Appendix A

Dataset complexes

A.1 Training data: PDBBind 2018 Refined set

10gs	184l	185l	186l	187l	188l	1a1e	1a28	1a4k	1a4r	1a4w	1a69
1a94	1a99	1a9m	1a9q	1aaq	1add	1adl	1ado	1afk	1afl	1ai4	1ai5
1ai7	1aid	1aj7	1ajn	1ajp	1ajq	1ajv	1ajx	1alw	1amk	1amw	1apv
1atl	1atr	1avn	1ax0	1azm	1b05	1b0h	1b1h	1b2h	1b32	1b38	1b3f
1b3g	1b3h	1b3l	1b40	1b46	1b4h	1b4z	1b51	1b52	1b55	1b57	1b58
1b5h	1b5i	1b5j	1b6h	1b6j	1b6k	1b6l	1b7h	1b8n	1b8o	1b8y	1b9j
1bai	1bcd	1bdq	1bgq	1bhf	1bhx	1bju	1bjv	1bm7	1bma	1bn1	1bn3
1bn4	1bnn	1bnq	1bnt	1bnu	1bnv	1bnw	1bp0	1bq4	1br6	1bty	1bv7
1bv9	1bwa	1bwb	1bxo	1bxq	1bxr	1bzj	1bzy	1c1r	1c1u	1c1v	1c3x
1c4u	1c5c	1c5n	1c5o	1c5p	1c5q	1c5s	1c5t	1c5x	1c5y	1c70	1c83
1c84	1c86	1c87	1c88	1cbx	1ceb	1cet	1cgl	1ciz	1cnw	1cnx	1cny
1cps	1ctt	1ctu	1d09	1d2e	1d3d	1d3p	1d4h	1d4i	1d4j	1d4k	1d4l
1d4p	1d4y	1d6v	1d6w	1d7i	1d7j	1d9i	1dar	1det	1df8	1dgm	1dhi
1dhj	1dif	1dl7	1dmp	1dqn	1drj	1drk	1drv	1dud	1duv	1dy4	1dzk
1e1v	1e1x	1e2k	1e2l	1e3g	1e3v	1e4h	1e5j	1e6q	1e6s	1eb2	1ebw
1ebz	1ec0	1ec1	1ec2	1ec3	1ec9	1ecq	1ecv	1efy	1egh	1ejn	1ela
1elb	1elc	1eld	1ele	1elr	1enu	1eoc	1epo	1erb	1ew8	1ew9	1ex8
1ez9	1ezq	1f0r	1f0s	1f0t	1f0u	1f3e	1f4e	1f4f	1f4g	1f4x	1f57
1f5k	1f5l	1f73	1f74	1f8b	1f8c	1f8d	1f8e	1fao	1fch	1fcx	1fcy
1fcz	1fd0	1fh7	1fh8	1fh9	1fhd	1fiv	1fjs	1fkb	1fkf	1fkg	1fkh
1fki	1fkn	1fkw	1fl3	1flr	1fm9	1fo0	1fpc	1fq5	1ft7	1ftm	1fv0
1fzj	1fzk	1fzm	1fzo	1fzq	1g1d	1g2l	1g2o	1g30	1g32	1g35	1g36
1g3d	1g3e	1g45	1g46	1g48	1g4o	1g52	1g53	1g54	1g74	1g7f	1g7g
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1hmt	1hn4	1hos	1hp5	1hpo	1hps	1hpv	1hpx	1hsh	1hsl	1hvh	1hvi
1hvj	1hvk	1hvl	1hvr	1hvs	1hwr	1hxb	1hxw	1hyo	1i1e	1i2s	1i37
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1ik4	1ikt	1ivp	1iy7	1izh	1izi	1j01	1j14	1j16	1j17	1j36	1j37
1j4r	1jak	1jao	1jaq	1jcx	1jet	1jeu	1jev	1jgl	1jlr	1jmf	1jmg
1jn4	1jq8	1jqy	1jsv	1jvu	1jyq	1jys	1jzs	1k1j	1k1l	1k1m	1k1n
1k1o	1k1y	1k21	1k22	1k27	1k4g	1k4h	1k6c	1k6p	1k6t	1k6v	1k9s
1kav	1kc7	1kdk	1kel	1kjr	1km3	1kmy	1koj	1kpm	1ksn	1kug	1kui
1kuk	1kv1	1kv5	1kyv	1kzk	1kzn	1l83	1l8g	1laf	1lag	1lah	1lan
1lbf	1lbk	1lcp	1lee	1lf2	1lgt	1lgw	1lhu	1li2	1li3	1li6	1lke
1lkk	1lkl	1lnm	1loq	1lpk	1lpz	1lrh	1lst	1lvu	1lyb	1lyx	1lzq
1m0b	1m0n	1m0o	1m0q	1m1b	1m2p	1m2q	1m2r	1m2x	1m48	1m4h	1m5w
1m7d	1m7i	1m7y	1m83	1mai	1mes	1met	1mfa	1mfd	1mfi	1mh5	1mjj
1mmq	1mmr	1moq	1mq5	1mrn	1mrs	1mrw	1mrx	1msm	1msn	1mtr	1mu6
1mu8	1mue	1my4	1n0s	1n1m	1n3i	1n46	1n4h	1n4k	1n51	1n5r	1ndv
1ndw	1ndy	1ndz	1nf8	1nfu	1nfw	1nfx	1nfy	1nh0	1nhu	1nhz	1nja
1njc	1njd	1nje	1njs	1nki	1nl9	1nli	1nm6	1nny	1no6	1np0	1nq7
1nt1	1nvr	1nvs	1nw4	1nw5	1nw7	1nwl	1nz7	1o0f	1o0m	1o0n	1o1s
1o2h	1o2j	1o2n	1o2o	1o2q	1o2r	1o2w	1o2z	1o30	1o33	1o35	1o36
1o38	1o3d	1o3i	1o3j	1o3l	1o5a	1o5c	1o5e	1o5g	1o5r	1o7o	1o86

A. Dataset complexes

```
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1sr7  1srg  1ssq  1stc  1str  1sv3  1sw2  1swg  1swr  1syh  1szd  1t31
1t32  1t4v  1t5f  1t7d  1t7j  1ta6  1tcx  1td7  1thz  1tjp  1tkb  1tlp
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1uwf  1uwt  1uwu  1uz1  1uz4  1uz8  1v0k  1v0l  1v11  1v16  1v1j  1v1m
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```

A. DATASET COMPLEXES

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5his	5hjq	5hrv	5hrw	5hrx	5htl	5htz	5hu9	5hva	5hvs	5hvt	5hwu
5hwv	5hz5	5hz6	5hz8	5hz9	5i1q	5i29	5i2e	5i2f	5i3a	5i3v	5i3w
5i3x	5i3y	5i7x	5i7y	5i80	5i88	5i8g	5i9x	5i9y	5i9z	5ia0	5ia1
5ia2	5ia3	5ia4	5ia5	5ie1	5igm	5ih9	5ihh	5ii2	5ikb	5ime	5ioz
5ipc	5ipj	5irr	5isz	5ito	5itp	5ivc	5ive	5ivv	5ivy	5iwg	5ix0
5izf	5izj	5j0d	5j1r	5j3l	5j41	5j6a	5j7q	5j7w	5j8z	5ja0	5jfp
5jfu	5jg1	5jhb	5ji8	5jop	5jox	5jq5	5js3	5jsg	5jsj	5jsq	5jss
5jt9	5jvi	5jxn	5jxq	5jy3	5jzi	5k03	5k0h	5k1d	5k1f	5k8s	5k9w
5ka1	5ka7	5ka9	5kab	5kad	5kat	5kax	5kbe	5kby	5kcb	5kej	5khm
5kly	5km9	5kma	5ko1	5kqx	5kqy	5kr0	5kr1	5kr2	5kva	5kz0	5l2s
5l30	5l3a	5l4i	5l4j	5l4m	5l7e	5l7g	5l7h	5l8a	5l9g	5l9i	5l9l
5l9o	5ld8	5ldm	5ldp	5lif	5ljq	5ljt	5lne	5lom	5lsg	5lsh
5lso	5lud	5lvd	5lvl	5lvq	5lvr	5lwd	5lwm	5lyn	5lyr	5lz4	5lz5
5lz7	5m04	5m17	5m23	5m25	5m28	5m4q	5m5d	5m77	5m7s	5m7u	5m9w
5ma7	5meh	5mek	5mes	5mg2	5mge	5mgf	5mgj	5mgk	5mjn	5mkr	5mks
5mn1	5mnr	5mo8	5mod	5mpz	5mqe	5mrb	5mrm	5mro	5mrp	5mxf	5my8
5mz8	5n0d	5n0e	5n0f	5n17	5n18	5n1r	5n1s	5n1z	5n24	5n25	5n2t
5n2z	5n31	5n34	5n3v	5n3y	5n6s	5n84	5n93	5n99	5n9r	5nbw	5ndf
5ne5	5nea	5neb	5nee	5ngz	5nih	5njz	5nk2	5nk3	5nk4	5nk6	5nk7
5nk8	5nk9	5nka	5nkb	5nkc	5nkd	5nkg	5nkh	5nki	5nn5	5nn6	5nvv
5nvw	5nvx	5nw07	5nw1	5nw2	5nwi	5o07	5o2d	5o4f	5o58	5oei	5oku
5oot	5op4	5op5	5oq8	5org	5orv	5orw	5os2	5os4	5os5	5ose	5ot8
5ot9	5ota	5otc	5ouh	5ovr	5ovx	5std	5sxm	5sym	5sz0	5sz1	5sz2
5sz3	5sz4	5sz5	5sz6	5sz7	5t19	5t7s	5t8o	5t8p	5t9u	5t9w	5t9z
5ta2	5ta4	5tb6	5tbe	5tbm	5tcj	5tcy	5tef	5tfx	5th4	5ti0	5tmp
5tp0	5tpx	5tt3	5ttw	5tuo	5tuz	5twj	5txy	5ty9	5tya	5u0d	5u0e
5u0f	5u0g	5u0w	5u0y	5u0z	5u11	5u12	5u13	5u14	5u28	5u49	5u4b
5u4d	5u6j	5u8c	5ueu	5uez	5uf0	5ufc	5uff	5ufp	5ufr	5ufs	5uk8
5ula	5uln	5ulp	5ult	5uoo	5uov	5upe	5upf	5upj	5upz	5ut6	5uv2

5uxf	5v0n	5v79	5v7a	5v82	5vb5	5vb6	5vb7	5vc3	5vc4	5vcv	5vcw
5vcy	5vcz	5vd0	5vd1	5vd2	5vd3	5vgy	5vi6	5vih	5vij	5vkc	5vo1
5voj	5vp9	5vsf	5vsj	5w1e	5wa8	5wa9	5wal	5wbm	5wbo	5wcm	5we9
5wex	5wl0	5wlo	5wp5	5wqc	5wuk	5wxh	5wyx	5wyz	5x54	5x62	5x74
5xg5	5yas	5yjm	6ayi	6b4l	6b4n	6b4u	6b7a	6b7b	6b96	6b97	6b98
6cpa	6en5	6ep4	6eqp	6equ	6euw	6eux	6ezq	6rnt	6std	6upj	7std
7upj	8a3h	8cpa	966c								

A.2 Validation data: PDBBind 2018 Core set

1a30	1bcu	1bzc	1e66	1eby	1g2k	1gpk	1gpn	1h22	1h23	1k1i	1lpg
1mq6	1nc1	1nc3	1nvq	1o0h	1o3f	1owh	1oyt	1p1n	1p1q	1ps3	1pxn
1q8t	1q8u	1qf1	1qkt	1r5y	1s38	1sqa	1syi	1u1b	1uto	1vso	1w4o
1y6r	1yc1	1ydr	1ydt	1z6e	1z95	1z9g	2al5	2br1	2brb	2c3i	2cbv
2cet	2fvd	2fxs	2hb1	2iwx	2j78	2j7h	2p15	2p4y	2pog	2qbp	2qbq
2qbr	2qe4	2qnq	2r9w	2v00	2v7a	2vkm	2vvn	2vw5	2w4x	2w66	2wbg
2wca	2weg	2wer	2wn9	2wnc	2wtv	2wvt	2x00	2xb8	2xbv	2xdl	2xii
2xj7	2xnb	2xys	2y5h	2yfe	2yge	2yki	2ymd	2zb1	2zcq	2zcr	2zda
2zy1	3acw	3ag9	3ao4	3arp	3arq	3b1m	3b27	3b5r	3b65	3b68	3bgz
3bv9	3cj4	3coy	3coz	3cyz	3d4z	3dd0	3dx1	3dx2	3e5a	3e92	3e93
3ebp	3ehy	3ejr	3f3c	3f3d	3f3e	3fcq	3fur	3fv1	3fv2	3g0w	3g2z
3g31	3gbb	3gc5	3ge7	3gnw	3gr2	3gv9	3gy4	3ivg	3jvr	3jvs	3jya
3k5v	3kgp	3kr8	3kwa	3lka	3mss	3myg	3n76	3n7a	3n86	3nq9	3nx7
3o9i	3oe4	3oe5	3ozs	3ozt	3p5o	3prs	3pww	3pyy	3qgy	3qqs	3r88
3rlr	3rr4	3rsx	3ryj	3tsk	3twp	3u5j	3u8k	3u8n	3u9q	3udh	3ueu
3uev	3uew	3uex	3ui7	3uo4	3up2	3uri	3utu	3uuo	3wtj	3wz8	3zdg
3zso	3zsx	3zt2	4abg	4agn	4agp	4agq	4bkt	4cig	4ciw	4cr9	4cra
4crc	4ddh	4ddk	4de1	4de2	4djv	4dld	4e5w	4e6q	4ea2	4eo8	4eor
4f09	4f2w	4f3c	4f9w	4gfm	4gid	4gkm	4gr0	4hge	4ih5	4ih7	4ivb
4ivc	4ivd	4j21	4j28	4j3l	4jfs	4jia	4jsz	4jxs	4k18	4k77	4kz6
4kzq	4kzu	4llx	4lzs	4m0y	4mgd	4mme	4mrw	4mrz	4msn	4ogj	4owm
4pcs	4qac	4qd6	4rfm	4tmn	4twp	4ty7	4w9c	4w9h	4w9i	4w9l	4wiv
5a7b	5aba	5c1w	5c28	5c2h	5dwr	5tmn					

A.3 Test set: CSAR HiQ

A.3.1 Set 1

1ax1	1swk	1vot	2add	2are	2b3f	2c1q	2cjp	2hr6	2ihk	2j4k	2jdy
2jgb	2nnq	2ou0	2p98	2pzv	2q6m	2qmj	2r3d	2rca	2v7t	2v7v	2v8y
2z4b	2zlz	3d2r	3f4j	1iup	1ukb	1w6o	2arb	2b1q	2bbf	2cem	2d2v
2idz	2ilz	2jbj	2jff	2jj3	2otz	2p3t	2pjo	2q3c	2qeh	2qvu	2r6w
2rde	2v7u	2v8q	2vhw	2z8f	3c7i	3ene					

A.3.2 Set 2

1ax2	1bcj	1gi9	1gx0	1gzc	1lhw	1q0y	1q6e	1rdi	1s50	1s9t	1tt1
1uld	1uzv	1x9d	1xw6	1y93	1z3t	2a3c	2dm5	2fai	2fv5	2hdq	2hj4
4ubp	1b6m	1bky	1gww	1gz9	1ha2	1ow4	1q4w	1q6g	1rdn	1s7y	1tr7
1txf	1urg	1w2g	1xl5	1y1m	1yxd	1zhx	2cji	2f5t	2ff1	2hd6	2hdr
2i0d											

A.4 Test set: CSAR 2014

fxa006	fxa102	fxa401	fxa422	syk222	syk224	syk226	syk249	trmd444	trmd446	trmd448	trmd450
trmd452	trmd454	trmd456	trmd458	trmd460	trmd462	trmd464	trmd466	trmd468	trmd470	trmd472	trmd474
fxa101	fxa398	fxa406	fxa441	syk223	syk225	syk233	syk250	trmd445	trmd447	trmd449	trmd451
trmd453	trmd455	trmd457	trmd459	trmd461	trmd463	trmd465	trmd467	trmd469	trmd471	trmd473	

Appendix B

Core set clusters

ID	PDB Codes	ID	PDB Codes
0	3ao4, 3zso, 3zsx, 3zt2, 4cig	30	1p1n, 1p1q, 1syi, 2al5
1	1a30, 1eby, 1g2k, 2qnq, 3o9i	31	1bcu, 1oyt, 2zda, 3bv9, 3utu
2	3oe4, 3oe5, 3ozs, 3ozt	32	3u8k, 3u8n, 3wtj, 3zdg, 4qac
3	2zb1, 3e92, 3e93, 4f9w	33	1e66, 1gpk, 1gpn, 1h22, 1h23
4	1bzc, 2hb1, 2qbp, 2qbq, 2qbr	34	1o0h, 1u1b, 1w4o
5	2weg, 3dd0, 3kwa, 3ryj, 4jsz	35	2zcq, 2zcr, 2zy1, 3acw, 4ea2
6	2vvn, 2w4x, 2w66, 2wca, 2xj7	36	1vso, 3fv1, 3fv2, 3gbb, 4dld
7	2wvt, 2xii, 4j28, 4jfs, 4pcs	37	3nq9, 3ueu, 3uev, 3uew, 3uex
8	1z95, 3b5r, 3b65, 3b68, 3g0w	38	3kr8, 4j21, 4j3l
9	2c3i, 3bgz, 3jya, 4k18, 5dwr	39	4e5w, 4ivb, 4ivc, 4ivd, 4k77
10	1k1i, 1o3f, 1uto, 3gy4, 4abg	40	3f3a, 3f3c, 3f3d, 3f3e, 4mme
11	2vkm, 3rsx, 3udh, 4djv, 4gid	41	2v7a, 3k5v, 3mss, 3pyy, 4twp
12	3arp, 3arq	42	1qf1, 1z9g, 3fcq, 4tmn, 5tmn
13	3ebp	43	3cyz
14	2v00, 3prs, 3pww, 3uri, 3wz8	44	2cbv, 2cet, 2j78, 2j7h, 2wbg
15	1qkt, 2p15, 2pog, 2qe4, 4mgd	45	2wtv, 3e5a, 3myg, 3uo4, 3up2
16	1r5y, 1s38, 3gc5, 3ge7, 3rr4	46	3ehy, 3lka, 3nx7, 3tsk, 4gr0
17	4agn, 4agp, 4agq, 5a7b, 5aba	47	3g2z, 3g31, 4de1, 4de2
18	1ps3, 3d4z, 3dx1, 3dx2, 3ejr	48	3ui7, 3uuo, 4llx, 4mrw, 4mrz, 4msn, 5c1w, 5c28, 5c2h
19	1pxn, 2fvd, 2xnb, 3pxf, 4eor	49	4bkt, 4w9c, 4w9h, 4w9i, 4w9l
20	1lpg, 1mq6, 1z6e, 2xbv, 2y5h	50	1yc1, 2xdl, 2yki, 3b27, 3rlr
21	3coy, 3coz, 3ivg, 4ddh, 4ddk	51	4e6q, 4f09, 4gfm, 4hge, 4jia
22	2wn9, 2wnc, 2x00, 2xys, 2ymd	52	4cr9, 4cra, 4crc, 4ty7
23	1nc1, 1nc3, 1y6r, 4f2w, 4f3c	53	3cj4, 3gnw, 4eo8, 4ih5, 4ih7
24	2fxs, 2iwx, 2vw5, 2wer, 2yge	54	2p4y, 2yfe, 3b1m, 3fur, 3u9q
25	3qgy, 4m0y, 4qd6, 4rfm	55	4kzq, 4kzu
26	1owh, 1sqa, 3kgp	56	3p5o, 3u5j, 4lzs, 4ogj, 4wiv
27	3qqs, 3r88, 3twp, 4gkm, 4owm	57	1q8t, 1q8u, 1ydr, 1ydt, 3ag9
28	1nvq, 2br1, 2brb, 3jvr, 3jvs	58	2xb8, 3n76, 3n7a, 3n86, 4ciw
29	2r9w, 3gr2, 3gv9, 4jxs, 4kz6		