**Supporting Information**

*Article*

# Investigation of the Molecular Details of the Interactions of Selenoglycosides and Human Galectin-3

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**Figure S1.** Chemical shift mapping for SeDG by $^{15}N$-$^{1}H$ HSQC NMR titration.

**Figure S2.** $^{15}N$-$^{1}H$ HSQC NMR titration for DSeDG.

**Figure S3.** Determination of $K_d$ values in the NMR titrations.

**Table S1.** Crystallographic data and refinement statistics.

**Table S2.** Energetic decomposition of binding enthalpy terms in MMGBSA and MMPBSA calculations.

**Figure S4.** The evolution of the C1-Se-Se-C1′ central dihedral angle in the DSeDG – hGal3 complex.

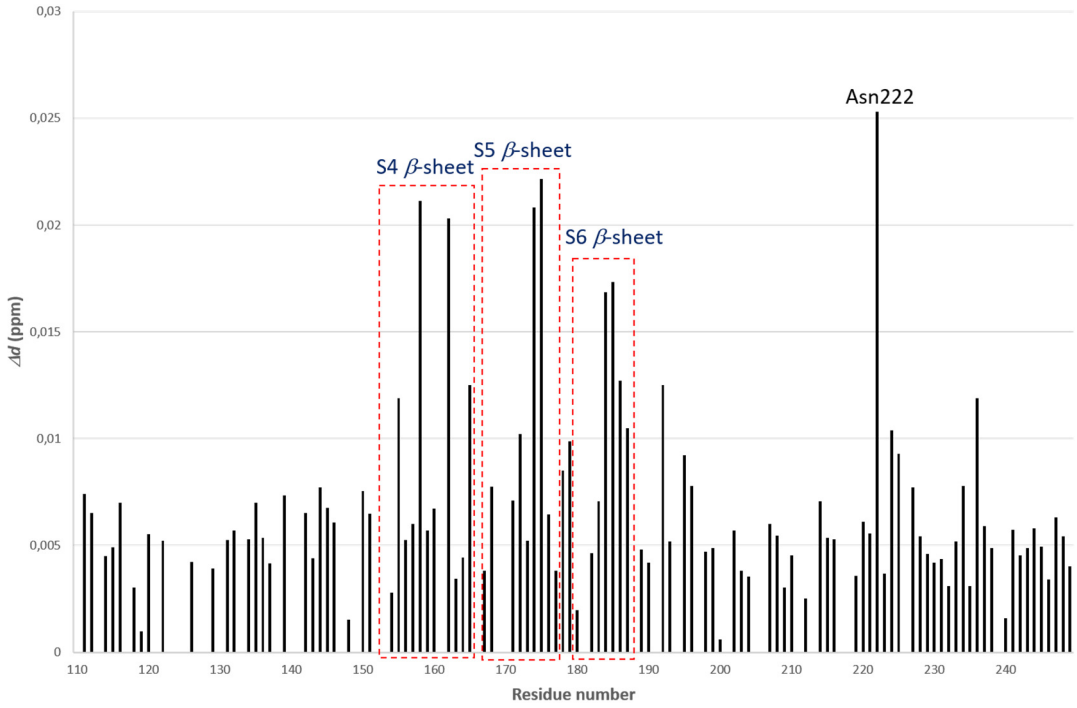



**Figure S1.** Euclidean weighted $^{15}$N- and $^{1}$H chemical shift changes ($\Delta d$) of *h*Gal-3 (CRD) determined between the end-points of titration with SeDG. $\Delta d$ values are plotted as a function of residue number of *h*Gal-3 (CRD).

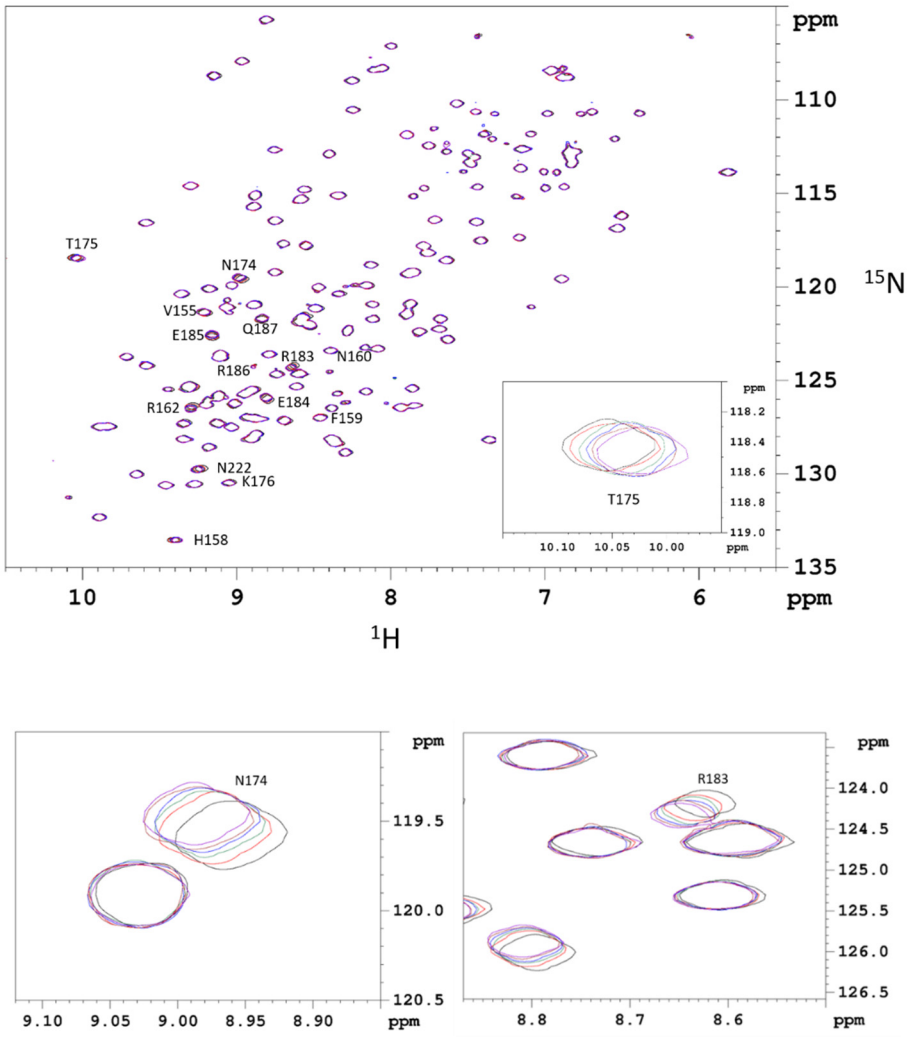
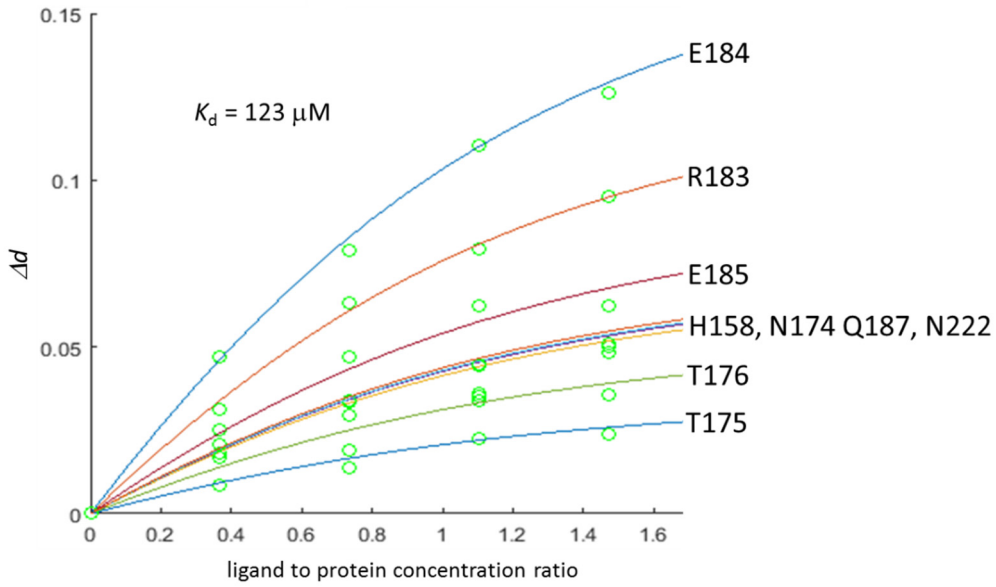



**Figure S2.** Overlay of $^{15}$N-$^{1}$H HSQC spectra for 0.27 mM $^{15}$N-labeled *h*Gal-3 (CRD) obtained upon titration with DSeDG (cc. of ligand: 0.0, 0.5, 1.0, 1.5, 2.0, and 2.5 mM). Cross peaks in black correspond to the reference HSQC-spectrum recorded in the absence of ligand DSeDG, while cross peaks in purple belong to the $^{15}$N-$^{1}$H correlation map acquired in the last titration step. Cross peaks showing the largest shifts upon complex formation are assigned. The expansions of Thr175, Asn174 (subsite *C*) and Arg183 (subsite *D*) cross peaks with the most shifted $^{15}$N- and $^{1}$H resonances are shown in the inset and below the full spectrum, respectively.

(A)




*(B)*

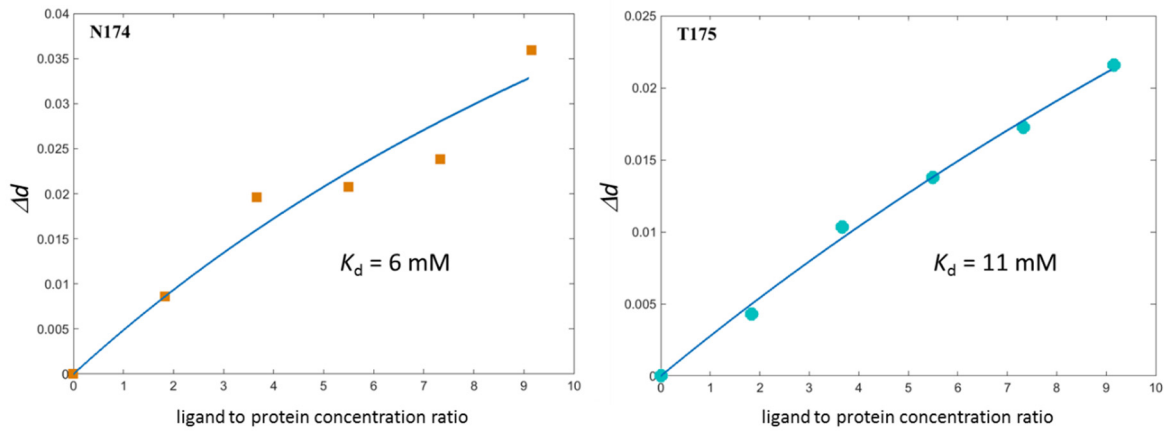



**Figure S3.** Evaluation of $K_d$ based on $^{15}N$,$^{1}H$ chemical shift changes for *h*Gal-3 (CRD) induced by adding ligand *(A)* SeDG and *(B)* DSeDG. $^{15}N$- and $^{1}H$ Euclidean weighted chemical shift changes (Δd) are plotted as a function of ligand to protein concentration ratio (A) for the 9 most affected residues and (B) the most shifted Asn174 and Thr175 residues. For fitting of binding curves the Optimization Toolbox of Matlab R2015a was used. During iterations the difference between the observed ($\Delta d_{obs}$) and calculated ($\Delta d_{calc}$) Δds was minimized with varying the values of $K_d$ and $\Delta d_{max}$.

**Table S1.** Crystallographic data and refinement statistics of *h*Gal-3 CRD structures with bound SeDG and DSeDG.

| Parameters | **hGal-3 CRD in complex with SeDG** | **hGal-3 CRD in complex with DSeDG** |
|---|---|---|
| Data collection | | |
| Resolution range (Å) | 30.84 - 1.96 (2.03 - 1.96) | 31.53 - 2.0 (2.07 - 2.0) |
| Space group | $P2_12_12_1$ | $P2_12_12_1$ |
| Unit cell | $a$ = 36.41, $b$ = 58.03, $c$ = 63.53 | $a$ = 34.90, $b$ = 58.36, $c$ = 63.05 |
| Total reflections | 39129 | 55226 |
| Unique reflections | 9282 (833) | 9123 (884) |
| Multiplicity | 4.2 | 6.0 |
| Completeness (%) | 91.46 (83.05) | 99.5 (97.6) |
| Mean I/sigma(I) | 20.54 (5.45) | 11.0 (7.9) |
| Wilson B-factor | 17.01 | 19.27 |
| R-merge (%) | 6.2 (13.9) | 13.3 (20.0) |
| CC (1/2) [%] | 99.9 (94.4) | 98.4 (96.9) |
| Refinement Statistics | | |
| R-work (%) | 15.82 (18.10) | 17.91 (15.59) |
| R-free (%) | 18.72 (24.11) | 23.09 (25.40) |
| RMS deviations | | |
| RMS (bonds) | 0.014 | 0.138 |
| RMS (angles) | 1.89 | 3.88 |
| Ramachandran plot statistics (%) | | |
| Favoured | 98.54 | 97.81 |
| Allowed | 1.46 | 2.19 |
| Outliers | 0.00 | 0.00 |
| PDB ID | 7RDP | 7RDO |

**Table S2.** Energy decomposition of the binding enthalpy according to MMGBSA and MMPBSA calculations. Residues with large negative contributions are highlighted in red, residues with large positive contributions are shown in green.

a) SeDGal

| | Res | VDW | Eel | PB | NPOL | **TOTAL** | VDW | Eel | PB | NPOL | **TOTAL** |
|---|---|---|---|---|---|---|---|---|---|---|---|
| SEG | 112 | -13.04 | -15.21 | 19.56 | -2.29 | **-10.98** | -13.04 | -15.21 | 13.34 | 0.00 | **-14.91** |
| GLY | 112 | 0.00 | 0.02 | -0.01 | 0.00 | **0.01** | 0.00 | 0.02 | -0.03 | 0.00 | **-0.01** |
| PRO | 113 | 0.00 | -0.01 | 0.01 | 0.00 | **0.00** | 0.00 | -0.01 | 0.01 | 0.00 | **0.00** |
| LEU | 114 | 0.00 | 0.00 | 0.00 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| ILE | 115 | 0.00 | -0.01 | 0.02 | 0.00 | **0.01** | 0.00 | -0.01 | 0.01 | 0.00 | **0.00** |
| VAL | 116 | -0.02 | 0.01 | 0.02 | 0.00 | **0.00** | -0.02 | 0.01 | 0.00 | 0.00 | **-0.01** |
| PRO | 117 | -0.05 | 0.03 | 0.01 | -0.01 | **-0.02** | -0.05 | 0.03 | -0.02 | 0.00 | **-0.05** |
| TYR | 118 | -0.01 | -0.03 | 0.03 | 0.00 | **-0.01** | -0.01 | -0.03 | 0.03 | 0.00 | **0.00** |
| ASN | 119 | -0.01 | 0.01 | 0.02 | 0.00 | **0.02** | -0.01 | 0.01 | -0.01 | 0.00 | **-0.01** |
| LEU | 120 | 0.00 | 0.00 | 0.01 | 0.00 | **0.00** | 0.00 | 0.00 | 0.01 | 0.00 | **0.00** |
| PRO | 121 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| LEU | 122 | 0.00 | 0.00 | 0.01 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| PRO | 123 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| GLY | 124 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| GLY | 125 | 0.00 | 0.00 | 0.00 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| VAL | 126 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| VAL | 127 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| PRO | 128 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.01 | 0.00 | **0.00** |
| ARG | 129 | 0.00 | -0.03 | 0.03 | 0.00 | **0.00** | 0.00 | -0.03 | 0.02 | 0.00 | **-0.01** |
| MET | 130 | 0.00 | 0.01 | 0.00 | 0.00 | **0.00** | 0.00 | 0.01 | -0.01 | 0.00 | **0.00** |
| LEU | 131 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| ILE | 132 | 0.00 | 0.01 | 0.00 | 0.00 | **0.01** | 0.00 | 0.01 | -0.01 | 0.00 | **0.00** |
| THR | 133 | 0.00 | 0.00 | 0.02 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| ILE | 134 | 0.00 | 0.01 | 0.00 | 0.00 | **0.01** | 0.00 | 0.01 | -0.01 | 0.00 | **0.00** |
| LEU | 135 | 0.00 | 0.00 | 0.01 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| GLY | 136 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| THR | 137 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| VAL | 138 | 0.00 | -0.01 | 0.04 | 0.00 | **0.02** | 0.00 | -0.01 | 0.02 | 0.00 | **0.01** |
| LYS | 139 | -0.01 | -0.05 | 0.08 | 0.00 | **0.02** | -0.01 | -0.05 | 0.05 | 0.00 | **0.00** |
| PRO | 140 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | -0.01 | 0.00 | **0.00** |
| ASN | 141 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| ALA | 142 | -0.01 | -0.01 | 0.04 | 0.00 | **0.03** | -0.01 | -0.01 | 0.03 | 0.00 | **0.01** |
| ASN | 143 | -0.04 | 0.03 | 0.01 | 0.00 | **0.00** | -0.04 | 0.03 | -0.02 | 0.00 | **-0.03** |
| ARG | 144 | -0.63 | -1.12 | 1.32 | -0.14 | **-0.56** | -0.63 | -1.12 | 1.80 | 0.00 | **0.05** |
| ILE | 145 | -0.19 | 0.12 | -0.19 | 0.00 | **-0.26** | -0.19 | 0.12 | -0.24 | 0.00 | **-0.31** |
| ALA | 146 | -0.53 | -0.08 | -0.02 | -0.08 | **-0.71** | -0.53 | -0.08 | 0.11 | 0.00 | **-0.50** |
| LEU | 147 | -0.12 | 0.05 | -0.03 | 0.00 | **-0.10** | -0.12 | 0.05 | -0.09 | 0.00 | **-0.16** |
| ASP | 148 | -0.18 | -1.15 | 1.52 | -0.04 | **0.16** | -0.18 | -1.15 | 2.20 | 0.00 | **0.87** |
| PHE | 149 | -0.02 | -0.01 | 0.00 | 0.00 | **-0.03** | -0.02 | -0.01 | 0.01 | 0.00 | **-0.02** |
| GLN | 150 | -0.03 | 0.06 | -0.04 | 0.00 | **-0.01** | -0.03 | 0.06 | -0.09 | 0.00 | **-0.06** |
| ARG | 151 | -0.01 | 0.03 | 0.01 | 0.00 | **0.03** | -0.01 | 0.03 | -0.03 | 0.00 | **0.00** |
| GLY | 152 | 0.00 | -0.01 | 0.02 | 0.00 | **0.01** | 0.00 | -0.01 | 0.01 | 0.00 | **0.00** |
| ASN | 153 | -0.01 | -0.03 | 0.06 | 0.00 | **0.02** | -0.01 | -0.03 | 0.03 | 0.00 | **-0.01** |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ASP | 154 | -0.01 | -0.11 | 0.08 | 0.00 | **-0.04** | -0.01 | -0.11 | 0.10 | 0.00 | **-0.02** |
| VAL | 155 | -0.14 | 0.02 | -0.14 | -0.01 | **-0.28** | -0.14 | 0.02 | -0.02 | 0.00 | **-0.14** |
| ALA | 156 | -0.01 | 0.02 | -0.01 | 0.00 | **0.00** | -0.01 | 0.02 | -0.03 | 0.00 | **-0.01** |
| PHE | 157 | -0.05 | -0.06 | -0.05 | 0.00 | **-0.17** | -0.05 | -0.06 | 0.08 | 0.00 | **-0.04** |
| HIE | 158 | -1.62 | -1.54 | 1.54 | -0.18 | **-1.80** | -1.62 | -1.54 | 2.02 | 0.00 | **-1.14** |
| PHE | 159 | -0.18 | -0.04 | -0.14 | 0.00 | **-0.36** | -0.18 | -0.04 | -0.02 | 0.00 | **-0.23** |
| ASN | 160 | -1.27 | 0.11 | -0.25 | -0.07 | **-1.48** | -1.27 | 0.11 | 0.15 | 0.00 | **-1.01** |
| PRO | 161 | -0.07 | 0.09 | 0.08 | 0.00 | **0.10** | -0.07 | 0.09 | -0.19 | 0.00 | **-0.17** |
| ARG | 162 | -1.10 | -3.71 | 3.60 | -0.26 | **-1.48** | -1.10 | -3.71 | 3.89 | 0.00 | **-0.92** |
| PHE | 163 | -0.02 | -0.02 | 0.04 | 0.00 | **0.00** | -0.02 | -0.02 | 0.04 | 0.00 | **0.00** |
| ASN | 164 | -0.01 | -0.03 | 0.08 | 0.00 | **0.04** | -0.01 | -0.03 | 0.04 | 0.00 | **0.00** |
| GLU | 165 | -0.08 | 0.45 | -0.43 | 0.00 | **-0.06** | -0.08 | 0.45 | -0.54 | 0.00 | **-0.17** |
| ASN | 166 | -0.01 | -0.01 | 0.03 | 0.00 | **0.02** | -0.01 | -0.01 | 0.01 | 0.00 | **-0.01** |
| ASN | 167 | 0.00 | -0.01 | 0.03 | 0.00 | **0.02** | 0.00 | -0.01 | 0.01 | 0.00 | **0.00** |
| ARG | 168 | -0.01 | -0.12 | 0.18 | 0.00 | **0.05** | -0.01 | -0.12 | 0.14 | 0.00 | **0.01** |
| ARG | 169 | -0.01 | -0.20 | 0.25 | 0.00 | **0.05** | -0.01 | -0.20 | 0.23 | 0.00 | **0.02** |
| VAL | 170 | -0.02 | 0.04 | -0.08 | 0.00 | **-0.07** | -0.02 | 0.04 | -0.06 | 0.00 | **-0.05** |
| ILE | 171 | -0.04 | -0.05 | -0.09 | 0.00 | **-0.18** | -0.04 | -0.05 | 0.07 | 0.00 | **-0.02** |
| VAL | 172 | -0.76 | 0.00 | -0.25 | -0.04 | **-1.04** | -0.76 | 0.00 | 0.23 | 0.00 | **-0.53** |
| CYS | 173 | -0.30 | -0.11 | -0.19 | 0.00 | **-0.61** | -0.30 | -0.11 | 0.13 | 0.00 | **-0.28** |
| ASN | 174 | -0.70 | -1.79 | 0.25 | -0.06 | **-2.30** | -0.70 | -1.79 | 1.41 | 0.00 | **-1.07** |
| THR | 175 | -0.10 | 0.09 | -0.14 | 0.00 | **-0.16** | -0.10 | 0.09 | -0.09 | 0.00 | **-0.10** |
| LYS | 176 | -0.18 | 0.37 | -0.04 | -0.01 | **0.14** | -0.18 | 0.37 | -0.02 | 0.00 | **0.16** |
| LEU | 177 | -0.01 | -0.01 | 0.03 | 0.00 | **0.01** | -0.01 | -0.01 | 0.00 | 0.00 | **-0.02** |
| ASP | 178 | -0.01 | -0.07 | 0.09 | 0.00 | **0.02** | -0.01 | -0.07 | 0.06 | 0.00 | **-0.02** |
| ASN | 179 | -0.03 | -0.03 | 0.11 | 0.00 | **0.05** | -0.03 | -0.03 | 0.04 | 0.00 | **-0.02** |
| ASN | 180 | -0.07 | 0.02 | 0.03 | 0.00 | **-0.02** | -0.07 | 0.02 | 0.02 | 0.00 | **-0.03** |
| TRP | 181 | -3.03 | -0.70 | 1.16 | -0.38 | **-2.95** | -3.03 | -0.70 | 0.86 | 0.00 | **-2.87** |
| GLY | 182 | -0.15 | -0.11 | 0.25 | -0.01 | **-0.03** | -0.15 | -0.11 | 0.22 | 0.00 | **-0.05** |
| ARG | 183 | -0.15 | 0.03 | -0.08 | -0.01 | **-0.21** | -0.15 | 0.03 | 0.02 | 0.00 | **-0.10** |
| GLU | 184 | -0.15 | -5.98 | 5.89 | -0.12 | **-0.36** | -0.15 | -5.98 | 7.31 | 0.00 | **1.18** |
| GLU | 185 | -0.06 | 0.24 | -0.21 | 0.00 | **-0.02** | -0.06 | 0.24 | -0.31 | 0.00 | **-0.12** |
| ARG | 186 | -0.15 | 0.14 | 0.01 | -0.01 | **-0.01** | -0.15 | 0.14 | -0.05 | 0.00 | **-0.05** |
| GLN | 187 | -0.01 | 0.01 | 0.01 | 0.00 | **0.01** | -0.01 | 0.01 | -0.02 | 0.00 | **-0.02** |
| SER | 188 | 0.00 | 0.01 | 0.00 | 0.00 | **0.00** | 0.00 | 0.01 | -0.01 | 0.00 | **0.00** |
| VAL | 189 | 0.00 | 0.02 | -0.01 | 0.00 | **0.01** | 0.00 | 0.02 | -0.03 | 0.00 | **-0.01** |
| PHE | 190 | -0.01 | -0.01 | 0.00 | 0.00 | **-0.02** | -0.01 | -0.01 | 0.02 | 0.00 | **0.00** |
| PRO | 191 | 0.00 | -0.01 | 0.01 | 0.00 | **0.00** | 0.00 | -0.01 | 0.01 | 0.00 | **0.00** |
| PHE | 192 | -0.01 | 0.00 | -0.02 | 0.00 | **-0.02** | -0.01 | 0.00 | 0.00 | 0.00 | **0.00** |
| GLU | 193 | 0.00 | 0.14 | -0.13 | 0.00 | **0.01** | 0.00 | 0.14 | -0.14 | 0.00 | **0.00** |
| SER | 194 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| GLY | 195 | 0.00 | -0.01 | 0.01 | 0.00 | **0.00** | 0.00 | -0.01 | 0.01 | 0.00 | **0.00** |
| LYS | 196 | 0.00 | -0.08 | 0.08 | 0.00 | **0.00** | 0.00 | -0.08 | 0.06 | 0.00 | **-0.02** |
| PRO | 197 | 0.00 | 0.01 | 0.00 | 0.00 | **0.00** | 0.00 | 0.01 | -0.01 | 0.00 | **0.00** |
| PHE | 198 | 0.00 | 0.00 | -0.01 | 0.00 | **-0.02** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| LYS | 199 | 0.00 | -0.06 | 0.07 | 0.00 | **0.02** | 0.00 | -0.06 | 0.03 | 0.00 | **-0.02** |
| ILE | 200 | 0.00 | -0.01 | 0.02 | 0.00 | **0.01** | 0.00 | -0.01 | 0.01 | 0.00 | **0.00** |
| GLN | 201 | 0.00 | 0.01 | 0.00 | 0.00 | **0.01** | 0.00 | 0.01 | -0.01 | 0.00 | **0.00** |
| VAL | 202 | 0.00 | -0.01 | 0.02 | 0.00 | **0.01** | 0.00 | -0.01 | 0.01 | 0.00 | **0.00** |
| LEU | 203 | 0.00 | 0.01 | 0.00 | 0.00 | **0.00** | 0.00 | 0.01 | -0.01 | 0.00 | **0.00** |
| VAL | 204 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| GLU | 205 | 0.00 | 0.06 | -0.06 | 0.00 | **0.00** | 0.00 | 0.06 | -0.05 | 0.00 | **0.01** |
| PRO | 206 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| ASP | 207 | 0.00 | 0.06 | -0.06 | 0.00 | **0.00** | 0.00 | 0.06 | -0.06 | 0.00 | **0.00** |
| HIE | 208 | 0.00 | 0.00 | 0.02 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| PHE | 209 | 0.00 | 0.01 | -0.02 | 0.00 | **-0.02** | 0.00 | 0.01 | -0.01 | 0.00 | **-0.01** |
| LYS | 210 | 0.00 | -0.09 | 0.10 | 0.00 | **0.01** | 0.00 | -0.09 | 0.08 | 0.00 | **-0.01** |
| VAL | 211 | 0.00 | 0.00 | 0.02 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| ALA | 212 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| VAL | 213 | 0.00 | 0.00 | 0.02 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| ASN | 214 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| ASP | 215 | 0.00 | 0.06 | -0.06 | 0.00 | **0.00** | 0.00 | 0.06 | -0.04 | 0.00 | **0.02** |
| ALA | 216 | 0.00 | 0.01 | 0.00 | 0.00 | **0.00** | 0.00 | 0.01 | -0.01 | 0.00 | **0.00** |
| HIE | 217 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| LEU | 218 | 0.00 | 0.00 | 0.03 | 0.00 | **0.02** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| LEU | 219 | -0.01 | -0.01 | 0.02 | 0.00 | **0.00** | -0.01 | -0.01 | 0.01 | 0.00 | **0.00** |
| GLN | 220 | 0.00 | 0.01 | 0.02 | 0.00 | **0.02** | 0.00 | 0.01 | -0.01 | 0.00 | **0.00** |
| TYR | 221 | -0.03 | 0.02 | -0.04 | 0.00 | **-0.05** | -0.03 | 0.02 | -0.02 | 0.00 | **-0.02** |
| ASN | 222 | 0.00 | 0.02 | -0.01 | 0.00 | **0.01** | 0.00 | 0.02 | -0.02 | 0.00 | **0.00** |
| HIE | 223 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | -0.01 | 0.00 | **0.00** |
| ARG | 224 | -0.02 | -0.35 | 0.52 | 0.00 | **0.15** | -0.02 | -0.35 | 0.35 | 0.00 | **-0.02** |
| VAL | 225 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| LYS | 226 | 0.00 | -0.04 | 0.05 | 0.00 | **0.00** | 0.00 | -0.04 | 0.04 | 0.00 | **0.00** |
| LYS | 227 | 0.00 | 0.00 | 0.00 | 0.00 | **0.01** | 0.00 | 0.00 | -0.01 | 0.00 | **-0.01** |
| LEU | 228 | 0.00 | 0.00 | 0.01 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| ASN | 229 | 0.00 | 0.00 | 0.01 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| GLU | 230 | 0.00 | -0.03 | 0.04 | 0.00 | **0.01** | 0.00 | -0.03 | 0.04 | 0.00 | **0.00** |
| ILE | 231 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| SER | 232 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| LYS | 233 | -0.01 | 0.18 | -0.14 | 0.00 | **0.04** | -0.01 | 0.18 | -0.19 | 0.00 | **-0.02** |
| LEU | 234 | -0.01 | 0.00 | -0.03 | 0.00 | **-0.04** | -0.01 | 0.00 | -0.02 | 0.00 | **-0.02** |
| GLY | 235 | -0.02 | 0.05 | -0.05 | 0.00 | **-0.02** | -0.02 | 0.05 | -0.03 | 0.00 | **0.00** |
| ILE | 236 | -0.03 | -0.02 | 0.00 | 0.00 | **-0.06** | -0.03 | -0.02 | 0.04 | 0.00 | **-0.02** |
| SER | 237 | -0.29 | -0.05 | 0.18 | -0.05 | **-0.21** | -0.29 | -0.05 | 0.22 | 0.00 | **-0.11** |
| GLY | 238 | -0.13 | -0.10 | 0.14 | -0.02 | **-0.10** | -0.13 | -0.10 | 0.16 | 0.00 | **-0.07** |
| ASP | 239 | -0.05 | 0.18 | -0.17 | 0.00 | **-0.04** | -0.05 | 0.18 | -0.27 | 0.00 | **-0.13** |
| ILE | 240 | -0.02 | 0.00 | 0.02 | 0.00 | **0.00** | -0.02 | 0.00 | 0.01 | 0.00 | **-0.02** |
| ASP | 241 | 0.00 | 0.04 | -0.04 | 0.00 | **0.00** | 0.00 | 0.04 | -0.04 | 0.00 | **-0.01** |
| LEU | 242 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| THR | 243 | 0.00 | 0.00 | 0.01 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| SER | 244 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | -0.01 | 0.00 | **0.00** |
| ALA | 245 | 0.00 | 0.00 | 0.01 | 0.00 | **0.01** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| SER | 246 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| TYR | 247 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| THR | 248 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| MET | 249 | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** | 0.00 | 0.00 | 0.00 | 0.00 | **0.00** |
| ILE | 250 | 0.00 | 0.02 | -0.02 | 0.00 | **0.00** | 0.00 | 0.02 | -0.01 | 0.00 | **0.01** |

b) DSeDGal A binding mode

| | Res. | VDW | Eel | PB | NPOL | TOTAL | VDW | Eel | PB | NPOL | TOTAL |
|---|---|---|---|---|---|---|---|---|---|---|---|
| SES | 112 | -10.45 | -13.36 | 18.19 | -1.93 | -7.54 | -10.45 | -13.36 | 11.97 | 0.00 | -11.84 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| GLY | 112 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 |
| PRO | 113 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LEU | 114 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ILE | 115 | 0.00 | -0.01 | 0.01 | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 | 0.00 | 0.00 |
| VAL | 116 | -0.01 | 0.01 | 0.01 | 0.00 | 0.01 | -0.01 | 0.01 | -0.01 | 0.00 | -0.01 |
| PRO | 117 | -0.02 | 0.01 | 0.00 | 0.00 | -0.02 | -0.02 | 0.01 | -0.01 | 0.00 | -0.03 |
| TYR | 118 | -0.01 | -0.03 | 0.03 | 0.00 | -0.01 | -0.01 | -0.03 | 0.03 | 0.00 | -0.01 |
| ASN | 119 | -0.03 | -0.02 | 0.04 | 0.00 | -0.01 | -0.03 | -0.02 | 0.02 | 0.00 | -0.02 |
| LEU | 120 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 |
| PRO | 121 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | -0.01 |
| LEU | 122 | -0.01 | -0.01 | 0.01 | 0.00 | 0.00 | -0.01 | -0.01 | 0.01 | 0.00 | -0.01 |
| PRO | 123 | -0.02 | -0.01 | 0.01 | 0.00 | -0.02 | -0.02 | -0.01 | 0.01 | 0.00 | -0.01 |
| GLY | 124 | -0.02 | -0.02 | 0.03 | -0.01 | -0.02 | -0.02 | -0.02 | 0.03 | 0.00 | -0.01 |
| GLY | 125 | -0.02 | 0.00 | 0.01 | 0.00 | 0.00 | -0.02 | 0.00 | 0.00 | 0.00 | -0.02 |
| VAL | 126 | -0.02 | 0.01 | -0.01 | 0.00 | -0.01 | -0.02 | 0.01 | 0.00 | 0.00 | 0.00 |
| VAL | 127 | -0.04 | -0.02 | 0.01 | -0.01 | -0.06 | -0.04 | -0.02 | 0.02 | 0.00 | -0.04 |
| PRO | 128 | -0.08 | -0.02 | 0.04 | -0.01 | -0.07 | -0.08 | -0.02 | 0.02 | 0.00 | -0.08 |
| ARG | 129 | -0.01 | -0.04 | 0.04 | 0.00 | 0.00 | -0.01 | -0.04 | 0.03 | 0.00 | -0.01 |
| MET | 130 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LEU | 131 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ILE | 132 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 |
| THR | 133 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ILE | 134 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 |
| LEU | 135 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| GLY | 136 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| THR | 137 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| VAL | 138 | 0.00 | -0.01 | 0.02 | 0.00 | 0.01 | 0.00 | -0.01 | 0.01 | 0.00 | 0.00 |
| LYS | 139 | -0.01 | -0.05 | 0.07 | 0.00 | 0.01 | -0.01 | -0.05 | 0.05 | 0.00 | -0.01 |
| PRO | 140 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 |
| ASN | 141 | -0.03 | -0.01 | 0.03 | -0.01 | -0.01 | -0.03 | -0.01 | 0.03 | 0.00 | 0.00 |
| ALA | 142 | -0.01 | -0.04 | 0.05 | 0.00 | 0.00 | -0.01 | -0.04 | 0.03 | 0.00 | -0.01 |
| ASN | 143 | -0.05 | 0.01 | 0.02 | -0.01 | -0.02 | -0.05 | 0.01 | 0.00 | 0.00 | -0.04 |
| ARG | 144 | -0.28 | -0.58 | 0.74 | -0.06 | -0.18 | -0.28 | -0.58 | 0.84 | 0.00 | -0.02 |
| ILE | 145 | -0.07 | 0.10 | -0.11 | 0.00 | -0.08 | -0.07 | 0.10 | -0.13 | 0.00 | -0.10 |
| ALA | 146 | -0.23 | -0.07 | 0.01 | -0.04 | -0.32 | -0.23 | -0.07 | 0.06 | 0.00 | -0.24 |
| LEU | 147 | -0.10 | 0.08 | -0.04 | 0.00 | -0.06 | -0.10 | 0.08 | -0.05 | 0.00 | -0.06 |
| ASP | 148 | -0.03 | -2.15 | 2.12 | -0.03 | -0.09 | -0.03 | -2.15 | 2.77 | 0.00 | 0.58 |
| PHE | 149 | -0.02 | -0.01 | 0.00 | 0.00 | -0.04 | -0.02 | -0.01 | 0.01 | 0.00 | -0.02 |
| GLN | 150 | -0.12 | 0.05 | -0.01 | -0.02 | -0.10 | -0.12 | 0.05 | -0.04 | 0.00 | -0.12 |
| ARG | 151 | -0.07 | -0.06 | 0.15 | -0.01 | 0.01 | -0.07 | -0.06 | 0.07 | 0.00 | -0.07 |
| GLY | 152 | -0.04 | -0.04 | 0.07 | -0.01 | -0.03 | -0.04 | -0.04 | 0.07 | 0.00 | -0.02 |
| ASN | 153 | -0.09 | -0.25 | 0.26 | -0.03 | -0.11 | -0.09 | -0.25 | 0.27 | 0.00 | -0.07 |
| ASP | 154 | -0.09 | -0.24 | 0.23 | 0.00 | -0.12 | -0.09 | -0.24 | 0.38 | 0.00 | 0.04 |
| VAL | 155 | -0.22 | 0.02 | -0.04 | -0.03 | -0.28 | -0.22 | 0.02 | 0.01 | 0.00 | -0.20 |
| ALA | 156 | -0.02 | 0.03 | 0.00 | 0.00 | 0.02 | -0.02 | 0.03 | -0.04 | 0.00 | -0.03 |
| PHE | 157 | -0.03 | -0.05 | 0.02 | 0.00 | -0.06 | -0.03 | -0.05 | 0.07 | 0.00 | -0.01 |
| HIE | 158 | -0.82 | -0.60 | 0.68 | -0.08 | -0.83 | -0.82 | -0.60 | 0.96 | 0.00 | -0.46 |
| PHE | 159 | -0.07 | -0.01 | -0.03 | 0.00 | -0.12 | -0.07 | -0.01 | 0.02 | 0.00 | -0.07 |
| ASN | 160 | -0.58 | 0.18 | -0.23 | -0.04 | -0.66 | -0.58 | 0.18 | -0.03 | 0.00 | -0.43 |
| PRO | 161 | -0.03 | 0.05 | 0.02 | 0.00 | 0.03 | -0.03 | 0.05 | -0.08 | 0.00 | -0.06 |
| ARG | 162 | -0.56 | -1.92 | 2.19 | -0.12 | -0.42 | -0.56 | -1.92 | 2.10 | 0.00 | -0.38 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| PHE | 163 | -0.02 | -0.03 | 0.03 | 0.00 | -0.02 | -0.02 | -0.03 | 0.03 | 0.00 | -0.02 |
| ASN | 164 | -0.06 | -0.07 | 0.10 | -0.01 | -0.03 | -0.06 | -0.07 | 0.10 | 0.00 | -0.02 |
| GLU | 165 | -0.10 | -0.05 | 0.03 | -0.01 | -0.13 | -0.10 | -0.05 | 0.12 | 0.00 | -0.04 |
| ASN | 166 | -0.09 | -0.07 | 0.13 | -0.02 | -0.05 | -0.09 | -0.07 | 0.13 | 0.00 | -0.03 |
| ASN | 167 | -0.05 | -0.06 | 0.09 | -0.01 | -0.02 | -0.05 | -0.06 | 0.07 | 0.00 | -0.03 |
| ARG | 168 | -0.17 | -0.20 | 0.31 | -0.03 | -0.10 | -0.17 | -0.20 | 0.29 | 0.00 | -0.09 |
| ARG | 169 | -0.06 | -0.23 | 0.27 | -0.01 | -0.02 | -0.06 | -0.23 | 0.26 | 0.00 | -0.03 |
| VAL | 170 | -0.11 | -0.01 | -0.02 | -0.01 | -0.14 | -0.11 | -0.01 | 0.00 | 0.00 | -0.11 |
| ILE | 171 | -0.03 | -0.01 | -0.01 | 0.00 | -0.06 | -0.03 | -0.01 | 0.02 | 0.00 | -0.03 |
| VAL | 172 | -0.30 | -0.02 | -0.06 | -0.02 | -0.39 | -0.30 | -0.02 | 0.07 | 0.00 | -0.25 |
| CYS | 173 | -0.08 | -0.01 | -0.02 | 0.00 | -0.11 | -0.08 | -0.01 | 0.04 | 0.00 | -0.05 |
| ASN | 174 | -0.33 | -0.68 | 0.28 | -0.03 | -0.77 | -0.33 | -0.68 | 0.53 | 0.00 | -0.48 |
| THR | 175 | -0.15 | 0.00 | 0.01 | -0.01 | -0.14 | -0.15 | 0.00 | 0.00 | 0.00 | -0.14 |
| LYS | 176 | -0.26 | -0.40 | 0.69 | -0.03 | 0.00 | -0.26 | -0.40 | 0.72 | 0.00 | 0.06 |
| LEU | 177 | -0.26 | -0.13 | 0.14 | -0.03 | -0.27 | -0.26 | -0.13 | 0.18 | 0.00 | -0.20 |
| ASP | 178 | -0.06 | -0.58 | 0.66 | -0.02 | 0.00 | -0.06 | -0.58 | 0.79 | 0.00 | 0.14 |
| ASN | 179 | -0.08 | -0.01 | 0.09 | -0.01 | -0.01 | -0.08 | -0.01 | 0.06 | 0.00 | -0.03 |
| ASN | 180 | -0.13 | -0.26 | 0.21 | -0.02 | -0.20 | -0.13 | -0.26 | 0.19 | 0.00 | -0.20 |
| TRP | 181 | -1.54 | -0.33 | 0.48 | -0.21 | -1.60 | -1.54 | -0.33 | 0.59 | 0.00 | -1.28 |
| GLY | 182 | -0.21 | -0.21 | 0.25 | -0.03 | -0.20 | -0.21 | -0.21 | 0.33 | 0.00 | -0.09 |
| ARG | 183 | -0.28 | -0.23 | 0.32 | -0.04 | -0.23 | -0.28 | -0.23 | 0.34 | 0.00 | -0.16 |
| GLU | 184 | -0.05 | -2.56 | 2.27 | -0.05 | -0.40 | -0.05 | -2.56 | 3.08 | 0.00 | 0.47 |
| GLU | 185 | -0.05 | 0.14 | -0.09 | 0.00 | 0.01 | -0.05 | 0.14 | -0.11 | 0.00 | -0.02 |
| ARG | 186 | -0.27 | -0.35 | 0.47 | -0.04 | -0.19 | -0.27 | -0.35 | 0.45 | 0.00 | -0.17 |
| GLN | 187 | -0.12 | -0.02 | 0.03 | -0.01 | -0.12 | -0.12 | -0.02 | 0.06 | 0.00 | -0.08 |
| SER | 188 | -0.12 | -0.10 | 0.15 | -0.03 | -0.10 | -0.12 | -0.10 | 0.16 | 0.00 | -0.07 |
| VAL | 189 | -0.02 | 0.02 | -0.02 | 0.00 | -0.01 | -0.02 | 0.02 | -0.03 | 0.00 | -0.02 |
| PHE | 190 | -0.01 | -0.01 | 0.01 | 0.00 | -0.02 | -0.01 | -0.01 | 0.02 | 0.00 | -0.01 |
| PRO | 191 | 0.00 | -0.01 | 0.01 | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 | 0.00 | 0.00 |
| PHE | 192 | 0.00 | 0.00 | -0.01 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| GLU | 193 | 0.00 | 0.11 | -0.10 | 0.00 | 0.01 | 0.00 | 0.11 | -0.10 | 0.00 | 0.01 |
| SER | 194 | -0.01 | -0.01 | 0.01 | 0.00 | 0.00 | -0.01 | -0.01 | 0.01 | 0.00 | 0.00 |
| GLY | 195 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 |
| LYS | 196 | 0.00 | -0.07 | 0.07 | 0.00 | 0.00 | 0.00 | -0.07 | 0.06 | 0.00 | -0.01 |
| PRO | 197 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 |
| PHE | 198 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LYS | 199 | 0.00 | -0.04 | 0.05 | 0.00 | 0.01 | 0.00 | -0.04 | 0.03 | 0.00 | -0.01 |
| ILE | 200 | 0.00 | -0.01 | 0.01 | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 | 0.00 | 0.00 |
| GLN | 201 | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 |
| VAL | 202 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LEU | 203 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| VAL | 204 | -0.01 | 0.00 | 0.01 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | -0.01 |
| GLU | 205 | -0.01 | 0.06 | -0.06 | 0.00 | -0.01 | -0.01 | 0.06 | -0.04 | 0.00 | 0.01 |
| PRO | 206 | -0.07 | -0.04 | 0.07 | -0.01 | -0.05 | -0.07 | -0.04 | 0.10 | 0.00 | -0.02 |
| ASP | 207 | -0.03 | -0.05 | 0.09 | 0.00 | 0.01 | -0.03 | -0.05 | 0.12 | 0.00 | 0.04 |
| HIE | 208 | -0.01 | -0.01 | 0.02 | 0.00 | 0.00 | -0.01 | -0.01 | 0.01 | 0.00 | -0.01 |
| PHE | 209 | -0.01 | 0.00 | -0.02 | 0.00 | -0.02 | -0.01 | 0.00 | 0.00 | 0.00 | -0.01 |
| LYS | 210 | 0.00 | -0.07 | 0.08 | 0.00 | 0.01 | 0.00 | -0.07 | 0.05 | 0.00 | -0.01 |
| VAL | 211 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ALA | 212 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| VAL | 213 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ASN | 214 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ASP | 215 | 0.00 | 0.05 | -0.05 | 0.00 | 0.00 | 0.00 | 0.05 | -0.04 | 0.00 | 0.01 |
| ALA | 216 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| HIE | 217 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LEU | 218 | 0.00 | 0.00 | 0.02 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LEU | 219 | -0.01 | -0.01 | 0.02 | 0.00 | 0.00 | -0.01 | -0.01 | 0.01 | 0.00 | -0.01 |
| GLN | 220 | -0.01 | 0.00 | 0.02 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 | 0.00 | -0.01 |
| TYR | 221 | -0.03 | -0.01 | 0.01 | 0.00 | -0.03 | -0.03 | -0.01 | 0.03 | 0.00 | -0.01 |
| ASN | 222 | -0.06 | -0.03 | 0.04 | -0.01 | -0.05 | -0.06 | -0.03 | 0.03 | 0.00 | -0.05 |
| HIE | 223 | -0.07 | -0.03 | 0.07 | 0.00 | -0.03 | -0.07 | -0.03 | 0.05 | 0.00 | -0.04 |
| ARG | 224 | -0.29 | -0.47 | 0.62 | -0.05 | -0.19 | -0.29 | -0.47 | 0.74 | 0.00 | -0.02 |
| VAL | 225 | -0.07 | -0.04 | 0.07 | 0.00 | -0.04 | -0.07 | -0.04 | 0.07 | 0.00 | -0.04 |
| LYS | 226 | -0.15 | -0.37 | 0.44 | -0.03 | -0.12 | -0.15 | -0.37 | 0.42 | 0.00 | -0.11 |
| LYS | 227 | -0.15 | -0.18 | 0.23 | -0.02 | -0.13 | -0.15 | -0.18 | 0.27 | 0.00 | -0.06 |
| LEU | 228 | -0.12 | -0.04 | 0.02 | -0.01 | -0.14 | -0.12 | -0.04 | 0.07 | 0.00 | -0.09 |
| ASN | 229 | -0.13 | -0.17 | 0.22 | -0.02 | -0.11 | -0.13 | -0.17 | 0.26 | 0.00 | -0.04 |
| GLU | 230 | -0.07 | -0.11 | 0.18 | -0.01 | -0.01 | -0.07 | -0.11 | 0.23 | 0.00 | 0.06 |
| ILE | 231 | -0.02 | 0.00 | 0.02 | 0.00 | 0.00 | -0.02 | 0.00 | 0.01 | 0.00 | -0.01 |
| SER | 232 | -0.03 | -0.01 | 0.03 | 0.00 | -0.01 | -0.03 | -0.01 | 0.02 | 0.00 | -0.01 |
| LYS | 233 | -0.03 | 0.09 | 0.00 | 0.00 | 0.05 | -0.03 | 0.09 | -0.08 | 0.00 | -0.03 |
| LEU | 234 | -0.01 | 0.02 | -0.03 | 0.00 | -0.02 | -0.01 | 0.02 | -0.03 | 0.00 | -0.02 |
| GLY | 235 | -0.02 | 0.00 | 0.00 | 0.00 | -0.02 | -0.02 | 0.00 | 0.01 | 0.00 | -0.01 |
| ILE | 236 | -0.03 | -0.02 | 0.01 | 0.00 | -0.03 | -0.03 | -0.02 | 0.02 | 0.00 | -0.02 |
| SER | 237 | -0.08 | 0.03 | 0.04 | -0.01 | -0.03 | -0.08 | 0.03 | 0.03 | 0.00 | -0.02 |
| GLY | 238 | -0.03 | -0.03 | 0.05 | 0.00 | -0.01 | -0.03 | -0.03 | 0.05 | 0.00 | -0.01 |
| ASP | 239 | -0.01 | 0.17 | -0.16 | 0.00 | -0.01 | -0.01 | 0.17 | -0.17 | 0.00 | -0.02 |
| ILE | 240 | -0.01 | 0.00 | 0.01 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | -0.01 |
| ASP | 241 | 0.00 | 0.05 | -0.05 | 0.00 | 0.00 | 0.00 | 0.05 | -0.04 | 0.00 | 0.01 |
| LEU | 242 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| THR | 243 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| SER | 244 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ALA | 245 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| SER | 246 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| TYR | 247 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| THR | 248 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| MET | 249 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ILE | 250 | 0.00 | 0.02 | -0.02 | 0.00 | 0.00 | 0.00 | 0.02 | -0.01 | 0.00 | 0.01 |

c) DSeDGal B binding mode

| | Res | VDW | Eel | PB | NPOL | TOTAL | VDW | Eel | PB | NPOL | TOTAL |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | - | - | | | |
| SES | 111 | -11.71 | -12.89 | 17.84 | -2.07 | -8.84 | 11.71 | 12.89 | 11.99 | 0.00 | -12.61 |
| GLY | 112 | 0.00 | -0.04 | 0.06 | 0.00 | 0.02 | 0.00 | -0.04 | 0.03 | 0.00 | -0.02 |
| PRO | 113 | -0.01 | -0.01 | 0.01 | 0.00 | -0.01 | -0.01 | -0.01 | 0.01 | 0.00 | -0.01 |
| LEU | 114 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ILE | 115 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| VAL | 116 | -0.02 | -0.01 | 0.01 | 0.00 | -0.01 | -0.02 | -0.01 | 0.01 | 0.00 | -0.02 |
| PRO | 117 | -0.03 | 0.00 | 0.01 | -0.01 | -0.02 | -0.03 | 0.00 | 0.00 | 0.00 | -0.03 |
| TYR | 118 | -0.01 | -0.01 | 0.01 | 0.00 | 0.00 | -0.01 | -0.01 | 0.01 | 0.00 | 0.00 |
| ASN | 119 | 0.00 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| LEU | 120 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| PRO | 121 | -0.01 | 0.00 | -0.01 | 0.00 | -0.02 | -0.01 | 0.00 | 0.00 | 0.00 | -0.01 |
| LEU | 122 | -0.01 | -0.02 | 0.02 | 0.00 | -0.02 | -0.01 | -0.02 | 0.02 | 0.00 | -0.02 |
| PRO | 123 | -0.02 | 0.00 | 0.01 | 0.00 | -0.02 | -0.02 | 0.00 | 0.01 | 0.00 | -0.01 |
| GLY | 124 | -0.02 | -0.01 | 0.02 | 0.00 | -0.02 | -0.02 | -0.01 | 0.03 | 0.00 | -0.01 |
| GLY | 125 | -0.02 | 0.00 | 0.00 | 0.00 | -0.01 | -0.02 | 0.00 | -0.01 | 0.00 | -0.03 |
| VAL | 126 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| VAL | 127 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| PRO | 128 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ARG | 129 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | -0.02 | 0.00 | -0.02 |
| MET | 130 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LEU | 131 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ILE | 132 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| THR | 133 | -0.01 | -0.01 | 0.03 | 0.00 | 0.00 | -0.01 | -0.01 | 0.01 | 0.00 | -0.01 |
| ILE | 134 | -0.02 | 0.01 | -0.02 | 0.00 | -0.03 | -0.02 | 0.01 | -0.01 | 0.00 | -0.02 |
| LEU | 135 | -0.25 | -0.04 | 0.00 | -0.04 | -0.33 | -0.25 | -0.04 | 0.03 | 0.00 | -0.27 |
| GLY | 136 | -0.11 | -0.01 | 0.02 | 0.00 | -0.10 | -0.11 | -0.01 | 0.09 | 0.00 | -0.03 |
| THR | 137 | -0.08 | -0.02 | 0.06 | -0.01 | -0.04 | -0.08 | -0.02 | 0.05 | 0.00 | -0.05 |
| VAL | 138 | -0.02 | -0.01 | 0.03 | 0.00 | 0.00 | -0.02 | -0.01 | 0.01 | 0.00 | -0.02 |
| LYS | 139 | -0.01 | -0.07 | 0.10 | 0.00 | 0.02 | -0.01 | -0.07 | 0.07 | 0.00 | -0.02 |
| PRO | 140 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ASN | 141 | 0.00 | -0.01 | 0.02 | 0.00 | 0.01 | 0.00 | -0.01 | 0.01 | 0.00 | 0.00 |
| ALA | 142 | -0.01 | 0.00 | 0.02 | 0.00 | 0.01 | -0.01 | 0.00 | 0.01 | 0.00 | 0.00 |
| ASN | 143 | -0.06 | 0.05 | 0.01 | -0.01 | -0.01 | -0.06 | 0.05 | 0.00 | 0.00 | -0.01 |
| ARG | 144 | -0.49 | -0.54 | 0.82 | -0.10 | -0.31 | -0.49 | -0.54 | 1.02 | 0.00 | -0.01 |
| ILE | 145 | -0.10 | 0.10 | -0.11 | 0.00 | -0.12 | -0.10 | 0.10 | -0.14 | 0.00 | -0.14 |
| ALA | 146 | -0.21 | -0.04 | 0.01 | -0.03 | -0.27 | -0.21 | -0.04 | 0.03 | 0.00 | -0.22 |
| LEU | 147 | -0.05 | 0.04 | -0.01 | 0.00 | -0.03 | -0.05 | 0.04 | -0.03 | 0.00 | -0.05 |
| ASP | 148 | -0.08 | -0.42 | 0.60 | -0.01 | 0.09 | -0.08 | -0.42 | 1.01 | 0.00 | 0.51 |
| PHE | 149 | -0.01 | 0.00 | -0.01 | 0.00 | -0.02 | -0.01 | 0.00 | 0.00 | 0.00 | -0.01 |
| GLN | 150 | -0.02 | 0.02 | -0.01 | 0.00 | -0.01 | -0.02 | 0.02 | -0.04 | 0.00 | -0.04 |
| ARG | 151 | -0.13 | -0.08 | 0.12 | -0.01 | -0.10 | -0.13 | -0.08 | 0.03 | 0.00 | -0.18 |
| GLY | 152 | -0.07 | -0.04 | 0.05 | -0.01 | -0.07 | -0.07 | -0.04 | 0.06 | 0.00 | -0.05 |
| ASN | 153 | -0.04 | -0.05 | 0.07 | -0.01 | -0.03 | -0.04 | -0.05 | 0.06 | 0.00 | -0.03 |
| ASP | 154 | -0.03 | -0.13 | 0.15 | 0.00 | -0.01 | -0.03 | -0.13 | 0.31 | 0.00 | 0.15 |
| VAL | 155 | -0.06 | 0.01 | -0.03 | 0.00 | -0.08 | -0.06 | 0.01 | -0.01 | 0.00 | -0.06 |
| ALA | 156 | -0.01 | 0.01 | 0.01 | 0.00 | 0.01 | -0.01 | 0.01 | -0.01 | 0.00 | -0.01 |
| PHE | 157 | -0.02 | -0.01 | -0.02 | 0.00 | -0.06 | -0.02 | -0.01 | 0.03 | 0.00 | 0.00 |
| HIE | 158 | -0.84 | -0.54 | 0.74 | -0.10 | -0.75 | -0.84 | -0.54 | 1.14 | 0.00 | -0.24 |
| PHE | 159 | -0.07 | 0.02 | -0.09 | 0.00 | -0.14 | -0.07 | 0.02 | -0.02 | 0.00 | -0.08 |
| ASN | 160 | -0.68 | -0.12 | -0.02 | -0.05 | -0.87 | -0.68 | -0.12 | 0.17 | 0.00 | -0.63 |
| PRO | 161 | -0.05 | 0.08 | 0.00 | 0.00 | 0.04 | -0.05 | 0.08 | -0.12 | 0.00 | -0.09 |
| ARG | 162 | -0.98 | -2.37 | 2.55 | -0.18 | -0.98 | -0.98 | -2.37 | 2.63 | 0.00 | -0.72 |
| PHE | 163 | -0.02 | -0.02 | 0.03 | 0.00 | -0.02 | -0.02 | -0.02 | 0.04 | 0.00 | -0.01 |
| ASN | 164 | -0.03 | -0.03 | 0.07 | 0.00 | 0.01 | -0.03 | -0.03 | 0.07 | 0.00 | 0.01 |
| GLU | 165 | -0.11 | 0.26 | -0.23 | -0.01 | -0.09 | -0.11 | 0.26 | -0.19 | 0.00 | -0.03 |
| ASN | 166 | -0.01 | 0.00 | 0.02 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 | 0.00 | -0.01 |
| ASN | 167 | -0.01 | -0.01 | 0.03 | 0.00 | 0.01 | -0.01 | -0.01 | 0.02 | 0.00 | 0.00 |
| ARG | 168 | -0.02 | -0.11 | 0.16 | 0.00 | 0.03 | -0.02 | -0.11 | 0.10 | 0.00 | -0.03 |
| ARG | 169 | -0.03 | -0.19 | 0.24 | 0.00 | 0.02 | -0.03 | -0.19 | 0.20 | 0.00 | -0.01 |
| VAL | 170 | -0.02 | 0.03 | -0.05 | 0.00 | -0.03 | -0.02 | 0.03 | -0.05 | 0.00 | -0.03 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ILE | 171 | -0.02 | -0.03 | -0.02 | 0.00 | -0.07 | -0.02 | -0.03 | 0.04 | 0.00 | -0.01 |
| VAL | 172 | -0.39 | -0.02 | -0.08 | -0.02 | -0.52 | -0.39 | -0.02 | 0.21 | 0.00 | -0.20 |
| CYS | 173 | -0.14 | 0.03 | -0.11 | 0.00 | -0.22 | -0.14 | 0.03 | 0.07 | 0.00 | -0.04 |
| ASN | 174 | -0.32 | -1.12 | 0.33 | -0.04 | -1.15 | -0.32 | -1.12 | 0.90 | 0.00 | -0.54 |
| THR | 175 | -0.06 | 0.05 | -0.06 | 0.00 | -0.07 | -0.06 | 0.05 | -0.06 | 0.00 | -0.07 |
| LYS | 176 | -0.10 | 0.10 | 0.08 | 0.00 | 0.07 | -0.10 | 0.10 | -0.01 | 0.00 | -0.01 |
| LEU | 177 | -0.01 | 0.00 | 0.01 | 0.00 | 0.00 | -0.01 | 0.00 | -0.01 | 0.00 | -0.02 |
| ASP | 178 | -0.01 | -0.05 | 0.07 | 0.00 | 0.02 | -0.01 | -0.05 | 0.10 | 0.00 | 0.04 |
| ASN | 179 | -0.02 | -0.01 | 0.06 | 0.00 | 0.03 | -0.02 | -0.01 | 0.02 | 0.00 | -0.02 |
| ASN | 180 | -0.04 | -0.01 | 0.05 | 0.00 | 0.00 | -0.04 | -0.01 | 0.02 | 0.00 | -0.03 |
| TRP | 181 | -1.81 | -0.48 | 0.46 | -0.23 | -2.06 | -1.81 | -0.48 | 0.59 | 0.00 | -1.70 |
| GLY | 182 | -0.07 | 0.02 | 0.04 | 0.00 | -0.01 | -0.07 | 0.02 | 0.02 | 0.00 | -0.03 |
| ARG | 183 | -0.05 | -0.05 | 0.04 | 0.00 | -0.06 | -0.05 | -0.05 | 0.03 | 0.00 | -0.07 |
| GLU | 184 | -0.17 | -2.57 | 2.69 | -0.07 | -0.12 | -0.17 | -2.57 | 3.78 | 0.00 | 1.04 |
| GLU | 185 | -0.03 | 0.13 | -0.12 | 0.00 | -0.02 | -0.03 | 0.13 | -0.16 | 0.00 | -0.06 |
| ARG | 186 | -0.08 | -0.10 | 0.21 | 0.00 | 0.03 | -0.08 | -0.10 | 0.10 | 0.00 | -0.07 |
| GLN | 187 | -0.01 | 0.01 | 0.01 | 0.00 | 0.01 | -0.01 | 0.01 | -0.01 | 0.00 | -0.01 |
| SER | 188 | -0.01 | 0.01 | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 | 0.00 | 0.00 | -0.01 |
| VAL | 189 | -0.05 | 0.00 | 0.01 | -0.01 | -0.05 | -0.05 | 0.00 | 0.00 | 0.00 | -0.05 |
| PHE | 190 | -0.05 | -0.04 | 0.05 | -0.01 | -0.05 | -0.05 | -0.04 | 0.08 | 0.00 | -0.01 |
| PRO | 191 | -0.12 | -0.24 | 0.24 | -0.02 | -0.15 | -0.12 | -0.24 | 0.17 | 0.00 | -0.18 |
| PHE | 192 | -0.07 | -0.02 | 0.02 | 0.00 | -0.07 | -0.07 | -0.02 | 0.08 | 0.00 | -0.01 |
| GLU | 193 | -0.08 | 0.15 | -0.12 | -0.01 | -0.06 | -0.08 | 0.15 | -0.12 | 0.00 | -0.05 |
| SER | 194 | -0.01 | 0.01 | 0.01 | 0.00 | 0.01 | -0.01 | 0.01 | -0.01 | 0.00 | -0.01 |
| GLY | 195 | -0.01 | 0.00 | 0.03 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 | 0.00 | -0.01 |
| LYS | 196 | -0.22 | -0.53 | 0.64 | -0.04 | -0.14 | -0.22 | -0.53 | 0.63 | 0.00 | -0.12 |
| PRO | 197 | -0.56 | -0.25 | 0.27 | -0.10 | -0.64 | -0.56 | -0.25 | 0.36 | 0.00 | -0.45 |
| PHE | 198 | -0.34 | -0.14 | 0.12 | -0.02 | -0.37 | -0.34 | -0.14 | 0.19 | 0.00 | -0.29 |
| LYS | 199 | -0.50 | -0.02 | 0.23 | -0.05 | -0.34 | -0.50 | -0.02 | 0.14 | 0.00 | -0.38 |
| ILE | 200 | -0.02 | 0.01 | 0.00 | 0.00 | -0.01 | -0.02 | 0.01 | -0.01 | 0.00 | -0.03 |
| GLN | 201 | -0.02 | -0.01 | 0.04 | 0.00 | 0.01 | -0.02 | -0.01 | 0.01 | 0.00 | -0.02 |
| VAL | 202 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LEU | 203 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 |
| VAL | 204 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| GLU | 205 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 | 0.00 | 0.01 | 0.02 | 0.00 | 0.03 |
| PRO | 206 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ASP | 207 | 0.00 | 0.03 | -0.03 | 0.00 | 0.00 | 0.00 | 0.03 | 0.00 | 0.00 | 0.03 |
| HIE | 208 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| PHE | 209 | 0.00 | 0.00 | -0.01 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 |
| LYS | 210 | 0.00 | -0.01 | 0.02 | 0.00 | 0.01 | 0.00 | -0.01 | -0.02 | 0.00 | -0.03 |
| VAL | 211 | -0.01 | -0.01 | 0.03 | 0.00 | 0.01 | -0.01 | -0.01 | 0.01 | 0.00 | -0.01 |
| ALA | 212 | -0.01 | 0.03 | -0.02 | 0.00 | -0.01 | -0.01 | 0.03 | -0.03 | 0.00 | -0.01 |
| VAL | 213 | -0.06 | -0.08 | 0.06 | 0.00 | -0.08 | -0.06 | -0.08 | 0.09 | 0.00 | -0.04 |
| ASN | 214 | -0.63 | -0.28 | 0.38 | -0.08 | -0.62 | -0.63 | -0.28 | 0.53 | 0.00 | -0.38 |
| ASP | 215 | 0.01 | -2.39 | 2.20 | -0.04 | -0.23 | 0.01 | -2.39 | 2.53 | 0.00 | 0.14 |
| ALA | 216 | -0.04 | -0.01 | 0.02 | -0.01 | -0.04 | -0.04 | -0.01 | 0.01 | 0.00 | -0.04 |
| HIE | 217 | -0.02 | -0.08 | 0.09 | 0.00 | -0.01 | -0.02 | -0.08 | 0.08 | 0.00 | -0.02 |
| LEU | 218 | -0.04 | -0.01 | 0.03 | 0.00 | -0.03 | -0.04 | -0.01 | 0.01 | 0.00 | -0.04 |
| LEU | 219 | -0.01 | -0.01 | 0.02 | 0.00 | 0.00 | -0.01 | -0.01 | 0.01 | 0.00 | 0.00 |
| GLN | 220 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| TYR | 221 | -0.01 | 0.01 | -0.03 | 0.00 | -0.04 | -0.01 | 0.01 | -0.01 | 0.00 | -0.02 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ASN | 222 | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | -0.01 | 0.00 | 0.00 |
| HIE | 223 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ARG | 224 | -0.01 | -0.23 | 0.34 | 0.00 | 0.10 | -0.01 | -0.23 | 0.21 | 0.00 | -0.03 |
| VAL | 225 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LYS | 226 | 0.00 | -0.04 | 0.04 | 0.00 | 0.01 | 0.00 | -0.04 | 0.01 | 0.00 | -0.03 |
| LYS | 227 | -0.01 | -0.02 | 0.04 | 0.00 | 0.01 | -0.01 | -0.02 | 0.00 | 0.00 | -0.03 |
| LEU | 228 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 |
| ASN | 229 | -0.02 | -0.03 | 0.04 | 0.00 | -0.02 | -0.02 | -0.03 | 0.07 | 0.00 | 0.01 |
| GLU | 230 | -0.10 | -0.08 | 0.10 | -0.02 | -0.09 | -0.10 | -0.08 | 0.24 | 0.00 | 0.06 |
| ILE | 231 | -0.02 | -0.01 | 0.01 | 0.00 | -0.02 | -0.02 | -0.01 | 0.02 | 0.00 | -0.01 |
| SER | 232 | -0.06 | -0.05 | 0.07 | -0.01 | -0.05 | -0.06 | -0.05 | 0.08 | 0.00 | -0.02 |
| LYS | 233 | -0.02 | 0.02 | 0.02 | 0.00 | 0.03 | -0.02 | 0.02 | -0.03 | 0.00 | -0.03 |
| LEU | 234 | -0.01 | 0.00 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 | -0.01 | 0.00 | -0.01 |
| GLY | 235 | -0.01 | 0.02 | -0.02 | 0.00 | -0.01 | -0.01 | 0.02 | -0.01 | 0.00 | 0.00 |
| ILE | 236 | -0.02 | -0.02 | 0.02 | 0.00 | -0.02 | -0.02 | -0.02 | 0.03 | 0.00 | -0.01 |
| SER | 237 | -0.10 | -0.04 | 0.10 | -0.02 | -0.07 | -0.10 | -0.04 | 0.11 | 0.00 | -0.04 |
| GLY | 238 | -0.06 | -0.03 | 0.07 | -0.01 | -0.03 | -0.06 | -0.03 | 0.08 | 0.00 | -0.01 |
| ASP | 239 | -0.02 | -0.11 | 0.09 | -0.01 | -0.05 | -0.02 | -0.11 | 0.18 | 0.00 | 0.05 |
| ILE | 240 | -0.01 | -0.01 | 0.02 | 0.00 | 0.00 | -0.01 | -0.01 | 0.01 | 0.00 | -0.02 |
| ASP | 241 | -0.01 | 0.09 | -0.09 | 0.00 | -0.02 | -0.01 | 0.09 | -0.07 | 0.00 | 0.01 |
| LEU | 242 | -0.02 | -0.02 | 0.02 | 0.00 | -0.02 | -0.02 | -0.02 | 0.02 | 0.00 | -0.02 |
| THR | 243 | -0.10 | -0.09 | 0.13 | -0.02 | -0.08 | -0.10 | -0.09 | 0.13 | 0.00 | -0.06 |
| SER | 244 | -0.01 | 0.01 | 0.00 | 0.00 | 0.00 | -0.01 | 0.01 | -0.01 | 0.00 | -0.01 |
| ALA | 245 | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| SER | 246 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| TYR | 247 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| THR | 248 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| MET | 249 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ILE | 250 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.02 | 0.00 | 0.02 |

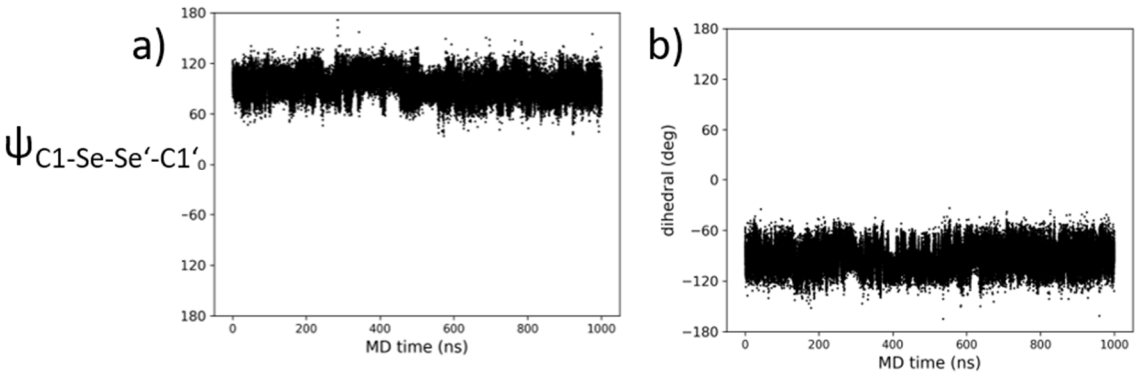



**Figure S4.** The evolution of the C1-Se-Se-C1′ central dihedral angle in the DSeDGal – *h*Gal3 complex in the MD simulation starting from binding mode A (a) and in B (b).