Supporting Information

Engineering DszC mutants from transition state macrodipole considerations and evolutionary sequence analysis

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Modeling of the QM/MM model of the DszC:DBT complex

The DszC:DBT complex was modelled in the catalytically-competent homodimeric form (chain A and F, with 417 residues each, from PDB ID 3X0Y with 2.3 Å resolution), in complex with the FMN cofactor in the oxidized form and with all X-ray waters within 6 Å of each catalytic site.[1] The FMN cofactor was modelled as C^{4a}-hydroperoxyflavin intermediate (C^{4a}OOH), as there was a well-defined electronic density for FMN in the active site of DszC that suggested a tight-binding of FMN to the active site of DszC. The binding pose of DBT was modelled as in the TdsC homolog enzyme from *Paenibacillus sp.* (64% identity and identical active site residues) binding oxidized FMN and DBT (PDB ID: 5XDE),[2] after aligning the conserved FMN cofactor and the backbone of catalytic residues His92, Ser163, His391 of both DszC and TdsC. As predicted by the Propka3.1 program,[3] physiological protonation states were attributed to all residues except His92, His388 and His391: His92 and His388 were protonated as δ-tautomers and His391 was doubly-protonated as in the imidazolium form.

The DszC homodimer was described with the ff10 force field[4], whereas DBT and C^{4a}OOH were parameterized with the GAFF[5] and with RESP charges derived after geometry optimization of each molecule at the HF/6-31G* level – using the Antechamber module available in AMBER12 and the Gaussian software for QM calculations[6]. The Xleap module of AMBER12 was used to add 33 Na^+ ions to counteract the overall positive charge of the system, and to add TIP3P waters[7] to fill a rectangular box with faces at a minimum distance of 12 Å from the solute. Afterwards, a four-step molecular mechanics (MM) energy minimization protocol was applied to remove bad contacts in the system: (1) positional harmonic restraints of 50 kcal·mol^{-1} were applied to water molecules; (2) positional harmonic restraints of 50 kcal·mol^{-1} were applied to all heavy atoms; (3) positional harmonic restraints of 10 kcal·mol^{-1} were applied backbone atoms of the solute; and (4) no restraints were applied.

The QM/MM model proceeding for ONIOM calculations was taken from the final minimized structure of the MM protocol. It comprised one monomer binding C^{4a}OOH and DBT, all residues of the second monomer within a radius of 18 Å from the His92, Tyr96, Asn129, Ser163, His388 and His391, C^{4a}OOH and DBT in the first monomer, and the water molecules at least 6 Å away from the catalytic site – in a total of 7238 atoms and total charge of -15. The QM layer included all atoms of DBT, the isoalloxazine ring (except for the two methyl groups in the phenyl moiety), the N^{10}-bound hydroxymethyl of the ribitol tail of C^{4a}OOH, and the side chains of residues His92, Tyr96, Asn129, Ser163, His388 and His391 – a total of 112 atoms, zero total charge and singlet multiplicity – whereas the MM layer comprised all the remaining atoms of the model. All atoms beyond a radius of 15 Å from the molecules composing the QM layer were kept rigid throughout the ONIOM calculations. All ONIOM calculations were ran with the Gaussian software.

All QM/MM calculations were carried out at the B3LYP/6-31G(d):ff10 level of theory,[8-16] with the Coulomb QM/MM interactions calculated with the electrostatic embedding scheme, as implemented in Gaussian 09.[6] The B3LYP/6-31G(d) level has been successfully employed in other QM/MM studies of the catalytic mechanism of enzymes.[17-20] In particular, to study the triplet-singlet spin inversion taking place upon formation of the C^{4a}OOH, we allowed break of the symmetry of the singlet configuration by accepting the inclusion of imaginary coefficients and/or mixed-spin orbitals in the wavefunction.[21-23] We used hydrogens as link atoms to complete the valence of the bonds in the boundary of the two layers.[24-27]

Transition state macrodipole calculations with different density functionals and basis sets

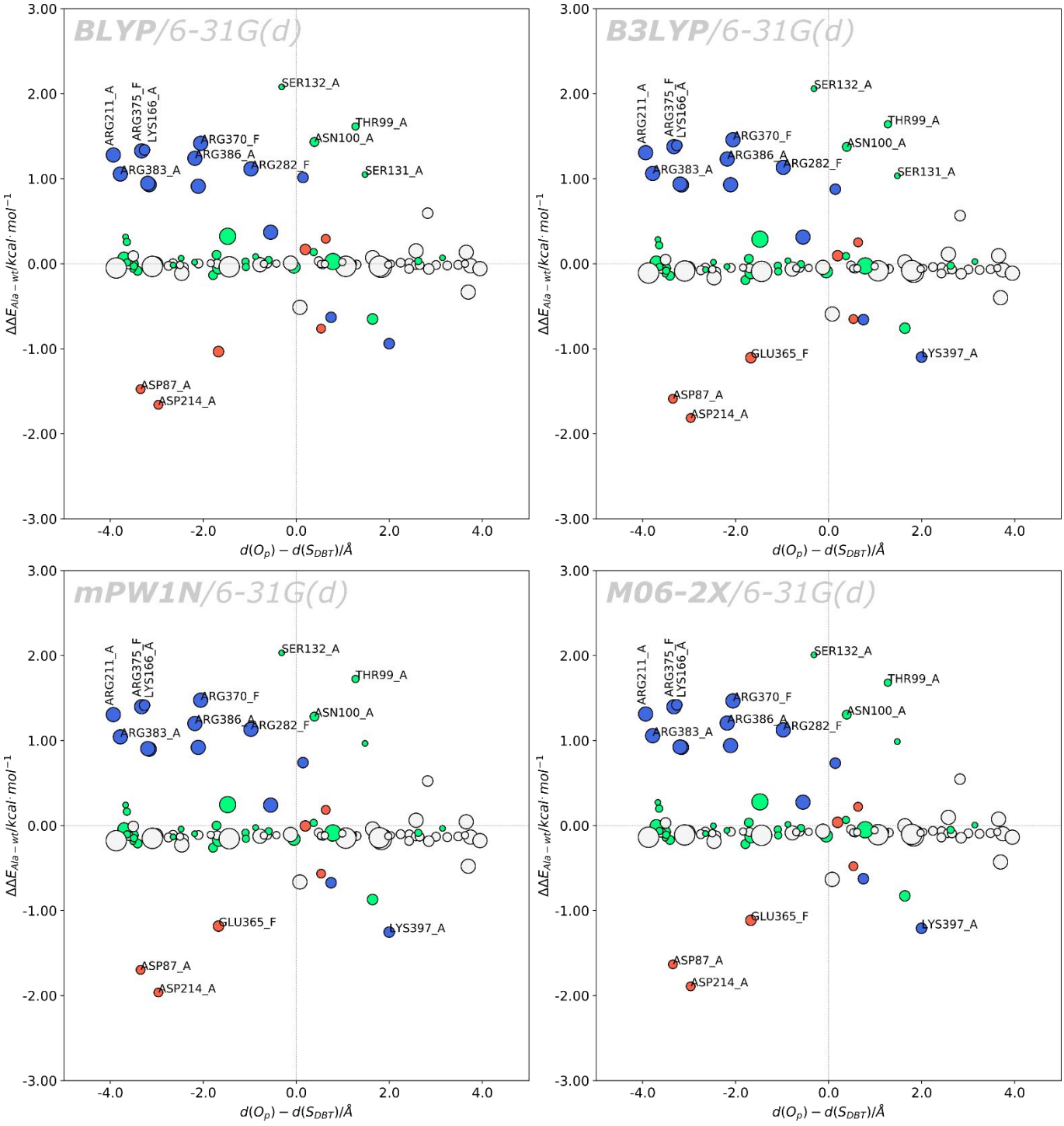

Figure S1. Activation energy differences upon alanine mutation for different density functionals (BLYP, B3LYP, mPW1N and M06-2X) as a function of the relative proximity of each residue to the O_p and the S_{DBT} atoms. Activation energy differences are calculated relatively to the activation energy of the wild-type form at the same level of theory; to determine the representative position of charged residues, only the heavy atoms of the charged group were considered to describe the position of the residue relatively to the active site, whereas the heavy atoms of the whole sidechain were considered for the remaining residues. Larger markers represent bulkier amino acids. Residues whose mutation provides a change larger than |1.0 kcal·mol-1| in the activation energy are labelled. Residues colored in blue and red correspond to positively and negatively charged residues, and those colored in green and gray correspond to polar and apolar residues. All calculations were performed at the ONIOM(DFT/6-31G(d):AMBER) level of theory.

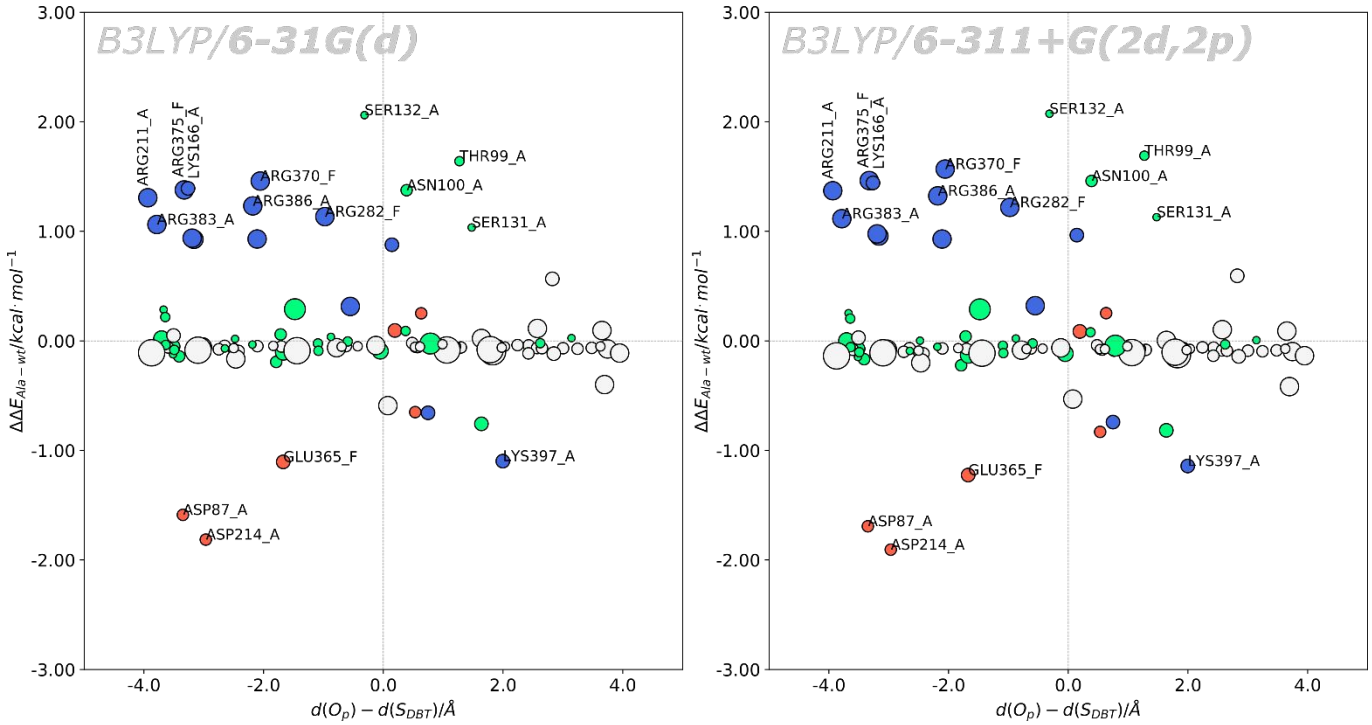

Figure S2. Activation energy differences upon alanine mutation for different basis sets (6-31G(d) and 6-311+G(2d,2p)) as a function of the relative proximity of each residue to the O_p and the S_{DBT} atoms. Activation energy differences are calculated relatively to the activation energy of the wild-type form at the same level of theory; to determine the representative position of charged residues, only the heavy atoms of the charged group were considered to describe the position of the residue relatively to the active site, whereas the heavy atoms of the whole sidechain were considered for the remaining residues. Larger markers represent bulkier amino acids. Residues whose mutation provides a change larger than |1.0 kcal·mol-1| in the activation energy are labelled. Residues colored in blue and red correspond to positively and negatively charged residues, and those colored in green and gray correspond to polar and apolar residues. All calculations were performed at the ONIOM(B3LYP:AMBER) level of theory.

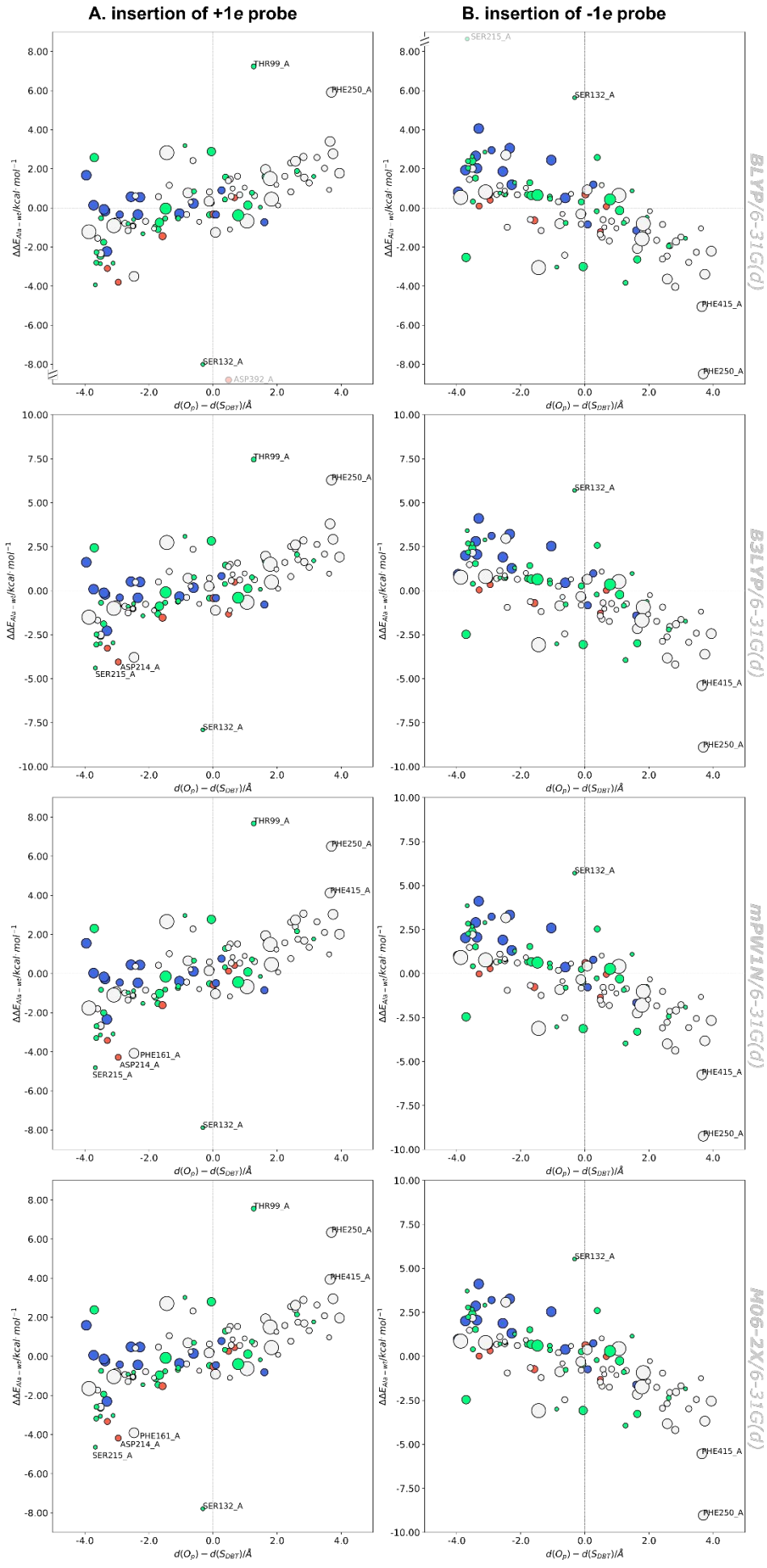
A. insertion of +1e probe
B. insertion of -1e probe
BLYP/6-31G(d)
B3LYP/6-31G(d)
mPWIN/6-31G(d)
M06-2X/6-31G(d)
THR99_A
PHE250_A
SER132_A
ASP392_A
SER215_A
PHE415_A
ASP214_A
PHE161_A
$\Delta\Delta E_{Ala-wt}$/kcal mol^{-1}
$d(O_p) - d(S_{DBT})$/Å

Figure S3. Activation energy differences for different density functionals (BLYP, B3LYP, mPW1N and M06-2X) upon insertion of a unitary probe charge in the geometric centre of the sidechain of the residues within 10 Å of the active site of DszC, as a function of the distance of the sidechain centre of mass to the O_p and S_{DBT} atoms. Larger markers represent bulkier amino acids. Since most residues are composed of C, N and O, we assumed for simplicity that the geometric center of each sidechain should closely resemble their centre of mass. Residues in which the probe insertion leads to a change larger than 50% of the maximum energy difference relative to the activation energy are labelled. Residues colored in blue and red correspond to positively and negatively charged residues, and those colored in green and gray correspond to polar and apolar residues.

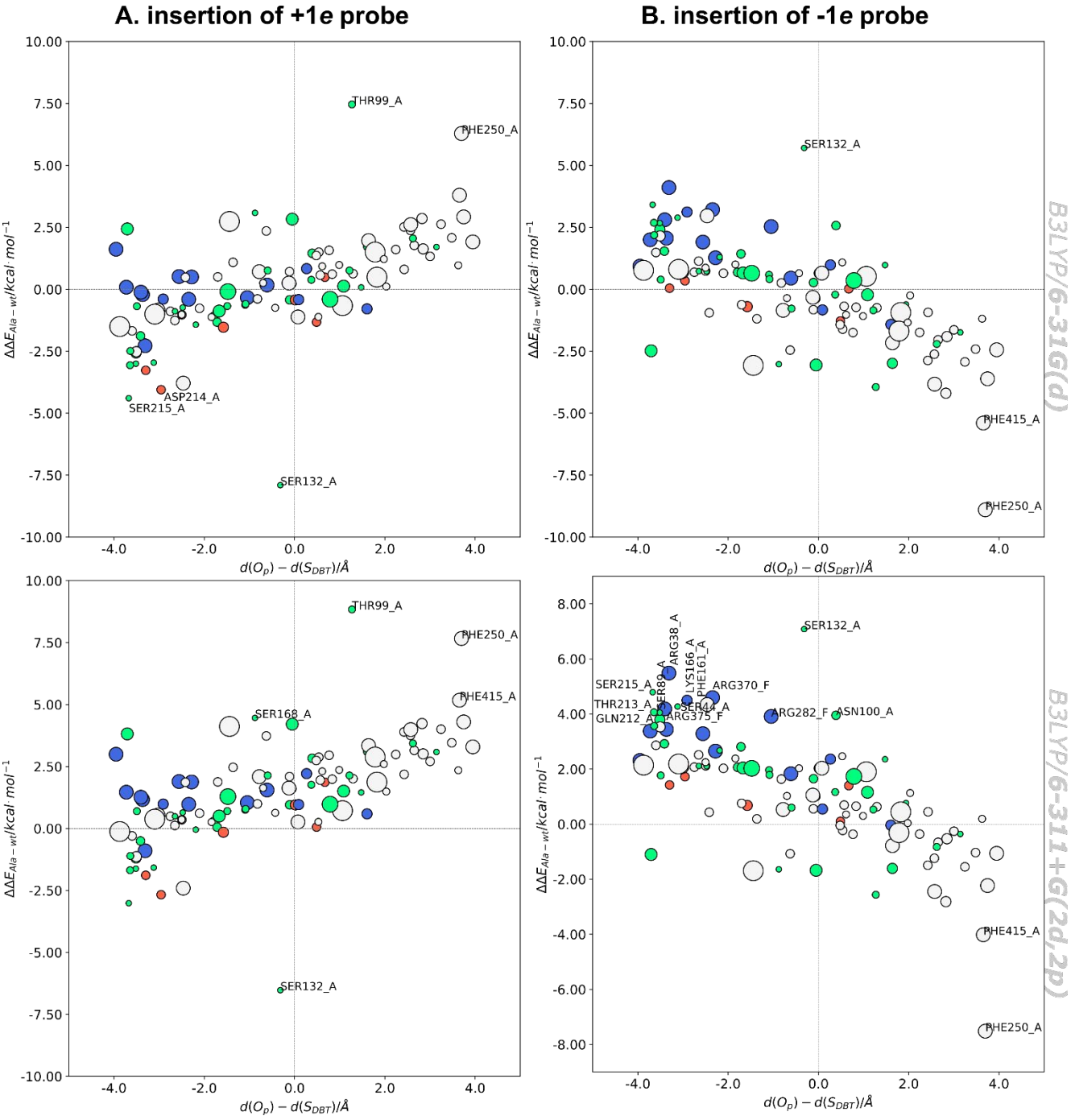

Figure S4. Activation energy differences for different basis sets (6-31G(d) and 6-311+G(2d,2p)) upon insertion of a unitary probe charge in the geometric centre of the sidechain of the residues within 10 Å of the active site of DszC, as a function of the distance of the sidechain centre of mass to the O_p and S_{DBT} atoms. Larger markers represent bulkier amino acids. Since most residues are composed of C, N and O, we assumed for simplicity

that the geometric center of each sidechain should closely resemble their centre of mass. Residues in which the probe insertion leads to a change larger than 50% of the maximum energy difference relative to the activation energy are labelled. Residues colored in blue and red correspond to positively and negatively charged residues, and those colored in green and gray correspond to polar and apolar residues.

Positional conservation scores obtained from the ConSurf server

	pos	ALA	CYS	ASP	GLU	PHE	GLY	HIS	ILE	LYS	LEU	MET	ASN	PRO	GLN	ARG	SER	THR	VAL	TRP	TYR	MAX AA	ConSurf Grade
MET	1											100.0										M 100.000	6*
THR	2																	100.0				T 100.000	8*
LEU	3										100.0											L 100.000	7*
SER	4																40.0	60.0				T 60.000	7*
PRO	5													80.0					20.0			P 80.000	6*
GLU	6	20.0			40.0									20.0				20.0				E 40.000	3*
LYS	7			20.0				20.0		40.0						20.0						K 40.000	3*
GLN	8					20.0									40.0			20.0		20.0		Q 40.000	1*
HIS	9							50.0							16.7		16.7	16.7				H 50.000	4*
VAL	10			12.5			12.5				12.5							25.0	37.5			V 37.500	2*
ARG	11	20.0					10.0			10.0						40.0	10.0	10.0				R 40.000	2*
PRO	12	16.7		8.3										66.7				8.3				P 66.667	5
ARG	13	25.0		12.5			6.3							6.3	6.3	25.0		12.5			6.3	AR 25.000	1
ASP	14	18.2		9.1		4.5	4.5				9.1		4.5	36.4	4.5	4.5		4.5				P 36.364	1
ALA	15	53.3		3.3	3.3		3.3	3.3						10.0		6.7	16.7					A 53.333	5
ALA	16	20.5		28.2	7.7		2.6								2.6	7.7	7.7	20.5	2.6			D 28.205	3
ASP	17	12.2		34.1	4.9	2.4	2.4	4.9			7.3		2.4	4.9	4.9	7.3	4.9	7.3				D 34.146	1
ASN	18	32.1		9.4	5.7	3.8				5.7			9.4	7.5	9.4	1.9	5.7	5.7	1.9		1.9	A 32.075	1
ASP	19	4.7		40.6	20.3		4.7	3.1					4.7	3.1	3.1	1.6	6.3	7.8				D 40.625	4
PRO	20	25.4				1.5		1.5	3.0		3.0			29.9			1.5		1.5	26.9	6.0	P 29.851	3
VAL	21	1.4		1.4		2.7			20.5		57.5		1.4		1.4	1.4			9.6	2.7		L 57.534	2
ALA	22	52.1		6.4	6.4		1.1	1.1		1.1	2.1		1.1	2.1	9.6	8.5	3.2	3.2	2.1			A 52.128	4
VAL	23	8.9		1.0					17.8	5.0	4.0	1.0		1.0	3.0	15.8	4.0	9.9	28.7			V 28.713	3
ALA	24	84.2				0.9			0.9		4.4							1.8	7.9			A 84.211	8
ARG	25	16.4		12.3	13.9		3.3	3.3	1.6	3.3					11.5	26.2	2.5	4.1	1.6			R 26.230	1
GLY	26	19.4		11.6	27.9	1.6	2.3	0.8		3.1	3.1				8.5	9.3	10.9	1.6				E 27.907	1
LEU	27	3.7				0.7			3.0		56.3	0.7						2.2	33.3			L 56.296	7
ALA	28	74.6	0.7				0.7		3.6		2.2					6.5	6.5	1.4	3.6			A 74.638	7
GLU	29	36.7		18.0	17.3		0.7	0.7		1.4	0.7		1.4	2.2	10.1	4.3	2.2	2.9	1.4			A 36.691	1
LYS	30	12.7		8.5	21.8		1.4	1.4	7.7	4.2	2.8		0.7		7.0	12.7	2.1	8.5	7.7		0.7	E 21.831	1
TRP	31	0.7				33.8			2.1		61.3									2.1		L 61.268	7
ARG	32	59.4		1.4	2.8		0.7	2.1		0.7					0.7	22.4	4.2	3.5	0.7		1.4	A 59.441	6
ALA	33	34.2		0.7	10.3				1.4	6.8	6.2			4.1	4.8	9.6	3.4	8.9	9.6			A 34.247	1
THR	34			32.7			7.5						2.7			4.1	8.8	44.2				T 44.218	7
ALA	35	93.9					1.4		0.7		0.7				0.7				2.7			A 93.878	9
VAL	36	35.6	0.7	0.7	0.7		1.3		2.0		7.4		1.3	4.0			4.7	0.7	40.9			V 40.940	4
GLU	37	22.8		4.7	51.0		0.7	1.3		2.0	2.7				5.4	1.3	0.7	4.0	3.4			E 51.007	3
ARG	38										4.7					95.3						R 95.302	9
ASP	39			92.6	7.4																	D 92.617	9
ARG	40	9.4			4.0			2.7	1.3	13.4	1.3				14.8	51.0	0.7	0.7			0.7	R 51.007	4
ALA	41	41.6		2.7	16.8		0.7	0.7	0.7	4.7	5.4				10.7	10.7	1.3	2.7	1.3			A 41.611	3
GLY	42	3.4		0.7			66.4				0.7		19.5		0.7	8.1		0.7				G 66.443	7
GLY	43	14.8			0.7		52.3		0.7	12.1	4.0				3.4	10.7		0.7	0.7			G 52.349	6
SER	44	6.0		2.7	2.7			16.8	0.7		8.7		4.0	9.4	1.3	5.4	9.4	30.9	1.3		0.7	T 30.872	6
ALA	45	27.5												72.5								P 72.483	8
THR	46	14.1	0.7	1.3	1.3	8.7		4.0		20.8	10.1				1.3	16.1	2.7	6.0	6.7	1.3	4.7	K 20.805	1
ALA	47	47.7		10.7	9.4	2.0	1.3	3.4	2.0	3.4	1.3		1.3	1.3	4.0	4.7	2.0	2.0	2.0		1.3	A 47.651	1
GLU	48	2.0		0.7	89.9						0.7				6.7							E 89.933	9
ARG	49	2.7							20.8	6.0	9.4					38.3			22.8			R 38.255	7
GLU	50	14.8		26.8	22.1		2.0		1.3	0.7			1.3		14.8	8.1	4.0	1.3	2.7			D 26.846	3
ASP	51	10.7		1.3	1.3			1.3	0.7	4.0	54.4	1.3			1.3	15.4	0.7	0.7	0.7	6.0		L 54.362	4
LEU	52					2.7			23.5		72.5	0.7							0.7			L 72.483	7
ARG	53	4.7								25.5						61.7	6.7	1.3				R 61.745	8
ALA	54	20.8		20.1	18.1		2.0	8.7		3.4			4.0		14.8	4.7	2.0	0.7			0.7	A 20.805	1

Table S1. Per residue variety for each position in the sequence of DszC, after the multi-sequence analysis performed by the ConSurf server

SER	**55**	22.1			0.7		0.7	3.4			1.3		1.3		1.3		67.8		0.7		0.7	S 67.785	7
GLY	**56**			4.0			94.6			0.7						0.7						G 94.631	9
LEU	**57**										100.0											L 100.000	9
LEU	**58**	0.7					0.7				81.2		1.3	2.0	0.7			2.7	9.4	1.3		L 81.208	8
SER	**59**	18.9		2.7	1.4		7.4	0.7		10.1	1.4		7.4	3.4	3.4	4.1	12.2	26.4			0.7	T 26.351	2
LEU	**60**	8.1				1.4			5.4		68.9	0.7							15.5			L 68.919	7
LEU	**61**	17.8				0.7	2.7		4.8		33.6	1.4			2.7		21.9	11.0	2.7	0.7		L 33.562	6
VAL	**62**	2.7		1.4	4.1	0.7	14.4	4.8	38.4		2.7		0.7				0.7	2.7	26.7			I 38.356	6
PRO	**63**	6.8					0.7				0.7			89.7			1.4			0.7		P 89.726	8
ARG	**64**	22.6	0.7		3.4		3.4	0.7		17.1			0.7	6.2	2.7	21.2	0.7	10.3	10.3			A 22.603	2
GLU	**65**	21.9	0.7	3.4	47.9		0.7	0.7		6.2			0.7	0.7	10.3	3.4	2.1	0.7		0.7		E 47.945	3
TYR	**66**	2.1			0.7	21.9		21.2	4.8		9.6		0.7				0.7		2.1	1.4	34.9	Y 34.932	2
GLY	**67**			0.7			98.6								0.7							G 98.630	9
GLY	**68**			0.7			99.3															G 99.315	9
TRP	**69**	19.2		2.7	4.8	0.7	26.7	4.8	0.7		13.0	0.7	0.7	0.7	13.0	1.4	3.4	1.4	0.7	3.4	2.1	G 26.712	1
GLY	**70**	2.1		6.8	11.6		76.0			0.7			0.7		1.4		0.7					G 76.027	5
ALA	**71**	40.5			7.4		8.1	1.4	0.7	0.7	14.2				17.6		0.7	0.7	7.4	0.7		A 40.541	5
ASP	**72**	2.0		26.2	2.7		6.0	2.0					9.4	15.4	0.7	7.4	20.8	7.4				D 26.174	1
TRP	**73**	4.0				2.7		1.3			4.0			0.7	1.3			0.7	0.7	79.2	5.4	W 79.195	7
PRO	**74**	13.4		3.4	5.4		2.7	2.0	2.7	2.0	4.7			20.1	8.1	3.4	18.1	5.4	8.7			P 20.134	1
THR	**75**	3.4		12.1	11.4	0.7			2.7		7.4		0.7		10.7	1.3	2.7	38.3	8.7			T 38.255	4
ALA	**76**	30.2				2.0	9.4		17.5		10.7	0.7			1.3		2.0	16.1	10.1			A 30.201	6
ILE	**77**	7.4	0.7			11.4		2.7	1.3		35.6	2.0	0.7		4.0		1.3	1.3	1.3		30.2	L 35.570	4
GLU	**78**	10.1		4.0	17.5		3.4	4.0		14.8	2.7		1.3		13.4	26.8	1.3	0.7				R 26.846	2
VAL	**79**	10.7	0.7				1.3	1.3	25.5		8.7							8.7	43.0			V 42.953	4
VAL	**80**	1.3				6.0	1.3		26.2		4.0		0.7				3.4	7.4	49.7			V 49.664	5
ARG	**81**	1.3					0.7			0.7					3.4	93.3		0.7				R 93.289	9
GLU	**82**	5.4			31.5		0.7	0.7	18.1	2.0	8.7				4.0	21.5		4.7	2.7			E 31.544	3
ILE	**83**					18.8			30.9		28.2	2.0							20.1			I 30.872	5
ALA	**84**	88.6					3.4										8.1					A 88.591	9
ALA	**85**	22.1			4.0					18.8					8.7	36.9	5.4	3.4	0.7			R 36.913	4
ALA	**86**	40.3					19.5				0.7						1.3	5.4	32.9			A 40.268	6
ASP	**87**			95.3	4.7																	D 95.302	9
GLY	**88**	8.1					36.2							3.4			47.0	5.4				S 46.980	8
SER	**89**	18.8											2.0				79.2					S 79.195	9
LEU	**90**	0.7				0.7			43.0		40.9	0.7					0.7		13.4			I 42.953	6
GLY	**91**	61.7					38.3															A 61.745	8
HIS	**92**							59.7				6.7			33.6							H 59.732	9
LEU	**93**								9.4		65.1								25.5			L 65.101	7
PHE	**94**					29.5			3.4		44.3			8.1					2.7		12.1	L 44.295	6
GLY	**95**	19.5					66.4				1.3				8.1		3.4	0.7	0.7			G 66.443	6
TYR	**96**		2.0			36.9		0.7					6.0				5.4				49.0	Y 48.993	8
HIS	**97**							82.6					0.7		15.4			1.3				H 82.550	8
LEU	**98**		2.7			16.1		35.6	1.3		10.7				1.3			0.7	0.7		30.9	H 35.570	6
THR	**99**	5.4				3.4	2.0	0.7	0.7		65.8		1.3				4.7	2.0	13.4		0.7	L 65.772	6
ASN	**100**		2.0				3.4	4.0			13.4	11.4	12.1	4.0	26.8		2.0			14.8	6.0	Q 26.846	6
ALA	**101**	6.0			0.7	2.7	3.4		10.1		28.9	0.7	1.3		3.4		17.5	3.4	22.1			L 28.859	6
PRO	**102**	34.2		0.7	0.7	0.7	2.0	2.0	4.0	0.7	1.3		8.1	1.3	7.4	4.0	0.7	8.1	9.4	14.1	0.7	A 34.228	5
MET	**103**	9.4				0.7	4.7	0.7	7.4		3.4	2.0	6.0			4.0	15.4	30.2	8.1	3.4	4.7	T 30.201	6
ILE	**104**	22.1				0.7	2.0		18.1		7.4	0.7		9.4			2.7	6.0	30.9			V 30.872	4
GLU	**105**	4.0		5.4	6.0		4.7	8.7	2.0		10.7	0.7	6.0		7.4	30.2	3.4	2.0	2.7		6.0	R 30.201	2
LEU	**106**	1.3				9.4	0.7		10.7		51.0	0.7				6.7		1.3	10.7	7.4		L 51.007	6
ILE	**107**	6.7			0.7	36.9	1.3	0.7	0.7		5.4	0.7			6.0	4.7	2.7	1.3	16.1	4.7	11.4	F 36.913	5
GLY	**108**	15.3		2.0	1.3	0.7	70.7		0.7		2.0				0.7	0.7	4.7	0.7	0.7			G 70.667	5
SER	**109**	3.4		5.4	4.0		3.4		0.7	1.3			7.4	0.7	4.0	11.4	22.8	34.2	1.3			T 34.228	3
GLN	**110**	12.8		10.1	10.7		2.7	0.7		0.7	2.0		0.7	47.7	2.7	5.4	1.3	2.7				P 47.651	1
GLU	**111**	31.8		8.1	45.3	0.7	2.7	1.4			0.7			0.7	3.4	1.4	1.4	1.4	1.4			E 45.270	3
GLN	**112**	0.7			0.7		0.7	1.4		0.7	5.4				82.4	4.7		2.0	1.4			Q 82.432	8
GLU	**113**	23.0			1.4		2.0	3.4	6.8	8.8	0.7				12.8	14.2	1.4	0.7	4.1	16.9	4.1	A 22.973	5
GLU	**114**	18.2		7.4	35.8		0.7	2.7		3.4			0.7	1.4	15.5	9.5	1.4	1.4	0.7	1.4		E 35.811	1
HIS	**115**	15.5		4.1	4.1	8.8		6.1		2.7	0.7		2.7	10.1	4.1	33.1	2.0	2.7	0.7		2.7	R 33.108	1
LEU	**116**	0.7				18.9	0.7	1.4	8.8		20.9	0.7			0.7	0.7	0.7	2.0	7.4	25.0	11.5	W 25.000	1

TYR	**117**	4.7		1.4	10.1	18.9	4.7	1.4	2.0		26.4				8.1	0.7	6.8	2.0		0.7	12.2	L 26.351	3
THR	**118**	10.8		1.4	15.5		6.8			8.8	0.7			1.4	2.7	35.1	5.4	9.5	2.0			R 35.135	2
GLN	**119**	10.0		4.0	22.0	1.3	11.3	2.7	1.3	2.7	11.3		0.7	2.7	11.3	16.0	0.7		0.7	1.3		E 22.000	1
ILE	**120**	8.0				0.7	0.7		9.3		2.7		4.0				12.7	51.3	8.0		2.7	T 51.333	7
ALA	**121**	36.7	0.7				2.7		8.7		9.3	0.7				0.7	0.7	9.3	30.7			A 36.667	5
GLN	**122**	22.0		2.7	23.3		1.3	1.3		4.0			2.0		8.7	20.0	10.0	4.7				E 23.333	1
ASN	**123**	2.0		1.3	18.0	0.7	18.7	10.7		8.7	2.0		22.7	0.7	9.3	4.0	1.3					N 22.667	2
ASN	**124**	2.0		5.3	1.3		9.3	2.0		7.3	0.7		32.7		9.3	25.3	4.0	0.7				N 32.667	3
TRP	**125**	0.7	0.7			0.7	0.7	1.3			22.0		0.7	0.7	1.3	8.0		0.7		54.7	8.0	W 54.667	4
TRP	**126**		3.3			71.3			0.7		9.3								2.0	8.7	4.7	F 71.333	7
THR	**127**					8.0		0.7	1.4						3.6			1.4	5.8	77.5	1.4	W 77.536	8
GLY	**128**	5.3	2.7				88.0										4.0					G 88.000	8
ASN	**129**	4.7		3.3			29.3						60.0				2.0	0.7				N 60.000	9
ALA	**130**	70.7					5.3		2.0								4.7	6.7	10.7			A 70.667	8
SER	**131**	2.7				4.7	4.0		2.0		33.3	0.7	0.7		10.0		8.7	2.7	30.7			L 33.333	6
SER	**132**	3.3		0.7				6.7					86.7		0.7		2.0					N 86.667	9
GLU	**133**	5.4			1.3		0.7							75.8		2.0	5.4	2.0	7.4			P 75.839	7
ASN	**134**												100.0									N 100.000	6*
ASN	**135**												100.0									N 100.000	6*
SER	**136**																100.0					S 100.000	6*
HIS	**137**							100.0														H 100.000	6*
VAL	**138**																		100.0			V 100.000	6*
LEU	**139**	3.3				2.7		0.7			40.0	2.0	1.3		8.0	38.7		0.7	2.7			L 40.000	7
ASP	**140**			84.7	3.3		4.7						1.3		0.7		4.7				0.7	D 84.667	9
TRP	**141**	9.3		2.7	1.3		5.3		6.7	12.0	2.7		3.3	18.7	2.7	12.0	5.3	16.0	0.7	1.3		P 18.667	2
LYS	**142**	4.7		18.0	1.3		10.0	2.0		2.7			0.7	2.0	1.3	46.7	6.7	3.3		0.7		R 46.667	6
VAL	**143**	5.3	0.7	0.7			1.3	0.7	1.3		43.3						6.7	30.0	10.0			L 43.333	6
ARG	**144**	2.7			7.3	2.0		0.7	6.7	10.7	4.0	0.7			6.0	17.3	2.7	20.7	18.7			T 20.667	1
ALA	**145**	30.7	1.3				4.7		14.0		33.3	1.3					2.0		12.7			L 33.333	6
THR	**146**	7.3		0.7	6.0		0.7	2.0	1.3	7.3	2.0		0.7		4.0	12.0	7.3	45.3	2.7		0.7	T 45.333	3
PRO	**147**	8.0		10.0	10.7		0.7	1.3		7.3	1.3		0.7	22.0	3.3	24.7	6.7	1.3	0.7	1.3		R 24.667	1
THR	**148**	3.3		26.7	10.0	5.3	1.3	2.7	1.3	0.7	3.3		1.3		4.0	12.7	3.3	14.7	8.7		0.7	D 26.667	1
GLU	**149**	12.5			6.3		25.0						3.1	37.5		6.3	9.4					P 37.500	1
ASP	**150**	8.0		28.7	8.7		42.7			2.0			2.0	4.7	0.7		2.0	0.7				G 42.667	1
GLY	**151**	1.3		28.0	10.0		41.3	1.3		2.0			7.3	0.7	1.3		1.3	4.7			0.7	G 41.333	1
GLY	**152**	1.3		6.0	5.3	0.7	48.7	7.3	0.7	1.3			4.7		2.0	1.3	7.3	3.3		8.7	1.3	G 48.667	1
TYR	**153**		0.7			20.7		4.0	6.7		12.7				0.7	5.3	0.7		2.0	11.3	35.3	Y 35.333	1
VAL	**154**	3.3			10.7	2.0			6.7		12.7				1.3	26.7	0.7	2.0	32.7		1.3	V 32.667	1
LEU	**155**					27.3			5.3		52.0								11.3		4.0	L 52.000	6
ASN	**156**	1.3		24.0	2.0			5.3		0.7			37.3		3.3	1.3	16.0	8.0	0.7			N 37.333	5
GLY	**157**						100.0															G 100.000	9
THR	**158**	4.0		4.0	2.7	6.7		2.7	4.7	13.3	4.0		0.7	1.3	4.7	26.7	4.7	5.3	13.3		1.3	R 26.667	1
LYS	**159**									83.3					3.3	13.3						K 83.333	9
HIS	**160**	0.7				5.3	10.0	10.7					2.7	6.0		2.7	46.0	15.3			0.7	S 46.000	6
PHE	**161**					86.7															13.3	F 86.667	9
CYS	**162**	20.7	40.7				2.0						6.0				28.0	1.3	1.3			C 40.667	7
SER	**163**	1.3															54.7	44.0				S 54.667	9
GLY	**164**	2.7					96.0						1.3									G 96.000	9
ALA	**165**	55.3					9.3										20.7	8.7	6.0			A 55.333	7
LYS	**166**	8.0			0.7		2.0	9.3	4.0	8.7	18.0	1.3	1.3	0.7	2.0	10.7	13.3	3.3	16.0		0.7	L 18.000	3
GLY	**167**	0.7	0.7	26.0		8.0	18.7		12.0		2.7						0.7	1.3	29.3			V 29.333	6
SER	**168**	31.3					5.3										63.3					S 63.333	8
ASP	**169**			78.0	8.0			4.0							8.7		1.3					D 78.000	8
LEU	**170**	2.7	0.7					0.7	6.0		13.3	17.3			4.7	20.0			15.3	10.0	9.3	R 20.000	4
LEU	**171**								19.3		53.3	7.3	0.7			1.3	0.7	14.7	2.7			L 53.333	7
PHE	**172**	2.0				0.7		0.7	12.0		13.3	0.7	7.3	10.0	2.0		4.7	20.0	25.3	0.7	0.7	V 25.333	6
VAL	**173**	16.0	2.7			2.0			10.7		18.7							2.0	48.0			V 48.000	6
PHE	**174**	3.3			14.7	1.3	3.3				8.7		5.3			4.7	49.3	8.7		0.7		S 49.333	8
GLY	**175**	64.0				0.7	23.3		0.7		2.0								4.0	5.3		A 64.000	7
VAL	**176**	6.7		2.0	4.0	2.0		6.0	6.0		6.0			2.0	6.0	8.7	4.7	7.3	24.7	8.7	5.3	V 24.667	1
VAL	**177**					10.0			20.0		30.0							10.0	30.0			LV 30.000	2*
GLN	**178**	20.0			20.0		20.0								40.0							Q 40.000	4*

ASP	**179**			66.7									33.3									D 66.667	6*
ASP	**180**			60.0			40.0															D 60.000	5*
SER	**181**	7.5		25.6	2.3	1.5	4.5	10.5	1.5	3.8	15.8	0.8	5.3	0.8	3.8	7.5	1.5	4.5	1.5		1.5	D 25.564	1
PRO	**182**	10.9		10.9	35.7		3.9		0.8	3.1			1.6	13.2	6.2	1.6	5.4	3.9	2.3		0.8	E 35.659	2
GLN	**183**	12.1		22.7	9.1	3.0	20.5	1.5	0.8	1.5	6.1		3.0	3.8	1.5	0.8	6.1	3.8	3.0		0.8	D 22.727	1
GLN	**184**	6.8	1.5	11.3	3.0		14.3	2.3	1.5		0.8		3.0	3.8	2.3	1.5	10.5	36.1	1.5			T 36.090	1
GLY	**185**	4.0		21.5	8.1		46.3			2.0			3.4		5.4	2.0	5.4	2.0				G 46.309	1
ALA	**186**	12.0		10.7	15.3		5.3			19.3			3.3		8.7	14.0	4.7	6.0	0.7			K 19.333	1
ILE	**187**	4.7		0.7		4.0	0.7	14.7	6.0	4.0	36.0	0.7		12.7		9.3	0.7	1.3	4.7			L 36.000	4
ILE	**188**	6.7						6.0	14.7		30.0					3.3	0.7	1.3	32.0	2.7	2.7	V 32.000	4
ALA	**189**	6.0				28.7	2.0	1.3	21.3		5.3	1.3	2.7		0.7		2.7	8.0	18.0		2.0	F 28.667	4
ALA	**190**	57.3				11.3	9.3				11.3						0.7	1.3	7.3		1.3	A 57.333	6
ALA	**191**	29.3	0.7			4.7		1.3	12.0		7.3				2.0		3.3	2.7	30.0		6.7	V 30.000	4
ILE	**192**	1.3							30.7		17.3							0.7	50.0			V 50.000	6
PRO	**193**	1.3		9.3	3.3					2.7				82.0		0.7		0.7				P 82.000	7
THR	**194**	13.3			0.7		6.0	0.7		2.7	0.7			4.0		8.7	13.3	49.3			0.7	T 49.333	5
SER	**195**	9.3		28.7	2.7	0.7	14.7	2.0	0.7	3.3	0.7		8.7	0.7	6.0	10.0	8.0	4.0				D 28.667	1
ARG	**196**	12.7		0.7				2.7	0.7	0.7	0.7				13.3	60.0	4.0	3.3	1.3			R 60.000	7
ALA	**197**	18.0		12.7	18.7		0.7	3.3		2.0				29.3	3.3	0.7	6.0	5.3				P 29.333	1
GLY	**198**	1.3					98.7															G 98.667	9
VAL	**199**					5.3			47.3		12.0								30.7		4.7	I 47.333	5
THR	**200**	5.3	0.7	0.7	2.0		3.3	2.0	3.3	1.3	2.7		1.3		10.0	8.0	8.7	35.3	14.7		0.7	T 35.333	1
PRO	**201**	6.0	0.7			22.0		2.7	16.7	0.7	7.3			4.0		1.3	1.3	0.7	32.7		4.0	V 32.667	5
ASN	**202**	7.3		2.0	5.3	0.7	10.7	17.3	4.0	0.7	18.7	0.7	14.0	0.7	6.0	2.7	1.3	1.3	5.3		1.3	L 18.667	1
ASP	**203**	2.7		50.7	1.3		17.3	10.7					7.3	2.7	4.0	1.3	1.3				0.7	D 50.667	3
ASP	**204**			95.3			1.3						3.3									D 95.333	9
TRP	**205**	2.0					1.3													96.7		W 96.667	9
ALA	**206**	2.0		80.7	0.7			2.7		0.7			12.0				1.3					D 80.667	7
ALA	**207**	15.3					14.0	0.7					55.3	7.3			4.7	2.0			0.7	N 55.333	8
ILE	**208**					18.0			39.3		16.7	20.7							5.3			I 39.333	6
GLY	**209**						100.0															G 100.000	9
MET	**210**										6.0	2.0			92.0							Q 92.000	9
ARG	**211**									2.0						96.7		1.3				R 96.667	9
GLN	**212**	0.7	0.7								37.3				50.7	2.7		7.3	0.7			Q 50.667	9
THR	**213**	3.3															12.0	84.7				T 84.667	9
ASP	**214**	22.0		54.0	16.0		6.0										0.7		1.3			D 54.000	8
SER	**215**				0.7		2.7										96.7					S 96.667	9
GLY	**216**			1.3			97.3						1.3									G 97.333	9
SER	**217**	1.3					10.0						4.0		0.7	1.3	52.7	30.0				S 52.667	7
THR	**218**	4.7				1.3			5.3		0.7						2.7	2.7	82.0		0.7	V 82.000	8
ASP	**219**	2.0		4.0	17.3	1.3	0.7	6.0	4.7	5.3	2.0		2.7		3.3	15.3	10.7	18.0	6.7			T 18.000	1
PHE	**220**					74.0			12.0		10.7								1.3		2.0	F 74.000	8
HIS	**221**	4.7		28.0	29.3			8.7		4.0			9.3		2.7	4.7	1.3	4.0	3.3			E 29.333	2
ASN	**222**	4.7		24.7	0.7		14.0	1.3		4.7			21.3		12.0	12.7	4.0					D 24.667	2
VAL	**223**	2.7				4.0			1.3		2.7							2.7	86.0		0.7	V 86.000	9
LYS	**224**	6.7			8.7	2.7		2.0	0.7	6.7	8.0			12.7	2.0	37.3	2.7	4.7	4.7		0.7	R 37.333	1
VAL	**225**	3.3							15.3		13.3							2.0	66.0			V 66.000	6
GLU	**226**	12.0		6.0	24.0	2.0	2.7	2.7		3.3	2.7			23.3	1.3	6.0	4.0	3.3			6.7	E 24.000	1
PRO	**227**	18.9		10.1	12.8	0.7	1.4	6.1		5.4	0.7		2.0	16.2	0.7	6.1	2.0	1.4	0.7	14.9		A 18.919	1
ASP	**228**	12.8		35.1	12.2	0.7	3.4	8.1		2.7	0.7		4.1		1.4	1.4	13.5	3.4	0.7			D 35.135	1
GLU	**229**	7.3		22.7	50.0			1.3			1.3		1.3		4.7	6.0	4.0			1.3		E 50.000	6
VAL	**230**	15.3	0.7			4.7			18.0		18.7	1.3				1.3			40.0			V 40.000	6
LEU	**231**	7.3				4.0			5.3		78.0	0.7							4.7			L 78.000	7
GLY	**232**	5.3		2.0	0.7	1.3	42.7	4.0	1.3	1.3	13.3		1.3	8.7	6.0	2.0	3.3	4.7	2.0			G 42.667	3
ALA	**233**	10.2	0.7	12.2	6.1	6.8	2.7	6.1			2.0	0.7	6.8	9.5	2.7	6.8	8.2	0.7	4.1	8.2	5.4	D 12.245	1
PRO	**234**	4.1		8.8	2.0	0.7	3.4	8.8	0.7	0.7	9.5		0.7	43.2	1.4	1.4	4.1	1.4	8.8		0.7	P 43.243	4
ASN	**235**	8.8		14.3	8.2		32.7	1.4			6.8		2.0	9.5	0.7	1.4	8.2	3.4	2.7			G 32.653	1
ALA	**236**	15.4		3.7	7.4	2.9	0.7	2.9	1.5	8.1	2.2		1.5	24.3	8.1	2.9	6.6	7.4	4.4			P 24.265	1
PHE	**237**	6.9		6.2	6.9	1.5	4.6		1.5	3.8	21.5		2.3	18.5	4.6	1.5	6.2	7.7	3.8	0.8	1.5	L 21.538	1
VAL	**238**	6.2		8.5	6.2	8.5	10.0		0.8	9.2	2.3		0.8	13.1	1.5	0.8	23.8	3.8	2.3	1.5	0.8	S 23.846	2
LEU	**239**	15.4		13.5	3.8		11.5			17.3	1.9		1.9	3.8	17.3	7.7		3.8	1.9			KQ 17.308	1
ALA	**240**	17.6		5.9	7.8				2.0					45.1			7.8	7.8	5.9			P 45.098	2

PHE	241			50.0		16.7			16.7		8.3					8.3							D 50.000	3*
ILE	242								15.4		76.9				7.7								L 76.923	6
GLN	243	5.4				3.6	7.1			3.6	16.1	1.8			16.1	5.4	5.4	12.5	19.6	3.6			T 19.643	1
SER	244	1.3		3.3	4.7	6.7	0.7	2.0	4.7	2.0	2.7		2.7		4.0		7.3	22.0	34.7	1.3			T 34.667	4
GLU	245	8.0		1.3	3.3	0.7	0.7	0.7	1.3		1.3				59.3	2.7	4.7	0.7	2.0	12.7		0.7	P 59.333	4
ARG	246	2.0				34.7	6.0	0.7	0.7	0.7	4.7					4.0	26.0	1.3		0.7	2.0	16.7	F 34.667	4
GLY	247	40.0		4.0	2.7		3.3	1.3	2.0	0.7			8.0	9.3	5.3	0.7	17.3	4.0	1.3				A 40.000	4
SER	248	4.0	10.7				4.0	0.7			1.3					9.3		24.7	45.3				T 45.333	6
LEU	249		0.7			8.0			3.3		83.3	0.7							0.7	3.3			L 83.333	8
PHE	250	4.0	0.7	1.3		2.0	0.7	6.7	3.3		8.7		12.7				46.7	1.3	2.0	10.0			R 46.667	6
ALA	251	10.7				0.7	10.0		0.7		8.0		3.3	20.7				14.0	22.0	10.0			T 22.000	5
PRO	252	6.0	7.3					2.0	2.7		34.0	2.7		34.7	7.3				1.3	1.3		0.7	P 34.667	5
ILE	253	6.0				6.0	3.3	4.0	20.7		26.7	0.7			1.3		0.7	12.0	18.0		0.7		L 26.667	3
ALA	254	39.3				4.0	5.3	1.3	22.0		0.7	0.7			4.7		14.7	2.7	0.7	4.0			A 39.333	7
GLN	255							1.3							94.7	3.3						0.7	Q 94.667	9
LEU	256	4.7							3.3		81.3	0.7			0.7		8.0	0.7	0.7				L 81.333	7
ILE	257	6.0					0.7	2.0	26.7		10.7	1.3	2.7				0.7	3.3	46.0				V 46.000	6
PHE	258					40.7		6.7	2.0	2.0	40.0	3.3			1.3	0.7	3.3						F 40.667	8
ALA	259	31.3					4.0		2.7		4.0						9.3	20.7	28.0				A 31.333	5
ASN	260	8.7	0.7		2.7	0.7		14.0			0.7		59.3		8.0	0.7	2.7	0.7			1.3		N 59.333	7
VAL	261					27.3			27.3		30.0	3.3							12.0				L 30.000	6
TYR	262	0.7	2.7	8.0		20.0					4.0					1.3					63.3		Y 63.333	7
LEU	263	10.0							10.0		58.7				0.7			1.3	19.3				L 58.667	6
GLY	264	3.3					96.7																G 96.667	9
ILE	265								64.0		7.3	2.0	3.3				6.0	12.0	5.3				I 64.000	8
ALA	266	92.0					5.3										1.3	0.7	0.7				A 92.000	9
HIS	267	3.3		0.7	53.3	0.7	2.7	2.7	0.7	0.7	6.0	0.7			18.7	6.0	1.3	0.7	0.7	1.3			E 53.333	5
GLY	268	2.7		0.7			96.0						0.7										G 96.000	8
ALA	269	92.0					1.3		1.3		0.7						1.3	0.7	2.7				A 92.000	9
LEU	270			0.7		23.3		0.7	0.7		72.0				1.3	0.7			0.7				L 72.000	7
ASP	271	28.0		16.0	24.7		0.7	0.7	0.7	4.0			2.7		11.3	4.0	2.7	4.0	0.7				A 28.000	1
ALA	272	22.0		5.3	44.0	4.7	0.7		0.7				0.7		7.3	1.3	0.7	8.7	3.3		0.7		E 44.000	4
ALA	273	91.3				0.7	6.7											0.7	0.7				A 91.333	9
ARG	274	14.7	1.3		0.7	0.7		1.3	2.0	12.7	13.3		1.3		0.7	36.0	7.3	1.3	6.0	0.7			R 36.000	4
GLU	275	10.7		22.0	27.3		4.0	4.0		6.0			2.7	1.3	6.0	11.3	2.0	2.7					E 27.333	1
TYR	276	1.3				12.0		2.7			2.0	1.3				1.3		2.0		4.7	72.7		Y 72.667	7
THR	277	2.0				1.3	0.7		2.7		4.0						2.7	62.0	24.7				T 62.000	7
ARG	278	2.7					0.7	2.7		6.0	17.3	0.7	1.3		4.7	50.0	2.0	6.0	6.0				R 50.000	4
THR	279	12.3		6.2	15.8		2.1	2.1		8.2	2.7		2.1		3.4	5.5	4.1	35.6					T 35.616	2
GLN	280	4.7		1.3	13.3		2.7	9.3		12.0			5.3		14.7	9.3	8.7	14.7	1.3	1.3	1.3		QT 14.667	1
ALA	281	20.1		0.7			11.4	2.0		0.7	0.7			1.3	2.7	3.4	23.5	31.5	2.0				T 31.544	5
ARG	282	0.7					1.4			8.1			0.7		2.7	79.7	6.1		0.7				R 79.730	8
PRO	283	23.0						0.7			0.7			73.0			2.0		0.7				P 72.973	6
TRP	284					2.0											0.7			97.3			W 97.279	9
THR	285	3.4			4.1	20.4	0.7	4.8	16.3	0.7	12.9	1.4		17.7	2.0	1.4	2.7	2.0	8.8		0.7		F 20.408	2
PRO	286	16.8		2.7	10.1	5.4	2.0	9.4	0.7	3.4	8.1	1.3	2.0	4.0		3.4	4.7	15.4	2.0		8.7		A 16.779	3
ALA	287	14.7		1.3	0.7	0.7	13.3							0.7			66.7	2.0					S 66.667	7
GLY	288	2.7		6.7	0.7		67.3	2.0	0.7	0.7	3.3		4.0	2.0	1.3	0.7	3.3	2.0		2.0	0.7		G 67.333	2
ILE	289	16.0		9.3	2.0	1.3		2.0	2.0		6.7			3.3		0.7	2.7	0.7	52.7		0.7		V 52.667	5
GLN	290	16.0		16.7	42.7		0.7	0.7			0.7		2.7	0.7	7.3	1.3	4.7	4.0	1.3		0.7		E 42.667	1
GLN	291	5.3	0.7	4.7	3.3		2.0	4.7	0.7	6.7	0.7		0.7		8.7	34.7	16.7	10.7					R 34.667	1
ALA	292	69.3					3.3	5.3	1.3		0.7		0.7	4.7	0.7		5.3	2.7	4.7		1.3		A 69.333	7
THR	293	16.7		0.7	3.3		4.7	2.0	4.7	0.7	0.7		2.0	3.3	5.3	4.0	12.7	23.3	16.0				T 23.333	1
GLU	294	2.7		46.0	28.7		0.7	1.3		0.7	1.3		3.3		12.7	2.0			0.7				D 46.000	4
ASP	295	0.7		84.0	14.7								0.7										D 84.000	9
PRO	296					7.3	0.7	0.7			0.7			86.7		0.7			0.7	2.7			P 86.667	8
TYR	297					6.0	0.7	1.3			13.3				2.0					4.7	72.0		Y 72.000	7
THR	298	2.0						3.3	39.3		13.3	0.7	1.3		1.3			10.7	28.0				I 39.333	4
ILE	299	0.7						0.7	10.7	2.7	58.7				19.3	3.3			4.0				L 58.667	6
ARG	300	10.7		4.7	18.0		3.3	8.7		4.0	4.0		0.7		18.7	15.3	4.7	3.3	2.7		1.3		Q 18.667	4
SER	301	5.3		0.7	0.7		4.7	24.0	1.3	3.3	6.7		2.0		4.0	32.7	0.7	12.0	2.0				R 32.667	4
TYR	302	2.7				25.3		0.7	2.0		3.3	0.7						0.7	8.0		56.7		Y 56.667	5

GLY	**303**	4.7					95.3																	G 95.333	9
GLU	**304**			19.3	54.0		2.0			0.7				10.0		4.7	7.3	0.7	1.3					E 54.000	5
PHE	**305**					33.3			1.3		52.7	11.3								0.7		0.7		L 52.667	7
THR	**306**	9.3		1.3	0.7	5.3	0.7	5.3	0.7	0.7	0.7	0.7				6.7	10.0	5.3	9.3	6.0	33.3	4.0		W 33.333	3
ILE	**307**	22.7					0.7		9.3		14.0							15.3	4.0	34.0				V 34.000	5
ALA	**308**	14.7		3.3	7.3		9.3	8.0		14.0	5.3			0.7	0.7	17.3	13.3	4.0	2.0					Q 17.333	2
LEU	**309**	6.7					0.7		8.0		58.0								9.3	16.7		0.7		L 58.000	5
GLN	**310**	6.7		1.3	14.0	0.7		0.7		7.3	3.3			1.3		14.0	34.0	2.7	1.3	4.7	8.0			R 34.000	6
GLY	**311**	66.7	0.7				12.7								4.0			16.0						A 66.667	7
ALA	**312**	66.0		2.0			3.3				1.3							10.0	4.7	12.7				A 66.000	7
ASP	**313**	13.3		7.3	26.7		2.7		8.0	1.3	0.7			0.7		3.3	19.3	5.3	8.0	3.3				E 26.667	3
ALA	**314**	62.7	0.7		2.7		0.7				23.3							2.0	0.7	7.3				A 62.667	7
ALA	**315**	2.0						1.3	0.7		94.7	0.7				0.7								L 94.667	9
ALA	**316**	60.0					0.7		1.3		11.3			0.7				2.7	12.0	10.7		0.7		A 60.000	6
ARG	**317**	1.3		64.0	14.0		0.7	0.7		1.3				5.3		2.7	7.3	0.7	1.3	0.7				D 64.000	5
GLU	**318**	10.0		2.0	10.7			4.0	2.0	8.0	5.3			2.0		10.7	34.0	6.0	2.0	2.7		0.7		R 34.000	1
ALA	**319**	86.0					1.3											2.0	2.0	8.7				A 86.000	8
ALA	**320**	51.3		0.7	0.7		26.0		1.3		4.7	0.7	3.3			1.3	1.3	1.3	3.3	4.0				A 51.333	4
HIS	**321**	19.3		10.0	16.0		3.3	6.0	1.3	1.3	6.7			1.3		7.3	18.7	4.7	0.7	2.7		0.7		A 19.333	1
LEU	**322**	37.3			14.0		0.7	0.7	1.3	4.7	9.3	1.3				10.7	6.7	6.0	4.0	3.3				A 37.333	2
LEU	**323**	2.7				12.7	2.0		11.3		48.7	2.0				0.7				18.7	0.7	0.7		L 48.667	4
GLN	**324**	1.3	0.7	38.7	9.3		0.7	0.7			2.0	0.7	0.7			32.0	2.7	6.0	2.7	1.3	0.7			D 38.667	4
THR	**325**	35.3	0.7	6.7	10.0		4.7	4.7	0.7	4.7	0.7			4.0		12.7	4.7	3.3	5.3	0.7	1.3			A 35.333	1
VAL	**326**	64.7	0.7		0.7		5.3	1.3	6.0		10.0							0.7	4.0	6.7				A 64.667	7
TRP	**327**	2.9	0.7	0.7		7.2		8.6	2.9		21.6			0.7			0.7	1.4	1.4	1.4	40.3	9.4		W 40.288	4
ASP	**328**	35.3		15.8	12.2	1.4	4.3	2.2	0.7		4.3			3.6	0.7	4.3	7.2	7.2		0.7				A 35.252	1
LYS	**329**	6.5	0.7	5.0	2.2	1.4		0.7	3.6	22.3	10.1			1.4	2.2	10.8	27.3	2.9	1.4	1.4				R 27.338	1
GLY	**330**	3.4		2.0	7.4		62.2	0.7		2.7					2.0	2.7	16.2	0.7						G 62.162	4
ASP	**331**	17.6		16.2	14.9	1.4	2.7	4.7		1.4	2.0			2.0	12.8	2.0	6.1	6.1	4.1	1.4	4.7			A 17.568	1
ALA	**332**	34.7		20.7	6.7		9.3	1.3		3.3	2.0			7.3		3.3	0.7	9.3	1.3					A 34.667	1
LEU	**333**					0.7			4.0		73.3				2.0				0.7	19.3				L 73.333	7
THR	**334**	1.3		3.3	1.3		3.3			0.7		0.7	1.3					12.0	76.0					T 76.000	7
PRO	**335**	49.3		9.3	18.7	4.0	0.7	1.3							7.3	0.7	1.3	2.0	0.7	1.3	2.0	1.3		A 49.333	4
GLU	**336**	16.0		22.7	29.3		2.0	1.3						1.3	0.7	9.3	12.0	2.0	2.0	1.3				E 29.333	1
ASP	**337**	9.3		8.7	43.3	0.7	2.0		0.7	1.3	0.7	0.7	1.3			18.7	2.0	7.3	3.3					E 43.333	4
ARG	**338**	6.0	1.3			0.7		0.7									84.7	0.7		1.3	3.3	1.3		R 84.667	9
GLY	**339**	27.3					71.3	0.7						0.7										G 71.333	8
GLU	**340**	12.0		6.0	60.0				0.7	3.3	1.3					2.7	9.3	2.0	0.7	2.0				E 60.000	4
LEU	**341**	28.0	4.0			1.3		2.0	7.3		20.7					0.7			5.3	30.7				V 30.667	4
MET	**342**	74.0			3.3		0.7					1.3						18.7	1.3	0.7				A 74.000	8
VAL	**343**	4.0	0.7		7.3				34.0		14.0	2.0							2.7	35.3				V 35.333	4
LYS	**344**	48.7	0.7	4.0	8.7			1.3		1.3	10.0						8.0	5.3	6.0	0.7	5.3			A 48.667	5
VAL	**345**	6.7					1.3		41.3		1.3							0.7	2.0	46.7				V 46.667	6
SER	**346**	68.0		3.3		2.7	2.7							0.7	0.7			14.0				8.0		A 68.000	7
GLY	**347**	38.7			20.7		1.3			0.7		2.0				6.0		10.7	19.3	0.7				A 38.667	7
VAL	**348**	84.7					0.7		0.7		3.3							1.3	2.0	7.3				A 84.667	8
LYS	**349**	0.7			3.3					86.7				6.0			3.3							K 86.667	9
ALA	**350**	14.7	0.7						10.0		2.7					2.7		1.3	3.3	60.7		4.0		V 60.667	6
LEU	**351**	22.0				2.7		6.0	2.0		16.7	1.3	2.0			6.7	7.3	2.0	2.7	25.3	1.3	2.0		V 25.333	4
ALA	**352**	68.0	0.7						2.0									11.3	15.3	2.7				A 68.000	7
THR	**353**	12.7					6.7	12.7	2.0					2.0		3.3		13.3	43.3	4.0				T 43.333	7
ASN	**354**	0.7		17.3	12.7		0.7	2.7		13.3				6.7		4.7	40.0	1.3						R 40.000	4
ALA	**355**	31.3	0.7	2.7					6.0		3.3	0.7	2.0			1.3		0.7	21.3	30.0				A 31.333	5
ALA	**356**	46.0					32.0											18.7	1.3	2.0				A 46.000	6
LEU	**357**								2.7		80.0		2.7			3.3			1.3	10.0				L 80.000	8
ASN	**358**	3.3		33.3	40.7	2.0		2.7		1.3	1.3	0.7	2.7			2.0	8.7		0.7			0.7		E 40.667	4
ILE	**359**	10.7							27.3		7.3		1.3					2.7	3.3	47.3				V 47.333	4
SER	**360**	15.3	6.7				12.7						0.7	0.7				15.3	48.0	0.7				T 48.000	5
SER	**361**	9.3	0.7	0.7	8.0		1.3	3.3					10.0			6.7		49.3	10.0	0.7				S 49.333	5
GLY	**362**	12.0		2.0	8.0		11.3			11.3			3.3			9.3	40.7	0.7	1.3					R 40.667	5
VAL	**363**	3.3							30.0		32.0	10.0								24.7				L 32.000	5
PHE	**364**					88.7					6.0											5.3		F 88.667	8

GLU	365			16.0	78.0											6.0								E 78.000	8
VAL	366	10.7				2.0	0.7		6.7		22.7	0.7				1.3	0.7		0.7	53.3	0.7			V 53.333	6
ILE	367	10.0	5.3				1.3		2.7		4.7	20.0				4.0		4.0	42.7	5.3				T 42.667	6
GLY	368						100.0																	G 100.000	9
ALA	369	80.0					1.3							0.7				6.7	11.3					A 80.000	8
ARG	370	1.3		0.7			0.7	0.7		2.7	0.7					0.7	88.0	4.0	0.7					R 88.000	8
GLY	371	57.3					4.7											36.0	1.3				0.7	A 57.333	7
THR	372	16.7									1.3							3.3	78.0	0.7				T 78.000	8
HIS	373	36.0		0.7			0.7	14.0		2.0	8.0		1.3	0.7	1.3	0.7	16.7	16.0	2.0				A 36.000	5
PRO	374	37.3		4.7	1.3		4.0	1.3	0.7	1.3	2.0		12.7	1.3	1.3	7.3	17.3	6.7	0.7					A 37.333	4
ARG	375	19.3		2.7	2.0		6.0	3.3		22.0			0.7	8.0	5.3	12.0	18.0	0.7						K 22.000	2
TYR	376	2.7			1.3	6.7		7.3			36.0		2.7		0.7	2.0		1.3	14.0			25.3		L 36.000	3
GLY	377	4.7	0.7				67.3	0.7					10.7			16.0								G 67.333	7
PHE	378					37.3		0.7			55.3	1.3								1.3		4.0		L 55.333	5
ASP	379			93.3				6.0					0.7											D 93.333	9
ARG	380							0.7	4.7		3.3					90.7				0.7				R 90.667	9
PHE	381					60.7		20.0														19.3		F 60.667	6
TRP	382					0.7															99.3			W 99.333	9
ARG	383															100.0								R 100.000	9
ASN	384			16.0									84.0											N 84.000	9
VAL	385	32.7							8.0		24.0				0.7					34.7				V 34.667	7
ARG	386															100.0								R 100.000	9
THR	387								2.0		0.7								82.7	14.7				T 82.667	9
HIS	388					4.0		80.0			6.0				9.3							0.7		H 80.000	9
SER	389																	15.3	84.7					T 84.667	9
LEU	390										94.0								2.0	4.0				L 94.000	9
HIS	391		0.7					96.7								0.7						2.0		H 96.667	9
ASP	392			90.7	2.7								6.0							0.7				D 90.667	9
PRO	393													98.7	0.7		0.7							P 98.667	9
VAL	394	10.1							12.1		20.1			0.7					1.3	55.7				V 55.705	6
SER	395	23.5		42.3	7.4	4.7		0.7						2.7	2.0	8.1	4.7	0.7	3.4					D 42.282	7
TYR	396							5.4						1.3						0.7	8.1	84.6		Y 84.564	8
LYS	397									85.2						14.8								K 85.235	9
ILE	398	16.1			0.7	0.7		0.7	14.8	4.7	28.9		6.0		2.7	6.7	1.3	2.7	10.1			4.0		L 28.859	3
ALA	399	2.7						5.4	0.7	8.7	2.7		0.7		15.4	61.1	0.7	0.7	0.7			0.7		R 61.074	6
ASP	400	4.0		25.5	54.4		0.7	6.7			0.7		3.4		0.7			3.4	0.7					E 54.362	8
VAL	401								19.5		37.6								43.0					V 42.953	7
GLY	402						100.0																	G 100.000	9
LYS	403	7.4		21.5	13.4					2.7	0.7		9.4		5.4	34.2	1.3	2.7	1.3					R 34.228	4
HIS	404	0.7				15.4		18.1													40.3	25.5		W 40.268	4
THR	405	41.6			1.3	10.7			0.7		10.1	0.7			4.7	1.3		5.4	20.1			3.4		A 41.611	5
LEU	406					0.7			1.3		95.3							0.7	2.0					L 95.302	9
ASN	407	0.7		3.4	1.3			1.3	1.3	2.0	12.8		43.0			3.4	7.4	23.5						N 42.953	5
GLY	408	1.3		14.1	3.4		60.4	3.4					4.0		5.4	6.0	1.3					0.7		G 60.403	1
GLN	409	9.4		2.7	25.5			1.3	3.4	5.4	0.7		1.3	0.7	12.8	12.1	2.7	16.1	6.0					E 25.503	1
TYR	410	6.1			0.7	7.5		8.8	10.2	1.4	21.8			4.8		9.5	0.7		13.6	1.4	13.6			L 21.769	1
PRO	411													100.0										P 100.000	9
ILE	412	10.8		5.9	36.3			2.9	5.9	8.8	2.0		2.0	2.0	1.0	2.0	2.9	13.7	3.9					E 36.275	1
PRO	413	2.2				1.1		1.1						94.6			1.1							P 94.565	8
GLY	414	2.6		1.3			11.8						2.6			3.9	39.5	38.2						S 39.474	6
PHE	415					70.2	2.1		4.3		4.3								2.1	17.0				F 70.213	6
THR	416																	6.5				93.5		Y 93.548	8
SER	417																100.0							S 100.000	6*

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