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Journal:	<i>Molecular Physics</i>
Manuscript ID:	TMPH-2008-0163.R1
Manuscript Type:	Full Paper
Date Submitted by the Author:	16-Jul-2008
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Keywords:	LMP2, conformations, peptides
Note: The following files were submitted by the author for peer review, but cannot be converted to PDF. You must view these files (e.g. movies) online.	
conformers.tex conformers.bbl

The accuracy of local MP2 methods for conformational energies

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Abstract

The relative energies of 95 conformers of four peptide models are studied using MP2 and LMP2 methods and correlation consistent basis sets ranging from double-zeta to augmented quintuple-zeta quality. It is found that both methods yield quite similar results, and the differences between MP2 and LMP2 decrease systematically with increasing basis set. Due to reduced intramolecular basis set superposition effects (BSSE) the LMP2 results converge more slowly to basis set limit for most of these rather small systems. However, for larger peptides, the BSSE has a very large effect on the energy difference between extended and helical structures, leading to a very strong basis set dependence of the canonical MP2 results. It is demonstrated for alanine octapeptides that the basis set error exceeds 30 and 20 kJ/mol, respectively, if augmented double-zeta and triple-zeta basis sets are used. On the other hand, the LMP2 results are only slightly affected by the basis set size, and even with augmented double-zeta basis sets reasonably accurate results are obtained. Furthermore, for the larger systems the computation times for the LMP2 calculations are shown to be up to one order or magnitude shorter than for canonical MP2 calculations with the same basis set.

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I. INTRODUCTION

Sampling the low-energy region of the phase-space is an essential element for simulating the behavior of macromolecules at finite temperature conditions. The only realistic energy functions for large-scale simulations are of the force field type, but it is desirable to establish the inherent accuracy of these methods. Two of us have recently shown that most force fields in common use have problems reproducing geometries and relative energies of conformations of small peptide models, typically accounting for only half of the conformations.¹ These conclusions were obtained by generating a reference set of structures and energies by a hierarchy of electronic structure methods, with geometry optimizations at the MP2/aug-cc-pVDZ level and relative energies obtained by extrapolating MP2 energies to the basis set limit and adding corrections for higher order electron correlation effects calculated at the CCSD(T) level. For molecules with localized bonding it is anticipated that relative energies of conformations will be insensitive to electron correlation beyond MP2, and it was found that the MP2/aug-cc-pVTZ level represented a suitable compromise between accuracy and computational cost, producing a typical accuracy of 1 kJ/mol for relative energies. We note that Hartree-Fock and density functional methods will be of limited use for systems with several degrees of conformational freedom, as the inadequacy of describing intramolecular dispersion will lead to artifacts in the resulting energy surface.

Having settled on the MP2 method as a suitable level of theory for generating reliable reference data for parameterizing force fields, there remains a question of the computationally most efficient formulation of MP2 theory. The conventional approach is based on canonical molecular orbitals, which leads to a formal $\mathcal{O}(\mathcal{N}^5)$ scaling of computer time with system size. The local MP2 (LMP2) method²⁻⁹ employs a localization scheme of the molecular orbitals prior to the MP2 step, and by utilizing the locality in the selection of correlating orbitals, the LMP2 method will approach linear scaling for large systems. An additional strategy to reduce the computational requirements is to expand products of functions in an auxiliary basis set,¹⁰⁻¹² a procedure usually called resolution of identity (RI) or density fitting (DF). Both of these procedures involve additional approximations beyond the regular MP2. In the current work we present extensive benchmark data to investigate the accuracy of these approximations relative to conventional MP2. An earlier study on the use of LMP2 for the calculation of conformational energies can be found in Ref. 13.

In section II we summarize the computational details of our calculations. In section III A we report a comparison of MP2, DF-MP2, and DF-LMP2 methods for 95 conformations of small glycine, alanine, serine and cysteine model peptide systems. Finally, in section III B the accuracy and computational savings of the local approximations are investigated for extended and folded structures of larger alanine peptide chains.

II. METHOD

All geometries used in Section III A have been taken as the MP2/aug-cc-pVDZ optimized reported previously,¹ and the performance for energies relative to the lowest energy conformations was evaluated as the mean and maximum absolute deviations (MAD and MAX) relative to the canonical MP2 results using the cc-pVnZ¹⁴ and aug-cc-pVnZ¹⁵ ($n = 2 - 5$) basis set families. As will be shown below, the additional diffuse functions in the augmented basis sets are essential for achieving rapid basis set convergence at both the Hartree-Fock (HF) and the MP2 levels. These functions are particularly important for the description of the nitrogen and oxygen lone pairs. However, the diffuse functions on the hydrogen atoms have only a rather small effect on the relative energies. Therefore, as a cost effective compromise we recommend mixed basis sets, where the cc-pVnZ sets are used for the hydrogen atoms, and the aug-cc-pVnZ sets for all other atoms. These basis sets will be denoted aug'-cc-pVnZ. For each of the 95 conformers, the MP2 complete basis set limit (CBS) has been estimated using an exponential extrapolation of the HF/aug'-cc-pVnZ energies ($n = 3 - 5$), and a two-point n^{-3} extrapolation of the MP2/aug'-cc-pVnZ ($n = 4 - 5$) correlation energies.¹⁶ These estimates will be denoted MP2/CBS[45].

In Section III B, the initial extended and helical structures of alanine tetra-, hexa- and octapeptide were created in Maestro, the graphic interface program of the MacroModel package.¹⁷ Three, five and seven aminoacid units, respectively, were used for the construction of our peptides. In addition, acetyl and N-methyl functional groups were added to the C-terminus and N-terminus to mimic the environment in a longer peptide chain. Geometries were first pre-optimized at the MM level with the MMFFs¹⁸ force field. The structures were then refined using the B-P86 density functional^{19,20} in combination with the TZVP basis set.²¹ Since no extensive search of the PES was made, there is no guarantee that the optimized structures are the global minima. However, for the purpose of the present

benchmarks this is of no relevance.

Density fitting approximations^{11,12} have been employed in the HF as well as the MP2/LMP2 steps, using, respectively, the cc-pVnZ/JKFIT and cc-pVnZ/MP2FIT or aug-cc-pVnZ/MP2FIT auxiliary basis sets of Weigend et al.^{22,23} In each case n corresponds to the orbital basis. Local density fitting approximations^{11,12} were disabled, except when otherwise noted. All calculations have been carried out using the MOLPRO²⁴ program package.

III. RESULTS AND DISCUSSION

A. Small peptide model systems

By comparison of the MP2 and DF-MP2 results it was found that typical errors due to the density fitting approximation are ~ 0.01 kJ/mol. The maximum deviations never exceeded 0.1 kJ/mol and are therefore well within the 1 kJ/mol target accuracy. Thus, **in agreement with earlier investigations on conformational energies²⁵ and other properties**, the errors introduced by density fitting are negligible. Therefore, density fitting was used in all further calculations. For simplicity, the prefix DF will be omitted in the following.

The LMP2 method involves two distinct approximations: first, the excitations are restricted to pair-specific domains of projected atomic orbitals (PAOs). Secondly, distant pairs can be treated by multipole approximations^{7,8,26} or neglected. Both approximations together lead to linear scaling of the computational cost with molecular size.^{7,8,11} In this benchmark set, however, the systems were rather small and all pairs have always been included, i.e., distant pair approximations were not applied. The impact of pair approximations will be discussed for larger systems in Section III B.

When computing small energy differences using local methods it is essential to make sure that consistent domains are employed for all conformers. In most previous local correlation calculations a method proposed by Boughton and Pulay²⁷ (BP) has been used to determine the domains automatically. Unfortunately, the domains generated by this procedure are sensitive to the basis set and may also change as a function of the geometry. The former problem may lead to an erratic basis set convergence, the latter to small steps on potential energy surfaces^{28–30} and to unbalanced results.³⁰ This also happens when considering different conformers, and we found that in the present benchmark the BP method leads

to quite unsatisfactory results, with maximum errors of up to about 10 kJ/mol relative to canonical MP2. Since the geometry changes between different conformers are substantial, the problem cannot be avoided by simply freezing the domains. We also tested the LMP2 implementation of the JAGUAR program³¹ for the cc-pVDZ and cc-pVTZ basis sets, and in these cases the average and maximum errors were even somewhat larger than with the BP procedure in MOLPRO.

Recently, two of us have developed an alternative method³² to determine the domains. This procedure is based on the natural population analysis (NPA) and natural localized molecular orbitals (NLMOs) proposed originally by Reed and Weinhold.^{33,34} It yields domains that are much more stable with respect to the basis set and geometry than the BP method. In the present work we have applied this NLMO/NPA method in LMP2 calculations for all 95 conformers using 10 different basis sets ranging from cc-pVDZ to aug'-cc-pV5Z. The NPA domain selection criterion³² was chosen to be 0.03. For each of the four model peptides the domains were consistent (i.e. the same atoms were selected for each orbital domain) for all conformers and 10 different basis sets. This confirms the superior stability of the new NLMO/NPA method.

The results are summarized in Table I, which shows the mean and maximum absolute deviations of the LMP2 and MP2 results for each basis set relative to the MP2/CBS[45] results. In addition, in the last two columns the mean and maximum absolute deviations between the LMP2 and MP2 results for each basis set are presented. The geometries and individual energies can be found in the supplementary material. The canonical MP2 method with an aug-cc-pVTZ basis is capable of reproducing the basis set limiting values within ≈ 1 kJ/mol. For the aug'-cc-pVnZ basis sets, in which the diffuse functions on the hydrogen atoms are omitted, the errors for MP2 are larger, while for LMP2 they perform almost as well as the full sets. On the other hand, the errors of both MP2 and LMP2 increase significantly if the diffuse functions are entirely omitted, at least for the smaller basis sets. These findings can be rationalized by the different contribution of basis set superposition effects (BSSE), as discussed below. It should be noted that the results for the double-zeta basis sets are rather strongly affected by errors of the HF contribution, and these basis sets are clearly too small for obtaining reliable energy differences.

The LMP2 results display convergence towards nearly the same limiting values as the canonical MP2 method. For the aug'-cc-pVnZ basis sets, the absolute deviations of the

LMP2 results from the MP2/CBS[45] reference values are typically twice as large as those of the canonical MP2. Without diffuse functions, the differences between MP2 and LMP2 results are even larger. The different convergence of the two methods with increasing basis set is attributed to the BSSE, which will be discussed below.

A closer inspection of the results for the two glycine conformers (Fig. 1) is presented in Fig. 2. The upper panel shows the convergence of the Hartree-Fock energy differences for the cc-pVnZ and aug'-cc-pVnZ basis sets. It is obvious that the inclusion of diffuse functions is essential to achieve rapid convergence. With the aug'-cc-pVDZ basis sets the error still amounts to 1.4 kJ/mol, but for all larger aug'-cc-pVnZ sets the HF values are very close to the estimated basis set limit. Note that in the present case the HF energy differences are negative, i.e., the energetic order of the two conformers is opposite than for MP2.

The lower panel of Fig. 2 shows the MP2 and LMP2 correlation energy contributions to the energy difference of the two conformers. The energetically lower conformer has a folded structure which is stabilized by hydrogen bonding, while the higher one has a stretched structure. At the more compact folded structure the dynamical correlation energy is larger, and therefore the correlation contribution to the energy difference is positive. This effect should increase with increasing basis set. However, as can be seen in the figure, the MP2 correlation contribution decreases with increasing cardinal number n . This can be attributed to the BSSE, which should decrease with n . Apparently, in the present case the decrease of the BSSE overcompensates the increase of the correlation contribution, leading overall to a decrease of the energy difference.

The behavior is entirely different for the LMP2 method, in which the BSSE is strongly reduced.^{6,35,36} When standard NPA domains are used, the correlation contribution converges from below to the basis set limit, as one would anticipate in the absence of BSSE. The convergence is slower than for MP2, because there is no compensation of the incomplete basis set error by the BSSE. If the domains are extended by including the PAOs at the first shell of neighboring atoms (LMP2(ext)), part of the BSSE is re-introduced, and in this case the basis set convergence dependence is remarkably weak. The total (HF + LMP2) triple-zeta value differs only by 0.01 kJ/mol from the quintuple-zeta one. However, the quintuple-zeta result is still 0.2 kJ/mol below the MP2/CBS[45] limit. This may be due to the two missing classes of ionic excitations, which are excluded in the LMP2 ansatz by construction.³⁶ Interestingly, the extrapolated LMP2(ext) result differs by less than 0.05

kJ/mol from the MP2 one. However, the extrapolation of local correlation energies should be considered with care, since the domains become more complete with increasing cardinal number, and this may lead to a different asymptotic basis set convergence than in the canonical case. Furthermore, it is of course essential that the domains are consistent for all basis sets. In the present applications, this is the case with the NLMO/NPA method, but not with the BP procedure.

The glycine case discussed above demonstrates well the different basis set convergence of MP2 and LMP2, but it is somewhat special in the sense that the MP2 correlation contribution converges from above to the basis set limit. In most other cases of the present benchmark set the MP2 correlation contributions converge from below to the basis set limit (still being positive if the energetically lowest conformer is taken as the reference), indicating that the BSSE is less dominant than in the glycine case. But the BSSE still improves the MP2 results, in particular for the small basis sets, and therefore the convergence of the LMP2 results is slower. This effect is reduced when extended domains are used: For LMP2(ext)/aug'-cc-pVTZ the average and maximum absolute deviations from the MP2/CBS[45] limits are 1.41 and 2.77 kJ/mol, respectively. These values are only 0.4-0.5 kJ/mol larger than the corresponding canonical MP2 values.

B. Alanine peptides

In order to demonstrate the accuracy and computational savings of the LMP2 method for larger peptides, alanine tetra-, hexa- and octapeptides were chosen as model systems. For each of these peptides, an extended and an α -helix conformer were optimized using density functional theory, as described in section III A. The optimized alpha-helix structures are shown in Fig. 3. At these structures, the HF, MP2 and LMP2 conformational energies were computed using aug'-cc-pVnZ basis sets ($n = 2 - 4$). The MP2/CBS[34] basis set limits were estimated by extrapolation of the triple-zeta and quadruple-zeta correlation energies. In these calculations the HF energies were not extrapolated, and the aug'-cc-pVQZ values were taken as the reference. The results are summarized in Table II.

As for the smaller model systems, the MP2 and LMP2 results converge to approximately the same basis set limits. However, the basis set convergence of the two methods is very different. The most striking result in Table II is the slow basis set convergence of the MP2

results for the octapeptide folding energy. The MP2/aug'-cc-pVTZ result has a deviation of 20 kJ/mol relative to the CBS[34] reference. This amounts to 31% of the total folding energy. On the other hand, the LMP2 results show a remarkably low basis set dependence. For the aug'-cc-pVDZ basis set this is partly due to error compensation of the HF and correlation contributions, but nevertheless for all three peptides the LMP2/aug'-cc-pVDZ results are already very close to the aug'-cc-pVQZ ones. Very likely, the strong basis set dependence of the canonical MP2 results is mainly due to BSSE effects, which over-stabilize the folded structure. The BSSE is largely eliminated in the LMP2, and this leads to the much better basis set stability, very similar to the case shown in Fig. 1 for the glycine conformers. **The same effect was observed by Head-Gordon and coworkers, while investigating the stability of 27 alanine tetrapeptides.**²⁵

The effect is most pronounced for the octapeptide, since the smaller structures, after optimization, tend to distort significantly from the ideal helix conformation, as shown in Fig. 3. In the hexamer, only half of the chain is folded, the other section is extended. In the case of the tetrapeptide, the **polypeptide** chain is too small and the backbone is approximately planar. However, even in this case, the LMP2 results are almost independent of the basis set, while the MP2 ones change by more than 40% from aug'-cc-pVDZ to the CBS[34] limit. Although these examples are simplified models, **the present results confirm earlier findings made for the alanine tetrapeptide.**²⁵ Large basis sets are needed when computing folding energies with canonical correlation methods, since BSSE starts to play a crucial role in larger peptides. As the chain size increases, the errors accumulate, and at least quadruple-zeta quality basis set are necessary in order to obtain reasonably accurate results with MP2.³⁷ On the other hand, local correlation methods allow to use much smaller basis sets; moreover, for a given basis set the computational effort is drastically reduced, as will be demonstrated in the following.

The computation times of MP2 and LMP2 calculations for the octapeptides are shown in Table III. The savings made by the local approximations are quite dramatic. As compared to the canonical calculation, the total computational time for the extended structure is reduced by one order of magnitude. As expected, the LMP2 calculations for the α -helix conformer with a more more three-dimensional structure are slower than for the extended peptide, especially for the iterations, but the savings are still significant. The longer computation times for the helix structure are mainly caused by the larger number of pairs included in

the calculation (see below).

Further savings are possible through the use of local density fitting approximations, which asymptotically lead to linear scaling of the computational cost with system size.¹¹ In the local density fitting method, the 4-index exchange integrals $K_{rs}^{ij} = (ri|sj)$ are decomposed into sums of products of 2- and 3-index integrals

$$K_{rs}^{ij} \approx \sum_{A \in [i]_{\text{fit}}} D_{ri}^A (sj|A) + \sum_{B \in [j]_{\text{fit}}} (ri|B) D_{sj}^B - \sum_{A \in [i]_{\text{fit}}} \sum_{B \in [j]_{\text{fit}}} D_{ri}^A J_{AB} D_{sj}^B, \quad (1)$$

where the indices $\{A, B\}$ refer to the auxiliary basis set and D_{ri}^A are the fitting coefficients obtained by solving systems of linear equations

$$(ri|A) = \sum_{B \in [i]_{\text{fit}}} J_{AB} D_{ri}^B \quad (2)$$

(for further details see Ref. 11). Note that this *robust* fitting approximation is slightly different than the less symmetric approximation described in Ref. 11.

In a conventional implementation, the summations in eqs. (1) and (2) would run over the full fitting basis, leading to $\mathcal{O}(\mathcal{N}^5)$ scaling. The last two terms in eq. (1) then cancel. In a local calculation, it is possible to use for each orbital pair ij a truncated fitting basis, in which only the auxiliary function in the vicinity of the localized orbitals i and j are included. The default in MOLPRO is to include in the domain $[i]_{\text{fit}}$ the fitting functions at all atoms that are separated from the atoms in the orbital domain $[i]$ by at most 3 bonds ($l_f = 3$). Using this value the effect of the local density fitting approximation on the relative energies is negligible. In fact, in the current case even smaller fitting domains with only the atoms that are separated by at most one bond ($l_f = 1$) from the atoms in the domain $[i]$ are sufficient to obtain accurate results (cf. Table III).

The number of pairs included in the LMP2 and therefore onset of linear scaling and the CPU-time depends on the the distance criterium R_{vd} for neglecting very distant pairs.^{6,7} Orbital pairs ij are neglected if the closest distance R_{ij} between an atom in the orbital domain $[i]$ and an atom in the orbital domain $[j]$ is larger than R_{vd} . Reducing this distance criterion below its default value of 15 bohr leads to significant savings, but increases the error in the energy difference (cf. Table III). If the distance criterion is set to 12 bohr the errors already exceed 1 kJ/mol. The sensitivity of the energy difference is due to the

different three-dimensional arrangement of the conformers. In the helix structure, more pairs are removed when R_{vd} is decreased: if R_{vd} is reduced from 15 to 12 bohr, about 800 pairs are removed in the helix case, while in the extended conformer only 500 pairs are removed. Therefore, the helix energy is more affected than the energy of the extended conformer, and the energy difference decreases.

Optionally, the integrals for distant pairs ($R_d < R_{ij} \leq R_{vd}$) can be approximated by multipole approximations, which also reduce the overall cost.^{8,26} However, as shown in Table III for various choices of R_d , this approximation leads to rather large errors. As already pointed out in Ref. 26, this is due to the neglect of certain exchange contributions, and such approximations are therefore not recommended in the study of intermolecular forces or for cases in which long-range interactions play a crucial role.

Finally, it should be noted that the CPU-time for the Hartree-Fock calculation (about 8.3 hours, using density fitting and the aug'-cc-pVTZ basis) exceeds that of the LMP2 step. The differences are even greater when the aug'-cc-pVQZ basis (3860 contracted functions) is used. The HF and MP2 calculations took about 85 and 110 hours, respectively, while the LMP2 calculation took only 28 hours (helix structure, without local density fitting approximations).

IV. CONCLUSIONS

We have investigated the effect of local approximations on the relative energies of different conformers. In order to obtain reliable LMP2 energy differences it is important that the orbital domains of the different conformers are defined consistently. This can be achieved using a recently proposed method that is based on natural population analysis.³² With this method consistent domains were obtained for all conformers and all basis sets studied in this work, and a smooth convergence with increasing basis set size to the basis set limit was always achieved.

For all model systems studied, the MP2 and LMP2 methods yield very similar results at the basis set limit. However, due to the reduced BSSE in the LMP2, the convergence of MP2 and LMP2 with increasing basis sets is different. For most of the small systems in the benchmark set the convergence of the LMP2 results is found to be somewhat slower than for MP2, since in these systems the BSSE partly compensates for other basis set deficiencies.

However, the BSSE increases with system size, and our calculations for larger peptide chains demonstrate that canonical MP2 may strongly over-stabilize helical structures. For the alanine-octapeptide the basis set error was found to be more than 30 and 20 kJ/mol, with augmented double-zeta and triple-zeta basis sets, respectively. In contrast, the LMP2 results are only weakly basis set dependent, and already with augmented double-zeta sets results close to the basis set limit are obtained. Moreover, the local approximations reduce the computation times by up to one order of magnitude.

Acknowledgements This work was supported by grants from the Danish Natural Science Research Council, the Danish Center for Scientific Computing, an EU Marie Curie training grant, the Grant Agency of the Academy of Sciences of the Czech Republic (IAA400550702), and the German Fonds der Chemischen Industrie.

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Tables

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TABLE I: Mean (MAD) and maximum (MAX) absolute deviations of relative energies (in kJ/mol) for 91 conformations of four model peptide systems.

Basis set	MP2 ^a		LMP2 ^a		LMP2 ^b	
	MAD	MAX	MAD	MAX	MAD	MAX
cc-pVDZ	3.02	10.55	2.34	7.21	2.39	6.02
cc-pVTZ	0.91	3.48	1.94	4.43	2.20	5.36
cc-pVQZ	0.34	0.86	1.23	2.78	1.16	3.02
cc-pV5Z	0.20	0.47	0.82	2.00	0.67	1.71
aug-cc-pVDZ	1.68	4.30	3.03	5.58	1.99	5.14
aug-cc-pVTZ	0.64	1.64	1.77	3.48	1.38	3.36
aug'-cc-pVDZ ^c	2.13	5.48	3.00	5.51	1.50	4.02
aug'-cc-pVTZ ^c	0.92	2.38	1.85	3.61	1.10	2.79
aug'-cc-pVQZ ^c	0.38	0.89	0.85	1.80	0.54	1.30
aug'-cc-pV5Z ^c	0.19	0.45	0.49	1.06	0.33	0.79
CBS[45] ^d	(0.0)	(0.0)	0.12	0.33	0.12	0.33

a) Relative to the MP2/CBS[45] values.

b) Relative to MP2 values for each basis set.

c) aug' indicates that diffuse functions are included only on non-hydrogen atoms.

d) Basis set limits estimated from extrapolations of the aug'-cc-pVnZ energies, see text.

TABLE II: Energy difference $E_{\alpha\text{-helix}} - E_{\text{extended}}$ (in kJ/mol) between the helical and extended conformers of the alanine peptides. The HF contribution is included in the MP2 and LMP2 values.

Peptide	Basis	HF	MP2	LMP2
(ala) ₄	aug'-cc-pVDZ	27.69	12.58	18.21
	aug'-cc-pVTZ	29.71	15.74	18.61
	aug'-cc-pVQZ	30.71	17.26	19.06
	CBS[34] ^a	—	18.03	19.06
(ala) ₆	aug'-cc-pVDZ	42.84	47.29	46.15
	aug'-cc-pVTZ	41.47	45.55	44.27
	aug'-cc-pVQZ	41.61	45.62	45.18
	CBS[34] ^a	—	45.57	45.75
(ala) ₈	aug'-cc-pVDZ	-15.32	-94.49	-60.08
	aug'-cc-pVTZ	-2.38	-84.03	-63.19
	aug'-cc-pVQZ	-0.87	-71.78	-60.84
	CBS[34] ^a	—	-63.95	-60.22

a) Calculated from the aug'-cc-pVTZ and aug'-cc-pVQZ correlation energies and the aug'-cc-pVQZ HF value.

TABLE III: CPU-times (in minutes, using 2.8 **GHz** opteron processors) for conventional and local correlation calculations^a with the aug'-cc-pVTZ basis set on the extended/helix conformers of the alanine octapeptide. The conformational energies (in kJ/mol) $\Delta E = E(\alpha\text{-helix}) - E(\text{extended})$ are also shown.

Method	l_f	R_{vd}	R_d	Integrals ^b	Iterations ^c	Total	ΔE
MP2	—	—	—	—	—	1509/1514	-84.03
LMP2	—	—	—	162/176	413/413	590/604	-63.01
LMP2	—	15	—	106/149	95/283	214/448	-63.19
LMP2	1	15	—	45/84	95/283	152/380	-63.13
LMP2	1	12	—	44/78	68/219	124/310	-61.91
LMP2	1	10	—	39/65	43/135	94/212	-58.19
LMP2	1	15	12	44/75	94/256	152/347	-62.30
LMP2	1	15	10	37/70	78/242	128/328	-60.40
LMP2	1	15	8	32/52	70/198	114/264	-52.48

- a) R_{vd} and R_d (in bohr) are the distance criteria for neglecting very distant pairs and for using multipole approximations, respectively;
 l_f determines the size of the local fitting domains, see text.
b) CPU-time for integral evaluation and transformation.
c) CPU-time to solve the first-order LMP2 equations.

Figure Captions

Figure 1: **Ball-and-stick** representation of the two glycine tripeptide conformers discussed in the text and Fig. 2. The upper structure corresponds to the minimum energy conformation.

Figure 2: Hartree-Fock (upper panel) and correlation contributions (lower panel) to the relative energy of the glycine conformers as a function of cardinal number n of the basis set.

Figure 3: **Ball-and-stick** representation of the alanine tetra-, hexa- and octapeptide optimized helical conformers.

Figures

For Peer Review Only

FIG. 1: Jakub et al., Molecular Physics

FIG. 2: Jakub et al., Molecular Physics

FIG. 3: Jakub et al., Molecular Physics

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For

This file contains:

- 1.) DF-HF results
- 2.) DF-MP2 results
- 3.) DF-LMP2 results
- 4.) Geometries (xyz format)

Basis sets:

DZ: cc-pVDZ

TZ: cc-pVTZ

QZ: cc-pVQZ

5Z: cc-pV5Z

ADZ: aug-cc-pVDZ

ATZ: aug-cc-pVTZ

(A)DZ: (aug)-cc-pVTZ

(A)TZ: (aug)-cc-pVTZ

(A)QZ: (aug)-cc-pVTZ

(A)5Z: (aug)-cc-pVTZ

The (aug)-cc-pVnZ basis sets do not include diffuse function on H-atoms.

All results obtained with density fitting, using the cc-pVnZ/JKFIT sets for DF-HF

the cc-pVnZ/MP2FIT for MP2/cc-pVnZ, and aug-cc-pVnZ/MP2FIT for both MP2/aug-cc-pVnZ and MP2/(aug)-cc-pVnZ

All relative energies in kJ/mol

DF-HF results

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	DZ	TZ	QZ	5Z	ADZ	ATZ	(A)DZ	(A)TZ	(A)QZ	(A)5Z	XPOL	REF
Glycine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-2.839	-5.361	-5.925	-6.112	-4.822	-5.984	-4.656	-6.071	-6.119	-6.170	-6.208	-6.208
Alanine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1.447	-1.511	-1.840	-1.935	-0.646	-1.767	-0.554	-1.804	-1.916	-1.944	-1.957	-1.957
3	13.250	12.498	12.605	12.609	12.507	12.483	12.606	12.547	12.588	12.610	12.624	12.624
4	13.187	10.404	10.202	10.252	10.718	10.320	10.597	10.290	10.258	10.264	10.272	10.272
5	18.994	20.741	21.444	21.691	20.905	21.692	20.718	21.653	21.712	21.730	21.739	21.739
6	19.124	18.738	19.200	19.311	18.436	19.196	18.248	19.114	19.307	19.330	19.330	19.330
7	23.513	23.057	23.325	23.496	23.671	23.574	23.886	23.563	23.569	23.539	23.513	23.513
Serine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	13.844	10.698	9.746	9.448	10.145	9.502	10.348	9.537	9.444	9.428	9.424	9.424
3	12.472	9.426	8.723	8.424	8.994	8.519	9.020	8.494	8.430	8.395	8.371	8.371
4	17.834	13.502	12.334	11.921	13.667	12.030	14.015	12.091	11.922	11.873	11.848	11.848
5	20.647	22.421	23.008	23.141	21.749	22.941	21.653	22.931	23.131	23.173	23.187	23.187
6	15.426	12.122	11.262	10.867	11.820	10.977	11.857	10.974	10.868	10.826	10.802	10.802
7	23.339	19.539	18.701	18.308	18.518	18.281	18.642	18.364	18.304	18.268	18.244	18.244
8	23.679	20.370	19.553	19.204	19.529	19.194	19.677	19.225	19.194	19.167	19.147	19.147
9	29.021	28.362	28.327	28.249	28.126	28.140	28.188	28.135	28.235	28.258	28.267	28.267
10	22.293	17.524	16.577	16.260	17.495	16.411	17.598	16.382	16.282	16.241	16.215	16.215

16.215												
11	27.520	23.690	22.624	22.275	22.546	22.325	22.803	22.354	22.285	22.241	22.210	22.210
12	23.642	18.392	17.537	17.219	18.566	17.366	18.665	17.363	17.230	17.186	17.162	17.162
13	25.152	19.858	18.632	18.239	19.599	18.397	19.359	18.354	18.250	18.211	18.188	18.188
14	27.222	27.371	27.328	27.276	26.983	27.333	26.994	27.316	27.283	27.283	27.286	27.286
15	38.663	32.597	31.414	30.935	31.446	30.807	31.690	30.867	30.890	30.879	30.866	30.866
16	30.655	25.646	25.066	24.864	25.280	24.915	25.198	24.875	24.886	24.861	24.838	24.838
17	36.766	30.626	29.399	28.889	29.370	28.739	29.523	28.811	28.846	28.842	28.835	28.835
18	30.755	23.365	21.634	21.011	23.179	21.175	23.246	21.144	20.991	20.947	20.925	20.925
19	34.717	31.625	31.148	30.920	31.248	30.792	31.669	30.853	30.909	30.901	30.888	30.888
20	39.578	33.338	32.094	31.570	32.100	31.451	32.364	31.490	31.522	31.520	31.516	31.516
21	32.233	26.920	26.226	25.941	26.242	25.980	26.179	25.978	25.957	25.928	25.905	25.905
22	27.087	25.817	25.797	25.743	25.532	25.824	25.560	25.756	25.790	25.766	25.742	25.742
23	33.156	28.584	27.570	27.159	27.746	27.224	27.976	27.144	27.153	27.110	27.071	27.071
24	37.647	35.761	35.374	35.160	34.759	35.076	34.809	35.104	35.162	35.161	35.154	35.154
25	30.682	30.470	30.622	30.493	29.559	30.393	29.511	30.360	30.480	30.481	30.469	30.469
26	33.773	31.498	31.098	30.845	29.987	30.730	29.709	30.704	30.827	30.820	30.800	30.800
27	33.596	33.537	33.620	33.505	32.648	33.427	32.621	33.375	33.488	33.495	33.489	33.489
28	33.054	35.697	36.546	36.734	36.020	36.639	35.749	36.538	36.732	36.770	36.782	36.782

29	32.716	28.178	27.494	27.161	27.544	27.267	27.407	27.193	27.185	27.150	27.119
30	40.237	38.007	37.389	37.236	38.169	37.370	38.650	37.410	37.289	37.245	37.220
31	37.942	34.582	33.696	33.370	34.231	33.460	34.239	33.464	33.381	33.358	33.347
32	39.473	36.612	36.154	35.896	35.278	35.806	35.040	35.734	35.879	35.872	35.852
33	42.574	38.401	37.711	37.420	37.265	37.393	37.069	37.364	37.386	37.371	37.357
34	42.537	38.410	37.812	37.540	36.939	37.501	36.874	37.436	37.537	37.528	37.509
35	48.278	45.415	45.006	44.905	45.541	44.969	46.022	44.999	44.971	44.910	44.861
36	58.549	53.979	53.472	53.094	54.125	52.971	54.265	53.031	53.049	53.060	53.068
37	54.922	53.327	53.121	52.909	52.726	52.870	52.556	52.837	52.870	52.901	52.924
38	61.061	55.832	54.797	54.415	55.292	54.556	55.371	54.544	54.418	54.383	54.366
39	68.255	60.615	58.704	58.068	60.266	58.412	60.424	58.425	58.107	58.026	57.991

Cysteine

1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	6.037	1.573	0.607	0.260	1.298	0.505	1.028	0.388	0.261	0.225	0.209
3	4.561	2.863	2.382	2.244	3.007	2.440	2.904	2.274	2.234	2.210	2.194
4	12.161	9.829	9.338	9.181	9.751	9.361	9.180	9.152	9.092	9.075	9.066
5	6.315	4.609	4.200	4.134	4.500	4.307	4.387	4.217	4.144	4.124	4.114
6	7.893	6.097	5.630	5.466	6.107	5.687	5.750	5.570	5.443	5.426	5.424
7	7.516	2.751	2.033	1.774	3.217	2.167	2.821	1.947	1.780	1.726	1.698
8	9.627	7.264	6.689	6.567	7.328	6.695	7.223	6.679	6.542	6.521	6.516
9	10.283	7.886	7.342	7.221	8.226	7.494	7.902	7.374	7.198	7.164	7.154
10	10.677	7.418	6.686	6.437	7.569	6.762	7.094	6.453	6.383	6.352	6.333
11	11.006	8.186	7.769	7.654	9.238	7.996	8.968	7.856	7.675	7.634	7.618

12	19.615	15.998	15.397	15.202	15.995	15.303	15.750	15.202	15.137	15.140	15.148
13	11.807	8.434	8.031	7.912	9.609	8.280	9.436	8.040	7.923	7.877	7.851
14	17.211	14.253	13.795	13.622	14.379	13.721	14.021	13.599	13.560	13.569	13.580
15	14.672	11.860	11.371	11.294	11.945	11.553	11.633	11.360	11.272	11.244	11.230
16	16.248	12.213	11.544	11.381	13.403	11.670	13.391	11.553	11.379	11.341	11.327
17	17.014	13.658	13.304	13.235	13.596	13.450	13.029	13.300	13.245	13.231	13.224
18	22.606	19.782	19.367	19.277	19.564	19.247	19.808	19.287	19.232	19.239	19.250
19	23.240	22.114	21.813	21.694	21.978	21.820	21.751	21.724	21.662	21.671	21.684
20	18.705	14.050	13.240	13.036	15.010	13.261	14.946	13.128	13.005	12.961	12.936
21	25.047	22.563	21.875	21.607	22.505	21.830	22.084	21.663	21.559	21.555	21.562
22	18.202	18.118	18.293	18.339	17.794	18.466	17.102	18.268	18.306	18.313	18.315
23	21.532	19.960	19.884	19.867	19.783	20.079	19.212	19.887	19.831	19.823	19.822
24	22.109	17.811	17.297	17.264	17.827	17.387	17.645	17.344	17.251	17.239	17.238
25	21.793	15.770	14.566	14.212	16.669	14.636	16.249	14.387	14.159	14.094	14.064
26	29.758	27.651	27.441	27.366	27.791	27.519	27.664	27.398	27.399	27.372	27.350
27	22.834	22.484	22.672	22.795	22.113	22.815	22.063	22.797	22.796	22.797	22.798
28	23.435	24.919	25.254	25.382	25.147	25.523	24.853	25.392	25.361	25.364	25.370
29	31.672	28.385	27.649	27.445	28.200	27.457	28.202	27.411	27.358	27.365	27.375
30	27.913	27.231	27.222	27.104	26.477	27.163	25.955	27.001	27.089	27.093	27.087

1												
2												
3	31	29.731	27.816	27.743	27.758	28.067	27.939	27.863	27.778	27.793	27.769	27.748
4	27.748											
5												
6	32	37.791	36.611	36.412	36.254	36.170	36.342	36.044	36.181	36.210	36.231	36.247
7	36.247											
8												
9	33	30.291	28.257	27.869	27.909	28.627	28.102	28.472	28.051	27.899	27.890	27.899
10	27.899											
11												
12	34	29.825	28.981	29.045	29.033	27.980	28.916	27.876	28.890	29.019	29.034	29.032
13	29.032											
14												
15	35	43.592	44.209	44.525	44.642	42.943	44.341	43.171	44.468	44.632	44.687	44.715
16	44.715											
17												
18	36	32.642	36.044	36.830	37.002	36.345	37.058	35.916	36.829	36.986	37.020	37.033
19	37.033											
20												
21	37	44.943	43.157	43.349	43.310	44.162	43.365	44.080	43.254	43.313	43.313	43.306
22	43.306											
23												
24	38	34.631	30.509	29.519	29.199	30.511	29.563	30.102	29.401	29.219	29.181	29.167
25	29.167											
26												
27	39	35.958	35.367	35.257	35.189	35.517	35.506	34.666	35.187	35.083	35.061	35.053
28	35.053											
29												
30	40	37.001	34.033	33.453	33.363	34.663	33.710	34.631	33.554	33.387	33.337	33.313
31	33.313											
32												
33	41	46.626	45.445	45.085	44.829	44.072	44.877	43.335	44.588	44.762	44.766	44.752
34	44.752											
35												
36	42	42.164	38.284	37.451	37.255	38.631	37.644	37.984	37.332	37.178	37.132	37.111
37	37.111											
38												
39	43	42.729	38.386	37.465	37.232	38.498	37.463	38.369	37.347	37.218	37.176	37.154
40	37.154											
41												
42	44	43.975	41.187	40.341	40.192	41.761	40.455	42.000	40.415	40.216	40.176	40.163
43	40.163											
44												
45	45	50.252	50.674	50.588	50.505	49.967	50.570	49.451	50.284	50.401	50.405	50.398
46	50.398											
47												
48	46	44.696	42.275	41.789	41.650	42.540	41.947	42.534	41.800	41.663	41.619	41.597
49	41.597											
50												
51	47	51.553	46.740	45.349	44.985	47.109	45.431	46.807	45.196	44.942	44.875	44.845
52	44.845											
53												
54	MAD											
55												
56	1	3.735	0.837	0.254	0.047	0.865	0.188	0.886	0.128	0.041	0.016	0.000
57												
58	MaxAD											
59												
60												

1 10.264 2.625 0.713 0.149 2.605 0.586 2.433 0.434 0.116 0.049 0.000

DF-MP2 results (using DF-HF reference functions)

	DZ	TZ	QZ	5Z	ADZ	ATZ	(A)DZ	(A)TZ	(A)QZ	(A)5Z	XPOL	REF
Glycine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	7.957	6.321	5.194	4.900	7.348	5.729	7.155	5.418	4.895	4.783	4.680	4.680
Alanine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	8.645	6.555	5.806	5.699	7.115	6.268	7.005	6.025	5.695	5.631	5.582	5.582
3	11.780	9.992	9.945	10.014	9.522	9.526	9.877	9.752	9.928	10.014	10.095	10.095
4	15.921	13.388	12.865	13.005	12.947	12.789	12.652	12.679	12.929	13.022	13.121	13.121
5	17.219	18.962	19.774	20.242	18.582	19.785	18.301	19.705	20.168	20.321	20.471	20.471
6	20.622	20.111	20.314	20.457	18.110	19.754	17.577	19.444	20.222	20.385	20.531	20.531
7	24.756	25.839	26.546	27.002	26.881	26.651	27.017	26.629	27.042	27.117	27.201	27.201
Serine												
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	18.352	14.933	13.810	13.471	13.939	13.491	14.045	13.469	13.436	13.483	13.546	13.546
3	19.039	16.685	15.493	15.076	16.195	15.244	15.755	15.110	15.039	15.006	14.985	14.985
4	23.293	19.992	18.288	17.776	19.809	18.195	19.960	18.217	17.849	17.769	17.712	17.712
5	15.919	17.941	18.623	19.024	17.218	18.291	17.000	18.295	19.046	19.158	19.246	19.246
6	24.248	20.709	19.182	18.618	20.179	19.064	19.707	18.930	18.604	18.557	18.526	18.526

1												
2												
3		18.526										
4												
5	7	30.796	26.215	24.645	24.089	23.463	23.958	23.641	23.867	23.951	24.013	24.091
6		24.091										
7												
8	8	29.240	26.175	24.899	24.427	23.795	24.197	23.842	24.021	24.275	24.351	24.439
9		24.439										
10												
11	9	28.942	27.567	27.393	27.563	25.725	26.581	26.037	26.648	27.457	27.674	27.887
12		27.887										
13												
14	10	30.767	27.039	25.699	25.354	26.142	25.553	25.880	25.286	25.327	25.348	25.389
15		25.389										
16												
17	11	33.022	30.003	28.897	28.540	27.410	28.327	27.549	28.242	28.471	28.528	28.603
18		28.603										
19												
20	12	32.966	28.572	27.180	26.849	27.485	27.130	27.318	26.833	26.738	26.771	26.828
21		26.828										
22												
23	13	35.386	29.632	27.642	27.147	27.296	27.277	26.608	26.889	26.970	27.038	27.127
24		27.127										
25												
26	14	28.518	29.384	29.536	29.653	28.001	29.316	27.768	29.141	29.557	29.733	29.921
27		29.921										
28												
29	15	41.581	34.244	32.498	31.967	30.185	31.032	30.746	31.107	31.671	31.878	32.095
30		32.095										
31												
32	16	36.451	32.610	31.906	31.775	30.427	31.236	29.693	30.840	31.570	31.792	32.030
33		32.030										
34												
35	17	42.603	34.648	32.647	32.063	30.530	31.367	30.689	31.333	31.837	32.027	32.223
36		32.223										
37												
38	18	43.046	35.972	33.358	32.516	33.430	32.832	32.905	32.419	32.302	32.385	32.497
39		32.497										
40												
41	19	36.722	32.738	31.928	31.764	31.080	31.195	31.842	31.350	31.704	31.812	31.921
42		31.921										
43												
44	20	43.729	36.482	34.606	34.043	32.479	33.370	32.726	33.293	33.834	34.018	34.209
45		34.209										
46												
47	21	39.861	34.791	33.760	33.503	31.982	32.995	31.426	32.683	33.286	33.518	33.769
48		33.769										
49												
50	22	33.788	34.035	34.164	34.284	33.219	34.156	32.744	33.793	34.214	34.316	34.425
51		34.425										
52												
53	23	39.815	36.868	35.783	35.430	34.144	35.216	33.835	34.720	35.262	35.388	35.526
54		35.526										
55												
56	24	38.437	36.847	36.468	36.360	34.504	35.560	34.545	35.664	36.254	36.426	36.601
57		36.601										
58												
59												
60												

25 37.089 36.755 36.802 36.670 33.839 35.864 33.237 35.500 36.304 36.557 36.809
36.809

26 41.671 38.574 37.609 37.305 34.145 36.557 33.661 36.175 36.975 37.223 37.471
37.471

27 37.472 38.249 38.409 38.329 35.462 37.457 34.880 37.052 37.978 38.232 38.484
38.484

28 32.449 36.773 37.914 38.316 34.995 37.287 33.995 36.836 38.000 38.316 38.619
38.619

29 44.335 41.179 40.494 40.270 37.826 39.959 36.633 39.193 40.070 40.288 40.524
40.524

30 40.752 40.301 40.088 40.214 40.242 40.055 40.589 40.028 40.270 40.390 40.537
40.537

31 43.815 41.110 40.189 39.859 38.883 39.708 38.529 39.379 39.728 39.851 39.993
39.993

32 45.850 42.879 41.942 41.677 38.645 40.837 38.116 40.405 41.343 41.605 41.865
41.865

33 48.272 43.064 41.950 41.615 39.155 40.895 38.904 40.621 41.307 41.523 41.751
41.751

34 47.703 43.999 43.154 42.942 39.676 42.018 39.112 41.647 42.616 42.884 43.156
43.156

35 51.056 49.640 49.749 49.975 49.848 49.529 50.290 49.562 50.018 50.119 50.241
50.241

36 59.537 54.486 53.666 53.360 52.099 52.722 51.936 52.582 53.193 53.407 53.627
53.627

37 55.494 54.607 54.558 54.461 50.661 53.240 49.659 52.764 53.975 54.388 54.813
54.813

38 65.537 61.912 61.306 61.117 59.223 60.394 58.639 59.957 60.863 61.208 61.591
61.591

39 77.596 71.888 70.286 69.769 69.614 69.935 69.116 69.451 69.676 69.836 70.053
70.053

Cysteine

1 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

2 12.862 10.062 8.688 8.239 9.145 8.807 8.748 8.543 8.281 8.247 8.232 8.232

3 9.129 9.710 9.657 9.640 9.013 9.816 8.072 9.237 9.537 9.646 9.770 9.770

4 14.261 12.434 12.032 11.939 11.592 11.734 10.845 11.273 11.637 11.790 11.960
11.960

1												
2												
3	5	11.784	11.669	11.364	11.346	11.353	11.568	10.729	11.090	11.291	11.339	11.401
4	11.401											
5												
6	6	12.885	13.472	13.360	13.300	12.953	13.521	12.209	13.021	13.231	13.311	13.411
7	13.411											
8												
9	7	16.126	14.092	13.268	13.120	13.154	13.781	12.315	13.083	13.056	13.095	13.164
10	13.164											
11												
12	8	16.735	16.168	15.970	15.965	15.702	16.120	15.089	15.537	15.844	15.950	16.079
13	16.079											
14												
15	9	16.025	16.316	16.516	16.659	15.996	16.807	15.061	16.366	16.573	16.686	16.830
16	16.830											
17												
18	10	17.513	17.349	17.235	17.241	16.303	17.407	14.831	16.439	17.032	17.215	17.421
19	17.421											
20												
21	11	17.417	16.329	16.100	16.100	16.938	16.533	16.028	15.925	16.070	16.129	16.219
22	16.219											
23												
24	12	21.976	18.728	18.305	18.317	16.583	17.717	16.204	17.423	18.033	18.305	18.596
25	18.596											
26												
27	13	19.525	17.918	17.546	17.535	17.498	18.064	16.671	17.265	17.450	17.498	17.571
28	17.571											
29												
30	14	21.413	19.140	19.008	19.093	17.669	18.757	16.848	18.289	18.888	19.128	19.382
31	19.382											
32												
33	15	21.544	20.718	20.564	20.709	20.594	20.831	19.766	20.134	20.590	20.721	20.874
34	20.874											
35												
36	16	24.041	22.804	22.214	22.154	22.482	22.664	21.514	22.058	22.063	22.109	22.183
37	22.183											
38												
39	17	22.111	21.790	22.109	22.331	20.841	22.080	19.416	21.491	22.237	22.482	22.748
40	22.748											
41												
42	18	25.978	23.423	23.330	23.512	21.889	23.007	21.605	22.574	23.285	23.542	23.815
43	23.815											
44												
45	19	22.670	23.667	24.076	24.237	22.284	23.747	21.701	23.465	24.080	24.327	24.590
46	24.590											
47												
48	20	27.296	24.485	23.737	23.649	24.116	23.992	23.180	23.095	23.416	23.544	23.701
49	23.701											
50												
51	21	26.992	26.232	26.086	25.994	24.554	25.723	23.479	25.180	25.766	26.024	26.306
52	26.306											
53												
54	22	23.575	25.409	26.053	26.379	23.607	26.127	22.223	25.327	26.143	26.407	26.678
55	26.678											
56												
57	23	25.902	25.559	25.915	26.194	23.791	25.855	22.768	25.280	25.963	26.213	26.482
58	26.482											
59												
60												

24	29.345	27.632	27.496	27.743	26.493	27.463	25.462	26.877	27.598	27.838	28.101
28.101											
25	33.274	30.431	29.575	29.458	29.825	30.003	27.939	28.821	29.154	29.299	29.489
29.489											
26	29.391	28.486	28.322	28.346	26.707	27.832	26.824	27.634	28.260	28.398	28.548
28.548											
27	28.015	28.777	29.445	29.826	27.193	29.453	26.465	28.810	29.612	29.865	30.131
30.131											
28	24.727	28.825	29.902	30.374	28.205	30.145	26.871	29.566	30.174	30.419	30.678
30.678											
29	33.764	32.050	31.887	31.919	30.311	31.375	29.739	30.894	31.598	31.914	32.250
32.250											
30	31.308	32.721	33.083	33.027	30.047	32.393	29.449	32.029	32.813	33.042	33.272
33.272											
31	31.846	31.686	31.850	32.126	30.728	31.681	30.503	31.295	32.083	32.243	32.414
32.414											
32	36.645	34.830	34.261	34.200	32.108	33.541	31.827	33.253	33.973	34.197	34.425
34.425											
33	31.530	31.977	32.439	32.826	32.003	32.637	31.238	32.265	32.747	32.956	33.192
33.192											
34	34.835	35.497	35.837	35.884	32.346	35.079	31.941	34.705	35.625	35.872	36.116
36.116											
35	36.253	35.647	35.699	35.822	32.143	34.637	32.945	34.934	35.733	35.953	36.156
36.156											
36	29.985	35.045	35.891	36.190	33.010	35.436	31.626	34.595	35.807	36.128	36.441
36.441											
37	40.619	39.187	39.392	39.565	38.931	39.209	38.578	38.900	39.566	39.723	39.882
39.882											
38	41.100	40.950	40.881	40.840	39.402	40.928	38.203	40.100	40.715	40.964	41.253
41.253											
39	38.481	40.856	41.524	41.870	39.328	41.434	37.366	40.442	41.398	41.762	42.159
42.159											
40	39.739	40.359	40.694	41.000	39.954	40.799	39.548	40.395	40.890	41.116	41.382
41.382											
41	44.276	43.635	43.223	43.004	38.971	41.629	37.794	40.891	42.402	42.834	43.270
43.270											
42	45.193	44.781	45.010	45.222	43.867	44.733	42.198	43.731	44.791	45.185	45.623
45.623											

1													
2													
3	43	47.666	47.318	47.409	47.534	46.099	47.274	45.159	46.449	47.287	47.608	47.968	
4	47.968												
5													
6	44	47.003	47.626	47.551	47.641	46.908	47.586	46.602	47.219	47.570	47.731	47.929	
7	47.929												
8													
9	45	47.884	50.067	50.202	50.368	46.862	49.399	45.207	48.344	49.748	50.189	50.639	
10	50.639												
11													
12	46	48.344	49.642	49.966	50.268	48.650	49.946	47.972	49.554	50.037	50.278	50.554	
13	50.554												
14													
15	47	57.296	56.224	55.879	55.901	55.221	55.838	53.951	54.847	55.568	55.853	56.193	
16	56.193												
17													
18	MAD												
19													
20	1	3.024	0.908	0.343	0.203	1.681	0.636	2.128	0.920	0.375	0.194	0.000	
21													
22	MaxAD												
23													
24	1	10.549	3.475	0.861	0.474	4.299	1.640	5.475	2.378	0.891	0.450	0.000	
25													
26													
27													
28	=====												
29	=====												
30													
31	DF-LMP2 results, standard NLMP/NPA domains, npasel=0.03, DF-HF reference functions												
32													
33	Last column: LMP2(ext)/(A)TZ												
34													
35	-----												
36													
37		DZ	TZ	QZ	5Z	ADZ	ATZ	(A)DZ	(A)TZ	(A)QZ	(A)5Z	XPOL	REF
38	LMP2(ext)												
39													
40	Glycine												
41													
42	1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
43	0.000												
44													
45	2	5.041	3.953	4.048	4.277	4.455	4.286	4.616	4.155	4.379	4.464	4.568	4.680
46	4.595												
47													
48	Alanine												
49													
50	1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
51	0.000												
52													
53	2	6.733	4.608	4.822	5.093	5.149	5.068	5.252	5.015	5.203	5.337	5.495	5.582
54	5.345												
55													
56	3	11.850	10.262	10.194	10.154	9.991	10.036	10.071	10.116	10.127	10.146	10.158	
57	10.095	10.071											
58													
59													
60													

4 14.753 12.026 12.355 12.758 12.054 12.268 11.910 12.225 12.744 12.923 13.113
13.121 12.338

5 17.285 18.875 19.928 20.310 19.100 19.803 18.865 19.762 20.251 20.366 20.477
20.471 19.669

6 21.430 20.111 20.451 20.493 19.312 19.792 19.083 19.732 20.316 20.435 20.535
20.531 19.675

7 23.553 24.278 25.718 26.517 25.148 25.760 25.427 25.829 26.658 26.898 27.155
27.201 26.020

Serine

1 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
0.000

2 15.934 13.560 13.181 13.156 12.803 12.868 13.044 12.930 13.217 13.368 13.540
13.546 13.116

3 15.501 13.659 14.012 14.326 12.638 13.706 12.807 13.723 14.423 14.675 14.953
14.985 14.257

4 19.868 17.657 17.410 17.446 17.555 17.182 18.011 17.297 17.511 17.646 17.816
17.712 17.608

5 16.615 18.897 19.652 19.732 18.715 19.197 18.264 19.208 19.559 19.584 19.580
19.246 18.943

6 20.427 17.595 17.579 17.776 16.090 17.184 16.232 17.175 17.884 18.151 18.451
18.526 17.925

7 27.190 23.252 23.132 23.247 20.786 22.475 21.026 22.531 23.320 23.617 23.942
24.091 23.283

8 25.736 23.234 23.400 23.631 21.432 22.834 21.734 22.892 23.695 23.991 24.311
24.439 23.463

9 28.360 27.707 28.038 28.020 26.845 27.157 26.834 27.232 27.814 27.949 28.076
27.887 27.130

10 27.282 23.806 24.137 24.522 23.121 23.736 23.412 23.760 24.604 24.927 25.284
25.389 24.247

11 29.602 27.098 27.339 27.663 25.173 26.638 25.692 26.735 27.749 28.100 28.483
28.603 27.331

12 28.300 24.607 25.288 25.817 23.907 24.903 24.168 24.928 25.908 26.281 26.695
26.828 25.600

13 31.322 26.038 25.682 25.982 23.770 25.080 23.679 24.994 26.105 26.480 26.892
27.127 25.812

14 26.955 28.215 29.159 29.484 27.671 28.703 27.641 28.698 29.438 29.691 29.960
29.921 28.774

1												
2												
3	15	38.580	32.211	31.716	31.563	29.541	30.414	29.954	30.541	31.412	31.728	32.059
4		32.095	30.895									
5												
6	16	32.951	29.107	30.118	30.821	27.616	29.349	27.675	29.338	30.846	31.341	31.864
7		32.030	29.876									
8												
9	17	39.436	32.386	31.616	31.504	29.055	30.412	29.349	30.500	31.428	31.789	32.165
10		32.223	31.050									
11												
12	18	38.846	32.124	31.370	31.421	29.735	30.514	30.033	30.491	31.434	31.845	32.301
13		32.497	31.289									
14												
15	19	34.446	31.501	31.568	31.658	31.136	31.050	31.535	31.171	31.680	31.856	32.035
16		31.921	31.296									
17												
18	20	40.432	34.025	33.515	33.484	31.173	32.367	31.607	32.463	33.414	33.801	34.203
19		34.209	32.911									
20												
21	21	36.349	31.334	31.987	32.518	29.081	31.041	29.131	31.024	32.534	33.028	33.554
22		33.769	31.736									
23												
24	22	30.458	31.199	32.828	33.583	30.854	32.470	30.888	32.452	33.654	34.004	34.373
25		34.425	32.819									
26												
27	23	36.096	33.310	33.848	34.301	31.558	33.115	32.012	33.103	34.386	34.841	35.325
28		35.526	33.786									
29												
30	24	36.023	34.906	35.625	35.949	33.377	34.847	33.567	34.991	35.989	36.305	36.630
31		36.601	35.294									
32												
33	25	35.060	34.864	35.762	36.078	32.408	34.784	32.336	34.742	35.971	36.311	36.655
34		36.809	35.302									
35												
36	26	38.476	35.859	36.325	36.574	32.490	35.015	32.358	34.970	36.428	36.857	37.296
37		37.471	35.549									
38												
39												
40	27	35.800	36.540	37.506	37.837	34.459	36.519	34.445	36.501	37.712	38.047	38.386
41		38.484	36.898									
42												
43	28	32.848	36.546	38.136	38.474	36.271	37.229	35.860	37.121	38.184	38.418	38.637
44		38.619	37.046									
45												
46	29	40.728	37.575	38.519	39.121	35.176	37.563	35.180	37.455	39.158	39.725	40.328
47		40.524	38.243									
48												
49	30	38.128	38.310	39.337	39.950	38.566	39.038	39.057	39.162	40.035	40.327	40.655
50		40.537	39.345									
51												
52	31	40.861	38.087	38.396	38.813	35.750	37.635	35.872	37.637	38.913	39.363	39.848
53		39.993	38.494									
54												
55	32	42.455	39.882	40.580	40.923	37.095	39.302	37.061	39.264	40.787	41.248	41.717
56		41.865	39.747									
57												
58	33	44.519	40.230	40.696	40.938	37.535	39.413	37.578	39.415	40.740	41.176	41.633
59												
60												

41.751 39.918

34 45.592 41.848 42.275 42.456 39.310 40.939 39.375 40.939 42.276 42.683 43.101
43.156 41.209

35 48.047 47.186 48.581 49.397 47.785 48.156 48.482 48.327 49.538 49.870 50.234
50.241 48.492

36 56.316 52.093 52.673 52.903 50.476 51.661 50.542 51.683 52.822 53.259 53.713
53.627 52.334

37 54.432 53.090 53.850 54.066 50.532 52.485 50.233 52.407 53.813 54.277 54.755
54.813 52.881

38 61.648 58.243 59.353 60.085 56.173 58.296 56.571 58.316 60.109 60.745 61.433
61.591 59.008

39 71.576 66.527 67.270 68.055 64.475 66.578 65.098 66.666 68.381 69.070 69.842
70.053 67.740

Cysteine

1 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
0.000

2 10.076 7.357 7.447 7.644 6.632 7.278 6.603 7.162 7.725 7.962 8.232 8.232
7.592

3 7.566 7.867 8.538 8.912 7.091 8.333 7.143 8.135 8.911 9.241 9.597 9.770
8.657

4 13.235 11.619 11.577 11.644 10.796 11.150 10.474 10.889 11.388 11.616 11.865
11.960 11.136

5 9.442 9.357 10.086 10.650 9.102 10.029 9.055 9.902 10.710 10.992 11.299 11.401
10.185

6 10.840 11.348 12.203 12.640 10.906 12.164 10.696 11.991 12.680 12.986 13.323
13.411 12.497

7 13.192 10.855 11.611 12.129 10.243 11.493 10.169 11.267 12.189 12.582 13.022
13.164 11.981

8 13.974 13.775 14.540 15.108 13.113 14.584 13.121 14.392 15.156 15.504 15.887
16.079 15.033

9 13.664 13.923 15.093 15.749 13.431 14.970 13.538 14.872 15.810 16.212 16.659
16.830 15.562

10 14.932 14.701 15.681 16.228 13.605 15.295 13.412 14.914 16.143 16.653 17.203
17.421 15.645

11 14.918 14.021 14.897 15.428 14.280 14.865 14.244 14.695 15.412 15.754 16.141
16.219 15.151

12 20.548 17.654 17.861 18.003 15.928 17.118 15.984 17.035 17.805 18.155 18.528

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18.596	17.344											
13	17.195	15.602	16.338	16.814	15.573	16.172	15.605	15.924	16.755	17.098	17.478	
17.571	16.426											
14	19.451	17.734	18.338	18.658	16.399	17.802	16.178	17.611	18.495	18.902	19.331	
19.382	18.056											
15	18.296	17.976	19.063	19.835	17.486	18.847	17.456	18.631	19.805	20.242	20.716	
20.874	19.091											
16	21.248	19.766	20.565	21.085	19.653	20.469	19.983	20.373	21.168	21.559	21.996	
22.183	21.090											
17	20.079	19.257	20.818	21.631	18.682	20.404	18.233	20.221	21.613	22.108	22.637	
22.748	20.597											
18	24.603	22.413	22.775	23.131	20.745	22.301	21.054	22.209	22.966	23.331	23.717	
23.815	22.582											
19	21.855	22.425	23.392	23.787	21.231	22.881	21.308	22.833	23.769	24.147	24.547	
24.590	23.219											
20	24.211	21.670	22.169	22.716	21.199	21.844	21.258	21.563	22.567	23.016	23.510	
23.701	22.257											
21	25.520	24.775	25.269	25.485	23.178	24.621	22.937	24.409	25.378	25.793	26.241	
26.306	24.919											
22	21.481	23.400	25.069	25.767	22.295	24.583	21.745	24.290	25.627	26.068	26.525	
26.678	24.753											
23	23.851	23.820	25.091	25.650	22.564	24.495	22.349	24.313	25.491	25.908	26.353	
26.482	24.726											
24	26.436	24.506	25.908	26.840	23.735	25.557	23.658	25.404	26.818	27.346	27.912	
28.101	25.944											
25	28.717	26.284	27.187	27.931	25.637	26.919	25.463	26.525	27.890	28.506	29.189	
29.489	27.570											
26	28.606	27.236	27.852	28.130	26.669	27.167	26.706	27.102	28.051	28.320	28.608	
28.548	27.191											
27	26.460	27.254	28.593	29.300	25.911	28.195	25.919	28.000	29.163	29.554	29.965	
30.131	28.397											
28	23.604	27.270	29.067	29.786	26.630	28.785	26.430	28.611	29.710	30.107	30.526	
30.678	29.035											
29	31.828	30.277	30.843	31.265	28.647	30.145	28.809	29.987	31.095	31.578	32.088	
32.250	30.591											
30	30.864	31.617	32.517	32.738	30.271	31.722	30.027	31.609	32.668	32.959	33.255	
33.272	31.852											

31	30.159	29.720	30.970	31.661	29.540	30.538	29.492	30.433	31.644	32.029	32.437
32	32.414	30.702									
32	35.572	34.402	34.427	34.319	32.569	33.460	32.523	33.335	34.052	34.294	34.541
33	34.425	33.640									
33	29.725	29.850	31.247	32.096	29.727	31.149	29.759	31.136	32.171	32.593	33.053
34	33.192	31.531									
34	33.774	34.119	35.096	35.481	32.335	34.298	32.370	34.201	35.383	35.713	36.043
35	36.116	34.510									
35	38.007	36.764	36.684	36.507	35.584	35.863	35.851	36.100	36.366	36.410	36.429
36	36.156	35.658									
36	31.115	35.123	36.236	36.353	34.400	35.362	33.930	35.084	36.028	36.255	36.469
37	36.441	35.026									
37	39.659	38.595	39.452	39.721	38.675	39.036	38.627	38.922	39.601	39.854	40.114
38	39.882	39.203									
38	37.948	37.161	38.666	39.540	35.853	38.154	35.744	37.952	39.622	40.298	41.034
39	41.253	38.844									
39	36.497	38.646	40.355	41.064	37.220	39.622	36.727	39.220	40.737	41.324	41.956
40	42.159	39.823									
40	37.290	37.264	39.000	40.004	37.112	38.674	37.569	38.639	40.072	40.598	41.177
41	41.382	39.212									
41	45.268	43.632	43.383	43.123	41.172	41.839	40.555	41.500	42.627	42.969	43.309
42	43.270	41.456									
42	42.399	41.762	43.243	44.143	40.871	42.570	40.522	42.197	43.933	44.622	45.371
43	45.623	42.850									
43	44.406	43.541	45.185	46.231	42.432	44.544	42.588	44.363	46.204	46.920	47.693
44	47.968	45.271									
44	44.518	44.482	45.727	46.512	43.991	45.411	44.712	45.494	46.706	47.216	47.781
45	47.929	46.218									
45	47.650	49.257	50.010	50.233	47.384	48.754	46.917	48.361	49.719	50.134	50.556
46	50.639	48.491									
46	44.881	46.301	48.255	49.188	45.371	47.722	45.681	47.647	49.193	49.752	50.362
47	50.554	48.440									
47	53.198	52.145	53.442	54.386	51.180	52.865	51.340	52.619	54.397	55.136	55.952
48	56.193	53.622									

MAD

1	2.342	1.936	1.232	0.816	3.032	1.773	2.998	1.853	0.851	0.488	0.123
1.410											

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MaxAD

1 7.212 4.427 2.783 1.998 5.578 3.475 5.509 3.605 1.796 1.057 0.334
2.774

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Geometries (xyz format, in Angstrom)

GLYCINE

glycine_1 -455.33935359386 a.u.
C 3.033948 0.370630 0.782112
C 1.802176 0.176200 -0.078235
O 1.443213 1.023317 -0.915523
H 2.905568 1.288005 1.374728
H 3.227794 -0.476299 1.455992
H 3.899914 0.514703 0.119925
N 1.111247 -0.986642 0.108032
C -0.095431 -1.292651 -0.659826
C -1.342397 -0.616305 -0.075338
O -2.228810 -1.261832 0.504760
H 1.378305 -1.602044 0.866193
H 0.073761 -0.960981 -1.696110
H -0.262854 -2.376884 -0.636398
N -1.378961 0.732275 -0.243586
C -2.451943 1.520840 0.348622
H -0.553035 1.176987 -0.642171
H -3.426608 1.141059 0.010760
H -2.426858 1.467394 1.448811

H -2.335331 2.564465 0.029241

glycine_2 -455.33656092531 a.u.

C 3.408842 0.915890 0.000064

C 2.340217 -0.161251 0.000005

O 2.612265 -1.371075 0.000060

H 4.041608 0.780273 0.889226

H 4.041946 0.780036 -0.888820

H 2.991492 1.933220 -0.000146

N 1.048372 0.279676 -0.000106

C -0.049249 -0.659777 -0.000081

C -1.356984 0.129111 -0.000043

O -1.382383 1.368707 -0.000024

H 0.800691 1.264838 -0.000066

H -0.001905 -1.315939 -0.886760

H -0.001854 -1.315948 0.886590

N -2.490703 -0.622673 -0.000073

C -3.805383 0.011417 0.000114

H -2.412975 -1.631614 0.000163

H -3.927408 0.644016 -0.891310

H -4.571278 -0.774406 -0.000424

H -3.927709 0.643093 0.892160

ALANINE

alanine_1 -494.53336002632 a.u.

C -3.077696 -0.614096 0.770471

C -1.837634 -0.380064 -0.068647

O -1.529867 -1.134105 -1.009779

1				
2				
3	H	-3.014507	-1.617365	1.215958
4				
5	H	-3.206763	0.133018	1.566818
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7	H	-3.954515	-0.593649	0.106906
8				
9	N	-1.085637	0.711655	0.257557
10				
11	C	0.134480	1.069664	-0.474965
12				
13	C	1.315236	0.235479	0.061169
14				
15	O	2.168922	0.706249	0.827271
16				
17	C	0.403704	2.563351	-0.339710
18				
19	H	-1.323813	1.247033	1.085193
20				
21	H	-0.048397	0.794167	-1.526080
22				
23	H	1.304426	2.833869	-0.908633
24				
25	H	-0.452033	3.137886	-0.725363
26				
27	H	0.588562	2.826041	0.712895
28				
29	N	1.317422	-1.054402	-0.372498
30				
31	C	2.279406	-2.008300	0.166327
32				
33	H	0.475135	-1.379089	-0.847767
34				
35	H	3.295361	-1.603282	0.062520
36				
37	H	2.097251	-2.207952	1.235029
38				
39	H	2.199387	-2.944809	-0.400683
40				
41				
42				
43	alanine_2	-494.53065171909	a.u.	
44				
45	C	-3.366859	-1.142124	-0.000615
46				
47	C	-2.312419	-0.081812	-0.258627
48				
49	O	-2.578516	1.000523	-0.803466
50				
51	H	-3.848821	-1.395499	-0.955887
52				
53	H	-2.955258	-2.053815	0.456102
54				
55	H	-4.134449	-0.716837	0.662522
56				
57	N	-1.045153	-0.392395	0.146127
58				
59				
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2
3 C 0.048393 0.545547 -0.030045
4
5 C 1.345438 -0.255900 0.070600
6
7 O 1.409581 -1.318680 0.708184
8
9 C 0.026939 1.650336 1.041756
10
11 H -0.818215 -1.277259 0.590800
12
13 H -0.052176 1.003826 -1.028869
14
15 H 0.839074 2.375615 0.874530
16
17 H -0.936851 2.176524 0.993300
18
19 H 0.150928 1.200185 2.038820
20
21 N 2.431426 0.303145 -0.528727
22
23 C 3.738664 -0.341795 -0.453976
24
25 H 2.301697 1.120310 -1.111200
26
27 H 3.996958 -0.535949 0.596426
28
29 H 3.737782 -1.301254 -0.993345
30
31 H 4.485960 0.328646 -0.897293
32
33
34
35
36
37 alanine_3 -494.52972984894 a.u.
38
39 C -3.146922 -0.743545 -0.625882
40
41 C -1.820406 -0.349990 -0.003653
42
43 O -1.408225 -0.898737 1.035189
44
45 H -3.136531 -1.826777 -0.812937
46
47 H -3.943901 -0.534397 0.102892
48
49 H -3.364878 -0.210896 -1.562710
50
51 N -1.127197 0.629874 -0.651936
52
53 C 0.129782 1.254654 -0.203070
54
55 C 1.371000 0.356162 -0.357228
56
57 O 2.382815 0.779386 -0.940581
58
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2				
3	C	0.032758	1.824145	1.220232
4				
5	H	-1.515910	0.967340	-1.523689
6				
7	H	0.312087	2.080949	-0.905353
8				
9	H	0.977631	2.335378	1.461016
10				
11	H	-0.788844	2.554629	1.278311
12				
13	H	-0.143915	1.028890	1.955771
14				
15	N	1.294828	-0.871052	0.213667
16				
17	C	2.436246	-1.775408	0.163178
18				
19	H	0.435499	-1.118684	0.706234
20				
21	H	2.729193	-1.966991	-0.880054
22				
23	H	3.302787	-1.342201	0.686066
24				
25	H	2.151896	-2.720297	0.644002
26				
27				
28				
29	alanine_4	-494.52842446812	a.u.	
30				
31	C	3.210523	-0.662723	-0.460988
32				
33	C	1.902501	-0.329339	0.234014
34				
35	O	1.592619	-0.795233	1.335459
36				
37	H	3.389166	-1.743558	-0.378568
38				
39	H	3.222393	-0.364554	-1.519893
40				
41	H	4.026069	-0.143867	0.065737
42				
43	N	1.063614	0.528567	-0.445477
44				
45	C	-0.109890	1.105277	0.209381
46				
47	C	-1.337755	0.182224	0.216490
48				
49	O	-2.351017	0.508207	0.848319
50				
51	C	-0.482221	2.429954	-0.463158
52				
53	H	1.409974	0.975421	-1.287344
54				
55	H	0.136098	1.268574	1.271371
56				
57	H	-1.380114	2.839518	0.018698
58				
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2
3 H 0.339979 3.156370 -0.369155
4
5 H -0.702916 2.270943 -1.532093
6
7 N -1.258725 -0.945502 -0.543219
8
9 C -2.326397 -1.937418 -0.487791
10
11 H -0.338347 -1.214934 -0.868032
12
13 H -3.291321 -1.432334 -0.626834
14
15 H -2.174863 -2.666844 -1.294361
16
17 H -2.343712 -2.457830 0.483431
18
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20
21 alanine_5 -494.52628258390 a.u.
22

23 C -3.025482 -1.075360 -0.074147
24
25 C -1.673961 -0.442820 0.205604
26
27 O -1.111030 -0.527053 1.302023
28
29 H -3.062202 -2.059331 0.412476
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31 H -3.806005 -0.443439 0.377657
32
33 H -3.233647 -1.183722 -1.148990
34
35 N -1.092705 0.222116 -0.855711
36
37 C 0.054423 1.117537 -0.645550
38
39 C 1.294468 0.361408 -0.131136
40
41 O 2.172619 0.945485 0.512583
42
43 C -0.280066 2.308181 0.258116
44
45 H -1.670731 0.386489 -1.672458
46
47 H 0.331884 1.486839 -1.648165
48
49 H 0.603106 2.952842 0.360338
50
51 H -1.105078 2.888571 -0.183820
52
53 H -0.572888 1.953842 1.255792
54
55 N 1.406073 -0.939392 -0.533569
56
57 C 2.470132 -1.767548 0.024114
58
59
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1				
2				
3	H	0.552975	-1.387601	-0.845018
4				
5	H	3.433815	-1.263280	-0.124568
6				
7	H	2.326646	-1.934370	1.104246
8				
9	H	2.478743	-2.731755	-0.501390
10				
11				
12				
13	alanine_6	-494.52646519902	a.u.	
14				
15	C	2.974570	-1.116271	-0.062307
16				
17	C	1.699117	-0.341278	-0.322664
18				
19	O	0.989887	-0.535484	-1.318870
20				
21	H	3.492270	-1.280126	-1.016614
22				
23	H	3.644318	-0.603055	0.642957
24				
25	H	2.699141	-2.097859	0.354607
26				
27	N	1.364186	0.601008	0.624654
28				
29	C	0.009715	1.164399	0.603282
30				
31	C	-1.004825	0.000252	0.591930
32				
33	O	-0.935240	-0.881154	1.457888
34				
35	C	-0.140797	2.221470	-0.495396
36				
37	H	1.801116	0.496087	1.533801
38				
39	H	-0.133757	1.649062	1.582859
40				
41	H	-1.141871	2.678966	-0.455125
42				
43	H	0.604554	3.014913	-0.338257
44				
45	H	0.029587	1.782705	-1.489211
46				
47	N	-1.993273	0.042415	-0.348935
48				
49	C	-2.865522	-1.120675	-0.496527
50				
51	H	-1.785949	0.576737	-1.184520
52				
53	H	-3.318936	-1.352210	0.475711
54				
55	H	-3.655464	-0.879325	-1.219954
56				
57	H	-2.302117	-2.004139	-0.838343
58				
59				
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alanine_7 -494.52311928750 a.u.

C	-3.057032	-1.512273	-0.105575
C	-2.243919	-0.229609	-0.088498
O	-2.768991	0.886557	-0.142497
H	-3.803773	-1.462314	0.699722
H	-3.596440	-1.570359	-1.062559
H	-2.442470	-2.415128	0.023446
N	-0.875702	-0.395257	0.013556
C	0.014347	0.758107	-0.185154
C	1.450466	0.285311	-0.403506
O	2.211983	0.847603	-1.196767
C	-0.021042	1.713028	1.019355
H	-0.513940	-1.305681	-0.254458
H	-0.282336	1.307966	-1.092609
H	0.671677	2.549888	0.840346
H	-1.037116	2.106567	1.151393
H	0.285158	1.186088	1.937333
N	1.840930	-0.791555	0.357429
C	3.247337	-1.189335	0.368071
H	1.265703	-1.024883	1.159878
H	3.583566	-1.338467	-0.666165
H	3.885179	-0.418690	0.830030
H	3.343311	-2.131957	0.922704

SERINE

serine_1 -569.60448066 a.u.

C	-3.218678	0.093386	-0.805734
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1				
2				
3	C	-1.985847	0.256377	0.058699
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5	O	-1.867557	1.197354	0.867710
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7	H	-3.359884	1.012328	-1.392661
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9	H	-3.155270	-0.770492	-1.482476
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11	H	-4.091405	-0.023707	-0.146631
12				
13	N	-1.018521	-0.691316	-0.087241
14				
15	C	0.211863	-0.676130	0.700726
16				
17	C	1.227497	0.305061	0.085748
18				
19	O	2.232960	-0.090240	-0.537938
20				
21	C	0.787063	-2.092439	0.726876
22				
23	O	0.958958	-2.592093	-0.603138
24				
25	H	-1.077728	-1.392311	-0.820258
26				
27	H	1.637259	-2.006543	-0.988627
28				
29	H	-0.047199	-0.342743	1.719776
30				
31	H	1.739484	-2.088721	1.283149
32				
33	H	0.080530	-2.769095	1.230128
34				
35	N	0.927618	1.611613	0.269056
36				
37	C	1.728101	2.653416	-0.364879
38				
39	H	0.010191	1.818727	0.668264
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41	H	2.787348	2.512916	-0.109304
42				
43	H	1.630566	2.620989	-1.461786
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45	H	1.387550	3.628379	0.006040
46				
47				
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49	serine_2	-569.59916816	a.u.	
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55	O	2.042449	0.571328	-1.099767
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57	H	3.809040	0.552463	0.949173
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5 H 4.123005 -0.876749 -0.061139
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9 C -0.297874 -0.764813 -0.296104
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11 C -1.053575 0.502802 0.146948
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13 O -2.080619 0.446149 0.851479
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15 C -1.109166 -2.017738 0.050015
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17 O -2.400124 -1.984675 -0.542770
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19 H 1.087691 -1.381118 1.215297
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21 H -2.856568 -1.247352 -0.101124
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23 H -0.124679 -0.715953 -1.383091
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25 H -0.592296 -2.902798 -0.350518
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27 H -1.177967 -2.112014 1.150915
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29 N -0.512085 1.662834 -0.288678
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31 C -1.083991 2.945885 0.102637
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33 H 0.369481 1.604309 -0.799509
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35 H -0.998178 3.103035 1.189175
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37 H -0.546122 3.742082 -0.427296
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39 H -2.149417 2.979640 -0.166131
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43 serine_3 -569.59831430 a.u.
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45 C -3.557316 -1.122781 0.178641
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47 C -2.433710 -0.157088 -0.142845
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49 O -2.628431 0.925398 -0.716508
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51 H -0.983564 -1.509072 0.507958
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53 N -1.180561 -0.540859 0.260039
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57 C 1.199094 -0.684661 -0.071571
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9	H	0.591568	2.896329	-0.572500
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11	H	2.389038	0.943388	-0.340747
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13	N	2.390135	-0.072505	-0.282339
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15	C	3.636388	-0.821017	-0.162544
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17	H	-3.210822	-2.012232	0.723865
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19	H	-4.312078	-0.595699	0.779833
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21	H	-4.032047	-1.431511	-0.764340
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23	H	-0.170729	0.562056	-1.204575
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25	H	-0.871779	1.955437	0.835001
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27	H	0.520540	1.228519	1.703497
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29	H	3.801965	-1.159622	0.872260
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31	H	3.601839	-1.706220	-0.812792
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33	H	4.464182	-0.170877	-0.473035
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37	serine_4	-569.59692849	a.u.	
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41	C	-2.233766	-0.480919	-0.176863
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43	O	-2.656332	0.638924	-0.526217
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47	H	-3.669700	-1.881570	-0.905924
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51	N	-0.912615	-0.733646	0.010917
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53	C	0.125363	0.262036	-0.202379
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57	O	1.523889	-1.568255	0.576779
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23 H 4.100016 -0.501581 0.834369
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25 H 3.972918 -1.343348 -0.733121
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27 H 4.627244 0.326712 -0.667878
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31 serine_5 -569.59791795 a.u.

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33 C 3.088244 -1.111930 -0.434288
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41 H 3.629090 -1.197573 0.519061
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51 O -0.834122 -1.804691 0.759098
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53 C -0.226784 1.913919 0.734464
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55 O -0.480536 2.163843 -0.649908
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57 H 1.669480 -0.727407 1.610360
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5	H	-0.187546	0.383171	2.206538
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7	H	-1.109325	2.287871	1.276608
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9	H	0.656244	2.477611	1.085594
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11	N	-2.039996	-0.103097	-0.200370
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13	C	-2.981463	-1.025163	-0.828065
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15	H	-1.894941	0.827203	-0.596593
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17	H	-3.360123	-1.727187	-0.073285
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19	H	-3.816429	-0.444928	-1.241756
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21	H	-2.501064	-1.607291	-1.631095
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31	O	-2.655824	0.915859	-0.745891
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33	H	-4.333516	-0.597829	0.742387
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35	H	-3.987290	-1.495995	-0.752547
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37	H	-3.193592	-1.984968	0.781955
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39	N	-1.184145	-0.506323	0.265965
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41	C	-0.028681	0.255104	-0.167871
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43	C	1.189917	-0.675612	-0.053277
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45	O	1.061820	-1.878215	0.236689
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47	C	0.104818	1.529231	0.677308
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49	O	1.093120	2.370246	0.042464
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51	H	-0.980022	-1.466725	0.538188
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53	H	1.091608	3.228207	0.487255
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55	H	-0.159477	0.569916	-1.219381
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57	H	-0.876199	2.027139	0.691250
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3 H 0.411111 1.267125 1.705749
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5 N 2.390165 -0.098615 -0.302121
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7 C 3.619476 -0.873990 -0.181428
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9 H 2.413729 0.913811 -0.392797
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19 serine_7 -569.59554335 a.u.
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23 C -1.386441 -1.325637 -0.020786
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27 H -2.279656 -2.960008 1.027762
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29 H -2.970861 -1.368976 1.491645
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31 H -3.369346 -2.110817 -0.093034
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35 C -0.107240 0.763369 -0.341706
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43 O -1.801696 2.434332 -0.367993
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53 H 0.243305 2.854314 -0.689849
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55 N 1.795515 -0.759357 -0.325855
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57 C 3.119521 -1.219929 0.072559
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5	H	3.189648	-1.337199	1.165826
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7	H	3.313127	-2.184834	-0.413235
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9	H	3.879943	-0.491322	-0.242465
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15	C	-2.519650	-2.018617	0.691781
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19	O	-0.738368	-1.899531	-0.935906
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21	H	-1.722558	0.401694	1.004005
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23	N	-1.061938	-0.075542	0.398691
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25	C	-0.117239	0.768628	-0.336044
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27	C	1.337353	0.467597	0.079689
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29	O	2.003650	1.267061	0.756375
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31	C	-0.438062	2.237092	-0.051212
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33	O	-1.825547	2.533882	-0.273713
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35	H	-2.001005	2.457260	-1.222416
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37	H	1.128479	-1.360592	-0.783087
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39	N	1.809156	-0.724419	-0.364618
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41	C	3.127269	-1.191458	0.047524
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43	H	-3.294466	-2.264567	-0.049109
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45	H	-2.152050	-2.961294	1.121863
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47	H	-2.957063	-1.400088	1.488315
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49	H	-0.234349	0.542996	-1.412283
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51	H	-0.244236	2.460133	1.006453
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53	H	0.222751	2.877741	-0.655899
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55	H	3.881333	-0.427179	-0.186762
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57	H	3.163275	-1.388194	1.131164
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serine_9 -569.59467924 a.u.

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O -1.547512 -0.297165 1.208270

H -1.468706 0.013290 -1.939512

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O 2.448657 0.221768 -1.122489

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H -0.333942 1.028476 1.706690

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N 1.142857 -1.119316 0.205589

C 2.289947 -1.909321 0.645627

H -3.386474 -0.958174 -1.476979

H -3.045221 -2.136856 -0.168207

H -3.986836 -0.672357 0.191239

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H 1.001482 2.697899 -0.128309

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serine_10 -569.59451888 a.u.

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7	O	-2.644249	0.467487	-1.204042
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9	H	-4.248313	-0.481482	0.750243
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11	H	-3.803155	-1.862299	-0.277234
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13	H	-3.015751	-1.656031	1.322765
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15	N	-1.094650	-0.367448	0.250708
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17	C	0.010525	0.254244	-0.459983
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19	C	1.281189	-0.503850	-0.052210
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21	O	1.251642	-1.429183	0.773531
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23	C	0.102851	1.743596	-0.090808
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25	O	0.451137	1.918807	1.283630
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27	H	-0.829078	-1.144709	0.854308
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29	H	-0.232832	1.467976	1.802495
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31	H	-0.156869	0.169165	-1.549947
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33	H	0.893245	2.244772	-0.670942
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35	H	-0.860455	2.219732	-0.337249
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37	N	2.427563	-0.107840	-0.664507
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39	C	3.711799	-0.676974	-0.265732
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41	H	2.409409	0.720129	-1.245555
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43	H	3.970144	-0.389346	0.765067
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45	H	3.658896	-1.772699	-0.319586
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47	H	4.484211	-0.314022	-0.955703
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50	serine_11 -569.59403494 a.u.			
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52	C	-2.162173	-2.277649	0.819050
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54	C	-1.291874	-1.392197	-0.049447
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56	O	-0.810226	-1.788123	-1.121775
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5 N -1.089312 -0.111164 0.408908
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11 O 1.865091 1.211972 0.980818
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13 C -0.581341 2.242469 0.021452
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15 O -1.871375 2.546855 -0.519878
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17 H -2.475929 1.846179 -0.233339
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21 N 1.828920 -0.555408 -0.483636
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23 C 3.148367 -1.035076 -0.088191
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25 H -2.531450 -1.767649 1.720295
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27 H -3.017722 -2.619253 0.218562
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31 H -0.301453 0.607596 -1.361541
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33 H -0.544673 2.418441 1.111307
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35 H 0.128591 2.933270 -0.452541
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37 H 3.865962 -0.203954 -0.121820
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39 H 3.140069 -1.441063 0.936305
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41 H 3.461444 -1.817639 -0.791117
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49 C 2.441949 -0.188591 0.251538
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51 O 2.631201 0.787285 0.991175
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53 H 1.023452 -1.330645 -0.785074
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55 N 1.197525 -0.498360 -0.228684
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57 C 0.035962 0.278175 0.153516
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5	O	-1.177063	-1.570516	-0.837682
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7	C	-0.044298	1.561211	-0.705116
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9	O	-1.108705	2.430831	-0.302740
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11	H	-1.935637	2.052821	-0.633435
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13	H	-2.235732	0.528577	1.284536
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23	H	4.011551	-1.562463	0.717352
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25	H	0.131155	0.580052	1.210266
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27	H	0.889102	2.119907	-0.554291
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29	H	-0.129208	1.274874	-1.768592
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31	H	-3.786488	-1.151576	-0.586365
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33	H	-3.464373	-1.935533	0.982126
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35	H	-4.375989	-0.388267	0.926027
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39	C	3.382938	0.237140	-0.014381
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41	C	1.890335	0.095646	0.219638
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43	O	1.352324	0.370460	1.296531
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45	H	3.720863	1.183113	0.430315
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47	H	3.895813	-0.584744	0.508488
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49	H	3.656027	0.208801	-1.079461
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51	N	1.151005	-0.338232	-0.865183
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53	C	-0.241930	-0.760868	-0.699821
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55	C	-1.129027	0.369559	-0.152318
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57	O	-2.125359	0.116973	0.544396
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5 O -1.684566 -2.583478 0.057672
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9 H -2.276722 -1.885360 0.391749
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13 H 0.326889 -2.782289 -0.195331
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17 N -0.813634 1.628493 -0.556283
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19 C -1.514091 2.770626 0.023106
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21 H 0.117573 1.760685 -0.932985
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23 H -2.596307 2.621182 -0.083444
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25 H -1.278527 2.881797 1.093728
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27 H -1.215958 3.677605 -0.518823
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31 serine_14 -569.59297755 a.u.

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35 C 1.568943 -0.910238 0.032302
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37 O 1.183610 -1.035156 -1.147255
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39 H 2.410354 -2.801531 0.555465
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41 H 3.579392 -1.623814 -0.079653
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43 H 2.991667 -1.471666 1.609913
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45 N 0.992236 -0.035089 0.901421
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47 C -0.081507 0.916785 0.584865
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49 C -1.476793 0.280399 0.462397
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51 O -2.445022 0.749098 1.081205
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53 C 0.215602 1.769781 -0.665891
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55 O 1.492505 2.406519 -0.583293
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9	H	-0.536298	2.572543	-0.696810
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11	N	-1.567702	-0.773814	-0.388162
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13	C	-2.852578	-1.423694	-0.616166
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15	H	-0.732849	-1.048347	-0.906220
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17	H	-3.276018	-1.775578	0.336218
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19	H	-3.570990	-0.724919	-1.071756
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21	H	-2.695412	-2.278502	-1.286432
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23				
24				
25	serine_15 -569.59288500 a.u.			
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27	C	2.877630	-1.628808	-0.386827
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29	C	1.591186	-1.102213	0.221581
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31	O	1.013025	-1.660412	1.159156
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33	H	2.798082	-2.718977	-0.495857
34				
35	H	3.104758	-1.172077	-1.361041
36				
37	H	3.703814	-1.417922	0.309742
38				
39	N	1.079412	0.046043	-0.356683
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41	C	0.044774	0.792243	0.351608
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43	C	-1.344670	0.147036	0.310979
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45	O	-2.226707	0.537149	1.086958
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47	C	-0.074601	2.183137	-0.285477
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49	O	1.193560	2.855321	-0.343599
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51	H	1.721996	0.612673	-0.905612
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53	H	1.428448	3.121504	0.557102
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55	H	0.300255	0.879985	1.422751
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57	H	-0.400772	2.082229	-1.332059
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59				
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5 N -1.552201 -0.766146 -0.676625
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7 C -2.803536 -1.514011 -0.726835
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9 H -0.725431 -1.139283 -1.128419
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11 H -3.642950 -0.811279 -0.644701
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13 H -2.861810 -2.043230 -1.687026
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15 H -2.872872 -2.238795 0.100401
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19 serine_16 -569.59284583 a.u.
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29 H 3.672626 -1.183303 -0.027402
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31 H 3.007413 -1.479075 1.608471
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33 N 0.991913 -0.062690 0.891991
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35 C -0.056597 0.901191 0.528820
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37 C -1.480036 0.323892 0.431302
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39 O -2.428384 0.907313 0.981551
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41 C 0.281692 1.682609 -0.743519
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43 O 1.536132 2.339328 -0.498572
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45 H 1.527331 0.166995 1.720278
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47 H 1.807916 2.777071 -1.316506
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49 H -0.103931 1.620703 1.358638
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51 H 0.351123 1.002793 -1.606300
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53 H -0.528409 2.414224 -0.910700
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55 N -1.618527 -0.797653 -0.315490
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57 C -2.933617 -1.398891 -0.495908
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7	H	-2.817890	-2.315522	-1.088422
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9	H	-3.379176	-1.644629	0.479647
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13	serine_17	-569.59174969	a.u.	
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15	C	-3.448900	-1.071357	0.480615
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19	O	-2.655105	0.488600	-1.191900
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21	H	-4.186382	-0.370540	0.898143
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23	H	-3.966702	-1.712141	-0.247913
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27	N	-1.106306	-0.439816	0.196678
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29	C	-0.001341	0.221804	-0.460635
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33	O	1.271131	-1.429782	0.786136
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35	C	0.075273	1.705852	-0.083030
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37	O	0.504457	1.776174	1.282510
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39	H	-0.861258	-1.116258	0.914522
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41	H	0.265269	2.644350	1.632642
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43	H	-0.142496	0.158568	-1.554861
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45	H	0.790222	2.228724	-0.747485
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47	H	-0.923387	2.145971	-0.229199
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49	N	2.417214	-0.113884	-0.682781
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53	H	2.380826	0.713175	-1.264710
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55	H	3.687226	-1.738576	-0.294702
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57	H	4.478910	-0.278157	-0.966976
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serine_18 -569.59263641 a.u.

C 3.487401 0.279265 -0.331846

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O 1.636955 0.565601 1.190398

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H 3.674825 -0.055856 -1.361964

N 1.205718 -0.453257 -0.812332

C -0.193631 -0.829873 -0.587730

C -1.215286 0.307070 -0.460072

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C -0.383697 -1.774612 0.624678

O -1.638795 -2.447107 0.542666

H 1.611641 -0.738338 -1.694840

H -2.300738 -1.787772 0.266947

H -0.504275 -1.398101 -1.477379

H 0.397245 -2.550019 0.594218

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H -1.227683 3.461563 0.576080

serine_19 -569.59210256 a.u.

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9	H	1.546789	0.168114	1.710395
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11	N	1.016816	-0.054245	0.877047
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13	C	-0.049383	0.891636	0.520447
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15	C	-1.469703	0.305710	0.432327
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17	O	-2.419302	0.908797	0.960657
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21	O	1.498104	2.413755	-0.636724
22				
23	H	1.320984	3.193485	-0.092073
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25	H	-0.775791	-1.207070	-0.749464
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27	N	-1.606705	-0.833972	-0.284939
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29	C	-2.924531	-1.428224	-0.470125
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31	H	3.041801	-1.460968	1.592735
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33	H	2.819557	-2.696744	0.305831
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35	H	3.685587	-1.182294	-0.054757
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37	H	-0.108733	1.606257	1.355552
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39	H	0.418369	0.988698	-1.603787
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41	H	-0.579729	2.341294	-0.984099
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43	H	-3.391911	-1.627813	0.505450
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45	H	-3.585893	-0.751788	-1.033471
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47	H	-2.806172	-2.370209	-1.020783
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56	O	0.960386	-1.697748	1.122853
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9 N 1.079689 0.042190 -0.353055
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11 C 0.052021 0.791658 0.366616
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13 C -1.346294 0.165091 0.305826
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15 O -2.234303 0.565729 1.069395
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17 C -0.051378 2.189077 -0.240773
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19 O 1.273634 2.753746 -0.225730
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21 H 1.749461 0.615821 -0.860539
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23 H 1.220259 3.654972 -0.571624
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27 H -0.428986 2.115172 -1.277003
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29 H -0.754901 2.780301 0.364946
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31 N -1.552206 -0.748038 -0.682338
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33 C -2.807742 -1.488244 -0.737934
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35 H -0.723609 -1.133184 -1.120413
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37 H -3.643765 -0.779842 -0.671132
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39 H -2.859670 -2.026560 -1.693457
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41 H -2.890016 -2.204513 0.095601
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45 serine_21 -569.59182483 a.u.
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49 C 1.902472 -0.842759 0.235314
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51 O 2.228513 -0.437775 1.355491
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53 H 0.608990 -0.673724 -1.327362
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55 N 0.656805 -0.571332 -0.315819
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57 C -0.123461 0.529307 0.244211
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3	C	-1.632051	0.305941	0.125255
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5	O	-2.428933	1.249312	0.219811
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9	O	1.689991	2.049967	-0.408276
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11	H	2.024094	1.896661	0.489325
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13	H	-1.315843	-1.702457	-0.022314
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15	N	-2.025758	-0.982088	-0.087774
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17	C	-3.442926	-1.327577	-0.078888
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21	H	2.264528	-2.307639	-1.345426
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23	H	3.477783	-1.000374	-1.191420
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25	H	0.121132	0.550406	1.319853
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27	H	-0.055642	1.914664	-1.435093
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29	H	-0.239796	2.689360	0.160964
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31	H	-3.556041	-2.362457	-0.427078
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33	H	-3.876010	-1.227017	0.929011
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35	H	-3.984633	-0.651774	-0.754406
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43	C	2.061561	-0.225220	-0.153356
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45	O	1.971459	0.410743	-1.215804
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47	H	1.052193	-1.219244	1.340311
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49	N	0.991240	-0.900189	0.378506
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51	C	-0.336415	-0.768235	-0.222914
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53	C	-0.981868	0.534850	0.277301
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55	O	-1.647952	0.576185	1.320128
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57	C	-1.199365	-1.979317	0.125655
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5 H -2.252234 -2.116208 -1.518185
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7 H 0.056124 1.516819 -1.161651
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9 N -0.708906 1.621999 -0.498122
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17 H 3.656861 0.687948 0.934709
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19 H -0.178689 -0.720025 -1.312451
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21 H -0.629879 -2.902796 -0.082513
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23 H -1.465681 -1.945947 1.192111
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25 H -2.154975 2.949642 0.229192
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27 H -0.510241 3.264737 0.841687
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29 H -0.925576 3.667423 -0.860526
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39 O 1.523968 -0.537806 -1.247116
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41 H 3.690331 -0.237032 1.254926
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43 H 3.535622 -1.663313 0.175610
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47 N 1.271611 0.457991 0.805346
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49 C -0.123939 0.896566 0.655632
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53 O -1.793877 -0.557454 1.645424
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55 C -0.305181 1.837787 -0.548814
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57 O -1.663877 2.273868 -0.635402
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13	N	-1.200831	-0.962312	-0.537884
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17	H	-0.379297	-0.880270	-1.141845
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19	H	-3.017674	-1.969298	-0.242921
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21	H	-2.040026	-2.525664	-1.639894
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23	H	-1.577403	-2.979573	0.037362
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29	C	-3.368232	-0.697605	-0.005877
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31	C	-2.044779	-0.023753	0.287920
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33	O	-1.582025	0.086522	1.426521
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35	H	-4.014268	-0.622803	0.877715
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37	H	-3.871624	-0.258975	-0.880328
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39	H	-3.165531	-1.761470	-0.209930
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41	N	-1.378254	0.480070	-0.820537
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43	C	0.063347	0.678185	-0.710789
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45	C	0.752395	-0.664955	-0.371925
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47	O	0.187176	-1.747456	-0.580849
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49	C	0.409001	1.829697	0.242811
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53	H	-1.673375	0.064693	-1.699466
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H	-0.313497	2.645681	0.079739
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N	2.012849	-0.565238	0.121370
C	2.786644	-1.766373	0.409616
H	2.429266	0.359853	0.179781
H	2.243591	-2.401946	1.123922
H	2.963479	-2.351768	-0.506152
H	3.748763	-1.466145	0.844722
serine_25 -569.59147579 a.u.			
C	-2.298150	-2.206374	-0.045689
C	-1.173185	-1.221967	0.209726
O	-0.549658	-1.170848	1.274720
H	-2.136371	-3.100163	0.570135
H	-3.247728	-1.737991	0.259419
H	-2.372354	-2.487088	-1.106940
N	-0.867875	-0.382972	-0.850072
C	-0.114319	0.849221	-0.593627
C	1.316832	0.582489	-0.106396
O	1.913930	1.411359	0.591411
C	-0.842794	1.782666	0.372318
O	-2.149696	1.990623	-0.204110
H	-1.588321	-0.303609	-1.561586
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H	-0.279868	2.724265	0.450280
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5	H	1.262252	-1.256855	-0.952739
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7	H	3.897224	-0.142026	-0.136463
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9	H	3.116779	-1.274059	1.002736
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11	H	3.554611	-1.822937	-0.653616
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15	serine_26	-569.59097222	a.u.	
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17	C	-3.365625	-0.664387	0.016355
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19	C	-2.024299	-0.024972	0.304893
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21	O	-1.522386	0.013097	1.430844
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23	H	-1.708016	0.160547	-1.684808
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25	N	-1.385237	0.532836	-0.796138
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27	C	0.062488	0.710077	-0.711620
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29	C	0.739112	-0.650642	-0.414875
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31	O	0.173044	-1.716945	-0.695004
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33	C	0.437816	1.841261	0.264401
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35	O	1.810007	2.259018	0.086308
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37	H	1.875721	2.725536	-0.759103
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39	H	2.395588	0.328823	0.275979
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41	N	1.982807	-0.586843	0.122096
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43	C	2.717777	-1.810415	0.418795
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45	H	-3.184390	-1.716010	-0.259233
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47	H	-3.980037	-0.636950	0.924852
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51	H	0.397421	1.019723	-1.718753
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55	H	0.358847	1.498261	1.301435
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5 H 3.677072 -1.537960 0.877454
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23 N 1.013513 -0.277358 1.009439
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25 C 0.043823 0.821603 0.962536
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31 C 0.635807 2.105708 0.368111
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33 O 1.195401 1.899935 -0.923659
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39 H -0.261965 1.032327 2.003800
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45 N -1.803338 -0.759658 0.630890
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21	C 0.948338 -0.319405 0.175617
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23	O 0.682315 -0.627100 1.339808
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25	C 0.585106 2.036046 -0.684979
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27	O 0.555834 2.518630 0.666643
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29	H -1.392782 1.096748 0.768550
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31	H 0.829259 3.445714 0.665419
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33	H -0.006516 0.230311 -1.692487
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35	H 1.614931 2.033067 -1.082784
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37	H -0.059816 2.649008 -1.338440
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39	N 2.095486 -0.719118 -0.458693
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41	C 2.983345 -1.674846 0.199203
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43	H 2.103541 -0.676379 -1.471064
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45	H 3.244392 -1.291690 1.194232
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47	H 2.502106 -2.658503 0.320844
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49	H 3.896388 -1.779811 -0.401515
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52	serine_29 -569.58914106 a.u.
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11 N 0.701436 -0.692555 0.270381
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13 C -0.112451 0.516692 0.480220
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15 C -1.595314 0.135149 0.453333
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17 O -2.424065 0.703371 1.171490
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19 C 0.101714 1.617701 -0.591567
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21 O 1.162618 2.507653 -0.303826
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23 H 0.304650 -1.554458 0.632035
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27 H 0.084667 0.966611 1.467127
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31 H -0.812406 2.230593 -0.615872
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33 N -1.938572 -0.839096 -0.446965
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35 C -3.347612 -1.140230 -0.687990
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37 H -1.242358 -1.121641 -1.127647
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39 H -3.839905 -1.351070 0.270601
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41 H -3.865516 -0.291638 -1.162137
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43 H -3.413515 -2.023863 -1.335926
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47 serine_30 -569.58967453 a.u.
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49 C 3.120214 -1.062621 -1.125943
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51 C 2.276523 -0.430251 -0.034762
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53 O 2.772866 0.070824 0.983023
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55 H 3.827923 -0.310085 -1.502676
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57 H 3.702620 -1.883094 -0.682018
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9	C	-1.382747	-0.447859	0.553388
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11	O	-1.859133	-1.218111	1.396025
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15	O	-0.275028	2.061592	-0.762286
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23	H	-0.679304	2.133670	1.305476
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55	N	-0.880662	-0.385583	-0.843230
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57	C	-0.138070	0.850099	-0.570972
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17 H -1.017581 1.228751 1.371161
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19 H -0.301198 2.668626 0.596165
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21 N 1.889604 -0.535642 -0.590219
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23 C 3.193185 -0.943158 -0.076611
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25 H 1.261713 -1.244139 -0.951920
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27 H 3.889396 -0.098032 -0.153681
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31 H 3.566027 -1.778882 -0.683364
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39 C -1.243826 -1.174527 0.209494
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43 H -1.471793 -0.370793 -1.667727
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45 N -0.896382 -0.343169 -0.834101
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51 O 1.999023 1.409182 0.461219
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53 C -0.757341 1.857994 0.345597
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55 O -2.077971 2.188122 -0.114630
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57 H -2.683390 1.518210 0.229287
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9	H	-2.602266	-2.232751	-1.158278
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13	H	-3.127596	-2.128697	0.555107
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15	H	0.000033	1.347900	-1.599042
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17	H	-0.771579	1.450944	1.366716
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19	H	-0.174430	2.786743	0.343097
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21	H	3.884205	-0.298166	-0.177292
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23	H	3.098716	-1.264119	1.101931
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25	H	3.445822	-2.005642	-0.499790
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29	serine_33 -569.58936549 a.u.			
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31	C	2.475785	-2.053480	-0.104962
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33	C	1.430630	-0.983725	-0.338442
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35	O	0.705849	-0.954067	-1.338906
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37	H	2.873627	-2.382786	-1.073295
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39	H	3.295058	-1.704336	0.540484
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43	N	1.324283	-0.020564	0.651226
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45	C	0.113913	0.808349	0.675184
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47	C	-1.128049	-0.100300	0.578995
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49	O	-1.236876	-1.073151	1.334345
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53	O	1.383708	2.745174	-0.085455
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57	H	2.137020	2.134424	-0.081052
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5 H 0.260523 1.533240 -1.373092
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17 H -3.959323 -0.133415 -1.173905
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19 H -2.905630 -1.579494 -0.970407
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23 serine_34 -569.58548889 a.u.
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27 C 2.364738 -0.306753 0.074195
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31 H 0.758195 -1.548332 0.196578
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33 N 1.009359 -0.591784 -0.039184
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23	O	-1.335686	-1.137270	0.936529
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25	H	-3.509933	-1.888000	-0.302829
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27	H	-3.918624	-0.257450	0.282748
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29	H	-3.536420	-0.503888	-1.448592
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31	N	-1.164516	0.271937	-0.893674
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35	C	1.405317	0.081023	-0.532562
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37	O	2.486328	0.545880	-0.935722
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39	C	0.117762	2.083065	0.264366
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41	O	-0.098032	1.521891	1.562812
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43	H	-1.718366	0.618575	-1.667605
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55	C	2.468403	-1.880646	0.412939
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57	H	0.387657	-1.279798	0.578270
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21 H 3.803833 -0.430807 0.328313
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31 O -0.902710 -1.443946 1.361609
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43 H -1.342684 2.408299 0.744201
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45 H 0.399447 2.853530 0.794747
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6	C	-3.448036	-0.344564	-0.374990
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10	O	-1.856220	0.649850	1.155911
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12	H	-3.948946	0.627191	-0.482656
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14	H	-3.420352	-0.856961	-1.347981
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16	H	-4.033544	-0.950370	0.333526
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18	N	-1.034945	-0.815241	-0.386210
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20	C	0.278519	-0.858125	0.257787
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22	C	0.939590	0.527594	0.331762
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24	O	1.677284	0.837070	1.267507
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26	C	1.149593	-1.821887	-0.556702
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28	O	2.390796	-1.966897	0.127289
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30	H	-1.286792	-1.578661	-1.006624
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32	H	2.988924	-2.474568	-0.437233
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34	H	0.201738	-1.210573	1.299345
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36	H	0.624539	-2.795018	-0.634847
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38	H	1.290441	-1.408890	-1.572572
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40	N	0.726851	1.327695	-0.763051
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42	C	1.183755	2.713781	-0.717124
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44	H	-0.096990	1.110952	-1.313221
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46	H	2.254866	2.728948	-0.477342
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48	H	1.025182	3.171529	-1.702782
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53	serine_38	-569.57795927	a.u.	
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3 O 2.488694 -0.392232 1.176244
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5 H 3.237631 -2.508755 -0.281146
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17 O -1.842558 -0.603319 1.584499
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19 C -0.157711 1.888221 -0.283546
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33 N -2.172442 -0.282018 -0.649916
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35 C -3.512169 -0.862667 -0.599564
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39 H -3.460397 -1.851761 -0.125035
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41 H -4.201879 -0.235396 -0.013122
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43 H -3.888815 -0.967942 -1.625446
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CYSTEINE

cysteine_1 -892.21081947086 a.u.

50 C -2.250475 -2.429025 -0.803597
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52 C -1.705008 -1.313294 0.063364
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54 O -2.443769 -0.622773 0.792264
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56 H -2.718237 -3.179529 -0.149367
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3	H	-3.032565	-2.016087	-1.456741
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7	N	-0.358239	-1.117616	0.006890
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9	C	0.327371	-0.108090	0.807715
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11	C	0.238126	1.293364	0.164326
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13	O	1.241303	1.917042	-0.224971
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15	C	1.782348	-0.525004	1.040149
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17	S	2.681147	-0.977895	-0.500053
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19	H	0.208275	-1.609646	-0.680558
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21	H	2.610078	0.269090	-1.021316
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23	H	-0.196100	-0.063949	1.779520
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25	H	2.322010	0.287929	1.544295
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27	H	1.809625	-1.424789	1.673800
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29	N	-1.023164	1.778410	0.075788
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31	C	-1.278214	3.070030	-0.550455
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33	H	-1.784325	1.183804	0.407467
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35	H	-0.717473	3.862809	-0.033882
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37	H	-0.966190	3.061603	-1.606209
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39	H	-2.353453	3.279909	-0.487142
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49	O	-2.620707	0.938535	-0.747450
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51	H	-4.452654	-0.407498	0.761596
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53	H	-4.306892	-1.213791	-0.816389
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55	H	-3.535755	-1.945305	0.631419
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57	N	-1.352565	-0.699240	0.196431
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3 C -0.119117 -0.022078 -0.146425
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5 C 1.009726 -1.055123 -0.017833
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7 O 0.800504 -2.187716 0.449573
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9 C 0.091440 1.194582 0.785608
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11 S 1.272374 2.441199 0.126578
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13 H -1.259249 -1.652596 0.540139
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15 H 0.468274 2.854183 -0.879441
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17 H -0.187717 0.343966 -1.185900
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19 H -0.878258 1.684709 0.941265
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21 H 0.493774 0.871713 1.758979
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23 N 2.231351 -0.644850 -0.440111
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25 C 3.397387 -1.506892 -0.273791
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27 H 2.344417 0.336802 -0.680404
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29 H 3.617403 -1.680981 0.791061
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31 H 3.210186 -2.478909 -0.750785
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33 H 4.257597 -1.023032 -0.753620
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37 cysteine_3 -892.20737742594 a.u.

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41 C 2.215467 -0.757578 -0.175347
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43 O 2.279015 -0.126889 -1.244419
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45 H 3.980631 -1.956834 -0.166067
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47 H 4.118577 -0.433174 0.740149
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49 H 3.227096 -1.818487 1.455760
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51 N 1.018490 -1.034948 0.428544
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53 C -0.249306 -0.560703 -0.136710
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55 C -0.480714 0.899623 0.294913
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57 O -1.222700 1.198054 1.246003
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9	H	-3.136455	0.129468	0.206984
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11	H	-0.147099	-0.611156	-1.231629
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13	H	-1.175579	-2.501094	0.042784
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15	H	-1.509875	-1.397143	1.420737
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17	N	0.218742	1.806260	-0.432477
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19	C	0.221985	3.214254	-0.052476
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21	H	0.930343	1.436487	-1.062197
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23	H	-0.813087	3.564270	0.060312
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25	H	0.745933	3.373398	0.903930
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27	H	0.718843	3.789427	-0.844161
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31	cysteine_4	-892.20640260508	a.u.	
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33	C	-2.291869	-2.368868	-0.833364
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35	C	-1.726852	-1.292512	0.070467
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37	O	-2.453325	-0.612504	0.819979
38				
39	H	-2.796282	-3.119221	-0.206945
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41	H	-3.047684	-1.914303	-1.489990
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43	H	-1.521974	-2.862129	-1.443667
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45	N	-0.374682	-1.123872	0.024483
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51	O	1.269319	1.864880	-0.225919
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53	C	1.774584	-0.530576	1.043904
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55	S	2.656412	-0.847426	-0.549478
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57	H	0.171391	-1.566894	-0.710937
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5 H -0.200222 -0.072622 1.797671
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9 H 1.815272 -1.443416 1.654074
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17 H -0.644374 3.864488 -0.065454
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19 H -0.918925 3.046218 -1.624405
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21 H -2.296179 3.316595 -0.503977
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33 H 3.871696 -1.432341 -1.011211
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35 H 2.953812 -0.208472 -1.955245
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37 H 4.114303 0.297748 -0.685406
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39 N 1.047243 -0.085495 -0.267561
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41 C 0.007599 0.170911 0.718670
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43 C -1.302774 -0.564928 0.402333
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45 O -2.383883 -0.185360 0.878618
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47 C -0.263415 1.670818 0.881924
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49 S -0.786072 2.457067 -0.698267
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51 H 0.965721 0.437521 -1.137125
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53 H -2.000968 1.862636 -0.724410
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57 H -1.038589 1.835246 1.641390
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11	H	-3.147766	-1.876232	-1.142113
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13	H	-2.050574	-3.274650	-1.391310
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25	O	-0.690372	2.052903	-0.968863
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27	H	1.281345	0.720300	1.118803
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29	N	0.503515	0.738546	0.466546
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31	C	0.223084	-0.492953	-0.272537
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33	C	-1.174454	-1.029581	0.112049
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35	O	-1.320801	-2.006065	0.862881
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39	S	3.002304	-0.996643	-0.188787
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41	H	2.871023	-0.603975	-1.476046
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43	H	-1.962230	0.549163	-0.891267
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45	N	-2.200983	-0.337961	-0.445065
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47	C	-3.576880	-0.638358	-0.066306
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53	H	1.182970	3.787182	-0.002332
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55	H	0.226305	-0.242218	-1.348600
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13 cysteine_7 -892.20580222661 a.u.
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33 O -0.880461 -1.789497 -1.013853
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35 C -0.024274 1.314855 -0.639102
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37 S -1.471709 2.333269 -0.146445
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41 H -2.404214 1.601387 -0.795068
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15	H	-0.256886	3.788183	1.015600
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17	H	1.171159	2.901798	1.649942
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19	H	1.248428	3.743788	0.068395
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21	N	0.503318	0.733003	0.473793
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23	C	0.227606	-0.510795	-0.249291
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25	C	-1.177173	-1.039704	0.111889
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27	O	-1.343899	-2.030771	0.839090
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29	C	1.273842	-1.566086	0.094121
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31	S	2.942421	-0.894069	-0.312602
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33	H	1.153666	0.700979	1.251855
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35	H	3.629099	-1.994624	0.062770
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37	H	0.256589	-0.270305	-1.326244
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39	H	1.209732	-1.825116	1.160255
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41	H	1.074607	-2.467631	-0.499881
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43	N	-2.188496	-0.320146	-0.436614
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53	H	-4.229677	-0.005824	-0.724105
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9 H 0.706373 0.818919 1.478874
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11 N 0.433370 0.815702 0.500816
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13 C 0.316083 -0.477656 -0.176940
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17 O -1.166572 -2.032246 0.982722
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21 S 3.089934 -0.823637 -0.378985
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23 H 2.986488 0.437990 0.094291
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27 N -2.086424 -0.567853 -0.527118
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35 H 0.611758 3.946538 0.209557
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39 H 1.477481 -1.518234 1.337117
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41 H 1.304908 -2.390646 -0.194713
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43 H -4.124357 -0.510023 -0.968679
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45 H -3.542067 -2.059804 -0.279259
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47 H -3.757017 -0.646087 0.784944
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51 cysteine_10 -892.20459812865 a.u.
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15	O	-1.063848	1.216797	1.367845
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17	C	-1.421082	-1.409217	0.400509
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29	H	-1.578355	-1.231642	1.475383
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31	N	0.162751	1.811242	-0.481082
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35	H	0.821974	1.432875	-1.158986
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37	H	-0.789666	3.569869	0.140340
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53	H	4.261090	-0.158955	-0.906999
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13 S -0.613220 2.245827 -0.659492
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15 H 0.912858 -0.986768 -1.128682
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17 H 0.433348 1.848674 -1.417430
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21 H -0.846358 1.545780 1.604720
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53 N -0.602772 0.593979 0.966319
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55 C 0.065116 -0.679141 0.674272
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57 C 1.587886 -0.564253 0.469417
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27	H	3.526845	1.356668	-1.435968
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29	H	3.982103	0.722969	0.180705
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33 cysteine_13 -892.20415032168 a.u.

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39	O	2.556463	-0.695091	1.342571
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41	H	0.814157	-0.634445	-1.324296
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53	S	0.162540	2.361761	-0.327196
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55	H	-0.945523	1.963799	-0.993715
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35 H -1.521403 3.644854 0.137582
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37 H -2.842236 2.447224 0.108481
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23	C	3.192541	-1.034334	-0.980308
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27	O	2.491306	-0.972619	1.330322
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29	H	3.597561	-2.051811	-0.884016
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31	H	2.749346	-0.909425	-1.979055
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33	H	4.027928	-0.328565	-0.860615
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35	N	0.932756	-0.411746	-0.259641
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37	C	-0.024861	0.089923	0.716751
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39	C	-1.460446	-0.352915	0.399169
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41	O	-2.435691	0.262942	0.850339
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43	C	0.030804	1.614361	0.867502
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45	S	-0.281874	2.477235	-0.732086
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15 cysteine_16 -892.20224663189 a.u.
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23 H 0.415775 -1.221016 -1.274249
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25 N 0.684644 -0.785833 -0.397013
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27 C -0.242731 0.172088 0.165083
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29 C -1.658990 -0.270842 -0.210302
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31 O -1.894141 -0.803026 -1.305330
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33 C -0.038045 1.603119 -0.370722
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35 S 1.687163 2.211342 -0.185581
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37 H 1.949135 1.531995 0.955329
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39 H -2.356736 0.339865 1.616196
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41 N -2.631119 0.022961 0.694850
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43 C -4.025435 -0.319221 0.427509
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55 H -0.736648 2.282156 0.143127
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19	H	-0.988650	3.142145	-1.357313
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21	H	-1.254308	3.716862	0.317785
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23	N	-0.485023	0.838241	-0.335903
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25	C	-0.290036	-0.412864	0.388467
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27	C	1.148036	-0.947427	0.325091
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29	O	1.521025	-1.807845	1.131803
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31	C	-1.193933	-1.508285	-0.193742
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33	S	-2.976794	-1.060434	-0.230077
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35	H	-1.374075	0.918885	-0.827127
36				
37	H	-3.105728	-0.889853	1.105247
38				
39	H	-0.504349	-0.275514	1.463201
40				
41	H	-0.925575	-1.698798	-1.245924
42				
43	H	-1.046234	-2.433486	0.378882
44				
45	N	1.903435	-0.503547	-0.716930
46				
47	C	3.313999	-0.866989	-0.798765
48				
49	H	1.571364	0.327150	-1.193236
50				
51	H	3.410987	-1.952732	-0.668661
52				
53	H	3.696682	-0.581179	-1.787383
54				
55	H	3.904484	-0.367173	-0.013957
56				
57				
58				
59				
60				

cysteine_18 -892.20247180682 a.u.

C	-1.915259	2.588281	0.523677
C	-0.928778	1.542406	0.047740
O	-0.447263	1.567506	-1.098996
H	-1.616718	3.565682	0.122766
H	-2.904952	2.332243	0.113894
H	-1.987546	2.639593	1.619943
N	-0.619431	0.563102	0.950585
C	0.073417	-0.693437	0.633114
C	1.598734	-0.573253	0.450689
O	2.356831	-1.374793	1.020331
C	-0.538606	-1.415001	-0.578138
S	-2.353633	-1.576706	-0.293676
H	-1.060445	0.617825	1.860749
H	-2.556299	-2.547124	-1.210376
H	-0.050717	-1.336525	1.516484
H	-0.357136	-0.854166	-1.503521
H	-0.083716	-2.414229	-0.639822
N	2.024393	0.407388	-0.381048
C	3.446356	0.566422	-0.658716
H	1.316786	0.965331	-0.862182
H	3.850484	-0.322876	-1.166906
H	3.578372	1.447881	-1.299195
H	4.003568	0.706015	0.279357

cysteine_19 -892.20231698181 a.u.

C	-3.679907	-0.450545	0.165650
C	-2.205160	-0.330866	-0.165787

1				
2				
3	O	-1.822551	-0.010798	-1.305738
4				
5	H	-1.739638	-0.791304	1.768909
6				
7	N	-1.340975	-0.607079	0.856154
8				
9	C	0.129463	-0.579356	0.761866
10				
11	C	0.668484	0.862168	0.660991
12				
13	O	1.256814	1.391340	1.614500
14				
15	C	0.645849	-1.506201	-0.349434
16				
17	S	2.477012	-1.615591	-0.340097
18				
19	H	2.686659	-0.335371	-0.721133
20				
21	H	-0.230188	1.058213	-1.151173
22				
23	N	0.479547	1.471449	-0.543095
24				
25	C	0.847094	2.875086	-0.702147
26				
27	H	-4.165617	0.509580	-0.060281
28				
29	H	-4.120019	-1.214613	-0.491659
30				
31	H	-3.870213	-0.720181	1.214268
32				
33	H	0.506520	-0.945657	1.727735
34				
35	H	0.287784	-2.530418	-0.157771
36				
37	H	0.289973	-1.194797	-1.338520
38				
39	H	0.706968	3.155239	-1.754210
40				
41	H	0.235746	3.530087	-0.060057
42				
43	H	1.900786	3.012023	-0.422899
44				
45				
46				
47	cysteine_20 -892.20163042237 a.u.			
48				
49	C	3.479346	-0.888263	-0.870725
50				
51	C	2.412063	-0.595657	0.165546
52				
53	O	2.682368	-0.354207	1.352719
54				
55	H	4.155660	-1.656612	-0.470709
56				
57	H	3.060956	-1.224672	-1.830207
58				
59				
60				

1
2
3 H 4.065095 0.028812 -1.034233
4
5 N 1.123925 -0.605420 -0.288984
6
7 C 0.024941 -0.276074 0.589453
8
9 C -1.266650 -0.700044 -0.117565
10
11 O -1.296904 -0.929661 -1.335607
12
13 C -0.013279 1.223978 0.947729
14
15 S -0.386986 2.212774 -0.563396
16
17 H 0.890591 -0.773483 -1.263767
18
19 H -0.029836 3.400649 -0.029123
20
21 H 0.148106 -0.833841 1.535061
22
23 H -0.786653 1.404467 1.711058
24
25 H 0.971106 1.501810 1.347598
26
27 N -2.371880 -0.767536 0.669966
28
29 C -3.684277 -1.022402 0.082661
30
31 H -2.290142 -0.552605 1.655309
32
33 H -3.946051 -0.230024 -0.634438
34
35 H -3.680127 -1.985184 -0.447742
36
37 H -4.427817 -1.051283 0.889174
38
39
40
41 cysteine_21 -892.20145215785 a.u.
42
43 C -3.693405 -0.396087 0.184280
44
45 C -2.218737 -0.300921 -0.155609
46
47 O -1.836793 -0.008109 -1.302870
48
49 H -4.146305 -1.165264 -0.458242
50
51 H -3.882438 -0.645664 1.238129
52
53 H -4.167753 0.566369 -0.055471
54
55 N -1.353617 -0.564722 0.868933
56
57 C 0.115631 -0.567374 0.766358
58
59
60

1				
2				
3	C	0.708038	0.851315	0.652950
4				
5	O	1.396978	1.321994	1.570578
6				
7	C	0.599671	-1.525517	-0.333687
8				
9	S	2.426816	-1.553283	-0.464477
10				
11	H	-1.752094	-0.728227	1.785546
12				
13	H	2.663247	-1.951139	0.805956
14				
15	H	0.481852	-0.933104	1.737947
16				
17	H	0.213643	-2.537248	-0.136177
18				
19	H	0.240178	-1.203056	-1.320130
20				
21	N	0.434276	1.508875	-0.501591
22				
23	C	0.921511	2.868386	-0.698389
24				
25	H	-0.273836	1.108046	-1.116607
26				
27	H	2.012372	2.893185	-0.565200
28				
29	H	0.668765	3.184122	-1.718824
30				
31	H	0.470965	3.565546	0.026215
32				
33				
34				
35	cysteine_22 -892.20181857175 a.u.			
36				
37	C	1.102074	2.986967	-0.082923
38				
39	C	0.395113	1.677871	0.208287
40				
41	O	-0.164081	1.433290	1.282163
42				
43	H	0.666512	3.774438	0.544863
44				
45	H	2.166680	2.876093	0.179745
46				
47	H	1.033139	3.267708	-1.144632
48				
49	N	0.399579	0.758925	-0.829690
50				
51	C	0.111965	-0.648988	-0.542765
52				
53	C	-1.343870	-0.875941	-0.093951
54				
55	O	-1.649089	-1.865230	0.582963
56				
57	C	1.078943	-1.266243	0.478613
58				
59				
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2
3 S 2.832761 -1.131610 -0.052328
4
5 H 1.091604 0.923634 -1.554785
6
7 H 2.781317 -2.097734 -0.996712
8
9 H 0.219825 -1.185380 -1.501871
10
11 H 1.007476 -0.723694 1.431939
12
13 H 0.815217 -2.315622 0.657635
14
15 N -2.256044 0.009730 -0.583171
16
17 C -3.635841 -0.045061 -0.112187
18
19 H -1.889206 0.882283 -0.944236
20
21 H -4.013033 -1.070033 -0.223074
22
23 H -3.709471 0.241756 0.949397
24
25 H -4.243928 0.635610 -0.722440
26
27
28

29 cysteine_23 -892.20174893625 a.u.

30
31 C 1.165494 2.962890 -0.106197
32
33 C 0.485616 1.643621 0.210875
34
35 O 0.005282 1.387380 1.320361
36
37 H 0.583272 3.777753 0.345083
38
39 H 2.163034 2.962912 0.360529
40
41 H 1.277298 3.138321 -1.186217
42
43 N 0.415747 0.739381 -0.831326
44
45 C 0.074991 -0.661819 -0.575068
46
47 C -1.384582 -0.849926 -0.120908
48
49 O -1.723655 -1.869404 0.492397
50
51 C 1.016793 -1.349234 0.425911
52
53 S 2.772860 -1.279169 -0.103036
54
55 H 1.004767 0.922295 -1.636892
56
57 H 2.996190 -0.001762 0.276982
58
59
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1				
2				
3	H	0.166044	-1.177935	-1.545889
4				
5	H	0.908750	-0.913088	1.426702
6				
7	H	0.753936	-2.414391	0.481359
8				
9	N	-2.263221	0.109146	-0.524333
10				
11	C	-3.640460	0.074542	-0.044303
12				
13	H	-1.867723	0.985872	-0.840926
14				
15	H	-4.059014	-0.924029	-0.225637
16				
17	H	-3.694850	0.285201	1.036007
18				
19	H	-4.225277	0.821632	-0.596829
20				
21				
22				
23	cysteine_24 -892.20071350906 a.u.			
24				
25	C	-0.700967	3.252451	-0.399680
26				
27	C	-0.110184	2.000100	0.219215
28				
29	O	0.667381	2.019533	1.177572
30				
31	H	0.051507	4.051570	-0.373923
32				
33	H	-1.042541	3.089962	-1.432567
34				
35	H	-1.560350	3.570609	0.211432
36				
37	N	-0.489935	0.806304	-0.372007
38				
39	C	-0.253376	-0.441141	0.350650
40				
41	C	1.203752	-0.926259	0.294445
42				
43	O	1.581467	-1.829728	1.050390
44				
45	C	-1.119725	-1.560623	-0.236225
46				
47	S	-2.900288	-1.102148	-0.067983
48				
49	H	-1.317757	0.829108	-0.963887
50				
51	H	-3.375026	-2.030378	-0.925814
52				
53	H	-0.477197	-0.304377	1.423341
54				
55	H	-0.878337	-1.698436	-1.301680
56				
57	H	-0.910710	-2.484895	0.317554
58				
59				
60				

1
2
3 N 1.981211 -0.372206 -0.674707
4
5 C 3.406209 -0.678810 -0.729775
6
7 H 1.629521 0.471811 -1.111277
8
9 H 3.539649 -1.767393 -0.679602
10
11 H 3.813078 -0.302940 -1.677726
12
13 H 3.948788 -0.221716 0.113408
14
15
16

17 cysteine_25 -892.19944915731 a.u.
18

19 C 2.644242 -2.266022 -0.408406
20
21 C 1.777603 -1.241269 0.296839
22
23 O 2.046150 -0.802208 1.422550
24
25 H 2.913081 -3.053715 0.308562
26
27 H 2.152185 -2.711070 -1.285636
28
29 H 3.570299 -1.767072 -0.732348
30
31 N 0.689138 -0.803963 -0.415471
32
33 C -0.228931 0.174084 0.129812
34
35 C -1.651409 -0.265089 -0.221494
36
37 O -1.907919 -0.790861 -1.314840
38
39 C -0.009772 1.575851 -0.468698
40
41 S 1.674041 2.172532 -0.018913
42
43 H 0.421180 -1.244093 -1.290236
44
45 H 1.618499 3.279596 -0.792797
46
47 H -0.066081 0.202003 1.220290
48
49 H -0.104645 1.511404 -1.563264
50
51 H -0.770152 2.266642 -0.071884
52
53 N -2.605009 0.020334 0.706094
54
55 C -4.002746 -0.328655 0.467849
56
57 H -2.310195 0.326133 1.624988
58
59
60

1				
2				
3	H	-4.313353	0.060347	-0.511382
4				
5	H	-4.146829	-1.420068	0.469568
6				
7	H	-4.617323	0.125941	1.255289
8				
9				
10				
11	cysteine_26 -892.20064029699 a.u.			
12				
13	C	2.997166	-1.471871	-1.030993
14				
15	C	2.196993	-0.702582	0.004229
16				
17	O	2.735085	0.003574	0.868071
18				
19	H	3.649177	-0.765687	-1.565193
20				
21	H	3.640774	-2.193271	-0.506496
22				
23	H	2.366236	-2.007008	-1.755452
24				
25	N	0.834747	-0.821345	-0.086871
26				
27	C	-0.060805	-0.227290	0.900822
28				
29	C	-1.510056	-0.605592	0.585785
30				
31	O	-2.292031	-0.970305	1.470991
32				
33	C	0.076456	1.312631	1.005437
34				
35	S	0.084613	2.194992	-0.605102
36				
37	H	0.439818	-1.471153	-0.756823
38				
39	H	1.360818	1.879629	-0.919300
40				
41	H	0.154288	-0.634948	1.903169
42				
43	H	-0.788182	1.702673	1.566151
44				
45	H	0.996777	1.567002	1.543636
46				
47	N	-1.860062	-0.505105	-0.737223
48				
49	C	-3.265306	-0.665128	-1.109404
50				
51	H	-1.283486	0.127704	-1.291508
52				
53	H	-3.628964	-1.627920	-0.727667
54				
55	H	-3.893384	0.134090	-0.683562
56				
57	H	-3.341604	-0.652989	-2.204410
58				
59				
60				

cysteine_27 -892.20045719276 a.u.

C	1.395409	2.832856	-0.071384
C	0.576057	1.592403	0.222169
O	0.054880	1.365135	1.317757
H	1.053463	3.648326	0.578418
H	2.449427	2.613423	0.163544
H	1.327900	3.137496	-1.126717
N	0.433694	0.708960	-0.836803
C	0.029455	-0.677895	-0.580035
C	-1.434745	-0.802448	-0.122554
O	-1.815489	-1.804292	0.495025
C	0.939683	-1.397236	0.425644
S	2.681440	-1.166521	-0.135869
H	1.033629	0.865015	-1.640868
H	3.208517	-2.177729	0.585743
H	0.099300	-1.199420	-1.550026
H	0.805299	-0.976403	1.429700
H	0.685287	-2.464026	0.428771
N	-2.268085	0.194581	-0.528880
C	-3.643358	0.228504	-0.043498
H	-1.828212	1.052683	-0.839148
H	-4.105307	-0.753763	-0.207407
H	-3.684187	0.458815	1.033463
H	-4.197547	0.991279	-0.606084

cysteine_28 -892.20006965072 a.u.

C	3.018038	-1.952719	-0.036010
C	1.794409	-1.092053	0.216812

1				
2				
3	O	1.571803	-0.544687	1.300881
4				
5	H	3.901587	-1.431520	0.357881
6				
7	H	2.903378	-2.893029	0.524570
8				
9	H	3.169196	-2.184678	-1.100415
10				
11	N	0.939501	-0.926912	-0.856925
12				
13	C	-0.384177	-0.323594	-0.659753
14				
15	C	-0.257860	1.107647	-0.098122
16				
17	O	-1.085136	1.571848	0.695213
18				
19	C	-1.300808	-1.183841	0.225661
20				
21	S	-3.082925	-0.844698	-0.046198
22				
23	H	1.063643	-1.537121	-1.657694
24				
25	H	-3.028530	0.407878	0.458861
26				
27	H	-0.841901	-0.237231	-1.659801
28				
29	H	-1.163042	-2.242463	-0.046425
30				
31	H	-1.047083	-1.048462	1.284945
32				
33	N	0.769014	1.843480	-0.612363
34				
35	C	1.063642	3.153483	-0.039594
36				
37	H	1.515327	1.325028	-1.060535
38				
39	H	0.158933	3.774461	-0.072972
40				
41	H	1.389650	3.066924	1.009547
42				
43	H	1.853243	3.628572	-0.636480
44				
45				
46				
47	cysteine_29 -892.19926080892 a.u.			
48				
49	C	-3.687937	-0.466515	0.228138
50				
51	C	-2.223020	-0.334585	-0.140763
52				
53	O	-1.871304	-0.023942	-1.292916
54				
55	H	-4.188287	0.487734	0.009261
56				
57	H	-4.136878	-1.238240	-0.414087
58				
59				
60				

1
2
3 H -3.849961 -0.732066 1.282556
4
5 N -1.332676 -0.584404 0.865062
6
7 C 0.133033 -0.559711 0.742845
8
9 C 0.709168 0.866353 0.627777
10
11 O 1.477430 1.305373 1.497638
12
13 C 0.622574 -1.490337 -0.377789
14
15 S 2.465221 -1.529892 -0.303614
16
17 H -1.710280 -0.769675 1.786259
18
19 H 2.613610 -2.337789 -1.375952
20
21 H 0.521468 -0.931271 1.703455
22
23 H 0.220442 -2.499258 -0.201310
24
25 H 0.296299 -1.124262 -1.358319
26
27 N 0.343063 1.561180 -0.476933
28
29 C 0.836513 2.916813 -0.684105
30
31 H -0.369671 1.155138 -1.082988
32
33 H 0.475738 3.596180 0.104248
34
35 H 1.935918 2.921961 -0.664324
36
37 H 0.484360 3.268830 -1.662271
38
39
40
41 cysteine_30 -892.19936668052 a.u.
42
43 C 3.659957 -0.258078 -0.009699
44
45 C 2.188227 -0.442957 0.291014
46
47 O 1.710921 -0.334725 1.423458
48
49 H 4.243191 -0.492837 0.889445
50
51 H 3.992831 -0.884238 -0.850830
52
53 H 3.818656 0.800947 -0.270460
54
55 N 1.393876 -0.755620 -0.805614
56
57 C -0.037762 -0.475640 -0.694136
58
59
60

1				
2				
3	C	-0.233149	1.032294	-0.384812
4				
5	O	0.664071	1.846854	-0.641227
6				
7	C	-0.698692	-1.463363	0.289351
8				
9	S	-2.515023	-1.666499	0.064104
10				
11	H	1.803122	-0.486195	-1.696078
12				
13	H	-2.474693	-2.022626	-1.239782
14				
15	H	-0.463215	-0.651294	-1.698386
16				
17	H	-0.214396	-2.443401	0.178140
18				
19	H	-0.565497	-1.126520	1.325842
20				
21	N	-1.433295	1.397580	0.133242
22				
23	C	-1.722747	2.805662	0.381026
24				
25	H	-2.168386	0.699437	0.200886
26				
27	H	-1.709703	3.383826	-0.556153
28				
29	H	-2.714083	2.879773	0.846695
30				
31	H	-0.966461	3.228840	1.057303
32				
33				
34				
35	cysteine_31 -892.19910741984 a.u.			
36				
37	C	3.216666	-1.248422	-1.017932
38				
39	C	2.359884	-0.524992	0.004034
40				
41	O	2.845101	0.145817	0.923009
42				
43	H	3.816796	-0.502161	-1.558968
44				
45	H	3.908019	-1.915961	-0.483864
46				
47	H	2.626823	-1.830259	-1.741011
48				
49	N	0.999114	-0.637116	-0.171850
50				
51	C	0.084487	-0.108422	0.836319
52				
53	C	-1.328161	-0.658767	0.649883
54				
55	O	-2.068003	-0.868038	1.617205
56				
57	C	0.061248	1.434819	0.837093
58				
59				
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2
3 S -0.471741 2.194602 -0.752174
4
5 H 0.655646 -1.361136 -0.793002
6
7 H -1.798192 2.185412 -0.492070
8
9 H 0.415970 -0.421152 1.841539
10
11 H -0.590132 1.790434 1.648842
12
13 H 1.083216 1.794758 1.018045
14
15 N -1.705349 -0.893239 -0.651962
16
17 C -3.102497 -1.235562 -0.919576
18
19 H -1.225721 -0.316084 -1.341628
20
21 H -3.377923 -2.105661 -0.310203
22
23 H -3.783891 -0.407309 -0.663483
24
25 H -3.205648 -1.486206 -1.983348
26
27
28

29 cysteine_32 -892.19858623738 a.u.

30
31 C 3.489315 -0.677007 -0.065923
32
33 C 2.047336 -0.217198 -0.154329
34
35 O 1.533332 0.088361 -1.246687
36
37 H 1.852271 -0.508948 1.843052
38
39 N 1.362175 -0.175007 1.022329
40
41 C -0.031390 0.247487 1.234112
42
43 C -1.119418 -0.703936 0.709375
44
45 O -2.183851 -0.797406 1.336439
46
47 C -0.321822 1.710213 0.800895
48
49 S -1.086806 1.991050 -0.843192
50
51 H -0.037374 1.532066 -1.560153
52
53 H -0.086605 -1.010630 -1.005236
54
55 N -0.841667 -1.387123 -0.432686
56
57 C -1.918893 -2.123618 -1.088027
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59
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3	H	4.124737	0.090772	-0.530138
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5	H	3.828471	-0.858313	0.963888
6				
7	H	3.594290	-1.601281	-0.652841
8				
9	H	-0.159935	0.218430	2.327311
10				
11	H	-1.066053	2.118941	1.501310
12				
13	H	0.600260	2.303687	0.894445
14				
15	H	-1.493860	-2.696120	-1.922811
16				
17	H	-2.378181	-2.812936	-0.367337
18				
19	H	-2.699282	-1.440835	-1.462551
20				
21				
22				
23	cysteine_33	-892.19861635228	a.u.	
24				
25	C	-3.470899	-1.367935	-0.309820
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27	C	-2.216876	-0.733676	0.262301
28				
29	O	-2.204691	-0.095698	1.318115
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31	H	-4.306094	-0.663535	-0.196814
32				
33	H	-3.362637	-1.650029	-1.367554
34				
35	H	-3.704777	-2.268638	0.278576
36				
37	N	-1.063224	-0.898307	-0.484277
38				
39	C	0.230841	-0.566759	0.117524
40				
41	C	0.454163	0.948220	0.227674
42				
43	O	1.310871	1.406831	0.998970
44				
45	C	1.344560	-1.185076	-0.746214
46				
47	S	2.980324	-1.237262	0.083438
48				
49	H	-1.078484	-1.582403	-1.234112
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51	H	2.880421	0.008938	0.607567
52				
53	H	0.280688	-0.962180	1.145085
54				
55	H	1.096439	-2.240209	-0.950414
56				
57	H	1.416997	-0.648775	-1.706319
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59				
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2
3 N -0.258387 1.721854 -0.633909
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5 C -0.175725 3.175846 -0.544286
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7 H -1.055832 1.288692 -1.084112
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9 H 0.878847 3.480123 -0.572540
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11 H -0.705599 3.612106 -1.401037
12
13 H -0.619701 3.544499 0.394208
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15
16

17 cysteine_34 -892.19849231317 a.u.
18

19 C 3.659020 -0.286207 -0.014330
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21 C 2.185758 -0.446939 0.292448
22
23 O 1.712045 -0.316390 1.424710
24
25 H 4.241792 -0.526845 0.883599
26
27 H 3.978952 -0.920360 -0.854396
28
29 H 3.834157 0.769180 -0.279229
30
31 N 1.383605 -0.763547 -0.795252
32
33 C -0.044207 -0.476832 -0.674032
34
35 C -0.236091 1.035769 -0.391618
36
37 O 0.640122 1.851085 -0.710172
38
39 C -0.708634 -1.424009 0.345757
40
41 S -2.481380 -1.673223 -0.125866
42
43 H 1.786582 -0.511453 -1.693506
44
45 H -2.876606 -2.217282 1.045461
46
47 H -0.479569 -0.671832 -1.671206
48
49 H -0.191173 -2.391773 0.310998
50
51 H -0.646844 -1.008563 1.357737
52
53 N -1.413723 1.402383 0.175009
54
55 C -1.703509 2.812716 0.408705
56
57 H -2.131721 0.698361 0.321071
58
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2				
3	H	-0.934628	3.251711	1.060693
4				
5	H	-1.714645	3.374146	-0.538285
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7	H	-2.684749	2.889882	0.894743
8				
9				
10				
11	cysteine_35 -892.19856656126 a.u.			
12				
13	C	3.313770	-0.639440	-0.482950
14				
15	C	1.872911	-0.190529	-0.374524
16				
17	O	1.116007	-0.144500	-1.355380
18				
19	H	2.076928	-0.096543	1.641855
20				
21	N	1.448739	0.155408	0.886964
22				
23	C	0.020943	0.193241	1.227822
24				
25	C	-0.703024	-1.001582	0.561878
26				
27	O	-0.245605	-2.141051	0.715611
28				
29	C	-0.597348	1.595442	1.116612
30				
31	S	-0.847063	2.293054	-0.578894
32				
33	H	0.038743	1.458636	-1.185841
34				
35	H	-1.989794	0.217202	-0.422882
36				
37	N	-1.874625	-0.734224	-0.074339
38				
39	C	-2.543287	-1.817259	-0.791525
40				
41	H	3.711517	-0.331657	-1.458255
42				
43	H	3.942914	-0.235181	0.323721
44				
45	H	3.329355	-1.739778	-0.429291
46				
47	H	-0.024962	-0.053191	2.304050
48				
49	H	-1.590673	1.580229	1.593890
50				
51	H	0.044410	2.286676	1.683290
52				
53	H	-3.500208	-1.441707	-1.176760
54				
55	H	-1.923442	-2.185961	-1.624739
56				
57	H	-2.727585	-2.650701	-0.100836
58				
59				
60				

cysteine_36 -892.19825551109 a.u.

C	-1.638194	2.710046	-0.050439
C	-0.674815	1.541096	-0.100495
O	-0.033348	1.243683	-1.111340
H	-1.312283	3.471962	-0.769756
H	-2.631725	2.342376	-0.353854
H	-1.715867	3.150452	0.955158
N	-0.544040	0.843211	1.092119
C	-0.010776	-0.519126	1.136910
C	1.242107	-0.668985	0.250108
O	1.383663	-1.632901	-0.508593
C	-1.051442	-1.608315	0.834442
S	-2.028502	-1.351892	-0.692907
H	-1.219394	1.075735	1.814195
H	-0.957566	-1.322127	-1.517481
H	0.341146	-0.685805	2.172565
H	-0.541381	-2.581569	0.795022
H	-1.796143	-1.633211	1.647204
N	2.217996	0.262047	0.481182
C	3.314880	0.363514	-0.479826
H	1.889344	1.127996	0.896719
H	3.798070	-0.616930	-0.575279
H	2.945741	0.676186	-1.470589
H	4.045320	1.092776	-0.105240

cysteine_37 -892.19598788871 a.u.

C	3.138837	-1.351654	0.332765
C	1.690349	-0.987975	0.061231

1				
2				
3	O	1.152220	-1.303815	-1.012003
4				
5	H	1.670468	-0.152412	1.887361
6				
7	N	1.072605	-0.314177	1.084513
8				
9	C	-0.173014	0.469915	1.133394
10				
11	C	-1.495245	-0.122648	0.604438
12				
13	O	-2.546810	0.350299	1.071594
14				
15	C	-0.001101	1.901446	0.583490
16				
17	S	0.598784	1.998709	-1.145304
18				
19	H	-0.368292	1.217913	-1.677610
20				
21	H	-0.549292	-1.313798	-0.757845
22				
23	N	-1.460491	-1.080561	-0.343883
24				
25	C	-2.709796	-1.612557	-0.875239
26				
27	H	3.338119	-2.343535	-0.093252
28				
29	H	3.773882	-0.618037	-0.188324
30				
31	H	3.395552	-1.347117	1.402383
32				
33	H	-0.389848	0.582849	2.209024
34				
35	H	-0.958668	2.431277	0.698031
36				
37	H	0.765395	2.431467	1.172499
38				
39	H	-2.469591	-2.422584	-1.575802
40				
41	H	-3.332524	-2.003099	-0.057214
42				
43	H	-3.284001	-0.830132	-1.396004
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45				
46				
47	cysteine_38 -892.19580040690 a.u.			
48				
49	C	3.699460	-1.054154	-0.412018
50				
51	C	2.584355	-0.121854	0.021817
52				
53	O	2.797750	0.982882	0.535043
54				
55	H	1.155034	-1.518215	-0.541246
56				
57	N	1.304815	-0.579738	-0.188601
58				
59				
60				

1
2
3 C 0.158904 0.186678 0.303670
4
5 C -1.015003 -0.772722 0.524535
6
7 O -1.383677 -1.110222 1.652587
8
9 C -0.153936 1.353322 -0.644845
10
11 S -1.668702 2.267055 -0.154048
12
13 H -1.214966 2.637571 1.064195
14
15 H -1.412496 -0.788062 -1.481767
16
17 N -1.557312 -1.303768 -0.621329
18
19 C -2.764773 -2.122979 -0.519349
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21 H 4.398897 -0.492797 -1.047229
22
23 H 4.244706 -1.382760 0.485291
24
25 H 3.334507 -1.937026 -0.956797
26
27 H 0.418109 0.594441 1.293208
28
29 H 0.711709 2.029189 -0.678644
30
31 H -0.339795 0.992276 -1.670317
32
33 H -2.993954 -2.536755 -1.510070
34
35 H -2.581087 -2.943308 0.186331
36
37 H -3.620573 -1.533908 -0.152562
38
39
40
41 cysteine_39 -892.19583377205 a.u.
42
43 C 3.083231 -1.872603 -0.026662
44
45 C 1.833021 -1.047972 0.217587
46
47 O 1.597757 -0.490333 1.293623
48
49 H 3.951528 -1.311952 0.346486
50
51 H 3.006093 -2.802525 0.557079
52
53 H 3.233731 -2.124470 -1.086667
54
55 N 0.968833 -0.930592 -0.854262
56
57 C -0.366768 -0.352017 -0.673240
58
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2				
3	C	-0.282486	1.077211	-0.100630
4				
5	O	-1.103021	1.484298	0.726245
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7	C	-1.277461	-1.212300	0.215015
8				
9	S	-3.046633	-0.731801	0.032153
10				
11	H	1.116952	-1.540362	-1.650973
12				
13	H	-3.421414	-1.836686	-0.650785
14				
15	H	-0.815647	-0.274471	-1.677662
16				
17	H	-1.170852	-2.270185	-0.064892
18				
19	H	-0.996211	-1.082940	1.268032
20				
21	N	0.695154	1.864719	-0.641232
22				
23	C	0.961909	3.169236	-0.041642
24				
25	H	1.455746	1.378932	-1.102503
26				
27	H	0.032468	3.753010	-0.023064
28				
29	H	1.331513	3.067832	0.991809
30				
31	H	1.707743	3.692680	-0.654359
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33				
34				
35	cysteine_40 -892.19558730201 a.u.			
36				
37	C	3.651888	-1.157321	-0.141174
38				
39	C	2.536053	-0.149817	0.066103
40				
41	O	2.750704	1.039777	0.315944
42				
43	H	1.140579	-1.655584	-0.001178
44				
45	N	1.252293	-0.648013	-0.058928
46				
47	C	0.111924	0.183734	0.345219
48				
49	C	-1.131198	-0.690557	0.510732
50				
51	O	-1.911446	-0.563097	1.461064
52				
53	C	-0.150904	1.269836	-0.717046
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55	S	-1.420065	2.487573	-0.200937
56				
57	H	-2.336712	1.585029	0.217626
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59				
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3 H -0.790062 -1.515223 -1.337313
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5 N -1.328264 -1.616169 -0.483533
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7 C -2.570878 -2.385086 -0.520610
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9 H 4.356376 -0.751384 -0.880629
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11 H 4.192159 -1.277996 0.809724
12
13 H 3.288822 -2.138349 -0.480411
14
15 H 0.310744 0.670320 1.312959
16
17 H 0.772891 1.849406 -0.854501
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19 H -0.427883 0.804429 -1.676647
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21 H -2.483820 -3.158095 -1.295119
22
23 H -2.726469 -2.861141 0.456278
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25 H -3.439154 -1.741493 -0.733990
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27
28

29 cysteine_41 -892.19597944300 a.u.
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31 C 3.095863 -1.155546 -0.553282
32
33 C 1.729342 -0.532301 -0.364109
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35 O 0.932130 -0.359383 -1.292781
36
37 H 3.502099 -0.831279 -1.520106
38
39 H 3.795358 -0.891409 0.253382
40
41 H 2.972926 -2.249933 -0.576956
42
43 N 1.407828 -0.166552 0.925568
44
45 C 0.017090 0.144988 1.257321
46
47 C -0.929709 -0.873275 0.578854
48
49 O -0.765144 -2.079348 0.795781
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51 C -0.315369 1.637775 1.120156
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53 S -0.124236 2.305389 -0.596576
54
55 H 1.982752 -0.552206 1.665910
56
57 H -0.594666 3.530918 -0.266097
58
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2				
3	H	-0.094799	-0.078925	2.332631
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5	H	-1.353778	1.796074	1.450834
6				
7	H	0.362659	2.196962	1.781733
8				
9	N	-1.969696	-0.367026	-0.144268
10				
11	C	-2.791701	-1.303213	-0.908968
12				
13	H	-1.805923	0.548811	-0.559485
14				
15	H	-3.194190	-2.066824	-0.230862
16				
17	H	-3.620238	-0.747517	-1.367450
18				
19	H	-2.200323	-1.806559	-1.691250
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21				
22				
23	cysteine_42 -892.19409950680 a.u.			
24				
25	C	-3.568131	-1.153410	-0.356039
26				
27	C	-2.286367	-0.601206	0.239651
28				
29	O	-2.261412	0.096488	1.256473
30				
31	H	-4.328377	-0.360416	-0.352918
32				
33	H	-3.435352	-1.535908	-1.378813
34				
35	H	-3.927980	-1.969983	0.288602
36				
37	N	-1.122106	-0.912458	-0.439725
38				
39	C	0.169900	-0.637610	0.191039
40				
41	C	0.478497	0.863378	0.282986
42				
43	O	1.250326	1.287142	1.149442
44				
45	C	1.252812	-1.348987	-0.632395
46				
47	S	2.919951	-1.067585	0.101392
48				
49	H	-1.165162	-1.636266	-1.150182
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51	H	3.504864	-2.059445	-0.608000
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53				
54	H	0.174522	-1.003910	1.230938
55				
56	H	1.046491	-2.430927	-0.626680
57				
58	H	1.231373	-0.971892	-1.667659
59				
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3 N -0.056343 1.640040 -0.703260
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5 C 0.103494 3.089340 -0.642122
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7 H -0.841128 1.247569 -1.210396
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9 H 1.166783 3.324425 -0.503405
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11 H -0.246715 3.524167 -1.587603
12
13 H -0.461941 3.522798 0.198689
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15
16
17 cysteine_43 -892.19324683884 a.u.
18

19 C 3.702306 -1.063987 -0.308642
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21 C 2.583930 -0.099248 0.038732
22
23 O 2.793892 1.050417 0.440262
24
25 H 4.394433 -0.563646 -1.000394
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27 H 4.255450 -1.299595 0.612777
28
29 H 3.339848 -1.997791 -0.762615
30
31 N 1.305071 -0.582581 -0.128481
32
33 C 0.158290 0.198513 0.340504
34
35 C -1.040741 -0.735521 0.535075
36
37 O -1.599364 -0.874049 1.626728
38
39 C -0.148266 1.335749 -0.648492
40
41 S -1.676638 2.200993 -0.088816
42
43 H 1.171850 -1.570904 -0.312999
44
45 H -1.582105 3.218381 -0.972014
46
47 H 0.387924 0.632636 1.325983
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49 H 0.701886 2.030639 -0.650518
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51 H -0.292785 0.928310 -1.662036
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53 N -1.413865 -1.438354 -0.585449
54
55 C -2.649850 -2.220061 -0.554608
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57 H -1.105183 -1.075244 -1.480866
58
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2				
3	H	-2.609221	-2.919020	0.290685
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5	H	-3.531909	-1.572152	-0.428298
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7	H	-2.732667	-2.784575	-1.492483
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10				
11	cysteine_44 -892.19294326763 a.u.			
12				
13	C	2.259781	-2.393616	-0.826023
14				
15	C	1.686580	-1.310332	0.066121
16				
17	O	2.261939	-0.923770	1.090861
18				
19	H	0.041402	-1.157854	-1.173813
20				
21	N	0.496031	-0.767271	-0.356988
22				
23	C	-0.194029	0.256556	0.417544
24				
25	C	-1.682595	-0.108350	0.514079
26				
27	O	-2.199093	-0.507298	1.561623
28				
29	C	0.020639	1.681638	-0.118447
30				
31	S	1.796855	2.139905	-0.263720
32				
33	H	2.217851	1.367342	0.764884
34				
35	H	-1.998935	0.528507	-1.417022
36				
37	N	-2.382586	-0.032340	-0.666159
38				
39	C	-3.816708	-0.316405	-0.673592
40				
41	H	2.556542	-3.244026	-0.196640
42				
43	H	1.555739	-2.733890	-1.599510
44				
45	H	3.163587	-1.996223	-1.311875
46				
47	H	0.202336	0.194337	1.441901
48				
49	H	-0.386238	1.794739	-1.137512
50				
51	H	-0.502493	2.390377	0.543589
52				
53	H	-4.169455	-0.317450	-1.713168
54				
55	H	-3.989119	-1.304535	-0.227078
56				
57	H	-4.379786	0.429076	-0.090162
58				
59				
60				

cysteine_45 -892.19297152350 a.u.

C	-1.680035	2.688722	0.011972
C	-0.742441	1.502958	-0.088041
O	-0.198027	1.160399	-1.140763
H	-1.394487	3.433233	-0.742035
H	-2.698601	2.334525	-0.214667
H	-1.678175	3.146136	1.012896
N	-0.513801	0.828724	1.102639
C	0.035725	-0.528134	1.109742
C	1.312042	-0.653338	0.251509
O	1.555067	-1.682077	-0.383851
C	-0.988464	-1.629044	0.791760
S	-1.957836	-1.295422	-0.742595
H	-1.122888	1.070416	1.878199
H	-2.944452	-2.164320	-0.427954
H	0.377554	-0.715098	2.144497
H	-0.441610	-2.576652	0.685773
H	-1.697921	-1.697179	1.630727
N	2.200277	0.379019	0.389475
C	3.330399	0.447891	-0.534221
H	1.796266	1.257580	0.695446
H	3.881020	-0.500517	-0.496242
H	2.990768	0.618125	-1.569245
H	3.992896	1.265391	-0.220084

cysteine_46 -892.19227693245 a.u.

C	2.332237	-2.747840	-0.021593
C	1.839087	-1.317023	0.082037

1				
2				
3	O	2.611505	-0.353099	0.147900
4				
5	H	-0.096989	-1.969637	0.265300
6				
7	N	0.472239	-1.150794	0.074678
8				
9	C	-0.111405	0.162157	0.375459
10				
11	C	-1.630720	0.031223	0.479385
12				
13	O	-2.285978	0.633460	1.334282
14				
15	C	0.229326	1.205620	-0.734138
16				
17	S	1.216676	2.634609	-0.158540
18				
19	H	2.297986	1.885159	0.155563
20				
21	H	-1.647939	-1.050635	-1.263420
22				
23	N	-2.212818	-0.779199	-0.465619
24				
25	C	-3.669093	-0.812591	-0.586794
26				
27	H	3.044757	-2.812046	-0.856066
28				
29	H	2.872781	-2.997017	0.903669
30				
31	H	1.520686	-3.473519	-0.176007
32				
33	H	0.249890	0.534136	1.346490
34				
35	H	0.752624	0.701748	-1.559672
36				
37	H	-0.696483	1.649656	-1.134243
38				
39	H	-3.945218	-1.597551	-1.302844
40				
41	H	-4.104993	-1.042885	0.394090
42				
43	H	-4.070685	0.156656	-0.923240
44				
45				
46	cysteine_47 -892.18977633428 a.u.			
47				
48	C	2.256111	-2.433423	-0.804541
49				
50	C	1.690433	-1.328668	0.067554
51				
52	O	2.274201	-0.904520	1.068383
53				
54	H	2.586519	-3.256410	-0.155902
55				
56	H	1.535442	-2.811925	-1.544469
57				
58				
59				
60				

H	3.137703	-2.038165	-1.331355
N	0.487439	-0.803470	-0.355372
C	-0.187234	0.248941	0.395944
C	-1.676047	-0.102542	0.515551
O	-2.184492	-0.484571	1.572976
C	0.029574	1.641684	-0.217416
S	1.818892	2.073842	-0.128694
H	0.007650	-1.233647	-1.137221
H	1.691490	3.233962	-0.811874
H	0.223717	0.226020	1.416363
H	-0.278995	1.651029	-1.275737
H	-0.562738	2.380873	0.345166
N	-2.388886	-0.037140	-0.658292
C	-3.825468	-0.307376	-0.645347
H	-2.007071	0.507787	-1.421823
H	-4.002274	-1.287846	-0.183851
H	-4.374954	0.450821	-0.065237
H	-4.190527	-0.318674	-1.680648

ALANINE PEPTIDES

Tetrapeptide (extended)

C	-1.7307169	-1.9998193	2.4398450
C	-1.7097793	-0.8547348	1.4381148
O	-2.7331081	-0.2460801	1.1122687
H	0.3399725	-1.1321307	1.1057528
N	-0.4815890	-0.5546139	0.9193524
C	-0.3049099	0.4209427	-0.1429185
C	0.9752746	0.0212053	-0.9041798

1				
2				
3	O	1.7890205	-0.7821991	-0.4277562
4				
5	C	-0.2141688	1.8598615	0.4020435
6				
7	H	-2.3492830	-1.7082871	3.2978703
8				
9	H	-2.2065653	-2.8728977	1.9702484
10				
11	H	-0.7316886	-2.2903146	2.7925998
12				
13	H	-1.1764994	0.3562927	-0.8156046
14				
15	H	-0.1251338	2.5918091	-0.4138146
16				
17	H	-1.1259607	2.0849493	0.9697891
18				
19	H	0.6558929	1.9666558	1.0649776
20				
21	H	0.5042038	1.3318417	-2.4600477
22				
23	N	1.1499928	0.6211133	-2.1075591
24				
25	C	2.3618694	0.4597004	-2.8985189
26				
27	C	2.4705975	1.7126959	-3.7914620
28				
29	O	1.4961277	2.4520774	-3.9871938
30				
31	C	2.3387540	-0.8315821	-3.7387636
32				
33	H	3.2183819	0.4169620	-2.2060526
34				
35	H	3.2732523	-0.9541708	-4.3048091
36				
37	H	2.2232795	-1.6947458	-3.0713953
38				
39	H	1.4994302	-0.8145745	-4.4482407
40				
41	H	4.4664927	1.2745949	-4.2320421
42				
43	N	3.6863544	1.9265814	-4.3491845
44				
45	C	3.9380344	2.9938027	-5.3061713
46				
47	C	5.1903624	2.5711036	-6.1053237
48				
49	O	5.9213548	1.6565450	-5.7116738
50				
51	C	4.1392074	4.3548152	-4.6123572
52				
53	H	4.7616485	4.0125554	-7.4966754
54				
55	N	5.4266357	3.2904298	-7.2357533
56				
57	C	6.5940226	3.0779876	-8.0828869
58				
59				
60				

H	3.0676617	3.0633957	-5.9800374
H	4.2826566	5.1607312	-5.3464066
H	3.2498130	4.5912478	-4.0150548
H	5.0178897	4.3245858	-3.9534336
H	7.1639666	2.2445437	-7.6570785
H	6.2929684	2.8199577	-9.1082906
H	7.2323661	3.9735146	-8.1091971

Tetrapeptide (alpha-helix)

C	-5.2517434	-2.0228398	0.7780798
C	-4.8625137	-0.5517560	0.7325422
O	-5.5925336	0.3304254	1.1814779
H	-3.2468464	-1.0469982	-0.4047796
N	-3.6131928	-0.3039855	0.1936698
C	-3.1178851	1.0615508	-0.0685251
C	-1.7262370	0.9878734	-0.7290987
O	-1.4639211	1.5783618	-1.7734027
C	-3.0555640	1.9271467	1.2022938
H	-6.2949817	-2.1176460	0.4506971
H	-4.6105689	-2.6679419	0.1636226
H	-5.2045696	-2.3636619	1.8226802
H	-3.7643212	1.5600933	-0.8077555
H	-2.6139898	2.9036408	0.9575397
H	-4.0642812	2.0735442	1.6015975
H	-2.4399311	1.4514300	1.9803264
H	-1.0743581	-0.1370730	0.8696851
N	-0.8053020	0.2230847	-0.0443091
C	0.5751754	0.0423786	-0.4887049

1				
2				
3	C	0.8320892	-1.3386175	-1.1474921
4				
5	O	1.9299767	-1.6255600	-1.6274862
6				
7	C	1.5748296	0.2853630	0.6460407
8				
9	H	0.7306093	0.7793531	-1.2916747
10				
11	H	2.5927162	0.1043997	0.2795442
12				
13	H	1.5024151	1.3187428	1.0101867
14				
15	H	1.3903442	-0.3988468	1.4890283
16				
17	H	-1.1402482	-1.8183899	-0.8301867
18				
19	N	-0.2371053	-2.1786707	-1.1385930
20				
21	C	-0.3020475	-3.4272486	-1.8714773
22				
23	C	-1.7869380	-3.6163954	-2.2563637
24				
25	O	-2.6893041	-2.9937801	-1.6767274
26				
27	C	0.2240130	-4.6168323	-1.0456462
28				
29	H	-1.2182257	-4.9588337	-3.6846560
30				
31	N	-2.0199070	-4.5168943	-3.2440336
32				
33	C	-3.3540002	-4.8607962	-3.7221645
34				
35	H	0.3135974	-3.3248260	-2.7813050
36				
37	H	0.2042205	-5.5504236	-1.6266284
38				
39	H	1.2623667	-4.4172411	-0.7507604
40				
41	H	-0.3826724	-4.7565815	-0.1400023
42				
43	H	-4.0694367	-4.2025039	-3.2174844
44				
45	H	-3.4263386	-4.7057978	-4.8077443
46				
47	H	-3.6022480	-5.9065505	-3.4893921
48				
49				
50	Hexapeptide (extended)			
51				
52	C	-0.3608532	-1.6602936	0.6496324
53				
54	C	-0.1276226	-0.5560681	-0.3627130
55				
56	O	-0.6332025	-0.5884094	-1.4949245
57				
58				
59				
60				

H	1.1136119	0.4378538	0.9547199
N	0.6655882	0.4785102	0.0434593
C	0.9183939	1.6653896	-0.7855861
C	2.0432127	1.3826641	-1.8183614
O	3.1668942	1.9025595	-1.7305239
C	1.2518372	2.8647625	0.0934572
H	-1.4405553	-1.7411778	0.8344402
H	-0.0308438	-2.6144382	0.2175455
H	0.1539205	-1.5005216	1.6061688
H	-0.0114654	1.8462696	-1.3484788
H	1.3957978	3.7592300	-0.5247347
H	0.4352338	3.0558902	0.8028889
H	2.1887511	2.7007938	0.6438141
H	0.7477894	0.1077843	-2.7435510
N	1.6836146	0.5323857	-2.8110937
C	2.6441820	-0.0159074	-3.7813257
C	2.9052129	0.9682584	-4.9560747
O	2.6590893	0.6709650	-6.1352698
C	2.1639305	-1.3705320	-4.2885396
H	3.6043398	-0.1265423	-3.2480599
H	2.8886842	-1.7857816	-4.9990594
H	2.0459071	-2.0703850	-3.4503032
H	1.2059472	-1.2761816	-4.8172679
H	3.6489079	2.2922453	-3.5813462
N	3.4488557	2.1518179	-4.5813551
C	3.7113546	3.2378847	-5.5347050
C	5.0764346	3.0156435	-6.2388999
O	6.0670616	3.7212666	-6.0045546

1				
2				
3	C	3.6596470	4.5903524	-4.8345397
4				
5	H	2.9260912	3.1728707	-6.3057079
6				
7	H	3.8304095	5.3960568	-5.5592767
8				
9	H	2.6775127	4.7377128	-4.3651184
10				
11	H	4.4454649	4.6677181	-4.0713944
12				
13	H	4.2282191	1.4191696	-7.1967284
14				
15	N	5.0832175	1.9840880	-7.1221608
16				
17	C	6.3178694	1.5017346	-7.7554772
18				
19	C	6.6420725	2.3252622	-9.0346569
20				
21	O	6.5579031	1.8469197	-10.1691426
22				
23	C	6.2064926	0.0150805	-8.0722042
24				
25	H	7.1311247	1.6834701	-7.0336599
26				
27	H	7.1394001	-0.3453565	-8.5223731
28				
29	H	6.0109312	-0.5569795	-7.1547789
30				
31	H	5.4025361	-0.1718295	-8.7963133
32				
33	H	7.0371163	3.9398624	-7.8015823
34				
35	N	7.0364581	3.6029448	-8.7736644
36				
37	C	7.3528233	4.5441033	-9.8391315
38				
39	C	8.5474872	5.4037628	-9.3875122
40				
41	O	8.6185333	5.8621288	-8.2470668
42				
43	C	6.1558599	5.4501898	-10.1861235
44				
45	H	9.3690370	5.1932384	-11.2592796
46				
47	N	9.4824237	5.6454142	-10.3574375
48				
49	C	10.6466073	6.4905728	-10.1345023
50				
51	H	7.6123680	3.9350113	-10.7187164
52				
53	H	6.4075892	6.1408801	-11.0044347
54				
55	H	5.3047415	4.8317078	-10.5016124
56				
57	H	5.8641729	6.0424284	-9.3081541
58				
59				
60				

1
2
3 H 11.5798958 5.9257748 -10.2774155
4
5 H 10.6456082 7.3588508 -10.8106350
6
7 H 10.5980034 6.8434755 -9.0977057
8
9
10

11 Hexapeptide (alpha-helix)
12

13 C -1.8566174 0.1013342 -1.9406248
14
15 C -0.6159223 0.8384601 -1.4770731
16
17 O -0.0408217 1.6717919 -2.1748291
18
19 H -0.7847461 -0.0470457 0.3731835
20
21 N -0.1532925 0.4972252 -0.2114070
22
23 C 0.8350031 1.3237120 0.4864251
24
25 C 2.1262977 0.5703329 0.8770376
26
27 O 2.9514878 1.0810749 1.6339012
28
29 C 0.2317379 2.0336121 1.7032682
30
31 H -1.6721523 -0.3443433 -2.9291980
32
33 H -2.1894172 -0.6807089 -1.2432468
34
35 H -2.6683791 0.8330278 -2.0611781
36
37 H 1.1506859 2.0733709 -0.2589486
38
39 H 1.0093333 2.6136293 2.2138784
40
41 H -0.5759802 2.7080001 1.3894721
42
43 H -0.1741294 1.3075339 2.4253439
44
45 H 1.6311483 -0.9320797 -0.4098080
46
47 N 2.3012168 -0.6625102 0.3077921
48
49 C 3.5930601 -1.3591072 0.4159509
50
51 C 3.7708568 -2.3936471 -0.7078489
52
53 O 4.7768092 -2.4192256 -1.4070539
54
55 C 3.7831743 -2.0094174 1.7979309
56
57 H 4.3929224 -0.6202898 0.2663661
58
59
60

1				
2				
3	H	4.7582001	-2.5140905	1.8461581
4				
5	H	3.7524435	-1.2309259	2.5699467
6				
7	H	2.9942150	-2.7459844	2.0106728
8				
9	H	2.0708731	-3.3635589	-0.0808724
10				
11	N	2.7285183	-3.2972024	-0.8580411
12				
13	C	2.8919019	-4.5149742	-1.6671273
14				
15	C	1.8199460	-4.6737204	-2.7714605
16				
17	O	1.6536886	-5.7503863	-3.3444868
18				
19	C	2.9637108	-5.7710448	-0.7946527
20				
21	H	3.8503666	-4.3767379	-2.1940940
22				
23	H	3.0454878	-6.6573026	-1.4346774
24				
25	H	3.8351909	-5.7240078	-0.1282801
26				
27	H	2.0545032	-5.8837677	-0.1832286
28				
29	H	1.3207904	-2.7068747	-2.5343001
30				
31	N	1.1260131	-3.5406179	-3.0837727
32				
33	C	0.0703038	-3.5090196	-4.0983918
34				
35	C	0.0687065	-2.1310410	-4.8073730
36				
37	O	-0.9571256	-1.4494301	-4.9121580
38				
39	C	-1.3040347	-3.8524465	-3.5232059
40				
41	H	0.3478475	-4.2785249	-4.8380595
42				
43	H	-2.0667795	-3.8256912	-4.3116260
44				
45	H	-1.2747678	-4.8592363	-3.0865012
46				
47	H	-1.5992763	-3.1298349	-2.7501844
48				
49	H	2.0843882	-2.3666941	-5.2885405
50				
51	N	1.2744435	-1.7407302	-5.2958974
52				
53	C	1.4595059	-0.5220795	-6.0717129
54				
55	C	2.6441301	-0.7914453	-7.0248753
56				
57	O	3.4413066	-1.7099068	-6.8136647
58				
59				
60				

C	1.7365610	0.7024881	-5.1780155
H	2.0391566	0.7889611	-8.1806001
N	2.7494898	0.0710105	-8.0738173
C	3.8488613	0.0275524	-9.0286965
H	0.5356948	-0.3472868	-6.6474843
H	1.8358314	1.6173242	-5.7804419
H	0.9126422	0.8546859	-4.4686694
H	2.6693302	0.5604624	-4.6144159
H	3.4771353	-0.1394299	-10.0501367
H	4.4310723	0.9606611	-9.0052481
H	4.4986555	-0.8072828	-8.7438783

Octapeptide (extended)

C	-1.6015296	-1.8805714	2.3774044
C	-1.5896908	-0.7306424	1.3785058
O	-2.6094311	-0.1101131	1.0646801
H	0.4556586	-1.0288983	1.0302893
N	-0.3629157	-0.4451823	0.8465530
C	-0.1794910	0.5369091	-0.2084299
C	1.1185258	0.1575073	-0.9505692
O	1.9276758	-0.6496631	-0.4719438
C	-0.1122078	1.9732887	0.3469699
H	-2.4978417	-1.7947855	3.0002755
H	-1.6439709	-2.8405352	1.8406806
H	-0.7068681	-1.8864723	3.0156836
H	-1.0368833	0.4670951	-0.8989338
H	-0.0087441	2.7105548	-0.4620455
H	-1.0380597	2.1876806	0.8958275

1				
2				
3	H	0.7423157	2.0803974	1.0299777
4				
5	H	0.6506303	1.4733871	-2.5038881
6				
7	N	1.3119669	0.7847594	-2.1358599
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9	C	2.5276427	0.6390056	-2.9237133
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11	C	2.5803622	1.8540920	-3.8747794
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13	O	1.5727058	2.5395584	-4.0979809
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15	C	2.5523364	-0.6834855	-3.7136442
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17	H	3.3904430	0.6609613	-2.2378115
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19	H	3.4887864	-0.7862934	-4.2799114
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21	H	2.4747221	-1.5255520	-3.0143948
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23	H	1.7099749	-0.7244231	-4.4187203
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25	H	4.5947864	1.4836750	-4.2814716
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27	N	3.7822829	2.0825615	-4.4532108
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29	C	4.0017993	3.0977434	-5.4750496
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31	C	5.3102714	2.7037495	-6.1961988
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33	O	6.0905495	1.8786016	-5.6991653
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35	C	4.0973451	4.5142943	-4.8773453
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37	H	3.1590616	3.0665025	-6.1853032
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39	H	4.2357462	5.2659153	-5.6670283
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41	H	3.1694611	4.7438782	-4.3386000
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43	H	4.9439464	4.5806466	-4.1796563
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45	H	4.9024601	4.0383758	-7.7515172
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47	N	5.5418904	3.3356261	-7.3688287
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49	C	6.7739321	3.1809251	-8.1318552
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51	C	6.8272164	4.3793928	-9.1060793
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53	O	5.8233301	5.0736310	-9.3219788
54				
55	C	6.8269205	1.8408566	-8.8890685
56				
57	H	7.6258549	3.2303409	-7.4337131
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3	H	7.7727365	1.7372440	-9.4389300
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5	H	6.7508317	1.0140720	-8.1719565
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7	H	5.9968311	1.7716675	-9.6060509
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9	H	8.8297231	3.9797614	-9.5463669
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11	N	8.0208922	4.5872271	-9.7062894
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13	C	8.2344116	5.5960364	-10.7358215
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15	C	9.5282188	5.1865242	-11.4736300
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17	O	10.3026473	4.3482072	-10.9915355
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19	C	8.3504851	7.0139539	-10.1455658
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21	H	7.3820528	5.5678200	-11.4344996
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23	H	8.4850147	7.7613994	-10.9399236
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25	H	7.4320060	7.2549652	-9.5958989
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27	H	9.2069816	7.0755026	-9.4597313
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29	H	9.1279535	6.5496705	-13.0041748
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31	N	9.7525629	5.8208360	-12.6466286
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33	C	10.9785868	5.6640012	-13.4178378
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35	C	11.0588900	6.8969748	-14.3444767
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37	O	10.0769264	7.6332401	-14.5210763
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39	C	11.0003841	4.3498742	-14.2203810
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41	H	11.8321066	5.6692899	-12.7200418
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43	H	11.9440695	4.2406624	-14.7729617
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45	H	10.9046496	3.5016692	-13.5311966
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47	H	10.1694126	4.3231249	-14.9393564
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49	H	13.0357480	6.4413992	-14.8414239
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51	N	12.2537178	7.0944159	-14.9452741
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53	C	12.4856634	8.1405319	-15.9308424
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55	C	13.7511292	7.7163324	-16.7111764
56				
57	O	14.4710101	6.7967250	-16.3084263
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3	C	12.6550890	9.5246106	-15.2767141
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5	H	13.3539844	9.1700411	-18.0953314
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7	N	14.0068515	8.4372266	-17.8345002
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9	C	15.1824831	8.2211709	-18.6692389
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11	H	11.6200916	8.1724511	-16.6143716
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13	H	12.7903922	10.3102774	-16.0338891
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15	H	11.7563733	9.7630731	-14.6944967
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17	H	13.5287121	9.5317528	-14.6105597
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19	H	15.7486604	7.3902307	-18.2337197
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21	H	14.8913797	7.9584096	-19.6962512
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23	H	15.8196219	9.1173292	-18.6931048
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25				
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27	Octapeptide (alpha-helix)			
28				
29	C	-2.8430480	-2.3803383	3.9023715
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31	C	-3.0538594	-1.8363243	2.5035294
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33	O	-2.7836173	-2.4919837	1.4915857
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35	H	-3.8569117	-0.1003200	3.2723942
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37	N	-3.5583057	-0.5598854	2.4154666
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39	C	-4.0665677	-0.0190382	1.1489268
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41	C	-2.9781513	0.1647379	0.0729983
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43	O	-3.2931440	0.2072438	-1.1207359
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45	C	-4.7978553	1.3039449	1.3958417
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47	H	-3.5787775	-3.1779732	4.0794207
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49	H	-1.8470415	-2.8361068	3.9648552
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51	H	-2.9494038	-1.6242085	4.6915507
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53	H	-4.7616677	-0.7488252	0.7041859
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55	H	-5.1666415	1.7006690	0.4423677
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57	H	-5.6604154	1.1541580	2.0611183
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3	H	-4.1279579	2.0525977 1.8442321
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5	H	-1.5187619	0.1861333 1.5068839
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7	N	-1.6976340	0.2892916 0.5104867
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9	C	-0.5705616	0.4094077 -0.4107890
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11	C	-0.4052511	-0.8021026 -1.3554030
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13	O	0.2573997	-0.6656526 -2.3925774
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15	C	0.7260205	0.6646916 0.3631593
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17	H	-0.7663353	1.2529362 -1.0892194
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19	H	1.5610473	0.7455489 -0.3427813
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21	H	0.6610323	1.6026213 0.9326422
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23	H	0.9432099	-0.1607753 1.0581392
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25	H	-1.5759524	-2.0382463 -0.1599737
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27	N	-0.9962036	-1.9723041 -1.0035100
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29	C	-0.9045453	-3.1394802 -1.8810718
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31	C	-1.5550713	-2.9226893 -3.2641194
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33	O	-1.2128669	-3.6405593 -4.2140314
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35	C	-1.4960212	-4.3777593 -1.2012488
36			
37	H	0.1567165	-3.3149260 -2.1130279
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39	H	-1.4248723	-5.2318548 -1.8855582
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41	H	-0.9435179	-4.6159463 -0.2820716
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43	H	-2.5517991	-4.2218969 -0.9387775
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45	H	-2.7105766	-1.3358022 -2.5898847
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47	N	-2.4949418	-1.9487594 -3.3811631
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49	C	-3.1223837	-1.6775833 -4.6749696
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53	O	-2.4309332	-1.2794123 -6.9479043
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55	C	-4.2808358	-0.6891345 -4.5172831
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57	H	-3.4986878	-2.6289977 -5.0790550
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3	H	-4.7222552	-0.4925332	-5.5021290
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5	H	-5.0576208	-1.1043722	-3.8600946
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7	H	-3.9355262	0.2621456	-4.0886080
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9	H	-0.7259529	-0.6400848	-4.3227596
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11	N	-0.9638933	-0.6267951	-5.3186576
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13	C	0.0485349	-0.1458367	-6.2551487
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15	C	0.9465330	-1.2563850	-6.8576035
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17	O	1.8287855	-0.9534608	-7.6635438
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19	C	0.9010784	0.9546998	-5.6196850
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21	H	-0.4910589	0.2567826	-7.1265873
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23	H	1.6847703	1.2537409	-6.3257611
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25	H	0.2805202	1.8291576	-5.3803149
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27	H	1.3771904	0.6000622	-4.6942200
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29	H	-0.0166890	-2.7273855	-5.7475537
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31	N	0.6675057	-2.5417732	-6.4865284
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33	C	1.3989015	-3.6755369	-7.0373421
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35	C	0.5984915	-4.4755708	-8.0878659
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37	O	1.1001815	-5.4945528	-8.5978532
38				
39	C	1.9147072	-4.6080238	-5.9346112
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41	H	2.2485835	-3.2437092	-7.5896835
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47	H	1.0850109	-4.9676360	-5.3093718
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49	H	-0.9622809	-3.1393469	-8.0083769
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51	N	-0.6273129	-4.0102510	-8.4252799
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53	C	-1.5129296	-4.7137892	-9.3649903
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55	C	-1.1573292	-4.3740252	-10.8448140
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57	O	-1.9268554	-3.7587794	-11.5859216
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3 C -2.9707169 -4.3989073 -9.0537608
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5 H 0.6317408 -5.2948489 -10.4899651
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7 N 0.0644358 -4.8470018 -11.2203689
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9 C 0.6387883 -4.5803014 -12.5280619
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11 H -1.3120784 -5.7884185 -9.2228596
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13 H -3.6241623 -4.9180967 -9.7657089
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15 H -3.2191039 -4.7242166 -8.0341439
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17 H -3.1703845 -3.3231642 -9.1448066
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19 H -0.1334391 -4.1065456 -13.1456395
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21 H 1.5036959 -3.9014689 -12.4570813
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23 H 0.9638790 -5.5150307 -13.0090573
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