Supporting Materials

Pre-orientation of protein and RNA just before contacting

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Table S1. Predicted protein-RNA binding sites of 23 protein-RNA complexes from two prediction methods: LEDock and BindN server.

Complex PDBid ^a	Protein PDBid ^a	LEDock ^b	BindN Server ^b	Native Binding Sites ^c
1E7K_A:C	2JNB_A	41GLU 33LYS 48ARG 44LYS 35LEU 36ARG 37LYS 97ARG 94GLY 96SER 95VAL 40ASN 34GLN 107LYS 30CYS 38GLY 105THR 32TYR 108GLU 50ILE 93CYS 31ASN 45THR 47ASN 43THR 109GLY 103SER 98PRO 49GLY 39ALA	9LYS 20LYS 31ASN 32TYR 33LYS 34GLN 36ARG 37LYS 40ASN 41GLU 43THR 44LYS 45THR 47ASN 48ARG 80TYR 84ARG 86LYS 87GLN 91ARG 97ARG 105THR 107LYS 110SER 111GLN 113LYS 125ARG	37LYS 38GLY 39ALA 40ASN 41GLU 44LYS 48ARG 59ASP 60ALA 61GLU 65ILE 86LYS 95VAL 96SER 97ARG 98PRO 99VAL 100ILE 101ALA
1F7U_A:B	1F7U_B	58ASN 62ARG 70PRO 71ARG 73ARG 74ILE 75LYS 76GLY 77ALA 78ASN 79PRO 80LYS 102ASN 103GLY 104PRO 105PHE 315LYS 323THR 324LYS 325PHE 326ASN 327LYS 328LYS 372ASP 373LEU 402GLN 462LYS 464ILE 465ASN 466ASN	8LYS 19LYS 21SER 32ARG 41LYS 43SER 62ARG 71ARG 73ARG 75LYS 76GLY 78ASN 80LYS 125THR 126ARG 127LYS 129ASP 130TYR 132SER 134LYS 152LYS 160ARG 181ARG 190LYS 201ARG 202TYR 238GLN 239SER 240THR 241ASN 242GLY 243LYS 245ARG 246GLU 247TYR 250ARG 263LYS 264ARG 266ARG 277TYR 279ARG 283LYS 287TYR 288SER 290GLU 291SER 292GLN 295LYS 311THR 315LYS 324LYS 326ASN 327LYS 328LYS 331LYS 336LYS 337SER 338ASP 340THR 341THR 343TYR 346ARG 354ARG	55GLU 59THR 62ARG 66LEU 68PRO 70PRO 71ARG 73ARG 105PHE 149ASN 186GLY 189GLY 190LYS 191GLN 290GLU 315LYS 317ALA 319LEU 328LYS 331LYS 333ILE 336LYS 337SER 342LEU 343TYR 346ARG 369SER 370GLN 371GLN 373LEU 374HIE 400MET 402GLN 425MET 428VAL 429MET 432ASN 435LYS 449VAL 460GLN 461GLY 462LYS 464ILE 465ASN 466ASN 473ARG 477PHE 478GLU 479GLY 480ASP 483PRO 484TYR 487TYR 490SER 491ARG

			357LYS 405SER 406THR 407ARG 408LYS 410THR 422LYS 430LYS 431LYS 432ASN 433GLU 434ASN 435LYS 436TYR 438GLN 460GLN 462LYS 463ARG 465ASN 466ASN 481THR 484TYR 486GLN 487TYR 489HIE 490SER 491ARG 493ARG 494SER 496GLU 497ARG 500SER 521LYS 525ARG 535ARG 539LYS 540THR 541HIE 542GLU 544THR 548THR 575THR 577ARG 581TYR 585ARG 589TYR 593ARG 602ARG	494SER 495VAL 498ASN 544THR 548THR 552LYS 555HIE 558SER 559SER 561TYR 562ASP 564LEU 565TRP 566VAL 567ALA 581TYR 602ARG 603MET
1JBS_B:D	1AQZ_A	10LEU 33ASP 34GLY 35LYS 36THR 37GLY 38SER 39SER 40TYR 42HIE 43TRP 45THR 49ASP 55ILE 56LYS 57GLY 58ARG 76GLN 103LYS 104LYS 105PRO 106LYS 108ASN 109PRO 131ARG 132GLY 133ASN 134GLN 135GLY 136ASP	14ARG 17TYR 19GLN 21LYS 23GLU 24SER 25ASN 26SER 28HIE 32SER 33ASP 34GLY 35LYS 36THR 37GLY 38SER 39SER 40TYR 42HIE 51ASN 53LYS 56LYS 58ARG 59THR 62LYS 65LYS 67ASP 69ASP 70ARG 71PRO 72PRO 73LYS 74HIE 75SER 76GLN 77ASN 78GLY 81LYS 98TYR 99LYS 101ASP 102SER 103LYS 104LYS 105PRO 106LYS 107GLU 108ASN 109PRO 113ARG 116TYR 121LYS 131ARG 133ASN 134GLN 138ARG	34GLY 35LYS 36THR 37GLY 38SER 39SER 40TYR 43TRP 45THR 48TYR 55ILE 58ARG 74HIE 76GLN 103LYS 106LYS 129HIE 133ASN 135GLY 136ASP
1KQ2_A,B,H, I,K,M:R	1KQ1_A, B,H,I,K,Z	4ASP 36LYS 37TYR 61ASN 62ILE 63GLN 64ASP 65LYS 95ASP 96LYS 97TYR 113HIE 122MET 123ILE 124ALA 126GLU 127ASN 130ASP 160TYR 161ASP 162LYS 163TYR 188ASN 191ASP 223LYS 224TYR 248ASN 283LYS 284TYR 300HIE	11LYS 14GLN 40SER 42ASN 43SER 44GLN 46LYS 47GLN 57THR 58TYR 71LYS 74GLN 100SER 102ASN 103SER 104GLN 106LYS 107GLN 137LYS 140GLN 166SER 168ASN 169SER 170GLN 172LYS 173GLN 183THR 198LYS 201GLN 227SER 229ASN 230SER 231GLN 233LYS 234GLN 244THR 245TYR 258LYS 261GLN 287SER 289ASN 290SER 291GLN 293LYS 294GLN	3GLN 22LEU 36LYS 37TYR 51TYR 52LYS 53HIE
1LNG_A:B	1LNG_A	2ILE 4TRP 7TYR 13SER	7TYR 9ASP 10LYS 11LYS	1MET 2ILE 4TRP 7TYR

		14ARG 15ARG 17GLY 18ARG 19LYS 21PRO 22GLU 23GLU 51LYS 52ARG 53TYR 54PRO 55ARG 57HIE 65GLU 67ASP 68TYR 69LYS 70GLY 71ASN 72LYS 73LEU 74GLN 77LYS 78GLU 81LYS	12LYS 13SER 14ARG 15ARG 16GLU 17GLY 18ARG 19LYS 32LYS 39LYS 40LYS 46LYS 49ARG 50ASP 51LYS 52ARG 53TYR 54PRO 55ARG 69LYS 71ASN 72LYS 84LYS 86LYS	12LYS 13SER 14ARG 15ARG 18ARG 19LYS 21PRO 22GLU 23GLU 50ASP 51LYS 52ARG 53TYR 54PRO 55ARG 57HIE 58TRP 66VAL 67ASP 68TYR 69LYS 71ASN 72LYS 73LEU 74GLN 77LYS
100A_A:C	100A_A	17ARG 19ARG 21VAL 22CYS 23GLU 24GLY 25PRO 26SER 27HIE 28GLY 29GLY 37LYS 38ASN 40LYS 99ASN 108LYS 212LYS 214VAL 215ARG 216MET 217ASP 218ARG 219THR 232LEU 234ASP 235LYS 268ARG 270PHE 306LYS 307PRO	12LYS 13GLN 14ARG 15GLY 17ARG 19ARG 26SER 27HIE 31PRO 33ALA 34SER 35SER 36GLU 37LYS 38ASN 39LYS 40LYS 41SER 42TYR 44GLN 46LYS 55LYS 65LYS 66ASN 68HIE 77LYS 87THR 106THR 107LYS 108LYS 109LYS 120GLU 124ARG 126TYR 138TYR 147ARG 148GLN 150THR 154LYS 158ARG 166LYS 174ARG 185THR 187SER 188PHE 189THR 190ARG 191ARG 194PRO 204LYS 207ASN 209SER 212LYS 215ARG 218ARG 219THR 224THR 264THR 268ARG 275LYS 276THR 277PRO 278LYS 279TYR 280LYS 285THR 286LYS 289SER 295ARG 296ARG 297LYS 298SER 299ASP 301GLU 302THR 303SER 306LYS	17ARG 19ARG 20TYR 22CYS 23GLU 25PRO 26SER 27HIE 28GLY 29GLY 40LYS 104HIE 105VAL 106THR 107LYS 108LYS 204LYS 205ALA 206PRO 207ASN 212LYS 214VAL
1P6V_A:B	1K8H_A	3SER 4ASP 5LYS 26GLU 28GLY 30VAL 31LEU 32LYS 33GLY 34SER 35GLU 37LYS 56ASN 70LYS 73THR 75GLU 76ASN 77HIE 81ARG 82LYS 83ARG 84LYS 86LEU 88HIE 89LYS 114LYS 115ASN 116ASN 117LYS 119LYS	2LYS 5LYS 13LYS 16LYS 18LYS 32LYS 34SER 35GLU 37LYS 38SER 40ARG 42LYS 44THR 46SER 53ARG 81ARG 82LYS 83ARG 84LYS 86LEU 90ARG 94ARG 98LYS 102LYS 110LYS 112TYR 114LYS 115ASN 117LYS 119LYS 126LYS 128LYS 129LYS 131TYR 133ARG	26GLU 27ALA 28GLY 29ILE 30VAL 31LEU 32LYS 33GLY 34SER 36VAL 37LYS 40ARG 58GLU 71HIE 85LEU 86LEU 87LEU 88HIE 89LYS 90ARG 91GLU 92ILE 113TRP 115ASN 116ASN 117LYS 118VAL 119LYS
1SZ1_A:E	1R8A_A	197ARG 198ARG 212GLU 213GLU 299ARG 302ARG 303LYS 306GLU 309GLU 310ARG 344ARG 345MET 346GLY 347PRO 348GLN 351ASP 353ARG 354ASN	22ARG 23LYS 25ARG 32ARG 37GLU 47SER 48TYR 50ARG 51ASN 52THR 55LYS 76ARG 84LYS 93ARG 94TYR 105LYS 116LYS 118LYS 121LYS 122ASN 124LYS 125SER 126ALA	59GLU 61ASP 91GLU 93ARG 95ALA 96GLU 99TYR 101HIE 108GLU 110ASP 163ALA 164GLU 165TYR 224ARG 228ALA 229ASN 289VAL 291ASP 292ASN

		357LYS 360SER 361ARG 373ARG 395THR 396HIE 397TRP 398HIE 399THR 401GLY 402LYS 409ARG	129ARG 130THR 140ARG 142LYS 144LYS 149ARG 152LYS 156LYS 161TYR 166LYS 168ARG 190LYS 191ASN 192ALA 193ARG 194ARG 195TRP 196THR 197ARG 198ARG 205LYS 207GLU 209ARG 210LYS 224ARG 237ARG 255LYS 266ARG 268ARG 269LYS 276THR 282LYS 284ARG 299ARG 301SER 302ARG 317ARG 318SER 321LYS 339SER 340ARG 343ARG 344ARG 348GLN 356LYS 357LYS 361ARG 362ASN 363ARG 366ARG 373ARG 381LYS 387GLU 388GLY 390ARG 392TYR 394SER 395THR 398HIE 399THR 402LYS 406GLU 409ARG 419LYS	295PRO 296GLN 299ARG 302ARG 303LYS 310ARG 345MET 346GLY 347PRO 348GLN 351ASP 354ASN 357LYS 358PHE 361ARG 363ARG 373ARG 392TYR 396HIE 398HIE 399THR 401GLY 402LYS 403ASN
1TFW_B:E,H	1R8A_A	299ARG 302ARG 303LYS 306GLU 310ARG 311GLU 344ARG 345MET 346GLY 347PRO 348GLN 351ASP 353ARG 354ASN 357LYS 358PHE 360SER 361ARG 373ARG 378GLU 381LYS 392TYR 395THR 396HIE 397TRP 398HIE 399THR 401GLY 402LYS 409ARG	22ARG 23LYS 25ARG 32ARG 37GLU 47SER 48TYR 50ARG 51ASN 52THR 55LYS 76ARG 84LYS 93ARG 94TYR 105LYS 116LYS 118LYS 121LYS 122ASN 124LYS 125SER 126ALA 129ARG 130THR 140ARG 142LYS 144LYS 149ARG 152LYS 156LYS 161TYR 166LYS 168ARG 190LYS 191ASN 192ALA 193ARG 194ARG 195TRP 196THR 197ARG 198ARG 205LYS 207GLU 209ARG 210LYS 224ARG 237ARG 255LYS 266ARG 268ARG 269LYS 276THR 282LYS 284ARG 299ARG 301SER 302ARG 317ARG 318SER 321LYS 339SER 340ARG 343ARG 344ARG 348GLN 356LYS 357LYS 361ARG 362ASN 363ARG 366ARG 373ARG 381LYS 387GLU	165TYR 292ASN 295PRO 296GLN 299ARG 302ARG 401GLY 402LYS

			388GLY 390ARG 392TYR 394SER 395THR 398HIE 399THR 402LYS 406GLU 409ARG 419LYS	
1WPU_A:C	1WPV_A	2LEU 4LYS 7ARG 9GLY 10ARG 13VAL 14LEU 39GLY 40LYS 41VAL 42GLY 43SER 44MET 45ASP 47HIE 48LYS 51ALA 52ALA 54GLU 55THR 56ALA 59LYS 65SER 100GLY 131PRO 132ILE 133LYS 140PHE 142VAL 144ILE	1THR 4LYS 6ARG 7ARG 10ARG 27GLU 28GLU 31ARG 40LYS 43SER 55THR 56ALA 57SER 58LYS 59LYS 60SER 64GLN 65SER 66GLU 68TYR 69ARG 72HIE 86THR 87ARG 97ARG 98THR 102ARG 107ARG 109ASN 111TYR 133LYS	40LYS 41VAL 42GLY 43SER 44MET 51ALA 52ALA 55THR 56ALA 59LYS 96LEU 98THR 99VAL 100GLY 101LEU 102ARG 127THR 130ALA 131PRO 132ILE 133LYS 134GLY 135LEU 136GLU
1WSUA:E	1LVA_A	122ALA 155GLN 158SER 160LYS 161GLU 164GLY 165SER 192GLU 218LEU 219ALA 220GLU 222ARG 223ASP 226GLY 228SER 229ARG 230LYS 231TYR 233LEU 234PRO 237GLU 241GLN 243LYS 246ARG 247ARG 248VAL 249GLY 250ASP 255VAL 256GLY	2SER 5LYS 26ARG 28SER 30SER 35ARG 36LYS 39GLN 47THR 50ARG 59SER 60THR 62ARG 63TYR 72ARG 80ARG 81TYR 84ARG 85PRO 89ARG 91GLU 93ARG 94SER 95ARG 96TYR 98SER 99ARG 103ARG 114ARG 117ARG 131THR 133SER 135SER 136GLU 137THR 139LYS 140LYS 143LYS 150ARG 152SER 153ARG 155GLN 156PRO 182ARG 204ARG 208LYS 212SER 213THR 222ARG 227SER 228SER 229ARG 230LYS 231TYR 243LYS 246ARG 247ARG 252ARG	218LEU 219ALA 222ARG 227SER 228SER 229ARG 230LYS 231TYR 233LEU 237GLU 247ARG 250ASP 252ARG
2ADC_A:B	1QM9_A	38PHE 40LYS 42GLU 43ASN 63GLY 72ARG 74THR 77LYS 78HIE 79GLN 80ASN 115ASN 116ILE 117PHE 118PRO 149LYS 150GLY 151PHE 152LYS 153PHE 154PHE 155GLN 156LYS 157ASP 158ARG 162LEU 164GLN 196SER 197THR 198ILE	15ARG 17THR 33ARG 35LYS 55GLN 64HIE 65LYS 67HIE 69LYS 72ARG 74THR 82GLN 85ARG 94THR 95LYS 96ASP 97TYR 99ASN 100SER 101PRO 103HIE 104ARG 106LYS 107LYS 108PRO 109GLY 110SER 111LYS 122THR 131SER 149LYS 152LYS 158ARG 190ARG 192SER 195LYS	101PRO 102LEU 112ASN 114GLN 115ASN 117PHE 124HIE 126SER 127ASN 152LYS 153PHE 154PHE 155GLN 156LYS 159LYS 160MET 162LEU 179HIE 186ASN 187HIE 190ARG 191VAL 192SER 193PHE 194SER 195LYS 196SER 197THR
2ASB_A:B	1K0R_A	1VAL 2SER 3ARG 4ARG 5HIE 6MET 7ASN 8ILE 9ASP 11ALA 14HIE 15ALA 86ARG 87ILE 90THR	2SER 3ARG 4ARG 20ARG 32LYS 33SER 37THR 40ARG 42THR 43GLN 45HIE 46GLN 47THR 50ARG 55ARG 57THR	214ARG 227ASN 229LYS 230GLY 233ILE 234GLY 236MET 237GLY 240VAL 241ARG 244MET 251LYS

		91THR 93ARG 94GLN 97LEU 98GLN 100PHE 101ARG 214ARG 233ILE 236MET 241ARG 251LYS 271PRO 273LYS 302LYS	61ARG 65ARG 86ARG 90THR 91THR 93ARG 94GLN 101ARG 104GLU 105SER 106THR 107ARG 118ARG 120SER 121ARG 123ASN 125ARG 131ARG 134THR 136THR 137LYS 139SER 154TYR 156HIE 157GLY 158ASN 159ARG 161ARG 168THR 169ARG 172ARG 177THR 179SER 180ARG 181THR 183PRO 184ASN 187ARG 209ARG 211ALA 213HIE 214ARG 216LYS 220ARG 222ASN 225GLY 229LYS 238GLN 239ARG 241ARG 242ASN 263ARG 270SER 273LYS 276SER 285ARG 288ARG 302LYS 305GLN 306ASN 308ARG 312ARG 314THR 317ARG 321ARG	252ILE 253ASP 254ILE 255ILE 270SER 271PRO 294PHE 295GLN 296LEU 297SER 298LEU 300ILE
2AZX_A:C	1O5T_A	8ASP 9LYS 11ILE 12VAL 13ARG 14PHE 15GLY 16SER 17SER 18LYS 20ASP 21LYS 22GLU 23LEU 26ARG 29ARG 47HIE 48ARG 49ASP 51ASN 52GLN 55ASP 59ASN 209ASP 225ARG 229ASP 232PRO 233ARG 235GLY 238LYS	3LYS 13ARG 16SER 17SER 18LYS 21LYS 26ARG 29ARG 30ALA 31THR 33GLN 34ARG 36HIE 37HIE 40ARG 60LYS 61LYS 64TYR 66TYR 67THR 69ARG 70GLY 71PRO 72SER 73SER 117GLN 119TYR 138LYS 151SER 152SER 156LYS 160LYS 163LYS 184LYS 195SER 197SER 198ASN 202GLN 205ARG 207ARG 228ARG 233ARG 236TYR 238LYS 254GLN 255THR 256LYS 258SER 259ALA 260SER 261ASP 263ASN 264SER 265SER 273LYS 274GLN 276LYS 277THR 278LYS 281LYS 285SER 288ARG 290THR 295ARG 324ARG 325LYS 327TYR 328THR 329SER 334THR 338LYS 339LYS 353GLN 355ARG 356ARG 357LYS 371ARG 372LYS	178ASP 179SER 262PRO 263ASN 280ASN 281LYS 282HIE 283ALA 284PHE 285SER 287GLY 288ARG 289ASP 290THR 291ILE 292GLU 294HIE 333LEU 334THR 335GLY 338LYS
2BH2_A:C	1UWV_A	13PHE 41THR 42GLU 43ASP 44LYS 45LYS 46GLN 47TYR	15GLN 19ARG 20HIE 21ASN 22GLY 23LYS 24THR 41THR	9ASP 11ASP 13PHE 15GLN 17VAL 19ARG 21ASN

		49ARG 117ARG 121ASN 124PRO 125LYS 133ARG 135ALA 136GLY 137SER 138SER 139ASP 188ARG 190THR 218SER 323GLU 344ALA 345ARG 346ALA 347GLY 368ASN 370ALA 374ARG	44LYS 45LYS 46GLN 47TYR 49ARG 51LYS 54ARG 55ARG 59SER 60PRO 61GLU 62ARG 63GLU 64THR 65PRO 66ARG 77GLN 82SER 86GLN 87GLN 88ARG 89SER 90LYS 91SER 92ALA 96ARG 98LYS 110TRP 112TYR 113ARG 114ARG 115ARG 116ALA 117ARG 119SER 122TYR 125LYS 128GLN 129LEU 130GLN 133ARG 134LYS 136GLY 137SER 138SER 161ARG 166SER 168GLN 170ARG 182SER 184THR 188ARG 194SER 195SER 197ASP 198ARG 199GLU 200LYS 203ARG 233ASN 236ARG 238THR 242ARG 253GLN 254LYS 257ARG 285THR 289SER 302LYS 304GLN 305GLN 306ASN 308ARG 328LYS 331TRP 333LYS 345ARG 361ARG 364TYR 371THR 374ARG 381LYS 384TYR 385THR 388ARG 406ARG	22GLY 23LYS 24THR 26PHE 44LYS 45LYS 46GLN 47TYR 49ARG 74GLY 75GLY 77GLN 96ARG 97LEU 113ARG 115ARG 116ALA 117ARG 120LEU 121ASN 132PHE 133ARG 134LYS 135ALA 136GLY 137SER 138SER 172LEU 173GLY 174HIE 188ARG 190THR 242ARG 247VAL 295GLY 296VAL 321ASN 323GLU 344ALA 345ARG 368ASN 370ALA 371THR 374ARG 393PHE 396THR 398HIE
2CZJ_A:B	1J1H_A	1MET 2ALA 3PRO 11ARG 21GLU 23GLY 25ALA 26LEU 27LYS 28GLY 29THR 32LYS 35ARG 52GLU 63TYR 70ASN 72ASP 74ARG 76LYS 77ARG 78LYS 80LEU 104LYS 106TYR 108ASN 109GLU 110ARG 111GLY 112TYR 114LYS	8ARG 9ARG 11ARG 27LYS 29THR 30GLU 32LYS 33SER 35ARG 38LYS 44SER 47ARG 65LYS 67SER 68TYR 70ASN 71VAL 72ASP 73PRO 74ARG 75ARG 76LYS 77ARG 78LYS 87ARG 88ARG 92LYS 95GLN 96LYS 99THR 110ARG 112TYR 114LYS 121ARG 123LYS	21GLU 22ALA 23GLY 24ILE 25ALA 26LEU 27LYS 28GLY 29THR 31VAL 32LYS 35ARG 52GLU 63TYR 65LYS 66GLY 67SER 68TYR 78LYS 79LEU 80LEU 81LEU 82HIE 83LYS 86LEU 110ARG 111GLY 112TYR 113ALA 114LYS
2DRA_A:B	1R8A_A	212GLU 299ARG 302ARG 303LYS 306GLU 310ARG 344ARG 345MET 346GLY 347PRO 348GLN 351ASP 353ARG 354ASN 357LYS 358PHE 360SER 361ARG 362ASN 373ARG 381LYS 392TYR 395THR 396HIE 397TRP 398HIE 399THR 401GLY 402LYS 409ARG	22ARG 23LYS 25ARG 32ARG 37GLU 47SER 48TYR 50ARG 51ASN 52THR 55LYS 76ARG 84LYS 93ARG 94TYR 105LYS 116LYS 118LYS 121LYS 122ASN 124LYS 125SER 126ALA 129ARG 130THR 140ARG 142LYS 144LYS 149ARG 152LYS 156LYS 161TYR 166LYS 168ARG 190LYS 191ASN	59GLU 61ASP 63PHE 93ARG 94TYR 95ALA 96GLU 97HIE 99TYR 110ASP 112VAL 126ALA 127VAL 129ARG 130THR 163ALA 164GLU 165TYR 224ARG 228ALA 229ASN 291ASP 292ASN 295PRO 296GLN 299ARG 302ARG 303LYS 310ARG 344ARG 345MET 346GLY

			192ALA 193ARG 194ARG 195TRP 196THR 197ARG 198ARG 205LYS 207GLU 209ARG 210LYS 224ARG 237ARG 255LYS 266ARG 268ARG 269LYS 276THR 282LYS 284ARG 299ARG 301SER 302ARG 317ARG 318SER 321LYS 339SER 340ARG 343ARG 344ARG 348GLN 356LYS 357LYS 361ARG 362ASN 363ARG 366ARG 373ARG 381LYS 387GLU 388GLY 390ARG 392TYR 394SER 395THR 398HIE 399THR 402LYS 406GLU 409ARG 419LYS	347PRO 354ASN 357LYS 358PHE 361ARG 363ARG 373ARG 392TYR 396HIE 398HIE 399THR 401GLY 402LYS 403ASN
2HVY_D:E	1PXW_A	32ARG 33ASP 34THR 35GLY 36LYS 37ILE 38ARG 39LYS 40GLY 42ASN 43GLU 46LYS 47ALA 49GLU 50ARG 51GLY 52GLN 54LYS 78LYS 93ALA 95ALA 96GLY 97ILE 98GLU 99VAL 100ALA 107ILE 108GLU 110GLY 113ARG	8LYS 10SER 11TYR 13LYS 32ARG 34THR 35GLY 36LYS 38ARG 39LYS 40GLY 41THR 42ASN 43GLU 44THR 45THR 46LYS 49GLU 50ARG 52GLN 54LYS 82TYR 84TYR 88LYS 89LYS 111LYS 113ARG 124ARG	38ARG 39LYS 40GLY 41THR 42ASN 43GLU 46LYS 50ARG 61ASP 62VAL 63ASP 64PRO 67ILE 88LYS 97ILE 99VAL 100ALA 101ALA 102ALA 103SER
2JOS_A:E	2HXY_A	1PRO 2THR 4ASP 5THR 6MET 23LYS 25SER 26ALA 27ILE 29GLN 30ARG 33LYS 46GLN 47SER 48GLY 49THR 204VAL 205LYS 206ARG 272GLY 273ASP 274MET 275PRO 276GLN 279ARG 299VAL 301ALA 302ARG 303GLY 305ASP	5THR 9ARG 14ARG 19TYR 23LYS 25SER 30ARG 33LYS 46GLN 47SER 48GLY 49THR 50GLY 51LYS 52THR 54THR 68ARG 79ARG 87LYS 107THR 114ARG 118TYR 126THR 129ARG 135ARG 136ARG 137ARG 138SER 140ARG 141THR 142ARG 145LYS 161LYS 197THR 201ARG 249THR 250LYS 251ARG 252LYS 261ARG 264ASN 268SER 273ASP 275PRO 276GLN 277LYS 279ARG 280GLU 287ARG 288SER 289GLY 291SER 292ARG 302ARG 321ARG 324TYR 327ARG 329GLY 330ARG 331SER	77PRO 78THR 79ARG 104ILE 105GLY 106GLY 107THR 109VAL 126THR 127PRO 128GLY 129ARG 132ASP 135ARG 154GLU 160PHE 163GLN 248ASN 249THR 250LYS 271HIE 272GLY 279ARG 297THR 298ASP 299VAL 319ASN

			332GLY 333ARG 334TYR 335GLY 336ARG 337LYS 345LYS	
2PJP_A:B	2PJP_A	22TRP 24ARG 25ASP 28LYS 34GLU 35GLN 38ARG 42ARG 46GLN 52ALA 54VAL 55LYS 56ASP 57ARG 83ALA 84ALA 87ARG 91GLY 92VAL 93GLY 94ARG 95LYS 96LEU 98ILE 99GLN 102GLU 106ARG 112ARG 114GLY 115ASN	28LYS 32THR 38ARG 40THR 42ARG 43GLN 51THR 55LYS 57ARG 58TYR 59TYR 60ARG 63ARG 72ARG 80SER 89ARG 94ARG 95LYS 106ARG 110THR 111ARG 112ARG 113ARG 115ASN 116ASP	22TRP 23VAL 24ARG 34GLU 38ARG 55LYS 56ASP 57ARG 83ALA 87ARG 93GLY 94ARG 95LYS 98ILE 102GLU 112ARG 115ASN 117HIE
2PXV_A:B	2PXV_A	21THR 22LYS 23GLU 26LYS 27PRO 28GLU 29ILE 30ILE 31LYS 32GLY 33SER 34ARG 35LYS 36ARG 37ARG 40ALA 44GLN 45VAL 46GLN 47ASP 49ASN 50ARG 52LEU 53LYS 56ASP 57ASP 58GLN 59ARG 60LYS 61LYS	20SER 21THR 22LYS 23GLU 24ARG 26LYS 31LYS 32GLY 33SER 34ARG 35LYS 36ARG 37ARG 38ILE 39ALA 40ALA 41GLY 42SER 44GLN 46GLN 50ARG 53LYS 58GLN 59ARG 60LYS 61LYS	10LYS 13VAL 14ARG 16ALA 19ASN 20SER 21THR 22LYS 23GLU 24ARG 33SER 34ARG 37ARG 40ALA 41GLY 42SER 43GLY
2QUX_A:C	2QUD_A	23GLN 25THR 26ALA 27ASP 28ARG 30ILE 39VAL 40GLY 43ARG 45THR 47SER 49ARG 50GLN 51ASN 52GLY 53ALA 58ARG 60ASN 62LYS 64ASP 66ALA 75LYS 76VAL 77ARG 78TYR 79THR 80GLN 81VAL 83SER 85ASP	3SER 5SER 6LYS 16THR 17ARG 20THR 21GLU 24SER 25THR 28ARG 41ARG 43ARG 45THR 47SER 49ARG 50GLN 51ASN 52GLY 54LYS 55THR 57TYR 58ARG 62LYS 75LYS 77ARG 78TYR 79THR 80GLN 92SER 93THR 94GLU 95ALA 96SER 97ARG 98LYS 101TYR 110THR 125ARG	49ARG 51ASN 52GLY 53ALA 55THR 56ALA 58ARG 62LYS 81VAL 83SER 85ASP 86VAL 87THR 89VAL
3BX2_A:C	3BWT_A	1SER 2ARG 3PHE 4ALA 5ASP 20LYS 21ASP 22GLN 23HIE 26ARG 29GLN 30LYS 33ASP 34ILE 58SER 59PHE 62TYR 65GLN 66LYS 69GLU 94PRO 95HIE 98ARG 101GLN 102LYS 105GLU 131LEU 135HIE 143ARG 175ARG	2ARG 17SER 23HIE 26ARG 38LYS 76ARG 81LYS 94PRO 95HIE 97THR 98ARG 101GLN 121ARG 124THR 129LYS 143ARG 145LYS 165THR 167ARG 181THR 182THR 215LYS 216GLU 218GLU 219LYS 220ASN 221LYS 222TYR 224TYR 233LYS 243LYS 246SER 254LYS 273THR 276GLN 283TYR 295SER 297LYS 300ASP 301TYR 303TYR 319ARG 320ASN 321THR 322PRO 323HIE 325LYS 326ARG	22GLN 26ARG 29GLN 58SER 61ASN 62TYR 65GLN 94PRO 95HIE 97THR 98ARG 101GLN 131LEU 132ASN 135HIE 167ARG 170CYS 171CYS 174GLN 203PRO 204PHE 206ASN 207TYR 210GLN 243LYS 244PHE 246SER 247ASN 250GLU 282SER 283TYR 285ASN 286TYR 289GLN 322PRO 323HIE 326ARG

^a PDB codes and chain identifier of the complex structure and the corresponding protein subunit used for binding sites prediction. Chain identifiers of receptor and ligand are separated by a colon.

^b Predicted binding residues of the protein subunit of the second column. The sequence number of residue and residue type are listed.

^c Native binding-site residues of the complex are mapped onto the protein subunit listed in the second column.