Electronic Supplementary Material (ESI) for ChemComm.

Molecular tweezers target a protein-protein interface and thereby modulate complex formation

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Supporting information

Content

1. Supplementary Information SI1: Experimental section.

1.1 Cloning, Expression and Purification of proteins

UBXD1-N (1-133 aa) sequence was cloned into a modified pET-41 vector with an N-terminal GST-tag as described before,[1] restriction enzymes *Apa*I and *Xho*I were purchased from Fermentas (Fast Digest, Germany), DreamTaq DNA polymerase from Thermoscientific/VWR (Germany). p97-N (1-199 aa) in a pProEx vector with an N-terminal 6xHis-tag was kindly provided by Prof. Freemont. The constructs were transformed into *E. coli* BL21(DE3)T1r (Sigma-Aldrich, Germany) for expression.

UBXD1-N was expressed by inoculating LB medium with an overnight culture, grown up to OD_{600} 0.8 and induction with 0.2 mM IPTG for 6 hours at 30 °C. UBXD1-N was isotopically labelled by resuspending cells from 1 L LB medium with an OD_{600} of 0.8 in 4 L M9 minimal medium supplemented with 1 g/l [^{15}N]ammonium chloride and grown up to OD_{600} 0.8 with subsequent induction of protein expression using 0.2 mM IPTG for 6 h at 30 °C. For isotope-labelling of p97-N, cells from 1 L LB medium with an OD_{600} of 0.8 were resuspended in 4 L M9 minimal medium supplemented with 1 g/l [^{15}N]ammonium chloride and grown up to OD_{600} 0.8 with subsequent induction of protein expression using 0.2 mM IPTG overnight at 30 °C. Cells were pelleted and lysed with lysozyme in low salt buffer (20 mM Tris, 50 mM NaCl, 1 mM PMSF, pH 7.4) and sonication. The cell lysate was centrifuged (95,000 xg, 70 min, 4 °C) and filtrated supernatant was used for further purification.

Protein mixture containing UBXD1-N was applied to a GSH column (Macherey & Nagel) in buffer 1 (20 mM Tris, 150 mM NaCl, pH 7.4) and GST-tagged protein was eluted using buffer 1 supplemented with 20 mM glutathione. Separation of UBXD1-N and the GST-tag was done by cleaving off the tag with PreScission protease and subsequent analytical size exclusion chromatography with a Superdex 75PG 26/600 column (GE Healthcare) in 50 mM KP_i buffer, 150 mM KCl, pH 6.5. The protein mixture containing p97-N was applied onto an anion exchange column (HiTrap Q HP, GE Healthcare) in buffer 2 (20 mM Bis-Tris, pH 6.6) and eluted with buffer 2 containing 500 mM NaCl. Subsequently, the eluted protein mixture was loaded onto a Ni-NTA column in buffer 3 (50 mM NaH_2PO_4, 300 mM NaCl, pH 8.0) containing 10 mM imidazole and then eluted after a washing step using buffer 3 supplemented with 500 mM imidazole. Finally, proteins were dialyzed for NMR spectroscopy against 50 mM KP_i buffer (pH 6.5 for UBXD1-N or pH 7.2 for p97-N).

1.2 Molecular Dynamics (MD) simulations and Quantum Mechanics/Molecular Mechanics (QM/MM) calculations

The coordinates of the N-terminal segment of the p97 protein (p97-N) were taken from the crystal structure reported by Hänzelmann *et al.* (PDB code 3QQ7),[2] which includes residues 20 to 187 without the flexible termini. MD simulations were performed for the protein without ligand and for the inclusion complexes formed between p97-N and the hydrogen phosphate tweezers with a 1:1 ratio. This way, all lysine and arginine residues present in the crystal structure of p97-N were investigated as tentative binding sites for the tweezers. MD simulations (60 ns) in explicit water were performed with the NAMD2.9 code using the CHARMM22 force field for the protein and ligand and the TIP3P model for water.[3-5] The CHARMM parameters for the tweezers were generated using Swissparam and tested by

us.[6-8] All simulations were performed at 300 K in the NPT ensemble with a time step of 2 fs. The PME method was used to handle the electrostatic interactions.[9] Of the 11 lysine and 15 arginine residues found in p97-N (20-187 aa), only six lysines (K20, K60, K62, K63, K109, K112) and seven arginines (R22, R53, R64, R86, R95, R113 and R159) formed conserved inclusion complexes during the MD simulations. In addition, MD simulations with five tweezer molecules bound to p97-N were performed to explore the possibility of simultaneous binding of multiple tweezers. The tweezers were initially placed forming inclusion complexes with K20, K63, R89 and R159. The fifth tweezers molecule was placed near K148 as in the 1:1 complex. Three independent replicas of 50 ns each were performed under the same conditions as the 1:1 complexes.

QM/MM optimizations of five randomly selected snapshots from the MD simulations of the conserved 1:1 complexes were performed to estimate the relative preference of tweezers toward specific residues on the protein surface. We used the program ChemShell v3.4 (ChemShell, see www.chemshell.org) with Turbomole 5.10 for the QM region and DL_POLY as driver of the CHARMM22 force field in the MM region.[10-12] The QM region, which included all atoms of tweezers and some lateral chain atoms of lysine and arginine (Figure S3), was treated at the B3LYP-D2/SVP level of theory.[13–15] Open valences at the QM/MM border were saturated using hydrogen link atoms and an electrostatic embedding scheme was used.[16,17] To avoid over-polarization of the QM region at the boundary, a charge shift scheme was applied.[18] No electrostatic cut offs were used. The optimization was performed with the HDLC optimizer.[19] The active region consisted of a 13 Å sphere centered on the middle ring of the hydrogen phosphate tweezers. All atoms within the active region were allowed to freely move in each optimization step. The lowest energy of the QM region (E) for each type of amino acid was set to 0 kcal/mol and taken as a reference. Analysis of the relative averaged energy values allows assigning the preferred amino acid binding site in all patches (Table S2).

1.3 Nuclear Magnetic Resonance (NMR) spectroscopy

NMR experiments were performed on a 700 MHz Ultrashield NMR spectrometer (Bruker, Germany) equipped with a cryoprobe (Bruker Biospin). NMR samples contained 260 µM of ^{15}N-labeled p97-N (H2O:D2O/ 90 %:10 %) or 320 µM of ^{15}N-labeled UBXD1-N. ^{1}H-^{15}N-HSQC spectra were recorded with 24 scans and 2k x 0.256k data points. Data were processed with Topspin 3.0 (Bruker). Titration experiments with hydrogen phosphate tweezers were performed at 27 °C by stepwise addition of 0, 10, 20, 50, 100, 150 and 200 µM of the hydrogen phosphate tweezers to p97-N or up to 130 µM hydrogen phosphate tweezers to UBXD1-N. Intensity changes of the signals were analyzed and ^{1}H- and ^{15}N-shifts were combined according to the following equation.[20]

$$\delta\Delta_{total} = \sqrt{(\delta\Delta_H)^2 + (0.154 \cdot \delta\Delta_N)^2}$$

1.4 Isothermal Titration Calorimetry (ITC)

For ITC experiments, 10 µM of p97-N was titrated in 29 steps with up to 1 mM hydrogen phosphate tweezers in 50 mM KP_i, pH 7.2 at 25 °C. The resulting titration curves were subjected to nonlinear regression and hence produced K_a values (Fit-Parameter: N = 0,190, K = 1,75E5, DH = -5,238, DS = -152). Complexation entropy terms ($-T\cdot\Delta S$) were subsequently derived from free binding energies (ΔG) and complexation enthalpies (ΔH). ITC experiments were carried out on a micro-calorimeter VP-ITC (Malvern, UK).

1.5 Fluorescence anisotropy

For fluorescence anisotropy, UBXD1-N was labeled with $ATTO_{594}$ according to the manufacturer's instructions. The tweezers were pre-incubated with p97-N in different protein/ligand ratios ranging from 1:0 to 1:0.5 and titrated in several steps until a final concentration ratio of 450 µM p97-tweezers complex to 1 µM UBXD1-N was reached. Fluorescence anisotropy was measured at a Cary Eclipse Fluorescence spectrometer (Agilent Technologies, Germany) in 50 mM KP_i, pH 7.2 with 0.05 % Tween at 21 °C.

1.6 ELISA

For an ELISA, we have coated wells (nunc, Maxisorp) with the indicated concentrations of UBXD1-N 1-133 (30-210 nM) in NaP_i buffer (50 mM NaP_i, pH 7.3) at 30 °C for 1 h, followed by 3 wash steps with NaP_iT (+ 0.1 % tween, 5 min each). Blocking was done with 5 % milk powder in NaP_iT at 30 °C for 1 h. Afterwards 1.2 µM p97-N and various tweezers concentrations (0-50 µM) in NaP_iT with 1 % milk powder were added simultaneously and incubated at 30 °C for 1 h. 3 wash steps (5 min each) followed with NaP_iT. For detection of the complex wells were incubated with an α-pentaHis antibody (1:4000, Qiagen) in NaP_iT with 1 % milk powder at 30 °C for 1 h. After another 3 wash steps with NaP_iT (5 min each), 50 µl/well TMB (Pierce) substrate for 15 min was added and the reaction was stopped with 50 µl/well 2N H_2SO_4. The TMB absorption was measured at 450 nm with an ELISA plate reader (BioTek Synergy HT).

1.7 Bio-Layer Interferometry (BLI)

Bio-Layer Interferometry (BLI) experiments were performed on an Octet Red 96 (Pall/Fortebio) instrument at 25°C. Ni-NTA coated biosensors (Pall/Fortebio) were loaded with His_6-tagged p97-N (55 µg/ml) in BLI buffer (50 mM KP_i, pH 7.2 with 150 mM NaCl and 0.05 % Tween), followed by blocking with 1 % BSA. UBXD1-N titrations (0 – 5 µM) in the absence and presence of different tweezers concentrations (0 µM, 0.5 µM, 5 µM and 50 µM) were performed. For each titration point, a control experiment at the same UBXD1-N concentration with buffer only in the loading step (no p97-N) was carried out and subtracted to account for remaining non-specific binding of UBXD1-N to the sensor surface. Furthermore, all data were referenced with p97-N loaded biosensors incubated in BLI buffer instead of UBXD1-N. Steady state data analysis was performed using the following steady state model for one-site binding:

$$R = \frac{R_{max} \cdot [UBXD1]}{K_D + [UBXD1]}$$

R: BLI response; R_{max}: maximum BLI response; K_D: dissociation constant; [UBXD1]: UBXD1-N concentration**.**For an ELISA, we have coated wells (nunc, Maxisorp) with the indicated concentrations of

2. Supplementary information SI2

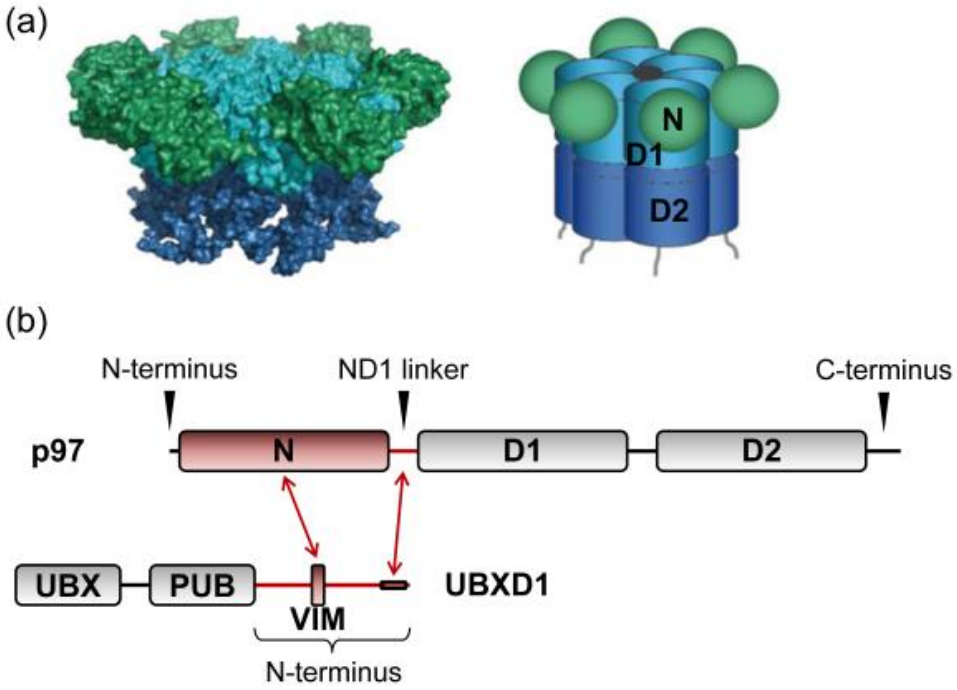


Figure SI2: Domain structure and interaction sites of the hexameric p97 barrel. The valosin-containing protein (VCP)/p97 is an abundant AAA (ATPase associated with diverse cellular activities)-type ATPase. It is involved in multiple cellular functions such as cell cycle regulation and DNA repair, protein degradation by the ubiquitin-proteasome system and autophagy as well as protein sorting at the endosome.[21-23] Missense mutations in p97 cause a multisystem neuromuscular degenerative disease characterized by inclusion body myopathy associated with Paget's disease of the bone and frontotemporal dementia (IBMPFD) and amyotrophic lateral sclerosis (ALS).[24,25] (a) Schematic presentation of p97 and its domain architecture. p97 acts as a macromolecular hexameric barrel complex. Each protomer consists of two AAA domains (D1 and D2) for ATP binding and hydrolysis (light/dark blue). The N-domain (green) at the N-terminus (p97-N) and the unstructured C-terminus of each protomer mediate the interaction of p97 with its adaptors and cofactors. The overall architecture of p97 can be described as two stacked hexameric rings formed by the D1- and D2-domains with the peripheral N-domain next to the D1-ring.[26] (b) Distinct cofactor proteins direct the p97 machinery to different tasks in the cell. One of these adaptors is UBXD1. The N-terminus of UBXD1 (UBXD1-N) exhibits two binding epitopes: a VCP interacting motif (VIM) which interacts with the VIM groove located on p97-N, and a binding site targeting the ND1-linker which connects the N- and D1-domain of p97.[1,27] Arrows are highlighting the sites of interaction between p97 and UBXD1. As IBMPFD/ALS mutations of p97 differentially affect individual cofactors and lead to unbalanced p97-cofactor interactions, chemically modulating these interactions may represent a novel strategy to restore p97 function in the disease.[28,29]

3. Supplementary Figure S1

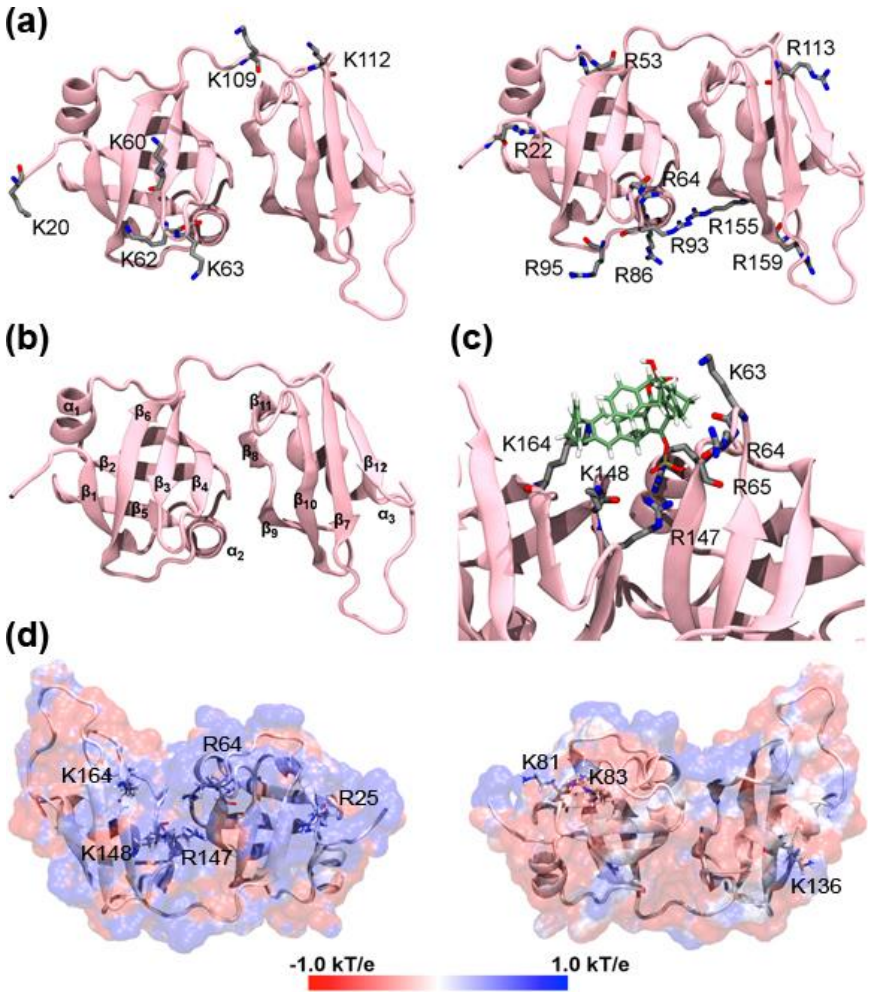


Figure S1: Structural overview of p97-N. (a) Relevant lysine (left) and arginine (right) residues of p97-N interacting with the tweezers. (b) p97-N regions classified by secondary structure motifs. (c) Positively charged residues near K148 in p97-N. (d) Left: In the case of K148 the tweezers does not form inclusion complexes but will remain at the protein surface due to the positive electrostatic potential. Right: In regions of less positive electrostatic potential, the tweezer does not establish inclusion complexes and moves away from the protein to the bulk solvent.

4. Supplementary Figure S2

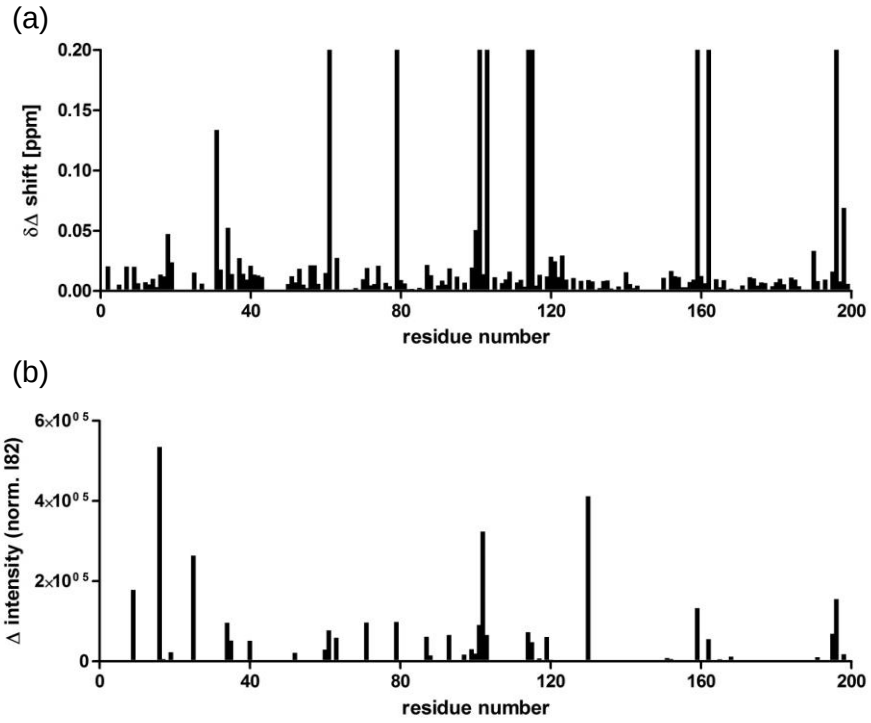


Figure S2: Shift- and intensity-differences of p97-N after titration with hydrogen phosphate tweezers. (a) Shift analysis of signals of ^{15}N-labeled p97-N from a ^{1}H-^{15}N-HSQC-spectra after addition of 100 µM hydrogen phosphate tweezers. (b) Intensity analysis of signals of ^{15}N-labeled p97-N from a ^{1}H-^{15}N-HSQC-spectra after addition of 100 µM tweezers. Shifts of specific N_H-signals and differences in intensity changes reveal a specific interaction between the hydrogen phosphate tweezers and p97-N.

5. Supplementary Figure S3

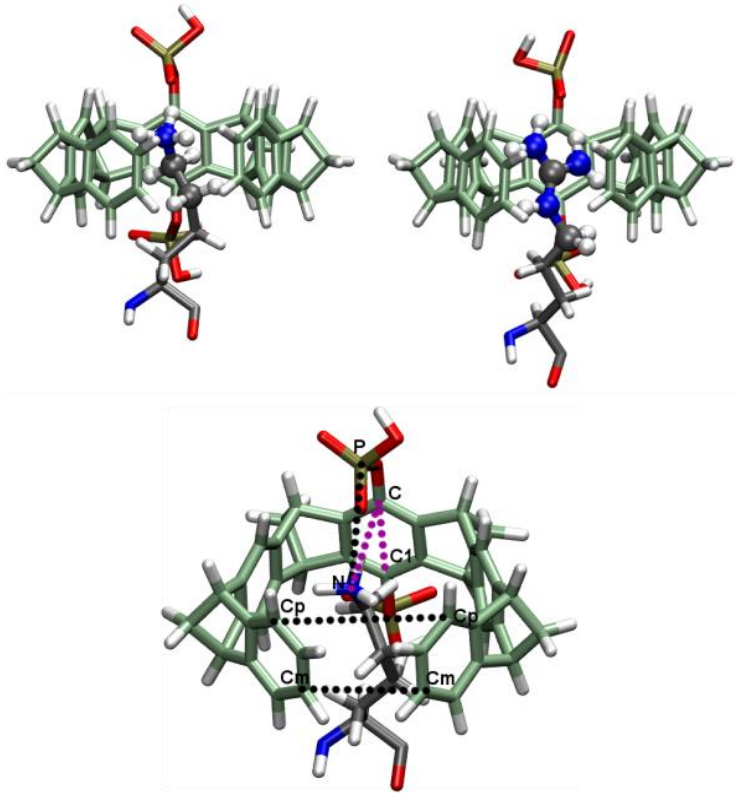


Figure S3: QM regions used for QM/MM calculations and selected geometrical parameters. Top: The QM region (QM/MM optimizations) includes all atoms of the hydrogen phosphate tweezers ($C_{42}H_{30}O_8P_2$) and the atoms of the lateral chain of lysine or arginine shown as spheres. Bottom: Relevant distances (black dash lines) and angle (violet dash line) reported in supplementary Table S1.

6. Supplementary Figure S4

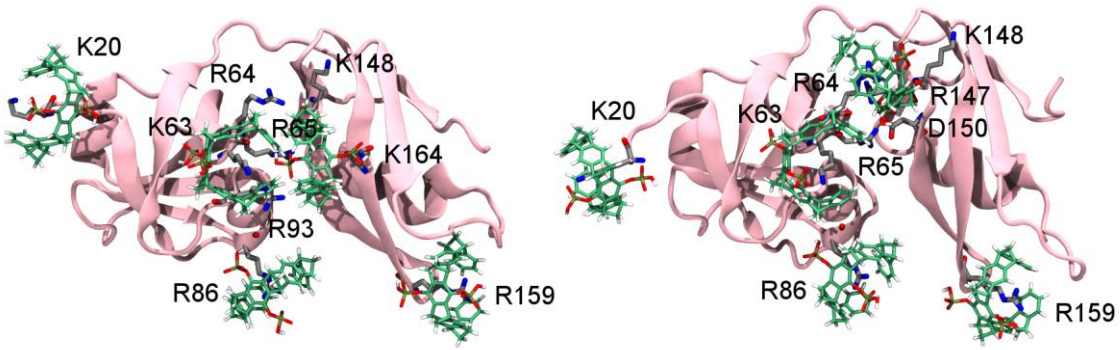
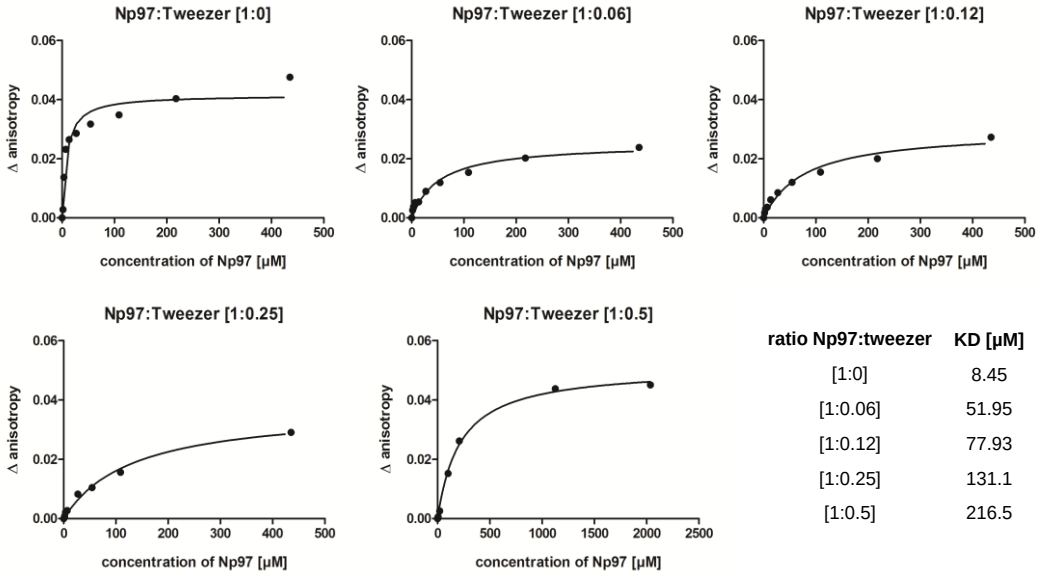


Figure S4: MD simulations with multiple tweezers. Additional MD simulations corroborated that the inclusion complexes were conserved in all cases. The last frame for the MD simulations (in total 3 independent replicas were performed, see figure 3, main text) is shown. The inclusion complexes with K20, K63, R86 and R159 were conserved. The fifth tweezers molecule around K148 remains in the central canyon of the domain. R64 (which is a favored residue according to the QM/MM calculations) can also form an inclusion complex with the tweezers.

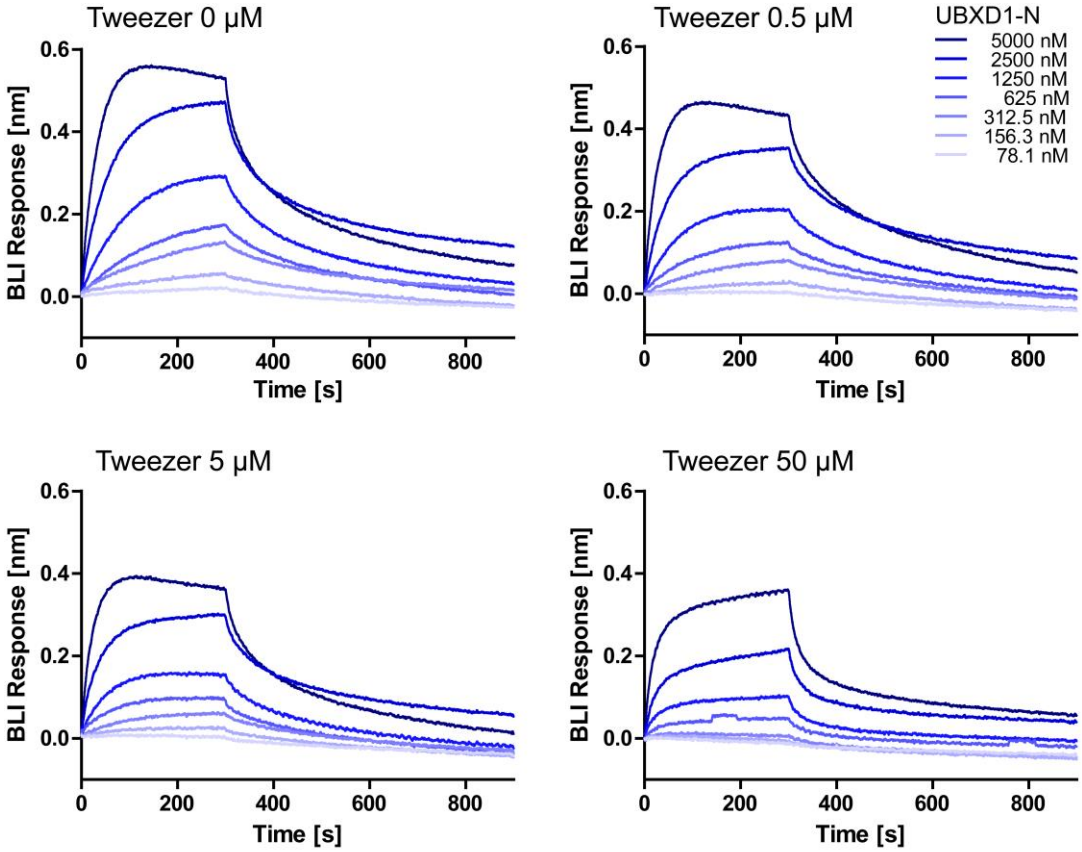
7. Supplementary Figure S5



ratio Np97:tweezer	KD [µM]
[1:0]	8.45
[1:0.06]	51.95
[1:0.12]	77.93
[1:0.25]	131.1
[1:0.5]	216.5

Figure S5: Titration curves of different hydrogen phosphate tweezers:p97-N ratios with UBXD1-N. Fluorescence anisotropy was measured of ATTO-labelled UBXD1-N in the presence of different p97-N:tweezers ratios as indicated. The preferred tweezers binding sites on the surface of p97-N are mainly next two the ND1-linker and hence the tweezers turns the two site binding site of the UBXD1-p97 complex into a one site binding complex mediated by the VIM groove. For a better comparison in respect to the final one site binding state we decided to choose a one site specific binding fit (GraphPad Prism) also for the initial state. The affinity between UBXD1-N and p97-N ascends with increasing hydrogen phosphate tweezers concentrations.

8. Supplementary Figure S6



Tweezer [µM]	K_D [µM]
0	2.1 ± 0.3
0.5	3.1 ± 0.5
5.0	3.8 ± 0.8
50	21 ± 10

Figure S6: BLI association and dissociation curves for the titrations of p97-N with UBXD1-N in the presence of different tweezers concentrations (0 µM, 0.5 µM, 5 µM, 50 µM) and K_D values obtained from steady-state data analysis (bottom).

9. Supplementary Figure S7

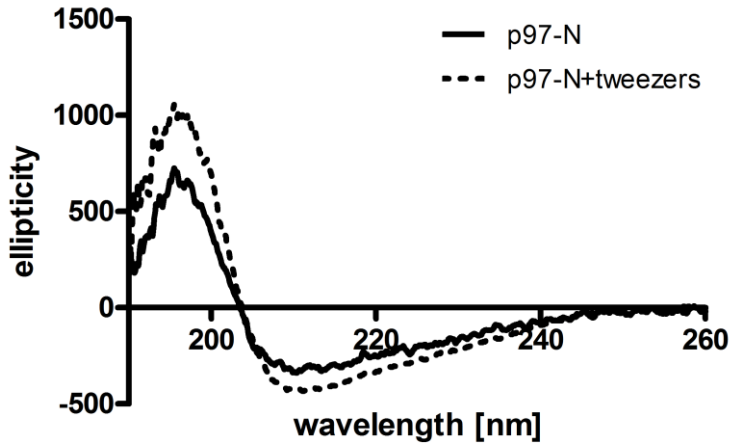


Figure S7: CD spectra of p97-N with bound tweezers. CD spectra of 0.15 mg/ml p97-N in the absence (solid line) and in the presence of tweezers (dashed line) were recorded in 50 mM KP_i, pH 7.2 at 25 °C with a CD spectrometer (J-710, Jasco). Secondary structure prediction from CD spectra by CDSSTR tool yields no significant changes in the secondary structure of p97-N upon binding of tweezers at sub-stoichiometric conditions.

10. Supplementary Figure S8

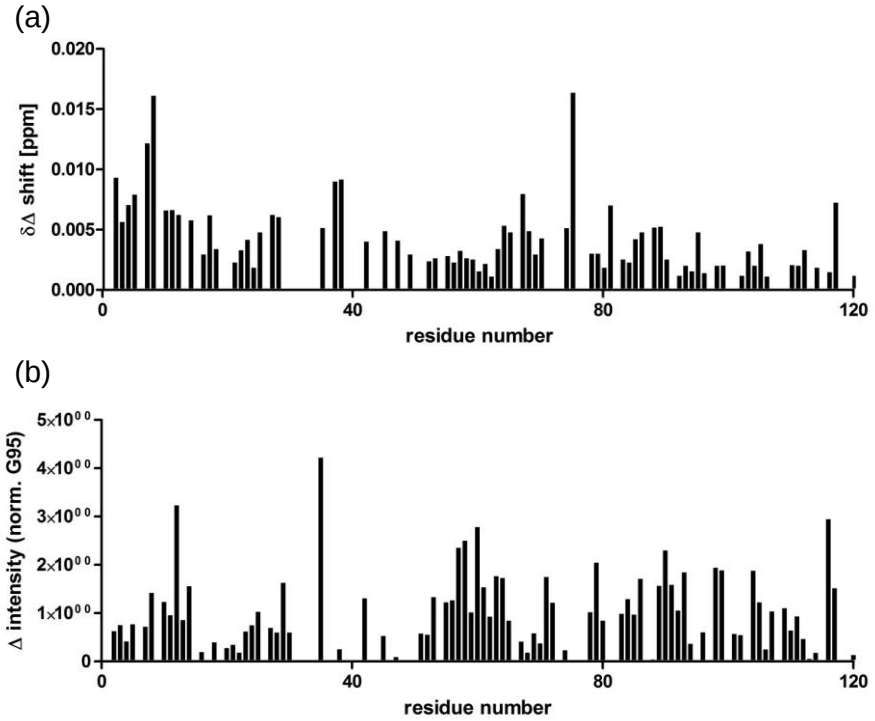


Figure S8: Shift- and intensity-differences of UBXD1-N after titration with hydrogen phosphate tweezers. (a) Shift analysis of signals of 320 µM ^{15}N-labeled UBXD1-N from a ^{1}H-^{15}N-HSQC-spectra after addition of 130 µM hydrogen phosphate tweezers. (b) Intensity analysis of signals of ^{15}N-labeled UBXD1-N from a ^{1}H-^{15}N-HSQC-spectra after addition of 130 µM tweezers.

11. Supplementary Table S1

Table S1: Selected geometrical parameters from MD simulations indicating if the tweezers are deformed upon inclusion and the degree of threading of the amino acid side chain inside the tweezers' cavity.

Residues	Cp – Cp [a]	Cm – Cm [a]	X – P [b]	ω [c]
K20	5.62 ± 0.41	4.05 ± 0.42	3.96 ± 0.17	90.0 ± 4.9
K63	5.85 ± 0.44	4.21 ± 0.46	3.92 ± 0.18	94.7 ± 5.9
K62	5.61 ± 0.47	4.05 ± 0.45	4.03 ± 0.31	87.2 ± 7.9
K60	5.33 ± 0.30	3.75 ± 0.28	4.05 ± 0.14	78.2 ± 3.5
K112	5.50 ± 0.33	3.87 ± 0.29	3.97 ± 0.14	87.6 ± 4.2
K109	5.55 ± 0.46	3.98 ± 0.46	4.01 ± 0.14	84.7 ± 5.3
R86	6.04 ± 0.64	4.43 ± 0.85	5.15 ± 0.70	74.4 ± 7.9
R95	5.94 ± 0.43	4.26 ± 0.50	4.85 ± 0.54	80.1 ± 10.1
R64	5.89 ± 0.40	4.25 ± 0.45	4.80 ± 0.52	78.3 ± 11.6
R22	5.73 ± 0.34	4.03 ± 0.35	4.44 ± 0.20	74.0 ± 4.4
R159	5.83 ± 0.35	4.07 ± 0.36	5.18 ± 0.72	81.5 ± 7.9
R53	5.77 ± 0.35	4.02 ± 0.36	4.92 ± 0.77	74.1 ± 5.7
R113	7.66 ± 1.19	6.61 ± 1.50	4.55 ± 0.20	85.4 ± 9.6

[a] Cp – Cp, Cm – Cm: intramolecular distances (Å) between the p- and m- carbon atoms, respectively in the last benzene units of each arm of the tweezers. [b] X – P: distance (Å) between the heavy atom of the lateral chain of Lys/Arg and the closest phosphorus atom of the tweezers. [c] ω: angle (°) formed by p-positions of the central benzene ring in tweezers and the X atoms described in [b] (for more details, see supplementary Figure S3).

12. Supplementary Table S2

Table S2: Relative QM energies [kcal/mol] from the QM/MM optimizations of inclusion complexes.

residue	E	σ [a]	residue	E	σ [a]
K20	0	9	R86	0	13
K63	6	2	R95	5	1
K62	19	9	R64	11	10
K60	26	3	R22	30	11
K112	44	18	R159	41	11
K109	50	7	R53	43	12
			R113	75	3

[a] Standard deviation.

13. Cartesian coordinates and QM energies of the inclusion complexes

Cartesian coordinates of the QM regions of the tweezers- amino acid inclusion complexes optimized at the QM/MM level of theory. Representative snapshot, the energy is given in Hartree. Only heavy atoms are reported.

Lys20-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	-21.62	-7.584	-16.956	C	-17.643	-3.769	-21.582
C	-20.251	-9.298	-18.816	C	-18.7	-2.406	-20.084
C	-20.244	-7.466	-17.185	C	-17.328	-2.431	-20.835
C	-22.288	-8.58	-17.675	C	-18.978	-3.373	-22.216
C	-21.61	-9.439	-18.555	C	-21.497	-2.334	-22.793
C	-19.582	-8.303	-18.106	C	-19.567	-3.681	-23.436
C	-22.645	-10.391	-19.142	C	-19.637	-2.539	-21.287
C	-23.509	-9.529	-20.051	C	-20.896	-2.022	-21.558
C	-25.256	-7.688	-21.142	C	-20.842	-3.149	-23.719
C	-23.657	-9.521	-21.437	C	-19.195	-6.457	-16.704
C	-24.201	-8.626	-19.214	C	-17.936	-7.378	-16.716
C	-25.071	-7.668	-19.752	O	-22.344	-6.756	-16.122
C	-24.567	-8.603	-21.963	P	-22.148	-6.618	-14.48
C	-25.051	-8.366	-23.395	O	-21.212	-5.289	-14.332
C	-24.557	-6.978	-23.803	O	-21.302	-7.768	-13.971
C	-24.132	-4.25	-24.129	O	-23.521	-6.309	-13.92
C	-23.641	-6.557	-24.764	O	-19.612	-10.133	-19.707
C	-25.247	-6.049	-22.992	P	-19.214	-9.67	-21.248
C	-25.04	-4.684	-23.142	O	-19.482	-11.112	-21.993
C	-23.44	-5.168	-24.925	O	-17.725	-9.402	-21.301
C	-26.16	-6.869	-22.073	O	-20.225	-8.671	-21.769
C	-26.541	-8.002	-23.083	N	-25.21	-2.577	-16.786
C	-23.77	-8.952	-17.772	C	-23.957	-3.311	-17.148
C	-23.609	-10.501	-17.915	C	-23.945	-3.701	-18.655
C	-18.137	-7.825	-18.196	C	-22.812	-4.689	-18.987
C	-18.209	-6.446	-18.851	C	-22.671	-5.043	-20.462
C	-18.636	-3.789	-19.443	C	-21.552	-6.06	-20.651
C	-18.855	-5.6	-17.925	N	-21.276	-6.329	-22.1
C	-17.783	-5.992	-20.101	C	-22.69	-2.547	-16.81
C	-17.992	-4.637	-20.37	O	-21.743	-3.121	-16.284
C	-19.092	-4.253	-18.206				
E_{QM} = -3036.268988							

Lys63-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	7.426	-9.278	-17.594	C	1.29	-11.995	-15.038
C	6.696	-11.711	-18.962	C	1.694	-9.983	-14.029
C	6.142	-9.472	-18.117	C	0.442	-10.797	-14.499
C	8.337	-10.319	-17.797	C	2.095	-12.293	-13.768
C	7.986	-11.513	-18.461	C	3.475	-12.175	-11.35
C	5.793	-10.661	-18.783	C	2.568	-13.477	-13.211
C	9.216	-12.424	-18.414	C	2.332	-11.05	-13.139
C	9.416	-12.793	-16.943	C	3.035	-10.973	-11.942
C	9.918	-12.79	-14.22	C	3.246	-13.405	-11.975
C	9.371	-14.018	-16.275	C	4.872	-8.617	-18.063
C	9.732	-11.596	-16.266	C	4.254	-9.016	-19.441
C	9.955	-11.561	-14.886	O	7.727	-8.169	-16.843
C	9.668	-13.995	-14.91	P	8.786	-6.946	-17.239
C	9.761	-15.118	-13.875	O	8.225	-5.882	-16.155
C	8.546	-14.903	-12.981	O	8.463	-6.45	-18.635
C	6.577	-13.894	-11.295	O	10.224	-7.328	-16.928
C	7.345	-15.592	-12.875	O	6.343	-12.838	-19.67
C	8.77	-13.7	-12.269	P	5.781	-14.213	-18.968
C	7.799	-13.198	-11.412	O	7.2	-14.896	-18.545
C	6.349	-15.063	-12.028	O	5.052	-15.004	-20.025
C	10.124	-13.163	-12.748	O	4.996	-13.846	-17.707
C	10.871	-14.516	-12.954	N	7.852	-7.613	-11.251
C	9.773	-10.494	-17.322	C	7.045	-7.89	-12.424
C	10.32	-11.326	-18.527	C	6.73	-9.402	-12.53
C	4.318	-10.55	-19.145	C	6.399	-9.894	-13.938
C	3.577	-10.57	-17.808	C	6.222	-11.403	-13.962
C	2.488	-9.986	-15.338	C	5.913	-11.954	-15.338
C	3.897	-9.364	-17.149	N	5.678	-13.43	-15.268
C	2.762	-11.539	-17.22	C	5.827	-6.979	-12.564
C	2.219	-11.217	-15.973	O	4.682	-7.41	-12.72
C	3.357	-9.045	-15.901				
E_{QM} = -3036.262663							

Lys62-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	-24.53	3.925	-2.457	C	-20.78	-2.343	-2.507
C	-21.821	4.359	-3.296	C	-22.894	-2.612	-1.679
C	-23.915	3.116	-3.41	C	-21.921	-3.411	-2.61
C	-23.766	4.973	-1.938	C	-20.661	-2.283	-0.986
C	-22.436	5.171	-2.344	C	-21.099	-2.284	1.761
C	-22.591	3.328	-3.833	C	-19.573	-2.123	-0.14
C	-21.872	6.299	-1.486	C	-21.97	-2.44	-0.472
C	-21.845	5.75	-0.056	C	-22.207	-2.429	0.897
C	-22.47	4.774	2.456	C	-19.804	-2.134	1.251
C	-20.795	5.373	0.782	C	-24.399	1.854	-4.114
C	-23.189	5.595	0.343	C	-23.657	2.035	-5.471
C	-23.525	5.101	1.603	O	-25.843	3.733	-2.074
C	-21.125	4.896	2.052	P	-26.332	2.417	-1.201
C	-20.271	4.412	3.227	O	-27.587	3.089	-0.414
C	-20.556	2.916	3.366	O	-25.249	2.112	-0.181
C	-21.7	0.408	3.746	O	-26.861	1.319	-2.113
C	-19.769	1.789	3.178	O	-20.499	4.551	-3.627
C	-21.908	2.798	3.754	P	-20.038	5.279	-5.054
C	-22.498	1.555	3.933	O	-18.575	5.783	-4.552
C	-20.353	0.524	3.385	O	-20.903	6.501	-5.301
C	-22.453	4.22	3.878	O	-19.872	4.231	-6.145
C	-21.163	4.93	4.403	N	-15.73	1.842	-1.898
C	-24.046	6.014	-0.851	C	-16.934	2.661	-1.859
C	-23.152	7.181	-1.381	C	-18.028	1.9	-1.056
C	-22.253	2.2	-4.811	C	-19.462	2.436	-1.162
C	-22.24	0.911	-3.985	C	-20.469	1.566	-0.407
C	-22.887	-1.278	-2.432	C	-21.901	2.08	-0.473
C	-23.561	0.714	-3.528	N	-22.834	1.15	0.249
C	-21.219	0.009	-3.688	C	-16.697	4.063	-1.291
C	-21.579	-1.108	-2.93	O	-15.873	4.256	-0.398
C	-23.904	-0.359	-2.704				
E_{QM} = -3036.241484							

Lys60-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	-19.923	-2.746	2.168	C	-13.954	0.891	3.738
C	-17.653	-3.88	0.841	C	-15.848	1.808	4.62
C	-18.755	-3.052	2.861	C	-14.348	1.682	5.026
C	-19.96	-3.092	0.821	C	-14.47	1.902	2.709
C	-18.842	-3.615	0.151	C	-15.894	3.84	1.314
C	-17.646	-3.622	2.211	C	-13.97	2.355	1.497
C	-19.245	-3.72	-1.325	C	-15.662	2.441	3.245
C	-19.489	-2.281	-1.814	C	-16.395	3.392	2.553
C	-20.468	0.282	-2.238	C	-14.698	3.336	0.796
C	-18.817	-1.468	-2.731	C	-18.34	-2.829	4.308
C	-20.624	-1.805	-1.117	C	-17.437	-4.088	4.493
C	-21.118	-0.511	-1.29	O	-21.021	-2.149	2.757
C	-19.341	-0.187	-2.943	P	-21.04	-0.518	3.066
C	-18.905	0.949	-3.871	O	-20.647	-0.444	4.648
C	-18.415	2.084	-2.968	O	-22.465	-0.042	2.866
C	-18.185	4.202	-1.173	O	-19.908	0.161	2.314
C	-17.165	2.656	-2.766	O	-16.515	-4.318	0.209
C	-19.549	2.552	-2.264	P	-16.148	-5.934	0.05
C	-19.447	3.601	-1.356	O	-14.766	-5.711	-0.794
C	-17.062	3.732	-1.862	O	-17.183	-6.573	-0.857
C	-20.734	1.707	-2.731	O	-15.844	-6.572	1.391
C	-20.315	1.525	-4.225	N	-11.014	0.201	-1.895
C	-21.076	-2.933	-0.202	C	-11.877	-0.308	-0.84
C	-20.735	-4.146	-1.123	C	-13.374	-0.067	-1.179
C	-16.537	-3.758	3.261	C	-14.395	-0.578	-0.144
C	-16.131	-2.324	3.63	C	-15.825	-0.107	-0.433
C	-16.154	0.334	4.381	C	-16.793	-0.32	0.727
C	-17.265	-1.749	4.241	N	-18.176	0.119	0.343
C	-14.967	-1.578	3.412	C	-11.621	-1.794	-0.672
C	-14.992	-0.238	3.822	O	-11.844	-2.58	-1.593
C	-17.318	-0.402	4.592				
E_{QM} = -3036.239948							

Lys112-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	12.322	19.962	8.974	C	5.508	17.642	9.688
C	11.899	17.692	7.27	C	5.9	19.467	11.005
C	11.205	19.87	8.145	C	4.706	18.894	10.176
C	13.236	18.912	8.916	C	5.955	17.107	11.049
C	13.03	17.802	8.082	C	6.877	16.79	13.657
C	10.988	18.753	7.316	C	6.149	15.822	11.535
C	14.176	16.827	8.356	C	6.21	18.238	11.86
C	13.952	16.346	9.794	C	6.681	18.096	13.158
C	13.602	16.165	12.531	C	6.609	15.67	12.859
C	13.571	15.107	10.32	C	10.019	20.809	7.946
C	14.147	17.472	10.626	C	9.742	20.532	6.434
C	13.942	17.412	12.006	O	12.568	21.095	9.716
C	13.42	15.034	11.708	P	12.226	21.386	11.293
C	13.113	13.863	12.646	O	13.577	20.883	12.078
C	11.759	14.145	13.302	O	11.053	20.53	11.75
C	9.655	15.139	14.835	O	12.129	22.887	11.401
C	10.533	13.495	13.259	O	11.686	16.562	6.518
C	11.94	15.29	14.107	P	12.055	16.518	4.894
C	10.89	15.819	14.848	O	11.721	14.952	4.644
C	9.483	13.99	14.056	O	13.532	16.822	4.713
C	13.406	15.697	13.971	O	11.015	17.335	4.149
C	14.041	14.271	13.838	N	8.303	12.695	7.007
C	14.511	18.639	9.707	C	9.453	13.36	7.579
C	15.315	17.861	8.62	C	8.987	14.208	8.786
C	9.643	18.982	6.62	C	10.08	15.086	9.395
C	8.58	18.95	7.722	C	9.53	16.059	10.426
C	6.965	19.484	9.906	C	10.475	17.219	10.697
C	8.812	20.081	8.536	N	9.8	18.238	11.557
C	7.537	18.061	7.991	C	10.463	12.315	8.012
C	6.728	18.355	9.094	O	11.624	12.317	7.605
C	8.018	20.368	9.647				
E_{QM} = -3036.203527							

Lys109-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	-7.611	14.938	5.644	C	-7.431	8.334	7.928
C	-5.63	13.438	4.22	C	-9.056	9.531	8.997
C	-7.925	13.744	5.003	C	-8.818	8.048	8.578
C	-6.32	15.431	5.458	C	-6.751	9.057	9.093
C	-5.348	14.697	4.758	C	-6.094	10.771	11.187
C	-6.951	13.006	4.311	C	-5.421	9.17	9.471
C	-4.076	15.546	4.761	C	-7.755	9.796	9.755
C	-3.603	15.641	6.218	C	-7.446	10.651	10.806
C	-3.387	16.132	8.938	C	-5.099	10.046	10.527
C	-2.495	15.112	6.893	C	-9.217	12.935	4.949
C	-4.588	16.38	6.905	C	-9.045	12.294	3.536
C	-4.502	16.64	8.272	O	-8.554	15.615	6.383
C	-2.409	15.365	8.268	P	-8.546	15.588	8.027
C	-1.371	14.98	9.33	O	-9.642	14.389	8.312
C	-2.065	14.063	10.343	O	-9.072	16.93	8.459
C	-3.575	13.001	12.431	O	-7.205	15.077	8.552
C	-1.864	12.735	10.701	O	-4.655	12.639	3.691
C	-3.026	14.855	11.008	P	-4.321	12.493	2.065
C	-3.788	14.341	12.048	O	-4.145	10.88	1.953
C	-2.632	12.212	11.762	O	-2.985	13.18	1.846
C	-2.94	16.252	10.396	O	-5.545	12.89	1.266
C	-1.395	16.299	10.168	N	-1.27	9.203	3.95
C	-5.663	16.741	5.883	C	-1.327	10.442	4.696
C	-4.748	16.952	4.632	C	-2.53	10.342	5.676
C	-7.627	11.719	3.844	C	-2.95	11.624	6.407
C	-7.947	10.955	5.131	C	-4.37	11.519	6.963
C	-8.844	10.192	7.635	C	-4.863	12.762	7.689
C	-8.931	11.708	5.81	N	-6.317	12.635	8.045
C	-7.373	9.821	5.709	C	0.002	10.677	5.412
C	-7.851	9.448	6.968	O	0.837	9.779	5.542
C	-9.384	11.355	7.084				
E_{QM} = -3036.196731							

Arg86-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	14.218	-5.975	7.062	C	7.681	-5.803	8.351
C	14.482	-8.136	8.925	C	6.746	-6.907	8.932
C	13.361	-7.076	7.039	C	8.261	-6.201	10.602
C	15.253	-5.998	7.996	C	9.069	-3.621	11.261
C	15.395	-7.081	8.885	C	8.775	-5.967	11.87
C	13.469	-8.129	7.961	C	8.154	-5.154	9.658
C	16.669	-6.826	9.691	C	8.548	-3.86	9.973
C	16.395	-5.61	10.572	C	9.183	-4.658	12.192
C	15.87	-3.095	11.594	C	12.201	-7.417	6.102
C	16.289	-5.482	11.958	C	12.389	-8.965	6.062
C	16.231	-4.509	9.708	O	13.974	-4.931	6.202
C	15.955	-3.232	10.206	P	14.994	-4.297	5.065
C	16.027	-4.202	12.454	O	13.901	-3.986	3.896
C	15.779	-3.688	13.876	O	16.001	-5.331	4.607
C	14.295	-3.309	13.912	O	15.489	-2.945	5.546
C	11.777	-2.198	13.482	O	14.588	-9.115	9.89
C	13.195	-3.886	14.534	P	15.261	-10.588	9.553
C	14.144	-2.19	13.061	O	16.822	-10.204	9.224
C	12.893	-1.626	12.836	O	14.653	-11.145	8.294
C	11.927	-3.313	14.312	O	15.185	-11.366	10.859
C	15.534	-1.892	12.484	N	10.737	-0.059	4.906
C	16.399	-2.262	13.732	C	10.835	-1.486	5.2
C	16.419	-5.044	8.28	C	11.162	-1.674	6.708
C	17.513	-6.125	8.575	C	11.233	-3.13	7.185
C	12.354	-9.125	7.614	C	11.871	-3.299	8.562
C	11.022	-8.42	7.879	N	11.751	-4.693	8.971
C	8.868	-6.671	7.925	C	12.269	-5.225	10.082
C	10.929	-7.364	6.945	N	13.049	-4.506	10.896
C	10.036	-8.619	8.852	N	12.001	-6.489	10.406
C	8.962	-7.719	8.863	C	9.64	-2.355	4.802
C	9.853	-6.473	6.951	O	9.802	-3.436	4.234
C	7.84	-7.488	9.88				
E_{QM} = -3145.733993							

Arg95-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	-0.42	-9.732	17.488	C	-6.038	-13.347	15.939
C	0.082	-9.509	14.672	C	-6.848	-13.194	14.609
C	-1.429	-9.384	16.586	C	-4.976	-14.552	14.217
C	0.858	-9.924	16.956	C	-4.216	-16.777	15.711
C	1.096	-9.828	15.572	C	-4.272	-15.569	13.585
C	-1.185	-9.277	15.208	C	-5.285	-14.629	15.593
C	2.559	-10.191	15.347	C	-4.921	-15.735	16.35
C	2.675	-11.67	15.718	C	-3.892	-16.692	14.351
C	2.785	-14.106	17.017	C	-2.918	-9.121	16.792
C	2.887	-12.813	14.936	C	-3.126	-8.052	15.672
C	2.483	-11.752	17.115	O	-0.691	-9.989	18.806
C	2.55	-12.969	17.792	P	-0.784	-8.839	20.016
C	2.935	-14.039	15.617	O	-1.837	-9.615	20.986
C	3.079	-15.487	15.131	O	-1.396	-7.567	19.464
C	1.729	-16.158	15.406	O	0.547	-8.793	20.735
C	-0.582	-17.218	16.55	O	0.308	-9.468	13.312
C	0.734	-16.646	14.571	P	1.044	-8.16	12.607
C	1.583	-16.208	16.812	O	0.608	-8.431	11.067
C	0.433	-16.721	17.396	O	2.554	-8.323	12.651
C	-0.428	-17.192	15.158	O	0.4	-6.898	13.137
C	2.85	-15.584	17.4	N	-1.677	-12.359	9.194
C	3.884	-16.072	16.336	C	-0.855	-12.184	10.386
C	2.189	-10.328	17.6	C	-1.367	-13.046	11.572
C	3.153	-9.56	16.644	C	-0.636	-12.761	12.895
C	-2.523	-8.956	14.549	C	-1.209	-13.533	14.074
C	-3.411	-10.19	14.749	N	-0.599	-13.118	15.334
C	-5.055	-12.184	15.753	C	-1.141	-13.424	16.519
C	-3.661	-10.289	16.137	N	-2.222	-14.208	16.584
C	-3.948	-11.11	13.847	N	-0.636	-12.947	17.657
C	-4.784	-12.101	14.373	C	0.591	-12.516	10.082
C	-4.472	-11.297	16.664	O	1.464	-11.649	10.059
C	-5.569	-13.236	13.708				
E_{QM} = -3145.734168							

Arg64-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	-9.088	-11.867	9.839	C	-2.977	-13.629	11.938
C	-10.293	-13.568	11.814	C	-2.564	-14.049	13.384
C	-8.66	-11.855	11.167	C	-3.503	-15.9	12.303
C	-10.149	-12.718	9.534	C	-2.778	-16.873	9.796
C	-10.743	-13.559	10.488	C	-3.628	-17.259	12.053
C	-9.227	-12.717	12.124	C	-3.028	-15.019	11.305
C	-11.863	-14.314	9.754	C	-2.671	-15.488	10.045
C	-11.172	-15.211	8.718	C	-3.251	-17.743	10.784
C	-9.644	-16.217	6.621	C	-7.583	-11.044	11.885
C	-11.034	-16.6	8.609	C	-8.256	-10.939	13.292
C	-10.566	-14.347	7.776	O	-8.468	-11.16	8.839
C	-9.796	-14.829	6.715	P	-8.677	-9.543	8.56
C	-10.247	-17.088	7.551	O	-7.588	-9.478	7.357
C	-9.728	-18.494	7.223	O	-8.187	-8.746	9.753
C	-8.228	-18.444	7.547	O	-10.092	-9.298	8.034
C	-5.515	-17.821	7.695	O	-10.87	-14.335	12.794
C	-7.47	-18.991	8.574	P	-12.423	-14.07	13.348
C	-7.643	-17.579	6.596	O	-13.025	-15.575	13.119
C	-6.289	-17.27	6.653	O	-13.163	-13.131	12.417
C	-6.1	-18.667	8.643	O	-12.334	-13.745	14.826
C	-8.78	-17.083	5.699	N	-5.406	-13.108	5.118
C	-9.65	-18.379	5.667	C	-5.581	-12.051	6.101
C	-10.893	-12.927	8.221	C	-5.514	-12.593	7.559
C	-12.323	-13.166	8.798	C	-6.547	-13.7	7.827
C	-8.463	-12.481	13.432	C	-6.513	-14.238	9.252
C	-7.011	-12.933	13.179	N	-7.555	-15.246	9.455
C	-4.417	-13.206	12.226	C	-7.606	-16.086	10.495
C	-6.484	-12.041	12.221	N	-6.585	-16.192	11.345
C	-6.231	-13.976	13.691	N	-8.696	-16.846	10.69
C	-4.916	-14.084	13.21	C	-4.708	-10.812	5.849
C	-5.193	-12.168	11.714	O	-4.397	-10.034	6.753
C	-3.764	-15.044	13.545				
E_{QM} = -3145.721281							

Arg22-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	-16.295	-6.974	-20.35	C	-14.951	-4.663	-14.299
C	-18.637	-8.194	-19.221	C	-15.959	-4.463	-13.122
C	-17.219	-6.24	-19.601	C	-15.589	-6.765	-13.445
C	-16.582	-8.329	-20.544	C	-13.143	-8.061	-13.739
C	-17.731	-8.926	-19.991	C	-15.5	-8.105	-13.089
C	-18.361	-6.841	-19.048	C	-14.471	-6.075	-13.965
C	-17.701	-10.394	-20.409	C	-13.245	-6.707	-14.121
C	-16.498	-11.024	-19.703	C	-14.251	-8.749	-13.235
C	-13.987	-11.864	-18.937	C	-17.209	-4.789	-19.116
C	-16.413	-12.004	-18.712	C	-18.748	-4.529	-19.1
C	-15.347	-10.44	-20.275	O	-15.167	-6.379	-20.862
C	-14.067	-10.841	-19.885	P	-15.242	-5.763	-22.413
C	-15.135	-12.449	-18.371	O	-13.714	-5.194	-22.532
C	-14.641	-13.574	-17.446	O	-16.191	-4.589	-22.43
C	-13.911	-12.911	-16.281	O	-15.438	-6.908	-23.391
C	-12.216	-11.423	-14.651	O	-19.792	-8.721	-18.678
C	-14.168	-12.862	-14.916	P	-19.813	-9.888	-17.515
C	-12.787	-12.261	-16.835	O	-21.23	-9.559	-16.798
C	-11.945	-11.498	-16.034	O	-18.666	-9.628	-16.542
C	-13.299	-12.112	-14.095	O	-19.985	-11.239	-18.186
C	-12.785	-12.586	-18.332	N	-10.771	-7.103	-20.348
C	-13.388	-14.028	-18.268	C	-11.429	-6.144	-19.468
C	-15.84	-9.425	-21.312	C	-11.252	-6.483	-17.962
C	-17.084	-10.215	-21.835	C	-11.948	-7.769	-17.493
C	-19.061	-5.775	-18.213	C	-13.474	-7.698	-17.516
C	-18.1	-5.509	-17.052	N	-14.008	-8.895	-16.878
C	-15.95	-4.841	-15.446	C	-15.304	-9.114	-16.628
C	-16.964	-4.882	-17.606	N	-16.247	-8.295	-17.088
C	-18.16	-5.863	-15.704	N	-15.647	-10.165	-15.878
C	-17.068	-5.51	-14.912	C	-10.83	-4.766	-19.726
C	-15.867	-4.535	-16.809	O	-9.666	-4.699	-20.131
C	-16.753	-5.771	-13.439				
E_{QM} = -3145.691							

Arg159-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	14.086	-13.991	-1.629	C	13.624	-8.272	1.638
C	16.136	-14.862	0.159	C	14.025	-7.925	3.106
C	13.941	-13.889	-0.246	C	15.976	-8.263	1.837
C	15.281	-14.539	-2.099	C	16.576	-7.371	-0.731
C	16.281	-14.989	-1.223	C	17.31	-8.131	1.468
C	14.967	-14.271	0.633	C	14.941	-7.931	0.936
C	17.372	-15.625	-2.088	C	15.224	-7.487	-0.349
C	18.008	-14.494	-2.899	C	17.604	-7.681	0.164
C	18.538	-12.384	-4.608	C	12.786	-13.393	0.622
C	19.3	-13.96	-2.889	C	12.975	-14.349	1.845
C	17.008	-14.008	-3.767	O	13.1	-13.564	-2.482
C	17.25	-12.931	-4.629	P	11.937	-14.565	-3.129
C	19.555	-12.911	-3.779	O	10.622	-13.631	-2.897
C	20.809	-12.061	-4.028	O	11.87	-15.836	-2.301
C	20.494	-10.679	-3.45	O	12.152	-14.655	-4.626
C	19.416	-8.187	-2.85	O	17.048	-15.416	1.033
C	21.005	-9.974	-2.367	P	18.404	-14.601	1.515
C	19.45	-10.146	-4.24	O	17.791	-13.682	2.725
C	18.888	-8.912	-3.938	O	18.903	-13.703	0.405
C	20.461	-8.707	-2.079	O	19.297	-15.691	2.075
C	19.153	-11.181	-5.329	N	13.23	-10.307	-6.329
C	20.594	-11.736	-5.54	C	12.438	-10.833	-5.24
C	15.757	-14.859	-3.515	C	12.978	-10.362	-3.864
C	16.455	-16.224	-3.21	C	14.451	-10.727	-3.65
C	14.47	-13.972	2.052	C	14.918	-10.554	-2.215
C	14.312	-12.45	2.152	N	16.329	-10.922	-2.131
C	13.638	-9.797	1.732	C	17.005	-11.163	-1.005
C	13.28	-12.096	1.253	N	16.401	-11.111	0.182
C	15.015	-11.48	2.871	N	18.312	-11.452	-1.043
C	14.662	-10.144	2.642	C	10.994	-10.397	-5.396
C	12.931	-10.765	1.011	O	10.676	-9.455	-6.126
C	15.297	-8.824	3.093				
E_{QM} = -3145.678023							

Arg53-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	-3.823	-3.845	-21.248	C	0.395	-8.996	-21.586
C	-3.185	-3.588	-18.464	C	1.537	-9.39	-20.601
C	-2.501	-3.849	-20.798	C	-0.534	-9.676	-19.524
C	-4.818	-3.652	-20.283	C	-2.865	-10.837	-20.511
C	-4.503	-3.507	-18.919	C	-1.459	-10.189	-18.622
C	-2.194	-3.741	-19.432	C	-0.766	-9.739	-20.917
C	-5.82	-3.232	-18.191	C	-1.922	-10.319	-21.423
C	-6.657	-4.505	-18.293	C	-2.64	-10.772	-19.131
C	-8.215	-6.635	-19.131	C	-1.164	-3.924	-21.548
C	-7.096	-5.411	-17.322	C	-0.329	-2.984	-20.622
C	-6.988	-4.658	-19.66	O	-4.111	-4.02	-22.578
C	-7.785	-5.721	-20.1	P	-4.395	-2.698	-23.564
C	-7.873	-6.487	-17.771	O	-4.076	-3.391	-24.999
C	-8.474	-7.689	-17.035	O	-3.388	-1.613	-23.236
C	-7.704	-8.911	-17.549	O	-5.876	-2.378	-23.546
C	-6.559	-10.936	-19.084	O	-2.855	-3.519	-17.119
C	-6.797	-9.776	-16.951	P	-2.579	-2.055	-16.399
C	-8.044	-9.053	-18.914	O	-1.709	-2.566	-15.092
C	-7.475	-10.052	-19.695	O	-3.889	-1.476	-15.908
C	-6.225	-10.802	-17.732	O	-1.657	-1.212	-17.26
C	-9.028	-7.926	-19.242	N	-4.671	-8.128	-13.518
C	-9.782	-7.857	-17.876	C	-3.639	-7.148	-13.828
C	-6.34	-3.49	-20.406	C	-3.087	-7.288	-15.285
C	-6.534	-2.399	-19.306	C	-4.087	-7.069	-16.436
C	-0.672	-3.783	-19.323	C	-3.44	-7.155	-17.818
C	-0.26	-5.186	-19.773	N	-4.427	-6.98	-18.883
C	0.201	-7.53	-21.178	C	-4.126	-7.089	-20.182
C	-0.527	-5.261	-21.159	N	-5.068	-6.943	-21.124
C	0.205	-6.292	-19.057	N	-2.889	-7.379	-20.576
C	0.427	-7.47	-19.785	C	-4.048	-5.702	-13.562
C	-0.276	-6.423	-21.89	O	-4.994	-5.167	-14.138
C	0.771	-8.895	-19.336				
E_{QM} = -3145.66574							

Arg113-TWEEZERS:

Atomic Symbol	x	y	z	Atomic Symbol	x	y	z
C	-18.096	-3.344	16.979	C	-13.404	-6.893	13.664
C	-19.711	-5.693	16.973	C	-13.351	-8.456	13.623
C	-17.583	-4.579	17.394	C	-15.068	-7.7	12.206
C	-19.454	-3.297	16.637	C	-14.822	-5.79	10.197
C	-20.25	-4.454	16.648	C	-15.91	-7.774	11.106
C	-18.382	-5.732	17.373	C	-14.124	-6.657	12.332
C	-21.669	-4.035	16.292	C	-13.988	-5.704	11.33
C	-21.665	-3.556	14.843	C	-15.779	-6.804	10.091
C	-21.577	-2.008	12.555	C	-16.173	-5.039	17.809
C	-22.346	-4.026	13.718	C	-16.579	-6.184	18.792
C	-20.891	-2.378	14.81	O	-17.277	-2.262	16.83
C	-20.825	-1.586	13.659	P	-16.962	-1.032	17.896
C	-22.292	-3.224	12.573	O	-17.712	0.168	17.059
C	-22.999	-3.338	11.22	O	-15.469	-0.799	17.868
C	-21.91	-3.442	10.147	O	-17.686	-1.312	19.199
C	-19.858	-2.965	8.317	O	-20.458	-6.862	16.908
C	-21.517	-4.471	9.297	P	-20.532	-7.696	15.475
C	-21.256	-2.19	10.114	O	-21.948	-7.203	14.832
C	-20.247	-1.934	9.195	O	-20.59	-9.155	15.88
C	-20.475	-4.219	8.381	O	-19.453	-7.222	14.525
C	-21.893	-1.337	11.207	N	-15.712	-0.669	8.377
C	-23.369	-1.831	11.042	C	-15.031	-1.211	9.54
C	-20.385	-2.144	16.241	C	-15.892	-2.304	10.22
C	-21.671	-2.634	16.993	C	-17.14	-1.736	10.91
C	-17.49	-6.906	17.747	C	-18.088	-2.795	11.454
C	-16.496	-7.038	16.592	N	-17.473	-3.529	12.548
C	-14.441	-6.721	14.779	C	-18.074	-4.568	13.136
C	-15.651	-5.913	16.663	N	-19.296	-4.954	12.754
C	-16.389	-7.974	15.563	N	-17.459	-5.251	14.104
C	-15.345	-7.792	14.655	C	-13.689	-1.799	9.138
C	-14.59	-5.748	15.771	O	-13.601	-2.622	8.229
C	-14.898	-8.599	13.435				
E_{QM} = -3145.622101							

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