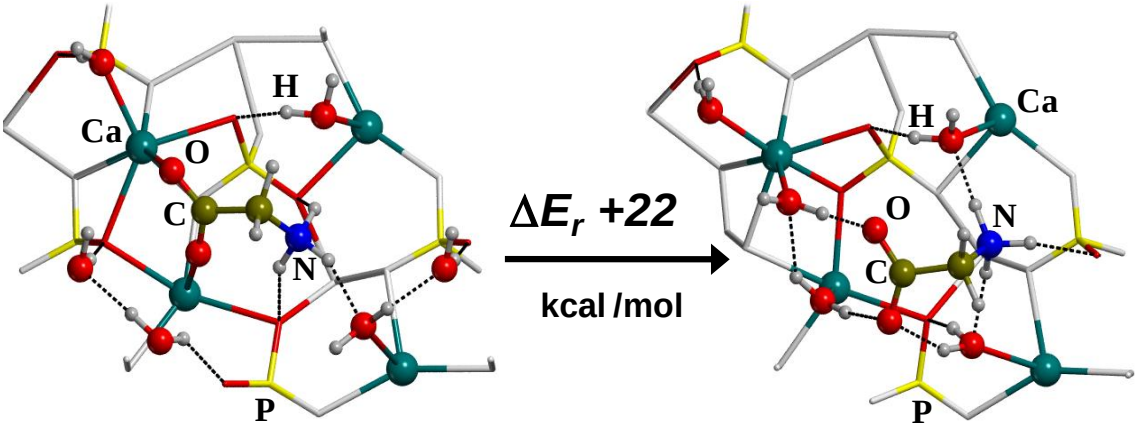
Supplementary Information

Title: Ab initio Modeling of Protein/biomaterial Interactions: Competitive Adsorption between Glycine and Water onto Hydroxyapatite Surfaces

Authors: Albert Rimola, Marta Corno, Claudio Marcelo Zicovich-Wilson, and Piero Ugliengo*



Acknowledgment. A. R. is indebted to the Ramón Areces Foundation for a postdoctoral fellowship. Financial support from MIUR (Project COFIN2006, Prot. 2006032335_005) is gratefully acknowledged. P. U. kindly acknowledges BSC-MN for the generous allowance of computing time through the "BCV-2008-2-0013: Simulation of peptide folding induced by inorganic materials" project.

Surface Models

The (001) surface of hexagonal hydroxyapatite has been fully optimized using the CRYSTAL06 code at the B3LYP level within the slab approach; *i.e.*, by selective cuts of the optimized bulk[1] ($[Ca_{10}(PO_4)_6(OH)_2]$, 44 atoms in the unit cell, space group $P6_3$). The considered bare surface exhibits *P3* layer group symmetry, is a non-defective (vacancies, steps or kink sites), uncharged, stoichiometric slab of thickness 13.5 Å. To avoid any possible bias, for the present work, the optimization was carried out within the *P1* symmetry.

The (001) surface derived from the hexagonal HA (shown in Figure 1) exhibits a dipolar character due to the ferroelectric orientation of the OH groups. In a previous work,[2] the effect of ferroelectricity on the surface energy as a function of the slab thickness was carefully checked. The structural and electronic characterization of these models, in terms of surface energy, geometry relaxation, band gap, field across the slab and electrostatic features in close proximity of the surface, has shown that the OH ferroelectricity does not prevent the formation of a (001) slab of thickness of at least 10 nm. For these reasons and for computational convenience, the HA double-layer slab is considered as a proper model of the HA (001) crystal face to study adsorption processes (see Reference[2] for details). Table 1 reports some significant features of the (001) double-layer model, including the surface energy (E_{surf} = 1.043 J m^{-2}), which is defined as

$$E_{surf} = (E_{sN} - N \cdot E_b)/2A$$

in which E_{sN} , N, E_b, and A are the energy of the slab unit cell, the number of bulk unit cell present in the considered slab model, the energy of the bulk and the unit cell area, respectively.

Table 1. B3LYP lattice parameters (Å), slab thickness (Å), unit cell surface area A (Å^2), surface energy E_{surf} (J m^{-2}) and average geometrical distances (Å) for the hexagonal (001) HA surface. The slab thickness is defined as the perpendicular distance between the most exposed Ca^{2+} surface ions.

surface	*a*	*b*	thickness	*A*	E_{surf}	<P-O>	<Ca-O>	<O-H>
(001)	9.307	9.307	13.5	75.0	1.043	1.551	2.385	0.9705

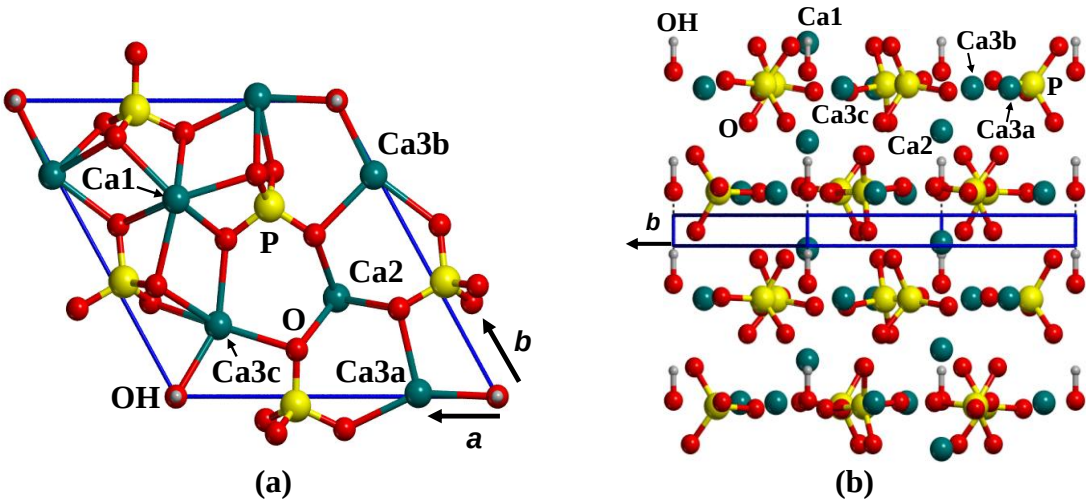


Figure 1. B3YP-fully optimized structure of the (001) hydroxyapatite surface: (a) top view, (b) lateral view.

The analysis of the electrostatic potential features was useful to predict the possible adsorption sites. Highly positive values of potential were found on top of the Ca^{2+} ions, suggesting compatible sites for the interaction with glycine electron rich groups. Deep negative zones are exhibited in close proximity of PO_4 groups so that it was expected that water and glycine donor hydrogen bond groups could easily interact with the (001) surface by exploiting rather strong H-bonds with the PO_4 groups.

In very recent works, the (001) HA surface's adsorptive capacity towards water[3] and glycine[4] have been investigated with the same computational parameters of the present work, considering Ca^{2+} as adsorption sites. In the surface's unit cell, different Ca ions are available to adsorbates and each of them has been investigated in interaction with water and glycine. For the case of water, the effect of increasing molecules loading was considered and the vibrational properties of the models were computed within the harmonic approximation at Γ point. Results showed that H_2O is molecularly adsorbed on the Ca ions of the (001) slab and, at higher water coverages, an important fraction of the interaction energy is due to inter-water H-bond. The average binding energy resulted about 90 kJ mol^{-1} $molecule^{-1}$. No water dissociation occurred; optimization starting from a pre-dissociated water molecule at the HA surface, reforms H_2O in a barrierless process. For the case of glycine, results showed that the adsorption is given in its zwitterionic state, in which the COO^- group interacts with two different Ca ions and the NH_3^+ establishes H-bond with the oxygen surface atoms.

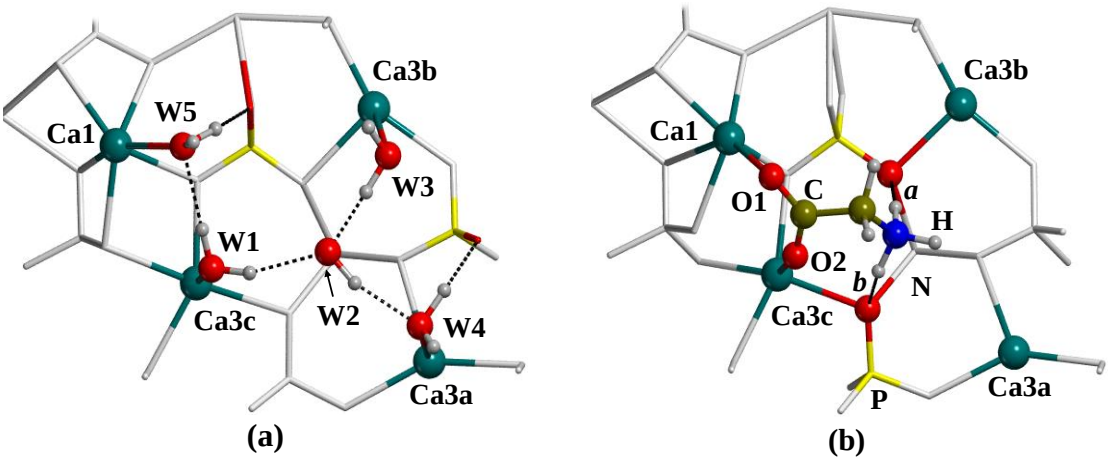


Figure 2. B3-LYP-fully optimized structure of the (001) hydroxyapatite surface: (a) in interaction with five H_2O molecules, (b) in interaction with glycine in the gas phase.

Among the various structures considered in this work, of particular relevance is structure **[Gly-5w]0w/HA** shown in Figure 3 below. It represents one glycine molecule adsorbed on a fully hydrated HA(001) surface originated from Figure 2a. This structure exhibits five H_2O molecules in contact with HA(001) surface and has been used as a further case in the discussion to prove that glycine prefers to contact HA(001) directly rather than through water molecules. Indeed **[Gly-5w]0w/HA** structure is 38 kJ/mol higher in energy than the most stable **[Gly-1w]4w/HA** structure.

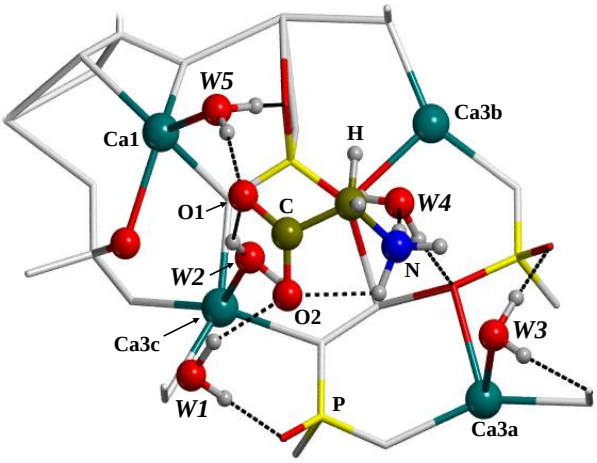


Figure 3. B3-LYP-fully optimized structure **[Gly-5w]0w/HA** of the (001) hydroxyapatite surface in direct interaction with five H_2O molecules and one glycine (zwitterion) only interacting with the water layer.

Computational Details

All calculations published in the present article have been carried out using a development version of the CRYSTAL06 periodic code,[5] which uses a local Gaussian basis set, allowing us to treat molecules, 1D periodic polymers, 2D periodic surfaces (slabs), and 3D crystals (bulks) with the same level of theory.[6] All calculations have been carried out on standard Linux boxes whereas graphical manipulations and vibration visualizations have been carried out with the molecular graphics program MOLDRAW[7] running on Microsoft Windows.

Basis Set. The details of the adopted Gaussian basis set are available on the CRYSTAL web site.[8] Here, the exponents of the outer sp and d shells in $Bohr^{-2}$ are explicitly given: H, 31G* (α_s= 0.161, α_p= 1.1); O, 6-31G* (α_{sp}= 0.27, α_d= 0.8); N, 6-31G* (α_{sp}= 0.212, α_d= 0.8); C, 6-31G* (α_{sp}= 0.1687, α_d= 0.8); P, (α_{sp}= 0.135, α_d= 0.7458); Ca, quasi-relativistic effective core potential of Hay and Wadt to represent the 10 innermost electrons, whereas a 31* (α_{sp}= 0.5) for the 8 outermost electrons and valence orbitals (basis [HAYWSC]-31G).

Hamiltonian and Computational Parameters. For systems in which hydrogen bond interactions are present, and in a periodic context, B3LYP has been proven to be rather accurate as far as structure, energetics, and vibrational frequency prediction are concerned.[9,10] It is now well established that standard GGA and hybrid functionals are unable to cope with dispersive interactions (London forces).[11-13] Because of that, the present absolute reaction energies should be considered underestimated by some amount. Because we mainly concern with the comparison between relative energies (ΔE_{rel} of Table 1 in the paper) of structures containing the same number of atoms we do not expect this deficiency to affect the general trend. For the same reason, the basis set superposition error BSSE has not been taken into account because, while affecting the absolute values of ΔE_{R1} ΔE_{R2} ΔE_{R3} it almost cancels out when computing the relative stability of the considered structures (ΔE_{rel} of Table 1 in the paper). The Hamiltonian matrix is diagonalized[5,14] in 10*k* points, corresponding to a shrinking factor of 4. Values of (6, 6, 6, 6, 14) for the tolerances controlling Coulomb and exchange series have been adopted for all calculations. The exchange and correlation functional is integrated numerically on a grid of points. Integration over radial and angular coordinates is performed through Gauss-Legendre and Lebedev schemes, respectively. A pruned grid consisting of 75 radial points and 5 subintervals with (86, 194, 350, 974, 350) angular points has been used for all calculations. This grid reduces the error to 3×10^{-5} electrons per unit cell in the total integrated electron

density (890 electrons). The SCF process was stopped when the energy difference between cycles was smaller than 10^{-8} in the geometry optimizations.

Geometry Optimization. A full relaxation of the atomic coordinates within the *P1* symmetry was performed while keeping fix the lattice parameters; *i.e.*, the unit cell is kept fixed to the optimized values of the free HA (001) surface whereas the internal coordinates are relaxed by means of analytical DFT energy gradients.[15,16] The geometry optimization was performed by means of a quasi-Newton algorithm in which the quadratic step (BFGS Hessian updating scheme) is combined with a linear one (parabolic fit) as proposed by Schlegel.[17] Convergence was tested on the rms and the absolute value of the largest component of the gradients and the estimated displacements. The thresholds for the maximum force, the rms force, the maximum atomic displacement, and the rms atomic displacement on all atoms were set to 0.00045, 0.00030, 0.00180, and 0.00120 au, respectively. The optimization was considered to be complete when the four conditions were simultaneously satisfied.[18]

Adopted strategy. The procedure adopted to study the micro-solvation of glycine adsorbed on the HA(001) surface is described in detail in the text. Here we would like to expand upon some of the difficulties related to approaches different from the present one which can be adopted to tackle the same problem.

Classical Molecular Dynamics (MD). One possibility is to adopt classical MD in order to consider the "bulk water" on top of the HA surface. This approach heavily relies, for the results to be physically meaningful, on a well developed force field. Reasonably accurate force fields exist for amino acids and proteins and bulk water when treated separately. For HA (both bulk and surfaces), far less exists and only quite recently a new force field has been developed by some of us.[19] The point is that there are no force fields which are capable to model the complex interactions between amino acids and the surface of HA in presence of water as this will require to cope with a variety of interactions spanning from electrostatic to H-bond. Indeed, in absence of accurate force fields any results will be almost useless for instance, in assessing the role of "bulk water" when adopting the most accurate B3LYP approach.

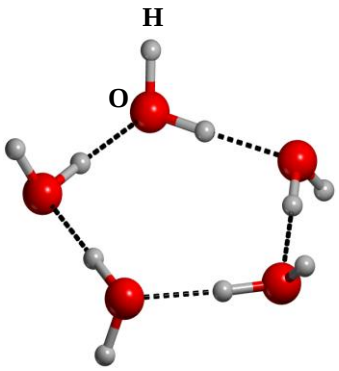
Ab inito Molecular Dynamics (AIMD). To study the process of moving glycine from bulk water towards a fully solvated (again in a bulk water) HA (001) surface one can adopt ab-initio molecular dynamics based on pseudo-potentials and plane-waves approach which is free from the points of weakness explained in the previous point. Let us summarize what are the difficulties which in our opinion hamper this straightforward approach. One should simulate a water slab on top of the HA(001) thick enough to be really representative of a

"bulk water". The interspace between the HA slabs (not needed in our work because Gaussian-type orbitals are adopted) should be large enough to allow glycine to be solvated as in the water bulk when detaching from the HA surface. The problem is then similar to what we got with our simplified microsolvated model: the surrounding of glycine and HA is distorted by the limited amount of water considered but at a much higher computational cost. There is a further drawback in this approach: the MD simulation should run by a very long time to allow glycine to desorb from the HA surface considering the very high energy of interaction (see column ΔE_{R1} of Table 1). The size of the system and the need for extremely long simulation time renders this approach at the limit of the top computational resources available in supercomputing centers.

Optimized Fractionary Coordinates

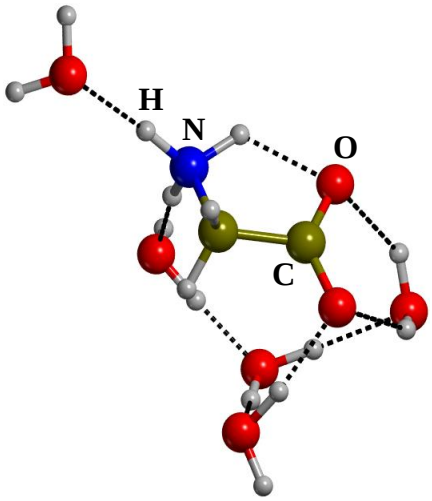
In the paper it has been adopted the notation [Gly-*X*w]*Y*w/HA to refer to a total of *X*+*Y* H_2O molecules of which *X* bridge Gly through the HA surface whereas *Y* interact only with the HA surface. Optimized fractionary coordinates have been written in the MOLDRAW format (MOLDRAW is freely available at http://www.moldraw.unito.it). Each coordinates block starts with a TITLE record and is terminated by a "-1 0 0 0" record. The coordinates of each structure can be copied and pasted in an ASCII editor and saved as a file with .MOL extension.

5w



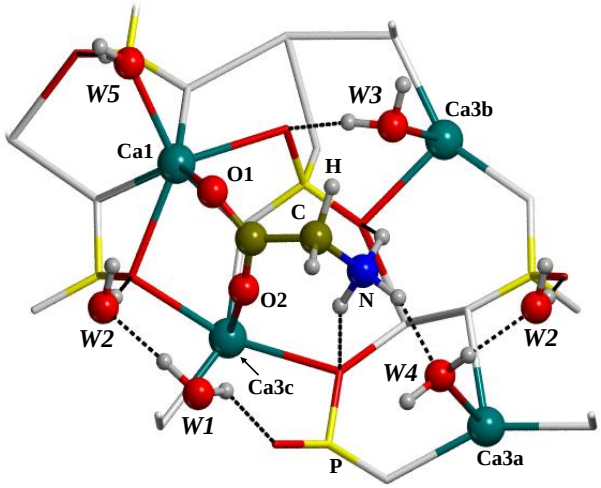

```
TITLE
5w IN CARTESIAN COORDINATES
CELL
1 1 1 90 90 90
COORD
 8   -0.546953190620   2.202170590071   -0.115334937794
 8   1.925487089135   1.202741960975   0.069283753406
 8   1.745672588923   -1.461782125029   0.017141640855
 8   -0.848026467430   -2.102022356810   0.044055314657
 8   -2.275807409426   0.154496056979   -0.056843911066
 1   -0.605935687586   2.796941797388   0.641737654378
 1   2.425456629811   1.410374228589   -0.729672666803
 1   2.084799073849   -1.853685352681   0.831122377157
 1   -1.096324608890   -2.562663246035   -0.766788275118
 1   -2.792598785791   0.278310268501   0.748220024725
 1   0.376815332905   1.833488236155   -0.073146168805
 1   1.873245870877   0.208400595673   0.080238302280
 1   0.782513268763   -1.713576806637   -0.001625454427
 1   -1.388862335592   -1.266505957585   0.032839065841
 1   -1.665022990249   0.938689394858   -0.101074442366
-1 0 0 0
```

Gly/5w




```
TITLE
Gly/5w IN CARTESIAN COORDINATES!
CELL
1 1 1 90 90 90
COORD
 8   1.520476904078   -0.782468516446   1.227319748146
 6   -0.538500607391   0.452605151052   1.133814402821
 6   0.974625574047   0.274705403890   0.818460039613
 8   1.486131345540   1.216726084962   0.160017942844
 1   -0.674809038343   0.796261488594   2.162641642999
 1   -1.083733621699   -0.481164695063   0.991918865470
 7   -1.040265672303   1.496690171477   0.190881062933
 1   -1.336248790942   1.025434595894   -0.722779376320
 1   -1.790350921140   2.084264548582   0.584040121107
 1   -0.164465527787   2.023802021767   -0.018434156125
 8   -1.611517730358   0.084707091701   -2.003773485924
 1   -0.923629799914   -0.663545079088   -1.965398204657
 8   0.179101340583   -1.782502245465   -1.833461796515
 1   1.109838594459   -1.462407407990   -1.767515850502
 1   -1.480928122583   0.497032031978   -2.866379614875
 1   0.024691414247   -2.283557748034   -1.002323818283
 8   2.761157155504   -0.853128027231   -1.317002472613
 1   2.590121786968   0.096667526262   -1.186326799085
 1   2.714728274383   -1.138844082694   -0.385487997205
 1   0.508739683584   -2.150468996192   1.072912727717
 8   -0.144542549755   -2.811560903006   0.726148613842
 1   0.239636609813   -3.678578841758   0.902852102538
 8   -3.136425476678   2.988040370738   1.491173720465
 1   -3.161866194600   3.951191916288   1.548205313735
 1   -4.048977299137   2.715655681776   1.332562957347
-1 0 0 0
```

[Gly-0w]5w/HA



No water molecules bridging the Gly-HA interaction.

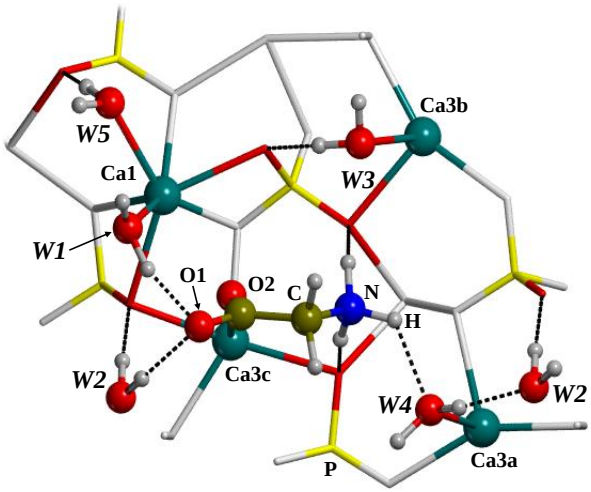
Fully direct contact between Gly and HA

```
TITLE
[Gly-0w]5w/HA
CELL
9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 20   0.323198038647   0.663660508487   7.183733577199
 8   0.615729438774   0.767951695420   6.714983238071
 8   0.219989489081   0.962979481180   6.651360481142
 8   0.084057658702   0.388745623955   6.726498178318
 1   0.982708259528   0.036754183967   6.649683526105
 8   0.972071838277   0.041294678906   5.689984364540
 8   0.673376777132   0.567740145221   5.399160892414
 8   0.449791353387   0.192767161740   5.336908300948
 8   0.818229990360   0.342487455995   5.574996191146
 15   0.588336050420   0.672271616771   5.370713641006
 15   0.337886110887   0.003965263143   5.428497608087
 15   0.007291651177   0.432867784603   5.522737854321
 20   0.723606929073   0.045950110021   5.518998774749
 20   0.964092554045   0.784496555818   5.381973775804
 20   0.230730869541   0.278024798552   5.349717368899
 8   0.397085362668   0.567117462066   5.220608902969
 8   0.431842237289   0.907131233873   5.595642005564
 8   0.093068843009   0.624471475187   5.580694773281
 8   0.656867088097   0.800178341725   4.236348066300
 8   0.228035860523   0.935117595864   4.169783990205
 8   0.067083544125   0.388998268083   4.223952331541
 20   0.294656204436   0.697618534292   3.702293869278
 20   0.655455817937   0.367832350099   3.793197680721
 8   0.290820470961   0.272444062729   3.123364405337
 8   0.715747670964   0.127997855728   3.288914033021
 8   0.890443227375   0.691276434761   3.186821144547
 1   0.975479451958   0.029854374819   3.114867234798
 8   0.971394933186   0.029216429573   2.146536978751
 8   0.295759108573   0.516610356946   1.966982952171
 8   0.489666029668   0.871486968790   2.059994904782
 8   0.133258600446   0.711558520333   1.895594413593
 15   0.367630111607   0.399066738392   1.983528423706
 15   0.607257409427   0.061150296902   2.019374034779
 15   0.943258544189   0.636168819476   1.920833169699
 20   0.219103919306   0.019584626460   1.909426627208
 20   0.986240404913   0.289103798877   1.982129655965
```

20	0.713524652383	0.785817415120	1.954569283895
8	0.558568706564	0.494445912161	2.143402680949
8	0.509342567501	0.154849520467	1.934087284842
8	0.851316067927	0.444411748882	1.942747635426
8	0.329560843505	0.299169389386	0.665820746877
8	0.723472116699	0.107327943450	0.800826642516
8	0.880678424840	0.689094050407	0.691789168724
20	0.631669612692	0.367365677468	0.274078203179
20	0.308049547885	0.699709863511	0.153628381321
8	0.596861710514	0.752760606457	-0.184835386094
8	0.235094782913	0.935361024241	-0.268407732474
8	0.075414841041	0.398028544442	-0.203691331840
1	0.981213752667	0.034973302003	-0.085055547035
8	0.978336522861	0.035780198277	-1.053248004525
8	0.644631379588	0.543786637953	-1.484471148095
8	0.449957884845	0.190108713737	-1.536165975611
8	0.809575291489	0.350192497944	-1.375633673496
15	0.575980500419	0.664602706525	-1.536489765867
15	0.339109452572	0.999116717783	-1.555175122181
15	0.000135715628	0.427115706660	-1.477112234701
20	0.734569348171	0.047528104268	-1.481519554944
20	0.957212612287	0.778103596028	-1.549275454159
20	0.230372112303	0.280154288716	-1.524197802310
8	0.388692159800	0.573343014412	-1.866315373846
8	0.441767377153	0.910755750356	-1.665374621165
8	0.088946763005	0.616321382656	-1.704387672230
8	0.676219803116	0.798758241674	-2.586435050931
8	0.217770579158	0.941292690680	-2.749479727005
8	0.039954163219	0.345465040405	-2.646308655527
20	0.292355594356	0.701261115276	-3.519353276740
20	0.645968926885	0.362710465299	-3.184081314565
8	0.289653953754	0.268598303836	-3.784853832965
8	0.717746574188	0.129337353800	-3.715073371772
8	0.876283387025	0.681095831223	-3.773921968402
1	0.965852908354	0.024129501436	-3.810584802314
8	0.962126753066	0.022516927497	-4.780687205095
8	0.264234302295	0.485397279533	-5.081088460956
8	0.517066177136	0.871512814938	-4.992293130301
8	0.122718245470	0.736581284139	-5.194437069801
15	0.354101979128	0.385252077866	-5.004870543994
15	0.610032780008	0.061783775415	-4.992397316962
15	0.933307816955	0.636661664185	-5.085435853801
20	0.209678214997	0.019885335843	-4.940865105149
20	0.977736751333	0.278652698173	-4.887311189769
20	0.709988370406	0.778280519292	-4.863873926621
8	0.545738303578	0.493263175619	-4.832019070013
8	0.493584672895	0.136948584001	-4.952532816494
8	0.861964456504	0.446103907486	-5.003791924281
8	0.332750936458	0.278714596749	-6.267347465779
8	0.721280211712	0.141951869008	-6.232840878468
8	0.839444771809	0.659511060155	-6.275030771990
20	0.630129971677	0.359910680843	-6.464346991501
8	0.331714823854	0.329573115589	7.556840976370
7	0.628618521886	0.369772445102	7.756103662135
6	0.411587476629	0.428053721433	8.490534443555
8	0.378752235869	0.530241519977	9.033389230389
6	0.563277464666	0.415429215082	8.945203302725
1	0.711714816369	0.474084514917	7.236899185562
1	0.679843913760	0.295472138742	7.941149170914
1	0.522249689785	0.316456461865	9.690337383076
1	0.661235208729	0.531752419899	9.355649714002

```
 1   0.533574124033   0.303065594344   7.071010845270
 8   0.990145010815   0.235672335352   8.980130212324
 1   0.061317775291   0.320994017639   9.606118460054
 1   0.026568491426   0.292398091340   8.074646696647
 8   0.684350311538   0.096646031627   7.919452536193
 1   0.579274163379   0.016568458829   8.334790093918
 1   0.775717243473   0.127608009697   8.556632508646
 8   0.868350939556   0.742420075166   7.697200855483
 1   0.943061687044   0.826816929208   8.341280506725
 1   0.770513212594   0.757085874645   7.564633376340
 8   0.336639084190   0.875088386113   8.557579918886
 1   0.289816178594   0.919322769879   7.824696835490
 1   0.290504896818   0.889631243583   9.377817701330
 8   0.107815186976   0.012048924329   9.076938991716
 1   0.172527686337   0.046514230461   8.251084680007
 1   0.067628026146   0.091048446775   9.165802497601
-1  0  0  0
```

[Gly-1w]4w/HA



1 water molecule bridging the Gly-HA interaction.

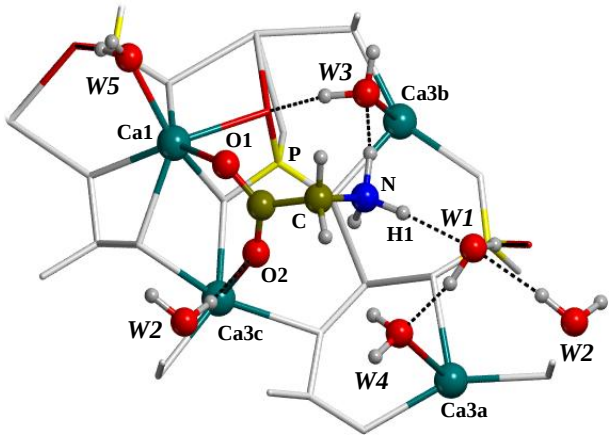
Contact between Gly and HA through W1, which interferes the O1-Ca1 interaction

```
TITLE
[Gly-1w]4w/HA
CELL
9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 20   0.319236715086   0.663507851663   7.218543927932
 8   0.612063397028   0.776116779565   6.736444179179
 8   0.226133479321   0.982942822102   6.630964367419
 8   0.082328870804   0.390806039697   6.687800992619
 1   0.989014996911   0.055749582729   6.572654223389
 8   0.977236007214   0.054488557959   5.608940285651
 8   0.675468294988   0.578052677666   5.456146475139
 8   0.452518126051   0.204483042181   5.282425964762
 8   0.819897394356   0.351403825356   5.540161578372
 15   0.589494390720   0.682427662642   5.390473368098
 15   0.339454033917   0.014326571708   5.394873399919
 15   0.009439993761   0.442696660772   5.511467024455
 20   0.727181224349   0.055574117393   5.481281120853
 20   0.966655631270   0.796909637612   5.397772945529
 20   0.238042681973   0.291518615445   5.374046055545
 8   0.399468288676   0.579033226756   5.185716076863
 8   0.434262090608   0.918957109631   5.558331861220
```

8	0.093679690365	0.634001472143	5.639548403692
8	0.664375751847	0.809902712138	4.259648468930
8	0.227710710349	0.943957319949	4.152713319891
8	0.071091901223	0.407076549392	4.185283194295
20	0.293290129447	0.706072140989	3.696682416250
20	0.662535645086	0.382205667993	3.765875754174
8	0.289933248304	0.283273264641	3.116596585458
8	0.720378540839	0.139460614061	3.269398974117
8	0.889777319246	0.691896025117	3.215013257320
1	0.977591344937	0.042769271069	3.126563941520
8	0.971374046624	0.037735982803	2.158342239659
8	0.299224337045	0.527912942268	1.940042553222
8	0.492693926908	0.880937676643	2.076103454779
8	0.135309109360	0.721988833093	1.891014434938
15	0.369198783192	0.408870951606	1.973437788079
15	0.608726224094	0.070768518098	2.019596771793
15	0.945281651616	0.645904074029	1.911413248714
20	0.219320572505	0.029869183223	1.901745582588
20	0.988458847447	0.298561526232	1.965951812268
20	0.714382693163	0.794534913433	1.963977906762
8	0.560213159691	0.503046419635	2.137801617750
8	0.509720049526	0.163425371426	1.952263205313
8	0.853597266789	0.454149640459	1.870425605868
8	0.331474363905	0.307900609111	0.659422050196
8	0.722187780099	0.117275664512	0.783043665445
8	0.885591908651	0.706587003880	0.715328272912
20	0.630902733815	0.371605209093	0.261668091185
20	0.310599863981	0.711019517843	0.150579122669
8	0.598633597442	0.763165301698	-0.184907569253
8	0.239627707338	0.947430806700	-0.270005747825
8	0.078081068244	0.404728900200	-0.226049985825
1	0.984118561639	0.048243328428	-0.098946657567
8	0.980723657868	0.047665855264	-1.067207409505
8	0.647294807451	0.552522526795	-1.461265631538
8	0.452635283145	0.199669374062	-1.565342428053
8	0.812691085177	0.358162323391	-1.391580970121
15	0.579333315644	0.673859924827	-1.528797374015
15	0.340608972112	0.008613193285	-1.572417554548
15	0.003654735266	0.438241778151	-1.482766855222
20	0.734686168672	0.055281350560	-1.482158731966
20	0.958093185789	0.788889139693	-1.549344627073
20	0.233164474280	0.290562618921	-1.541189519118
8	0.392740046794	0.583179689554	-1.878036008292
8	0.442128854062	0.919053975705	-1.692871451223
8	0.090670736676	0.628226956138	-1.656049408932
8	0.682499622075	0.807592830087	-2.573883874532
8	0.216948690967	0.950928395694	-2.749178083585
8	0.049041799647	0.366135171317	-2.688802567518
20	0.290337684556	0.704774422355	-3.521212654660
20	0.651538746206	0.373806640730	-3.188863523756
8	0.286647037627	0.276277514466	-3.811814842848
8	0.722969254336	0.137741880968	-3.713743008135
8	0.876101963895	0.684090702797	-3.769488092198
1	0.968278993860	0.031303834067	-3.823524549642
8	0.963620214173	0.028397534877	-4.793377209965
8	0.267283954117	0.494081500306	-5.133032917167
8	0.518056646683	0.878920929512	-4.962097352350
8	0.124291857612	0.745107107895	-5.193071191197
15	0.355729507888	0.392864345393	-5.028563586195
15	0.612310058425	0.069238433492	-4.975269246006
15	0.934897856723	0.643639319169	-5.092940752569

```
 20   0.212626519230   0.028047233627   -4.949018802390
 20   0.980754351592   0.285531917264   -4.902913331580
 20   0.710991323162   0.784975224245   -4.858136765993
 8   0.547044109680   0.499735594762   -4.829281707637
 8   0.497080605735   0.145896599218   -4.923893811982
 8   0.865487002968   0.453346893283   -5.035029068885
 8   0.336592305250   0.285781087860   -6.283686360394
 8   0.721386440969   0.147318145632   -6.229984563165
 8   0.840663046011   0.667356234581   -6.273899433584
 20   0.632002552971   0.366185991035   -6.466668009006
 8   0.363838039677   0.403999814991   7.644799805742
 7   0.626746110705   0.364746191817   7.522902439686
 6   0.392734605919   0.358084901040   8.747504521680
 8   0.308495675852   0.328310207038   9.809147058872
 6   0.547863074543   0.341605456953   8.841311293731
 1   0.670609706044   0.481134290510   7.103075348944
 1   0.717843961755   0.333162890680   7.508045439090
 1   0.514972477921   0.218945275082   9.218023533515
 1   0.635835800397   0.434812967342   9.536684788284
 1   0.542979497168   0.288903019054   6.780691628782
 8   0.991883040716   0.154161213899   8.542889171653
 1   0.083776747269   0.199885067214   9.179528076369
 1   0.024101781698   0.246102991010   7.885889309658
 8   0.694296408516   0.103038903747   7.847022230687
 1   0.586009069717   0.025614790151   8.225637568851
 1   0.782377173155   0.106851207852   8.413202807169
 8   0.875696929137   0.783318865042   7.740260629504
 1   0.939406790764   0.886591144393   8.224046989616
 1   0.768641579154   0.779926365519   7.538504687845
 8   0.350619109125   0.900528116502   8.456968856154
 1   0.295351319974   0.942734370383   7.751311115330
 1   0.299132349616   0.896373762378   9.303362830472
 8   0.259245657268   0.582711593655   9.518108198435
 1   0.303129131719   0.647878328953   10.318006549140
 1   0.257036171176   0.476694161998   9.710421154045
-1 0 0 0
```

[Gly-1w]4w-SI1/HA



1 water molecule bridging the Gly-HA interaction.

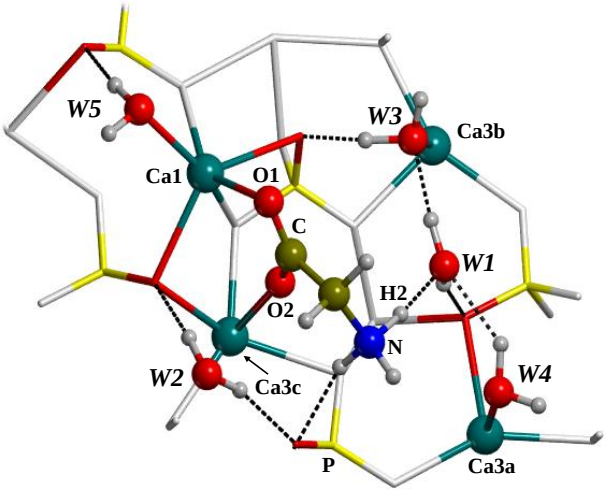
Contact between Gly and HA through W1, which interferes the NH1-surface interaction

```
TITLE
[Gly-1w]4w-SI1/HA
CELL
9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 20   0.315764569302   0.671717471234   7.028824181887
 8   0.609892968811   0.777993687658   6.566756532795
 8   0.212681452291   0.973072964796   6.399096644519
 8   0.086173599672   0.393664778320   6.576697643935
 1   0.979047787333   0.057232240314   6.459074172705
 8   0.966097781133   0.051818793559   5.495897161189
 8   0.668202155052   0.568680514228   5.384051826881
 8   0.450687929890   0.189214167333   5.094255991416
 8   0.813186769032   0.338689337035   5.491144632931
 15   0.584115424847   0.673848221741   5.263132073354
 15   0.329176839766   0.002732321101   5.182811887691
 15   0.002684405062   0.436138461168   5.406927021492
 20   0.712415496136   0.044220701179   5.311520161574
 20   0.956446287384   0.794107340168   5.214897998711
 20   0.235122101026   0.281333318241   5.293521365269
 8   0.393802983883   0.570293025518   5.089641509430
 8   0.416093615973   0.898871027662   5.346009891471
 8   0.078649838829   0.626702047052   5.511126163723
 8   0.660331001145   0.798425379184   4.113009012575
 8   0.215411554068   0.933993911753   3.951623007018
 8   0.062592059665   0.401127716612   4.069993245270
 20   0.281615616642   0.692837526479   3.544132930206
 20   0.659926866011   0.375413192136   3.670140361964
 8   0.276210345872   0.272522323463   2.994645641433
 8   0.712033616490   0.131491904405   3.128513323167
 8   0.879292136331   0.678591037335   3.071594049531
 1   0.970770566911   0.032903760368   2.980575712173
 8   0.961571529296   0.025578743941   2.014580880222
 8   0.290859157203   0.518081494860   1.803972898818
 8   0.484636885466   0.870358284521   1.952796236339
 8   0.125534777005   0.710873819373   1.734952705426
 15   0.359506062972   0.397867418973   1.855979558558
 15   0.600106611457   0.060360498425   1.879329046759
 15   0.935588119431   0.634030347909   1.763954245089
 20   0.210683913524   0.020619045784   1.737190294589
 20   0.980043310712   0.287380737737   1.842752413135
 20   0.704437132163   0.782745524419   1.816227658968
 8   0.550221464857   0.490830955340   2.035007408683
```

8	0.500620818637	0.152067733961	1.791593712069
8	0.844875257160	0.442402814504	1.727648852060
8	0.322804768417	0.297506376624	0.536849865353
8	0.714295545857	0.104702822420	0.649936115561
8	0.874264344575	0.693766055510	0.571717233460
20	0.621542048915	0.361640609455	0.129899065051
20	0.301690817921	0.700324629864	0.010799740639
8	0.588224975784	0.750652311368	-0.322773760584
8	0.228838601569	0.935967812844	-0.422055310529
8	0.069198095159	0.393451458337	-0.359009122600
1	0.975099201197	0.037557316426	-0.236150338743
8	0.972222146648	0.036836631294	-1.204579086155
8	0.636895817434	0.540548206020	-1.603512344778
8	0.442311983024	0.188613443377	-1.706714608985
8	0.803164041960	0.346801234317	-1.519217733829
15	0.569724139680	0.662491300041	-1.670993683266
15	0.331347901565	0.997431259578	-1.716686878054
15	0.994158240866	0.426890588160	-1.612515643231
20	0.726168237744	0.044542540768	-1.617944451343
20	0.948963888143	0.777912575335	-1.690195227168
20	0.224384049495	0.280289537948	-1.673532753438
8	0.383380819158	0.572623332321	-2.027762100391
8	0.433790006612	0.908741945308	-1.820744471594
8	0.081060106841	0.616854548238	-1.787061216994
8	0.674339661818	0.796901197367	-2.706767129206
8	0.208708026452	0.938138940042	-2.901492527605
8	0.039066197592	0.354768479715	-2.821311480895
20	0.279848947966	0.694130480726	-3.659798521120
20	0.642818602682	0.362324028103	-3.323827647222
8	0.274526019114	0.263920507463	-3.951029945455
8	0.713183613442	0.126931321158	-3.847490158975
8	0.866748271897	0.672424561463	-3.908375521961
1	0.958460960039	0.019280413692	-3.963918575602
8	0.953253119074	0.016265796076	-4.933609300311
8	0.257884612350	0.483320870509	-5.268150132513
8	0.508375960899	0.867628382299	-5.092686256465
8	0.114229592283	0.733875342003	-5.343617500748
15	0.345559084385	0.381384827473	-5.161095258138
15	0.602600159988	0.057937944590	-5.109598998415
15	0.924958237319	0.632035862313	-5.235379383724
20	0.202711864243	0.016688664324	-5.093363858813
20	0.971268351405	0.273897907107	-5.036135268963
20	0.700618861434	0.772882410301	-4.992757828762
8	0.536799899839	0.487456274426	-4.952775461654
8	0.487257810342	0.134493037677	-5.061372640387
8	0.856091586908	0.441863022531	-5.176079545529
8	0.326983156569	0.274876334029	-6.419339101506
8	0.711684306163	0.135642957813	-6.364236043921
8	0.829653625025	0.655164335341	-6.411298008771
20	0.621902248556	0.354670199711	-6.601614562425
8	0.359893739726	0.338189571740	7.519343481608
7	0.707541462758	0.475953274997	8.188019184304
6	0.426664195507	0.445207436245	8.442105540451
8	0.388450583279	0.550523359722	8.800453644966
6	0.571450790837	0.440596253848	9.163571253734
1	0.661680878007	0.438452879158	7.231812233802
1	0.786139961327	0.606109687255	8.087345268381
1	0.526296862816	0.316297963591	9.570245538263
1	0.622503965185	0.532190103624	9.964059856280
1	0.778580304847	0.422792038900	8.461182463274
8	0.871335799896	0.796274527584	7.599814958293

```
 1   0.765588571262   0.796308025840   7.355126641749
 1   0.938542351689   0.896355381436   8.147221847152
 8   0.054955642430   0.096526870287   8.809656921274
 1   0.006463661178   0.166385272039   9.000261359798
 1   0.158345826980   0.168732327547   8.337971365695
 8   0.612453230967   0.108385969599   7.465674459459
 1   0.509495587425   0.026330143880   7.916818718465
 1   0.580478881400   0.177746250707   6.961250535435
 8   0.302107214697   0.874819395145   8.316244324909
 1   0.255661405803   0.924103189359   7.562008064301
 1   0.266710747087   0.891283646156   9.179751705925
 8   0.902708049897   0.310452719679   8.775089188917
 1   0.975973578038   0.347168761031   7.966136300821
 1   0.798223387998   0.220449758183   8.417348878541
-1  0  0  0
```

[Gly-1w]4w-SI2/HA



1 water molecule bridging the Gly-HA interaction.

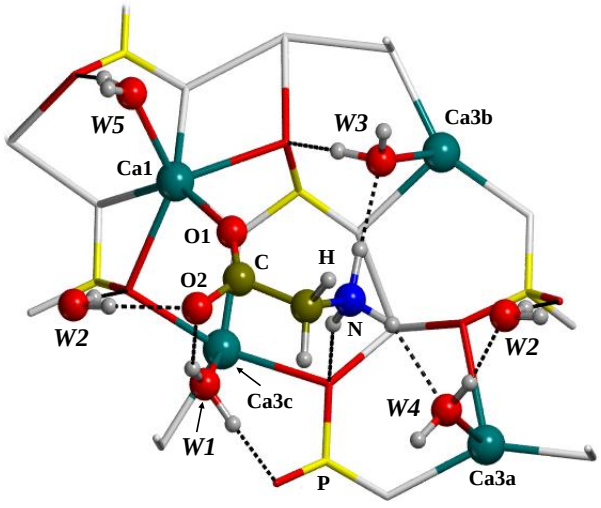
Contact between Gly and HA through W1, which interferes the NH2-surface interaction

```
TITLE
[Gly-1w]4w-SI2/HA
CELL
9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 20   0.345419708150   0.667478145345   7.165132644702
 8   0.638340767501   0.783199970720   6.577279213397
 8   0.232750526894   0.992655613088   6.620974463916
 8   0.097387965555   0.394055914597   6.664632737322
 1   0.980240791426   0.047472582055   6.393803150193
 8   0.986624192952   0.053917597172   5.429199467358
 8   0.694133191716   0.589102458623   5.190565230996
 8   0.469387650048   0.205990155875   5.292174631399
 8   0.834658456159   0.357210691510   5.506070931110
 15   0.603340988050   0.687097372922   5.211728164387
 15   0.355410504395   0.019681892238   5.434037786199
 15   0.026118472650   0.444577418007   5.467794904567
 20   0.736205896781   0.060251041067   5.378048865955
 20   0.982816509164   0.799043030326   5.270685182294
 20   0.252477990146   0.293213700464   5.279120749818
 8   0.412237252468   0.581429240008   5.126168236852
 8   0.444519626340   0.920296936471   5.702847549990
 8   0.108927096585   0.635835070447   5.533778360150
 8   0.658260681279   0.815592300586   4.084558525351
```

8	0.250284766842	0.946521078581	4.149504983637
8	0.082577963761	0.401128453692	4.156103358881
20	0.314560616941	0.716499135057	3.636384139113
20	0.663195530075	0.377768860210	3.701211475943
8	0.323577729447	0.293067504219	3.080861594955
8	0.726336780921	0.144814272516	3.191024054246
8	0.916762149496	0.727261010960	3.044380337034
1	0.992022854197	0.049044278094	3.044774944850
8	0.993008223402	0.053699112819	2.075464835352
8	0.310198132066	0.531212608997	1.928490255551
8	0.504177320132	0.890178581655	1.930019149341
8	0.151042809590	0.727229884258	1.812071089853
15	0.386686507563	0.417684705043	1.915389406210
15	0.623257498860	0.079484886227	1.891243357649
15	0.961711438806	0.655946055318	1.838094754531
20	0.236952749118	0.036563367164	1.859286156154
20	0.002678957415	0.309881743323	1.908080081862
20	0.734680892357	0.809339985061	1.835373378595
8	0.578277110842	0.517725095800	2.010564873607
8	0.527046279446	0.174479765938	1.776492172739
8	0.866733475516	0.464680850723	1.947952940580
8	0.341962487033	0.316080501000	0.607109751333
8	0.744664574351	0.125221732539	0.711215811203
8	0.896804586392	0.699652806272	0.568793506957
20	0.652148655452	0.394614788775	0.179482609537
20	0.325004784126	0.714801188129	0.073116686111
8	0.619459491902	0.774585963017	-0.303717860420
8	0.246701408612	0.948440808867	-0.341304275761
8	0.088871393064	0.422745623139	-0.267380916604
1	0.993484331915	0.044581740027	-0.171430929331
8	0.992407479845	0.047776128102	-1.139456069367
8	0.664681009462	0.568259799778	-1.645165251701
8	0.464799442104	0.209097815880	-1.540608940034
8	0.823576229326	0.372608572139	-1.473195997576
15	0.590246440269	0.684488419846	-1.655293946740
15	0.356456204173	0.018147844452	-1.593156038869
15	0.013255702294	0.443165645891	-1.577661581899
20	0.754351970395	0.068986015951	-1.598007601154
20	0.977329624557	0.793738120836	-1.643887673395
20	0.243852213488	0.295191330168	-1.579882912464
8	0.400474893750	0.588310160441	-1.884102921980
8	0.461305921336	0.932294901221	-1.695597640670
8	0.105936110286	0.629827338273	-1.917299128445
8	0.673961880729	0.816068602744	-2.757148746123
8	0.241428028129	0.963438607011	-2.826734411117
8	0.042956783579	0.342856390419	-2.656547934675
20	0.323660758990	0.733606725402	-3.605641548380
20	0.646551074529	0.372792770395	-3.270705033686
8	0.326210600835	0.295439225763	-3.806331868102
8	0.726600686464	0.149955479499	-3.828861933256
8	0.908999161225	0.732686346565	-3.909202718381
1	0.981536644212	0.052973296575	-3.901301762386
8	0.982037978679	0.056815057504	-4.871333158736
8	0.279548709734	0.505798758926	-5.040850572120
8	0.538305703866	0.897338279406	-5.205913579165
8	0.143610806442	0.755913928684	-5.288610495994
15	0.374245213066	0.410116509808	-5.044458148818
15	0.626705375105	0.087157643415	-5.147968043826
15	0.954326105421	0.665729054014	-5.151594265054
20	0.223111755293	0.041727825107	-5.003357487719
20	0.992523347645	0.309721753828	-4.941247983934

```
 20   0.732276419824   0.808129765551   -5.004137165350
 8    0.566342804896   0.523267377137   -4.956010076230
 8    0.506080314251   0.156981910607   -5.119319508790
 8    0.872533996230   0.474653937680   -4.954389761256
 8    0.345987319123   0.303648175610   -6.314281989500
 8    0.743927641674   0.177348477242   -6.340374250880
 8    0.862187978419   0.683891867473   -6.380584868375
 20   0.649684783706   0.388883507081   -6.548045269280
 8    0.376840951898   0.388206489158   7.455920809413
 7    0.475469012601   0.213069592263   8.751666477765
 6    0.401033731302   0.431578149422   8.668729174726
 8    0.401184022541   0.555369740704   9.160396200994
 6    0.426515229019   0.314046503308   9.593776608121
 1    0.597558692008   0.295602548551   8.368765167352
 1    0.473733951604   0.116117401843   9.244269053590
 1    0.309306185458   0.232452415537   10.098759393730
 1    0.523076001327   0.382918524057   10.334161161590
 1    0.397639452811   0.165322149304   7.930067945870
 8    0.750578071679   0.117230282183   7.799777641769
 1    0.815159687866   0.075871978503   8.247143258105
 1    0.812015868628   0.236462120368   7.958109571958
 8    0.873820239759   0.761693423954   7.611615411240
 1    0.922888410920   0.849254830313   8.270997940959
 1    0.767427240301   0.762099241563   7.310441889444
 8    0.229630020887   0.796618401062   8.452126195742
 1    0.222976470926   0.871833070850   7.752750953011
 1    0.116874770318   0.725761627146   8.749383938857
 8    0.777441850318   0.432432733433   7.920918486647
 1    0.782817068918   0.409315080927   6.948378218129
 1    0.803770762413   0.548877458439   7.944291362442
 1    0.073225070495   0.228559949373   7.903179272601
 1    0.129762254669   0.099049125811   7.860076219018
 8    0.056335117279   0.126770604252   8.351619441334
-1  0  0  0
```

[Gly-1w]4w-SI3/HA



1 water molecule bridging the Gly-HA interaction.

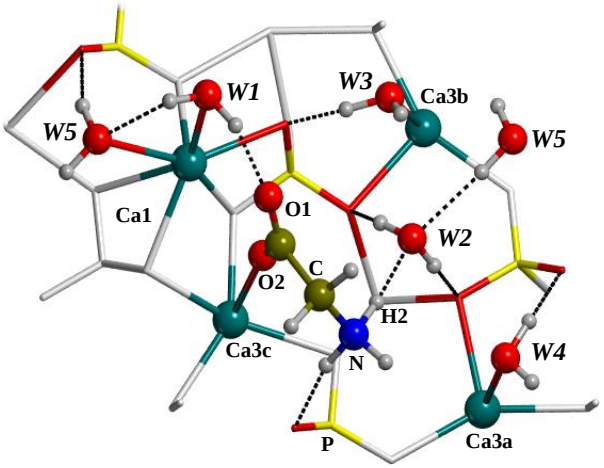
Contact between Gly and HA through W1, which interferes the O2-Ca3c interaction

```
TITLE
[Gly-1w]4w-SI3/HA
CELL
9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
```

20	0.335720082162	0.672525486962	7.033335231871
8	0.632714640718	0.782234358687	6.449602938128
8	0.218564768165	0.934468144387	6.634723976829
8	0.091843138117	0.403233874428	6.583815852535
1	0.984763553883	0.041545290498	6.349567694107
8	0.973361517699	0.031547026976	5.383451675698
8	0.679494128635	0.577869148225	5.102862331670
8	0.440997144407	0.196344777350	5.484887836484
8	0.823362881037	0.355151205330	5.420743684276
15	0.589433066455	0.676880073317	5.137929403128
15	0.342924379390	0.005122489256	5.426513476227
15	0.012310488942	0.437052023138	5.337069942619
20	0.736969424907	0.055983772884	5.324822812200
20	0.969122278836	0.779799506414	5.221009975431
20	0.226515999975	0.278215273143	5.239030572180
8	0.398302963797	0.564803134792	5.155132462458
8	0.447864943573	0.919908836817	5.517718253626
8	0.104952735762	0.628686480714	5.243134680554
8	0.631694092203	0.797554781103	3.963695769229
8	0.243810338494	0.949182532745	4.112697276523
8	0.060672878120	0.369678835891	4.114379310435
20	0.318612576114	0.716851223234	3.549019201217
20	0.634363807264	0.356606397649	3.683450952999
8	0.326559222751	0.289791729051	3.088571807350
8	0.709547615200	0.132672750545	3.135479073296
8	0.914327285269	0.737298301660	2.949372339335
1	0.978105593173	0.042339005519	2.976266779343
8	0.981551122907	0.052060057034	2.009297346663
8	0.297765026756	0.520824270079	1.915787983568
8	0.495504931377	0.883072234857	1.793090483844
8	0.140685968665	0.716545283090	1.784975389119
15	0.376421830313	0.409140731781	1.882088215969
15	0.611125366544	0.072812931976	1.813051456185
15	0.951911791620	0.650109540451	1.817748942490
20	0.221641771059	0.028533411404	1.815750028979
20	0.990289084184	0.306491162962	1.850612476887
20	0.725470103089	0.803080703084	1.757340489234
8	0.568054121506	0.511826766517	1.900035817874
8	0.511934695491	0.164965298012	1.728497460124
8	0.852705178177	0.459895923809	2.013791700735
8	0.322714059989	0.302778498895	0.599567422710
8	0.734359646777	0.127428448996	0.638358867231
8	0.887285695505	0.686398174478	0.506766522783
20	0.645288902005	0.387913167662	0.137838973599
20	0.313040250405	0.706163139050	0.016541468428
8	0.614128758466	0.772691007582	-0.383799542908
8	0.234661769417	0.939028062917	-0.381205304145
8	0.076507276304	0.418369714157	-0.314735472181
1	0.979541442827	0.034593517753	-0.220012178454
8	0.979808339171	0.037636844658	-1.188432359788
8	0.655401508320	0.562938343815	-1.706386432162
8	0.453743125038	0.202410277787	-1.554804831923
8	0.813214386346	0.367916323348	-1.548785171334
15	0.579113609142	0.677487731462	-1.714401724196
15	0.345400095440	0.011403931323	-1.625798939907
15	0.002447639045	0.436202958022	-1.644221374664
20	0.743235847137	0.061176923057	-1.658514948936
20	0.967391302856	0.784559374880	-1.693052008658
20	0.231817653288	0.285618610710	-1.613482787370
8	0.388418370223	0.578675385146	-1.885955120634
8	0.450338759666	0.925845663479	-1.743226522972

```
 8   0.096992865634   0.621984975506   -2.012686321764
 8   0.654187360086   0.805811500564   -2.850513565125
 8   0.231306331839   0.959493153208   -2.862710419467
 8   0.030326249262   0.331199666083   -2.690361451646
20   0.319010725238   0.729352007583   -3.656366621580
20   0.631822947352   0.363802806128   -3.318135408724
 8   0.320033400643   0.290603648956   -3.840644897117
 8   0.714556815645   0.142465312055   -3.887019200822
 8   0.901247261776   0.732154711032   -3.965885016276
 1   0.970363175285   0.047340504551   -3.955241324170
 8   0.972130724964   0.052821654814   -4.924825538861
 8   0.269035790308   0.499033497632   -5.067170145359
 8   0.529156065524   0.892012700127   -5.297291280071
 8   0.134204596171   0.748807998142   -5.322560582843
15   0.364460649467   0.404118602398   -5.086049643666
15   0.616489337057   0.081586814227   -5.215829322446
15   0.944944756266   0.660655741981   -5.188019670846
20   0.211973010853   0.035270627222   -5.044687556253
20   0.981874445717   0.305336169261   -4.981035416489
20   0.723086511857   0.803224598005   -5.076632602007
 8   0.556538756680   0.518337313562   -5.019519888218
 8   0.494881578255   0.150154454966   -5.182955269739
 8   0.860860542088   0.469658132322   -4.970225768879
 8   0.334346437805   0.297081712242   -6.353486603661
 8   0.735027092803   0.174632685553   -6.395269967335
 8   0.853813021687   0.678003534874   -6.429427474068
20   0.640367563680   0.383995367237   -6.595397952825
 8   0.279067675818   0.328345166313   9.915091195761
 7   0.618777909757   0.381246625353   7.789820546309
 6   0.400842373106   0.411537249315   9.152972901287
 8   0.429283700955   0.535171374819   8.454946799382
 6   0.526992752507   0.348225590083   9.083203285465
 1   0.697294065043   0.507458452109   7.626315186342
 1   0.688264995518   0.322561942036   7.763715539629
 1   0.461476140401   0.214581144610   9.250014683369
 1   0.619084401035   0.406423142979   9.879519269040
 1   0.540535080955   0.329560940937   6.969310413196
 8   0.981120890988   0.338198654287   9.057774452628
 1   0.069258567450   0.332418607766   9.543451094017
 1   0.024701433849   0.367052988314   8.126442831715
 8   0.716666829035   0.114180107242   7.730132393172
 1   0.622018896903   0.032875722875   8.238477508423
 1   0.810911758036   0.176218920270   8.360638992014
 8   0.849223847419   0.732086696881   7.500188597832
 1   0.899201725007   0.795142069521   8.301145632882
 1   0.755666989392   0.755648706264   7.231157495905
 8   0.356296337509   0.871590910886   8.591073902651
 1   0.300128159376   0.912969968918   7.950266399084
 1   0.318169059426   0.871522091788   9.486744316905
 1   0.194659110888   0.070234888150   7.406272698288
 1   0.178139651164   0.193688255993   8.463491349859
 8   0.176954762973   0.166092212003   7.523980835790
-1 0 0 0
```

[Gly-2w]3w/HA



2 water molecules bridging the Gly-HA interaction.

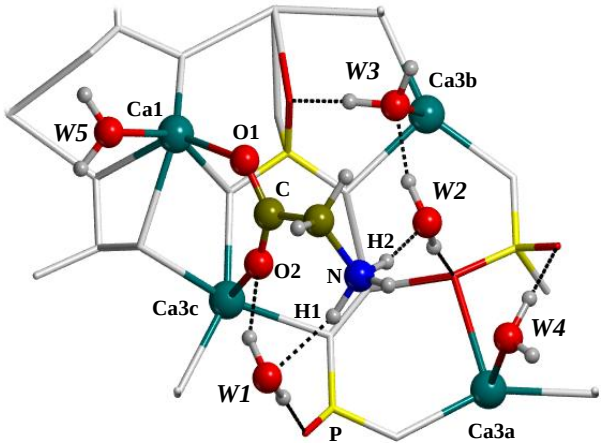
Contact between Gly and HA through W1 and W2, which interfere the O1-Ca1 and the NH2-surface interactions, respectively.

```
TITLE
[Gly-2w]3w/HA
CELL
9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 20   0.327009887593   0.666966162334   7.147785893280
 8   0.621443669502   0.779331582609   6.653286031619
 8   0.232550978607   0.977157144399   6.630390762009
 8   0.088862333235   0.393202102350   6.642930929887
 1   0.993727760574   0.046604977809   6.484898038190
 8   0.987528661974   0.053540658371   5.521686848747
 8   0.683988750343   0.578356900833   5.409581077997
 8   0.460838720265   0.199948664875   5.302768029002
 8   0.827497945909   0.347304336298   5.469847169516
 15   0.596555320545   0.681238241711   5.325450353654
 15   0.349166771596   0.011640891361   5.400705356571
 15   0.018596702652   0.439231690806   5.413981287881
 20   0.734883536236   0.052948679612   5.404480043771
 20   0.975461304796   0.798092231286   5.299199272051
 20   0.250275691848   0.290211335539   5.395153146383
 8   0.406528490723   0.576948803612   5.149866908322
 8   0.442534484797   0.914566652694   5.580835688015
 8   0.097688048278   0.630051130041   5.453270879448
 8   0.668658472045   0.806550234113   4.179055359750
 8   0.240070910266   0.941083092041   4.134661351972
 8   0.078449034268   0.395743778507   4.127952044155
 20   0.303485151578   0.706657615187   3.638939765549
 20   0.661713520333   0.375487030986   3.733515720971
 8   0.308168285251   0.284122061250   3.119708704714
 8   0.725192377090   0.135286596255   3.212274712732
 8   0.897842777883   0.697356681677   3.133811955613
 1   0.988077734850   0.042135052389   3.083014312418
 8   0.983075444253   0.038006978412   2.114137332363
 8   0.305060289391   0.524247646013   1.921192488080
 8   0.498642839195   0.879294582274   1.998366576904
 8   0.141938254759   0.719865878589   1.841553192240
 15   0.377753631402   0.407481934419   1.951115365665
 15   0.616843390371   0.068841587199   1.944834821600
 15   0.951815154335   0.643373960172   1.867153577645
 20   0.229998231396   0.028599110875   1.876864409571
 20   0.995681160540   0.296324405027   1.912996653934
 20   0.724637915174   0.795631589127   1.887712546782
```

8	0.569293224608	0.504518715955	2.071161956107
8	0.519732133522	0.163198760088	1.857474636167
8	0.860274705458	0.451688013912	1.885027699457
8	0.335943112332	0.304958799266	0.642525598223
8	0.733578337858	0.113510093156	0.732707502627
8	0.889397284948	0.696395173294	0.636502120052
20	0.640941480840	0.377288877308	0.215810415173
20	0.317105312866	0.707309900999	0.099960241373
8	0.606535471911	0.761276523013	-0.245416032664
8	0.243765447591	0.942839326243	-0.315449420139
8	0.084668249894	0.407512325063	-0.258115200835
1	0.989795547023	0.041548461685	-0.136186054515
8	0.986867099886	0.042774588345	-1.104193517546
8	0.654098907922	0.552987731434	-1.551113139013
8	0.458611280682	0.198780753522	-1.574530990472
8	0.818342521582	0.359303803075	-1.430544249134
15	0.584490874420	0.673074431728	-1.597310657493
15	0.348272588553	0.007684515433	-1.598802722474
15	0.008706242884	0.434803865778	-1.535976134341
20	0.744470340301	0.056496637886	-1.550462246262
20	0.966918982334	0.785782713722	-1.600870274901
20	0.239041291430	0.287814620673	-1.563934547046
8	0.396740894627	0.580914333722	-1.911366705918
8	0.451393749407	0.919873567748	-1.714389686707
8	0.098223242845	0.623662880586	-1.783537911545
8	0.682138962529	0.806865797147	-2.656148881856
8	0.227633637051	0.950430332407	-2.797877065257
8	0.046182331218	0.349138096670	-2.688085946194
20	0.303883434965	0.712161747984	-3.574074529927
20	0.652836075800	0.369972382139	-3.239415572703
8	0.302006426195	0.278391321376	-3.824069827510
8	0.725512821961	0.138313137482	-3.777509995166
8	0.887320582182	0.694081660550	-3.833275627092
1	0.974671465771	0.034166490398	-3.864144842530
8	0.971569474865	0.033246864928	-4.834364158760
8	0.273108145936	0.494215358559	-5.112723325912
8	0.526910390368	0.881072507389	-5.068800676668
8	0.132450391630	0.745365083707	-5.247953247148
15	0.363649903405	0.394624684561	-5.048290434343
15	0.619023180676	0.071288734817	-5.061327840268
15	0.942990188021	0.646697833014	-5.135855730807
20	0.218192884277	0.028945438848	-4.988256755039
20	0.986521714386	0.288912599357	-4.939791650425
20	0.719882470548	0.788294083580	-4.927489897670
8	0.555471611501	0.503381248617	-4.891786326354
8	0.501828281546	0.145504322231	-5.022541238056
8	0.870119491910	0.455939280525	-5.039480379780
8	0.340946611732	0.288089310313	-6.312777012873
8	0.731199910220	0.152989644628	-6.294655741055
8	0.849532597973	0.669020009640	-6.332029211615
20	0.639482265668	0.370039268638	-6.519300763383
8	0.366834678603	0.408833883650	7.714960845857
7	0.463043564232	0.183484511457	8.490098767173
6	0.398316807733	0.410905798207	8.947539242427
8	0.417244333668	0.517913879820	9.798518931768
6	0.412583329533	0.264568322150	9.525262319146
1	0.570913665478	0.278058426710	8.024778512426
1	0.493367141995	0.101112276550	8.898523538278
1	0.293131427588	0.172440122930	9.949209559152
1	0.504935390197	0.311344467466	10.321954762500
1	0.369077472916	0.117163303273	7.770916878491

```
 8    0.812377180125    0.138049562148    7.717697408033
 1    0.832262544550    0.062857148435    8.247318733495
 1    0.922290135070    0.238307237178    7.557788663649
 8    0.887308530167    0.827058746045    7.704189340824
 1    0.874470857464    0.765539383547    8.514405225460
 1    0.771584203378    0.801186546824    7.427829305272
 8    0.113841637081    0.702848956762    8.319505389764
 1    0.133617578235    0.801674371226    7.807131426231
 1    0.997818506469    0.619119309580    8.170251590210
 8    0.750796454766    0.454954029558    7.635186682144
 1    0.781410059465    0.399047824179    6.930341763005
 1    0.708235902251    0.509714138098    7.037909290994
 8    0.418300040227    0.798095481279    9.296561542746
 1    0.437552779808    0.709917065661    9.659914559455
 1    0.311890063639    0.773637134349    9.662829634092
-1  0  0  0
```

[Gly-2w]3w-SI1/HA



2 water molecules bridging the Gly-HA interaction.

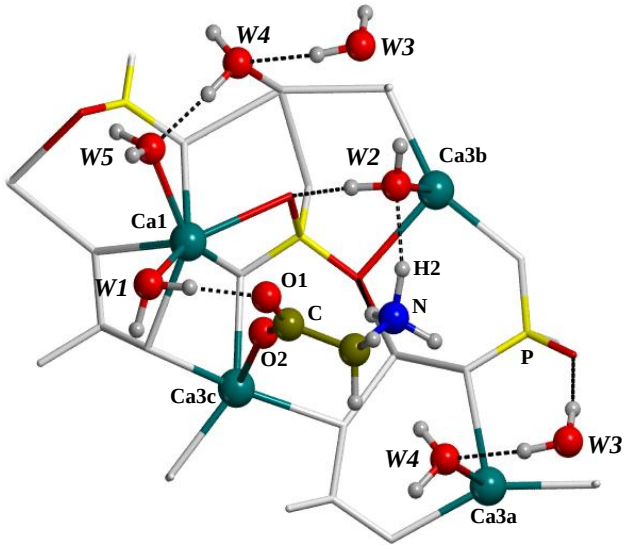
Contact between Gly and HA through W1 and W2, which interfere the NH1-surface and NH2-surface interactions, respectively.

```
TITLE
[Gly-2w]3w-SI1/HA
CELL
9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 20    0.314721251460    0.689047275955    6.993663561173
 8    0.642124838072    0.787022800670    6.508057738128
 8    0.230364487664    0.912112380610    6.590068521069
 8    0.084602349608    0.401480382761    6.630688652923
 1    0.981461126176    0.024629984459    6.537286140156
 8    0.997462604338    0.036468143892    5.581493295341
 8    0.681806224496    0.577868099139    5.150671643716
 8    0.442880221389    0.191536748244    5.514452792929
 8    0.821628300535    0.350637258779    5.439009421421
 15    0.594609299796    0.679849518686    5.207890748017
 15    0.352756796971    0.003097588046    5.407453923941
 15    0.011565576564    0.426755744141    5.312829326163
 20    0.754629402917    0.055173507788    5.250845208447
 20    0.978482647867    0.779616613831    5.202562458288
 20    0.246553204252    0.287945614309    5.390522721788
 8    0.402416197607    0.575747152470    5.214688526037
 8    0.466179945668    0.926287577730    5.425366780909
 8    0.103960919896    0.615986119605    5.084061077773
 8    0.643475199960    0.799061471303    4.003969452029
```

8	0.251855355703	0.945584475007	4.092177029298
8	0.048622476301	0.337945129538	4.190111971677
20	0.333213102990	0.727084769802	3.535528490180
20	0.633182617228	0.353449816589	3.731332811855
8	0.332902372650	0.292986612367	3.158685716152
8	0.718688457102	0.132689554275	3.104098275119
8	0.923074195220	0.744180352434	2.941209085456
1	0.981269646078	0.043808735951	2.950398634746
8	0.983596668037	0.052162154224	1.983970512349
8	0.301653143374	0.521716880078	1.973496852599
8	0.506105492181	0.884979820246	1.759960339724
8	0.146518881749	0.716029164143	1.794497838427
15	0.379177745656	0.408717096604	1.929645835280
15	0.617427565655	0.075513993959	1.798969696254
15	0.958178979772	0.650789646959	1.843944821760
20	0.224749005902	0.028985268651	1.850955920525
20	0.995689813813	0.308136442651	1.860973514608
20	0.729350401166	0.800910564027	1.766196727170
8	0.570952958067	0.510664956020	1.902790791209
8	0.514649835687	0.164166550318	1.772900728061
8	0.858237696584	0.461665266438	2.096859295951
8	0.319755043977	0.299829814262	0.662659352806
8	0.737773309993	0.137640955107	0.603683458655
8	0.891620237670	0.681927054175	0.520033444044
20	0.653387302398	0.387407698532	0.165749533693
20	0.318072023341	0.707070129000	0.025631729385
8	0.624108105894	0.777557365727	-0.387095304739
8	0.240252610746	0.939827100327	-0.349352620247
8	0.080847035073	0.420740327162	-0.295580531948
1	0.982382810473	0.033712270034	-0.209921990009
8	0.984013810399	0.036799427141	-1.178607734422
8	0.662368726109	0.565464882496	-1.695624344514
8	0.459381624591	0.204684298846	-1.508997376337
8	0.820107081421	0.372452805258	-1.558554206194
15	0.584307125973	0.678276693217	-1.699474632489
15	0.350878138096	0.013581058057	-1.593267004952
15	0.008829219285	0.438319809509	-1.637354617377
20	0.748736964215	0.061756990844	-1.657820590614
20	0.973469775212	0.784240621127	-1.670575453673
20	0.236469156851	0.284918388622	-1.581549622467
8	0.393159619506	0.577440781420	-1.822307766550
8	0.455703458202	0.928092561365	-1.726801893903
8	0.105643745524	0.623969163677	-2.012603298297
8	0.651530525944	0.803500016127	-2.863937086540
8	0.236800283832	0.963967116966	-2.826991207312
8	0.035937598691	0.331087028651	-2.666505359254
20	0.329560234996	0.731983864925	-3.637280141353
20	0.635764851125	0.364467882847	-3.297679640609
8	0.327951625986	0.293547023381	-3.814286136887
8	0.720058336347	0.143390637741	-3.876560102315
8	0.908792193266	0.737269733345	-3.947630868948
1	0.976030468571	0.050094068165	-3.938817990649
8	0.978191054071	0.055945809492	-4.908275395317
8	0.275431853956	0.500972711291	-5.041541554771
8	0.536257506515	0.894737060603	-5.309585835049
8	0.141165888703	0.750263314471	-5.285379822550
15	0.370819768401	0.406054885642	-5.065883711298
15	0.622793400139	0.084069209589	-5.210040774030
15	0.951886148388	0.663320366355	-5.157133699932
20	0.217506606521	0.037063563296	-5.015910823477
20	0.988167244451	0.308576790475	-4.959190566618

```
 20    0.729735449872    0.805627290322    -5.070431041753
 8    0.562905705386    0.520698175244    -5.012220325322
 8    0.500553310792    0.151823516197    -5.167787448043
 8    0.866353295501    0.472395133878    -4.929669290737
 8    0.339506894203    0.298334004028    -6.329495841032
 8    0.741901207719    0.179229291914    -6.381660742448
 8    0.861663212652    0.680427894811    -6.406708245414
 20    0.647332142836    0.386723071124    -6.575214324865
 8    0.322264151221    0.330485069933    7.781878264863
 7    0.514403307633    0.264440705696    9.349679601888
 6    0.396720882113    0.442355087600    8.652785750170
 8    0.408225775818    0.581354729649    8.734600886327
 6    0.483017739389    0.399956992620    9.782907647502
 1    0.613904081033    0.317826124630    8.610283664572
 1    0.554800814748    0.222598118540    10.125073855550
 1    0.404651211653    0.360627595966    10.676361949160
 1    0.601607052865    0.509487157300    10.023030822840
 1    0.405025702287    0.165898247568    8.983069124891
 8    0.169508043734    0.010571041030    8.728992649379
 1    0.199329959412    0.977496388343    7.828945544973
 1    0.185019770887    0.119826303529    8.507079818724
 8    0.822996992766    0.139202269626    7.613845089513
 1    0.842471174930    0.078303890641    8.299463435003
 1    0.929789611847    0.245829302940    7.469998882920
 8    0.868053271318    0.751988496405    7.518086201612
 1    0.942110185878    0.836466635680    8.147032235335
 1    0.768985713752    0.768339308799    7.260765881395
 8    0.120846690235    0.655219743057    8.733480084514
 1    0.107456715126    0.747212766607    9.015731181143
 1    0.008887879008    0.564017347756    8.540442977446
 8    0.778998821979    0.436316993195    7.904693331428
 1    0.780976936841    0.392373579187    6.992191696207
 1    0.792396207623    0.547502644735    7.739436937862
-1  0  0  0
```

[Gly-2w]3w-SI2/HA



2 water molecules bridging the Gly-HA interaction.

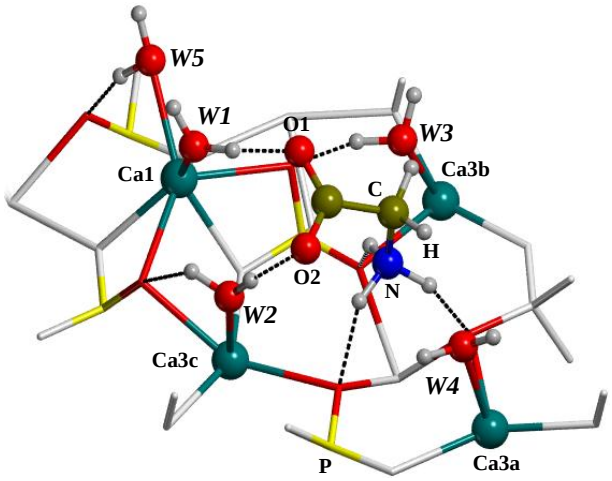
Contact between Gly and HA through W1 and W2, which interfere the O1-Ca1 and NH2-surface interactions, respectively.

```
TITLE
[Gly-2w]3w-SI2/HA
CELL
```

9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 20   0.313164733022   0.654168405819   7.152365832423
 8   0.610721992163   0.774134989596   6.635293150269
 8   0.221540915428   0.978623663291   6.501345466231
 8   0.085016798249   0.381462710549   6.536580360296
 1   0.981209043630   0.054939870276   6.454197773377
 8   0.975125055341   0.052608207313   5.486771558758
 8   0.669549047213   0.567176579807   5.431170939766
 8   0.454457171662   0.193364580333   5.163919585700
 8   0.813357488828   0.338913418653   5.562498841143
 15   0.585996537421   0.674255027813   5.313754872836
 15   0.336439381897   0.005758790511   5.280525573668
 15   0.003495298520   0.435573570087   5.447500389932
 20   0.721031136671   0.044214629810   5.343386057637
 20   0.963711918252   0.795533122965   5.287959833051
 20   0.246529344071   0.283523565244   5.397440901659
 8   0.396891379531   0.572592944560   5.094339974414
 8   0.425667319284   0.904388826152   5.441025490493
 8   0.080660293880   0.625020838102   5.658149678502
 8   0.667915544932   0.799784402976   4.182477989656
 8   0.222271958206   0.933464009109   4.045715916898
 8   0.058557878927   0.410254617856   4.058555311892
 20   0.284069071738   0.696585849679   3.613502725493
 20   0.663788242475   0.374711941553   3.705089357925
 8   0.279297964142   0.275156463880   3.072119972056
 8   0.716460519169   0.133490228313   3.182451339482
 8   0.883850580437   0.677419672981   3.149129460631
 1   0.974049880861   0.037344856780   3.057451655250
 8   0.964457581859   0.027584461104   2.091976619724
 8   0.295252887564   0.520636189049   1.863826164204
 8   0.488969238347   0.871652414695   2.023599608017
 8   0.129413337125   0.713094976453   1.793033108967
 15   0.362669751298   0.399545215700   1.926260199518
 15   0.603367734779   0.061570779255   1.940347399168
 15   0.939431341742   0.636025022251   1.821287724024
 20   0.213160467752   0.021760156819   1.823427220485
 20   0.983605763570   0.289652902064   1.882092462332
 20   0.707921311890   0.784019343290   1.880851978534
 8   0.553664197528   0.491780900870   2.097057518514
 8   0.503352427275   0.152839522869   1.865463173931
 8   0.847621547915   0.444568069570   1.745577841382
 8   0.325164992142   0.298120934635   0.610234545522
 8   0.716250488989   0.106484215489   0.703185733722
 8   0.879723754456   0.700218647598   0.649091388159
 20   0.622698447190   0.360763889627   0.186498830290
 20   0.305427346999   0.702302391977   0.075202920307
 8   0.591862513259   0.753013586430   -0.259469430695
 8   0.233323568682   0.939128399086   -0.349943364839
 8   0.073127563243   0.394862190367   -0.307643702058
 1   0.978636983450   0.039901601765   -0.176185624677
 8   0.975225061262   0.039205195123   -1.144501900026
 8   0.640817554871   0.542458307195   -1.531135059648
 8   0.445902441051   0.190569767516   -1.648370133318
 8   0.806784356187   0.348145140072   -1.463433021868
 15   0.573441155650   0.664229837937   -1.604225852096
 15   0.334369476082   0.999345745285   -1.651581696346
 15   0.997877427023   0.429281055550   -1.554903959244
 20   0.728797592427   0.045769818858   -1.558912044332
 20   0.952013918711   0.780105146252   -1.623131692910
 20   0.227721188349   0.282072071011   -1.609908327096

```
 8   0.387169641063   0.574186395757   -1.961674605710
 8   0.436338627410   0.910157816860   -1.763159982163
 8   0.084216270164   0.619407927052   -1.713237584136
 8   0.678028702150   0.798250877757   -2.642698145198
 8   0.210965563506   0.940468253914   -2.830488189512
 8   0.044377532205   0.359725336657   -2.772082535125
20   0.282583678016   0.694454232669   -3.594807706989
20   0.646435522004   0.364503659841   -3.262311854292
 8   0.277955996601   0.265944761373   -3.889404924729
 8   0.717205323643   0.128342707785   -3.785859942557
 8   0.869673422631   0.673313939850   -3.842978699085
 1   0.961967199390   0.021166844803   -3.900915175682
 8   0.956779264721   0.017887401159   -4.870595183089
 8   0.261422524061   0.484844905380   -5.215257135771
 8   0.511448136624   0.869005479520   -5.025196314686
 8   0.117631824701   0.735454321548   -5.274427730808
15   0.349030343030   0.382929015240   -5.102203643008
15   0.605945874024   0.059326442171   -5.044286259201
15   0.928309266920   0.633562839962   -5.171064446386
20   0.206258727319   0.018284647899   -5.026299263415
20   0.974738275276   0.275532556628   -4.978238735245
20   0.704081432531   0.774563573777   -4.929794034649
 8   0.540271575142   0.489127393309   -4.893466187958
 8   0.490908532444   0.136220859190   -4.992005810662
 8   0.859445066194   0.443362835422   -5.117270356317
 8   0.330565773180   0.275987981477   -6.357379409085
 8   0.714580581245   0.136748859416   -6.301788741740
 8   0.833388227583   0.657154432911   -6.347229638062
20   0.625275119184   0.355966709549   -6.539104633031
 8   0.378420611390   0.424992396065   7.639395129562
 7   0.705380575164   0.468455736705   7.877967237397
 6   0.448149202108   0.447144470794   8.773677896896
 8   0.429301056688   0.515738249568   9.779557081781
 6   0.572796505109   0.385115871071   8.906838564045
 1   0.658685345748   0.476104522026   6.927530064226
 1   0.785900008252   0.592792932764   8.113501556042
 1   0.509063746754   0.251719720365   8.725544169318
 1   0.629257930562   0.412406751982   9.897002127961
 1   0.772805393521   0.410519225203   7.719167702311
 8   0.875641641598   0.805404058797   7.684676427619
 1   0.766790879037   0.798493649922   7.425075395496
 1   0.933803935550   0.905898067063   8.219206894918
 8   0.964534990809   0.160312644744   8.514284821284
 1   0.849793592039   0.135075552995   8.471441399084
 1   0.015919517299   0.243082870186   7.784618839366
 8   0.652176887371   0.110850335895   7.581377419298
 1   0.543712829019   0.030241856770   7.974116445772
 1   0.631889653305   0.186523039686   7.053477244060
 8   0.339539116713   0.889325886278   8.332757464178
 1   0.280411785923   0.930602705280   7.662277530960
 1   0.288470656442   0.871537516066   9.202857224143
 8   0.166568335185   0.544016357052   9.248825177552
 1   0.081667731965   0.427635251992   9.199161316262
 1   0.259207788220   0.537167876120   9.679696180442
-1 0 0 0
```

[Gly-2w]3w-SI3/HA



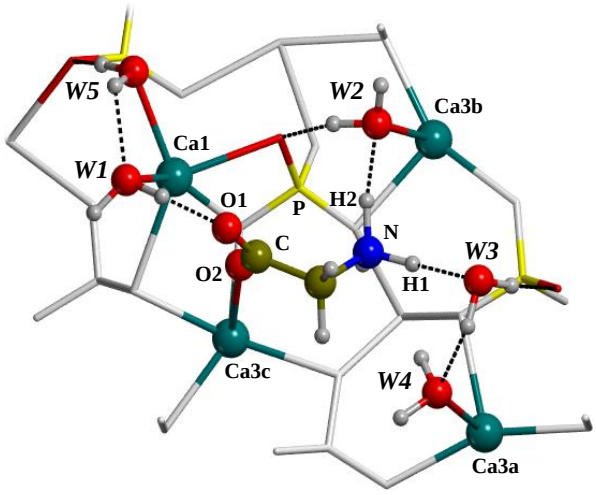
2 water molecules bridging the Gly-HA interaction.
Contact between Gly and HA through W1 and W2, which interfere the O1-Ca1 and O2-Ca3c surface interactions, respectively.

```
TITLE
[Gly-2w]3w-SI3/HA
CELL
9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 20   0.314449984725   0.693198191097   7.021146690006
 8   0.606922760133   0.767361229232   6.646787924445
 8   0.215348357638   0.948787662690   6.463914477271
 8   0.088686940890   0.404132634135   6.595402106057
 1   0.998769607173   0.051494001333   6.470298655965
 8   0.971629618613   0.044401787861   5.527947049243
 8   0.662921682312   0.563821369566   5.365043020041
 8   0.440966848640   0.194194511777   5.215577685638
 8   0.817591374820   0.342508461677   5.438390839756
 15   0.580866017745   0.672001132329   5.308277063671
 15   0.332814588902   0.004270720820   5.237939040382
 15   0.009066274786   0.437494956625   5.380379289158
 20   0.725928015432   0.047980247334   5.334845649812
 20   0.957986473742   0.788412818876   5.214994336410
 20   0.230055961510   0.281979737820   5.244595183436
 8   0.390526566119   0.570915491233   5.130019475108
 8   0.434484500449   0.913786023328   5.334424513699
 8   0.085741915765   0.628239998707   5.359189389948
 8   0.658091639366   0.797522717515   4.161147961031
 8   0.222756109011   0.938030483149   3.981598480495
 8   0.063918962530   0.389358459621   4.077039349976
 20   0.289248425640   0.697847903508   3.543257422935
 20   0.652540891396   0.369566047386   3.669938628387
 8   0.284271532323   0.273872195594   2.988650032756
 8   0.714917877397   0.129840764974   3.134411629367
 8   0.880818845800   0.683784834180   3.062397753935
 1   0.975562934520   0.035262860300   2.984440486182
 8   0.965208298749   0.028235025774   2.018928691158
 8   0.292852527237   0.518249595300   1.813333545916
 8   0.488138119660   0.871455797391   1.933435292295
 8   0.127738198491   0.711500981403   1.755675164900
 15   0.363082287444   0.399261825259   1.845141566428
 15   0.603309517197   0.061585135309   1.883983054034
 15   0.937619265959   0.635321350842   1.779196162353
 20   0.213574744201   0.020868176341   1.754927452967
 20   0.982380564213   0.289296448556   1.835432586824
```

20	0.708021620898	0.784370786422	1.841727041686
8	0.553800433398	0.493317185339	2.015260611320
8	0.503726652674	0.153599645255	1.820835642814
8	0.846529911920	0.443591681663	1.768199462274
8	0.325409372062	0.298617408224	0.529578246993
8	0.716809892063	0.108999601905	0.647315907081
8	0.877263648905	0.693188777996	0.568501537640
20	0.625841116108	0.363025162124	0.136063197257
20	0.304296526654	0.701295803368	0.014834161306
8	0.592724498848	0.753035516136	-0.313661166344
8	0.233177009852	0.936932908891	-0.406206740439
8	0.072139786500	0.395761899581	-0.356317011837
1	0.978306656383	0.038809525396	-0.228589118428
8	0.975188847028	0.038278436157	-1.196918437574
8	0.640098018816	0.542019689170	-1.598385363773
8	0.446399623014	0.189977571723	-1.693154699052
8	0.806743576298	0.348817908818	-1.523636547733
15	0.573149167143	0.664147553210	-1.659987714217
15	0.334654514419	0.998936074817	-1.706196881219
15	0.997658519595	0.428783506979	-1.615620774769
20	0.729004751663	0.045885461716	-1.614117268971
20	0.951922577580	0.779188837447	-1.683902785670
20	0.227530314382	0.281395897760	-1.672997558723
8	0.386537720688	0.574146316020	-2.009916316356
8	0.436460272600	0.909700688215	-1.826284624246
8	0.084734771034	0.618675719314	-1.793523155655
8	0.676824718606	0.798103467453	-2.702591326319
8	0.211215219357	0.941360319490	-2.884341677521
8	0.042933588094	0.356157289188	-2.818826198352
20	0.284301217511	0.695421818633	-3.655074870518
20	0.645261633017	0.364001135801	-3.320372381538
8	0.280669963157	0.266752855479	-3.943697763230
8	0.716876423202	0.128269151562	-3.845220309955
8	0.870040017580	0.674422262999	-3.902306772091
1	0.962560582366	0.022010579452	-3.954272371528
8	0.957646312279	0.018912383896	-4.924024648329
8	0.261195757062	0.484561430023	-5.263966507780
8	0.512081917337	0.869398214767	-5.093624630932
8	0.118214930596	0.735624816459	-5.327278455233
15	0.349688597723	0.383378603271	-5.160339544250
15	0.606309569319	0.059714853646	-5.107205401682
15	0.928828949342	0.634083730680	-5.226208946200
20	0.206610193547	0.018560160385	-5.082725902591
20	0.974715803807	0.276000126255	-5.034295748930
20	0.705023894046	0.775477990849	-4.988177776039
8	0.540991583005	0.490258641538	-4.961543163487
8	0.491074756217	0.136377831480	-5.056731160473
8	0.859477901070	0.443803472159	-5.168682823079
8	0.330506303356	0.276314303634	-6.415745463173
8	0.715433246038	0.137728066485	-6.361638618786
8	0.834523352323	0.657850847281	-6.406273384418
20	0.625949204966	0.356705097935	-6.598909370283
8	0.401522508107	0.218286616788	9.623777012459
7	0.652694547884	0.373467314770	7.502886874764
6	0.521411371728	0.367267255096	9.621189314984
8	0.518721610705	0.494838898484	9.974853917705
6	0.683125135884	0.393844003573	8.971834482974
1	0.656404438492	0.474340299785	7.024365980298
1	0.737173891621	0.354429043240	6.942832075887
1	0.713953610706	0.300595174214	9.292325846787
1	0.785598736509	0.518983984697	9.141805632826

```
 1   0.538883005759   0.274337499610   7.263724617881
 8   0.693939674087   0.085158333676   7.712867723729
 1   0.576715952086   0.023643356595   8.012503871173
 1   0.753558452119   0.054827052650   8.332955182393
 8   0.228915766267   0.254666372930   7.650454965785
 1   0.269698012111   0.227228381171   8.464026969742
 1   0.169492085117   0.311713801905   7.900033145728
 8   0.368981797490   0.933230880727   8.452716491033
 1   0.304224201923   0.954306182463   7.712387295226
 1   0.385594566564   0.018474437372   9.114797169697
 8   0.312870961513   0.589706688091   9.166677478586
 1   0.292902960645   0.639386165277   9.938141577505
 1   0.383131000241   0.543883127629   9.507628455003
 8   0.868517463319   0.759804248298   7.553359644672
 1   0.936323597626   0.837740870517   8.233334971787
 1   0.764453844277   0.765529112879   7.456297222574
-1  0  0  0
```

[Gly-3w]2w/HA



3 water molecules bridging the Gly-HA interaction.

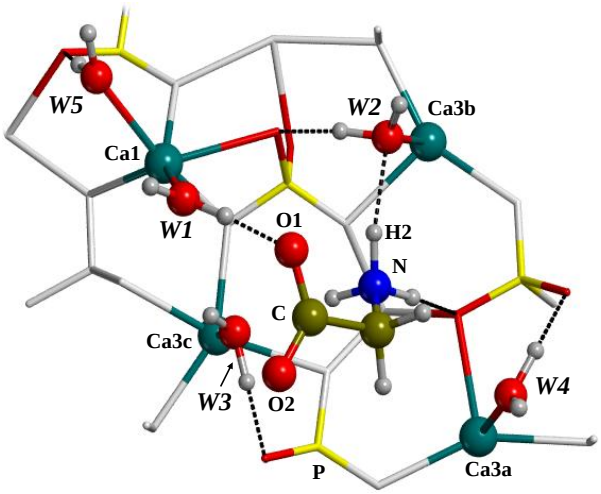
Contact between Gly and HA through W1, W2 and W3, which interfere the O1-Ca1, NH2-surface and NH1-surface interactions, respectively.

```
TITLE
[Gly-3w]2w/HA
CELL
9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 20   0.316635454545   0.665071809363   7.077098838932
 8   0.610725968739   0.774106887467   6.583209501275
 8   0.215471964084   0.975349360019   6.472853938796
 8   0.077496425021   0.385282152328   6.564018155390
 1   0.981673653956   0.056376973363   6.454086511612
 8   0.971645637451   0.052015527347   5.489865096852
 8   0.666060391347   0.565867219927   5.364812622031
 8   0.445464299818   0.195604434425   5.131372194900
 8   0.809540698470   0.339136315516   5.486966256123
 15   0.584274817904   0.673404207776   5.257519784016
 15   0.331493445660   0.007657930097   5.249322303321
 15   0.999750089845   0.435404348375   5.406318887333
 20   0.718490600493   0.043607471192   5.279928002051
 20   0.959518658445   0.793939689832   5.240952205530
 20   0.238930308865   0.287366598089   5.342699392764
 8   0.394493617232   0.575356467796   5.053956734872
 8   0.424168766834   0.908894536666   5.394795640609
```

8	0.079364620642	0.625863680410	5.552329311414
8	0.665366091289	0.800184350688	4.129613088599
8	0.217966727371	0.933853405551	4.009041789977
8	0.059451868840	0.402699173813	4.064091090266
20	0.280699302146	0.697597853108	3.571653100288
20	0.656014345020	0.373014371024	3.664641698487
8	0.275840495904	0.274963340792	3.021363309936
8	0.713288384678	0.133067518276	3.129732796611
8	0.880235720618	0.679657151552	3.092981881509
1	0.970481956189	0.035603291871	2.997141335283
8	0.960920904872	0.027385766970	2.031528267588
8	0.290391517430	0.520207710370	1.821703538403
8	0.485085341464	0.871740160745	1.972579804570
8	0.125438181391	0.712630004140	1.750517102905
15	0.358449135512	0.399506619271	1.875918531165
15	0.599785971066	0.061642237707	1.890268652290
15	0.935383865807	0.635491050397	1.778712872294
20	0.209966909062	0.021636419873	1.782603287556
20	0.980118831311	0.289523875333	1.842957881363
20	0.704431693841	0.783699693161	1.828084471190
8	0.549480899055	0.492071020140	2.043910759585
8	0.499956093460	0.153219163661	1.822518131717
8	0.844100461915	0.443895473442	1.729949048968
8	0.321025894216	0.298284086666	0.559932459347
8	0.712416241195	0.106895476282	0.651835343063
8	0.874583489755	0.696587537094	0.592333254663
20	0.620097568482	0.361662377128	0.143167381478
20	0.301395914462	0.702079539993	0.028731085075
8	0.587990930671	0.752879261522	-0.308227449573
8	0.229562574385	0.938862724859	-0.393002108691
8	0.068980084754	0.394844098284	-0.351243020255
1	0.974995547459	0.039836839656	-0.223458856255
8	0.971138066719	0.038709975588	-1.191691145458
8	0.636686192694	0.542210177858	-1.580936214375
8	0.442228078261	0.190464463012	-1.691251505150
8	0.803050681469	0.348390990035	-1.510209508985
15	0.569379123383	0.664004293272	-1.653032011872
15	0.330534057457	0.999269553010	-1.695443406373
15	0.994096311628	0.429203889198	-1.601075164645
20	0.724842269926	0.045595757345	-1.607304185868
20	0.948050508928	0.779704587807	-1.671293252673
20	0.223756118287	0.281667201633	-1.657551449697
8	0.383069534209	0.573921338573	-2.008815601473
8	0.432342057609	0.909934329230	-1.810177946420
8	0.080640879633	0.619314298152	-1.762230748835
8	0.673848931114	0.798030876475	-2.691836248356
8	0.207020368137	0.940704648156	-2.873760309517
8	0.040407609563	0.359245378092	-2.816619943869
20	0.278815805617	0.694223979040	-3.641984098573
20	0.642587343320	0.364293892287	-3.308551682759
8	0.273939576749	0.265765693063	-3.936995058979
8	0.713390392112	0.128345358019	-3.832653605607
8	0.865779227883	0.673088473418	-3.890107281089
1	0.957914018555	0.020759334618	-3.947773172994
8	0.952825653492	0.017582548625	-4.917501992460
8	0.257588824083	0.484702406152	-5.262959006313
8	0.507697240939	0.868908974726	-5.071944746344
8	0.113855766978	0.735395238983	-5.320133763164
15	0.345152881290	0.382739993437	-5.149692423592
15	0.602107335360	0.059216131974	-5.090839996611
15	0.924522948566	0.633383587160	-5.217803734078

```
 20    0.202409002012    0.018130363324    -5.071647395596
 20    0.970962477990    0.275293614894    -5.024077811197
 20    0.700163693909    0.774262864632    -4.977895709755
 8    0.536376332568    0.488854631508    -4.940307340885
 8    0.487010940160    0.136040120066    -5.038007442744
 8    0.855777202414    0.443216227206    -5.164012929610
 8    0.326705482792    0.275779824067    -6.404595853933
 8    0.710698389553    0.136671495810    -6.348472852619
 8    0.829574910952    0.656900190860    -6.394196740895
 20    0.621480506102    0.355750038319    -6.585669515489
 8    0.367850465133    0.428668017272    7.634685476541
 7    0.687163691809    0.453495021120    7.956326246870
 6    0.424585160983    0.427288813033    8.786856407355
 8    0.398378640641    0.479259908709    9.862705444598
 6    0.543922595483    0.358903585849    8.873566151392
 1    0.652653831598    0.443256503102    6.955409415913
 1    0.747121286122    0.581023778172    8.119605390320
 1    0.480632816394    0.228380855711    8.580733564053
 1    0.591456341875    0.371888428839    9.889172422805
 1    0.777987164740    0.420129899798    8.115855468743
 8    0.863435300342    0.788839299127    7.609027877601
 1    0.758794321752    0.793862514901    7.339131329417
 1    0.924380485281    0.872372205504    8.275541682349
 8    0.917482502861    0.363311456562    8.757569761970
 1    0.835282426384    0.245716278973    8.817262178324
 8    0.672843984168    0.101717504006    7.560263615762
 1    0.559128602806    0.030999230811    7.917348740227
 1    0.675489720084    0.198030186739    7.158055907796
 8    0.360505333169    0.911349225690    8.272668548808
 1    0.289916449519    0.942142175044    7.661406730147
 1    0.304708876621    0.858739694174    9.101851749380
 8    0.217375577941    0.613318128608    9.362074843044
 1    0.102036212371    0.526664842537    9.496189353930
 1    0.283408411365    0.563510724791    9.718229427778
 1    0.982205290623    0.366792556400    7.933473597843
-1  0  0  0
```

[Gly-3w]2w-SI1/HA



3 water molecules bridging the Gly-HA interaction.

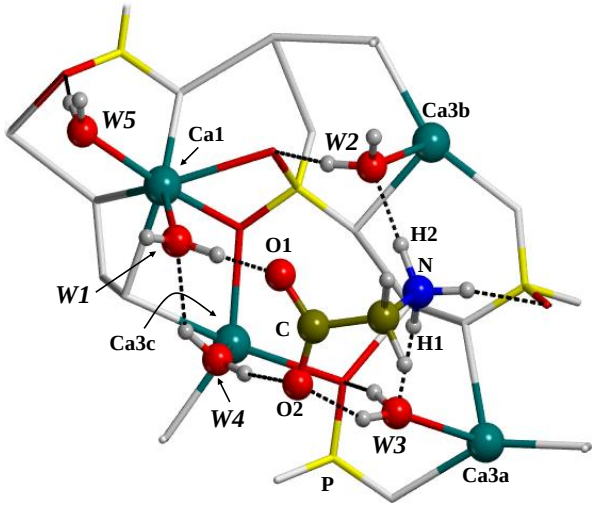
Contact between Gly and HA through W1, W2 and W3, which interfere the O1-Ca1, NH2-surface and O2-Ca3c interactions, respectively.

```
TITLE
[Gly-3w]2w-SI1/HA
CELL
```

9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 20   0.306690195046   0.673188149041   7.218020591565
 8   0.602570842382   0.769686960287   6.673972474377
 8   0.196855975632   0.967139349704   6.556980629324
 8   0.068026230797   0.386513661958   6.682999856267
 1   0.958297356173   0.038276244228   6.378885619011
 8   0.954786937967   0.036300372018   5.409727819512
 8   0.653977195833   0.567707548219   5.321889868483
 8   0.432159634508   0.192738881207   5.253676131020
 8   0.804527064530   0.342033534673   5.520543162520
 15   0.565291137937   0.668265201360   5.345895771912
 15   0.321887779960   0.004606391115   5.388001028729
 15   0.995805704378   0.434704853516   5.474725867072
 20   0.707089354801   0.041399311703   5.404689817788
 20   0.947609671352   0.781426255023   5.314754668419
 20   0.212919442627   0.276677624457   5.245356968325
 8   0.373760750469   0.562027915825   5.297980750083
 8   0.418523090474   0.912043093853   5.651530672368
 8   0.078335185159   0.625199489234   5.557887063562
 8   0.617379382689   0.789701155295   4.161609092146
 8   0.217698082918   0.929174300798   4.106387836104
 8   0.052837435900   0.392469490475   4.158394655151
 20   0.285163861973   0.700210809140   3.663892546735
 20   0.638395930337   0.367343819489   3.723903241418
 8   0.276113125205   0.273115665256   3.044565925339
 8   0.699320641849   0.128121603779   3.216581650060
 8   0.873148612339   0.690115191362   3.131211745563
 1   0.959173431319   0.031342858534   3.082965848960
 8   0.954604900482   0.029052451465   2.113353496696
 8   0.281526631204   0.517869895523   1.907611502767
 8   0.473963200631   0.872971714584   1.974445666555
 8   0.117451693877   0.710544586266   1.850112673028
 15   0.352652367434   0.399669329000   1.904167739482
 15   0.591215841546   0.062433729011   1.942419984778
 15   0.927685996636   0.636227231869   1.864709321447
 20   0.202563271809   0.018287143792   1.864928258061
 20   0.971089779444   0.289830681054   1.915830808773
 20   0.697129803718   0.785592326845   1.906717226800
 8   0.543462333643   0.494422835485   2.064136052752
 8   0.493245649017   0.155940634500   1.867352764573
 8   0.835135801059   0.444422003130   1.877634808236
 8   0.313440243547   0.299903811577   0.588537243671
 8   0.708058661084   0.110155464238   0.727938113508
 8   0.866812759316   0.691324326452   0.638633530215
 20   0.616535811239   0.366982669081   0.204630017981
 20   0.292346583202   0.700647610324   0.095145491676
 8   0.582103818237   0.754106132192   -0.244694978834
 8   0.220805885904   0.936801475276   -0.322175941579
 8   0.060193829471   0.397935895061   -0.271363272302
 1   0.966328279957   0.037344396064   -0.152085478694
 8   0.962748805847   0.037279138263   -1.120216763648
 8   0.630039855193   0.544641696300   -1.539116774803
 8   0.435418656783   0.190829180483   -1.603681040795
 8   0.795049245470   0.350690330738   -1.447980393257
 15   0.561251904325   0.665344765890   -1.593366819706
 15   0.323473605274   0.999878722664   -1.616425792737
 15   0.985760327527   0.428776872639   -1.541764500858
 20   0.718115087762   0.047496819861   -1.543901945950
 20   0.941415365143   0.779201016780   -1.608233886358
 20   0.215138115325   0.280724688390   -1.598687527634

```
 8   0.374101142335   0.573954229872   -1.926294228042
 8   0.425314753683   0.910678466922   -1.737562645480
 8   0.074000742472   0.618321907245   -1.747139299479
 8   0.661806020754   0.799176277898   -2.645088425923
 8   0.200965309301   0.943071577967   -2.802010345641
 8   0.028147435118   0.350965396966   -2.724664525675
20   0.276179363755   0.699542330121   -3.578678392006
20   0.631807548283   0.364217471396   -3.248454554809
 8   0.273965185578   0.269295940549   -3.857233733636
 8   0.703989386095   0.129812468657   -3.776046869856
 8   0.860078507077   0.679342038586   -3.831673602931
 1   0.951137589772   0.024461212581   -3.872661514785
 8   0.947264891824   0.022403166150   -4.842724907197
 8   0.249435774275   0.485708037715   -5.163314901131
 8   0.501649867967   0.871649695648   -5.042714745450
 8   0.107728869195   0.737081283358   -5.246826840613
15   0.339184017980   0.385537855668   -5.079025636113
15   0.595148361241   0.061933629462   -5.047335872052
15   0.918253501499   0.636693465310   -5.146515146373
20   0.195164990562   0.020273153021   -5.001558954658
20   0.963038144484   0.278691539851   -4.954945442287
20   0.694928776941   0.778477033659   -4.923373169138
 8   0.530717046602   0.493500189139   -4.900541031478
 8   0.479236570485   0.137743813514   -5.003063783006
 8   0.847422451601   0.446172229011   -5.076750498821
 8   0.318394954680   0.278508549525   -6.337176403170
 8   0.705614353451   0.141297491179   -6.293257851133
 8   0.824893472791   0.660366608760   -6.335078744605
20   0.615320650609   0.359697137935   -6.527998995948
 8   0.504524374024   0.420957617653   9.934859142907
 7   0.642629931629   0.374995167938   7.697601861663
 6   0.471190464522   0.272778014457   9.739907475148
 8   0.349090075343   0.140454294342   10.135583560420
 6   0.599280517940   0.258985489842   8.848814082837
 1   0.701205355403   0.497670417419   7.994100417770
 1   0.715414497419   0.361421769652   6.963136984878
 1   0.549651937918   0.133848867506   8.457470436970
 1   0.712835013205   0.292967467979   9.407025547533
 1   0.535602436651   0.351562450114   7.212069355077
 8   0.817480217358   0.127385851656   7.651818770636
 1   0.815362753846   0.092509100235   8.560140881392
 1   0.923482864394   0.235347548476   7.487656429913
 8   0.843227790440   0.736761406015   7.635737370802
 1   0.900327026957   0.794971357566   8.437259601606
 1   0.745272690908   0.753630847917   7.478133264900
 8   0.263001328551   0.846841223551   8.669750364447
 1   0.229740800212   0.896899932334   7.935198641860
 1   0.298269205152   0.931461544145   9.374463075349
 8   0.324666591428   0.546783921130   9.220092989747
 1   0.273884247510   0.557657375611   10.025981481390
 1   0.398158441725   0.502331450850   9.539866195113
 8   0.278219914664   0.260088579652   7.507570135970
 1   0.250809691180   0.287284582496   8.367006754143
 1   0.249799707622   0.142544864993   7.499698302061
-1 0 0 0
```

[Gly-4w]1w/HA



4 water molecules bridging the Gly-HA interaction.

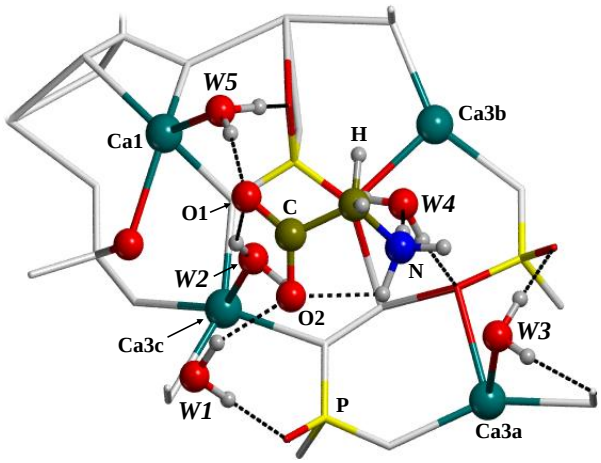
Contact between Gly and HA through W1, W2, W3, and W4, which interfere the O1-Ca1, NH2-surface, NH1-surface, and O2-Ca3c interactions, respectively.

```
TITLE
[Gly-4w]1w/HA
CELL
9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 20   0.291671644859   0.679123659815   7.022340831988
 8   0.585746473476   0.766711578052   6.628826022866
 8   0.177901870232   0.945316845250   6.444633219800
 8   0.051908388235   0.399383184144   6.684889571619
 1   0.956241521726   0.040266238206   6.518885705649
 8   0.934860665763   0.035739494261   5.567367305335
 8   0.638933784501   0.559857306656   5.333074014889
 8   0.417792277004   0.179321809999   5.253031779871
 8   0.788175259131   0.334814452162   5.401406955361
 15   0.553330110132   0.663004399266   5.307997170077
 15   0.297657869319   0.990215788526   5.245424568881
 15   0.977933918287   0.428926012909   5.384796830772
 20   0.686907456035   0.037372448890   5.358682260724
 20   0.926609421229   0.780656198058   5.190447964811
 20   0.200197292544   0.268769922699   5.310300344323
 8   0.361921843775   0.557615798757   5.213438972549
 8   0.391754338018   0.892394337543   5.332127552155
 8   0.055635323910   0.619876524152   5.339514908205
 8   0.617360572212   0.786645213267   4.135790512692
 8   0.190371464316   0.933173005999   3.978105292912
 8   0.040886037523   0.378674014061   4.140624533262
 20   0.263538285747   0.686183288114   3.556180578083
 20   0.619736692104   0.360842490849   3.686786613744
 8   0.264321105128   0.268058122612   3.047519592658
 8   0.683569956452   0.118826374895   3.145974959156
 8   0.852715230094   0.682909639191   3.036608068142
 1   0.947316703549   0.025413579287   2.999183003862
 8   0.939310423338   0.022317151902   2.032385214056
 8   0.261812445681   0.506822321959   1.844402203010
 8   0.457146663906   0.862999506615   1.918251181978
 8   0.099078347510   0.702347324938   1.778540314602
 15   0.335052569066   0.390370073667   1.874764918206
 15   0.574464866089   0.052914778985   1.880805952257
 15   0.909145817131   0.627317663696   1.793893465510
 20   0.186488398674   0.013315987514   1.754723878132
```

20	0.953408829695	0.281444526992	1.874446871740
20	0.680672530464	0.778564996623	1.834315276267
8	0.526201827081	0.487463626530	1.997671993265
8	0.476584936097	0.146579178085	1.803756085100
8	0.817753994111	0.435611168154	1.837488071536
8	0.293357799373	0.287527960528	0.568399978801
8	0.690785407249	0.099668452802	0.662698375787
8	0.847478970885	0.678832828121	0.550783544401
20	0.599737469590	0.359606065414	0.150961578028
20	0.274588260399	0.691249395760	0.025571447865
8	0.564341824997	0.744710587676	-0.310691802385
8	0.201929317997	0.925037175041	-0.399966819724
8	0.041892938454	0.390370822301	-0.322575432567
1	0.947344638283	0.025929288328	-0.206044557588
8	0.945728301519	0.026716412871	-1.174426253189
8	0.610644167179	0.534831334314	-1.612715841196
8	0.416285771753	0.181651623931	-1.651947400479
8	0.776415566903	0.342378182339	-1.504935663410
15	0.542702962170	0.656222581233	-1.661014104973
15	0.306339844303	0.990559022545	-1.683644687477
15	0.966852288193	0.418294669343	-1.603033130522
20	0.702455037232	0.039522869479	-1.613441478227
20	0.924425315137	0.769144915487	-1.679725993123
20	0.197548089476	0.271763573685	-1.639481402660
8	0.355146059921	0.565010274965	-1.984161296612
8	0.409621723678	0.902999925225	-1.799417810814
8	0.056225787012	0.607238314737	-1.846355346428
8	0.642451064561	0.790023726328	-2.715152022727
8	0.185176068826	0.933168475034	-2.878495997055
8	0.005535504804	0.334178698987	-2.760638075299
20	0.260397140929	0.693774637266	-3.647577545908
20	0.612071631004	0.353892914800	-3.309584208326
8	0.257890626988	0.260679159387	-3.903292317906
8	0.684399185048	0.121072308774	-3.844554252583
8	0.843574094675	0.673623578494	-3.902012095142
1	0.933117648844	0.016223726498	-3.934608314877
8	0.929375182433	0.014750736653	-4.904674926439
8	0.231087026552	0.477033897367	-5.196730458900
8	0.484462719598	0.863456004681	-5.126682385828
8	0.089878740231	0.728335432454	-5.320611152561
15	0.321245398020	0.377120937889	-5.125245873587
15	0.577123116530	0.053717488302	-5.124024056294
15	0.900462611231	0.628594488227	-5.210931360881
20	0.176633539456	0.011783388845	-5.067510553308
20	0.944697178909	0.270692446701	-5.009267377107
20	0.677332573355	0.770345511255	-4.991502533110
8	0.512939405172	0.485415831921	-4.959648490933
8	0.460411679679	0.128572108800	-5.084410345980
8	0.828820757828	0.438013619339	-5.125403573534
8	0.299341379330	0.270579653499	-6.388710625931
8	0.688667536981	0.134351658890	-6.362026900083
8	0.806706610756	0.651330992953	-6.402204484544
20	0.597239271952	0.352048777155	-6.590504984020
8	0.556115660705	0.493570807511	9.749616604190
7	0.811849233780	0.441273627240	8.191668559877
6	0.565073333338	0.364837291765	9.582656404560
8	0.447632706395	0.218414967374	9.359039978759
6	0.744124461328	0.391939319981	9.573593375085
1	0.819167626068	0.553686604850	7.923319900426
1	0.924317793715	0.446026254943	8.018303017861
1	0.744403487245	0.278171436936	9.832395206752

```
 1    0.823185813619    0.491859337876    10.258046281940
 1    0.734895281311    0.348896365881    7.520136833965
 8    0.578683963708    0.128562070390    7.322206868347
 1    0.518856965947    0.121442805187    8.148632502666
 1    0.527868714278    0.170943572407    6.669962796177
 8    0.835469650745    0.743923115159    7.558343239673
 1    0.900781541175    0.824951044991    8.230054317382
 1    0.729003287356    0.746909870085    7.412623685086
 8    0.220600803120    0.827921309971    8.553538011244
 1    0.200992933449    0.888801295278    7.775666163269
 1    0.276243706040    0.912129378872    9.229125712077
 8    0.326157375987    0.564695809390    9.056224671063
 1    0.288296322734    0.581544812428    9.907821501488
 1    0.413248022087    0.534618330811    9.283131169561
 8    0.228429138765    0.256143408192    7.684904151255
 1    0.205028462396    0.330662805282    8.192505906648
 1    0.296107208544    0.229465719126    8.271973725094
-1  0  0  0
```

[Gly-5w]0w/HA



Gly adsorption onto HA-5w surface.

5 water molecules bridging the Gly-HA interaction.

No contact between Gly and HA

```
TITLE
[Gly-5w]0w/HA
CELL
9.3066655000 9.3066655000 1.0000000000 90.000000 90.000000 120.000000
COORD
 8    0.359104508993    0.154944520544    13.953987672050
 7    0.679569384368    0.291678204228    13.769837059500
 6    0.432090312350    0.303379448984    14.351335069850
 8    0.374956862794    0.399990533371    14.416499429280
 6    0.617106461235    0.371100002134    14.729315135030
 1    0.710134599214    0.361530390917    12.842275890820
 1    0.779406345736    0.282565342340    14.070493871590
 1    0.626716487016    0.335410178313    15.752631765070
 1    0.690403232670    0.505556995848    14.624158241160
 1    0.580423308070    0.174449650260    13.595932012870
 20    0.282651280008    0.677044359989    11.044874275700
 8    0.614382903229    0.764892157652    10.672205186520
 8    0.193083378176    0.886713591192    10.730687522910
 8    0.062176283004    0.393765214950    10.766780001430
 1    0.974721017993    0.018357519287    10.706545174400
 8    0.969239162650    0.019415643681    9.738191120858
 8    0.649318254065    0.554260940176    9.308469560122
```

8	0.409071322061	0.170990618411	9.692782204899
8	0.792722802640	0.327221214384	9.573264402046
15	0.566659355217	0.662048605898	9.372965662552
15	0.317045188145	0.981757084751	9.572142234005
15	0.983443521485	0.410118025986	9.442763384290
20	0.724796391024	0.034280163464	9.479833093557
20	0.944679571674	0.763569936807	9.301078082528
20	0.215402681104	0.270872603332	9.447990380596
8	0.373827846976	0.561641640730	9.301649182690
8	0.434503645332	0.908675552551	9.566690104038
8	0.069336503558	0.598556009833	9.188560338256
8	0.624561353821	0.783355408875	8.176267787531
8	0.221154460859	0.928740056778	8.228868825657
8	0.022667046973	0.323569682279	8.318513885288
20	0.302883380166	0.709240131024	7.660285608912
20	0.602201545048	0.330838374162	7.869493424515
8	0.305558309290	0.273322280333	7.269347539363
8	0.689232628558	0.111706825221	7.266260837440
8	0.893852765903	0.725124252568	7.053693225943
1	0.953495944181	0.025394360898	7.083589489276
8	0.957081155290	0.034542899906	6.117425659999
8	0.273276568686	0.502332455077	6.101947206364
8	0.477718474677	0.864696938020	5.906504690416
8	0.117442575431	0.696381372627	5.920398881447
15	0.352294221260	0.390740898466	6.050748382525
15	0.589647693410	0.055327222987	5.952694984451
15	0.928875565024	0.630771130225	5.966121584117
20	0.196733707820	0.010059031643	5.974385153893
20	0.967048342705	0.289288959201	5.997559580138
20	0.701391964058	0.783418070795	5.908420893591
8	0.543813966944	0.493150259700	6.040643330313
8	0.486793834402	0.143979956473	5.909554458330
8	0.828848931216	0.441838254159	6.230469389973
8	0.295206015901	0.282771334029	4.778095812876
8	0.710335529771	0.116245155432	4.758930555222
8	0.862745698024	0.661137468700	4.638674903833
20	0.623521889517	0.367744515041	4.298491445627
20	0.289997746782	0.687591783455	4.157675092539
8	0.595272641100	0.757230184124	3.750442198813
8	0.211612454257	0.920533550885	3.778840520761
8	0.052780450794	0.400941974526	3.837890509151
1	0.954439904726	0.014501670408	3.924055994290
8	0.956097156028	0.017707964035	2.955403485650
8	0.633348553106	0.545310294134	2.434075211847
8	0.430813156771	0.184680797439	2.615498989230
8	0.791050172620	0.351470377437	2.584335442232
15	0.556124036946	0.658861762265	2.433244810033
15	0.322439964728	0.993626769942	2.535377206783
15	0.979977749324	0.418345287790	2.499408315440
20	0.720360077729	0.042346705837	2.483165889701
20	0.944783682863	0.764888313062	2.457689344274
20	0.208262004222	0.265960573928	2.546316635948
8	0.364989506151	0.558736311913	2.300926958086
8	0.427396302645	0.908178789849	2.411220778309
8	0.076166486411	0.603935421377	2.123143553467
8	0.625112442274	0.784928789832	1.275770454738
8	0.208691505108	0.943063944171	1.298695387371
8	0.007275369111	0.311637547403	1.466181943300
20	0.299883473115	0.712263863998	0.495207776665
20	0.607714620530	0.344716435396	0.834634015143
8	0.298633956514	0.273312824584	0.316376747558

```
 8   0.691379828056   0.123854830915   0.259213951778
 8   0.880505296706   0.717556948442   0.181323047250
 1   0.947261060453   0.030080630353   0.192135202812
 8   0.949447256179   0.036009814660   -0.777307960075
 8   0.246780714836   0.481257011844   -0.908883894683
 8   0.507426711571   0.874834515082   -1.170264550025
 8   0.112401541164   0.730471847455   -1.161501502579
 15   0.342103498334   0.386261441358   -0.932725257895
 15   0.594064778973   0.064208758932   -1.074035772394
 15   0.923169686500   0.643490831962   -1.029672668269
 20   0.188807496369   0.017220594613   -0.886338700063
 20   0.959462143611   0.288624863886   -0.826099657862
 20   0.700890560647   0.785711021403   -0.935497963169
 8   0.534200012769   0.500740503696   -0.874699849706
 8   0.471876574861   0.132042909323   -1.034626217688
 8   0.837848588955   0.452609746226   -0.800077828117
 8   0.311144773184   0.278845586613   -2.198007200961
 8   0.713108570017   0.159037752023   -2.246729860767
 8   0.832465627705   0.660348578380   -2.276779092286
 20   0.618407710138   0.366741894440   -2.442500776727
 8   0.430392602675   0.675376685118   12.911892085450
 8   0.040501956536   0.986172586186   12.633733254120
 1   0.421492385509   0.594322036403   13.578031654320
 1   0.131199167256   0.054727314067   13.244341278870
 1   0.530262458320   0.704391287346   12.376817639600
 1   0.095391996883   0.947108603085   12.011479033840
 8   0.811317328590   0.122947503659   11.885888851150
 8   0.333239686988   0.330569201799   11.623747199330
 1   0.912711382696   0.229295677543   11.656237360220
 1   0.305534146394   0.340248271601   12.543965086170
 1   0.854102450073   0.056730289576   12.294021643500
 1   0.378259803028   0.256478518096   11.644063543800
 8   0.754963219057   0.477209427453   11.613895214610
 1   0.671998533372   0.501984763768   11.259607176180
 1   0.760154236980   0.407154155498   10.868907006930
-1 0 0 0
```

Table 1. Absolute electronic energies (E) of the computed structures, in Hartrees. Relative energies (ΔE_{rel}), of the structures belonging to the Gly/5w/HA system, in kcal mol^{-1}. The notation [Gly-Xw]Yw/HA refers to a total of X+Y H_2O molecules of which X bridge Gly through the HA surface whereas Y interact only with the HA surface.

	structure	E (Hartrees)	ΔE_{rel} (kcal mol^{-1})
fragments	5w	-381.99201545	
	Gly	-284.28424845	
	5w/Gly	-666.29052606	
	HA	-8742.20219147	
	5w/HA	-9124.34623291	
	Gly/HA	-9026.47547860	
0 water at Gly/HA interface	[Gly-0w]5w/HA	-9408.70916978	0.0
1 water at Gly/HA interface	[Gly-1w]4w/HA	-9408.70726715	1.2
	[Gly-1w]4w-SI1/HA	-9408.69928672	6.2
	[Gly-1w]4w-SI2/HA	-9408.68988017	12.1
	[Gly-1w]4w-SI3/HA	-9408.68781288	13.4
2 water at Gly/HA interface	[Gly-2w]3w/HA	-9408.69632501	8.1
	[Gly-2w]3w-SI1/HA	-9408.69194824	10.8
	[Gly-2w]3w-SI2/HA	-9408.68869168	12.9
	[Gly-2w]3w-SI3/HA	-9408.67854284	19.2
3 water at Gly/HA interface	[Gly-3w]2w/HA	-9408.69291030	10.2
	[Gly-3w]2w-SI1/HA	-9408.69076107	11.6
4 water at Gly/HA interface	[Gly-4w]1w/HA	-9408.67477203	21.6
5 water at Gly/HA interface	[Gly-5w]0w/HA	-9408.64832359	38.1

Table 2. Absolute electronic energies (*E*) of the single-point energy calculations for the extraction of one H_2O molecule, in Hartrees. Reaction energies (ΔE_r) of the water extraction process, in kcal mol^{-1}.

[Gly-0w]5w/HA → [Gly-0w]4w/HA + W		
Extracted water W	E [Gly-0w]4w/HA (Hartrees)	ΔE_r (kcal mol^{-1})
W1	-9332.280751	31.1
W2	-9332.270294	37.6
W3	-9332.266350	40.1
W4	-9332.261874	42.9
W5	-9332.253153	48.4
[Gly-1w]4w/HA → [Gly-1w]3w/HA + W		
Extracted water W	E [Gly-1w]3w/HA (Hartrees)	ΔE_r (kcal mol^{-1})
W2	-9332.272848	36.0
W3	-9332.269555	38.1
W4	-9332.269102	38.4
W5	-9332.255208	47.1
[Gly-2w]3w/HA → [Gly-2w]2w/HA + W		
Extracted water W	E [Gly-2w]2w/HA (Hartrees)	ΔE_r (kcal mol^{-1})
W3	-9332.252563	48.7
W4	-9332.247052	52.2
W5	-9332.237212	58.4
[Gly-3w]2w/HA → [Gly-3w]1w/HA + W		
Extracted water W	E [Gly-3w]1w/HA (Hartrees)	ΔE_r (kcal mol^{-1})
W4	-9332.260724	43.6
W5	-9332.235398	59.5

References

(1) Corno, M.; Busco, C.; Civalleri, B.; Ugliengo, P. *Phys. Chem. Chem. Phys.* **2006**, *8*, 2464.

(2) Corno, M.; Orlando, R.; Civalleri, B.; Ugliengo, P. *Eur. J. Mineral.* **2007**, *19*, 757.

(3) Corno, M.; Busco, C.; Bolis, V.; Tosoni, S.; Ugliengo, P. *Langmuir* **2009**, *25*, 2188.

(4) Rimola, A.; Corno, M.; Zicovich-Wilson, C.; Ugliengo, P. *J. Am. Chem. Soc.* **2008**, *130*, 16181.

(5) Dovesi, R.; Saunders, V. R.; Roetti, C.; Orlando, R.; Zicovich-Wilson, C. M.; Pascale, F.; Civalleri, B.; Doll, K.; Harrison, N. M.; Bush, I. J.; D'Arco, P.; Llunell, M. CRYSTAL2006 User's Manual; http://www.crystal.unito.it; University of Torino: Torino, 2006.

(6) Dovesi, R.; Civalleri, B.; Orlando, R.; Roetti, C.; Saunders, V. R. *Rev. Comput. Chem.* **2005**, *21*, 1.

(7) Ugliengo, P. http://www.moldraw.unito.it: MOLDRAW: A molecular graphics program to display and manipulate molecular structures; H1 (32-bit) ed. Torino, 2005.

(8) http://www.crystal.unito.it/Basis_Sets/Ptable.html. CRYSTAL basis set library. Torino, 2005.

(9) Tosoni, S.; Pascale, F.; Ugliengo, P.; Orlando, R.; Saunders, V. R.; Dovesi, R. *Mol. Phys.* **2005**, *103*, 2549.

(10) Ugliengo, P.; Pascale, F.; Mérawa, M.; Labéguerie, P.; Tosoni, S.; Dovesi, R. *J. Phys. Chem. B.* **2004**, *108*, 13632.

(11) Walsh, T. *Phys. Chem. Chem. Phys.* **2005**, *7*, 443.

(12) Wu, X.; Vargas, M. C.; Nayak, S.; Lotrich, V.; Scoles, G. *J. Chem. Phys.* **2001**, *115*, 8748.

(13) Xu, X.; Goddard III, W. *Proc. Nat. Acad. Sci. USA* **2004**, *101*, 2673.

(14) Monkhorst, H. J.; Pack, J. D. *Phys. Rev. B.* **1976**, *8*, 5188.

(15) Doll, K. *Comput. Phys. Comm.* **2001**, *137*, 74.

(16) Doll, K.; Saunders, V. R.; Harrison, N. M. *Int. J. Quantum Chem.* **2001**, *82*, 1.

(17) Schlegel, H. B. *J. Comp. Chem.* **1982**, *3*, 214.

(18) Civalleri, B.; D'Arco, P.; Orlando, R.; Saunders, V. R.; Dovesi, R. *Chem. Phys. Lett.* **2001**, *348*, 131.

(19) Pedone, A.; Corno, M.; Civalleri, B.; Malavasi, G.; Menziani, M. C.; Segre, U.; Ugliengo, P. *J. Mater. Chem.* **2007**, *17*, 2061.