Supplementary Information

Extrinsic functions of lectin domains in O-GalNAc glycan biosynthesis

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Figure S-1: A: Crystal structure of soluble human ppGalNAc-T2 (without the short N-terminal cytoplasmic tail and small transmembrane anchor) (PDB: 2FFU) visualized with VMD (http://www.ks.uiuc.edu/Research/vmd/). **B:** Schematic representation of recombinant constructs: soluble human ppGalNAc-Ts (catalytic and lectin domain) and soluble human lectin domains of ppGalNAc-T with N-terminal 6x-His-tag. Recombinant proteins were expressed in Sf9 insect cells as soluble molecules, and proteins were purified by affinity chromatography using Co^{2+}-charged resin. **C:** Purity of proteins was analyzed by SDS-PAGE stained with Coomassie Brilliant Blue. Enzymes and lectin domains are shown as **1**: ppGalNAc-T2, **2**: ppGalNAc-T3, **3**: dC1GalT, **4:** T2lec, **5**: T3lec and **6**:T4lec.

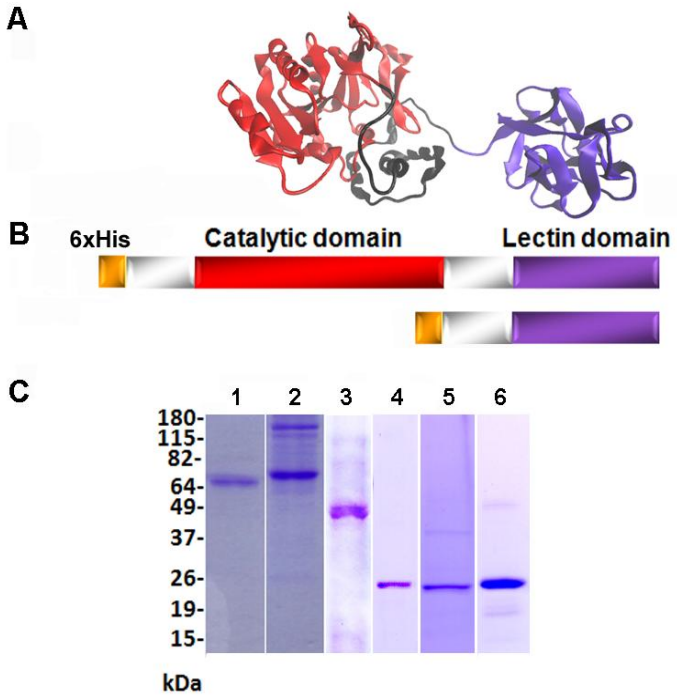


Table S-1: Kinetic parameters for the enzyme ppGalNAc-T2 in absence or presence of T3lec and T4lec using MUC1 and MUC2 as acceptor peptides.

Kinetic parameters (Best-fit values ± Std. Error)	ppGalNAc-T2/ MUC1	ppGalNAc-T2/ MUC1 +T3lec	ppGalNAc-T2/ MUC1 +T4lec	ppGalNAc-T2/ MUC2	ppGalNAc-T2/ MUC2 +T3lec	ppGalNAc-T2/ MUC2 +T4lec
Vmax **(nmol/mg.min)**	**29.8 ± 2.8**	**14.2 ± 2.1**	**28.4 ± 4.5**	**106.2 ± 3.4**	**79 ± 13**	**98 ± 13**
Km **(μM)**	**0.28 ± 0.10**	**0.32 ± 0.18**	**0.55 ± 0.28**	**0.067 ± 0.010**	**0.231 ± 0.080**	**0.094 ± 0.035**

Figure S-2: Kinetics plots of MUC2 peptide glycosylation assay under initial velocity condition of ppGalNAc-T2 enzymatic reaction (black). Effects of T3lec (**A,** blue) and T4lec (**C,** red) on ppGalNAc-T2 activity. Plots were fitted to Michaelis-Menten equation using GraphPad software program yielding R^2: 0.99 (black), 0.97 (blue) and 0.94 (red). Double reciprocal plots of enzyme activity without lectin domain (black) or in the presence of 0.16 µM T3lec (**B**) or T4lec (**D**) indicated the type of inhibition of ppGalNAc-T2 activity. Plots were fitted to linear regression using GraphPad software program yielding R^2: 0.99 (black), 0.99 (blue) and 0.99 (red).

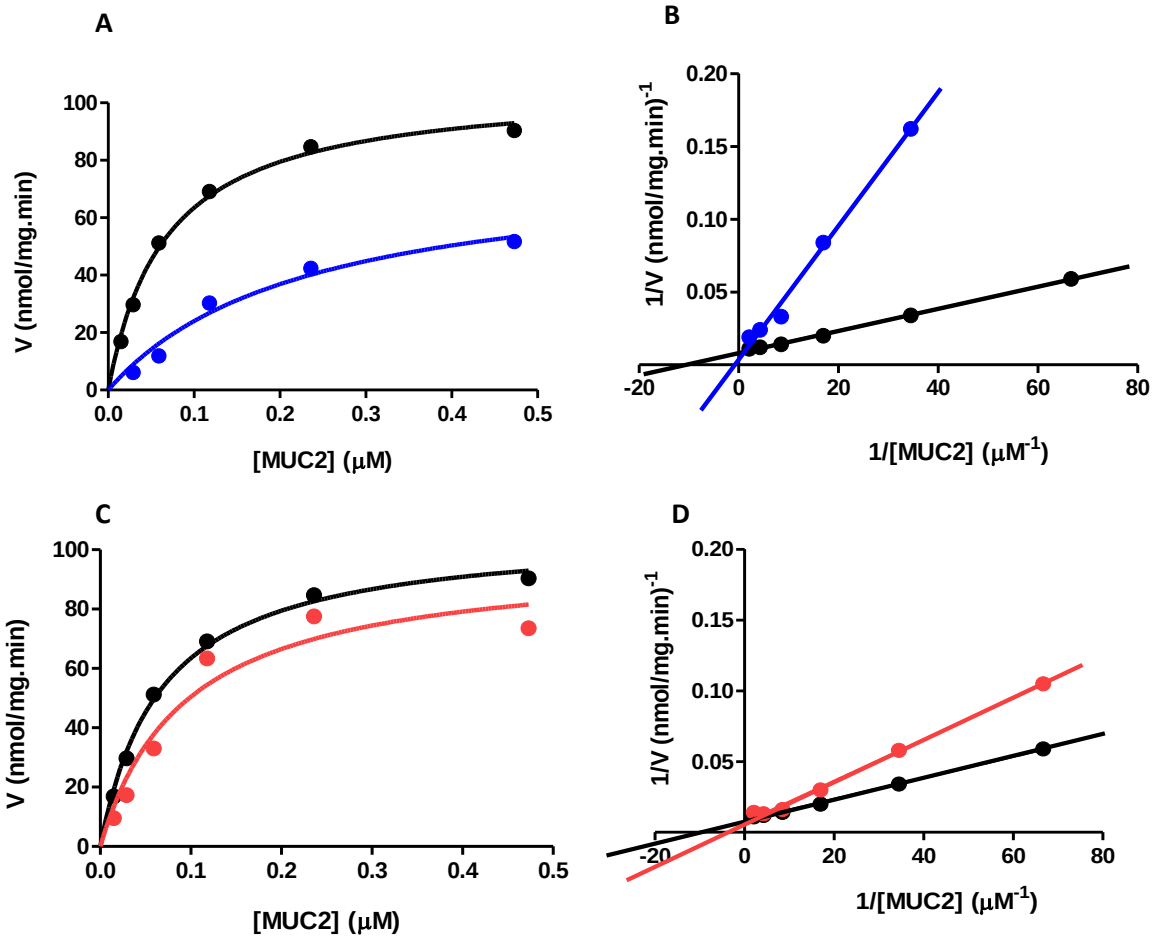


Table S-2: Kinetic parameters for the enzyme ppGalNAc-T3 in absence or presence of T3lec using MUC1 and MUC2 as acceptor peptides.

Kinetic parameters (Best-fit values ± Std. Error)	**ppGalNAc-T3/ MUC1**	**ppGalNAc-T3/ MUC1 +T3lec**	**ppGalNAc-T3/ MUC2**	**ppGalNAc-T3/ MUC2 +T3lec**
Vmax **(nmol/mg.min)**	**2.95 ± 0.58**	**2.07 ± 0.35**	**25.7 ± 3.3**	**24.1 ± 9.1**
Km **(µM)**	**0.36 ± 0.22**	**0.68 ± 0.30**	**0.183 ± 0.088**	**1.40 ± 0.81**

Table S-3: Determination of inhibition constants of T3lec and T4lec on the enzyme activity of ppGalNAc-T2 with MUC1 and MUC2 as acceptor peptides.

Inhibitory Characteristics (mean ± Std. error)	T3lec on MUC1/ ppGalNAc-T2	T4lec on MUC1/ ppGalNAc-T2	T3lec on MUC2/ ppGalNAc-T2	T4lec on MUC2/ ppGalNAc-T2
Type of inhibition	**Non-competitive**	**Competitive**	**Competitive**	**Competitive**
Ki	**-**	**0.17 ± 0.10**	**0.065 ± 0.024**	**0.40 ± 0.16**
Ki´	**0.146 ± 0.025**	**-**	**-**	**-**
(µM)				

Table S-4: Determination of inhibition constants of T3lec on the ppGalNAc-T3 enzyme activity with MUC1 and MUC2 as acceptor peptides.

Inhibitory Characteristics (mean ± Std. error)	T3lec on MUC1/ ppGalNAc-T3	T3lec on MUC2/ ppGalNAc-T3
Type of inhibition	**Mixed**	**Competitive**
Ki ***Ki´*** **(µM)**	**0.047 ± 0.037** **0.188 ± 0.049**	**0.0120 ± 0.0090** **-**

Table S-5: Kinetic parameters for the *Drosophila* Core 1 Gal-T (dC1GalT) enzyme in absence or presence of T3lec using desialylated ovine submaxillary mucin (dOSM) as acceptor glycoprotein.

Kinetic parameters (Best-fit values ± Std. Error)	dOSM/ dC1GalT	dOSM/ dC1GalT +T3lec
Vmax **(pmol/mg.min)**	**20.6 ± 3.6**	**13.2 ± 1.0**
Km **(μM)**	**1.21 ± 0.45**	**0.140 ± 0.040**

Table S-6: Kinetic parameters for the dC1GalT enzyme in absence or presence of ppGalNAc-T3 using ovine submaxillary mucin (OSM) as acceptor glycoprotein.

Kinetic parameters (Best-fit values ± Std. Error)	OSM/ dC1GalT	OSM/ dC1GalT + ppGalNAc-T3
Vmax **(pmol/mg.min)**	**33.1 ± 2.2**	**90 ± 17**
Km **(μM)**	**1.12 ± 0.18**	**4.2 ± 1.2**

Table S-7: PISA analysis of ppGalNAc-T2 assembly interface (PDB: 2FFV).

CCP4 on-line

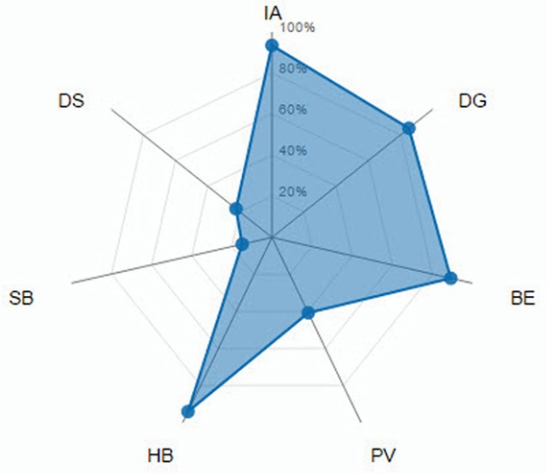
jsPISA 2.0.4 [PDB 2ffv]

Interface B || A

Summary

	Monomer 1		Monomer 2	
Monomer ID		B		A
Class		Protein		Protein
Symmetry operation		X,Y,Z		X,Y,Z
Symmetry ID		1_555		1_555
Interface atoms	181	4.7%	187	4.8%
Surface atoms	2073	53.7%	2097	53.5%
Total atoms	3859	100.0%	3921	100.0%
Interface residues	55	11.4%	58	11.9%
Surface residues	442	91.9%	445	91.0%
Total residues	481	100.0%	489	100.0%
BSA, Å²	1688.0	7.9%	1691.3	7.7%
ASA, Å²	21334.0	100.0%	21942.3	100.0%
Solvation energy, kcal/mol		-433.0		-433.5
SE gain, kcal/mol		-6.0		-4.8

Interaction radar



Interface parameters

IA	:	Interface area, Å²	1690
DG	:	Solvation Energy, kcal/mol	-10.81
BE	:	Total Binding Energy, kcal/mol	-19.69
PV	:	Hydrophobic P-value	0.2327
HB	:	Number of Hydrogen Bonds	20
SB	:	Number of Salt Bridges	0
DS	:	Number of Disulphide Bonds	0

Radar area, exceeding the 50% border line on most points, indicates that the interface is likely to be significant for biological assembly. Interfaces with radar area, fitting within the 50% border line, are more likely to be artefacts of crystal packing.

Interface B || A

Hydrogen bonds

	Monomer 1	Length	Monomer 2
1	B:GLN 262 [NE2]	3.3735	A:GLN 511 [OE1]
2	B:SER 267 [OG]	2.5091	A:ASP 494 [OD2]
3	B:ALA 268 [N]	2.9122	A:ASP 494 [OD1]
4	B:TYR 471 [OH]	3.6881	A:CYS 473 [O]
5	B:GLN 480 [NE2]	3.6245	A:TYR 284 [OH]
6	B:HIS 492 [NE2]	2.6628	A:TYR 284 [OH]
7	B:ASP 494 [N]	3.8026	A:ASP 269 [OD1]
8	B:GLN 511 [NE2]	2.8590	A:GLN 262 [OE1]
9	B:GLN 262 [OE1]	3.6659	A:GLN 511 [NE2]
10	B:TYR 263 [O]	3.6617	A:ARG 514 [NH2]
11	B:GLY 265 [O]	2.9381	A:GLY 512 [N]
12	B:ASP 269 [OD1]	3.8766	A:ASP 494 [N]
13	B:TYR 284 [OH]	3.0694	A:HIS 492 [NE2]
14	B:TYR 284 [OH]	3.7994	A:GLN 480 [NE2]
15	B:THR 368 [O]	3.7728	A:HIS 462 [ND1]
16	B:ASP 465 [OD2]	3.4028	A:ASN 257 [ND2]
17	B:CYS 473 [O]	3.4998	A:TYR 471 [OH]
18	B:ASP 494 [OD1]	2.6624	A:ALA 268 [N]
19	B:ASP 494 [OD2]	2.6704	A:SER 267 [OG]
20	B:GLN 511 [OE1]	3.4251	A:GLN 262 [NE2]

Salt bridges

No salt bridges found

Disulphide bonds

No disulphide bonds found

Covalent bonds

No covalent bonds found

Interface B || A

Residue table for Monomer 1

##	IS	Residue	HS	ASA	BSA	Delta G
1	s	B:LEU 74		114.62	0.00	0.00
2	s	B:LYS 75		117.91	0.00	0.00
3	s	B:VAL 76		45.97	0.00	0.00
4	s	B:ARG 77		155.45	0.00	0.00
5	s	B:TRP 78		40.11	0.00	0.00
6	s	B:PRO 79		84.78	0.00	0.00
7	s	B:ASP 80		99.30	0.00	0.00
8	s	B:PHE 81		20.32	0.00	0.00
9	s	B:ASN 82		84.23	0.00	0.00
10	s	B:GLN 83		44.35	0.00	0.00
11	s	B:GLU 84		125.81	0.00	0.00
12	s	B:ALA 85		65.38	0.00	0.00
13	s	B:TYR 86		0.18	0.00	0.00
14	s	B:VAL 87		39.58	0.00	0.00
15	s	B:GLY 88		70.27	0.00	0.00
16	s	B:GLY 89		78.55	0.00	0.00
17	s	B:PHE 104		99.79	0.00	0.00
18	s	B:ASN 105		54.73	0.00	0.00
19	s	B:GLN 106		105.76	0.00	0.00
20	s	B:VAL 107		112.42	0.00	0.00
21	s	B:GLU 108		57.86	0.00	0.00
22		B:SER 109		0.00	0.00	0.00
23	s	B:ASP 110		53.23	0.00	0.00
24	s	B:LYS 111		146.00	0.00	0.00
25	s	B:LEU 112		43.11	0.00	0.00
26	s	B:ARG 113		144.28	0.00	0.00
27	s	B:MET 114		11.56	0.00	0.00
28	s	B:ASP 115		25.80	0.00	0.00
29	s	B:ARG 116		31.84	0.00	0.00
30	s	B:ALA 117		91.47	0.00	0.00
31	s	B:ILE 118		20.30	0.00	0.00
32	I	B:PRO 119		77.96	33.41	0.53
33	I	B:ASP 120		56.94	1.59	-0.02
34	I	B:THR 121		30.24	7.53	0.12
35	s	B:ARG 122		17.39	0.00	0.00
36	s	B:HIS 123		81.17	0.00	0.00
37	I	B:ASP 124		87.74	22.55	0.09
38	s	B:GLN 125		68.50	0.00	0.00
39	s	B:CYS 126		0.37	0.00	0.00
40	s	B:GLN 127		84.78	0.00	0.00
41	s	B:ARG 128		169.89	0.00	0.00
42	s	B:LYS 129		73.68	0.00	0.00
43	s	B:GLN 130		165.26	0.00	0.00
44	s	B:TRP 131		45.90	0.00	0.00
45	s	B:ARG 132		102.48	0.00	0.00
46	s	B:VAL 133		143.47	0.00	0.00
47	s	B:ASP 134		79.06	0.00	0.00
48	s	B:LEU 135		14.33	0.00	0.00
49	s	B:PRO 136		37.73	0.00	0.00
50	s	B:ALA 137		29.28	0.00	0.00
51		B:THR 138		0.00	0.00	0.00
52		B:SER 139		0.00	0.00	0.00
53		B:VAL 140		0.00	0.00	0.00
54		B:VAL 141		0.00	0.00	0.00
55		B:ILE 142		0.00	0.00	0.00
56	s	B:THR 143		6.49	0.00	0.00
57	s	B:PHE 144		10.66	0.00	0.00
58	s	B:HIS 145		59.37	0.00	0.00
59	s	B:ASN 146		67.21	0.00	0.00
60	s	B:GLU 147		25.84	0.00	0.00
61	s	B:ALA 148		8.70	0.00	0.00
62	s	B:ARG 149		27.32	0.00	0.00
63	s	B:SER 150		3.73	0.00	0.00
64	s	B:ALA 151		3.46	0.00	0.00
65	s	B:LEU 152		1.01	0.00	0.00
66	s	B:LEU 153		3.02	0.00	0.00
67	s	B:ARG 154		5.98	0.00	0.00
68	s	B:THR 155		0.34	0.00	0.00
69	s	B:VAL 156		0.17	0.00	0.00
70	s	B:VAL 157		2.50	0.00	0.00
71	s	B:SER 158		7.69	0.00	0.00
72		B:VAL 159		0.00	0.00	0.00
73	s	B:LEU 160		16.64	0.00	0.00
74	s	B:LYS 161		89.82	0.00	0.00
75	s	B:LYS 162		35.82	0.00	0.00
76	s	B:SER 163		3.79	0.00	0.00
77	s	B:PRO 164		31.79	0.00	0.00
78	s	B:PRO 165		103.90	0.00	0.00
79	s	B:HIS 166		112.75	0.00	0.00
80	s	B:LEU 167		5.85	0.00	0.00
81	s	B:ILE 168		2.77	0.00	0.00
82	s	B:LYS 169		100.25	0.00	0.00
83	s	B:GLU 170		6.81	0.00	0.00
84		B:ILE 171		0.00	0.00	0.00
85		B:ILE 172		0.00	0.00	0.00
86	s	B:LEU 173		0.17	0.00	0.00
87		B:VAL 174		0.00	0.00	0.00
88	s	B:ASP 175		0.13	0.00	0.00
89	s	B:ASP 176		3.87	0.00	0.00
90	s	B:TYR 177		95.65	0.00	0.00
91	s	B:SER 178		0.37	0.00	0.00
92	s	B:ASN 179		120.82	0.00	0.00
93	s	B:ASP 180		50.29	0.00	0.00
94	s	B:PRO 181		64.44	0.00	0.00
95	s	B:GLU 182		71.15	0.00	0.00
96	s	B:ASP 183		15.97	0.00	0.00
97		B:GLY 184		0.00	0.00	0.00
98	s	B:ALA 185		48.58	0.00	0.00
99	s	B:LEU 186		38.66	0.00	0.00
100		B:LEU 187		0.00	0.00	0.00
101	s	B:GLY 188		16.21	0.00	0.00
102	s	B:LYS 189		94.85	0.00	0.00
103	s	B:ILE 190		2.68	0.00	0.00
104	s	B:GLU 191		27.49	0.00	0.00
105	s	B:LYS 192		62.70	0.00	0.00
106	s	B:VAL 193		0.37	0.00	0.00
107	s	B:ARG 194		86.27	0.00	0.00
108	s	B:VAL 195		48.13	0.00	0.00
109	s	B:LEU 196		27.53	0.00	0.00
110	s	B:ARG 197		77.57	0.00	0.00
111	s	B:ASN 198		9.55	0.00	0.00
112	s	B:ASP 199		132.50	0.00	0.00
113	s	B:ARG 200		150.63	0.00	0.00
114	s	B:ARG 201		118.51	0.00	0.00
115	s	B:GLU 202		41.83	0.00	0.00
116	s	B:GLY 203		2.18	0.00	0.00
117	s	B:LEU 204		50.57	0.00	0.00
118	s	B:MET 205		4.34	0.00	0.00
119	s	B:ARG 206		78.03	0.00	0.00
120		B:SER 207		0.00	0.00	0.00
121	s	B:ARG 208		1.15	0.00	0.00
122	s	B:VAL 209		2.51	0.00	0.00
123	s	B:ARG 210		100.38	0.00	0.00
124		B:GLY 211		0.00	0.00	0.00
125	s	B:ALA 212		1.33	0.00	0.00
126	s	B:ASP 213		82.03	0.00	0.00
127	s	B:ALA 214		29.92	0.00	0.00
128	s	B:ALA 215		6.99	0.00	0.00
129	s	B:GLN 216		123.24	0.00	0.00
130	s	B:ALA 217		12.80	0.00	0.00
131	s	B:LYS 218		154.64	0.00	0.00
132	s	B:VAL 219		4.02	0.00	0.00
133	s	B:LEU 220		0.17	0.00	0.00
134	s	B:THR 221		1.33	0.00	0.00
135		B:PHE 222		0.00	0.00	0.00
136	s	B:LEU 223		2.51	0.00	0.00
137	s	B:ASP 224		24.41	0.00	0.00
138	s	B:SER 225		8.21	0.00	0.00
139	s	B:HIS 226		41.13	0.00	0.00
140	s	B:CYS 227		1.25	0.00	0.00
141	s	B:GLU 228		8.65	0.00	0.00
142	s	B:CYS 229		0.57	0.00	0.00
143	s	B:ASN 230		0.49	0.00	0.00
144	s	B:GLU 231		68.00	0.00	0.00
145	s	B:HIS 232		75.45	0.00	0.00
146	s	B:TRP 233		0.62	0.00	0.00
147		B:LEU 234		0.00	0.00	0.00
148	s	B:GLU 235		8.39	0.00	0.00
149	s	B:PRO 236		2.54	0.00	0.00
150	s	B:LEU 237		1.33	0.00	0.00
151		B:LEU 238		0.00	0.00	0.00
152	s	B:GLU 239		41.91	0.00	0.00
153	s	B:ARG 240		41.78	0.00	0.00
154	s	B:VAL 241		4.78	0.00	0.00
155	s	B:ALA 242		28.33	0.00	0.00
156	s	B:GLU 243		114.98	0.00	0.00
157	s	B:ASP 244		50.54	0.00	0.00
158	s	B:ARG 245		126.34	0.00	0.00
159	s	B:THR 246		48.25	0.00	0.00
160	s	B:ARG 247		41.37	0.00	0.00
161	s	B:VAL 248		0.12	0.00	0.00
162		B:VAL 249		0.00	0.00	0.00
163	s	B:SER 250		9.74	0.00	0.00
164	s	B:PRO 251		6.19	0.00	0.00
165	s	B:ILE 252		8.05	0.00	0.00
166	s	B:ILE 253		6.83	0.00	0.00
167		B:ASP 254		0.00	0.00	0.00
168	I	B:VAL 255		39.13	30.09	0.48
169	s	B:ILE 256		0.90	0.00	0.00
170	I	B:ASN 257		41.12	21.63	-0.33
171	s	B:MET 258		40.47	0.00	0.00
172	s	B:ASP 259		85.09	0.00	0.00
173	I	B:ASN 260		81.66	8.59	-0.10
174	s	B:PHE 261		1.52	0.00	0.00
175	I	B:GLN 262	H	105.93	59.70	-0.70
176	I	B:TYR 263	H	7.42	3.81	-0.04
177	I	B:VAL 264		62.33	60.49	0.97
178	I	B:GLY 265	H	37.73	34.38	-0.17
179	I	B:ALA 266		23.08	17.24	0.16
180	I	B:SER 267	H	62.68	51.73	0.35
181	I	B:ALA 268	H	20.44	9.07	0.03
182	I	B:ASP 269	H	80.36	44.79	-0.20
183	I	B:LEU 270		41.53	34.96	0.56
184	s	B:LYS 271		5.27	0.00	0.00
185		B:GLY 272		0.00	0.00	0.00
186		B:GLY 273		0.00	0.00	0.00
187		B:PHE 274		0.00	0.00	0.00
188	s	B:ASP 275		51.54	0.00	0.00
189	s	B:TRP 276		9.16	0.00	0.00
190	s	B:ASN 277		50.07	0.00	0.00
191	s	B:LEU 278		10.72	0.00	0.00
192	s	B:VAL 279		37.05	0.00	0.00
193	s	B:PHE 280		30.06	0.00	0.00
194	s	B:LYS 281		50.64	0.00	0.00
195	I	B:TRP 282		77.29	30.30	0.36
196	s	B:ASP 283		25.92	0.00	0.00
197	I	B:TYR 284	H	184.16	75.39	0.13
198	s	B:MET 285		21.28	0.00	0.00
199	s	B:THR 286		39.05	0.00	0.00
200	I	B:PRO 287		79.01	8.71	0.14
201	I	B:GLU 288		112.44	2.19	-0.04
202	s	B:GLN 289		29.96	0.00	0.00
203	I	B:ARG 290		140.21	40.84	-1.21
204	I	B:ARG 291		137.99	2.03	-0.02
205	s	B:SER 292		62.62	0.00	0.00
206	s	B:ARG 293		19.49	0.00	0.00
207	s	B:GLN 294		147.07	0.00	0.00
208	s	B:GLY 295		68.01	0.00	0.00
209	s	B:ASN 296		59.21	0.00	0.00
210	s	B:PRO 297		51.84	0.00	0.00
211	s	B:VAL 298		10.60	0.00	0.00
212	s	B:ALA 299		10.38	0.00	0.00
213	s	B:PRO 300		50.05	0.00	0.00
214	s	B:ILE 301		6.70	0.00	0.00
215	s	B:LYS 302		83.09	0.00	0.00
216	s	B:THR 303		3.59	0.00	0.00
217	s	B:PRO 304		3.32	0.00	0.00
218	s	B:MET 305		4.41	0.00	0.00
219	s	B:ILE 306		4.78	0.00	0.00
220	s	B:ALA 307		22.40	0.00	0.00
221	s	B:GLY 308		12.10	0.00	0.00
222	s	B:GLY 309		19.07	0.00	0.00
223	s	B:LEU 310		1.18	0.00	0.00
224	s	B:PHE 311		4.82	0.00	0.00
225	s	B:VAL 312		0.34	0.00	0.00
226	s	B:MET 313		0.17	0.00	0.00
227	s	B:ASP 314		10.42	0.00	0.00
228	s	B:LYS 315		36.64	0.00	0.00
229	s	B:PHE 316		119.39	0.00	0.00
230	s	B:TYR 317		22.85	0.00	0.00
231	s	B:PHE 318		0.62	0.00	0.00
232	s	B:GLU 319		63.19	0.00	0.00
233	s	B:GLU 320		81.73	0.00	0.00
234	s	B:LEU 321		4.85	0.00	0.00
235	s	B:GLY 322		10.59	0.00	0.00
236	s	B:LYS 323		46.23	0.00	0.00
237	s	B:TYR 324		7.25	0.00	0.00
238	s	B:ASP 325		2.03	0.00	0.00
239	s	B:MET 326		87.98	0.00	0.00
240	s	B:MET 327		90.99	0.00	0.00
241	s	B:MET 328		18.05	0.00	0.00
242	s	B:ASP 329		33.45	0.00	0.00
243	s	B:VAL 330		55.22	0.00	0.00
244	s	B:TRP 331		173.65	0.00	0.00
245	s	B:GLY 332		12.82	0.00	0.00
246	s	B:GLY 333		31.67	0.00	0.00
247	s	B:GLU 334		21.92	0.00	0.00
248	s	B:ASN 335		43.20	0.00	0.00
249	s	B:LEU 336		10.20	0.00	0.00
250	s	B:GLU 337		1.79	0.00	0.00
251	s	B:ILE 338		2.68	0.00	0.00
252	s	B:SER 339		0.13	0.00	0.00
253		B:PHE 340		0.00	0.00	0.00
254	s	B:ARG 341		0.29	0.00	0.00
255		B:VAL 342		0.00	0.00	0.00
256	s	B:TRP 343		25.94	0.00	0.00
257	s	B:GLN 344		1.72	0.00	0.00
258	s	B:CYS 345		19.10	0.00	0.00
259	s	B:GLY 346		57.54	0.00	0.00
260	s	B:GLY 347		6.53	0.00	0.00
261	s	B:SER 348		12.73	0.00	0.00
262	s	B:LEU 349		1.34	0.00	0.00
263	s	B:GLU 350		1.46	0.00	0.00
264	s	B:ILE 351		13.73	0.00	0.00
265	s	B:ILE 352		7.54	0.00	0.00
266	s	B:PRO 353		5.16	0.00	0.00
267	s	B:CYS 354		4.16	0.00	0.00
268		B:SER 355		0.00	0.00	0.00
269	I	B:ARG 356		15.30	1.90	-0.07
270	s	B:VAL 357		0.17	0.00	0.00
271		B:GLY 358		0.00	0.00	0.00
272	s	B:HIS 359		13.53	0.00	0.00
273	s	B:VAL 360		8.82	0.00	0.00
274	s	B:PHE 361		11.70	0.00	0.00
275	s	B:ARG 362		141.11	0.00	0.00
276	s	B:LYS 363		155.25	0.00	0.00
277	s	B:GLN 364		81.86	0.00	0.00
278	s	B:HIS 365		36.21	0.00	0.00
279	s	B:PRO 366		35.57	0.00	0.00
280	I	B:TYR 367		17.14	9.59	0.05
281	I	B:THR 368	H	68.19	38.98	-0.12
282	I	B:PHE 369		102.25	16.73	0.27
283	I	B:PRO 370		81.60	46.53	0.74
284	s	B:GLY 371		41.63	0.00	0.00
285	s	B:GLY 372		9.34	0.00	0.00
286	s	B:SER 373		50.71	0.00	0.00
287	s	B:GLY 374		66.50	0.00	0.00
288	s	B:THR 375		88.13	0.00	0.00
289	s	B:VAL 376		82.38	0.00	0.00
290	s	B:PHE 377		108.99	0.00	0.00
291	s	B:ALA 378		1.61	0.00	0.00
292	s	B:ARG 379		49.23	0.00	0.00
293		B:ASN 380		0.00	0.00	0.00
294	s	B:THR 381		15.64	0.00	0.00
295	s	B:ARG 382		24.30	0.00	0.00
296	s	B:ARG 383		3.22	0.00	0.00
297		B:ALA 384		0.00	0.00	0.00
298	s	B:ALA 385		0.24	0.00	0.00
299	s	B:GLU 386		33.07	0.00	0.00
300	s	B:VAL 387		1.86	0.00	0.00
301	s	B:TRP 388		0.73	0.00	0.00
302		B:MET 389		0.00	0.00	0.00
303	s	B:ASP 390		41.41	0.00	0.00
304	s	B:GLU 391		111.16	0.00	0.00
305	s	B:TYR 392		31.58	0.00	0.00
306	s	B:LYS 393		54.36	0.00	0.00
307	s	B:ASN 394		62.17	0.00	0.00
308	s	B:PHE 395		18.44	0.00	0.00
309	s	B:TYR 396		1.14	0.00	0.00
310	s	B:TYR 397		3.71	0.00	0.00
311	s	B:ALA 398		7.70	0.00	0.00
312	s	B:ALA 399		25.59	0.00	0.00
313	s	B:VAL 400		18.57	0.00	0.00
314	s	B:PRO 401		83.47	0.00	0.00
315	s	B:SER 402		80.22	0.00	0.00
316	s	B:ALA 403		1.51	0.00	0.00
317	s	B:ARG 404		124.60	0.00	0.00
318	s	B:ASN 405		133.96	0.00	0.00
319	s	B:VAL 406		46.28	0.00	0.00
320	s	B:PRO 407		106.85	0.00	0.00
321	s	B:TYR 408		51.28	0.00	0.00
322	s	B:GLY 409		41.04	0.00	0.00
323	s	B:ASN 410		103.48	0.00	0.00
324	s	B:ILE 411		18.12	0.00	0.00
325	s	B:GLN 412		91.41	0.00	0.00
326	s	B:SER 413		75.30	0.00	0.00
327	s	B:ARG 414		20.09	0.00	0.00
328	s	B:LEU 415		62.05	0.00	0.00
329	s	B:GLU 416		108.80	0.00	0.00
330	s	B:LEU 417		21.77	0.00	0.00
331	s	B:ARG 418		38.60	0.00	0.00
332	s	B:LYS 419		168.06	0.00	0.00
333	s	B:LYS 420		153.81	0.00	0.00
334	s	B:LEU 421		35.46	0.00	0.00
335	s	B:SER 422		92.72	0.00	0.00
336	s	B:CYS 423		16.13	0.00	0.00
337	s	B:LYS 424		104.48	0.00	0.00
338	s	B:PRO 425		65.51	0.00	0.00
339		B:PHE 426		0.00	0.00	0.00
340	s	B:LYS 427		104.04	0.00	0.00
341	s	B:TRP 428		61.21	0.00	0.00
342		B:TYR 429		0.00	0.00	0.00
343	s	B:LEU 430		10.09	0.00	0.00
344	s	B:GLU 431		101.03	0.00	0.00
345	s	B:ASN 432		87.83	0.00	0.00
346	s	B:VAL 433		19.00	0.00	0.00
347	s	B:TYR 434		1.30	0.00	0.00
348	s	B:PRO 435		84.42	0.00	0.00
349	s	B:GLU 436		78.45	0.00	0.00
350	s	B:LEU 437		16.18	0.00	0.00
351	I	B:ARG 438		140.83	35.39	-0.37
352	s	B:VAL 439		61.56	0.00	0.00
353	s	B:PRO 440		7.09	0.00	0.00
354	s	B:ASP 441		85.96	0.00	0.00
355	s	B:HIS 442		150.77	0.00	0.00
356	s	B:GLN 443		90.51	0.00	0.00
357	s	B:ASP 444		11.07	0.00	0.00
358	s	B:ILE 445		48.83	0.00	0.00
359		B:ALA 446		0.00	0.00	0.00
360	s	B:PHE 447		9.04	0.00	0.00
361	s	B:GLY 448		2.09	0.00	0.00
362	s	B:ALA 449		15.84	0.00	0.00
363	s	B:LEU 450		0.31	0.00	0.00
364	s	B:GLN 451		61.03	0.00	0.00
365	s	B:GLN 452		32.23	0.00	0.00
366	s	B:GLY 453		66.71	0.00	0.00
367	s	B:THR 454		111.30	0.00	0.00
368	s	B:ASN 455		57.41	0.00	0.00
369	s	B:CYS 456		1.50	0.00	0.00
370	s	B:LEU 457		0.12	0.00	0.00
371	I	B:ASP 458		17.95	11.70	-0.13
372		B:THR 459		0.00	0.00	0.00
373	I	B:LEU 460		58.23	13.51	-0.11
374	I	B:GLY 461		44.30	32.06	-0.01
375	I	B:HIS 462		73.28	45.70	0.36
376	I	B:PHE 463		96.60	72.35	0.94
377	I	B:ALA 464		88.25	81.55	0.89
378	I	B:ASP 465	H	79.66	64.81	0.06
379	I	B:GLY 466		10.21	0.17	0.00
380	s	B:VAL 467		34.89	0.00	0.00
381	s	B:VAL 468		0.15	0.00	0.00
382	s	B:GLY 469		3.17	0.00	0.00
383	I	B:VAL 470		37.61	2.33	-0.03
384	I	B:TYR 471	H	121.94	96.60	0.87
385	I	B:GLU 472		126.82	52.00	-0.07
386	I	B:CYS 473	H	33.52	7.86	-0.09
387	I	B:HIS 474		123.02	82.11	0.44
388	I	B:ASN 475		152.57	24.37	-0.16
389	s	B:GLY 478		84.91	0.00	0.00
390	I	B:ASN 479		52.79	2.68	0.04
391	I	B:GLN 480	H	36.79	6.52	-0.03
392	s	B:GLU 481		61.70	0.00	0.00
393	s	B:TRP 482		1.63	0.00	0.00
394	s	B:ALA 483		9.87	0.00	0.00
395	s	B:LEU 484		5.19	0.00	0.00
396	s	B:THR 485		9.38	0.00	0.00
397	s	B:LYS 486		126.35	0.00	0.00
398	s	B:GLU 487		88.09	0.00	0.00
399	s	B:LYS 488		83.58	0.00	0.00
400	s	B:SER 489		9.63	0.00	0.00
401		B:VAL 490		0.00	0.00	0.00
402	s	B:LYS 491		53.28	0.00	0.00
403	I	B:HIS 492	H	28.25	12.68	0.36
404	I	B:MET 493		138.65	77.92	1.88
405	I	B:ASP 494	H	101.79	60.47	-0.56
406	I	B:LEU 495		22.93	22.59	0.36
407		B:CYS 496		0.00	0.00	0.00
408	s	B:LEU 497		0.51	0.00	0.00
409		B:THR 498		0.00	0.00	0.00
410	s	B:VAL 499		3.19	0.00	0.00
411	I	B:VAL 500		64.81	8.21	0.13
412	s	B:ASP 501		70.41	0.00	0.00
413	s	B:ARG 502		118.94	0.00	0.00
414	s	B:ALA 503		52.39	0.00	0.00
415	s	B:PRO 504		84.25	0.00	0.00
416	s	B:GLY 505		33.44	0.00	0.00
417	s	B:SER 506		19.45	0.00	0.00
418	s	B:LEU 507		54.55	0.00	0.00
419	s	B:ILE 508		0.37	0.00	0.00
420	I	B:LYS 509		38.74	5.39	-0.19
421		B:LEU 510		0.00	0.00	0.00
422	I	B:GLN 511	H	38.48	35.44	-0.05
423	I	B:GLY 512		45.89	30.75	0.18
424	s	B:CYS 513		44.06	0.00	0.00
425	I	B:ARG 514		176.11	58.46	-0.30
426	I	B:GLU 515		156.90	13.39	-0.24
427	s	B:ASN 516		132.43	0.00	0.00
428	s	B:ASP 517		22.06	0.00	0.00
429	s	B:SER 518		70.87	0.00	0.00
430	I	B:ARG 519		90.50	16.08	-0.38
431	s	B:GLN 520		2.62	0.00	0.00
432	s	B:LYS 521		50.56	0.00	0.00
433	s	B:TRP 522		1.09	0.00	0.00
434	s	B:GLU 523		42.25	0.00	0.00
435	s	B:GLN 524		34.26	0.00	0.00
436	s	B:ILE 525		25.43	0.00	0.00
437	s	B:GLU 526		120.20	0.00	0.00
438	s	B:GLY 527		65.05	0.00	0.00
439	s	B:ASN 528		30.27	0.00	0.00
440	s	B:SER 529		25.61	0.00	0.00
441	s	B:LYS 530		2.62	0.00	0.00
442	s	B:LEU 531		1.81	0.00	0.00
443	s	B:ARG 532		73.94	0.00	0.00
444	s	B:HIS 533		0.91	0.00	0.00
445	s	B:VAL 534		32.43	0.00	0.00
446	s	B:GLY 535		64.74	0.00	0.00
447	s	B:SER 536		32.02	0.00	0.00
448	s	B:ASN 537		91.41	0.00	0.00
449	s	B:LEU 538		4.01	0.00	0.00
450	s	B:CYS 539		0.16	0.00	0.00
451	s	B:LEU 540		0.58	0.00	0.00
452		B:ASP 541		0.00	0.00	0.00
453	s	B:SER 542		14.69	0.00	0.00
454	s	B:ARG 543		140.30	0.00	0.00
455	s	B:THR 544		24.43	0.00	0.00
456	s	B:ALA 545		37.53	0.00	0.00
457	s	B:LYS 546		204.27	0.00	0.00
458	s	B:SER 547		90.54	0.00	0.00
459	s	B:GLY 548		31.84	0.00	0.00
460	s	B:GLY 549		1.84	0.00	0.00
461	s	B:LEU 550		0.37	0.00	0.00
462		B:SER 551		0.00	0.00	0.00
463	s	B:VAL 552		0.17	0.00	0.00
464	s	B:GLU 553		23.84	0.00	0.00
465	s	B:VAL 554		75.71	0.00	0.00
466	s	B:CYS 555		37.70	0.00	0.00
467	s	B:GLY 556		26.50	0.00	0.00
468	s	B:PRO 557		133.36	0.00	0.00
469	s	B:ALA 558		22.75	0.00	0.00
470	s	B:LEU 559		145.06	0.00	0.00
471	s	B:SER 560		19.95	0.00	0.00
472	s	B:GLN 561		1.47	0.00	0.00
473	s	B:GLN 562		57.49	0.00	0.00
474	s	B:TRP 563		3.73	0.00	0.00
475	s	B:LYS 564		95.31	0.00	0.00
476	s	B:PHE 565		3.42	0.00	0.00
477	s	B:THR 566		51.13	0.00	0.00
478	s	B:LEU 567		7.70	0.00	0.00
479	s	B:ASN 568		14.10	0.00	0.00
480	s	B:LEU 569		55.89	0.00	0.00
481	s	B:GLN 570		145.34	0.00	0.00

Residue table for Monomer 2

##	IS	Residue	HS	ASA	BSA	Delta G
1	s	A:ASP 72		128.77	0.00	0.00
2	s	A:ALA 73		112.47	0.00	0.00
3	s	A:LEU 74		60.17	0.00	0.00
4	s	A:LYS 75		116.08	0.00	0.00
5	s	A:VAL 76		47.78	0.00	0.00
6	s	A:ARG 77		159.13	0.00	0.00
7	s	A:TRP 78		38.74	0.00	0.00
8	s	A:PRO 79		80.47	0.00	0.00
9	s	A:ASP 80		103.20	0.00	0.00
10	s	A:PHE 81		12.86	0.00	0.00
11	s	A:ASN 82		91.82	0.00	0.00
12	s	A:GLN 83		44.12	0.00	0.00
13	s	A:GLU 84		143.81	0.00	0.00
14	s	A:ALA 85		69.53	0.00	0.00
15	s	A:TYR 86		4.57	0.00	0.00
16	s	A:VAL 87		42.48	0.00	0.00
17	s	A:GLY 88		68.28	0.00	0.00
18	s	A:GLY 89		86.32	0.00	0.00
19	s	A:PRO 98		91.53	0.00	0.00
20	s	A:TYR 99		67.78	0.00	0.00
21	s	A:ALA 100		88.14	0.00	0.00
22	s	A:ARG 101		163.26	0.00	0.00
23	s	A:ASN 102		31.09	0.00	0.00
24	s	A:LYS 103		104.45	0.00	0.00
25	s	A:PHE 104		10.78	0.00	0.00
26	s	A:ASN 105		19.23	0.00	0.00
27	s	A:GLN 106		42.11	0.00	0.00
28	s	A:VAL 107		80.10	0.00	0.00
29	s	A:GLU 108		46.17	0.00	0.00
30		A:SER 109		0.00	0.00	0.00
31	s	A:ASP 110		54.67	0.00	0.00
32	s	A:LYS 111		138.22	0.00	0.00
33	s	A:LEU 112		48.65	0.00	0.00
34	s	A:ARG 113		139.21	0.00	0.00
35	s	A:MET 114		14.43	0.00	0.00
36	s	A:ASP 115		28.74	0.00	0.00
37	s	A:ARG 116		41.71	0.00	0.00
38	s	A:ALA 117		91.31	0.00	0.00
39	s	A:ILE 118		26.43	0.00	0.00
40	I	A:PRO 119		77.10	33.27	0.53
41	I	A:ASP 120		67.58	14.81	-0.11
42	I	A:THR 121		30.19	7.86	0.13
43	s	A:ARG 122		30.98	0.00	0.00
44	s	A:HIS 123		87.22	0.00	0.00
45	I	A:ASP 124		90.37	9.17	0.08
46	s	A:GLN 125		80.57	0.00	0.00
47	s	A:CYS 126		0.74	0.00	0.00
48	I	A:GLN 127		101.43	4.06	-0.06
49	s	A:ARG 128		174.41	0.00	0.00
50	s	A:LYS 129		78.52	0.00	0.00
51	s	A:GLN 130		163.32	0.00	0.00
52	s	A:TRP 131		35.71	0.00	0.00
53	s	A:ARG 132		106.96	0.00	0.00
54	s	A:VAL 133		123.74	0.00	0.00
55	s	A:ASP 134		96.10	0.00	0.00
56	s	A:LEU 135		8.50	0.00	0.00
57	s	A:PRO 136		39.15	0.00	0.00
58	s	A:ALA 137		32.41	0.00	0.00
59		A:THR 138		0.00	0.00	0.00
60		A:SER 139		0.00	0.00	0.00
61		A:VAL 140		0.00	0.00	0.00
62		A:VAL 141		0.00	0.00	0.00
63		A:ILE 142		0.00	0.00	0.00
64	s	A:THR 143		8.19	0.00	0.00
65	s	A:PHE 144		8.91	0.00	0.00
66	s	A:HIS 145		59.28	0.00	0.00
67	s	A:ASN 146		31.00	0.00	0.00
68	s	A:GLU 147		10.25	0.00	0.00
69	s	A:ALA 148		0.67	0.00	0.00
70	s	A:ARG 149		29.30	0.00	0.00
71	s	A:SER 150		3.47	0.00	0.00
72	s	A:ALA 151		4.38	0.00	0.00
73	s	A:LEU 152		0.67	0.00	0.00
74	s	A:LEU 153		1.51	0.00	0.00
75	s	A:ARG 154		7.50	0.00	0.00
76		A:THR 155		0.00	0.00	0.00
77	s	A:VAL 156		0.17	0.00	0.00
78	s	A:VAL 157		0.17	0.00	0.00
79	s	A:SER 158		10.87	0.00	0.00
80		A:VAL 159		0.00	0.00	0.00
81	s	A:LEU 160		19.33	0.00	0.00
82	s	A:LYS 161		92.16	0.00	0.00
83	s	A:LYS 162		47.64	0.00	0.00
84	s	A:SER 163		6.75	0.00	0.00
85	s	A:PRO 164		30.89	0.00	0.00
86	s	A:PRO 165		100.89	0.00	0.00
87	s	A:HIS 166		111.58	0.00	0.00
88	s	A:LEU 167		4.36	0.00	0.00
89	s	A:ILE 168		3.72	0.00	0.00
90	s	A:LYS 169		105.00	0.00	0.00
91	s	A:GLU 170		7.63	0.00	0.00
92		A:ILE 171		0.00	0.00	0.00
93		A:ILE 172		0.00	0.00	0.00
94		A:LEU 173		0.00	0.00	0.00
95		A:VAL 174		0.00	0.00	0.00
96	s	A:ASP 175		0.25	0.00	0.00
97	s	A:ASP 176		3.48	0.00	0.00
98	s	A:TYR 177		91.73	0.00	0.00
99	s	A:SER 178		0.94	0.00	0.00
100	s	A:ASN 179		129.87	0.00	0.00
101	s	A:ASP 180		55.78	0.00	0.00
102	s	A:PRO 181		65.82	0.00	0.00
103	s	A:GLU 182		76.76	0.00	0.00
104	s	A:ASP 183		8.18	0.00	0.00
105		A:GLY 184		0.00	0.00	0.00
106	s	A:ALA 185		44.09	0.00	0.00
107	s	A:LEU 186		52.26	0.00	0.00
108		A:LEU 187		0.00	0.00	0.00
109	s	A:GLY 188		25.46	0.00	0.00
110	s	A:LYS 189		92.64	0.00	0.00
111	s	A:ILE 190		0.17	0.00	0.00
112	s	A:GLU 191		32.13	0.00	0.00
113	s	A:LYS 192		60.78	0.00	0.00
114	s	A:VAL 193		5.52	0.00	0.00
115	s	A:ARG 194		93.92	0.00	0.00
116	s	A:VAL 195		46.94	0.00	0.00
117	s	A:LEU 196		20.40	0.00	0.00
118	s	A:ARG 197		93.37	0.00	0.00
119	s	A:ASN 198		11.81	0.00	0.00
120	s	A:ASP 199		137.85	0.00	0.00
121	s	A:ARG 200		139.92	0.00	0.00
122	s	A:ARG 201		97.96	0.00	0.00
123	s	A:GLU 202		46.10	0.00	0.00
124	s	A:GLY 203		4.86	0.00	0.00
125	s	A:LEU 204		58.17	0.00	0.00
126	s	A:MET 205		9.01	0.00	0.00
127	s	A:ARG 206		65.50	0.00	0.00
128	s	A:SER 207		1.00	0.00	0.00
129	s	A:ARG 208		2.04	0.00	0.00
130	s	A:VAL 209		19.38	0.00	0.00
131	s	A:ARG 210		94.23	0.00	0.00
132		A:GLY 211		0.00	0.00	0.00
133	s	A:ALA 212		1.34	0.00	0.00
134	s	A:ASP 213		102.02	0.00	0.00
135	s	A:ALA 214		26.44	0.00	0.00
136	s	A:ALA 215		3.32	0.00	0.00
137	s	A:GLN 216		122.74	0.00	0.00
138	s	A:ALA 217		9.18	0.00	0.00
139	s	A:LYS 218		139.62	0.00	0.00
140	s	A:VAL 219		6.00	0.00	0.00
141		A:LEU 220		0.00	0.00	0.00
142	s	A:THR 221		1.17	0.00	0.00
143		A:PHE 222		0.00	0.00	0.00
144	s	A:LEU 223		2.17	0.00	0.00
145	s	A:ASP 224		19.72	0.00	0.00
146	s	A:SER 225		6.77	0.00	0.00
147	s	A:HIS 226		40.15	0.00	0.00
148	s	A:CYS 227		1.11	0.00	0.00
149	s	A:GLU 228		8.70	0.00	0.00
150	s	A:CYS 229		1.91	0.00	0.00
151	s	A:ASN 230		0.98	0.00	0.00
152	s	A:GLU 231		63.37	0.00	0.00
153	s	A:HIS 232		73.44	0.00	0.00
154	s	A:TRP 233		0.62	0.00	0.00
155		A:LEU 234		0.00	0.00	0.00
156	s	A:GLU 235		7.07	0.00	0.00
157	s	A:PRO 236		2.95	0.00	0.00
158	s	A:LEU 237		1.51	0.00	0.00
159		A:LEU 238		0.00	0.00	0.00
160	s	A:GLU 239		48.89	0.00	0.00
161	s	A:ARG 240		44.16	0.00	0.00
162	s	A:VAL 241		5.95	0.00	0.00
163	s	A:ALA 242		41.59	0.00	0.00
164	s	A:GLU 243		115.58	0.00	0.00
165	s	A:ASP 244		51.90	0.00	0.00
166	s	A:ARG 245		100.89	0.00	0.00
167	s	A:THR 246		42.32	0.00	0.00
168	s	A:ARG 247		40.57	0.00	0.00
169	s	A:VAL 248		0.58	0.00	0.00
170		A:VAL 249		0.00	0.00	0.00
171	s	A:SER 250		11.37	0.00	0.00
172	s	A:PRO 251		5.04	0.00	0.00
173	s	A:ILE 252		8.37	0.00	0.00
174	s	A:ILE 253		6.55	0.00	0.00
175		A:ASP 254		0.00	0.00	0.00
176	I	A:VAL 255		35.74	27.55	0.44
177	s	A:ILE 256		1.61	0.00	0.00
178	I	A:ASN 257	H	44.49	24.47	-0.19
179	s	A:MET 258		43.37	0.00	0.00
180	s	A:ASP 259		72.29	0.00	0.00
181	I	A:ASN 260		79.41	0.44	-0.00
182	s	A:PHE 261		1.87	0.00	0.00
183	I	A:GLN 262	H	103.76	53.76	-0.62
184	s	A:TYR 263		10.46	0.00	0.00
185	I	A:VAL 264		60.51	57.34	0.92
186	I	A:GLY 265		39.42	32.44	-0.15
187	I	A:ALA 266		23.58	16.12	0.17
188	I	A:SER 267	H	55.90	46.09	0.38
189	I	A:ALA 268	H	23.34	9.46	0.04
190	I	A:ASP 269	H	70.86	43.64	-0.19
191	I	A:LEU 270		47.11	38.15	0.61
192	s	A:LYS 271		7.81	0.00	0.00
193		A:GLY 272		0.00	0.00	0.00
194		A:GLY 273		0.00	0.00	0.00
195	s	A:PHE 274		0.32	0.00	0.00
196	s	A:ASP 275		49.68	0.00	0.00
197	s	A:TRP 276		14.98	0.00	0.00
198	s	A:ASN 277		60.45	0.00	0.00
199	s	A:LEU 278		9.86	0.00	0.00
200	s	A:VAL 279		31.87	0.00	0.00
201	s	A:PHE 280		31.22	0.00	0.00
202	s	A:LYS 281		46.61	0.00	0.00
203	I	A:TRP 282		76.97	26.82	0.36
204	s	A:ASP 283		22.65	0.00	0.00
205	I	A:TYR 284	H	187.05	82.97	0.12
206	I	A:MET 285		24.38	1.40	0.00
207	s	A:THR 286		34.61	0.00	0.00
208	I	A:PRO 287		93.72	9.18	0.15
209	I	A:GLU 288		118.02	1.84	-0.03
210	s	A:GLN 289		25.51	0.00	0.00
211	I	A:ARG 290		148.87	31.61	-0.80
212	I	A:ARG 291		141.57	2.60	-0.05
213	s	A:SER 292		55.75	0.00	0.00
214	s	A:ARG 293		25.08	0.00	0.00
215	s	A:GLN 294		145.18	0.00	0.00
216	s	A:GLY 295		65.69	0.00	0.00
217	s	A:ASN 296		60.33	0.00	0.00
218	s	A:PRO 297		52.54	0.00	0.00
219	s	A:VAL 298		8.66	0.00	0.00
220	s	A:ALA 299		12.89	0.00	0.00
221	s	A:PRO 300		47.97	0.00	0.00
222	s	A:ILE 301		6.15	0.00	0.00
223	s	A:LYS 302		94.04	0.00	0.00
224	s	A:THR 303		4.17	0.00	0.00
225	s	A:PRO 304		2.82	0.00	0.00
226	s	A:MET 305		5.69	0.00	0.00
227	s	A:ILE 306		4.42	0.00	0.00
228	s	A:ALA 307		23.15	0.00	0.00
229	s	A:GLY 308		11.46	0.00	0.00
230	s	A:GLY 309		17.32	0.00	0.00
231	s	A:LEU 310		1.16	0.00	0.00
232	s	A:PHE 311		2.62	0.00	0.00
233	s	A:VAL 312		0.50	0.00	0.00
234	s	A:MET 313		1.17	0.00	0.00
235	s	A:ASP 314		21.31	0.00	0.00
236	s	A:LYS 315		35.55	0.00	0.00
237	s	A:PHE 316		132.90	0.00	0.00
238	s	A:TYR 317		8.97	0.00	0.00
239	s	A:PHE 318		2.21	0.00	0.00
240	s	A:GLU 319		58.81	0.00	0.00
241	s	A:GLU 320		84.53	0.00	0.00
242	s	A:LEU 321		3.18	0.00	0.00
243	s	A:GLY 322		11.86	0.00	0.00
244	s	A:LYS 323		72.76	0.00	0.00
245	s	A:TYR 324		4.93	0.00	0.00
246	s	A:ASP 325		2.84	0.00	0.00
247	s	A:MET 326		75.56	0.00	0.00
248	s	A:MET 327		85.43	0.00	0.00
249	s	A:MET 328		16.33	0.00	0.00
250	s	A:ASP 329		39.00	0.00	0.00
251	s	A:VAL 330		75.78	0.00	0.00
252	s	A:TRP 331		157.95	0.00	0.00
253	s	A:GLY 332		14.07	0.00	0.00
254	s	A:GLY 333		31.54	0.00	0.00
255	s	A:GLU 334		26.16	0.00	0.00
256	s	A:ASN 335		35.85	0.00	0.00
257	s	A:LEU 336		12.98	0.00	0.00
258	s	A:GLU 337		1.34	0.00	0.00
259	s	A:ILE 338		2.33	0.00	0.00
260		A:SER 339		0.00	0.00	0.00
261		A:PHE 340		0.00	0.00	0.00
262	s	A:ARG 341		1.16	0.00	0.00
263		A:VAL 342		0.00	0.00	0.00
264	s	A:TRP 343		23.45	0.00	0.00
265	s	A:GLN 344		0.49	0.00	0.00
266	s	A:CYS 345		18.85	0.00	0.00
267	s	A:GLY 346		61.30	0.00	0.00
268	s	A:GLY 347		3.85	0.00	0.00
269	s	A:SER 348		14.29	0.00	0.00
270	s	A:LEU 349		1.01	0.00	0.00
271	s	A:GLU 350		2.09	0.00	0.00
272	s	A:ILE 351		13.73	0.00	0.00
273	s	A:ILE 352		7.87	0.00	0.00
274	s	A:PRO 353		5.60	0.00	0.00
275	s	A:CYS 354		5.45	0.00	0.00
276		A:SER 355		0.00	0.00	0.00
277	I	A:ARG 356		18.20	2.19	-0.08
278		A:VAL 357		0.00	0.00	0.00
279		A:GLY 358		0.00	0.00	0.00
280	s	A:HIS 359		13.52	0.00	0.00
281	s	A:VAL 360		8.71	0.00	0.00
282	s	A:PHE 361		6.10	0.00	0.00
283	s	A:ARG 362		141.97	0.00	0.00
284	s	A:LYS 363		126.93	0.00	0.00
285	s	A:GLN 364		84.24	0.00	0.00
286	s	A:HIS 365		31.86	0.00	0.00
287	s	A:PRO 366		38.52	0.00	0.00
288	I	A:TYR 367		17.77	9.73	0.03
289	I	A:THR 368		64.60	35.63	0.12
290	I	A:PHE 369		94.58	13.92	0.22
291	I	A:PRO 370		76.25	46.70	0.75
292	s	A:GLY 371		46.07	0.00	0.00
293	s	A:GLY 372		8.12	0.00	0.00
294	s	A:SER 373		57.54	0.00	0.00
295	s	A:GLY 374		68.44	0.00	0.00
296	s	A:THR 375		85.26	0.00	0.00
297	s	A:VAL 376		85.43	0.00	0.00
298	s	A:PHE 377		117.23	0.00	0.00
299	s	A:ALA 378		4.77	0.00	0.00
300	s	A:ARG 379		56.70	0.00	0.00
301		A:ASN 380		0.00	0.00	0.00
302	s	A:THR 381		4.81	0.00	0.00
303	s	A:ARG 382		33.01	0.00	0.00
304	s	A:ARG 383		1.78	0.00	0.00
305		A:ALA 384		0.00	0.00	0.00
306		A:ALA 385		0.00	0.00	0.00
307	s	A:GLU 386		31.03	0.00	0.00
308	s	A:VAL 387		2.07	0.00	0.00
309	s	A:TRP 388		0.29	0.00	0.00
310		A:MET 389		0.00	0.00	0.00
311	s	A:ASP 390		40.21	0.00	0.00
312	s	A:GLU 391		118.58	0.00	0.00
313	s	A:TYR 392		38.79	0.00	0.00
314	s	A:LYS 393		51.73	0.00	0.00
315	s	A:ASN 394		65.67	0.00	0.00
316	s	A:PHE 395		18.43	0.00	0.00
317	s	A:TYR 396		4.43	0.00	0.00
318	s	A:TYR 397		3.46	0.00	0.00
319	s	A:ALA 398		6.80	0.00	0.00
320	s	A:ALA 399		24.27	0.00	0.00
321	s	A:VAL 400		37.67	0.00	0.00
322	s	A:PRO 401		85.55	0.00	0.00
323	s	A:SER 402		83.93	0.00	0.00
324	s	A:ALA 403		1.51	0.00	0.00
325	s	A:ARG 404		129.38	0.00	0.00
326	s	A:ASN 405		133.48	0.00	0.00
327	s	A:VAL 406		41.53	0.00	0.00
328	s	A:PRO 407		108.65	0.00	0.00
329	s	A:TYR 408		43.04	0.00	0.00
330	s	A:GLY 409		44.05	0.00	0.00
331	s	A:ASN 410		95.10	0.00	0.00
332	s	A:ILE 411		20.62	0.00	0.00
333	s	A:GLN 412		93.64	0.00	0.00
334	s	A:SER 413		77.01	0.00	0.00
335	s	A:ARG 414		19.35	0.00	0.00
336	s	A:LEU 415		66.04	0.00	0.00
337	s	A:GLU 416		101.08	0.00	0.00
338	s	A:LEU 417		27.18	0.00	0.00
339	s	A:ARG 418		38.54	0.00	0.00
340	s	A:LYS 419		164.22	0.00	0.00
341	s	A:LYS 420		143.79	0.00	0.00
342	s	A:LEU 421		40.32	0.00	0.00
343	s	A:SER 422		93.28	0.00	0.00
344	s	A:CYS 423		19.64	0.00	0.00
345	s	A:LYS 424		96.76	0.00	0.00
346	s	A:PRO 425		63.50	0.00	0.00
347		A:PHE 426		0.00	0.00	0.00
348	s	A:LYS 427		107.19	0.00	0.00
349	s	A:TRP 428		69.18	0.00	0.00
350		A:TYR 429		0.00	0.00	0.00
351	s	A:LEU 430		8.30	0.00	0.00
352	s	A:GLU 431		98.32	0.00	0.00
353	s	A:ASN 432		86.61	0.00	0.00
354	s	A:VAL 433		18.64	0.00	0.00
355	s	A:TYR 434		0.92	0.00	0.00
356	I	A:PRO 435		84.15	3.91	-0.04
357	I	A:GLU 436		79.25	0.33	0.01
358	s	A:LEU 437		9.99	0.00	0.00
359	I	A:ARG 438		154.36	35.95	-0.63
360	s	A:VAL 439		62.46	0.00	0.00
361	s	A:PRO 440		7.07	0.00	0.00
362	s	A:ASP 441		75.99	0.00	0.00
363	s	A:HIS 442		149.29	0.00	0.00
364	s	A:GLN 443		74.50	0.00	0.00
365	s	A:ASP 444		10.41	0.00	0.00
366	s	A:ILE 445		40.67	0.00	0.00
367		A:ALA 446		0.00	0.00	0.00
368	s	A:PHE 447		15.43	0.00	0.00
369	s	A:GLY 448		2.02	0.00	0.00
370	s	A:ALA 449		13.77	0.00	0.00
371		A:LEU 450		0.00	0.00	0.00
372	s	A:GLN 451		63.30	0.00	0.00
373	s	A:GLN 452		27.48	0.00	0.00
374	s	A:GLY 453		67.89	0.00	0.00
375	s	A:THR 454		113.13	0.00	0.00
376	s	A:ASN 455		53.94	0.00	0.00
377	s	A:CYS 456		2.32	0.00	0.00
378		A:LEU 457		0.00	0.00	0.00
379	I	A:ASP 458		22.35	9.18	-0.13
380	s	A:THR 459		0.24	0.00	0.00
381	I	A:LEU 460		59.57	13.41	-0.12
382	I	A:GLY 461		45.60	33.53	0.00
383	I	A:HIS 462	H	77.87	53.23	-0.36
384	I	A:PHE 463		96.67	72.48	0.87
385	I	A:ALA 464		83.72	79.46	0.90
386	I	A:ASP 465		79.24	62.02	0.06
387	I	A:GLY 466		9.69	0.17	0.00
388	s	A:VAL 467		40.44	0.00	0.00
389	s	A:VAL 468		0.17	0.00	0.00
390	s	A:GLY 469		3.34	0.00	0.00
391	I	A:VAL 470		40.81	3.56	-0.04
392	I	A:TYR 471	H	129.98	102.37	0.94
393	I	A:GLU 472		124.78	47.03	-0.01
394	I	A:CYS 473	H	29.01	7.72	-0.09
395	I	A:HIS 474		126.23	82.45	-0.40
396	I	A:ASN 475		155.01	24.95	-0.22
397	s	A:GLY 478		80.33	0.00	0.00
398	I	A:ASN 479		59.06	3.01	0.05
399	I	A:GLN 480	H	34.63	6.49	-0.04
400	s	A:GLU 481		57.56	0.00	0.00
401	s	A:TRP 482		1.97	0.00	0.00
402	s	A:ALA 483		11.71	0.00	0.00
403	s	A:LEU 484		0.33	0.00	0.00
404	s	A:THR 485		9.03	0.00	0.00
405	s	A:LYS 486		116.38	0.00	0.00
406	s	A:GLU 487		88.06	0.00	0.00
407	s	A:LYS 488		58.77	0.00	0.00
408	s	A:SER 489		12.78	0.00	0.00
409		A:VAL 490		0.00	0.00	0.00
410	s	A:LYS 491		52.63	0.00	0.00
411	I	A:HIS 492	H	26.82	12.38	0.48
412	I	A:MET 493		129.86	69.45	2.03
413	I	A:ASP 494	H	98.12	56.47	-0.49
414	I	A:LEU 495		20.90	20.73	0.33
415	s	A:CYS 496		0.17	0.00	0.00
416		A:LEU 497		0.00	0.00	0.00
417		A:THR 498		0.00	0.00	0.00
418	s	A:VAL 499		3.02	0.00	0.00
419	I	A:VAL 500		70.61	19.22	0.31
420	s	A:ASP 501		71.93	0.00	0.00
421	s	A:ARG 502		118.29	0.00	0.00
422	s	A:ALA 503		51.87	0.00	0.00
423	s	A:PRO 504		88.34	0.00	0.00
424	s	A:GLY 505		31.12	0.00	0.00
425	s	A:SER 506		20.66	0.00	0.00
426	s	A:LEU 507		60.16	0.00	0.00
427	s	A:ILE 508		0.50	0.00	0.00
428	I	A:LYS 509		41.04	7.05	-0.26
429	s	A:LEU 510		0.34	0.00	0.00
430	I	A:GLN 511	H	38.42	37.08	-0.10
431	I	A:GLY 512	H	40.70	31.21	0.16
432	s	A:CYS 513		43.81	0.00	0.00
433	I	A:ARG 514	H	146.21	73.12	-0.44
434	I	A:GLU 515		159.49	27.60	-0.42
435	s	A:ASN 516		130.23	0.00	0.00
436	s	A:ASP 517		21.78	0.00	0.00
437	s	A:SER 518		62.64	0.00	0.00
438	I	A:ARG 519		67.41	12.53	-0.31
439	s	A:GLN 520		2.83	0.00	0.00
440	s	A:LYS 521		51.71	0.00	0.00
441	s	A:TRP 522		0.15	0.00	0.00
442	s	A:GLU 523		45.77	0.00	0.00
443	s	A:GLN 524		36.50	0.00	0.00
444	s	A:ILE 525		26.75	0.00	0.00
445	s	A:GLU 526		119.99	0.00	0.00
446	s	A:GLY 527		70.33	0.00	0.00
447	s	A:ASN 528		35.19	0.00	0.00
448	s	A:SER 529		30.84	0.00	0.00
449	s	A:LYS 530		3.98	0.00	0.00
450	s	A:LEU 531		2.37	0.00	0.00
451	s	A:ARG 532		76.02	0.00	0.00
452	s	A:HIS 533		0.46	0.00	0.00
453	s	A:VAL 534		47.48	0.00	0.00
454	s	A:GLY 535		70.64	0.00	0.00
455	s	A:SER 536		26.18	0.00	0.00
456	s	A:ASN 537		94.91	0.00	0.00
457	s	A:LEU 538		9.03	0.00	0.00
458	s	A:CYS 539		0.17	0.00	0.00
459	s	A:LEU 540		0.12	0.00	0.00
460		A:ASP 541		0.00	0.00	0.00
461	s	A:SER 542		12.78	0.00	0.00
462	s	A:ARG 543		144.01	0.00	0.00
463	s	A:THR 544		26.61	0.00	0.00
464	s	A:ALA 545		37.71	0.00	0.00
465	s	A:LYS 546		205.87	0.00	0.00
466	s	A:SER 547		94.37	0.00	0.00
467	s	A:GLY 548		31.89	0.00	0.00
468	s	A:GLY 549		1.99	0.00	0.00
469		A:LEU 550		0.00	0.00	0.00
470		A:SER 551		0.00	0.00	0.00
471	s	A:VAL 552		0.17	0.00	0.00
472	s	A:GLU 553		20.80	0.00	0.00
473	s	A:VAL 554		78.72	0.00	0.00
474	s	A:CYS 555		37.06	0.00	0.00
475	s	A:GLY 556		21.97	0.00	0.00
476	s	A:PRO 557		132.44	0.00	0.00
477	s	A:ALA 558		26.91	0.00	0.00
478	s	A:LEU 559		144.13	0.00	0.00
479	s	A:SER 560		23.13	0.00	0.00
480	s	A:GLN 561		1.31	0.00	0.00
481	s	A:GLN 562		57.21	0.00	0.00
482	s	A:TRP 563		5.27	0.00	0.00
483	s	A:LYS 564		102.05	0.00	0.00
484	s	A:PHE 565		4.83	0.00	0.00
485	s	A:THR 566		57.55	0.00	0.00
486	s	A:LEU 567		2.68	0.00	0.00
487	s	A:ASN 568		18.01	0.00	0.00
488	s	A:LEU 569		50.73	0.00	0.00
489	s	A:GLN 570		148.39	0.00	0.00