$n \rightarrow \pi^*$ Interactions in Proteins

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Table S1 | Data used to generate Figure 2b.

ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\rightarrow\pi^*}$ (kcal/mol)
–20	–20	2.51833	137.777	1.34
–20	–25	2.51833	133.727	2.18
–20	–30	2.51833	129.571	2.99
–20	–35	2.51833	125.338	3.80
–20	–40	2.51833	121.047	4.52
–20	–45	2.51833	116.716	5.11
–20	–50	2.51833	112.356	5.51
–20	–55	2.51833	107.978	5.69
–20	–60	2.51833	103.591	5.74
–20	–65	2.51833	99.203	5.62
–20	–70	2.51833	94.821	5.26
–20	–75	2.51833	90.453	4.65
–20	–80	2.51833	86.108	3.86
–25	–10	2.56119	143.303	0.50
–25	–15	2.56119	139.361	1.08
–25	–20	2.56119	135.280	1.76
–25	–25	2.56119	131.100	2.49
–25	–30	2.56119	126.846	3.20
–25	–35	2.56119	122.540	3.84
–25	–40	2.56119	118.197	4.37
–25	–45	2.56119	113.829	4.68
–25	–50	2.56119	109.446	4.80
–25	–55	2.56119	105.058	4.81
–25	–60	2.56119	100.671	4.70
–25	–65	2.56119	96.294	4.39
–25	–70	2.56119	91.934	3.88
–25	–75	2.56119	87.598	3.23
–25	–80	2.56119	83.295	2.48
–30	0	2.61178	149.021	0.14
–30	–5	2.61178	145.227	0.38
–30	–10	2.61178	141.246	0.79
–30	–15	2.61178	137.131	1.32
–30	–20	2.61178	132.922	1.93
–30	–25	2.61178	128.647	2.54
–30	–30	2.61178	124.324	3.11
–30	–35	2.61178	119.968	3.58
–30	–40	2.61178	115.593	3.81
–30	–45	2.61178	111.207	3.88
–30	–50	2.61178	106.818	3.89
–30	–55	2.61178	102.435	3.79

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
–30	–60	2.61178	98.064	3.55
–30	–65	2.61178	93.714	3.15
–30	–70	2.61178	89.390	2.64
–30	–75	2.61178	85.102	2.06
–30	–80	2.61178	80.859	1.45
–35	0	2.66928	147.440	0.24
–35	–5	2.66928	143.414	0.53
–35	–10	2.66927	139.263	0.93
–35	–15	2.66928	135.024	1.39
–35	–20	2.66928	130.725	1.88
–35	–25	2.66928	126.385	2.39
–35	–30	2.66928	122.019	2.83
–35	–35	2.66927	117.637	2.98
–35	–40	2.66928	113.248	3.02
–35	–45	2.66928	108.862	3.04
–35	–50	2.66928	104.484	2.97
–35	–55	2.66927	100.122	2.79
–35	–60	2.66928	95.783	2.49
–35	–65	2.66928	91.475	2.13
–35	–70	2.66927	87.204	1.67
–35	–75	2.66928	82.981	1.21
–35	–80	2.66928	78.816	0.76
–40	0	2.73282	145.842	0.34
–40	–5	2.73282	141.651	0.60
–40	–10	2.73282	137.381	0.92
–40	–15	2.73282	133.059	1.27
–40	–20	2.73282	128.703	1.70
–40	–25	2.73282	124.327	2.14
–40	–30	2.73282	119.940	2.23
–40	–35	2.73282	115.552	2.27
–40	–40	2.73282	111.169	2.32
–40	–45	2.73282	106.799	2.27
–40	–50	2.73282	102.449	2.14
–40	–55	2.73282	98.125	1.93
–40	–60	2.73282	93.834	1.67
–40	–65	2.73282	89.584	1.34
–40	–70	2.73282	85.383	0.98
–40	–75	2.73282	81.243	0.64
–40	–80	2.73282	77.173	0.37
–45	0	2.80154	144.264	0.37
–45	–5	2.80154	139.963	0.57

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
–45	–10	2.80154	135.619	0.78
–45	–15	2.80154	131.249	1.08
–45	–20	2.80154	126.865	1.53
–45	–25	2.80154	122.476	1.69
–45	–30	2.80154	118.09	1.67
–45	–35	2.80154	113.715	1.71
–45	–40	2.80154	109.357	1.69
–45	–45	2.80154	105.021	1.60
–45	–50	2.80154	100.714	1.46
–45	–55	2.80154	96.443	1.28
–45	–60	2.80154	92.216	1.04
–45	–65	2.80154	88.040	0.77
–45	–70	2.80154	83.927	0.53
–45	–75	2.80154	79.885	0.33
–45	–80	2.80154	75.930	0.18
–50	0	2.87456	142.733	0.33
–50	–5	2.87456	138.369	0.45
–50	–10	2.87456	133.987	0.58
–50	–15	2.87456	129.599	0.96
–50	–20	2.87456	125.212	1.21
–50	–25	2.87456	120.834	1.24
–50	–30	2.87456	116.470	1.27
–50	–35	2.87456	112.126	1.26
–50	–40	2.87456	107.807	1.16
–50	–45	2.87456	103.521	1.07
–50	–50	2.87456	99.274	0.96
–50	–55	2.87456	95.072	0.78
–50	–60	2.87456	90.924	0.59
–50	–65	2.87456	86.838	0.42
–50	–70	2.87456	82.826	0.27
–50	–75	2.87456	78.900	0.15
–50	–80	2.87456	75.075	0.07
–55	0	2.95102	141.268	0.25
–55	–5	2.95102	136.880	0.28
–55	–10	2.95102	132.492	0.43
–55	–15	2.95102	128.112	0.83
–55	–20	2.95102	123.746	0.86
–55	–25	2.95103	119.397	0.88
–55	–30	2.95102	115.072	0.89
–55	–35	2.95102	110.776	0.85
–55	–40	2.95102	106.515	0.79

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
–55	–45	2.95103	102.293	0.69
–55	–50	2.95102	98.120	0.57
–55	–55	2.95102	94.001	0.44
–55	–60	2.95102	89.946	0.31
–55	–65	2.95102	85.965	0.22
–55	–70	2.95102	82.069	0.13
–55	–75	2.95102	78.273	0.07
–55	–80	2.95102	74.592	0.03
–60	0	3.03011	139.881	0.12
–60	–5	3.03011	135.502	0.14
–60	–10	3.03011	131.135	0.44
–60	–15	3.03011	126.787	0.58
–60	–20	3.03011	122.460	0.59
–60	–25	3.03011	118.160	0.59
–60	–30	3.03011	113.891	0.57
–60	–35	3.03011	109.659	0.54
–60	–40	3.03011	105.468	0.50
–60	–45	3.03011	101.326	0.41
–60	–50	3.03011	97.240	0.31
–60	–55	3.03011	93.218	0.23
–60	–60	3.03011	89.269	0.17
–60	–65	3.03011	85.405	0.11
–60	–70	3.03011	81.638	0.06
–60	–75	3.03011	77.984	0.03
–60	–80	3.03011	74.458	0.01
–65	0	3.11105	138.578	0.06
–65	–5	3.11105	134.236	0.09
–65	–10	3.11105	129.915	0.36
–65	–15	3.11105	125.618	0.38
–65	–20	3.11105	121.350	0.38
–65	–25	3.11105	117.115	0.37
–65	–30	3.11105	112.917	0.36
–65	–35	3.11105	108.763	0.32
–65	–40	3.11105	104.657	0.28
–65	–45	3.11105	100.607	0.21
–65	–50	3.11105	96.621	0.16
–65	–55	3.11105	92.708	0.12
–65	–60	3.11105	88.877	0.08
–65	–65	3.11105	85.141	0.05
–70	0	3.1931	137.363	0.02
–70	–5	3.1931	133.082	0.09

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
–70	–10	3.1931	128.826	0.22
–70	–15	3.1931	124.600	0.23
–70	–20	3.1931	120.407	0.23
–70	–25	3.1931	116.252	0.22
–70	–30	3.1931	112.140	0.20
–70	–35	3.1931	108.077	0.18
–70	–40	3.1931	104.068	0.14
–70	–45	3.1931	100.123	0.11
–70	–50	3.1931	96.248	0.08
–70	–55	3.1931	92.454	0.05
–70	–60	3.1931	88.751	0.03
–70	–65	3.1931	85.153	0.02
–75	0	3.27558	136.235	0.01
–75	–5	3.27558	132.036	0.07
–75	–10	3.27558	127.865	0.13
–75	–15	3.27558	123.726	0.12
–75	–20	3.27558	119.623	0.12
–75	–25	3.27558	115.562	0.11
–75	–30	3.27558	111.549	0.10
–75	–35	3.27558	107.588	0.09
–75	–40	3.27558	103.689	0.06
–75	–45	3.27558	99.858	0.04
–75	–50	3.27558	96.104	0.03
–75	–55	3.27558	92.439	0.02
–80	0	3.35785	135.193	0.01
–80	–5	3.35785	131.095	0.04
–80	–10	3.35785	127.025	0.06
–80	–15	3.35785	122.988	0.06
–80	–20	3.35785	118.989	0.06
–80	–25	3.35785	115.035	0.05
–80	–30	3.35785	111.132	0.04
–80	–35	3.35785	107.286	0.03
–80	–40	3.35785	103.505	0.02
–80	–45	3.35785	99.798	0.01
–80	–50	3.35785	96.174	0.01
–80	–55	3.35785	92.645	0.00
0	80	2.43688	100.261	8.21
0	85	2.43688	95.872	8.31
0	90	2.43688	91.486	8.07
0	95	2.43688	87.109	7.45
0	100	2.43688	82.749	6.46

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
0	105	2.43688	78.415	5.15
0	110	2.43688	74.117	3.65
0	115	2.43688	69.864	2.13
0	120	2.43688	65.670	0.89
0	125	2.43688	61.551	0.21
–5	80	2.4428	104.43	7.60
–5	85	2.4428	100.046	8.04
–5	90	2.4428	95.657	8.18
–5	95	2.4428	91.272	8.00
–5	100	2.4428	86.897	7.45
–5	105	2.4428	82.54	6.51
–5	110	2.4428	78.211	5.24
–5	115	2.4428	73.918	3.74
–5	120	2.4428	69.673	2.22
–5	125	2.4428	65.488	0.94
–5	130	2.4428	61.38	0.23
–10	80	2.45858	108.705	6.45
–10	85	2.45858	104.33	7.14
–10	90	2.45858	99.944	7.60
–10	95	2.45858	95.555	7.77
–10	100	2.45858	91.172	7.63
–10	105	2.45858	86.801	7.16
–10	110	2.45858	82.452	6.32
–10	115	2.45858	78.132	5.14
–10	120	2.45858	73.851	3.71
–10	125	2.45858	69.62	2.23
–10	130	2.45858	65.454	0.98
–10	135	2.45858	61.367	0.25
–15	80	2.48392	113.035	5.04
–15	85	2.48392	108.67	5.81
–15	90	2.48392	104.288	6.47
–15	95	2.48392	99.9	6.93
–15	100	2.48392	95.513	7.10
–15	105	2.48392	91.135	7.02
–15	110	2.48392	86.772	6.64
–15	115	2.48392	82.434	5.91
–15	120	2.48392	78.129	4.85
–15	125	2.48392	73.867	3.54
–15	130	2.48392	69.659	2.17
–15	135	2.48392	65.52	0.98
–15	140	2.48392	61.467	0.27

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
–20	80	2.51833	117.37	3.61
–20	85	2.51833	113.014	4.35
–20	90	2.51833	108.638	5.06
–20	95	2.51833	104.252	5.65
–20	100	2.51833	99.863	6.04
–20	105	2.51833	95.48	6.26
–20	110	2.51833	91.11	6.22
–20	115	2.51833	86.761	5.91
–20	120	2.51833	82.44	5.31
–20	125	2.51833	78.157	4.39
–20	130	2.51833	73.922	3.23
–20	135	2.51833	69.748	2.01
–20	140	2.51833	65.649	0.95
–20	145	2.51833	61.642	0.27
–20	150	2.51833	57.75	0.19
–25	80	2.56119	121.666	2.34
–25	85	2.56119	117.316	2.99
–25	90	2.56119	112.945	3.65
–25	95	2.56119	108.56	4.25
–25	100	2.56119	104.172	4.77
–25	105	2.56119	99.787	5.12
–25	110	2.56119	95.412	5.32
–25	115	2.56119	91.056	5.31
–25	120	2.56119	86.726	5.09
–25	125	2.56119	82.431	4.59
–25	130	2.56119	78.179	3.81
–25	135	2.56119	73.982	2.82
–25	140	2.56119	69.853	1.77
–25	145	2.56119	65.807	0.86
–25	150	2.56119	61.862	0.26
–25	155	2.56119	58.042	0.13
–30	80	2.61178	125.881	1.37
–30	85	2.61178	121.536	1.86
–30	90	2.61178	117.166	2.41
–30	95	2.61178	112.783	2.95
–30	100	2.61178	108.394	3.47
–30	105	2.61178	104.008	3.88
–30	110	2.61178	99.632	4.19
–30	115	2.61178	95.274	4.37
–30	120	2.61178	90.939	4.39
–30	125	2.61178	86.638	4.20

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
–30	130	2.61178	82.377	3.81
–30	135	2.61178	78.168	3.16
–30	140	2.61178	74.021	2.35
–30	145	2.61178	69.95	1.49
–30	150	2.61178	65.972	0.74
–30	155	2.61178	62.106	0.24
–30	160	2.61178	58.377	0.10
–35	80	2.66927	129.981	0.70
–35	85	2.66927	125.636	1.05
–35	90	2.66927	121.266	1.46
–35	95	2.66927	116.882	1.89
–35	100	2.66927	112.493	2.33
–35	105	2.66928	108.108	2.73
–35	110	2.66928	103.732	3.07
–35	115	2.66928	99.374	3.33
–35	120	2.66927	95.04	3.47
–35	125	2.66928	90.737	3.49
–35	130	2.66928	86.474	3.36
–35	135	2.66928	82.26	3.02
–35	140	2.66928	78.106	2.50
–35	145	2.66928	74.023	1.86
–35	150	2.66927	70.026	1.19
–35	155	2.66927	66.134	0.60
–35	160	2.66927	62.366	0.21
–35	165	2.66928	58.748	0.07
–40	80	2.73282	133.934	0.34
–40	85	2.73282	129.584	0.55
–40	90	2.73282	125.211	0.81
–40	95	2.73282	120.825	1.11
–40	100	2.73282	116.437	1.45
–40	105	2.73282	112.052	1.77
–40	110	2.73282	107.68	2.08
–40	115	2.73282	103.325	2.36
–40	120	2.73282	98.995	2.56
–40	125	2.73282	94.696	2.68
–40	130	2.73282	90.437	2.69
–40	135	2.73282	86.226	2.57
–40	140	2.73282	82.073	2.30
–40	145	2.73282	77.988	1.89
–40	150	2.73282	73.985	1.40
–40	155	2.73282	70.08	0.90

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
–40	160	2.73282	66.292	0.46
–40	165	2.73282	62.642	0.16
–40	170	2.73282	59.158	0.05
–45	80	2.80154	137.71	0.16
–45	85	2.80154	133.351	0.27
–45	90	2.80154	128.972	0.42
–45	95	2.80154	124.585	0.61
–45	100	2.80154	120.197	0.84
–45	105	2.80154	115.816	1.07
–45	110	2.80154	111.448	1.32
–45	115	2.80154	107.101	1.56
–45	120	2.80154	102.779	1.76
–45	125	2.80154	98.49	1.92
–45	130	2.80154	94.241	2.00
–45	135	2.80154	90.04	2.01
–45	140	2.80154	85.895	1.89
–45	145	2.80154	81.817	1.67
–45	150	2.80154	77.819	1.36
–45	155	2.80154	73.914	1.00
–45	160	2.80154	70.119	0.64
–45	165	2.80154	66.455	0.33
–45	170	2.80154	62.945	0.12
–45	175	2.80154	59.618	0.04
–45	180	2.80154	56.506	0.08
–50	80	2.87456	141.279	0.07
–50	85	2.87456	136.908	0.13
–50	90	2.87456	132.523	0.21
–50	95	2.87456	128.134	0.32
–50	100	2.87456	123.749	0.45
–50	105	2.87456	119.375	0.61
–50	110	2.87456	115.017	0.79
–50	115	2.87456	110.681	0.96
–50	120	2.87456	106.373	1.13
–50	125	2.87456	102.099	1.28
–50	130	2.87456	97.866	1.40
–50	135	2.87456	93.681	1.45
–50	140	2.87456	89.552	1.43
–50	145	2.87456	85.49	1.33
–50	150	2.87456	81.505	1.15
–50	155	2.87456	77.611	0.92
–50	160	2.87456	73.823	0.67

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
–50	165	2.87456	70.159	0.43
–50	170	2.87456	66.641	0.22
–50	175	2.87456	63.293	0.08
–50	180	2.87456	60.144	0.02
–55	85	2.95103	140.225	0.06
–55	90	2.95103	135.836	0.10
–55	95	2.95103	131.45	0.15
–55	100	2.95103	127.072	0.23
–55	105	2.95102	122.709	0.33
–55	110	2.95102	118.366	0.44
–55	115	2.95102	114.048	0.56
–55	120	2.95102	109.759	0.69
–55	125	2.95103	105.507	0.81
–55	130	2.95102	101.296	0.92
–55	135	2.95102	97.135	0.98
–55	140	2.95102	93.031	1.00
–55	145	2.95102	88.992	0.97
–55	150	2.95103	85.03	0.87
–55	155	2.95102	81.157	0.75
–55	160	2.95102	77.386	0.59
–55	165	2.95102	73.735	0.42
–55	170	2.95103	70.223	0.26
–55	175	2.95102	66.871	0.14
–55	180	2.95102	63.708	0.05
–60	85	3.03011	143.27	0.02
–60	90	3.03011	138.884	0.05
–60	95	3.03011	134.507	0.07
–60	100	3.03011	130.145	0.11
–60	105	3.03011	125.801	0.16
–60	110	3.03011	121.48	0.23
–60	115	3.03011	117.186	0.30
–60	120	3.03011	112.925	0.39
–60	125	3.03011	108.702	0.48
–60	130	3.03011	104.522	0.56
–60	135	3.03011	100.392	0.63
–60	140	3.03011	96.319	0.66
–60	145	3.03011	92.313	0.66
–60	150	3.03011	88.383	0.62
–60	155	3.03011	84.54	0.55
–60	160	3.03011	80.797	0.45
–60	165	3.03011	77.17	0.35

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
–60	170	3.03011	73.676	0.24
–60	175	3.03011	70.336	0.14
–60	180	3.03011	67.174	0.07
–65	85	3.11105	143.27	0.02
–65	90	3.11105	138.884	0.05
–65	95	3.11105	134.507	0.07
–65	100	3.11105	132.945	0.05
–65	105	3.11105	128.63	0.08
–65	110	3.11105	124.342	0.11
–65	115	3.11105	120.083	0.15
–65	120	3.11105	115.858	0.21
–65	125	3.11105	111.673	0.26
–65	130	3.11105	107.533	0.33
–65	135	3.11105	103.443	0.37
–65	140	3.11105	99.411	0.41
–65	145	3.11105	95.446	0.42
–65	150	3.11105	91.556	0.40
–65	155	3.11105	87.752	0.37
–65	160	3.11105	84.047	0.31
–65	165	3.11105	80.455	0.25
–65	170	3.11105	76.992	0.18
–65	175	3.11105	73.676	0.12
–65	180	3.11105	70.53	0.06
–70	100	3.1931	135.451	0.02
–70	105	3.1931	131.181	0.03
–70	110	3.1931	126.938	0.05
–70	115	3.1931	122.726	0.07
–70	120	3.1931	118.549	0.10
–70	125	3.1931	114.413	0.13
–70	130	3.1931	110.322	0.17
–70	135	3.1931	106.282	0.21
–70	140	3.1931	102.301	0.23
–70	145	3.1931	98.386	0.24
–70	150	3.1931	94.545	0.24
–70	155	3.1931	90.791	0.22
–70	160	3.1931	87.133	0.20
–70	165	3.1931	83.585	0.16
–70	170	3.1931	80.163	0.13
–70	175	3.1931	76.884	0.08
–70	180	3.1931	73.767	0.05
–75	100	3.27558	137.642	0.01

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
–75	105	3.27558	133.435	0.01
–75	110	3.27558	129.254	0.02
–75	115	3.27558	125.104	0.03
–75	120	3.27558	120.988	0.04
–75	125	3.27558	116.913	0.06
–75	130	3.27558	112.883	0.08
–75	135	3.27558	108.904	0.10
–75	140	3.27558	104.983	0.12
–75	145	3.27558	101.128	0.12
–75	150	3.27558	97.348	0.13
–75	155	3.27558	93.652	0.12
–75	160	3.27558	90.051	0.11
–75	165	3.27558	86.558	0.09
–75	170	3.27558	83.188	0.07
–75	175	3.27558	79.955	0.05
–75	180	3.27558	76.879	0.03
–80	100	3.35785	139.497	0.00
–80	105	3.35785	135.375	0.00
–80	110	3.35785	131.276	0.01
–80	115	3.35785	127.205	0.01
–80	120	3.35785	123.166	0.02
–80	125	3.35785	119.166	0.02
–80	130	3.35785	115.21	0.03
–80	135	3.35785	111.304	0.04
–80	140	3.35785	107.455	0.05
–80	145	3.35785	103.671	0.06
–80	150	3.35785	99.961	0.06
–80	155	3.35785	96.333	0.06
–80	160	3.35785	92.8	0.05
–80	165	3.35785	89.371	0.04
–80	170	3.35785	86.062	0.03
–80	175	3.35785	82.887	0.02
–80	180	3.35785	79.864	0.01
20	20	2.51123	137.379	1.31
20	25	2.51123	133.329	2.12
20	30	2.51123	129.174	2.96
20	35	2.51123	124.942	3.75
20	40	2.51123	120.653	4.51
20	45	2.51123	116.322	5.13
20	50	2.51123	111.963	5.63
20	55	2.51123	107.585	5.96

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
20	60	2.51123	103.199	6.11
20	65	2.51123	98.81	6.07
20	70	2.51123	94.428	5.79
20	75	2.51123	90.06	5.28
20	80	2.51123	85.714	4.51
25	20	2.55257	134.825	1.78
25	25	2.55257	130.647	2.53
25	30	2.55257	126.395	3.25
25	35	2.55257	122.09	3.88
25	40	2.55257	117.748	4.43
25	45	2.55257	113.381	4.84
25	50	2.55257	108.999	5.09
25	55	2.55257	104.611	5.19
25	60	2.55257	100.224	5.14
25	65	2.55257	95.846	4.90
25	70	2.55257	91.485	4.46
25	75	2.55257	87.148	3.83
25	80	2.55257	82.844	3.07
30	20	2.60178	132.414	2.06
30	25	2.60177	128.141	2.68
30	30	2.60178	123.82	3.22
30	35	2.60178	119.466	3.68
30	40	2.60178	115.091	4.00
30	45	2.60178	110.705	4.20
30	50	2.60178	106.317	4.26
30	55	2.60178	101.933	4.21
30	60	2.60178	97.561	4.01
30	65	2.60178	93.21	3.66
30	70	2.60178	88.885	3.16
30	75	2.60178	84.595	2.56
30	80	2.60178	80.349	1.90
35	20	2.65804	130.168	2.11
35	25	2.65804	125.83	2.56
35	30	2.65804	121.465	2.94
35	35	2.65804	117.084	3.18
35	40	2.65804	112.695	3.33
35	45	2.65804	108.308	3.38
35	50	2.65804	103.93	3.34
35	55	2.65804	99.567	3.19
35	60	2.65804	95.226	2.92
35	65	2.65804	90.916	2.56

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
35	70	2.65804	86.644	2.09
35	75	2.65804	82.418	1.59
35	80	2.65804	78.251	1.09
40	20	2.72053	128.102	1.96
40	25	2.72053	123.726	2.25
40	30	2.72053	119.34	2.44
40	35	2.72053	114.952	2.55
40	40	2.72053	110.569	2.61
40	45	2.72053	106.198	2.58
40	50	2.72053	101.846	2.46
40	55	2.72053	97.52	2.28
40	60	2.72053	93.226	2.01
40	65	2.72053	88.974	1.67
40	70	2.72053	84.771	1.30
40	75	2.72053	80.628	0.92
40	80	2.72053	76.556	0.58
45	20	2.78835	126.224	1.66
45	25	2.78835	121.835	1.80
45	30	2.78835	117.449	1.90
45	35	2.78835	113.073	1.95
45	40	2.78835	108.712	1.94
45	45	2.78835	104.374	1.86
45	50	2.78835	100.065	1.74
45	55	2.78835	95.792	1.55
45	60	2.78835	91.562	1.30
45	65	2.78835	87.383	1.02
45	70	2.78835	83.267	0.75
45	75	2.78835	79.223	0.50
45	80	2.78835	75.265	0.29
50	20	2.86063	124.537	1.29
50	25	2.86063	120.157	1.36
50	30	2.86063	115.791	1.42
50	35	2.86063	111.445	1.41
50	40	2.86063	107.124	1.36
50	45	2.86063	102.835	1.29
50	50	2.86063	98.584	1.17
50	55	2.86063	94.379	0.99
50	60	2.86063	90.227	0.79
50	65	2.86063	86.139	0.59
50	70	2.86063	82.124	0.42
50	75	2.86063	78.196	0.26

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
50	80	2.86063	74.369	0.13
55	20	2.93651	123.041	0.95
55	25	2.93651	118.689	0.99
55	30	2.93651	114.361	1.00
55	35	2.93651	110.062	0.98
55	40	2.93651	105.797	0.93
55	45	2.93651	101.572	0.85
55	50	2.93651	97.395	0.73
55	55	2.93651	93.272	0.58
55	60	2.93651	89.214	0.44
55	65	2.93651	85.229	0.33
55	70	2.93651	81.331	0.23
55	75	2.93651	77.533	0.13
55	80	2.93651	73.851	0.06
60	20	3.01517	121.731	0.68
60	25	3.01517	117.427	0.69
60	30	3.01517	113.153	0.67
60	35	3.01517	108.916	0.65
60	40	3.01517	104.721	0.60
60	45	3.01517	100.575	0.53
60	50	3.01517	96.485	0.42
60	55	3.01517	92.459	0.32
60	60	3.01517	88.506	0.25
60	65	3.01517	84.639	0.18
60	70	3.01517	80.871	0.11
60	75	3.01517	77.215	0.06
60	80	3.01517	73.69	0.02
65	20	3.09582	120.602	0.45
65	25	3.09582	116.361	0.44
65	30	3.09582	112.158	0.43
65	35	3.09582	107.997	0.40
65	40	3.09582	103.886	0.36
65	45	3.09582	99.832	0.29
65	50	3.09582	95.841	0.23
65	55	3.09582	91.923	0.18
65	60	3.09582	88.089	0.13
65	65	3.09582	84.351	0.08
65	70	3.09582	80.722	0.05
65	75	3.09582	77.219	0.04
65	80	3.09582	73.86	0.01
70	20	3.17771	119.645	0.28

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
70	25	3.17771	115.482	0.27
70	30	3.17771	111.364	0.26
70	35	3.17771	107.293	0.23
70	40	3.17771	103.279	0.20
70	45	3.17771	99.328	0.15
70	50	3.17771	95.448	0.12
70	55	3.17771	91.65	0.09
70	60	3.17771	87.944	0.06
70	65	3.17771	84.344	0.04
75	20	3.26016	118.852	0.16
75	25	3.26016	114.782	0.16
75	30	3.26016	110.76	0.14
75	35	3.26016	106.792	0.12
75	40	3.26016	102.886	0.10
75	45	3.26016	99.049	0.07
75	50	3.26016	95.29	0.05
75	55	3.26016	91.621	0.04
75	60	3.26016	88.052	0.02
80	20	3.34252	118.213	0.08
80	25	3.34252	114.249	0.08
80	30	3.34252	110.336	0.06
80	35	3.34252	106.481	0.05
80	40	3.34252	102.693	0.04
80	45	3.34252	98.98	0.03
80	50	3.34252	95.351	0.02
80	55	3.34252	91.818	0.01
20	–100	2.51123	100.023	6.17
20	–105	2.51123	95.638	6.36
20	–110	2.51123	91.266	6.19
20	–115	2.51123	86.912	5.81
20	–120	2.51123	82.587	5.09
20	–125	2.51123	78.298	4.12
20	–130	2.51123	74.055	2.98
20	–135	2.51123	69.872	1.81
20	–140	2.51123	65.761	0.81
20	–145	2.51123	61.742	0.22
20	–150	2.51123	57.833	0.21
25	–100	2.55257	104.343	5.08
25	–105	2.55257	99.956	5.41
25	–110	2.55257	95.579	5.51
25	–115	2.55257	91.22	5.42

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
25	–120	2.55257	86.884	5.00
25	–125	2.55257	82.582	4.38
25	–130	2.55257	78.322	3.55
25	–135	2.55257	74.115	2.57
25	–140	2.55257	69.974	1.59
25	–145	2.55257	65.914	0.75
25	–150	2.55257	61.953	0.20
25	–155	2.55257	58.113	0.14
30	–100	2.60178	108.584	3.93
30	–105	2.60178	104.197	4.3
30	–110	2.60178	99.819	4.57
30	–115	2.60178	95.456	4.64
30	–120	2.60178	91.116	4.51
30	–125	2.60178	86.807	4.15
30	–130	2.60178	82.537	3.61
30	–135	2.60178	78.317	2.91
30	–140	2.60178	74.157	2.12
30	–145	2.60178	70.072	1.33
30	–150	2.60178	66.076	0.63
30	–155	2.60178	62.19	0.19
30	–160	2.60178	58.438	0.09
35	–100	2.65804	112.709	2.84
35	–105	2.65804	108.322	3.24
35	–110	2.65804	103.943	3.55
35	–115	2.65804	99.58	3.74
35	–120	2.65804	95.24	3.78
35	–125	2.65804	90.929	3.64
35	–130	2.65804	86.657	3.32
35	–135	2.65804	82.432	2.86
35	–140	2.65804	78.263	2.30
35	–145	2.65804	74.165	1.68
35	–150	2.65804	70.15	1.05
35	–155	2.65804	66.236	0.51
35	–160	2.65804	62.444	0.16
35	–165	2.65804	58.799	0.06
35	–170	2.65804	55.33	0.28
40	–100	2.72053	116.684	1.96
40	–105	2.72053	112.297	2.30
40	–110	2.72053	107.921	2.61
40	–115	2.72053	103.561	2.84
40	–120	2.72053	99.224	2.97

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
40	–125	2.72053	94.916	2.98
40	–130	2.72053	90.647	2.83
40	–135	2.72053	86.423	2.57
40	–140	2.72053	82.255	2.19
40	–145	2.72053	78.154	1.74
40	–150	2.72053	74.132	1.26
40	–155	2.72053	70.205	0.79
40	–160	2.72053	66.391	0.39
40	–165	2.72053	62.712	0.12
40	–170	2.72053	59.196	0.04
45	–100	2.78835	120.479	1.28
45	–105	2.78835	116.096	1.57
45	–110	2.78835	111.724	1.82
45	–115	2.78835	107.37	2.04
45	–120	2.78835	103.04	2.20
45	–125	2.78835	98.741	2.28
45	–130	2.78835	94.48	2.25
45	–135	2.78835	90.265	2.13
45	–140	2.78835	86.105	1.91
45	–145	2.78835	82.009	1.61
45	–150	2.78835	77.99	1.27
45	–155	2.78835	74.062	0.92
45	–160	2.78835	70.241	0.57
45	–165	2.78835	66.548	0.27
45	–170	2.78835	63.004	0.08
45	–175	2.78835	59.639	0.02
50	–100	2.86063	124.072	0.8
50	–105	2.86063	119.693	1.01
50	–110	2.86063	115.329	1.21
50	–115	2.86063	110.985	1.39
50	–120	2.86063	106.668	1.54
50	–125	2.86063	102.382	1.64
50	–130	2.86063	98.136	1.67
50	–135	2.86063	93.936	1.64
50	–140	2.86063	89.791	1.53
50	–145	2.86063	85.709	1.36
50	–150	2.86063	81.703	1.14
50	–155	2.86063	77.785	0.89
50	–160	2.86063	73.97	0.62
50	–165	2.86063	70.275	0.38
50	–170	2.86063	66.722	0.19

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
50	–175	2.86063	63.336	0.05
55	–100	2.93651	127.438	0.49
55	–105	2.93651	123.068	0.63
55	–110	2.93651	118.717	0.77
55	–115	2.93651	114.389	0.91
55	–120	2.93651	110.089	1.03
55	–125	2.93651	105.824	1.12
55	–130	2.93651	101.599	1.17
55	–135	2.93651	97.421	1.19
55	–140	2.93651	93.298	1.14
55	–145	2.93651	89.239	1.05
55	–150	2.93651	85.255	0.91
55	–155	2.93651	81.356	0.76
55	–160	2.93651	77.557	0.57
55	–165	2.93651	73.874	0.40
55	–170	2.93651	70.327	0.24
55	–175	2.93651	66.937	0.11
55	–180	2.93651	63.73	0.03
60	–100	3.01517	130.555	0.29
60	–105	3.01517	126.202	0.38
60	–110	3.01517	121.871	0.48
60	–115	3.01517	117.566	0.58
60	–120	3.01517	113.292	0.66
60	–125	3.01517	109.053	0.73
60	–130	3.01517	104.857	0.79
60	–135	3.01517	100.709	0.81
60	–140	3.01517	96.616	0.79
60	–145	3.01517	92.588	0.76
60	–150	3.01517	88.633	0.68
60	–155	3.01517	84.763	0.58
60	–160	3.01517	80.991	0.46
60	–165	3.01517	77.332	0.35
60	–170	3.01517	73.802	0.23
60	–175	3.01517	70.423	0.13
60	–180	3.01517	67.217	0.05
65	–100	3.09582	133.402	0.16
65	–105	3.09582	129.076	0.22
65	–110	3.09582	124.774	0.28
65	–115	3.09582	120.501	0.34
65	–120	3.09582	116.261	0.40
65	–125	3.09582	112.059	0.46

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
65	–130	3.09582	107.9	0.49
65	–135	3.09582	103.79	0.52
65	–140	3.09582	99.737	0.52
65	–145	3.09582	95.748	0.51
65	–150	3.09582	91.832	0.46
65	–155	3.09582	88	0.41
65	–160	3.09582	84.264	0.34
65	–165	3.09582	80.638	0.26
65	–170	3.09582	77.138	0.19
65	–175	3.09582	73.783	0.12
65	–180	3.09582	70.593	0.06
70	–100	3.17771	135.956	0.09
70	–105	3.17771	131.671	0.12
70	–110	3.17771	127.412	0.15
70	–115	3.17771	123.183	0.20
70	–120	3.17771	118.988	0.23
70	–125	3.17771	114.832	0.27
70	–130	3.17771	110.721	0.30
70	–135	3.17771	106.659	0.32
70	–140	3.17771	102.654	0.32
70	–145	3.17771	98.713	0.31
70	–150	3.17771	94.846	0.30
70	–155	3.17771	91.061	0.27
70	–160	3.17771	87.371	0.22
70	–165	3.17771	83.789	0.18
70	–170	3.17771	80.329	0.14
70	–175	3.17771	77.009	0.09
70	–180	3.17771	73.847	0.06
75	–100	3.26016	138.195	0.04
75	–105	3.26016	133.968	0.06
75	–110	3.26016	129.768	0.07
75	–115	3.26016	125.598	0.11
75	–120	3.26016	121.462	0.13
75	–125	3.26016	117.365	0.15
75	–130	3.26016	113.312	0.16
75	–135	3.26016	109.309	0.17
75	–140	3.26016	105.362	0.18
75	–145	3.26016	101.48	0.18
75	–150	3.26016	97.671	0.17
75	–155	3.26016	93.943	0.17
75	–160	3.26016	90.309	0.15

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ϕ (°)	ψ (°)	d (Å)	θ (°)	$E_{n\square\pi^*}$ (kcal/mol)
75	–165	3.26016	86.78	0.13
75	–170	3.26016	83.37	0.11
75	–175	3.26016	80.096	0.09
75	–180	3.26016	76.975	0.06
80	–100	3.34252	140.095	0.02
80	–105	3.34252	135.951	0.02
80	–110	3.34252	131.829	0.03
80	–115	3.34252	127.735	0.05
80	–120	3.34252	123.673	0.06
80	–125	3.34252	119.649	0.07
80	–130	3.34252	115.667	0.08
80	–135	3.34252	111.735	0.08
80	–140	3.34252	107.859	0.09
80	–145	3.34252	104.045	0.09
80	–150	3.34252	100.304	0.08
80	–155	3.34252	96.644	0.08
80	–160	3.34252	93.075	0.00

Table S2 | Residues in Figure 2c with $d \leq 2.60$ Å.

PDB entry	Chain	Xaa	Yaa	d (Å)
1l7a	A	Asp203	Tyr204	2.30
1e87	A	Lys133	Arg134	2.41
1c4o	A	Pro248	Glu249	2.46
1e87	A	Tyr135	Ala136	2.48
2j0i	A	Leu490	Pro491	2.51
1t1u	A	Ser356	Asn357	2.52
2ggc	A	Arg189	Glu190	2.52
1ks8	A	Leu322	Ser323	2.53
1gvd	A	Lys113	Arg114	2.55
1h4x	A	Thr9	Arg10	2.55
1ro2	A	Ile153	Pro154	2.56
1kjq	A	Ala171	Glu172	2.58
2q4n	A	Val110	Asp111	2.58
1f1u	A	Asp279	Asn280	2.59
1d8w	A	Leu325	Phe326	2.60
1g6u	A	Phe17	Ser18	2.60
1h4x	A	Leu70	Glu71	2.60
2ce2	X	Met72	Arg73	2.60
2q3t	A	Arg106	Leu107	2.60

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Table S3 | Data used to generate Figure 4b.

	d (Å)											
θ (°)	2.4	2.6	2.8	3.0	3.2	3.4	3.6	3.8	4.0	4.2	4.4	4.6
0	0	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0	0	0	0	0	0
30	0	0	0	0	0	0	0	0	0	0	0	0
40	0	0	0	0	0	0	0	0	0	0	0	0
50	0	0	2	1	0	0	0	0	0	0	0	0
60	0	1	4	6	4	10	0	0	0	0	0	0
70	1	5	9	36	65	85	17	1	0	1	0	0
80	2	45	273	193	116	101	47	20	1	0	0	0
90	2	1300	25587	6919	651	240	128	76	4	0	0	0
100	2	1837	46755	18850	1588	560	282	155	65	8	0	0
110	2	182	6026	4928	1463	747	520	272	129	18	0	0
120	0	7	467	1821	1515	1050	643	464	116	15	0	0
130	0	2	6	180	1018	1510	713	252	162	12	0	0
140	0	1	3	12	99	403	370	242	243	1	0	0
150	0	0	1	1	21	42	56	171	54	0	1	1
160	0	0	0	0	34	43	11	2	0	0	1	0
170	0	0	0	3	27	11	0	0	0	0	0	0

Table S4 | Data used to generate Figure 4c.

	d (Å)											
θ (°)	2.4	2.6	2.8	3.0	3.2	3.4	3.6	3.8	4.0	4.2	4.4	4.6
0	0	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0	0	0	0	0	0
30	1	0	0	0	0	0	0	0	0	0	0	0
40	2	0	3	1	0	1	0	0	0	0	0	0
50	0	6	11	10	1	1	0	0	2	1	0	0
60	4	10	16	35	96	52	1	0	36	57	2	0
70	1	28	86	306	518	446	163	7	19	213	64	4
80	7	283	1939	2406	1626	838	428	260	19	126	84	10
90	26	2213	7511	5116	2726	1569	891	728	337	37	20	0
100	7	2020	9630	6096	3873	2757	2528	3068	4265	1399	11	0
110	3	348	7841	6504	5149	4719	5427	9750	17652	3135	11	1
120	4	26	2223	6614	6627	7165	9059	13245	7832	314	4	3
130	1	9	83	1361	4547	6735	6357	5007	1800	119	10	1
140	0	5	8	125	1035	2535	2706	2259	1195	24	25	3
150	0	1	5	52	572	513	499	729	128	11	99	12
160	1	0	6	36	731	337	105	7	1	5	158	7
170	0	0	0	24	584	180	2	0	0	0	0	0

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Table S5 | Proteins with high (>80%) or low (<10%) $n \rightarrow \pi^*$ content.

"Cartoon" image of protein [a]	PDB entry	Chain	Fraction of residues in $n \rightarrow \pi^*$ interaction (%)	Protein Name
	1jek	A	97	Envelope glycoprotein gp160
	1jcd	A	94	Major outer membrane lipoprotein
	1g6u	A	87	*De novo* domain swapped dimer
	1l2p	A	86	ATP synthase subunit *b* dimerization domain
	1n7s	B	83	Syntaxin-1A from a truncated neuronal snare complex
	1nkd	—	82	Regulatory protein Rop
	1n7s	C	82	Synaptosomal-associated protein 25 from a truncated neuronal snare complex
	2ic6	A	81	Coiled coil domain of the sin nombre virus nucleocapsid protein

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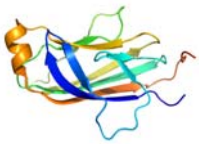
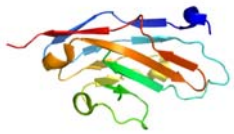
"Cartoon" image of protein [a]	PDB entry	Chain	Fraction of residues in $n \rightarrow \pi^*$ interaction (%)	Protein Name
	1nqj	A	9.8	Collagen binding domain of class 1 collagenase from *Clostridium histolyticum*
	1mqk	L	9.7	Fv fragment of the anti-cytochrome C oxidase antibody 7e2
	1d7p	M	9.7	C2 domain of human clotting factor VIII
	2or7	A	9.6	T-cell immunoglobulin and mucin-domain-containing protein 2
	2hew	F	9.6	Murine tumour necrosis factor ligand superfamily member 4
	1jov	A	9.5	Hl1317 *Haemophilus influenzae* protein of unknown function
	1nko	A	9.5	Sialic acid-binding Ig-like lectin 7
	1jxg	A	9.5	Plastocyanin A, chloroplastic

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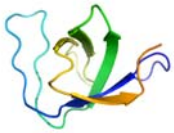
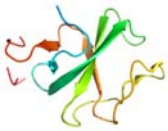
"Cartoon" image of protein [a]	PDB entry	Chain	Fraction of residues in $n \rightarrow \pi^*$ interactions (%)	Protein Name
	2o9s	A	9.4	Second SH3 domain from ponsin
	1mtp	B	9.4	Serine proteinase inhibitor
	2e3h	A	9.3	CAP-Gly domain-containing linker protein 1
	2f01	A	9.3	Streptavidin
	1mqk	H	9.2	Ig heavy chain V region 5–84 (Mouse)
	1tvg	A	9.2	Heat shock protein β-11
	2tnf	A	9.0	Murine tumor necrosis factor-α
	2h14	A	9.0	WD repeat-containing protein 5

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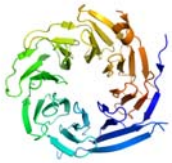
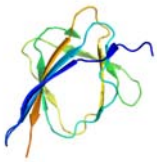
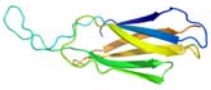
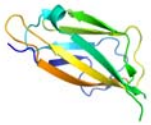
"Cartoon" image of protein [a]	PDB entry	Chain	Fraction of residues in $n \rightarrow \pi^*$ interaction (%)	Protein Name
	1r5m	A	8.9	SIR4-interacting protein SIF2
	2ozi	A	8.9	Putative uncharacterized protein from *Rhodopseudomonas palustris*
	2qfe	A	8.8	Distal c2-like domain of human calpain-7
	1v8h	A	8.8	Sulfur-oxidation protein SoxZ
	3bfo	A	8.6	Ig-like c2-type2 domain of mucosa-associated lymphoid tissue lymphoma translocation protein 1
	1dg6	A	8.6	Tumor necrosis factor ligand superfamily member 10 (Apo2l/trail)
	1lyq	A	8.5	Copper-resistance protein C
	2ic2	A	8.3	First FNIII domain of interference hedgehog

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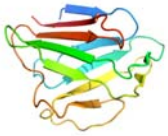
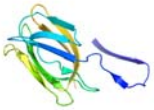
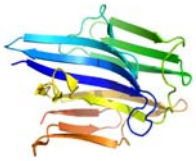
"Cartoon" image of protein [a]	PDB entry	Chain	Fraction of residues in $n \rightarrow \pi^*$ interaction (%)	Protein Name
	2ccv	A	8.3	Agglutinin
	1gvp	—	8.3	DNA-binding protein G5P
	1ifr	A	8.3	Globular domain of lamin-A/C
	2b4h	A	8.1	Rhesus rotavirus vp5 antigen domain
	2gud	A	7.8	Griffithsin
	2hlr	A	7.3	Extracellular domain of bone morphogenetic protein type II receptor
	1y43	B	7.2	Aspergillopepsin-2 light chain
	1uxz	A	7.1	Carbohydrate-binding module from cellulase B

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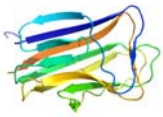
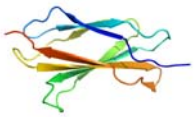
"Cartoon" image of protein [a]	PDB entry	Chain	Fraction of residues in $n \rightarrow \pi^*$ interaction (%)	Protein Name
	2bt9	A	7.0	Fucose-binding lectin protein
	1is3	A	6.9	Congerin-2
	1wck	A	6.8	C-Terminal domain of the BclA protein, *Bacillus anthracis* spore surface protein
	3bcw	A	6.5	Putative uncharacterized protein from *Bordetella bronchiseptica*
	1u2h	A	6.5	N-terminally truncated human apep1, a striated muscle preferentially expressed protein kinase
	1ugx	A	6.3	Agglutinin α chain
	2rb8	A	5.6	Tenascin

[a] Images were generated with the program PyMOL (Schrödinger, LLC).

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