

Additional file 1

PDB	Id	BSA	n1	n2	geometry		core-rim		core-surface		final	
1a0t	1	1,967.37	55	55	23	bio	0.60	bio	-3.11	bio	3	bio
1a0t	2	1,965.86	55	55	23	bio	0.62	bio	-3.10	bio	3	bio
1a0t	3	1,964.43	55	55	23	bio	0.61	bio	-3.02	bio	3	bio
1af6	1	1,844.06	77	77	23	bio	0.60	bio	-2.76	bio	3	bio
1af6	2	1,842.20	77	77	22	bio	0.60	bio	-2.76	bio	3	bio
1af6	3	1,840.30	77	77	23	bio	0.60	bio	-2.75	bio	3	bio
1ek9	1	2,441.63	96	96	4	xtal	0.74	bio	-1.35	bio	0	bio
1ek9	2	2,438.95	96	96	4	xtal	0.69	bio	-1.44	bio	0	bio
1ek9	3	2,430.41	96	96	5	xtal	0.70	bio	-1.47	bio	0	bio
1eys	1	4,828.53	83	102	57	bio	0.68	bio	-7.74	bio	0	bio
1jb0	1	3,967.59	105	107	78	bio	0.38	bio	-5.86	bio	0	bio
1jb0	5	1,105.55	49	105	8	bio	0.66	bio	NaN	bio	3	bio
1jb0	7	915.10	22	22	4	xtal	0.75	bio	-1.51	bio	2	bio
1k4c	2	1,081.94	9	9	10	bio	0.73	nopred	-2.59	nopred	1	bio
1ldf	1	1,581.38	102	102	23	bio	0.46	bio	-2.19	bio	3	bio
1lgh	1	940.40	12	8	3	xtal	0.27	bio	-3.85	bio	2	bio
1lgh	3	939.70	12	8	3	xtal	0.27	bio	-3.91	bio	2	bio
1lgh	5	600.77	8	8	2	xtal	1.09	nopred	-0.60	nopred	1	xtal
1lgh	8	581.01	8	8	1	xtal	1.50	nopred	-0.07	nopred	1	xtal
1ppj	14	1,115.12	67	79	3	xtal	0.73	bio	-0.39	xtal	2	xtal
1q16	7	824.59	74	74	0	xtal	1.24	xtal	-0.41	xtal	3	xtal
1qd6	1	1,441.46	92	92	3	xtal	0.39	bio	-2.18	bio	2	bio
1rwt	2	995.20	119	119	10	bio	0.63	bio	-1.90	bio	3	bio
1rwt	3	979.02	119	119	9	bio	0.57	bio	-1.68	bio	3	bio
1rwt	5	962.82	119	119	9	bio	0.64	bio	-1.82	bio	3	bio
1u7g	1	1,707.86	90	90	22	bio	0.94	xtal	-1.04	bio	2	bio
1uun	1	1,892.53	29	29	9	bio	0.62	bio	-1.51	bio	3	bio
1uun	2	1,891.08	29	29	10	bio	0.56	bio	-1.60	bio	3	bio
1v54	4	2,716.39	124	46	42	bio	0.35	bio	-4.46	bio	0	bio
1v54	6	1,904.80	82	124	17	bio	0.59	bio	NaN	xtal	2	bio
1v54	8	1,810.38	102	46	21	bio	0.70	bio	NaN	xtal	2	bio
1v54	15	1,372.85	118	124	13	bio	0.73	bio	-1.38	bio	3	bio
1v54	30	910.99	46	82	6	bio	1.31	xtal	1.46	xtal	2	xtal
1v54	31	718.29	33	102	1	xtal	0.90	nopred	-1.51	nopred	1	xtal
1yc9	1	2,581.47	11	11	11	bio	0.47	bio	-1.70	bio	0	bio
1z98	1	1,749.51	118	118	26	bio	0.37	bio	-3.32	bio	3	bio
1z98	2	1,744.76	118	118	23	bio	0.40	bio	-3.52	bio	3	bio
2b2f	1	1,905.34	31	31	35	bio	0.84	xtal	-1.35	bio	2	bio
2bhw	1	915.74	119	119	7	bio	0.53	bio	-1.73	bio	3	bio
2bhw	2	915.19	119	119	8	bio	0.53	bio	-1.71	bio	3	bio
2bhw	3	910.88	119	119	7	bio	0.53	bio	-1.72	bio	3	bio
2bs2	3	2,050.12	16	16	8	bio	0.81	xtal	-1.08	bio	2	bio
2f2b	1	1,764.89	24	24	26	bio	0.63	bio	-1.13	bio	3	bio
2fgr	1	1,232.88	10	10	15	bio	0.35	bio	-3.24	bio	3	bio
2gr8	2	1,089.95	8	8	11	bio	1.04	nopred	1.66	nopred	1	bio
2gr8	3	1,087.53	8	8	9	bio	0.86	nopred	1.78	nopred	1	bio
2gr8	4	1,082.06	8	8	10	bio	0.93	nopred	2.05	nopred	1	bio
2j1n	1	1,570.40	110	110	18	bio	0.72	bio	-0.69	xtal	2	bio
2j1n	2	1,566.71	110	110	18	bio	0.78	xtal	-0.66	xtal	2	xtal
2j1n	3	1,564.96	110	110	18	bio	0.69	bio	-0.89	xtal	2	bio
2j58	1	4,294.95	107	107	15	bio	0.56	bio	-5.60	bio	0	bio
2j58	2	4,285.26	107	107	20	bio	0.51	bio	-5.82	bio	0	bio
2j58	3	4,257.43	107	107	20	bio	0.53	bio	-6.00	bio	0	bio
2j58	4	4,256.53	107	107	17	bio	0.52	bio	-5.69	bio	0	bio
2j58	5	4,255.17	107	107	20	bio	0.50	bio	-5.96	bio	0	bio
2j58	6	4,248.70	107	107	19	bio	0.55	bio	-6.04	bio	0	bio
2j58	7	4,242.90	107	107	19	bio	0.51	bio	-5.94	bio	0	bio
2j58	8	4,200.38	107	107	20	bio	0.51	bio	-5.82	bio	0	bio
2j7a	23	671.21	9	9	4	xtal	0.69	nopred	-0.14	nopred	1	xtal
2j8c	1	4,808.45	75	106	79	bio	0.52	bio	-7.99	bio	0	bio
2j8s	1	3,320.38	106	106	14	bio	0.35	bio	-2.85	bio	0	bio
2j8s	2	3,145.04	106	106	10	bio	0.32	bio	-2.76	bio	0	bio
2j8s	3	2,818.52	106	106	10	bio	0.56	bio	-2.20	bio	0	bio
2mpr	1	1,877.41	76	76	23	bio	0.57	bio	-2.74	bio	3	bio
2mpr	2	1,873.89	76	76	23	bio	0.54	bio	-2.84	bio	3	bio
2mpr	3	1,868.01	76	76	22	bio	0.54	bio	-2.82	bio	3	bio
2o4v	1	2,018.80	27	27	17	bio	0.76	xtal	-2.78	bio	2	bio
2o4v	2	2,015.21	27	27	17	bio	0.77	xtal	-2.75	bio	2	bio

continued on next page

PDB	Id	BSA	n1	n2	geometry	core-rim	core-surface	final
2o4v	3	1,996.42	27	27	16 bio	0.75 xtal	-2.78 bio	2 bio
2o9d	1	1,829.57	101	101	30 bio	0.46 bio	-2.52 bio	3 bio
2o9d	2	1,717.59	101	101	29 bio	0.45 bio	-2.50 bio	3 bio
2qi9	1	1,882.77	94	94	6 bio	0.60 bio	-3.11 bio	3 bio
2w2e	1	2,553.53	14	14	28 bio	0.46 bio	-0.94 xtal	0 bio
2wgm	5	1,924.29	77	77	31 bio	0.81 xtal	NaN nopred	1 xtal
2wgm	8	1,922.22	77	77	31 bio	0.80 xtal	NaN nopred	1 xtal
2wgm	11	1,919.28	77	77	30 bio	0.86 xtal	NaN nopred	1 xtal
2wgm	19	1,915.75	77	77	31 bio	0.84 xtal	NaN nopred	1 xtal
2wgm	20	1,915.47	77	77	32 bio	0.79 xtal	NaN nopred	1 xtal
2wgm	21	1,914.82	77	77	31 bio	0.83 xtal	NaN nopred	1 xtal
2wgm	22	1,914.72	77	77	32 bio	0.85 xtal	NaN nopred	1 xtal
2wgm	33	1,900.78	77	77	30 bio	0.80 xtal	NaN nopred	1 xtal
2wgm	35	1,897.38	77	77	31 bio	0.80 xtal	NaN nopred	1 xtal
2wgm	38	1,895.48	77	77	31 bio	0.80 xtal	NaN nopred	1 xtal
2wgm	44	1,887.79	77	77	30 bio	0.79 xtal	NaN nopred	1 xtal
2wie	1	1,909.58	103	103	35 bio	1.19 xtal	NaN nopred	1 xtal
2wie	2	1,889.23	103	103	33 bio	1.20 xtal	NaN nopred	1 xtal
2wie	3	1,877.42	103	103	35 bio	1.22 xtal	NaN nopred	1 xtal
2wie	4	1,867.64	103	103	34 bio	1.21 xtal	NaN nopred	1 xtal
2wie	5	1,856.78	103	103	33 bio	1.36 xtal	NaN nopred	1 xtal
2wjn	1	4,693.27	18	102	57 bio	0.79 xtal	-4.95 bio	0 bio
2wlj	1	2,247.77	9	9	13 bio	0.86 nopred	-1.22 nopred	0 bio
2wlj	2	2,183.44	9	9	10 bio	0.61 nopred	-1.90 nopred	1 bio
2wsw	2	715.72	23	23	3 xtal	0.45 bio	-0.33 xtal	2 xtal
2zfg	1	1,440.50	104	104	19 bio	0.78 xtal	-1.74 bio	2 bio
3arc	1	6,054.21	101	82	111 bio	0.80 xtal	NaN nopred	0 bio
3arc	4	3,644.40	113	82	41 bio	2.05 xtal	NaN xtal	0 bio
3arc	5	3,250.90	101	102	29 bio	1.15 xtal	NaN bio	0 bio
3b9w	1	1,983.85	15	15	28 bio	0.49 bio	-4.20 bio	3 bio
3c02	1	1,591.30	6	6	22 bio	0.33 nopred	-1.82 nopred	1 bio
3cx5	6	1,491.21	28	104	5 xtal	1.03 xtal	-0.49 xtal	3 xtal
3d5k	1	2,739.74	102	102	7 bio	0.59 bio	-2.27 bio	0 bio
3d5k	2	2,738.93	102	102	10 bio	0.58 bio	-2.46 bio	0 bio
3d5k	3	2,726.55	102	102	8 bio	0.65 bio	-2.37 bio	0 bio
3d9s	1	1,558.88	87	87	22 bio	0.55 bio	-1.84 bio	3 bio
3d9s	2	1,547.05	87	87	21 bio	0.62 bio	-1.68 bio	3 bio
3d9s	3	1,542.02	87	87	22 bio	0.58 bio	-1.54 bio	3 bio
3d9s	4	1,527.44	87	87	24 bio	0.53 bio	-1.75 bio	3 bio
3gd8	1	1,515.83	35	35	16 bio	0.35 bio	-2.46 bio	3 bio
3hb3	1	3,887.81	30	106	26 bio	0.53 bio	-4.90 bio	0 bio
3jqo	1	2,342.02	10	10	4 xtal	0.83 xtal	1.78 xtal	0 bio
3jqo	2	2,336.49	10	10	5 xtal	0.85 xtal	NaN xtal	0 bio
3jqo	3	2,327.38	10	10	5 xtal	0.84 xtal	NaN xtal	0 bio
3jqo	4	2,323.32	10	10	6 bio	0.77 xtal	NaN xtal	0 bio
3jqo	5	2,306.63	10	10	5 xtal	0.78 xtal	NaN xtal	0 bio
3jqo	6	2,306.03	10	10	5 xtal	0.87 xtal	NaN xtal	0 bio
3jqo	7	2,299.34	10	10	5 xtal	0.88 xtal	NaN xtal	0 bio
3jqo	8	2,299.00	10	10	5 xtal	0.73 bio	NaN xtal	0 bio
3jqo	9	2,291.00	10	10	5 xtal	0.77 xtal	NaN xtal	0 bio
3jqo	10	2,288.86	10	10	5 xtal	0.81 xtal	2.37 xtal	0 bio
3jqo	11	2,280.57	10	10	5 xtal	0.79 xtal	NaN xtal	0 bio
3jqo	12	2,276.64	10	10	5 xtal	0.82 xtal	1.90 xtal	0 bio
3jqo	13	2,273.28	10	10	5 xtal	0.91 xtal	NaN xtal	0 bio
3jqo	14	2,227.60	10	10	5 xtal	0.79 xtal	1.02 xtal	0 bio
3k3f	1	1,689.32	0	0	12 bio	1,000.00 nopred	NaN nopred	1 bio
3kcu	1	1,615.51	111	111	16 bio	0.69 bio	-1.87 bio	3 bio
3kcu	2	1,581.06	111	111	16 bio	0.56 bio	-2.03 bio	3 bio
3kcu	3	1,491.53	111	111	17 bio	0.57 bio	-2.10 bio	3 bio
3kcu	4	1,487.20	111	111	17 bio	0.57 bio	-2.10 bio	3 bio
3kcu	5	1,426.85	111	111	16 bio	0.54 bio	-2.17 bio	3 bio
3kly	1	1,689.28	34	34	16 bio	0.64 bio	-1.27 bio	3 bio
3kly	2	1,646.64	34	34	17 bio	0.58 bio	-1.41 bio	3 bio
3kly	3	1,637.08	34	34	16 bio	0.57 bio	-1.45 bio	3 bio
3kly	4	1,631.44	34	34	16 bio	0.58 bio	-1.35 bio	3 bio
3kly	5	1,616.54	34	34	17 bio	0.56 bio	-1.51 bio	3 bio
3lde	1	821.44	3	3	5 xtal	0.30 nopred	-1.62 nopred	1 xtal
3m7l	1	1,490.55	11	11	10 bio	0.64 bio	-1.62 bio	3 bio
3pik	1	2,662.31	33	33	4 xtal	0.82 xtal	-0.82 xtal	0 bio
3rlf	1	3,993.60	103	89	30 bio	0.31 bio	-5.97 bio	0 bio

continued on next page

Additional file 1 - continued from previous page

PDB	Id	BSA	n1	n2	geometry		core-rim		core-surface		final	
3tdo	1	1,711.47	15	15	23	bio	0.72	bio	-2.71	bio	3	bio
3tdo	2	1,610.37	15	15	24	bio	0.63	bio	-2.94	bio	3	bio
3tdo	3	1,603.49	15	15	24	bio	0.57	bio	-3.06	bio	3	bio
3tdo	4	1,595.40	15	15	22	bio	0.62	bio	-2.92	bio	3	bio
3tdo	5	1,581.25	15	15	22	bio	0.62	bio	-2.89	bio	3	bio
3tij	1	1,259.18	105	105	10	bio	0.51	bio	-2.27	bio	3	bio
3vzt	1	1,452.94	78	78	14	bio	0.43	bio	-2.51	bio	3	bio
4a01	1	3,265.69	111	111	61	bio	0.32	bio	-5.68	bio	0	bio
4av3	1	2,838.90	10	10	47	bio	0.56	bio	-2.83	bio	0	bio
4f4s	1	1,633.16	107	107	28	bio	0.98	xtal	NaN	nopred	1	xtal
4f4s	5	1,577.73	107	107	28	bio	0.87	xtal	NaN	nopred	1	xtal
4f4s	6	1,567.80	107	107	29	bio	0.84	xtal	NaN	nopred	1	xtal
4f4s	7	1,553.88	107	107	26	bio	1.00	xtal	NaN	nopred	1	xtal
4f4s	9	1,545.24	107	107	28	bio	0.82	xtal	NaN	nopred	1	xtal
7ahl	1	2,817.31	3	3	11	bio	0.96	nopred	0.14	nopred	0	bio
7ahl	2	2,809.31	3	3	11	bio	1.07	nopred	0.83	nopred	0	bio
7ahl	3	2,793.55	3	3	13	bio	0.89	nopred	0.14	nopred	0	bio
7ahl	4	2,789.40	3	3	12	bio	0.85	nopred	0.15	nopred	0	bio
7ahl	5	2,785.36	3	3	12	bio	0.88	nopred	0.05	nopred	0	bio
7ahl	6	2,763.94	3	3	12	bio	0.90	nopred	0.16	nopred	0	bio
7ahl	7	2,745.04	3	3	12	bio	1.04	nopred	0.50	nopred	0	bio