Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The protein-water Nuclear Overhauser Effect (NOE) as an indirect microscope for molecular surface mapping of interaction patterns

Supplementary Information

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1 Equivalence of measuring $\sigma_{\mathrm{NOE}}/\sigma_{\mathrm{ROE}}$ or $f_I\{S\}$

In the main article, we claimed that one gets comparable information if using either the ratio $\sigma_{\mathrm{NOE}}/\sigma_{\mathrm{ROE}}$ employed by experimentalists[1,2] or else the NOE enhancement $f_I\{S\}$, then forming the difference.

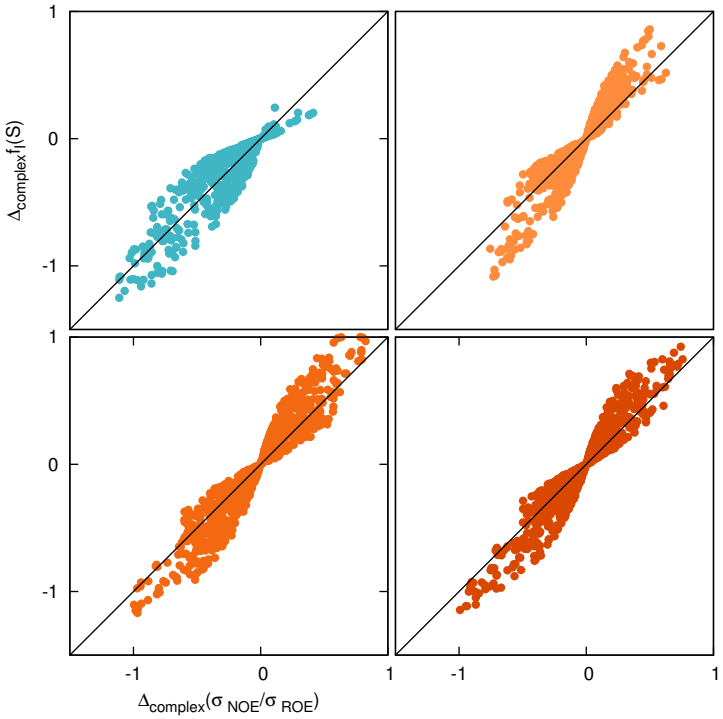
$$\Delta_{\mathrm{complex}}(\sigma_{\mathrm{NOE}}/\sigma_{\mathrm{ROE}}) \approx \Delta_{\mathrm{complex}}(f_I\{S\}) \quad (1)$$

$$\Delta_{\mathrm{confined}}(\sigma_{\mathrm{NOE}}/\sigma_{\mathrm{ROE}}) \approx \Delta_{\mathrm{confined}}(f_I\{S\}) \quad (2)$$

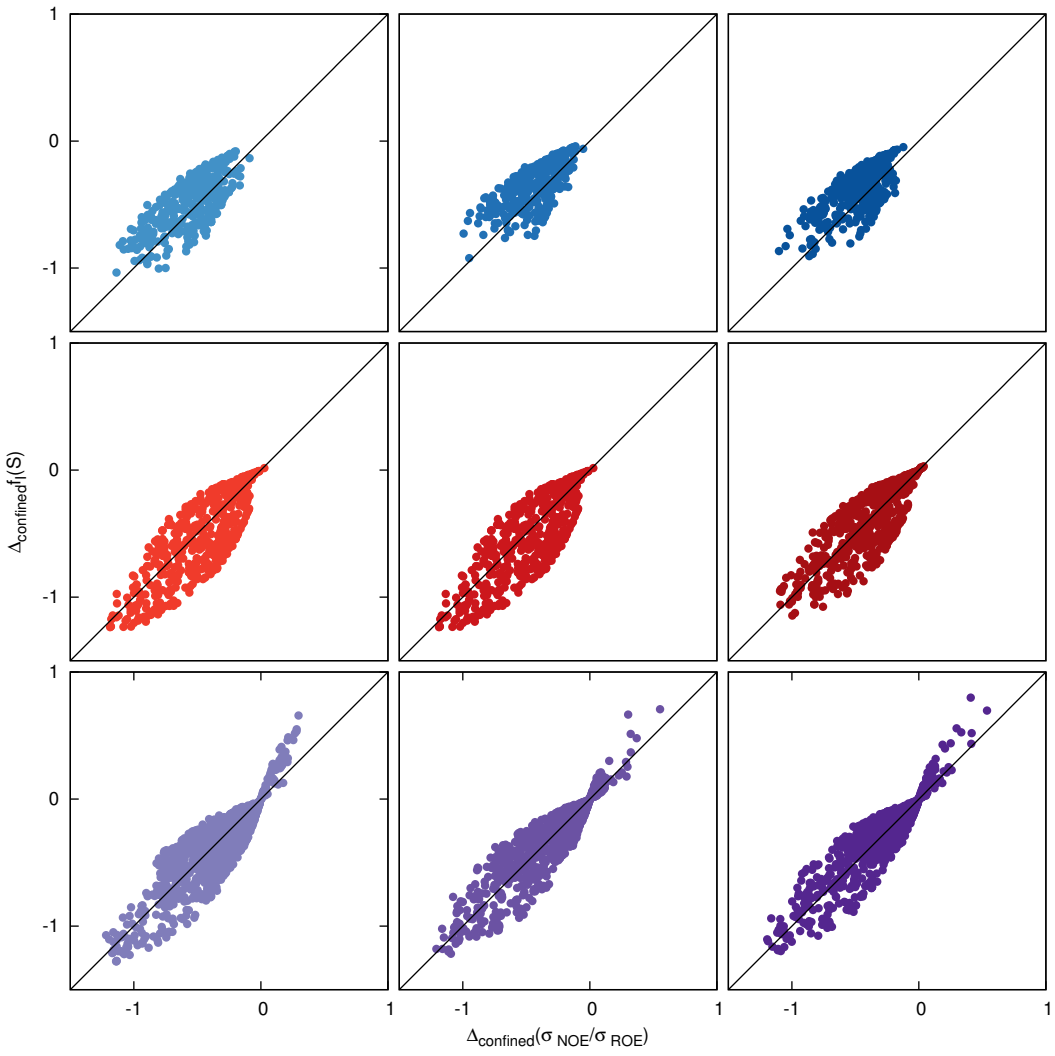
$$\Delta\Delta_{\mathrm{confined,\ complex}}(\sigma_{\mathrm{NOE}}/\sigma_{\mathrm{ROE}}) \approx \Delta\Delta_{\mathrm{confined,\ complex}}(f_I\{S\}) \quad (3)$$

Why are these two entities equivalent? Both of them were shown to be short-ranged NOE observables reporting on local hydration phenomena[3], thus they can be expected to present similar information if a difference of a test state (e.g. complex) and a reference state (e.g. free protein) is formed. In this section, we show that this is indeed the case by drawing correlation diagrams.

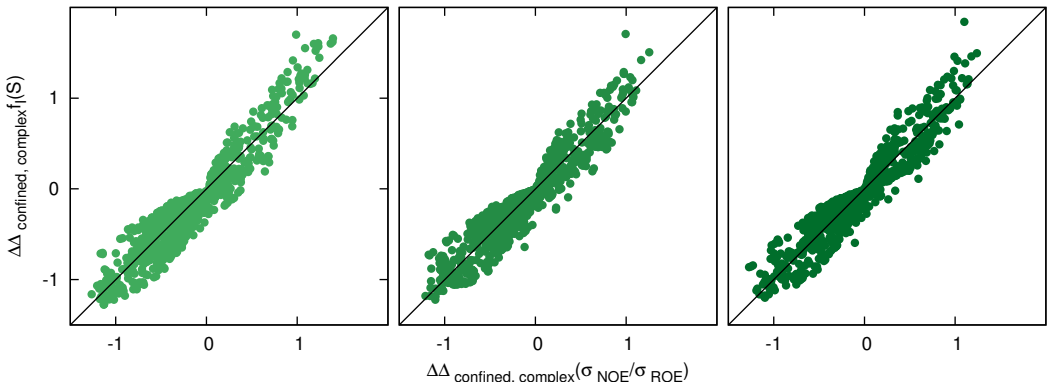
The NOE enhancement, typically obtained from the traditional saturation experiment, comes with the advantage of being one single experiment instead of two different ones. However, note that it also comes with caveats: Both spin diffusion and hydrogen exchange reactions can complicate the interpretation of the measurement.



Complex formation NOE difference $\Delta_{\mathrm{complex}}$ in bulk (turquoise), complex formation in micelle unscaled, half-scaled, fully scaled (orange, pale to dark). The black line marks equality of the two observables, showing that they are indeed strongly correlated.



Encapsulation NOE difference Δ_{confined} of the ligase (blue), ubiquitin (red) and the ligase-ubiquitin complex (purple) with unscaled, half-scaled and fully scaled parameters (pale to dark color)



Complexation-encapsulation distinction $\Delta\Delta_{\text{confined, complex}}$ of the unscaled (pale green), half-scaled (medium green) and the fully scaled (dark green) system.

2 Path dependence for calculating $\Delta\Delta_{\text{confined, complex}}$

In order to form this double difference, we need to either

- First form the protein complex from the isolated proteins in bulk dilution, then encapsulate the whole complex, or
- First encapsulate the isolated proteins separately, then form the complex within encapsulation

Looking at the corresponding paths in Fig. 1 in the main article, one may be tempted to think the choice of path does not matter. However, forming a difference along a path does not constitute a state function, as can be seen from a simple example:

Let A and C be states with a conserved quantity Q defined as Q(A) = 1 and Q(C) = 0. Furthermore, let there be alternative intermediate states B and B' with Q(B) = 0.5 and Q(B') = 0.1, such that two paths are possible: A→B→C and A→B'→C. The edges of this path contain the changes in Q with ΔQ(X,Y) = Q(X) - Q(Y).

Forming the sum

$$\Sigma\Delta Q(\mathrm{A},\mathrm{C}) = \Delta Q(\mathrm{A},\mathrm{B}^*) + \Delta Q(\mathrm{B}^*,\mathrm{C}) = Q(\mathrm{A}) - Q(\mathrm{C}) \tag{4}$$

over either path yields an identical change ΣΔQ(A,C) (0.5 + 0.5 = 1 = 0.9 + 0.1) reflective of initial and final states only, with no regard for the intermediate states.

Forming the difference

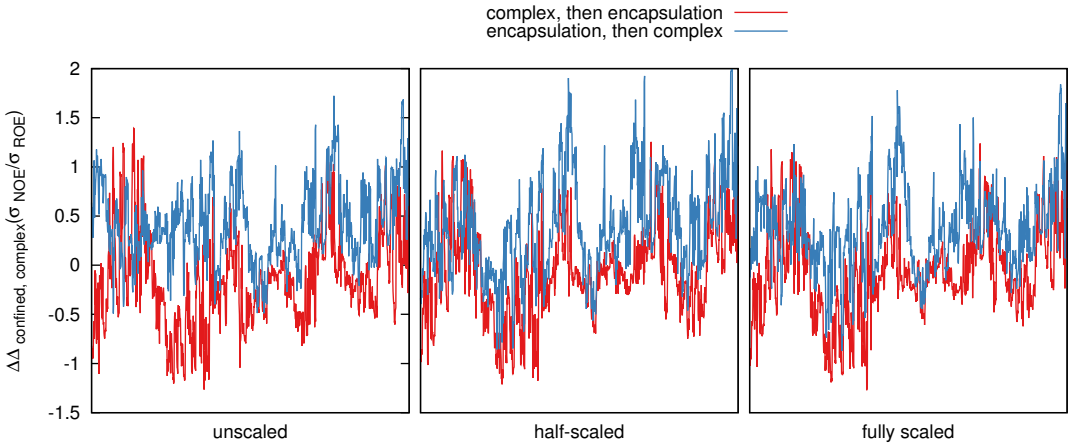
$$\Delta\Delta Q(\mathrm{A},\mathrm{C}) = \Delta Q(\mathrm{A},\mathrm{B}^*) - \Delta Q(\mathrm{B}^*,\mathrm{C}) = Q(\mathrm{A}) - 2\cdot Q(\mathrm{B}^*) + Q(\mathrm{C}) \tag{5}$$

over these paths yields vastly different values (0.5 - 0.5 = 0 ≠ 0.9 - 0.1 = 0.8), thus depending on the intermediate of the path.

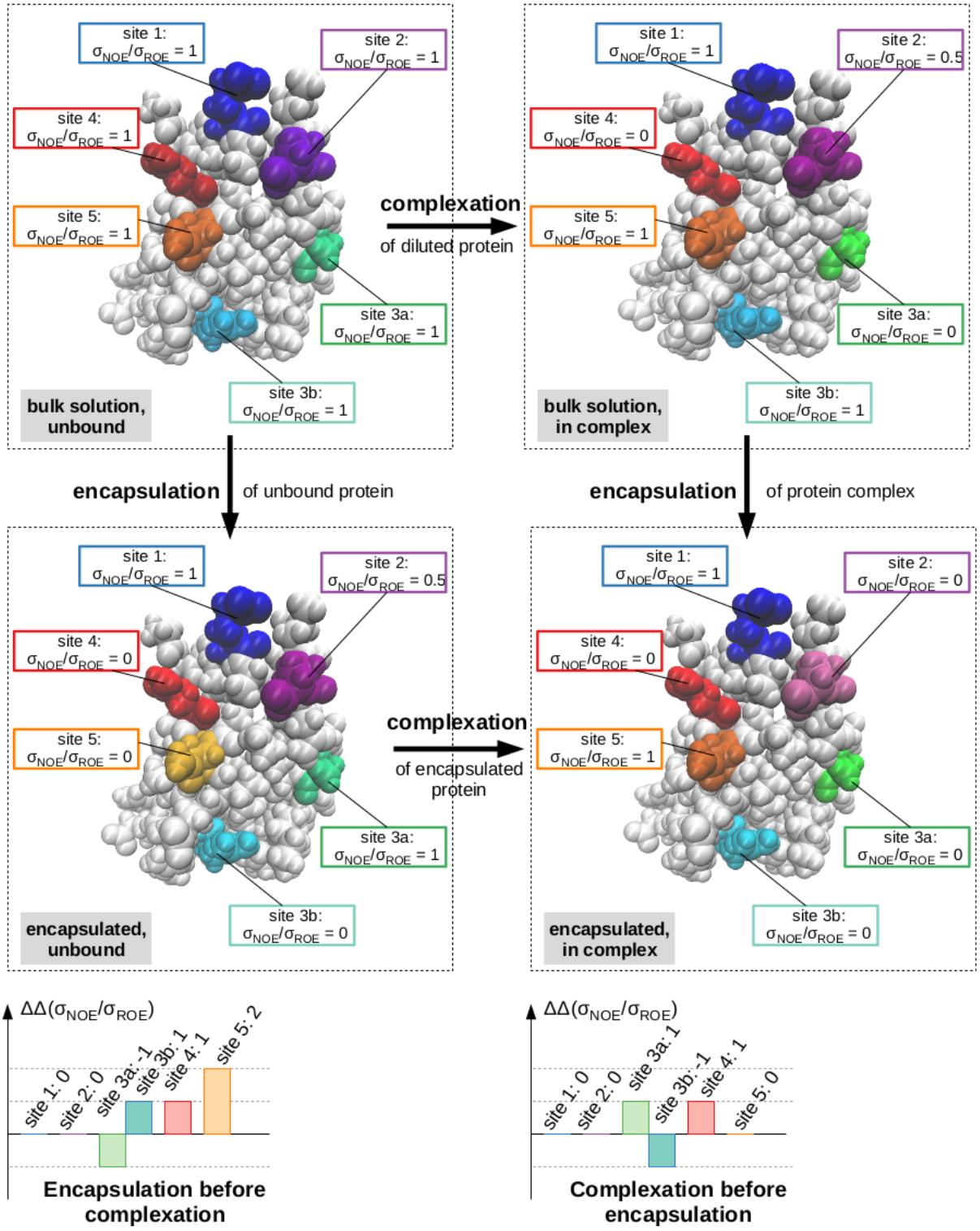
In fact, the double difference is sensitive to anisotropy of the intermediate with regards to the initial and final states. Intermediate Q(B) = 0.5 being the exact average of Q(A) and Q(B) yields a double difference of 0, while intermediate Q(B') is much closer to the final state C and yields almost the entire change in Q.

Let there be another alternative intermediate B" being much closer to the initial state A instead with Q(B") = 0.9. The double difference then yields -0.8. Thus the double difference is not only is a measure of intermediate anisotropy, but the sign also contains information about which state is more similar.

This sensitivity is precisely the reason why we devised the double difference $\Delta\Delta_{\text{confined, complex}}$ to account for two different influences of the environment on the studied biomolecule, e.g. complex formation and confinement. However, the considerations above raise the question which path to take, *i.e.* (1) complexation before encapsulation or (2) encapsulation before complexation. The figure below shows how these two double differences are clearly not state functions. The x-axis enumerates all protein hydrogen identities.



We want to comprehensively illustrate potential information and pitfalls inherent to the double difference. The figure below presents a fictional protein with six sites showing fundamentally different behavior upon complexation, confinement, or both. The NOE to ROE values selected here where chosen for the sake of mathematical simplicity.



In bulk dilution, the unbound protein shows fast hydration dynamics as can be expected[4] with NOE/ROE being 1 at all sites.

Site 1 represents a region that is entirely unaffected by either complex formation, encapsulation or both. Forming the double difference yields zero for sites of this type.

Site 2 is affected both by encapsulation and complex formation in equal measure. Since the double difference is a measure of intermediate anisotropy, it yields zero for this case.

Site 3a is affected by complex formation only while site 3b is affected selectively by the capsule wall. Forming the double difference (second difference minus first difference) yields positive values for the first difference and negative values for the second difference, thus

	sites mostly affected by complex	**sites mostly affected by confinement**
complexation before encapsulation	positive	negative
encapsulation before complexation	negative	positive

Looking at the bar diagram in above figure shows that this is indeed fulfilled. This is the optimal case where the double difference can reveal chemical information.

Site 4 is affected both by complex formation and encapsulation in equal measure. This is true e.g. for the binding region in ubiquitin (β-sheets, hydrophobic patch) which is the most interaction-prone part of ubiquitin, binding both to complex partners and the wall. Contrary to site 2, introducing the other environmental influence does not change the value further. This raises following question: If the protein is both encapsulated and bound to a partner, which one of these two selectively interacts with this region?

Looking at the bar diagrams at the bottom of above figure, we note that for both pathways, we obtain the same sign, which makes it impossible to tell apart which influence is predominant. Naive interpretation would yield

	positive sign observed	**negative sign observed**
complexation before encapsulation	complex	cell wall
encapsulation before complexation	cell wall	complex

In this case, the chosen path influences the interpretation. In our ubiquitin system (and probably most protein complex systems), the complex formation is more selective than the cell wall influence.

Consider the path encapsulation, then complexation: Unbound protein interacts with the cell wall, but upon introducing the complex partner, the same site interacts with the partner protein instead. However, the (retarded) dynamics do not change that much, thus this change is silent with regards to NOE/ROE measurement. Since the first process will be reflected more accurately by the double difference sign, we recommend to take the path "complexation before encapsulation", as complexation sites are more selective, thus avoiding silent changes, as we have done in the main article (cf. Fig. 5).

Site 5 presents a part of the protein affected by one influence introduced (e.g. encapsulation), but less (or not at all) affected when both influences are present. This is the case, e.g. when a residue of the free protein interacts with the surfactant wall, but upon forming a complex, the resulting geometry points the same residue away from the wall towards the bulk-like core of the reverse micelle. This is the case of reversible intermediates. Reversible intermediates will appear in the pathway including said intermediate, in this case the encapsulated, but unbound protein, yet not in the other path.

In summary, we recommend to use the path complexation, then encapsulation to study the influences of complex formation and confinement on a protein. Measuring the other path as well may help to identify, e.g., reversible intermediates (case 5).

3 Tables of computational NOE observables

This section lists the absolute observables σ_{NOE}, σ_{ROE} and their ratio for the systems considered in the main article. In analogy to a previous publication, we decided to show only the surface protons as decided by the σ_{ROE} being larger than or equal to the protein median σ_{ROE}.[4] For the encapsulated systems, we selected the half-scaled system as representative since it resembles the scaling strategy recommended by Best and Mittal most closely.[5] Note that the observables of hydrogen atoms attached to the same heavy atom can differ due to the asymmetric chemical environment of the protein.

Table 1: Ligase, unbound, in bulk solution

residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{\mathrm{NOE}}/\sigma_{\mathrm{ROE}}$	residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{\mathrm{NOE}}/\sigma_{\mathrm{ROE}}$
GLY-1	NH	10.41	14.67	0.71	GLY-1	NH	10.24	14.88	0.69
GLY-1	NH	10.29	14.93	0.69	GLY-1	H_α	7.62	11.56	0.66
GLY-1	H_α	7.03	11.33	0.62	SER-2	NH	8.22	15.27	0.54
SER-2	H_α	6.7	11.49	0.58	SER-2	H_β	8.35	11.28	0.74
SER-2	H_β	8.19	10.89	0.75	SER-2	H_γ	13.03	18.12	0.72
GLY-3	NH	8.98	13.72	0.65	PRO-4	H_α	6.7	10.37	0.65
GLU-5	NH	8.16	13.7	0.6	GLU-5	H_α	8.28	15.0	0.55
GLU-5	H_β	8.01	20.49	0.39	GLU-5	H_β	6.12	23.68	0.26
GLU-5	H_γ	6.85	24.82	0.28	GLU-5	H_γ	11.06	19.05	0.58
ALA-6	NH	9.62	19.3	0.5	ALA-6	H_α	8.04	12.16	0.66
ALA-6	H_β	8.58	13.08	0.66	ALA-6	H_β	8.77	13.07	0.67
ALA-6	H_β	8.61	12.91	0.67	ALA-7	NH	9.08	14.23	0.64
ALA-7	H_α	7.29	14.0	0.52	ALA-7	H_β	8.3	13.06	0.64
ALA-7	H_β	8.19	13.58	0.6	ALA-7	H_β	8.16	13.45	0.61
LEU-8	NH	8.15	16.11	0.51	LEU-8	H_α	3.72	12.75	0.29
LEU-8	H_β	5.2	12.42	0.42	LEU-8	H_γ	5.37	10.77	0.5
LEU-8	H_δ	6.62	10.56	0.63	LEU-8	H_δ	6.68	10.84	0.62
LEU-8	H_δ	6.76	10.65	0.63	GLU-9	NH	3.36	24.26	0.14
GLU-9	H_α	6.85	14.36	0.48	GLU-9	H_β	9.47	15.89	0.6
GLU-9	H_β	8.61	18.18	0.47	GLU-9	H_γ	10.33	15.96	0.65
GLU-9	H_γ	10.85	16.24	0.67	ASN-10	NH	2.12	19.63	0.11
ASN-10	H_α	6.47	12.16	0.53	ASN-10	H_β	5.15	13.71	0.38
ASN-10	H_β	3.51	18.3	0.19	ASN-10	H_δ	10.83	18.1	0.6
ASN-10	H_δ	10.48	17.64	0.59	VAL-11	NH	5.9	14.04	0.42
VAL-11	H_β	5.72	15.17	0.38	VAL-11	H_γ	4.35	11.69	0.37
VAL-11	H_γ	4.54	11.81	0.38	VAL-11	H_γ	4.6	11.99	0.38
ASP-12	NH	5.66	14.81	0.38	ASP-12	H_α	7.31	14.66	0.5
ASP-12	H_β	11.74	18.08	0.65	ASP-12	H_β	8.43	20.07	0.42
ALA-13	H_β	5.95	12.72	0.47	ALA-13	H_β	5.41	13.29	0.41
ALA-13	H_β	5.34	14.06	0.38	LYS-14	H_ϵ	2.91	12.71	0.23
LYS-14	H_ϵ	3.09	18.09	0.17	LYS-14	H_ζ	4.55	27.01	0.17
LYS-14	H_ζ	5.09	26.94	0.19	LYS-14	H_ζ	5.14	26.03	0.2
ALA-16	H_β	8.25	12.5	0.66	ALA-16	H_β	8.63	12.7	0.68
ALA-16	H_β	8.53	12.46	0.68	LYS-17	H_α	5.97	10.49	0.57
LYS-17	H_δ	5.85	10.71	0.55	LYS-17	H_δ	5.64	11.08	0.51
LYS-17	H_ϵ	5.83	13.8	0.42	LYS-17	H_ϵ	7.05	12.37	0.57
LYS-17	H_ζ	9.64	16.15	0.6	LYS-17	H_ζ	9.47	16.17	0.59
LYS-17	H_ζ	9.54	16.23	0.59	GLY-20	H_α	8.08	12.12	0.67
GLY-20	H_α	8.31	10.79	0.77	GLU-21	H_α	6.78	10.43	0.65
GLU-21	H_β	-0.85	29.26	-0.03	GLU-21	H_γ	5.24	17.41	0.3
GLU-21	H_γ	7.72	17.81	0.43	GLY-22	H_α	8.17	11.03	0.74
GLY-22	H_α	7.74	11.34	0.68	TYR-23	H_α	3.24	16.36	0.2
TYR-23	H_δ	0.5	28.74	0.02	TYR-23	H_ϵ	4.16	18.46	0.23
TYR-23	OH	-4.52	50.21	-0.09	TYR-23	H_ϵ	-5.08	22.82	-0.22
ALA-24	NH	-2.21	37.12	-0.06	ALA-24	H_α	8.63	17.79	0.49

ALA-24	H_β	8.29	19.33	0.43	ALA-24	H_β	8.19	19.05	0.43
ALA-24	H_β	8.05	19.08	0.42	PHE-25	NH	10.85	19.24	0.56
PHE-25	H_β	7.69	13.64	0.56	PHE-25	H_ζ	8.71	12.18	0.72
GLU-26	NH	7.36	16.69	0.44	GLU-26	H_β	10.36	19.88	0.52
GLU-26	H_β	10.4	17.61	0.59	GLU-26	H_γ	11.31	16.92	0.67
GLU-26	H_γ	11.06	17.46	0.63	GLU-27	H_α	3.68	12.06	0.31
GLU-27	H_β	2.52	22.21	0.11	GLU-27	H_β	-1.72	18.09	-0.1
GLU-27	H_γ	8.66	18.37	0.47	GLU-27	H_γ	10.16	18.4	0.55
LYS-29	H_β	5.67	12.53	0.45	LYS-29	H_ϵ	5.47	10.43	0.52
LYS-29	H_ζ	11.81	17.71	0.67	LYS-29	H_ζ	11.76	17.64	0.67
LYS-29	H_ζ	11.63	18.04	0.64	ARG-30	H_β	5.31	11.96	0.44
ARG-30	H_β	6.0	12.71	0.47	ARG-30	H_γ	5.9	11.06	0.53
ARG-30	H_γ	5.6	11.07	0.51	ARG-30	H_δ	8.49	14.43	0.59
ARG-30	H_δ	6.08	12.28	0.5	ARG-30	H_ϵ	9.57	17.47	0.55
ARG-30	H_η	9.19	20.34	0.45	ARG-30	H_η	11.36	17.28	0.66
ARG-30	H_η	10.72	17.32	0.62	ARG-30	H_η	11.36	16.13	0.7
GLU-33	H_α	6.34	13.17	0.48	GLU-33	H_β	6.17	12.37	0.5
GLU-33	H_β	9.59	19.0	0.5	GLU-33	H_γ	11.3	17.34	0.65
GLU-33	H_γ	9.09	15.35	0.59	GLN-36	H_β	8.41	12.79	0.66
GLN-36	H_ϵ	11.32	13.29	0.85	GLN-36	H_ϵ	8.6	10.63	0.81
ASN-37	H_β	0.66	11.32	0.06	ASN-37	H_β	4.99	13.46	0.37
ASN-37	H_δ	10.11	17.32	0.58	ASN-37	H_δ	8.96	16.68	0.54
ASN-38	H_α	1.47	25.36	0.06	ASN-38	H_β	6.42	12.12	0.53
ASN-38	H_δ	11.35	16.73	0.68	ASN-38	H_δ	10.45	16.41	0.64
VAL-39	NH	0.56	28.3	0.02	VAL-39	H_β	2.81	13.44	0.21
VAL-39	H_γ	2.55	11.48	0.22	VAL-39	H_γ	2.44	11.46	0.21
VAL-39	H_γ	2.48	11.37	0.22	GLU-40	NH	4.04	12.64	0.32
GLU-40	H_α	3.75	10.59	0.35	GLU-40	H_β	10.48	16.32	0.64
GLU-40	H_β	8.04	13.89	0.58	GLU-40	H_γ	11.16	19.06	0.59
GLU-40	H_γ	10.36	18.79	0.55	ARG-43	H_γ	-0.46	15.67	-0.03
ARG-43	H_δ	2.72	24.74	0.11	ARG-43	H_δ	6.72	17.74	0.38
ARG-43	H_ϵ	0.55	29.94	0.02	ARG-43	H_η	8.94	25.0	0.36
ARG-43	H_η	8.0	25.66	0.31	ARG-43	H_η	6.97	17.76	0.39
ARG-43	H_η	6.39	27.97	0.23	SER-44	H_α	6.32	12.35	0.51
SER-44	H_β	7.17	10.65	0.67	SER-44	H_β	7.84	12.52	0.63
SER-44	H_γ	14.3	19.56	0.73	ILE-45	H_α	5.24	10.55	0.5
LEU-46	H_α	-0.71	14.05	-0.05	LEU-46	H_β	-1.77	12.67	-0.14
LEU-46	H_δ	0.03	11.17	0.0	LEU-46	H_δ	0.23	11.12	0.02
LEU-46	H_δ	0.26	11.37	0.02	ARG-47	H_β	6.02	10.87	0.55
ARG-47	H_γ	6.91	11.7	0.59	ARG-47	H_δ	5.18	14.7	0.35
ARG-47	H_δ	2.62	10.46	0.25	ARG-47	H_ϵ	9.64	13.7	0.7
ARG-47	H_η	12.43	16.94	0.73	ARG-47	H_η	12.62	20.57	0.61
ARG-47	H_η	8.45	23.45	0.36	ARG-47	H_η	11.73	21.18	0.55
GLU-48	H_α	8.65	13.99	0.62	GLU-48	H_β	9.0	13.93	0.65
GLU-48	H_β	8.71	14.51	0.6	GLU-48	H_γ	11.14	15.82	0.7
GLU-48	H_γ	11.14	15.86	0.7	PHE-49	H_β	6.78	16.97	0.4
PHE-49	H_β	1.2	24.51	0.05	PHE-49	H_δ	5.03	10.69	0.47
PHE-49	H_ϵ	7.08	10.38	0.68	PHE-49	H_ζ	7.43	10.32	0.72
PHE-49	H_δ	4.97	10.93	0.45	ALA-50	NH	0.69	10.88	0.06
ALA-50	H_α	7.17	15.89	0.45	ALA-50	H_β	3.91	16.57	0.24
ALA-50	H_β	4.15	16.66	0.25	ALA-50	H_β	4.1	16.0	0.26
PHE-51	NH	8.15	13.34	0.61	PHE-51	H_α	6.77	15.37	0.44
PHE-51	H_β	7.13	10.36	0.69	PRO-52	H_δ	9.99	14.59	0.68
PRO-52	H_α	7.0	11.49	0.61	PRO-52	H_β	10.64	13.88	0.77

Table 2: Ligase, unbound, encapsulated

residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{NOE}/\sigma_{ROE}$	residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{NOE}/\sigma_{ROE}$
GLY-1	NH	8.75	18.46	0.47	GLY-1	NH	8.76	17.95	0.49
GLY-1	NH	8.66	18.12	0.48	GLY-1	H_α	6.29	15.62	0.4
GLY-1	H_α	6.17	13.4	0.46	SER-2	NH	6.21	17.61	0.35
SER-2	H_α	4.61	12.33	0.37	SER-2	H_β	5.32	10.85	0.49
SER-2	H_γ	8.72	16.92	0.52	GLY-3	NH	5.67	15.83	0.36
GLY-3	H_α	1.46	12.33	0.12	GLU-5	NH	1.37	17.56	0.08
GLU-5	H_α	-0.52	16.84	-0.03	GLU-5	H_β	2.42	21.96	0.11
GLU-5	H_β	3.23	22.71	0.14	GLU-5	H_γ	2.15	26.21	0.08
GLU-5	H_γ	4.1	24.05	0.17	ALA-6	NH	-2.45	22.63	-0.11
ALA-7	NH	-2.16	17.83	-0.12	ALA-7	H_α	-0.42	12.58	-0.03
ALA-7	H_β	1.69	15.32	0.11	ALA-7	H_β	1.73	15.54	0.11
ALA-7	H_β	1.62	15.91	0.1	LEU-8	NH	-2.94	20.18	-0.15
LEU-8	H_α	-1.39	13.85	-0.1	GLU-9	NH	-2.89	29.12	-0.1
GLU-9	H_α	-8.39	34.4	-0.24	GLU-9	H_β	-20.68	58.37	-0.35
GLU-9	H_β	-6.81	33.38	-0.2	GLU-9	H_γ	-3.51	28.11	-0.12
GLU-9	H_γ	-3.24	27.34	-0.12	ASN-10	NH	-14.47	49.22	-0.29
ASN-10	H_α	-2.2	24.98	-0.09	ASN-10	H_β	-4.99	22.18	-0.22
ASN-10	H_β	-2.59	18.87	-0.14	ASN-10	H_δ	2.93	21.16	0.14
ASN-10	H_δ	2.08	25.97	0.08	VAL-11	NH	-0.99	27.97	-0.04
VAL-11	H_α	-4.4	12.08	-0.36	VAL-11	H_β	3.1	19.44	0.16
VAL-11	H_γ	2.26	11.1	0.2	VAL-11	H_γ	2.08	11.09	0.19
VAL-11	H_γ	2.25	11.29	0.2	VAL-11	H_γ	-2.87	24.7	-0.12
VAL-11	H_γ	-2.64	24.71	-0.11	VAL-11	H_γ	-2.7	24.34	-0.11
ASP-12	NH	0.86	15.89	0.05	ASP-12	H_β	2.85	11.28	0.25
ASP-12	H_β	1.59	13.0	0.12	ALA-13	H_β	-0.94	14.01	-0.07
ALA-13	H_β	-1.64	15.08	-0.11	ALA-13	H_β	-1.42	15.09	-0.09
LYS-14	H_γ	-6.97	22.8	-0.31	LYS-14	H_γ	-3.37	16.47	-0.2
LYS-14	H_δ	-3.46	12.71	-0.27	LYS-14	H_δ	-6.73	18.67	-0.36
LYS-14	H_ϵ	-9.13	32.51	-0.28	LYS-14	H_ϵ	-6.46	33.51	-0.19
LYS-14	H_ζ	-14.85	60.49	-0.25	LYS-14	H_ζ	-13.94	59.93	-0.23
LYS-14	H_ζ	-13.31	57.35	-0.23	LYS-17	H_β	-5.48	17.1	-0.32
LYS-17	H_β	-2.18	14.37	-0.15	LYS-17	H_γ	-2.22	13.58	-0.16
LYS-17	H_δ	-0.61	12.59	-0.05	LYS-17	H_δ	-2.03	13.98	-0.15
LYS-17	H_ϵ	-2.36	20.86	-0.11	LYS-17	H_ϵ	-0.5	16.32	-0.03
LYS-17	H_ζ	-0.67	26.57	-0.03	LYS-17	H_ζ	-0.92	26.34	-0.03
LYS-17	H_ζ	-1.6	27.77	-0.06	LEU-18	H_α	-8.17	19.3	-0.42
MET-19	H_α	-5.4	15.85	-0.34	GLY-20	H_α	-0.89	11.44	-0.08
GLU-21	H_α	-2.71	15.98	-0.17	GLU-21	H_β	-22.13	57.48	-0.38
GLU-21	H_β	-5.61	15.44	-0.36	GLU-21	H_γ	-11.94	36.48	-0.33
GLU-21	H_γ	-6.77	28.91	-0.23	GLY-22	H_α	-0.57	12.1	-0.05
GLY-22	H_α	-1.59	12.99	-0.12	TYR-23	H_α	-6.55	28.39	-0.23
TYR-23	H_β	-4.94	14.2	-0.35	TYR-23	H_δ	-11.66	39.55	-0.29
TYR-23	H_ϵ	-7.87	31.31	-0.25	TYR-23	OH	-35.19	94.86	-0.37
TYR-23	H_ϵ	-17.36	44.15	-0.39	ALA-24	NH	-16.72	57.19	-0.29
ALA-24	H_α	-9.2	34.59	-0.27	ALA-24	H_β	-1.84	29.09	-0.06
ALA-24	H_β	-1.85	29.22	-0.06	ALA-24	H_β	-1.84	29.39	-0.06
PHE-25	NH	-13.73	49.99	-0.27	PHE-25	H_β	-4.06	23.08	-0.18
PHE-25	H_β	-1.89	11.46	-0.16	PHE-25	H_ζ	3.36	12.17	0.28
GLU-26	NH	-4.54	28.63	-0.16	GLU-26	H_β	7.57	21.86	0.35
GLU-26	H_β	2.83	25.45	0.11	GLU-26	H_γ	5.24	21.02	0.25
GLU-26	H_γ	2.22	23.13	0.1	GLU-27	H_α	2.65	16.36	0.16
GLU-27	H_β	-1.97	27.26	-0.07	GLU-27	H_β	-7.0	24.41	-0.29
GLU-27	H_γ	3.27	24.12	0.14	GLU-27	H_γ	5.59	22.99	0.24
LYS-29	H_β	3.86	14.35	0.27	LYS-29	H_ϵ	3.8	11.83	0.32
LYS-29	H_ζ	7.72	18.98	0.41	LYS-29	H_ζ	7.22	19.35	0.37
LYS-29	H_ζ	7.35	19.02	0.39	ARG-30	H_α	1.35	12.0	0.11
ARG-30	H_β	2.04	14.4	0.14	ARG-30	H_β	5.2	17.11	0.3
ARG-30	H_γ	5.32	15.54	0.34	ARG-30	H_δ	5.42	18.19	0.3

ARG-30	H_ϵ	4.14	18.81	0.22	ARG-30	H_η	5.11	16.79	0.3
ARG-30	H_η	4.84	17.36	0.28	ARG-30	H_η	4.55	17.52	0.26
ARG-30	H_η	4.47	14.92	0.3	GLU-33	H_α	2.9	16.27	0.18
GLU-33	H_β	6.24	21.06	0.3	GLU-33	H_γ	6.71	18.52	0.36
GLU-33	H_γ	2.9	10.94	0.27	GLN-36	H_ϵ	4.94	14.56	0.34
ASN-37	H_β	-9.52	29.29	-0.32	ASN-37	H_β	-7.9	35.56	-0.22
ASN-37	H_δ	5.08	23.21	0.22	ASN-37	H_δ	-5.75	39.85	-0.14
ASN-38	H_α	-9.42	39.03	-0.24	ASN-38	H_β	0.54	14.44	0.04
ASN-38	H_δ	2.22	23.67	0.09	ASN-38	H_δ	-1.16	31.19	-0.04
VAL-39	NH	-11.41	43.63	-0.26	VAL-39	H_β	-4.12	23.02	-0.18
VAL-39	H_γ	-2.74	15.94	-0.17	VAL-39	H_γ	-2.43	16.26	-0.15
VAL-39	H_γ	-2.62	16.33	-0.16	VAL-39	H_γ	-1.8	11.1	-0.16
VAL-39	H_γ	-2.08	11.62	-0.18	VAL-39	H_γ	-1.7	11.35	-0.15
GLU-40	NH	-4.3	23.08	-0.19	GLU-40	H_α	-5.0	23.41	-0.21
GLU-40	H_β	2.3	19.56	0.12	GLU-40	H_β	1.8	17.04	0.11
GLU-40	H_γ	1.6	26.94	0.06	GLU-40	H_γ	0.61	29.56	0.02
ARG-43	H_β	-3.04	17.2	-0.18	ARG-43	H_β	-5.11	15.07	-0.34
ARG-43	H_γ	-7.81	20.02	-0.39	ARG-43	H_γ	-3.64	15.14	-0.24
ARG-43	H_δ	-10.69	44.37	-0.24	ARG-43	H_δ	-6.63	33.12	-0.2
ARG-43	H_ϵ	-24.21	65.82	-0.37	ARG-43	H_η	-1.95	36.0	-0.05
ARG-43	H_η	-4.9	43.2	-0.11	ARG-43	H_η	-9.29	34.95	-0.27
ARG-43	H_η	-10.4	49.8	-0.21	SER-44	H_α	-0.21	16.83	-0.01
SER-44	H_β	2.41	11.62	0.21	SER-44	H_γ	4.1	23.68	0.17
LEU-46	H_α	-2.24	21.7	-0.1	LEU-46	H_β	-4.3	15.9	-0.27
LEU-46	H_δ	-1.84	14.76	-0.12	LEU-46	H_δ	-2.11	15.41	-0.14
LEU-46	H_δ	-1.99	14.97	-0.13	ARG-47	H_α	-2.61	17.54	-0.15
ARG-47	H_β	-1.48	21.41	-0.07	ARG-47	H_β	-1.18	16.29	-0.07
ARG-47	H_γ	-0.25	15.48	-0.02	ARG-47	H_γ	-1.68	13.13	-0.13
ARG-47	H_δ	-4.39	24.73	-0.18	ARG-47	H_δ	-5.5	21.66	-0.25
ARG-47	H_ϵ	-2.09	25.83	-0.08	ARG-47	H_η	-0.91	30.26	-0.03
ARG-47	H_η	-4.01	35.87	-0.11	ARG-47	H_η	-10.24	44.48	-0.23
ARG-47	H_η	-5.58	37.16	-0.15	GLU-48	NH	-3.88	18.83	-0.21
GLU-48	H_α	0.5	20.33	0.02	GLU-48	H_β	2.49	13.82	0.18
GLU-48	H_β	1.91	16.07	0.12	GLU-48	H_γ	3.65	18.24	0.2
GLU-48	H_γ	3.62	18.57	0.19	PHE-49	NH	-1.02	13.03	-0.08
PHE-49	H_β	-1.69	14.32	-0.12	PHE-49	H_β	-3.96	19.79	-0.2
ALA-50	NH	-3.67	16.47	-0.22	ALA-50	H_α	-4.81	26.58	-0.18
ALA-50	H_β	-3.9	24.96	-0.16	ALA-50	H_β	-4.42	26.65	-0.17
ALA-50	H_β	-4.27	26.37	-0.16	PHE-51	NH	-4.48	24.98	-0.18
PHE-51	H_α	-4.2	25.18	-0.17	PRO-52	H_δ	-3.94	20.25	-0.19
PRO-52	H_α	-1.85	13.89	-0.13	PRO-52	H_β	0.07	13.69	0.0

Table 3: Ligase, in complex with UBQ, in bulk solution

residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{NOE}/\sigma_{ROE}$	residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{NOE}/\sigma_{ROE}$
GLY-1	NH	10.39	13.25	0.78	GLY-1	NH	10.32	13.26	0.78
GLY-1	NH	10.46	13.19	0.79	GLY-1	H_α	7.68	10.92	0.7
SER-2	NH	9.14	13.12	0.7	SER-2	H_β	8.09	11.96	0.68
SER-2	H_β	7.95	11.52	0.69	SER-2	H_γ	12.92	18.01	0.72
GLY-3	NH	8.32	14.04	0.59	GLY-3	H_α	4.47	14.4	0.31
GLY-3	H_α	5.7	11.93	0.48	PRO-4	H_δ	4.37	13.25	0.33
PRO-4	H_δ	5.45	11.36	0.48	PRO-4	H_α	6.32	12.91	0.49
PRO-4	H_β	6.88	11.26	0.61	PRO-4	H_β	4.81	14.66	0.33
PRO-4	H_γ	5.29	13.6	0.39	GLU-5	NH	5.71	19.15	0.3
GLU-5	H_α	4.6	19.92	0.23	GLU-5	H_β	7.9	20.89	0.38
GLU-5	H_β	8.97	18.47	0.49	GLU-5	H_γ	10.05	18.43	0.55
GLU-5	H_γ	9.99	20.08	0.5	ALA-6	NH	4.71	26.29	0.18
ALA-6	H_α	5.51	17.72	0.31	ALA-6	H_β	5.65	17.25	0.33
ALA-6	H_β	5.49	17.07	0.32	ALA-6	H_β	5.85	17.02	0.34
ALA-7	NH	4.39	25.47	0.17	ALA-7	H_α	5.69	17.86	0.32
ALA-7	H_β	7.55	14.91	0.51	ALA-7	H_β	7.48	14.91	0.5
ALA-7	H_β	7.43	14.93	0.5	LEU-8	NH	2.15	24.35	0.09
LEU-8	H_α	3.47	13.12	0.26	LEU-8	H_β	4.51	13.46	0.34
GLU-9	NH	2.83	28.75	0.1	GLU-9	H_α	5.03	17.45	0.29
GLU-9	H_β	7.18	20.53	0.35	GLU-9	H_β	6.81	22.35	0.3
GLU-9	H_γ	7.79	19.86	0.39	GLU-9	H_γ	8.48	19.58	0.43
ASN-10	NH	-0.27	27.12	-0.01	ASN-10	H_α	2.81	21.46	0.13
ASN-10	H_β	1.34	22.01	0.06	ASN-10	H_β	1.04	23.8	0.04
ASN-10	H_δ	-1.39	46.33	-0.03	ASN-10	H_δ	-12.41	68.33	-0.18
VAL-11	NH	-5.19	40.4	-0.13	VAL-11	H_β	0.14	26.99	0.01
VAL-11	H_γ	2.2	11.62	0.19	VAL-11	H_γ	2.29	11.49	0.2
VAL-11	H_γ	2.22	11.58	0.19	VAL-11	H_γ	2.93	16.3	0.18
VAL-11	H_γ	3.04	15.85	0.19	VAL-11	H_γ	2.96	16.25	0.18
ASP-12	NH	-18.05	55.02	-0.33	ASP-12	H_β	-43.52	94.26	-0.46
ASP-12	H_β	-60.34	138.02	-0.44	ALA-13	NH	-3.08	11.74	-0.26
ALA-13	H_β	-0.5	20.1	-0.03	ALA-13	H_β	-0.11	19.97	-0.01
ALA-13	H_β	-0.01	19.46	-0.0	LYS-14	H_ϵ	2.65	14.22	0.19
LYS-14	H_ϵ	3.43	18.01	0.19	LYS-14	H_ζ	4.57	27.29	0.17
LYS-14	H_ζ	4.52	26.78	0.17	LYS-14	H_ζ	4.76	27.56	0.17
ALA-16	H_β	-3.73	11.63	-0.32	ALA-16	H_β	-3.61	11.38	-0.32
ALA-16	H_β	-3.78	11.47	-0.33	LYS-17	H_α	-0.58	13.28	-0.04
LYS-17	H_δ	3.51	11.5	0.31	LYS-17	H_δ	3.08	13.05	0.24
LYS-17	H_ϵ	5.25	14.41	0.36	LYS-17	H_ϵ	5.9	14.17	0.42
LYS-17	H_ζ	9.17	20.16	0.45	LYS-17	H_ζ	9.39	19.87	0.47
LYS-17	H_ζ	8.93	19.52	0.46	LEU-18	H_α	-5.87	18.52	-0.32
MET-19	H_α	-19.32	43.06	-0.45	MET-19	H_β	-19.39	43.23	-0.45
MET-19	H_γ	-28.91	62.75	-0.46	MET-19	H_ϵ	-14.14	34.42	-0.41
MET-19	H_ϵ	-13.99	34.79	-0.4	MET-19	H_ϵ	-13.6	33.81	-0.4
GLY-20	H_α	-0.03	19.63	-0.0	GLY-20	H_α	-1.92	21.48	-0.09
GLU-21	H_α	6.13	13.06	0.47	GLU-21	H_β	0.03	25.37	0.0
GLU-21	H_β	-6.05	22.54	-0.27	GLU-21	H_γ	1.12	23.85	0.05
GLU-21	H_γ	6.51	20.32	0.32	GLY-22	NH	-5.3	17.51	-0.3
GLY-22	H_α	2.83	16.83	0.17	GLY-22	H_α	-20.44	58.77	-0.35
TYR-23	NH	-7.34	18.79	-0.39	TYR-23	H_α	-9.06	36.24	-0.25
TYR-23	H_β	-5.8	16.57	-0.35	TYR-23	H_δ	-9.53	41.26	-0.23
TYR-23	H_ϵ	2.82	17.45	0.16	TYR-23	OH	0.55	38.17	0.01
TYR-23	H_δ	-4.22	12.06	-0.35	TYR-23	H_ϵ	-3.67	22.9	-0.16
ALA-24	NH	-23.51	75.61	-0.31	ALA-24	H_α	-115.05	252.8	-0.46
ALA-24	H_β	-2.0	39.91	-0.05	ALA-24	H_β	-1.88	39.16	-0.05
ALA-24	H_β	-1.12	38.54	-0.03	PHE-25	NH	-34.99	99.89	-0.35
PHE-25	H_β	-11.64	46.49	-0.25	PHE-25	H_β	-7.14	22.33	-0.32
PHE-25	H_δ	1.27	13.66	0.09	PHE-25	H_ϵ	5.94	14.25	0.42
GLU-26	NH	-5.87	39.76	-0.15	GLU-26	H_β	8.32	22.67	0.37

GLU-26	H_β	7.01	28.22	0.25	GLU-26	H_γ	7.37	24.71	0.3
GLU-26	H_γ	8.64	19.57	0.44	GLU-27	H_β	-1.26	17.77	-0.07
GLU-27	H_β	-5.46	23.71	-0.23	GLU-27	H_γ	2.95	28.43	0.1
GLU-27	H_γ	5.45	21.45	0.25	LYS-29	H_ϵ	6.01	12.15	0.49
LYS-29	H_ϵ	5.31	11.04	0.48	LYS-29	H_ζ	10.2	18.54	0.55
LYS-29	H_ζ	10.13	18.51	0.55	LYS-29	H_ζ	10.03	18.09	0.55
ARG-30	H_α	4.93	11.89	0.41	ARG-30	H_γ	5.6	11.16	0.5
ARG-30	H_γ	6.63	13.01	0.51	ARG-30	H_δ	4.6	12.18	0.38
ARG-30	H_δ	6.4	13.95	0.46	ARG-30	H_ϵ	8.79	18.85	0.47
ARG-30	H_η	7.99	26.36	0.3	ARG-30	H_η	11.32	18.06	0.63
ARG-30	H_η	10.55	16.88	0.63	ARG-30	H_η	11.43	18.66	0.61
GLU-33	H_α	6.17	13.04	0.47	GLU-33	H_β	7.39	13.98	0.53
GLU-33	H_β	8.9	18.05	0.49	GLU-33	H_γ	10.64	17.29	0.62
GLU-33	H_γ	10.22	17.78	0.57	GLN-36	H_β	8.78	13.0	0.68
GLN-36	H_ϵ	11.35	13.56	0.84	ASN-37	H_β	0.75	12.37	0.06
ASN-37	H_β	5.18	14.91	0.35	ASN-37	H_δ	10.33	18.0	0.57
ASN-37	H_δ	8.45	18.43	0.46	ASN-38	H_α	2.38	24.26	0.1
ASN-38	H_β	7.11	12.26	0.58	ASN-38	H_δ	11.34	16.29	0.7
ASN-38	H_δ	10.89	15.85	0.69	VAL-39	NH	1.1	28.24	0.04
VAL-39	H_β	3.42	14.62	0.23	GLU-40	NH	4.47	12.65	0.35
GLU-40	H_β	10.28	16.4	0.63	GLU-40	H_β	8.29	14.13	0.59
GLU-40	H_γ	11.3	19.0	0.59	GLU-40	H_γ	10.47	19.5	0.54
ARG-43	H_γ	-1.66	13.67	-0.12	ARG-43	H_γ	-1.47	15.56	-0.09
ARG-43	H_δ	4.18	19.24	0.22	ARG-43	H_δ	4.59	16.84	0.27
ARG-43	H_ϵ	-1.53	33.99	-0.05	ARG-43	H_η	9.06	23.96	0.38
ARG-43	H_η	9.32	22.89	0.41	ARG-43	H_η	7.97	23.55	0.34
ARG-43	H_η	6.4	21.33	0.3	SER-44	H_β	7.44	11.33	0.66
SER-44	H_β	7.46	12.01	0.62	SER-44	H_γ	14.57	20.28	0.72
ARG-47	H_α	2.98	13.0	0.23	ARG-47	H_ϵ	7.52	17.22	0.44
ARG-47	H_η	7.34	23.14	0.32	ARG-47	H_η	7.58	21.66	0.35
ARG-47	H_η	6.97	16.92	0.41	ARG-47	H_η	-0.02	34.04	-0.0
GLU-48	H_β	10.33	13.77	0.75	GLU-48	H_β	7.53	13.22	0.57
GLU-48	H_γ	8.99	14.58	0.62	GLU-48	H_γ	10.31	13.9	0.74
PHE-49	H_β	3.13	12.83	0.24	PHE-49	H_β	2.3	13.62	0.17
PHE-49	H_ϵ	6.69	11.05	0.61	ALA-50	H_α	5.35	15.19	0.35
ALA-50	H_β	7.84	12.09	0.65	ALA-50	H_β	7.65	11.92	0.64
ALA-50	H_β	7.68	12.07	0.64	PHE-51	NH	3.61	11.91	0.3
PHE-51	H_α	-0.74	10.96	-0.07	PHE-51	H_β	5.54	11.73	0.47
PRO-52	H_δ	0.86	13.07	0.07	PRO-52	H_δ	-1.6	18.65	-0.09
PRO-52	H_α	10.4	17.24	0.6	PRO-52	H_β	6.19	13.4	0.46
PRO-52	H_β	8.1	17.3	0.47	PRO-52	H_γ	4.45	17.99	0.25

Table 4: Ligase, in complex with UBQ, encapsulated

residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{NOE}/\sigma_{ROE}$	residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{NOE}/\sigma_{ROE}$
GLY-1	NH	-4.28	44.84	-0.1	GLY-1	NH	-5.0	45.98	-0.11
GLY-1	NH	-4.01	44.91	-0.09	GLY-1	H_α	-3.8	35.25	-0.11
GLY-1	H_α	-0.98	30.67	-0.03	SER-2	NH	-1.38	32.23	-0.04
SER-2	H_α	2.17	17.5	0.12	SER-2	H_γ	5.88	22.29	0.26
GLY-3	NH	2.31	22.0	0.11	GLY-3	H_α	-2.67	15.97	-0.17
PRO-4	H_α	-3.15	19.72	-0.16	GLU-5	NH	-10.18	40.88	-0.25
GLU-5	H_α	-9.95	35.92	-0.28	GLU-5	H_β	-15.9	58.68	-0.27
GLU-5	H_β	-16.32	59.37	-0.27	GLU-5	H_γ	-8.8	43.7	-0.2
GLU-5	H_γ	-9.98	51.95	-0.19	ALA-6	NH	-10.33	38.43	-0.27
ALA-6	H_α	-3.62	17.26	-0.21	ALA-7	NH	-5.51	25.58	-0.22
ALA-7	H_α	-34.09	81.99	-0.42	ALA-7	H_β	-21.9	61.1	-0.36
ALA-7	H_β	-20.7	59.77	-0.35	ALA-7	H_β	-23.38	64.41	-0.36
LEU-8	NH	-60.74	135.25	-0.45	LEU-8	H_β	-8.08	20.25	-0.4
LEU-8	H_β	-16.95	39.54	-0.43	LEU-8	H_γ	-6.6	16.56	-0.4
GLU-9	NH	-51.96	113.45	-0.46	GLU-9	H_α	-2.3	26.65	-0.09
GLU-9	H_β	-22.77	66.98	-0.34	GLU-9	H_β	-33.71	84.86	-0.4
GLU-9	H_γ	-10.72	39.98	-0.27	GLU-9	H_γ	-8.12	40.03	-0.2
ASN-10	NH	0.28	32.18	0.01	ASN-10	H_α	-23.75	67.82	-0.35
ASN-10	H_β	-4.21	35.79	-0.12	ASN-10	H_β	0.52	26.44	0.02
ASN-10	H_δ	-22.15	80.78	-0.27	ASN-10	H_δ	-13.95	64.77	-0.22
VAL-11	NH	-88.9	197.65	-0.45	VAL-11	H_α	-15.8	35.14	-0.45
VAL-11	H_β	-33.44	84.0	-0.4	VAL-11	H_γ	-9.69	32.06	-0.3
VAL-11	H_γ	-10.23	32.6	-0.31	VAL-11	H_γ	-10.17	32.47	-0.31
VAL-11	H_γ	-26.99	69.27	-0.39	VAL-11	H_γ	-24.98	64.47	-0.39
VAL-11	H_γ	-26.73	68.17	-0.39	ASP-12	NH	-77.68	168.42	-0.46
ASP-12	H_α	-8.36	22.97	-0.36	ASP-12	H_β	-27.14	66.6	-0.41
ASP-12	H_β	-35.52	89.65	-0.4	ALA-13	H_β	3.85	16.99	0.23
ALA-13	H_β	4.06	16.73	0.24	ALA-13	H_β	3.81	16.79	0.23
LYS-14	H_γ	-3.04	19.85	-0.15	LYS-14	H_γ	-1.07	15.34	-0.07
LYS-14	H_δ	-13.59	31.7	-0.43	LYS-14	H_ϵ	-13.46	43.98	-0.31
LYS-14	H_ϵ	-8.98	38.86	-0.23	LYS-14	H_ζ	-23.61	77.2	-0.31
LYS-14	H_ζ	-24.09	77.13	-0.31	LYS-14	H_ζ	-25.73	81.04	-0.32
LYS-17	H_ϵ	3.27	15.51	0.21	LYS-17	H_ζ	6.76	16.35	0.41
LYS-17	H_ζ	6.9	16.51	0.42	LYS-17	H_ζ	6.63	16.39	0.4
MET-19	H_α	-22.12	48.52	-0.46	MET-19	H_β	-17.51	39.11	-0.45
MET-19	H_γ	-27.41	58.95	-0.46	MET-19	H_ϵ	-26.04	58.69	-0.44
MET-19	H_ϵ	-27.31	61.22	-0.45	MET-19	H_ϵ	-25.48	57.31	-0.44
GLY-20	H_α	1.08	16.89	0.06	GLY-20	H_α	-2.2	20.27	-0.11
GLU-21	H_α	2.03	15.22	0.13	GLU-21	H_β	-10.95	41.44	-0.26
GLU-21	H_γ	1.59	16.46	0.1	GLU-21	H_γ	2.85	20.13	0.14
GLY-22	NH	-9.0	23.32	-0.39	GLY-22	H_α	-3.59	30.32	-0.12
GLY-22	H_α	-28.42	74.21	-0.38	TYR-23	NH	-5.9	15.21	-0.39
TYR-23	H_α	-10.89	38.8	-0.28	TYR-23	H_β	-8.06	20.96	-0.38
TYR-23	H_δ	-11.82	45.85	-0.26	TYR-23	H_ϵ	2.93	21.81	0.13
TYR-23	OH	-11.11	55.97	-0.2	TYR-23	H_ϵ	-11.72	33.62	-0.35
ALA-24	NH	-35.16	94.65	-0.37	ALA-24	H_α	-54.81	130.04	-0.42
ALA-24	H_β	-2.37	36.08	-0.07	ALA-24	H_β	-2.78	36.47	-0.08
ALA-24	H_β	-3.37	37.02	-0.09	PHE-25	NH	-47.76	123.24	-0.39
PHE-25	H_β	-20.94	59.53	-0.35	PHE-25	H_β	-32.08	72.06	-0.45
PHE-25	H_δ	-11.48	32.49	-0.35	PHE-25	H_ϵ	-1.65	16.98	-0.1
GLU-26	NH	-2.71	29.52	-0.09	GLU-26	H_α	-2.38	17.51	-0.14
GLU-26	H_β	3.57	28.61	0.12	GLU-26	H_β	4.27	25.74	0.17
GLU-26	H_γ	1.39	32.14	0.04	GLU-26	H_γ	-22.09	75.73	-0.29
GLU-27	H_α	-5.75	24.87	-0.23	GLU-27	H_β	-11.77	39.89	-0.3
GLU-27	H_β	-12.25	33.6	-0.36	GLU-27	H_γ	1.96	26.71	0.07
GLU-27	H_γ	-1.9	34.3	-0.06	LYS-29	H_α	-5.18	17.5	-0.3
LYS-29	H_β	-3.99	28.81	-0.14	LYS-29	H_β	-2.35	16.07	-0.15
LYS-29	H_δ	-3.42	17.61	-0.19	LYS-29	H_ϵ	-10.45	40.8	-0.26

LYS-29	H_{ϵ}	-7.62	31.72	-0.24	LYS-29	H_{ζ}	-6.74	41.84	-0.16
LYS-29	H_{ζ}	-7.26	41.98	-0.17	LYS-29	H_{ζ}	-7.58	42.3	-0.18
ARG-30	H_{α}	-4.71	18.08	-0.26	ARG-30	H_{β}	-5.23	21.23	-0.25
ARG-30	H_{β}	-2.3	19.93	-0.12	ARG-30	H_{γ}	-1.5	17.98	-0.08
ARG-30	H_{γ}	-3.15	24.6	-0.13	ARG-30	H_{δ}	-5.46	31.07	-0.18
ARG-30	H_{δ}	-4.2	21.5	-0.2	ARG-30	H_{ϵ}	-3.58	33.94	-0.11
ARG-30	H_{η}	-13.67	50.53	-0.27	ARG-30	H_{η}	-2.59	30.07	-0.09
ARG-30	H_{η}	-1.85	30.01	-0.06	ARG-30	H_{η}	-0.44	23.62	-0.02
LEU-32	H_{β}	-10.17	26.44	-0.38	LEU-32	H_{β}	-7.01	19.64	-0.36
GLU-33	NH	-5.51	16.09	-0.34	GLU-33	H_{α}	-8.47	33.29	-0.25
GLU-33	H_{β}	-6.89	24.15	-0.29	GLU-33	H_{β}	-7.63	36.99	-0.21
GLU-33	H_{γ}	-8.71	41.14	-0.21	GLU-33	H_{γ}	-10.23	37.33	-0.27
GLN-36	H_{α}	-10.31	29.38	-0.35	GLN-36	H_{β}	-10.88	27.37	-0.4
GLN-36	H_{ϵ}	-4.31	18.01	-0.24	ASN-37	H_{β}	-31.62	68.69	-0.46
ASN-37	H_{β}	-59.8	134.41	-0.44	ASN-37	H_{δ}	-22.47	75.43	-0.3
ASN-37	H_{δ}	-73.19	168.38	-0.43	ASN-38	H_{α}	-16.48	49.98	-0.33
ASN-38	H_{β}	-6.6	18.12	-0.36	ASN-38	H_{δ}	-6.41	31.12	-0.21
ASN-38	H_{δ}	-10.48	40.35	-0.26	VAL-39	NH	-16.33	53.57	-0.3
VAL-39	H_{β}	-4.07	28.8	-0.14	VAL-39	H_{γ}	-1.59	15.3	-0.1
VAL-39	H_{γ}	-1.26	15.01	-0.08	GLU-40	NH	-6.0	22.78	-0.26
GLU-40	H_{α}	-8.95	25.8	-0.35	GLU-40	H_{β}	-7.2	25.01	-0.29
GLU-40	H_{γ}	-1.25	22.61	-0.06	GLU-40	H_{γ}	0.03	26.97	0.0
ARG-43	H_{β}	-10.65	27.59	-0.39	ARG-43	H_{β}	-6.05	15.48	-0.39
ARG-43	H_{δ}	-7.6	35.25	-0.22	ARG-43	H_{δ}	-5.43	27.51	-0.2
ARG-43	H_{ϵ}	-9.17	42.03	-0.22	ARG-43	H_{η}	-8.57	45.29	-0.19
ARG-43	H_{η}	-1.29	38.28	-0.03	ARG-43	H_{η}	-2.03	40.4	-0.05
ARG-43	H_{η}	0.1	21.97	0.0	SER-44	NH	-9.7	23.08	-0.42
SER-44	H_{β}	-7.11	17.93	-0.4	SER-44	H_{γ}	-8.71	30.9	-0.28
ILE-45	H_{γ}	-5.39	16.58	-0.33	ILE-45	H_{γ}	-5.12	16.21	-0.32
ILE-45	H_{γ}	-5.71	17.3	-0.33	LEU-46	H_{α}	-11.08	37.33	-0.3
LEU-46	H_{β}	-4.01	17.79	-0.23	LEU-46	H_{δ}	-6.09	21.41	-0.28
LEU-46	H_{δ}	-5.97	21.12	-0.28	LEU-46	H_{δ}	-6.15	21.51	-0.29
ARG-47	H_{α}	1.88	19.9	0.09	ARG-47	H_{γ}	2.57	15.57	0.17
ARG-47	H_{γ}	-2.69	22.2	-0.12	ARG-47	H_{δ}	-1.77	21.2	-0.08
ARG-47	H_{δ}	2.63	19.39	0.14	ARG-47	H_{ϵ}	-4.31	21.82	-0.2
ARG-47	H_{η}	-5.08	26.3	-0.19	ARG-47	H_{η}	-8.67	47.04	-0.18
ARG-47	H_{η}	1.07	31.78	0.03	ARG-47	H_{η}	-0.92	33.85	-0.03
GLU-48	H_{α}	-5.11	23.24	-0.22	GLU-48	H_{γ}	-5.48	19.06	-0.29
ALA-50	H_{α}	-13.59	46.84	-0.29	ALA-50	H_{β}	-3.18	27.49	-0.12
ALA-50	H_{β}	-3.72	28.39	-0.13	ALA-50	H_{β}	-3.13	28.15	-0.11
PHE-51	NH	-8.91	40.16	-0.22	PHE-51	H_{β}	-0.65	21.13	-0.03

Table 5: UBQ, unbound, in bulk solution

residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{NOE}/\sigma_{ROE}$	residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{NOE}/\sigma_{ROE}$
MET-1	NH	9.98	22.15	0.45	MET-1	NH	9.78	21.87	0.45
MET-1	NH	9.85	21.82	0.45	MET-1	H_α	4.85	25.37	0.19
MET-1	H_β	6.81	16.86	0.4	MET-1	H_β	1.44	14.42	0.1
GLN-2	NH	-2.81	33.73	-0.08	GLN-2	H_β	2.01	11.31	0.18
GLN-2	H_γ	4.77	11.42	0.42	GLN-2	H_γ	3.52	14.17	0.25
GLN-2	H_ϵ	11.35	16.13	0.7	GLN-2	H_ϵ	10.05	15.9	0.63
PHE-4	H_ζ	8.82	11.86	0.74	LYS-6	H_ζ	10.66	14.74	0.72
LYS-6	H_ζ	10.64	14.74	0.72	LYS-6	H_ζ	10.64	14.76	0.72
THR-7	H_α	-2.78	13.34	-0.21	THR-7	H_β	-1.16	22.22	-0.05
THR-7	H_γ	-1.44	31.61	-0.05	LEU-8	NH	-8.11	38.94	-0.21
LEU-8	H_α	5.72	14.78	0.39	LEU-8	H_β	4.61	15.59	0.3
LEU-8	H_β	1.3	19.06	0.07	LEU-8	H_γ	2.18	14.31	0.15
LEU-8	H_δ	6.85	12.15	0.56	LEU-8	H_δ	6.96	12.2	0.57
LEU-8	H_δ	6.96	12.08	0.58	LEU-8	H_δ	6.98	11.53	0.6
LEU-8	H_δ	6.9	11.46	0.6	LEU-8	H_δ	6.8	11.38	0.6
THR-9	NH	3.09	19.04	0.16	THR-9	H_β	8.14	12.72	0.64
THR-9	H_γ	11.95	28.52	0.42	THR-9	H_γ	8.84	14.97	0.59
THR-9	H_γ	8.67	14.98	0.58	THR-9	H_γ	8.81	14.94	0.59
GLY-10	H_α	8.54	13.21	0.65	GLY-10	H_α	7.99	12.44	0.64
LYS-11	H_α	8.17	11.6	0.7	LYS-11	H_δ	6.69	13.96	0.48
LYS-11	H_δ	6.86	13.47	0.51	LYS-11	H_ϵ	7.74	13.35	0.58
LYS-11	H_ϵ	7.14	13.59	0.53	LYS-11	H_ζ	13.2	21.93	0.6
LYS-11	H_ζ	13.3	22.07	0.6	LYS-11	H_ζ	13.34	22.05	0.6
THR-12	NH	10.82	15.17	0.71	THR-12	H_β	9.05	12.84	0.7
THR-12	H_γ	15.03	21.21	0.71	ILE-13	H_α	7.59	14.61	0.52
THR-14	NH	10.71	19.05	0.56	THR-14	H_β	9.3	13.81	0.67
THR-14	H_γ	16.41	21.78	0.75	LEU-15	H_α	5.3	13.85	0.38
GLU-16	NH	8.19	26.39	0.31	GLU-16	H_β	12.97	20.79	0.62
GLU-16	H_β	12.42	22.41	0.55	GLU-16	H_γ	10.82	17.63	0.61
GLU-16	H_γ	9.67	15.47	0.63	VAL-17	H_α	-2.16	38.05	-0.06
VAL-17	H_β	-4.21	14.35	-0.29	GLU-18	NH	-1.55	38.73	-0.04
GLU-18	H_α	2.5	11.4	0.22	GLU-18	H_β	8.73	19.9	0.44
GLU-18	H_β	4.45	36.91	0.12	GLU-18	H_γ	12.32	30.28	0.41
GLU-18	H_γ	13.17	25.66	0.51	PRO-19	H_δ	7.94	15.42	0.51
PRO-19	H_δ	4.12	13.12	0.31	PRO-19	H_β	4.27	11.95	0.36
PRO-19	H_γ	8.42	12.86	0.66	PRO-19	H_γ	6.65	12.33	0.54
SER-20	H_β	11.91	17.0	0.7	SER-20	H_β	10.16	17.22	0.59
SER-20	H_γ	11.41	49.65	0.23	ASP-21	H_α	7.73	35.66	0.22
ASP-21	H_β	-11.92	42.34	-0.28	ASP-21	H_β	-4.69	17.13	-0.27
THR-22	NH	3.0	21.47	0.14	THR-22	H_γ	10.4	32.82	0.32
THR-22	H_γ	8.19	14.52	0.56	THR-22	H_γ	8.38	14.94	0.56
THR-22	H_γ	8.22	14.76	0.56	ILE-23	H_γ	-7.27	19.42	-0.37
ILE-23	H_γ	-6.55	17.82	-0.37	ILE-23	H_γ	-7.75	20.18	-0.38
GLU-24	H_α	0.49	12.25	0.04	GLU-24	H_β	9.31	19.48	0.48
GLU-24	H_β	5.27	16.96	0.31	GLU-24	H_γ	10.66	31.3	0.34
GLU-24	H_γ	10.43	20.72	0.5	ASN-25	H_β	-0.94	20.45	-0.05
ASN-25	H_β	2.57	14.62	0.18	ASN-25	H_δ	11.83	21.79	0.54
ASN-25	H_δ	11.51	21.46	0.54	LYS-27	H_β	0.52	12.26	0.04
LYS-27	H_δ	-6.85	25.8	-0.27	LYS-27	H_δ	-3.03	18.01	-0.17
LYS-27	H_ϵ	-5.46	21.88	-0.25	LYS-27	H_ϵ	-6.17	22.08	-0.28
LYS-27	H_ζ	-8.1	62.25	-0.13	LYS-27	H_ζ	-8.23	63.15	-0.13
LYS-27	H_ζ	-7.19	62.86	-0.11	ALA-28	H_β	8.71	15.82	0.55
ALA-28	H_β	8.88	16.02	0.55	ALA-28	H_β	8.84	15.96	0.55
LYS-29	H_α	4.79	11.99	0.4	LYS-29	H_γ	1.17	12.71	0.09
LYS-29	H_γ	4.35	15.06	0.29	LYS-29	H_δ	4.23	13.7	0.31
LYS-29	H_δ	1.34	16.39	0.08	LYS-29	H_ϵ	3.55	21.98	0.16
LYS-29	H_ϵ	6.69	17.04	0.39	LYS-29	H_ζ	3.83	36.45	0.1
LYS-29	H_ζ	4.75	36.36	0.13	LYS-29	H_ζ	4.28	36.44	0.12

GLN-31	H_γ	7.88	12.18	0.65	GLN-31	H_ϵ	12.46	15.84	0.79
GLN-31	H_ϵ	10.17	15.75	0.65	ASP-32	H_α	15.21	20.37	0.75
ASP-32	H_β	10.62	17.55	0.61	ASP-32	H_β	11.18	18.9	0.59
LYS-33	H_ϵ	7.54	13.38	0.56	LYS-33	H_ϵ	7.78	13.9	0.56
LYS-33	H_ζ	12.53	17.96	0.7	LYS-33	H_ζ	12.7	18.01	0.71
LYS-33	H_ζ	12.72	18.11	0.7	GLU-34	H_α	10.58	18.89	0.56
GLU-34	H_β	6.45	19.27	0.33	GLU-34	H_γ	1.92	13.3	0.14
GLU-34	H_γ	2.91	11.84	0.25	GLY-35	H_α	9.33	11.98	0.78
GLY-35	H_α	8.54	11.35	0.75	PRO-37	H_β	8.85	14.8	0.6
PRO-37	H_β	1.81	11.4	0.16	PRO-37	H_γ	7.71	11.6	0.66
PRO-37	H_γ	8.69	11.63	0.75	PRO-38	H_δ	8.14	13.49	0.6
PRO-38	H_β	2.2	13.26	0.17	PRO-38	H_β	6.28	19.5	0.32
PRO-38	H_γ	8.08	14.36	0.56	ASP-39	NH	6.13	17.12	0.36
ASP-39	H_α	4.33	33.84	0.13	ASP-39	H_β	9.61	19.53	0.49
ASP-39	H_β	11.44	19.66	0.58	GLN-40	NH	-3.33	13.27	-0.25
GLN-40	H_α	-1.71	13.61	-0.13	GLN-40	H_ϵ	9.76	15.25	0.64
GLN-40	H_ϵ	8.54	15.44	0.55	ARG-42	H_α	-17.44	49.47	-0.35
ARG-42	H_β	-4.71	21.76	-0.22	ARG-42	H_β	-2.31	11.27	-0.21
ARG-42	H_γ	-0.11	14.27	-0.01	ARG-42	H_γ	-2.95	16.23	-0.18
ARG-42	H_δ	-2.86	29.57	-0.1	ARG-42	H_δ	-5.72	34.84	-0.16
ARG-42	H_ϵ	0.46	30.86	0.01	ARG-42	H_η	1.19	28.71	0.04
ARG-42	H_η	6.59	21.97	0.3	ARG-42	H_η	6.04	22.09	0.27
ARG-42	H_η	7.63	21.68	0.35	LEU-43	NH	-38.62	96.97	-0.4
LEU-43	H_β	-6.24	15.81	-0.39	PHE-45	H_ϵ	7.66	13.9	0.55
PHE-45	H_ζ	9.45	15.67	0.6	PHE-45	H_δ	3.23	12.37	0.26
PHE-45	H_ϵ	7.79	13.67	0.57	ALA-46	NH	11.42	21.95	0.52
ALA-46	H_α	9.01	13.61	0.66	ALA-46	H_β	8.14	15.2	0.54
ALA-46	H_β	8.17	15.2	0.54	ALA-46	H_β	8.45	15.23	0.55
GLY-47	NH	8.93	15.76	0.57	GLY-47	H_α	9.18	11.68	0.79
GLY-47	H_α	8.14	11.45	0.71	LYS-48	H_α	7.71	11.38	0.68
LYS-48	H_β	7.68	12.97	0.59	LYS-48	H_β	7.48	15.76	0.47
LYS-48	H_γ	5.55	12.42	0.45	LYS-48	H_γ	5.84	11.49	0.51
LYS-48	H_δ	7.03	11.46	0.61	LYS-48	H_ϵ	7.15	11.65	0.61
LYS-48	H_ζ	11.26	17.52	0.64	LYS-48	H_ζ	11.11	17.38	0.64
LYS-48	H_ζ	11.12	17.55	0.63	GLN-49	NH	9.91	15.71	0.63
GLN-49	H_β	4.96	18.18	0.27	GLN-49	H_β	6.94	15.12	0.46
GLN-49	H_γ	3.25	15.87	0.2	GLN-49	H_γ	2.95	16.15	0.18
GLN-49	H_ϵ	8.05	23.55	0.34	GLN-49	H_ϵ	7.74	23.11	0.33
LEU-50	NH	-6.31	21.23	-0.3	LEU-50	H_β	-8.43	21.25	-0.4
GLU-51	H_α	1.19	31.62	0.04	GLU-51	H_β	12.27	23.63	0.52
GLU-51	H_β	4.52	11.89	0.38	GLU-51	H_γ	10.81	22.41	0.48
GLU-51	H_γ	12.71	22.18	0.57	ASP-52	NH	5.72	41.43	0.14
ASP-52	H_α	-7.07	23.46	-0.3	ASP-52	H_β	5.68	24.36	0.23
ASP-52	H_β	11.88	26.92	0.44	GLY-53	NH	11.82	22.03	0.54
GLY-53	H_α	10.8	16.21	0.67	GLY-53	H_α	8.54	13.99	0.61
ARG-54	H_α	5.93	16.01	0.37	ARG-54	H_γ	5.41	13.11	0.41
ARG-54	H_δ	6.38	11.96	0.53	ARG-54	H_δ	7.64	13.58	0.56
ARG-54	H_ϵ	9.48	19.47	0.49	ARG-54	H_η	12.71	21.57	0.59
ARG-54	H_η	12.82	16.67	0.77	ARG-54	H_η	13.79	20.56	0.67
ARG-54	H_η	13.12	16.42	0.8	THR-55	NH	3.14	18.13	0.17
THR-55	H_γ	11.05	21.75	0.51	THR-55	H_γ	8.5	14.42	0.59
THR-55	H_γ	8.32	14.31	0.58	THR-55	H_γ	8.29	14.0	0.59
SER-57	H_α	4.69	13.0	0.36	SER-57	H_β	9.42	14.54	0.65
SER-57	H_β	7.94	12.59	0.63	SER-57	H_γ	14.79	20.35	0.73
ASP-58	H_α	13.96	19.03	0.73	ASP-58	H_β	6.03	13.63	0.44
ASP-58	H_β	2.66	12.3	0.22	TYR-59	OH	13.3	32.2	0.41
TYR-59	H_δ	6.42	11.56	0.56	TYR-59	H_ϵ	8.58	16.81	0.51
ASN-60	H_β	8.88	12.78	0.7	ASN-60	H_β	9.45	13.6	0.69
ASN-60	H_δ	13.2	15.65	0.84	ASN-60	H_δ	11.37	14.63	0.78
GLN-62	NH	6.0	16.5	0.36	GLN-62	H_α	5.58	19.5	0.29
GLN-62	H_β	8.13	14.45	0.56	GLN-62	H_β	8.15	15.31	0.53

GLN-62	H_γ	9.04	13.08	0.69	GLN-62	H_γ	7.92	14.46	0.55
GLN-62	H_ϵ	11.02	16.71	0.66	GLN-62	H_ϵ	10.94	16.59	0.66
LYS-63	NH	7.41	17.05	0.43	LYS-63	H_β	4.06	12.11	0.34
LYS-63	H_β	1.04	15.98	0.07	LYS-63	H_γ	6.98	12.86	0.54
LYS-63	H_γ	7.71	14.02	0.55	LYS-63	H_δ	7.5	14.04	0.53
LYS-63	H_δ	7.18	14.85	0.48	LYS-63	H_ϵ	8.64	12.75	0.68
LYS-63	H_ϵ	8.21	13.6	0.6	LYS-63	H_ζ	12.89	16.43	0.78
LYS-63	H_ζ	12.82	16.45	0.78	LYS-63	H_ζ	12.89	16.52	0.78
GLU-64	H_β	10.26	14.05	0.73	GLU-64	H_β	11.65	15.94	0.73
GLU-64	H_γ	5.95	16.15	0.37	GLU-64	H_γ	6.53	11.57	0.56
SER-65	H_α	10.42	16.19	0.64	SER-65	H_γ	7.63	16.17	0.47
THR-66	NH	11.34	19.04	0.6	THR-66	H_β	8.95	15.41	0.58
THR-66	H_γ	17.64	25.84	0.68	HSD-68	H_δ	9.95	17.29	0.58
HSD-68	H_ϵ	12.39	17.74	0.7	HSD-68	H_δ	8.36	13.95	0.6
VAL-70	H_α	-3.37	23.92	-0.14	VAL-70	H_γ	4.97	11.71	0.42
VAL-70	H_γ	5.01	11.54	0.43	VAL-70	H_γ	5.06	11.58	0.44
LEU-71	NH	2.25	25.62	0.09	LEU-71	H_α	-7.92	20.99	-0.38
LEU-71	H_β	5.31	14.97	0.35	LEU-71	H_γ	-0.37	14.26	-0.03
LEU-71	H_δ	5.16	11.72	0.44	LEU-71	H_δ	5.1	11.56	0.44
LEU-71	H_δ	5.3	11.85	0.45	ARG-72	H_α	7.7	13.86	0.56
ARG-72	H_β	4.67	13.03	0.36	ARG-72	H_β	4.1	12.64	0.32
ARG-72	H_δ	4.51	12.67	0.36	ARG-72	H_δ	6.1	14.28	0.43
ARG-72	H_ϵ	5.23	22.55	0.23	ARG-72	H_η	4.45	32.62	0.14
ARG-72	H_η	11.25	19.06	0.59	ARG-72	H_η	7.79	24.73	0.32
ARG-72	H_η	11.8	19.01	0.62	LEU-73	NH	9.63	17.88	0.54
LEU-73	H_α	3.59	15.61	0.23	LEU-73	H_β	7.64	12.27	0.62
LEU-73	H_β	7.79	12.59	0.62	LEU-73	H_δ	8.47	11.32	0.75
LEU-73	H_δ	8.4	11.21	0.75	LEU-73	H_δ	8.64	11.77	0.73
LEU-73	H_δ	8.64	11.77	0.73	LEU-73	H_δ	8.75	11.84	0.74
ARG-74	NH	4.72	18.47	0.26	ARG-74	H_α	2.55	19.07	0.13
ARG-74	H_β	6.45	14.28	0.45	ARG-74	H_β	7.79	14.01	0.56
ARG-74	H_γ	5.91	14.44	0.41	ARG-74	H_γ	4.76	16.34	0.29
ARG-74	H_δ	6.62	14.7	0.45	ARG-74	H_δ	7.94	13.77	0.58
ARG-74	H_ϵ	9.65	17.88	0.54	ARG-74	H_η	10.93	20.52	0.53
ARG-74	H_η	11.26	21.21	0.53	ARG-74	H_η	11.52	20.76	0.56
ARG-74	H_η	8.79	24.62	0.36	GLY-75	NH	10.23	21.21	0.48
GLY-75	H_α	9.39	13.14	0.71	GLY-75	H_α	7.73	14.79	0.52
GLY-76	NH	12.02	19.24	0.62	GLY-76	H_α	12.29	16.4	0.75

Table 6: UBQ, unbound, encapsulated

residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{NOE}/\sigma_{ROE}$	residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{NOE}/\sigma_{ROE}$
MET-1	NH	7.23	16.9	0.43	MET-1	NH	7.29	17.12	0.43
MET-1	NH	7.15	17.84	0.4	MET-1	H_α	1.12	23.43	0.05
MET-1	H_β	4.32	13.89	0.31	MET-1	H_β	-0.78	13.96	-0.06
GLN-2	NH	-8.13	35.5	-0.23	GLN-2	H_γ	0.66	14.11	0.05
GLN-2	H_ϵ	8.2	15.86	0.52	GLN-2	H_ϵ	6.27	15.65	0.4
PHE-4	H_δ	-1.11	12.8	-0.09	PHE-4	H_ϵ	2.72	13.43	0.2
PHE-4	H_ζ	4.54	13.61	0.33	PHE-4	H_ϵ	3.0	12.98	0.23
LYS-6	H_β	-13.64	33.31	-0.41	LYS-6	H_β	-9.45	21.68	-0.44
LYS-6	H_γ	-8.8	23.88	-0.37	LYS-6	H_δ	-3.65	14.52	-0.25
LYS-6	H_ϵ	-2.66	17.56	-0.15	LYS-6	H_ϵ	-4.24	19.36	-0.22
LYS-6	H_ζ	-1.45	27.15	-0.05	LYS-6	H_ζ	-1.41	26.86	-0.05
LYS-6	H_ζ	-1.43	26.81	-0.05	THR-7	H_α	-14.96	31.89	-0.47
THR-7	H_β	-19.33	46.71	-0.41	THR-7	H_γ	-20.13	53.6	-0.38
THR-7	H_γ	-5.42	13.99	-0.39	THR-7	H_γ	-5.88	15.19	-0.39
THR-7	H_γ	-5.44	14.28	-0.38	LEU-8	NH	-22.65	51.67	-0.44
LEU-8	H_α	-16.34	36.33	-0.45	LEU-8	H_β	-9.63	22.18	-0.43
LEU-8	H_γ	-7.51	16.96	-0.44	THR-9	NH	-13.3	33.15	-0.4
THR-9	H_β	-4.33	12.8	-0.34	THR-9	H_γ	-22.47	72.98	-0.31
THR-9	H_γ	-5.53	14.94	-0.37	THR-9	H_γ	-5.68	15.08	-0.38
THR-9	H_γ	-5.69	15.43	-0.37	GLY-10	NH	-5.14	12.51	-0.41
GLY-10	H_α	-3.52	12.42	-0.28	GLY-10	H_α	-7.14	21.09	-0.34
LYS-11	H_α	-2.45	19.21	-0.13	LYS-11	H_β	-3.11	13.7	-0.23
LYS-11	H_β	-3.79	15.32	-0.25	LYS-11	H_γ	-1.32	13.6	-0.1
LYS-11	H_γ	-1.55	12.49	-0.12	LYS-11	H_δ	-4.31	23.83	-0.18
LYS-11	H_δ	-2.09	20.22	-0.1	LYS-11	H_ϵ	-0.89	19.32	-0.05
LYS-11	H_ϵ	-3.26	23.36	-0.14	LYS-11	H_ζ	0.76	39.07	0.02
LYS-11	H_ζ	1.4	38.27	0.04	LYS-11	H_ζ	0.88	38.26	0.02
THR-12	NH	-0.02	25.64	-0.0	THR-12	H_β	1.91	16.96	0.11
THR-12	H_γ	-0.51	34.06	-0.01	ILE-13	H_α	3.45	14.72	0.23
THR-14	NH	6.2	18.9	0.33	THR-14	H_β	5.93	13.69	0.43
THR-14	H_γ	10.46	22.42	0.47	GLU-16	NH	6.65	19.68	0.34
GLU-16	H_β	9.6	16.85	0.57	GLU-16	H_β	9.29	17.3	0.54
GLU-16	H_γ	7.63	14.18	0.54	GLU-16	H_γ	6.52	12.53	0.52
VAL-17	H_α	-6.82	38.94	-0.18	VAL-17	H_β	-7.43	19.42	-0.38
VAL-17	H_γ	-3.42	12.22	-0.28	VAL-17	H_γ	-3.61	13.23	-0.27
VAL-17	H_γ	-3.53	12.94	-0.27	GLU-18	NH	-5.27	37.13	-0.14
GLU-18	H_β	6.28	16.18	0.39	GLU-18	H_β	3.02	28.14	0.11
GLU-18	H_γ	8.86	23.45	0.38	GLU-18	H_γ	9.3	20.99	0.44
PRO-19	H_δ	5.89	12.25	0.48	SER-20	H_β	8.45	14.05	0.6
SER-20	H_β	7.38	14.23	0.52	SER-20	H_γ	8.15	37.53	0.22
ASP-21	H_α	4.58	29.88	0.15	ASP-21	H_β	-24.31	62.36	-0.39
ASP-21	H_β	-8.85	23.52	-0.38	THR-22	NH	0.76	20.43	0.04
THR-22	H_γ	5.8	27.45	0.21	THR-22	H_γ	5.32	12.2	0.44
THR-22	H_γ	5.61	12.38	0.45	THR-22	H_γ	5.35	12.21	0.44
ILE-23	H_β	-14.6	30.41	-0.48	ILE-23	H_γ	-66.35	136.84	-0.48
ILE-23	H_γ	-69.12	142.03	-0.49	ILE-23	H_γ	-70.81	145.24	-0.49
ILE-23	H_γ	-7.35	15.38	-0.48	GLU-24	H_α	-6.77	17.42	-0.39
GLU-24	H_β	4.38	17.69	0.25	GLU-24	H_β	-6.97	29.81	-0.23
GLU-24	H_γ	-16.15	57.63	-0.28	GLU-24	H_γ	5.02	19.02	0.26
ASN-25	H_β	-3.78	20.1	-0.19	ASN-25	H_β	1.16	13.95	0.08
ASN-25	H_δ	7.72	17.87	0.43	ASN-25	H_δ	7.46	18.91	0.39
LYS-27	H_γ	-9.38	19.38	-0.48	LYS-27	H_δ	-66.46	135.74	-0.49
LYS-27	H_δ	-11.48	24.71	-0.46	LYS-27	H_ϵ	-15.66	35.13	-0.45
LYS-27	H_ϵ	-52.26	108.35	-0.48	LYS-27	H_ζ	-62.86	144.87	-0.43
LYS-27	H_ζ	-62.83	144.72	-0.43	LYS-27	H_ζ	-63.47	145.61	-0.44
LYS-29	H_γ	2.76	12.7	0.22	LYS-29	H_δ	-1.97	18.77	-0.1
LYS-29	H_ϵ	-0.72	23.18	-0.03	LYS-29	H_ϵ	3.46	15.53	0.22
LYS-29	H_ζ	-3.16	38.98	-0.08	LYS-29	H_ζ	-2.95	38.96	-0.08

LYS-29	H_{ζ}	-3.63	40.75	-0.09
GLN-31	H_{ϵ}	7.99	16.44	0.49
ASP-32	H_{α}	8.6	20.29	0.42
ASP-32	H_{β}	7.06	15.92	0.44
LYS-33	H_{ζ}	8.96	15.98	0.56
LYS-33	H_{ζ}	8.82	15.96	0.55
GLU-34	H_{β}	-14.8	47.48	-0.31
GLU-34	H_{γ}	-3.48	16.68	-0.21
ILE-36	H_{δ}	-4.81	13.56	-0.35
ILE-36	H_{δ}	-4.56	12.6	-0.36
PRO-38	H_{δ}	2.42	17.25	0.14
PRO-38	H_{β}	-7.67	31.64	-0.24
ASP-39	NH	-4.07	28.52	-0.14
ASP-39	H_{β}	-6.98	35.55	-0.2
GLN-40	H_{α}	-12.39	27.3	-0.45
GLN-40	H_{ϵ}	-19.62	45.74	-0.43
ARG-42	H_{β}	-45.7	94.52	-0.48
ARG-42	H_{γ}	-24.26	52.25	-0.46
ARG-42	H_{δ}	-61.24	131.76	-0.46
ARG-42	H_{ϵ}	-65.26	155.89	-0.42
ARG-42	H_{η}	-55.24	132.87	-0.42
ARG-42	H_{η}	-9.64	47.85	-0.2
LEU-43	H_{β}	-24.61	50.14	-0.49
PHE-45	H_{α}	-14.93	37.07	-0.4
PHE-45	H_{ϵ}	-6.82	29.13	-0.23
PHE-45	H_{δ}	-11.28	30.65	-0.37
ALA-46	NH	-33.8	86.86	-0.39
ALA-46	H_{β}	-5.66	23.84	-0.24
ALA-46	H_{β}	-4.54	21.89	-0.21
LYS-48	H_{α}	-12.24	32.62	-0.38
LYS-48	H_{β}	-9.15	29.28	-0.31
LYS-48	H_{γ}	-6.11	21.08	-0.29
LYS-48	H_{δ}	-3.61	17.04	-0.21
LYS-48	H_{ϵ}	-2.02	16.86	-0.12
LYS-48	H_{ζ}	-5.72	42.2	-0.14
GLN-49	NH	-17.31	47.06	-0.37
GLN-49	H_{β}	-9.75	31.0	-0.31
GLN-49	H_{γ}	-9.2	24.12	-0.38
GLN-49	H_{ϵ}	-16.42	52.98	-0.31
LEU-50	H_{α}	-10.47	25.65	-0.41
LEU-50	H_{β}	-51.33	104.37	-0.49
GLU-51	H_{α}	-30.5	83.04	-0.37
GLU-51	H_{β}	-2.22	15.92	-0.14
GLU-51	H_{γ}	0.76	33.19	0.02
ASP-52	H_{α}	-76.63	157.76	-0.49
ASP-52	H_{β}	-1.91	45.68	-0.04
GLY-53	H_{α}	6.23	16.48	0.38
ARG-54	H_{α}	2.84	14.91	0.19
ARG-54	H_{δ}	2.3	13.94	0.17
ARG-54	H_{ϵ}	2.57	22.07	0.12
ARG-54	H_{η}	7.71	19.0	0.41
ARG-54	H_{η}	7.62	18.31	0.42
THR-55	H_{γ}	7.09	18.39	0.39
THR-55	H_{γ}	5.71	12.11	0.47
SER-57	H_{γ}	10.64	18.5	0.58
ASP-58	H_{β}	2.44	13.45	0.18
TYR-59	H_{β}	-3.63	14.91	-0.24
TYR-59	H_{δ}	-1.45	18.47	-0.08
ASN-60	H_{β}	2.53	15.58	0.16
ASN-60	H_{δ}	6.31	17.17	0.37
ILE-61	H_{α}	-6.26	24.73	-0.25
GLN-31	H_{γ}	3.4	12.41	0.27
GLN-31	H_{ϵ}	5.9	19.26	0.31
ASP-32	H_{β}	7.36	15.19	0.48
LYS-33	H_{β}	-0.13	15.65	-0.01
LYS-33	H_{ζ}	8.86	15.68	0.57
GLU-34	H_{α}	-2.35	30.07	-0.08
GLU-34	H_{γ}	-12.2	31.39	-0.39
GLY-35	H_{α}	2.03	12.63	0.16
ILE-36	H_{δ}	-4.41	12.41	-0.36
PRO-37	H_{β}	1.27	17.61	0.07
PRO-38	H_{β}	-3.61	13.05	-0.28
PRO-38	H_{γ}	2.72	15.37	0.18
ASP-39	H_{α}	-34.09	92.0	-0.37
ASP-39	H_{β}	-2.16	34.41	-0.06
GLN-40	H_{ϵ}	-20.43	50.86	-0.4
ARG-42	H_{α}	-73.95	151.38	-0.49
ARG-42	H_{β}	-26.62	56.72	-0.47
ARG-42	H_{γ}	-87.1	180.21	-0.48
ARG-42	H_{δ}	-53.87	115.28	-0.47
ARG-42	H_{η}	-54.39	127.93	-0.43
ARG-42	H_{η}	-22.78	84.25	-0.27
LEU-43	NH	-174.52	355.52	-0.49
LEU-43	H_{γ}	-10.41	21.19	-0.49
PHE-45	H_{δ}	-14.18	36.57	-0.39
PHE-45	H_{ζ}	-4.59	29.29	-0.16
PHE-45	H_{ϵ}	-5.27	27.51	-0.19
ALA-46	H_{α}	-9.28	26.92	-0.34
ALA-46	H_{β}	-5.27	23.63	-0.22
GLY-47	NH	-19.78	46.68	-0.42
LYS-48	H_{β}	-5.93	21.23	-0.28
LYS-48	H_{γ}	-8.27	24.26	-0.34
LYS-48	H_{δ}	-4.03	20.63	-0.2
LYS-48	H_{ϵ}	-3.81	20.02	-0.19
LYS-48	H_{ζ}	-5.45	41.43	-0.13
LYS-48	H_{ζ}	-7.35	43.32	-0.17
GLN-49	H_{β}	-11.19	29.73	-0.38
GLN-49	H_{γ}	-7.78	21.46	-0.36
GLN-49	H_{ϵ}	-18.78	55.61	-0.34
LEU-50	NH	-21.6	45.33	-0.48
LEU-50	H_{β}	-10.17	21.14	-0.48
GLU-51	NH	-7.73	19.85	-0.39
GLU-51	H_{β}	2.56	30.22	0.08
GLU-51	H_{γ}	-3.57	35.66	-0.1
ASP-52	NH	-31.88	96.71	-0.33
ASP-52	H_{β}	-16.63	53.98	-0.31
GLY-53	NH	4.07	26.56	0.15
GLY-53	H_{α}	4.62	12.72	0.36
ARG-54	H_{γ}	1.09	13.82	0.08
ARG-54	H_{δ}	2.55	15.32	0.17
ARG-54	H_{η}	5.54	24.05	0.23
ARG-54	H_{η}	6.56	22.95	0.29
THR-55	NH	0.34	16.03	0.02
THR-55	H_{γ}	5.81	12.3	0.47
SER-57	H_{β}	6.42	12.6	0.51
ASP-58	H_{α}	8.28	18.71	0.44
TYR-59	H_{α}	0.66	16.55	0.04
TYR-59	OH	-9.02	58.62	-0.15
TYR-59	H_{ϵ}	-4.0	29.25	-0.14
ASN-60	H_{β}	1.2	19.83	0.06
ASN-60	H_{δ}	7.23	16.95	0.43
GLN-62	NH	-11.06	42.45	-0.26

GLN-62	H_{α}	1.74	18.76	0.09	GLN-62	H_{β}	2.57	16.74	0.15
GLN-62	H_{β}	-2.39	25.66	-0.09	GLN-62	H_{γ}	2.81	16.43	0.17
GLN-62	H_{γ}	-1.19	23.54	-0.05	GLN-62	H_{ϵ}	5.89	18.47	0.32
GLN-62	H_{ϵ}	4.63	17.59	0.26	LYS-63	NH	3.19	16.94	0.19
LYS-63	H_{β}	-2.82	17.82	-0.16	LYS-63	H_{γ}	2.43	15.32	0.16
LYS-63	H_{γ}	3.63	14.97	0.24	LYS-63	H_{δ}	3.71	14.99	0.25
LYS-63	H_{δ}	3.26	16.46	0.2	LYS-63	H_{ϵ}	5.2	14.2	0.37
LYS-63	H_{ϵ}	4.44	15.25	0.29	LYS-63	H_{ζ}	8.41	17.25	0.49
LYS-63	H_{ζ}	8.11	17.68	0.46	LYS-63	H_{ζ}	8.58	17.82	0.48
GLU-64	H_{β}	3.24	17.86	0.18	GLU-64	H_{β}	4.37	20.11	0.22
GLU-64	H_{γ}	1.71	17.3	0.1	GLU-64	H_{γ}	2.5	12.72	0.2
SER-65	H_{α}	-4.43	30.87	-0.14	SER-65	H_{β}	-4.05	15.71	-0.26
SER-65	H_{γ}	-6.43	31.67	-0.2	THR-66	NH	-8.83	41.13	-0.21
THR-66	H_{β}	-8.96	35.49	-0.25	THR-66	H_{γ}	-6.74	53.84	-0.13
THR-66	H_{γ}	-4.77	20.27	-0.24	THR-66	H_{γ}	-4.97	21.09	-0.24
THR-66	H_{γ}	-4.63	20.56	-0.22	LEU-67	H_{α}	-8.85	21.08	-0.42
HSD-68	H_{α}	-11.08	23.56	-0.47	HSD-68	H_{β}	-18.48	40.7	-0.45
HSD-68	H_{β}	-5.3	12.63	-0.42	HSD-68	H_{δ}	-30.04	72.83	-0.41
HSD-68	H_{ϵ}	-12.98	43.49	-0.3	HSD-68	H_{δ}	-16.13	43.53	-0.37
LEU-69	NH	-49.85	106.66	-0.47	LEU-69	H_{β}	-12.73	27.03	-0.47
VAL-70	H_{γ}	-8.08	17.95	-0.45	VAL-70	H_{γ}	-9.19	19.52	-0.47
VAL-70	H_{γ}	-9.72	21.2	-0.46	ARG-72	H_{α}	-25.2	53.99	-0.47
ARG-72	H_{β}	-25.15	54.38	-0.46	ARG-72	H_{β}	-30.57	66.21	-0.46
ARG-72	H_{γ}	-8.95	19.56	-0.46	ARG-72	H_{γ}	-12.5	27.19	-0.46
ARG-72	H_{δ}	-11.47	26.15	-0.44	ARG-72	H_{δ}	-9.69	24.28	-0.4
ARG-72	H_{ϵ}	-38.86	85.2	-0.46	ARG-72	H_{η}	-24.06	63.55	-0.38
ARG-72	H_{η}	-27.3	87.23	-0.31	ARG-72	H_{η}	-42.16	100.36	-0.42
ARG-72	H_{η}	-17.6	64.81	-0.27	LEU-73	NH	-35.35	76.83	-0.46
LEU-73	H_{α}	-24.25	52.2	-0.46	LEU-73	H_{β}	-17.12	37.25	-0.46
LEU-73	H_{β}	-12.23	27.44	-0.45	ARG-74	NH	-56.23	121.2	-0.46
ARG-74	H_{α}	-14.38	36.0	-0.4	ARG-74	H_{β}	-5.95	20.98	-0.28
ARG-74	H_{β}	-16.41	39.53	-0.42	ARG-74	H_{γ}	-16.42	40.75	-0.4
ARG-74	H_{γ}	-9.33	29.16	-0.32	ARG-74	H_{δ}	-6.21	27.45	-0.23
ARG-74	H_{δ}	-7.82	30.03	-0.26	ARG-74	H_{ϵ}	-12.97	46.42	-0.28
ARG-74	H_{η}	4.26	26.05	0.16	ARG-74	H_{η}	-2.06	34.74	-0.06
ARG-74	H_{η}	-4.7	37.99	-0.12	ARG-74	H_{η}	4.36	24.02	0.18
GLY-75	NH	-11.82	46.33	-0.26	GLY-75	H_{α}	-1.37	15.5	-0.09
GLY-76	NH	-10.74	39.63	-0.27	GLY-76	H_{α}	-18.2	47.51	-0.38

Table 7: UBQ, in complex with ligase, in bulk solution

residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{\mathrm{NOE}}/\sigma_{\mathrm{ROE}}$	residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{\mathrm{NOE}}/\sigma_{\mathrm{ROE}}$
MET-1	NH	8.58	18.92	0.45	MET-1	NH	8.58	19.23	0.45
MET-1	NH	8.15	18.89	0.43	MET-1	H_α	3.1	23.82	0.13
MET-1	H_β	5.61	14.79	0.38	MET-1	H_β	0.64	13.74	0.05
GLN-2	NH	-4.9	33.34	-0.15	GLN-2	H_γ	4.38	11.29	0.39
GLN-2	H_γ	2.8	14.08	0.2	GLN-2	H_ϵ	8.55	14.75	0.58
GLN-2	H_ϵ	10.3	14.14	0.73	LYS-6	H_β	-4.17	16.52	-0.25
LYS-6	H_γ	-3.91	20.93	-0.19	LYS-6	H_γ	-0.75	17.1	-0.04
LYS-6	H_δ	1.8	12.45	0.14	LYS-6	H_δ	0.93	12.43	0.07
LYS-6	H_ϵ	3.45	14.84	0.23	LYS-6	H_ϵ	3.54	14.92	0.24
LYS-6	H_ζ	7.36	19.74	0.37	LYS-6	H_ζ	7.21	19.38	0.37
LYS-6	H_ζ	7.27	19.56	0.37	THR-7	H_α	-18.3	44.08	-0.42
THR-7	H_β	-3.8	27.09	-0.14	THR-7	H_γ	-4.47	34.54	-0.13
LEU-8	NH	-27.85	79.15	-0.35	LEU-8	H_α	-4.5	28.54	-0.16
LEU-8	H_β	1.43	19.95	0.07	LEU-8	H_β	-6.44	32.08	-0.2
LEU-8	H_γ	-7.77	29.0	-0.27	LEU-8	H_δ	0.13	13.28	0.01
LEU-8	H_δ	0.06	13.47	0.0	LEU-8	H_δ	0.01	13.33	0.0
LEU-8	H_δ	-0.3	14.34	-0.02	LEU-8	H_δ	-0.11	14.23	-0.01
LEU-8	H_δ	-0.67	15.06	-0.04	THR-9	NH	1.18	17.26	0.07
THR-9	H_α	5.88	11.54	0.51	THR-9	H_β	6.83	11.7	0.58
THR-9	H_γ	12.87	23.36	0.55	THR-9	H_γ	7.8	14.26	0.55
THR-9	H_γ	7.87	14.37	0.55	THR-9	H_γ	7.72	14.54	0.53
GLY-10	H_α	5.91	14.16	0.42	GLY-10	H_α	2.85	20.4	0.14
LYS-11	NH	1.75	11.64	0.15	LYS-11	H_α	6.7	11.31	0.59
LYS-11	H_δ	5.83	12.14	0.48	LYS-11	H_δ	6.08	11.73	0.52
LYS-11	H_ϵ	6.84	11.56	0.59	LYS-11	H_ϵ	6.29	12.41	0.51
LYS-11	H_ζ	11.83	19.49	0.61	LYS-11	H_ζ	11.8	19.54	0.6
LYS-11	H_ζ	11.94	19.49	0.61	THR-12	NH	9.06	14.63	0.62
THR-12	H_β	7.47	11.91	0.63	THR-12	H_γ	12.04	20.29	0.59
ILE-13	H_α	6.71	13.19	0.51	THR-14	NH	9.48	16.88	0.56
THR-14	H_β	7.81	11.84	0.66	THR-14	H_γ	14.29	19.63	0.73
LEU-15	H_α	4.58	12.1	0.38	GLU-16	NH	7.11	22.84	0.31
GLU-16	H_β	11.22	18.1	0.62	GLU-16	H_β	10.73	19.11	0.56
GLU-16	H_γ	9.49	15.96	0.59	GLU-16	H_γ	8.75	14.19	0.62
VAL-17	H_α	-3.93	37.22	-0.11	VAL-17	H_β	-4.66	14.14	-0.33
GLU-18	NH	-2.04	35.13	-0.06	GLU-18	H_β	7.83	17.77	0.44
GLU-18	H_β	4.73	31.8	0.15	GLU-18	H_γ	11.15	26.34	0.42
GLU-18	H_γ	11.59	22.5	0.52	PRO-19	H_δ	6.89	13.4	0.51
PRO-19	H_δ	3.57	11.35	0.31	PRO-19	H_γ	7.54	11.5	0.66
SER-20	H_β	10.5	15.01	0.7	SER-20	H_β	8.91	15.06	0.59
SER-20	H_γ	10.08	41.53	0.24	ASP-21	H_α	6.52	31.24	0.21
ASP-21	H_β	-13.27	41.52	-0.32	ASP-21	H_β	-4.94	16.48	-0.3
THR-22	NH	2.12	19.44	0.11	THR-22	H_γ	8.56	29.77	0.29
THR-22	H_γ	6.88	12.75	0.54	THR-22	H_γ	6.74	12.61	0.53
THR-22	H_γ	6.98	12.92	0.54	ILE-23	H_γ	-6.58	15.96	-0.41
ILE-23	H_γ	-6.23	15.28	-0.41	ILE-23	H_γ	-6.44	15.72	-0.41
GLU-24	H_α	-0.35	13.23	-0.03	GLU-24	H_β	7.69	17.04	0.45
GLU-24	H_β	3.87	15.69	0.25	GLU-24	H_γ	8.11	30.91	0.26
GLU-24	H_γ	9.03	18.42	0.49	ASN-25	H_β	-1.45	18.78	-0.08
ASN-25	H_β	2.11	13.2	0.16	ASN-25	H_δ	10.04	20.56	0.49
ASN-25	H_δ	9.68	17.78	0.54	LYS-27	H_β	-0.3	12.62	-0.02
LYS-27	H_δ	-8.11	25.84	-0.31	LYS-27	H_δ	-6.22	22.85	-0.27
LYS-27	H_ϵ	-13.3	33.44	-0.4	LYS-27	H_ϵ	-8.73	23.71	-0.37
LYS-27	H_ζ	-25.6	93.75	-0.27	LYS-27	H_ζ	-24.33	89.42	-0.27
LYS-27	H_ζ	-25.86	92.24	-0.28	ALA-28	H_β	7.58	14.15	0.54
ALA-28	H_β	7.54	13.98	0.54	ALA-28	H_β	7.32	14.05	0.52
LYS-29	H_γ	4.11	13.29	0.31	LYS-29	H_δ	3.59	11.67	0.31
LYS-29	H_δ	0.19	14.91	0.01	LYS-29	H_ϵ	2.19	20.54	0.11
LYS-29	H_ϵ	6.06	14.93	0.41	LYS-29	H_ζ	1.85	33.89	0.05

LYS-29	H_{ζ}	2.25	34.21	0.07	LYS-29	H_{ζ}	2.58	33.25	0.08
GLN-31	H_{ϵ}	10.19	14.08	0.72	GLN-31	H_{ϵ}	9.42	14.02	0.67
ASP-32	H_{α}	13.01	17.82	0.73	ASP-32	H_{β}	9.01	14.77	0.61
ASP-32	H_{β}	9.72	16.41	0.59	LYS-33	H_{ϵ}	6.42	11.6	0.55
LYS-33	H_{ϵ}	6.66	12.17	0.55	LYS-33	H_{ζ}	10.96	15.4	0.71
LYS-33	H_{ζ}	10.91	15.59	0.7	LYS-33	H_{ζ}	10.94	15.58	0.7
GLU-34	H_{α}	9.36	16.46	0.57	GLU-34	H_{β}	6.17	16.72	0.37
GLU-34	H_{γ}	1.49	12.45	0.12	PRO-37	H_{β}	7.19	11.77	0.61
PRO-37	H_{β}	-0.65	14.71	-0.04	PRO-38	H_{δ}	6.78	11.38	0.6
PRO-38	H_{β}	0.65	13.37	0.05	PRO-38	H_{β}	4.1	19.13	0.21
PRO-38	H_{γ}	6.76	12.97	0.52	ASP-39	NH	3.55	15.03	0.24
ASP-39	H_{α}	-3.33	42.23	-0.08	ASP-39	H_{β}	7.77	19.71	0.39
ASP-39	H_{β}	8.45	18.74	0.45	GLN-40	NH	-9.16	24.33	-0.38
GLN-40	H_{α}	-12.75	35.5	-0.36	GLN-40	H_{ϵ}	7.95	14.61	0.54
GLN-40	H_{ϵ}	8.82	15.43	0.57	GLN-41	NH	-13.34	31.29	-0.43
ARG-42	H_{α}	-42.73	94.11	-0.45	ARG-42	H_{β}	-9.47	22.14	-0.43
ARG-42	H_{γ}	-9.43	26.24	-0.36	ARG-42	H_{γ}	-10.55	25.32	-0.42
ARG-42	H_{δ}	-35.34	92.53	-0.38	ARG-42	H_{δ}	-19.89	56.87	-0.35
ARG-42	H_{ϵ}	-30.37	93.27	-0.33	ARG-42	H_{η}	-9.89	34.01	-0.29
ARG-42	H_{η}	-30.02	85.16	-0.35	ARG-42	H_{η}	-2.84	35.79	-0.08
ARG-42	H_{η}	-41.8	119.39	-0.35	LEU-43	NH	-71.8	156.01	-0.46
LEU-43	H_{β}	-13.2	28.66	-0.46	PHE-45	H_{α}	-40.87	92.97	-0.44
PHE-45	H_{β}	-7.27	16.72	-0.43	PHE-45	H_{δ}	-61.48	139.36	-0.44
PHE-45	H_{ϵ}	-7.4	42.14	-0.18	PHE-45	H_{ζ}	5.36	19.55	0.27
PHE-45	H_{ϵ}	4.77	14.4	0.33	ALA-46	NH	-19.07	69.2	-0.28
ALA-46	H_{α}	-10.65	58.21	-0.18	ALA-46	H_{β}	5.6	16.56	0.34
ALA-46	H_{β}	5.66	16.54	0.34	ALA-46	H_{β}	5.71	16.59	0.34
GLY-47	NH	-18.7	54.65	-0.34	GLY-47	H_{α}	5.1	16.26	0.31
LYS-48	H_{β}	4.79	13.52	0.35	LYS-48	H_{β}	3.02	15.14	0.2
LYS-48	H_{δ}	5.52	11.63	0.47	LYS-48	H_{ζ}	10.15	16.6	0.61
LYS-48	H_{ζ}	10.05	16.84	0.6	LYS-48	H_{ζ}	10.04	16.71	0.6
GLN-49	NH	3.13	15.81	0.2	GLN-49	H_{β}	0.35	17.48	0.02
GLN-49	H_{γ}	-11.38	31.32	-0.36	GLN-49	H_{γ}	-16.55	48.27	-0.34
GLN-49	H_{ϵ}	-7.21	58.22	-0.12	GLN-49	H_{ϵ}	4.5	27.89	0.16
LEU-50	NH	-14.56	32.93	-0.44	LEU-50	H_{β}	-15.1	33.31	-0.45
GLU-51	H_{α}	-5.39	38.94	-0.14	GLU-51	H_{β}	10.15	21.47	0.47
GLU-51	H_{β}	3.67	12.37	0.3	GLU-51	H_{γ}	7.57	24.25	0.31
GLU-51	H_{γ}	9.48	23.74	0.4	ASP-52	NH	2.13	44.62	0.05
ASP-52	H_{α}	-3.72	14.11	-0.26	ASP-52	H_{β}	3.7	23.64	0.16
ASP-52	H_{β}	9.18	24.44	0.38	GLY-53	NH	9.8	19.1	0.51
GLY-53	H_{α}	9.17	13.98	0.66	GLY-53	H_{α}	7.27	12.18	0.6
ARG-54	H_{α}	5.13	17.02	0.3	ARG-54	H_{γ}	5.13	14.17	0.36
ARG-54	H_{δ}	6.88	13.59	0.51	ARG-54	H_{ϵ}	7.91	18.33	0.43
ARG-54	H_{η}	11.05	16.68	0.66	ARG-54	H_{η}	11.65	15.12	0.77
ARG-54	H_{η}	10.09	21.76	0.46	ARG-54	H_{η}	11.15	15.85	0.7
THR-55	NH	1.7	20.15	0.08	THR-55	H_{γ}	9.31	19.44	0.48
THR-55	H_{γ}	6.79	12.31	0.55	THR-55	H_{γ}	6.89	12.32	0.56
THR-55	H_{γ}	6.88	12.25	0.56	SER-57	H_{α}	4.35	11.49	0.38
SER-57	H_{β}	7.82	11.97	0.65	SER-57	H_{γ}	13.0	17.95	0.72
ASP-58	H_{α}	11.68	16.01	0.73	ASP-58	H_{β}	3.66	12.69	0.29
ASP-58	H_{β}	2.88	16.57	0.17	TYR-59	OH	9.52	33.53	0.28
TYR-59	H_{ϵ}	5.31	14.2	0.37	ASN-60	H_{β}	7.69	11.57	0.66
ASN-60	H_{β}	8.02	12.65	0.63	ASN-60	H_{δ}	11.65	14.14	0.82
ASN-60	H_{δ}	9.77	12.93	0.76	GLN-62	NH	2.14	21.06	0.1
GLN-62	H_{α}	4.51	18.15	0.25	GLN-62	H_{β}	6.59	12.74	0.52
GLN-62	H_{β}	5.74	15.16	0.38	GLN-62	H_{γ}	7.61	11.77	0.65
GLN-62	H_{γ}	6.49	13.62	0.48	GLN-62	H_{ϵ}	11.43	17.58	0.65
GLN-62	H_{ϵ}	7.43	12.34	0.6	LYS-63	NH	6.18	15.71	0.39
LYS-63	H_{β}	-0.36	15.81	-0.02	LYS-63	H_{γ}	5.57	11.44	0.49
LYS-63	H_{γ}	6.41	12.68	0.51	LYS-63	H_{δ}	6.04	12.96	0.47
LYS-63	H_{δ}	5.71	13.52	0.42	LYS-63	H_{ϵ}	7.29	11.4	0.64

LYS-63	H_{ϵ}	6.61	12.68	0.52	LYS-63	H_{ζ}	10.83	14.52	0.75
LYS-63	H_{ζ}	11.07	14.71	0.75	LYS-63	H_{ζ}	10.89	14.59	0.75
GLU-64	H_{β}	8.34	13.55	0.62	GLU-64	H_{β}	9.25	14.37	0.64
GLU-64	H_{γ}	4.6	15.18	0.3	SER-65	H_{α}	6.66	17.42	0.38
SER-65	H_{γ}	3.03	18.15	0.17	THR-66	NH	3.87	28.79	0.13
THR-66	H_{β}	-3.79	37.55	-0.1	THR-66	H_{γ}	11.55	30.65	0.38
THR-66	H_{γ}	-0.53	19.46	-0.03	THR-66	H_{γ}	-0.23	18.36	-0.01
THR-66	H_{γ}	-0.81	19.33	-0.04	LEU-67	H_{α}	-30.97	68.0	-0.46
HSD-68	NH	-20.49	48.52	-0.42	HSD-68	H_{α}	-6.38	15.09	-0.42
HSD-68	H_{β}	-7.43	17.79	-0.42	HSD-68	H_{β}	-10.58	24.08	-0.44
HSD-68	H_{δ}	-60.99	143.52	-0.42	HSD-68	H_{ϵ}	-4.0	43.56	-0.09
HSD-68	H_{δ}	-9.64	36.31	-0.27	LEU-69	NH	-14.81	35.47	-0.42
LEU-69	H_{β}	-4.6	11.45	-0.4	LEU-69	H_{γ}	-4.03	12.16	-0.33
VAL-70	H_{α}	-19.24	52.15	-0.37	VAL-70	H_{γ}	-3.08	12.39	-0.25
VAL-70	H_{γ}	-2.93	12.52	-0.23	VAL-70	H_{γ}	-2.94	12.48	-0.24
LEU-71	NH	-4.07	35.77	-0.11	LEU-71	H_{β}	3.0	18.51	0.16
LEU-71	H_{γ}	-0.81	17.21	-0.05	LEU-71	H_{δ}	3.97	11.42	0.35
ARG-72	NH	-4.17	12.53	-0.33	ARG-72	H_{α}	-15.83	49.56	-0.32
ARG-72	H_{β}	-12.5	35.98	-0.35	ARG-72	H_{β}	-6.86	21.37	-0.32
ARG-72	H_{γ}	-17.87	44.34	-0.4	ARG-72	H_{γ}	-3.18	15.29	-0.21
ARG-72	H_{δ}	-10.86	35.58	-0.31	ARG-72	H_{δ}	-15.97	49.76	-0.32
ARG-72	H_{ϵ}	-131.28	285.0	-0.46	ARG-72	H_{η}	-24.78	85.94	-0.29
ARG-72	H_{η}	4.19	24.98	0.17	ARG-72	H_{η}	-31.27	96.08	-0.33
ARG-72	H_{η}	-0.17	33.32	-0.01	LEU-73	NH	-25.95	77.97	-0.33
LEU-73	H_{α}	-4.04	27.97	-0.14	LEU-73	H_{β}	3.53	15.48	0.23
LEU-73	H_{β}	2.39	18.68	0.13	LEU-73	H_{γ}	1.07	14.99	0.07
LEU-73	H_{δ}	6.02	12.45	0.48	LEU-73	H_{δ}	6.1	12.29	0.5
LEU-73	H_{δ}	6.19	12.22	0.51	LEU-73	H_{δ}	4.84	13.6	0.36
LEU-73	H_{δ}	4.76	13.32	0.36	LEU-73	H_{δ}	5.08	13.25	0.38
ARG-74	NH	-19.16	60.09	-0.32	ARG-74	H_{α}	-7.82	37.11	-0.21
ARG-74	H_{β}	2.55	18.35	0.14	ARG-74	H_{β}	-6.34	36.67	-0.17
ARG-74	H_{γ}	-1.83	24.02	-0.08	ARG-74	H_{γ}	-8.4	36.43	-0.23
ARG-74	H_{δ}	-1.63	28.0	-0.06	ARG-74	H_{δ}	4.42	16.35	0.27
ARG-74	H_{ϵ}	4.77	21.34	0.22	ARG-74	H_{η}	6.46	27.92	0.23
ARG-74	H_{η}	3.84	32.39	0.12	ARG-74	H_{η}	8.68	23.61	0.37
ARG-74	H_{η}	3.26	36.06	0.09	GLY-75	NH	4.78	27.65	0.17
GLY-75	H_{α}	7.18	14.48	0.5	GLY-75	H_{α}	3.57	21.47	0.17
GLY-76	NH	3.97	32.42	0.12	GLY-76	H_{α}	1.41	34.89	0.04

Table 8: UBQ, in complex with ligase, encapsulated

residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{\mathrm{NOE}}/\sigma_{\mathrm{ROE}}$	residue	proton	σ_{NOE}	σ_{ROE}	$\sigma_{\mathrm{NOE}}/\sigma_{\mathrm{ROE}}$
MET-1	NH	-0.14	30.3	-0.0	MET-1	NH	-0.48	30.52	-0.02
MET-1	NH	-0.21	29.09	-0.01	MET-1	H_α	-5.22	36.96	-0.14
MET-1	H_β	-2.21	25.06	-0.09	MET-1	H_β	-5.84	23.3	-0.25
GLN-2	NH	-18.82	55.68	-0.34	GLN-2	H_β	-3.72	18.62	-0.2
GLN-2	H_γ	0.44	16.99	0.03	GLN-2	H_γ	-2.52	21.43	-0.12
GLN-2	H_ϵ	3.73	19.92	0.19	GLN-2	H_ϵ	6.44	18.52	0.35
PHE-4	H_ζ	4.75	13.73	0.35	LYS-6	H_γ	-1.86	15.48	-0.12
LYS-6	H_γ	1.62	13.31	0.12	LYS-6	H_ϵ	4.13	12.45	0.33
LYS-6	H_ζ	6.21	15.13	0.41	LYS-6	H_ζ	6.32	15.14	0.42
LYS-6	H_ζ	6.39	15.04	0.42	THR-7	H_α	-11.46	29.1	-0.39
THR-7	H_β	-2.71	21.52	-0.13	THR-7	H_γ	-4.59	28.02	-0.16
THR-7	H_γ	-0.64	12.62	-0.05	LEU-8	NH	-21.5	60.01	-0.36
LEU-8	H_α	-2.95	22.76	-0.13	LEU-8	H_β	-2.18	21.21	-0.1
LEU-8	H_β	-6.28	25.73	-0.24	LEU-8	H_γ	-3.59	19.27	-0.19
LEU-8	H_δ	-0.15	12.34	-0.01	LEU-8	H_δ	0.91	12.93	0.07
LEU-8	H_δ	0.95	13.01	0.07	LEU-8	H_δ	0.95	13.01	0.07
THR-9	NH	-0.25	20.66	-0.01	THR-9	H_α	4.45	12.35	0.36
THR-9	H_γ	7.6	20.78	0.37	THR-9	H_γ	5.57	13.22	0.42
THR-9	H_γ	5.62	13.55	0.41	THR-9	H_γ	5.64	13.39	0.42
GLY-10	H_α	4.65	14.46	0.32	GLY-10	H_α	5.59	13.04	0.43
LYS-11	NH	2.29	13.14	0.17	LYS-11	H_δ	3.8	13.79	0.28
LYS-11	H_δ	4.27	12.87	0.33	LYS-11	H_ϵ	5.06	12.46	0.41
LYS-11	H_ϵ	4.27	13.08	0.33	LYS-11	H_ζ	9.29	18.85	0.49
LYS-11	H_ζ	8.78	19.2	0.46	LYS-11	H_ζ	9.1	19.0	0.48
THR-12	NH	6.93	14.26	0.49	THR-12	H_γ	9.52	20.35	0.47
ILE-13	H_α	3.77	13.65	0.28	THR-14	NH	5.92	18.3	0.32
THR-14	H_β	5.32	13.48	0.39	THR-14	H_γ	10.41	19.52	0.53
LEU-15	H_α	1.26	14.57	0.09	GLU-16	NH	-2.92	36.2	-0.08
GLU-16	H_β	5.29	25.5	0.21	GLU-16	H_β	3.96	28.51	0.14
GLU-16	H_γ	4.44	22.76	0.19	GLU-16	H_γ	3.79	20.67	0.18
VAL-17	H_α	-5.85	33.01	-0.18	GLU-18	NH	-6.73	33.88	-0.2
GLU-18	H_α	-4.64	18.17	-0.26	GLU-18	H_β	-3.27	30.2	-0.11
GLU-18	H_β	-5.45	37.91	-0.14	GLU-18	H_γ	1.31	34.34	0.04
GLU-18	H_γ	1.77	36.09	0.05	PRO-19	H_δ	-3.07	26.63	-0.12
PRO-19	H_δ	-4.76	21.88	-0.22	PRO-19	H_β	-5.21	22.52	-0.23
PRO-19	H_β	-2.41	18.57	-0.13	PRO-19	H_γ	-0.47	20.38	-0.02
PRO-19	H_γ	-2.04	20.29	-0.1	SER-20	NH	-3.26	19.15	-0.17
SER-20	H_α	-1.02	13.4	-0.08	SER-20	H_β	0.07	27.77	0.0
SER-20	H_β	1.4	22.55	0.06	SER-20	H_γ	-6.05	56.7	-0.11
ASP-21	H_α	0.05	31.87	0.0	ASP-21	H_β	-8.17	25.91	-0.32
ASP-21	H_β	-4.17	12.33	-0.34	THR-22	NH	-0.27	15.77	-0.02
THR-22	H_γ	5.12	24.6	0.21	THR-22	H_γ	4.11	14.92	0.28
THR-22	H_γ	4.07	14.75	0.28	THR-22	H_γ	4.13	14.66	0.28
ILE-23	H_γ	-11.72	26.92	-0.44	ILE-23	H_γ	-11.64	26.4	-0.44
ILE-23	H_γ	-12.53	28.28	-0.44	GLU-24	H_β	5.61	17.51	0.32
GLU-24	H_β	3.38	14.26	0.24	GLU-24	H_γ	7.83	24.72	0.32
GLU-24	H_γ	6.46	17.34	0.37	ASN-25	H_β	-2.6	20.73	-0.13
ASN-25	H_δ	7.6	21.78	0.35	ASN-25	H_δ	7.17	20.56	0.35
LYS-27	H_δ	-9.52	28.31	-0.34	LYS-27	H_δ	-12.12	33.35	-0.36
LYS-27	H_ϵ	-6.27	20.2	-0.31	LYS-27	H_ϵ	-6.29	19.83	-0.32
LYS-27	H_ζ	-11.72	59.55	-0.2	LYS-27	H_ζ	-9.59	54.25	-0.18
LYS-27	H_ζ	-11.1	57.23	-0.19	ALA-28	H_β	5.82	15.25	0.38
ALA-28	H_β	6.19	15.18	0.41	ALA-28	H_β	6.35	15.19	0.42
LYS-29	H_γ	-1.61	14.24	-0.11	LYS-29	H_γ	1.55	15.33	0.1
LYS-29	H_δ	1.36	14.32	0.1	LYS-29	H_δ	-0.37	14.72	-0.02
LYS-29	H_ϵ	1.16	19.69	0.06	LYS-29	H_ϵ	2.53	19.73	0.13
LYS-29	H_ζ	1.46	29.63	0.05	LYS-29	H_ζ	1.09	30.03	0.04
LYS-29	H_ζ	0.83	30.01	0.03	GLN-31	H_ϵ	8.57	14.35	0.6

GLN-31	H_ϵ	6.34	13.89	0.46
ASP-32	H_β	5.62	17.32	0.32
LYS-33	H_ϵ	3.67	14.74	0.25
LYS-33	H_ζ	7.8	16.85	0.46
LYS-33	H_ζ	7.77	17.28	0.45
GLU-34	H_β	4.38	16.71	0.26
PRO-37	H_β	5.88	13.62	0.43
PRO-38	H_β	3.91	16.33	0.24
ASP-39	NH	2.65	15.03	0.18
ASP-39	H_β	6.92	18.41	0.38
GLN-40	NH	-4.54	15.14	-0.3
GLN-40	H_ϵ	6.69	15.81	0.42
GLN-41	NH	-4.32	12.34	-0.35
ARG-42	H_β	-7.29	17.4	-0.42
ARG-42	H_γ	-10.49	25.13	-0.42
ARG-42	H_δ	-21.91	57.73	-0.38
ARG-42	H_η	-36.01	92.69	-0.39
ARG-42	H_η	-0.23	29.98	-0.01
LEU-43	NH	-57.92	126.63	-0.46
PHE-45	H_α	-25.85	60.46	-0.43
PHE-45	H_ϵ	-7.73	38.33	-0.2
PHE-45	H_δ	-3.3	17.55	-0.19
ALA-46	NH	-27.64	81.45	-0.34
ALA-46	H_β	-1.42	28.61	-0.05
ALA-46	H_β	-1.8	28.28	-0.06
GLY-47	H_α	-13.54	49.04	-0.28
LYS-48	H_α	-9.22	27.31	-0.34
LYS-48	H_β	-2.34	28.22	-0.08
LYS-48	H_γ	-3.77	24.64	-0.15
LYS-48	H_δ	-1.61	24.48	-0.07
LYS-48	H_ϵ	-0.06	20.68	-0.0
LYS-48	H_ζ	2.44	24.66	0.1
GLN-49	NH	-21.14	61.74	-0.34
GLN-49	H_β	-4.19	17.76	-0.24
GLN-49	H_γ	-6.79	26.54	-0.26
GLN-49	H_ϵ	1.09	29.32	0.04
LEU-50	H_β	-15.56	33.86	-0.46
GLU-51	H_β	7.12	20.3	0.35
GLU-51	H_γ	5.17	22.72	0.23
ASP-52	NH	-2.0	39.49	-0.05
ASP-52	H_β	3.28	20.33	0.16
GLY-53	NH	7.08	19.42	0.36
GLY-53	H_α	5.25	14.08	0.37
ARG-54	H_γ	0.97	21.74	0.04
ARG-54	H_ϵ	0.39	24.09	0.02
ARG-54	H_η	7.08	20.9	0.34
ARG-54	H_η	7.76	19.37	0.4
THR-55	H_γ	-1.93	31.85	-0.06
THR-55	H_γ	1.66	17.69	0.09
SER-57	H_α	-6.71	27.86	-0.24
SER-57	H_β	-1.45	21.05	-0.07
ASP-58	H_α	1.66	25.08	0.07
ASP-58	H_β	-5.65	30.96	-0.18
TYR-59	OH	5.43	29.5	0.18
TYR-59	H_ϵ	3.33	18.31	0.18
ASN-60	H_β	0.48	17.3	0.03
ASN-60	H_δ	1.79	22.62	0.08
ILE-61	H_α	-3.26	19.16	-0.17
GLN-62	H_α	-8.85	35.49	-0.25
GLN-62	H_β	-0.94	22.99	-0.04
GLN-62	H_γ	-0.73	21.17	-0.03
ASP-32	H_α	10.32	18.26	0.57
ASP-32	H_β	6.34	18.0	0.35
LYS-33	H_ϵ	4.33	15.58	0.28
LYS-33	H_ζ	7.59	17.61	0.43
GLU-34	H_α	7.34	14.99	0.49
GLU-34	H_γ	-0.08	12.38	-0.01
PRO-37	H_β	0.08	13.04	0.01
PRO-38	H_γ	5.62	12.9	0.44
ASP-39	H_α	1.9	32.94	0.06
ASP-39	H_β	6.75	20.29	0.33
GLN-40	H_α	-3.16	15.27	-0.21
GLN-40	H_ϵ	7.12	13.84	0.51
ARG-42	H_α	-24.19	55.49	-0.44
ARG-42	H_γ	-45.0	96.96	-0.46
ARG-42	H_δ	-28.42	73.63	-0.39
ARG-42	H_ϵ	-24.58	73.47	-0.33
ARG-42	H_η	-0.89	29.02	-0.03
ARG-42	H_η	5.39	26.63	0.2
LEU-43	H_β	-13.5	29.22	-0.46
PHE-45	H_δ	-42.67	97.98	-0.44
PHE-45	H_ζ	1.22	24.11	0.05
PHE-45	H_ϵ	0.29	21.13	0.01
ALA-46	H_α	-41.45	108.18	-0.38
ALA-46	H_β	-1.41	28.1	-0.05
GLY-47	NH	-57.46	129.56	-0.44
GLY-47	H_α	-11.05	32.24	-0.34
LYS-48	H_β	-1.09	25.15	-0.04
LYS-48	H_γ	-0.85	21.94	-0.04
LYS-48	H_δ	-0.66	20.95	-0.03
LYS-48	H_ϵ	-1.06	24.35	-0.04
LYS-48	H_ζ	2.23	24.74	0.09
LYS-48	H_ζ	2.27	24.39	0.09
GLN-49	H_β	-4.69	27.33	-0.17
GLN-49	H_γ	-6.38	20.32	-0.31
GLN-49	H_ϵ	-28.79	92.2	-0.31
LEU-50	NH	-10.43	24.54	-0.42
GLU-51	H_α	-8.16	40.12	-0.2
GLU-51	H_β	2.28	13.07	0.17
GLU-51	H_γ	7.24	21.46	0.34
ASP-52	H_α	-8.3	22.72	-0.37
ASP-52	H_β	7.22	24.19	0.3
GLY-53	H_α	6.87	15.89	0.43
ARG-54	H_α	-2.03	26.27	-0.08
ARG-54	H_δ	4.74	16.88	0.28
ARG-54	H_η	3.6	23.68	0.15
ARG-54	H_η	6.42	22.71	0.28
THR-55	NH	-8.7	34.93	-0.25
THR-55	H_γ	1.89	17.07	0.11
THR-55	H_γ	1.74	17.18	0.1
SER-57	H_β	-2.03	22.61	-0.09
SER-57	H_γ	0.21	31.26	0.01
ASP-58	H_β	-3.7	19.83	-0.19
TYR-59	H_α	1.44	15.14	0.1
TYR-59	H_δ	1.58	16.37	0.1
ASN-60	H_α	-4.66	22.01	-0.21
ASN-60	H_β	1.37	19.0	0.07
ASN-60	H_δ	1.54	21.38	0.07
GLN-62	NH	-5.65	32.55	-0.17
GLN-62	H_β	-2.27	24.68	-0.09
GLN-62	H_γ	1.03	17.48	0.06
GLN-62	H_ϵ	-2.65	34.3	-0.08

GLN-62	H_ϵ	-1.14	20.51	-0.06	LYS-63	NH	-6.26	31.6	-0.2
LYS-63	H_β	-3.77	19.71	-0.19	LYS-63	H_β	-7.68	24.63	-0.31
LYS-63	H_γ	-1.39	19.92	-0.07	LYS-63	H_γ	-1.42	22.15	-0.06
LYS-63	H_δ	-0.71	20.74	-0.03	LYS-63	H_δ	-0.7	21.44	-0.03
LYS-63	H_ϵ	1.57	19.05	0.08	LYS-63	H_ϵ	-0.77	23.95	-0.03
LYS-63	H_ζ	4.28	24.1	0.18	LYS-63	H_ζ	4.53	23.44	0.19
LYS-63	H_ζ	4.78	23.61	0.2	GLU-64	H_β	4.45	16.02	0.28
GLU-64	H_β	3.71	18.9	0.2	GLU-64	H_γ	-2.81	20.72	-0.14
GLU-64	H_γ	1.14	14.7	0.08	SER-65	H_α	3.68	18.78	0.2
SER-65	H_β	-1.35	13.81	-0.1	SER-65	H_γ	-1.52	22.73	-0.07
THR-66	NH	2.3	26.2	0.09	THR-66	H_β	-2.4	30.85	-0.08
THR-66	H_γ	9.36	27.79	0.34	THR-66	H_γ	0.81	15.01	0.05
THR-66	H_γ	0.34	14.94	0.02	THR-66	H_γ	0.45	15.5	0.03
LEU-67	H_α	-20.78	46.25	-0.45	HSD-68	NH	-11.41	27.03	-0.42
HSD-68	H_β	-6.28	17.3	-0.36	HSD-68	H_β	-6.76	17.56	-0.38
HSD-68	H_δ	-36.64	96.44	-0.38	HSD-68	H_ϵ	1.49	33.1	0.04
HSD-68	H_δ	-4.5	26.17	-0.17	LEU-69	NH	-12.16	28.19	-0.43
VAL-70	H_α	-13.19	38.35	-0.34	LEU-71	NH	-4.48	34.6	-0.13
LEU-71	H_β	2.16	19.22	0.11	LEU-71	H_γ	-1.64	15.68	-0.1
ARG-72	H_α	-22.84	57.26	-0.4	ARG-72	H_β	-26.27	60.16	-0.44
ARG-72	H_β	-40.09	88.35	-0.45	ARG-72	H_γ	-11.77	34.5	-0.34
ARG-72	H_γ	-8.47	25.08	-0.34	ARG-72	H_δ	-32.08	73.9	-0.43
ARG-72	H_δ	-40.21	92.24	-0.44	ARG-72	H_ϵ	-4.04	25.44	-0.16
ARG-72	H_η	1.95	24.3	0.08	ARG-72	H_η	1.63	29.28	0.06
ARG-72	H_η	-24.41	66.2	-0.37	ARG-72	H_η	-1.82	27.31	-0.07
LEU-73	NH	-57.9	133.41	-0.43	LEU-73	H_α	2.21	15.81	0.14
LEU-73	H_β	-0.29	17.95	-0.02	LEU-73	H_β	-4.54	26.13	-0.17
LEU-73	H_γ	0.53	14.29	0.04	LEU-73	H_δ	4.94	12.8	0.39
LEU-73	H_δ	4.72	12.7	0.37	LEU-73	H_δ	4.89	12.73	0.38
ARG-74	NH	-46.81	111.25	-0.42	ARG-74	H_α	1.84	16.56	0.11
ARG-74	H_β	0.47	19.69	0.02	ARG-74	H_β	-22.59	65.61	-0.34
ARG-74	H_γ	-5.13	29.15	-0.18	ARG-74	H_γ	-8.45	35.41	-0.24
ARG-74	H_δ	3.39	14.21	0.24	ARG-74	H_δ	3.06	16.13	0.19
ARG-74	H_ϵ	4.77	19.23	0.25	ARG-74	H_η	6.04	19.24	0.31
ARG-74	H_η	5.3	22.99	0.23	ARG-74	H_η	6.34	19.84	0.32
ARG-74	H_η	5.88	21.37	0.28	GLY-75	NH	1.7	20.09	0.08
GLY-75	H_α	4.54	15.24	0.3	GLY-75	H_α	0.14	17.96	0.01
GLY-76	NH	-4.97	40.21	-0.12	GLY-76	H_α	-25.93	84.24	-0.31

References

[1] N. V. Nucci, M. S. Pometun and A. J. Wand, *Nature Structural & Molecular Biology*, 2011, **18**, 245–249.

[2] N. V. Nucci, M. S. Pometun and A. J. Wand, *J. Am. Chem. Soc.*, 2011, **133**, 12326.

[3] P. Honegger and O. Steinhauser, *Phys. Chem. Chem. Phys.*, 2019, **21**, 14571–14582.

[4] D. Braun, M. Schmollngruber and O. Steinhauser, *J. Phys. Chem. Lett.*, 2017, **8**, 3421.

[5] R. B. Best, W. Zheng and J. Mittal, *J. Chem. Theory Comput.*, 2014, **10**, 5113–5124.