

Table 3. Change in solvent accessible surface area of HEWL and VHH residues upon VHH-HEWL complex formation ($> 1\text{\AA}^2 \Delta\text{ASA}$).

HEWL											
D2-L29		D2-L19		cAb-Lys2		D3-L11		cAb-Lys3		D2-L24	
Residue	ΔASA (\AA^2)	Residue	ΔASA (\AA^2)	Residue	ΔASA (\AA^2)	Residue	ΔASA (\AA^2)	Residue	ΔASA (\AA^2)	Residue	ΔASA (\AA^2)
		LYS 33	4.03					GLU 35	10.93	LYS 1	13.05
PHE 34	25.01	PHE 34	41.05	PHE 34	29.69	ASN 46	12.4	ASN 46	29.34	GLN 41	44.62
GLU 35	25.25	GLU 35	18.25	GLU 35	27.57			THR 47	51.63	THR 43	23.55
		ASN 37	40.61			ASP 48	16.59	ASP 48	54.28	TYR 53	15.95
THR 43	1.55							SER 50	1.12	ASN 65	27.08
ASN 44	63.02	ASN 44	54.3	ASN 44	23.27			ASP 52	20.82	ASP 66	37.43
ARG 45	110.14	ARG 45	105.39	ARG 45	116.62			GLN 57	12.68	GLY 67	43.42
ASN 46	44.31	ASN 46	40.88	ASN 46	49.35			ILE 58	3.38	ARG 68	45.81
THR 47	143.68	THR 47	146.45	THR 47	142.13	ASN 59	5.49	ASN 59	33.42	ASN 74	7.84
ASP 48	28.5	ASP 48	43.15	ASP 48	30.31	ARG 61	65.56	ARG 61	35.91	ASN 77	11.58
				SER 50	2.7	TRP 62	102.01	TRP 62	119.47	ILE 78	2.3
ASP 52	18.14	ASP 52	13.15	ASP 52	19.76	TRP 63	22.3	TRP 63	37.56	PRO 79	58.44
GLN 57	6.93	GLN 57	1.45	GLN 57	2.9	ARG 73	19.55	ARG 73	30.98	SER 81	79.27
				ASN 59	20.72	LEU 75	60.27	LEU 75	20.71	ALA 82	11.26
				ARG 61	13.08	LYS 97	11.07	LYS 97	1.5	LEU 84	46.06
				TRP 62	2.79			ILE 98	6.14	SER 85	26.74
ARG 68	2.97					ASP101	70.93			SER 86	31.86
				ASN103	2.02	GLY102	18.66				
				ASN106	21.87	ASN103	103.68	ASN103	43.95		
VAL109	77.2	VAL109	70.43	VAL109	69.61	ASN106	37.42	ASN106	14.17		
ALA110	21.23	ALA110	26.22	ALA110	18.88	ALA107	43.48	ALA107	52.2		
ARG112	45.66			ARG112	91.14			TRP108	13.98		
ASN113	78.18	ASN113	58.79	ASN113	53.21	VAL109	19.59	VAL109	42.11		
ARG114	67.55	ARG114	76.22	ARG114	45.12	ARG112	82.39	ARG112	53.01		
				LYS116	11.85	ASN113	21.48				
						LYS 116	14.85				

VHH

D2-L29		D2-L19		cAb-Lys2		D3-L11		cAb-Lys3		D2-L24	
Residue	Δ ASA (Å^2)	Residue	Δ ASA (Å^2)	Residue	Δ ASA (Å^2)	Residue	Δ ASA (Å^2)	Residue	Δ ASA (Å^2)	Residue	Δ ASA (Å^2)
TYR 29	26.21	GLU 44	2.6	ARG 45	17.4	ASP 29	28.85	THR 28	8.97	ASP 1	16.39
LYS 30	27.25	VAL 50	1.25	VAL 50	1.51	SER 30	9.37	ILE 29	58.18	TYR 27	61.84
ASN 31	20.06	ASP 52	4.95	ASP 52	4.09	GLU 32	33.69	GLY 30	12.38	SER 30	10.55
PHE 37	34.81	ARG 56	43.26	ASN 57	33.17	TYR 52	30.02	PRO 31	2.69	ARG 100	80.08
ASP 44	17.05	THR 57	11.37	THR 58	10.16	HIS 54	53.26	TYR 32	33.1	GLN 101	80.99
ARG 45	30.58	ALA 58	31.71	ALA 59	32.96	THR 55	31.2	MET 53	3.3	GLY 102	57.6
GLY 47	8.88	TYR 59	18.35	TYR 60	13.45	ASN 57	21.24	GLY 54	47.3	TRP 103	42.08
PHE 50	2.38	ALA 60	2.4	ASP 62	25.51	TYR 59	6.74	GLY 55	37.48	TYR 104	82.55
TYR 60	19.59	ASP 61	31.69	LYS 65	16.96	ARG 100	4.47	ILE 57	46.2	ILE 105	25.4
TYR 100	89.55	TRP 99	72.31	ASP 99	6.42	LYS 101	33.23	ASN 74	6.81	TYR 110	98.19
ARG 101	13.15	SER 101	22.58	THR 100	12.19	TYR 102	109.78	SER 100	1.27	GLY 111	11.08
ASN 102	34.07	SER 104	39.92	TRP 103	95.04	VAL 103	10.43	THR 101	33.3	ASN 113	24.99
TYR 103	19.76	CYS 105	18.24	ARG 105	35.4	PRO 104	65.55	ILE 102	76.17		
GLN 105	44.79	GLY 106	19.38	GLY 106	4.1	VAL 105	31.36	TYR 103	51.55		
CYS 106	18.22	THR 107	44.96	TYR 107	123.74	ARG 106	49.35	ALA 104	115.87		
ALA 107	22.76	ASN 108	58.41	CYS 108	24.3	PHE 107	56.78	SER 105	72.31		
THR 108	24.78	ARG 109	32.78	GLY 109	15.63	SER 112	16.57	TYR 106	102.05		
ARG 109	129.83	ASN 110	83.81	THR 110	20.39	SER 113	21.07	TYR 107	24.15		
TYR 110	18.18	ARG 111	84.22	ASN 111	41.09	ASP 115	34.31	GLU 108	7.19		
TRP 111	31.34	TYR 112	6.52	ASN 113	102.8			TYR 118	51.76		
		ASN 113	9.71	TYR 114	98.42						
				PHE 115	1.42						
				SER 116	33.43						