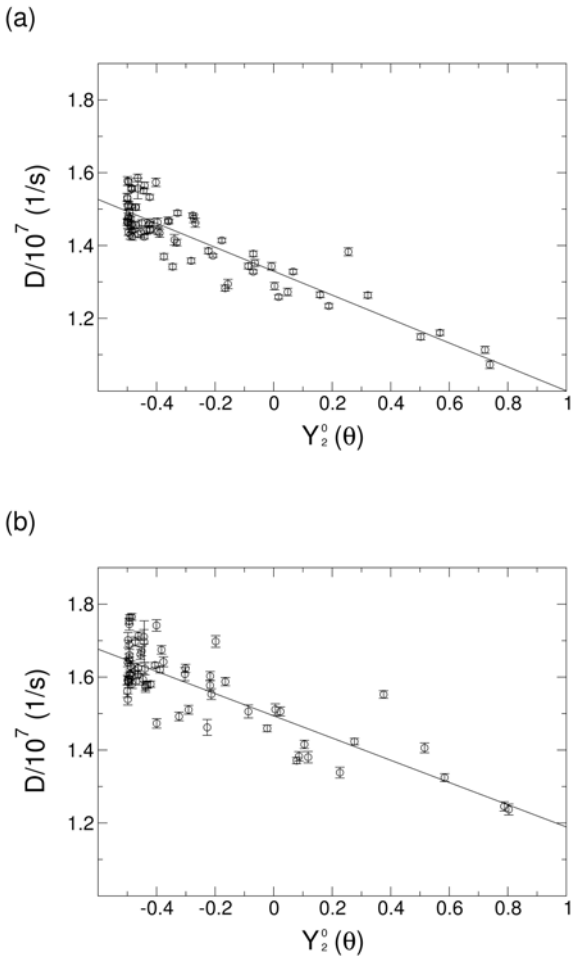
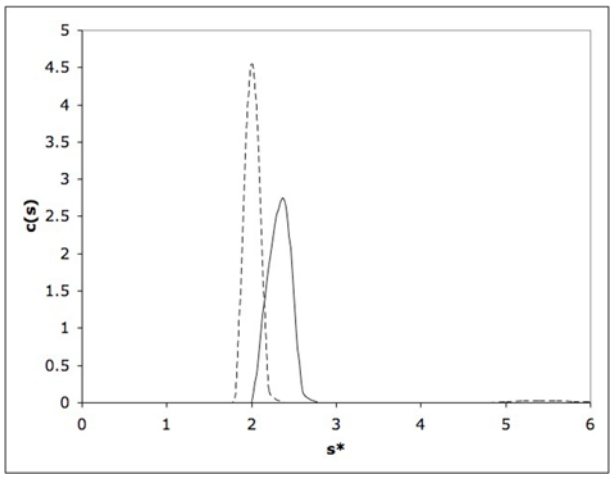


Supplementary Figure 1. The local diffusion constant D plotted as a function of the modified spherical harmonic function $Y_2^0(\theta) = (3\cos^2\theta - 1)/2$ for the Ca^{2+}-loaded state (a) and the apo state (b).



Supplementary Figure 2. Sedimentation coefficient distributions for the Ca^{2+}-bound and apo states (solid and dashed curves, respectively).

Supplementary Table 1

Residual dipolar couplings of Ca^{2+}-bound state of CBD1

Residue number	RDC_{exp}	RDC_{calc}	* = excluded from alignment tensor calculation
374	14.5300	12.2538	
376	12.3100	12.9651	
377	10.3800	8.6017	
378	15.1400	12.0369	
379	14.0100	14.3500	
381	14.2500	17.1610	
382	8.8400	2.5091	
383	7.7300	-1.0753	*
384	4.5000	9.3364	
385	-3.1600	-12.7485	*
387	12.6000	12.5166	
388	-6.8400	-12.2619	
389	20.8200	17.5183	
391	2.8700	1.9861	
392	8.5600	11.4870	
393	3.0700	3.7944	
394	6.1200	10.3184	
395	9.3600	9.6963	
396	17.0800	15.5061	
397	15.8500	16.5524	
399	9.4300	10.8409	
402	-1.9800	-4.1905	
403	5.5400	10.8448	
404	-7.7400	-10.1829	
405	6.1500	7.2970	
406	-2.8100	-8.5547	*
407	8.1200	7.4871	
408	6.7200	0.8896	*
409	12.2300	10.6986	
411	12.3200	10.8407	
412	15.6500	15.6950	
413	15.8400	14.8533	

414	2.0100	3.9757	
415	13.5500	12.8324	
416	-17.2500	-16.7920	
417	-19.0300	-17.5956	
418	1.0600	3.0736	
419	9.3700	12.6253	
420	-2.2200	-1.6789	
421	2.5200	-1.8993	
422	19.0900	17.6822	
423	17.3300	14.6332	
424	-3.2500	-5.2712	
425	11.8100	10.2714	
426	11.9300	9.4816	
427	11.5700	9.6603	
429	11.1700	11.4036	
430	-1.1500	-1.3851	
431	7.8400	13.7856	
432	-11.9800	-17.1148	
435	6.5800	5.5132	
437	9.6300	1.8224	*
438	10.0500	8.2749	
439	6.8800	5.5877	
440	6.0500	6.4996	
441	2.1400	3.1596	
442	9.7800	11.5967	
443	-0.2200	1.8344	
444	15.5800	15.4419	
445	11.6200	8.8501	
446	6.2200	4.5498	
447	12.0800	10.8214	
448	18.2100	17.1390	
449	-27.7400	-25.8975	
450	-23.9300	-20.5249	
451	17.4100	17.9195	
452	15.0200	17.8318	
453	3.3800	2.8566	
454	12.9700	12.6706	
455	12.3600	13.7958	
456	15.6100	16.2144	
457	16.8100	15.0909	
458	14.5100	12.1979	
459	9.6400	9.5928	
460	12.1700	10.1736	
462	12.7600	11.7565	

463	10.6500	9.7690	
464	1.3800	-0.4525	
465	9.4400	6.9469	
466	6.2000	13.2348	*
483	9.7500	5.2295	*
484	16.3400	15.2782	
486	1.8800	12.6271	*
487	5.3200	8.6159	
488	5.8300	4.5769	
491	-2.3200	11.2033	*
492	13.8900	11.4472	
493	13.6600	14.4600	
494	17.8900	15.8748	
496	15.9600	14.6205	
497	-0.2600	-2.4164	
498	8.5200	10.6147	
500	3.7700	5.3605	
501	0.2200	9.1342	*
502	2.9900	9.0488	*

Supplementary Table 2

Residual dipolar couplings of apo state of CBD1

Residue number	RDC_{exp}	RDC_{calc}	* = excluded from alignment tensor calculation
374	14.4200	10.8218	
376	19.8700	18.5840	
377	13.7900	11.9350	
378	13.0600	11.2819	
379	11.7600	8.3939	
380	15.0900	14.9404	
383	13.2500	3.7784	*
386	9.7700	2.5865	*
387	19.1900	18.2645	
388	-3.7300	-7.3918	
389	13.7000	14.4769	
391	-6.3900	-8.5701	
392	3.2200	6.8340	

393	1.4000	2.2135	
395	15.8100	15.8462	
397	19.0800	19.0204	
399	12.3700	11.6737	
402	3.4200	0.0281	
403	3.9600	10.6811	
405	4.5100	3.2596	
406	-3.1000	-11.8109	*
407	12.6800	10.8633	
408	12.0100	2.3581	*
412	9.8900	8.9276	
413	7.8300	7.4956	
414	3.3300	6.0192	
416	-11.7700	-12.3699	
417	-20.8900	-21.2509	
418	2.6400	4.0522	
419	14.0300	15.8259	
420	-0.7300	2.1518	
421	1.7500	-7.8711	*
422	18.1000	17.0725	
423	16.9600	15.9336	
424	1.3800	-0.3767	
425	16.9400	13.9744	
427	16.4400	14.6723	
429	16.8800	16.8033	
430	0.7500	-2.8022	
431	7.3900	16.8732	*
432	-18.0400	-20.5685	
437	11.2100	2.3720	*
438	15.7100	12.6143	
439	9.9200	9.6703	
441	-4.3800	-6.5959	
442	4.0400	2.6067	
443	-9.4500	-8.9018	
444	21.3600	19.1135	
445	18.5500	12.2134	*
446	8.7700	6.6960	
447	6.2000	11.8173	
449	-10.3500	-30.4495	*
450	-10.7700	-16.2959	
451	-13.2600	15.8645	*
452	-2.9500	14.6385	*
456	16.5100	18.3535	
457	15.6400	13.8859	

458	12.8900	11.3360	
459	14.8900	10.8519	*
460	12.3300	7.2442	
462	19.5600	17.3834	
463	16.1600	14.3674	
464	0.5600	-0.9967	
465	6.6400	5.3581	
466	0.5200	5.9554	
483	8.4700	8.2258	
484	12.0100	9.1817	
486	14.2000	7.8525	*
487	10.5400	13.5054	
488	8.4700	8.4463	
490	15.6800	16.9016	
492	11.4200	7.9277	
493	15.1800	13.2421	
494	16.4200	17.2107	
496	17.5000	19.2918	
497	3.9900	3.7752	
502	-0.5800	11.4015	*

Supplementary Table 3

^{15}N backbone relaxation of Ca^{2+}-bound CBD1

Residue number	T_1 (s)	T_2 (s)	NOE
373	1.2186±0.0099	0.0528±0.0005	0.8017±0.0194
374	1.2989±0.0123	0.0572±0.0006	0.8307±0.0221
376	1.2279±0.0103	0.0503±0.0005	0.8708±0.0186
377	1.1537±0.0098	0.0576±0.0006	0.8212±0.0190
378	1.1730±0.0056	0.0540±0.0002	0.8241±0.0110
379	1.2157±0.0111	0.0616±0.0005	0.8224±0.0162
381	1.2207±0.0077	0.0609±0.0004	0.8357±0.0150
382	1.3738±0.0079	0.0565±0.0003	0.7860±0.0136
383	1.2297±0.0059	0.0528±0.0003	0.8375±0.0116
384	1.4094±0.0101	0.0518±0.0004	0.8385±0.0162
385	1.3362±0.0105	0.0531±0.0005	0.8263±0.0165
387	1.1888±0.0066	0.0516±0.0003	0.8473±0.0119
388	1.3742±0.0100	0.0447±0.0004	0.8611±0.0151
389	1.3034±0.0054	0.0550±0.0002	0.8337±0.0098

391	1.4539±0.0089	0.0473±0.0003	0.8364±0.0152
392	1.3046±0.0090	0.0568±0.0004	0.8124±0.0162
393	1.4474±0.0096	0.0548±0.0004	0.8099±0.0151
394	1.2101±0.0100	0.0532±0.0004	0.8684±0.0174
395	1.2118±0.0098	0.0524±0.0004	0.8499±0.0182
396	1.2724±0.0097	0.0538±0.0004	0.8303±0.0178
397	1.1380±0.0079	0.0540±0.0004	0.8262±0.0167
399	1.1827±0.0207	0.0339±0.0006	0.8093±0.0291
402	1.2151±0.0146	0.0445±0.0006	0.8402±0.0231
403	1.1011±0.0121	0.0540±0.0007	0.7904±0.0241
404	1.5480±0.0122	0.0428±0.0004	0.7846±0.0177
405	1.3161±0.0097	0.0506±0.0004	0.8556±0.0167
406	1.4941±0.0121	0.0462±0.0004	0.8125±0.0193
407	1.2716±0.0091	0.0497±0.0004	0.8352±0.0182
408	1.2715±0.0095	0.0487±0.0004	0.8800±0.0189
409	1.2015±0.0078	0.0501±0.0004	0.8470±0.0146
411	1.1969±0.0092	0.0502±0.0004	0.8011±0.0160
412	1.2249±0.0069	0.0583±0.0004	0.8190±0.0126
413	1.3063±0.0096	0.0496±0.0004	0.8863±0.0158
414	1.4418±0.0133	0.0538±0.0005	0.8322±0.0174
415	1.2950±0.0121	0.0560±0.0006	0.8511±0.0189
416	1.4689±0.0114	0.0406±0.0004	0.8593±0.0155
417	1.8064±0.0209	0.0430±0.0006	0.8422±0.0212
418	1.3191±0.0129	0.0484±0.0005	0.8502±0.0181
419	1.3091±0.0106	0.0547±0.0005	0.8611±0.0172
420	1.3477±0.0089	0.0500±0.0003	0.7216±0.0128
421	1.3172±0.0132	0.0510±0.0006	0.8582±0.0196
422	1.1574±0.0056	0.0510±0.0003	0.8510±0.0109
423	1.1423±0.0084	0.0562±0.0004	0.8412±0.0159
424	1.4263±0.0112	0.0468±0.0004	0.8416±0.0171
425	1.2038±0.0093	0.0519±0.0004	0.8616±0.0174
426	1.2997±0.0068	0.0537±0.0003	0.8246±0.0133
427	1.2234±0.0060	0.0528±0.0002	0.8278±0.0124
429	1.2070±0.0083	0.0553±0.0004	0.8323±0.0155
430	1.5330±0.0092	0.0483±0.0004	0.8093±0.0166
431	1.2995±0.0101	0.0552±0.0004	0.8121±0.0163
432	1.7525±0.0178	0.0447±0.0006	0.8647±0.0240
435	1.3208±0.0087	0.0489±0.0004	0.8161±0.0142
437	1.2155±0.0077	0.0515±0.0004	0.8233±0.0135
438	1.2340±0.0065	0.0598±0.0004	0.8286±0.0142
439	1.3492±0.0066	0.0592±0.0003	0.8004±0.0120
440	1.2337±0.0070	0.0556±0.0004	0.8121±0.0142

441	1.4819±0.0079	0.0536±0.0003	0.8252±0.0141
442	1.3208±0.0075	0.0589±0.0004	0.8269±0.0137
443	1.4144±0.0128	0.0469±0.0005	0.8403±0.0194
444	1.2229±0.0087	0.0548±0.0004	0.8391±0.0158
445	1.2067±0.0127	0.0524±0.0005	0.8294±0.0186
446	1.2596±0.0092	0.0507±0.0004	0.8404±0.0157
447	1.4459±0.0067	0.0626±0.0003	0.7270±0.0101
448	1.2182±0.0148	0.0575±0.0007	0.8273±0.0194
449	1.7550±0.0114	0.0396±0.0004	0.8391±0.0149
450	1.5618±0.0200	0.0400±0.0005	0.8726±0.0208
451	1.1969±0.0136	0.0525±0.0006	0.8564±0.0218
452	1.2519±0.0072	0.0615±0.0003	0.7987±0.0129
453	1.3795±0.0067	0.0535±0.0003	0.7919±0.0107
454	1.2500±0.0109	0.0590±0.0006	0.7296±0.0150
455	1.3050±0.0128	0.0548±0.0005	0.8558±0.0183
456	1.1795±0.0075	0.0517±0.0003	0.8474±0.0140
457	1.2060±0.0105	0.0519±0.0005	0.8250±0.0166
458	1.2863±0.0076	0.0554±0.0003	0.8452±0.0139
459	1.2737±0.0107	0.0530±0.0006	0.8489±0.0193
460	1.2692±0.0134	0.0537±0.0006	0.7928±0.0214
462	1.1744±0.0108	0.0589±0.0006	0.8172±0.0183
463	1.1913±0.0057	0.0583±0.0003	0.8257±0.0141
464	1.4071±0.0184	0.0412±0.0006	0.8548±0.0318
465	1.3063±0.0111	0.0468±0.0005	0.7709±0.0254
466	1.1875±0.0099	0.0497±0.0005	0.7637±0.0215
469	0.8818±0.0046	0.1105±0.0006	0.4530±0.0097
470	0.9278±0.0064	0.1361±0.0010	0.3455±0.0109
472	0.8504±0.0035	0.1233±0.0005	0.4218±0.0080
473	0.8534±0.0039	0.1339±0.0007	0.3724±0.0089
475	0.8151±0.0025	0.1028±0.0003	0.4492±0.0076
476	0.8753±0.0030	0.1085±0.0004	0.4180±0.0080
477	0.9313±0.0056	0.0993±0.0006	0.4788±0.0123
480	1.0535±0.0093	0.0693±0.0006	0.6211±0.0172
483	1.0570±0.0144	0.0490±0.0008	0.7420±0.0319
484	1.1818±0.0077	0.0521±0.0004	0.7957±0.0202
486	1.2804±0.0130	0.0534±0.0007	0.8445±0.0255
487	1.2985±0.0159	0.0530±0.0008	0.8292±0.0270
488	1.6279±0.0199	0.0565±0.0007	0.7886±0.0222
490	1.1966±0.0288	0.0584±0.0014	0.8281±0.0312
492	1.2089±0.0092	0.0541±0.0004	0.8434±0.0162
493	1.3254±0.0095	0.0552±0.0004	0.8263±0.0160
494	1.1766±0.0087	0.0541±0.0004	0.8179±0.0151

496	1.2280±0.0104	0.0564±0.0005	0.8469±0.0166
497	1.3576±0.0125	0.0462±0.0005	0.8324±0.0175
498	1.2096±0.0145	0.0523±0.0007	0.8333±0.0210
500	1.4140±0.0104	0.0477±0.0004	0.8381±0.0152
501	0.9909±0.0049	0.0738±0.0003	0.6468±0.0093
502	0.9375±0.0102	0.1029±0.0011	0.5573±0.0149
503	0.9288±0.0089	0.1633±0.0017	0.3512±0.0118
504	0.8847±0.0016	0.1536±0.0003	0.4689±0.0037
505	0.7926±0.0020	0.1953±0.0006	0.2433±0.0045
506	0.8314±0.0041	0.2629±0.0018	0.0808±0.0070
507	0.8334±0.0024	0.2997±0.0014	0.0149±0.0047
508	0.8640±0.0016	0.3723±0.0014	-0.0920±0.0037

Supplementary Table 4

^{15}N backbone relaxation of apo state of CBD1

Residue number	T_1 (s)	T_2 (s)	NOE
374	1.2234±0.0138	0.0698±0.0009	0.8779±0.0359
376	1.1658±0.0122	0.0590±0.0007	0.8219±0.0281
377	1.0917±0.0111	0.0665±0.0008	0.7834±0.0287
378	1.1308±0.0069	0.0611±0.0004	0.8432±0.0200
379	1.1916±0.0156	0.0692±0.0010	0.8434±0.0307
380	1.1404±0.0068	0.0580±0.0004	0.8179±0.0194
383	1.1356±0.0098	0.0550±0.0007	0.8498±0.0305
384	1.2527±0.0119	0.0557±0.0006	0.7886±0.0307
385	1.2430±0.0093	0.0610±0.0005	0.7868±0.0246
387	1.0769±0.0085	0.0576±0.0006	0.8567±0.0252
388	1.1602±0.0127	0.0479±0.0007	0.8491±0.0306
389	1.2335±0.0070	0.0618±0.0004	0.8414±0.0193
391	1.3755±0.0108	0.0527±0.0005	0.8389±0.0267
392	1.2706±0.0115	0.0641±0.0007	0.7972±0.0286
393	1.3569±0.0114	0.0627±0.0006	0.8206±0.0260
394	1.1461±0.0120	0.0620±0.0007	0.8800±0.0317
395	1.1400±0.0116	0.0625±0.0007	0.8678±0.0302
396	1.2006±0.0121	0.0649±0.0007	0.8254±0.0288
397	1.0874±0.0093	0.0623±0.0006	0.8013±0.0245
399	1.1639±0.0245	0.0382±0.0009	0.8079±0.0425
400	1.1208±0.0109	0.0579±0.0007	0.7967±0.0288
403	1.0595±0.0145	0.0616±0.0010	0.7963±0.0356

404	1.4053±0.0124	0.0508±0.0005	0.7997±0.0251
405	1.2618±0.0118	0.0584±0.0006	0.7927±0.0259
406	1.3797±0.0143	0.0535±0.0006	0.9245±0.0326
407	1.2041±0.0096	0.0608±0.0006	0.8464±0.0270
408	1.1898±0.0105	0.0555±0.0005	0.8298±0.0260
409	1.1412±0.0096	0.0578±0.0006	0.8482±0.0245
411	1.1348±0.0100	0.0589±0.0006	0.8328±0.0258
412	1.1773±0.0094	0.0663±0.0006	0.8103±0.0229
413	1.2475±0.0107	0.0563±0.0006	0.8229±0.0249
414	1.3412±0.0155	0.0622±0.0008	0.8126±0.0322
415	1.2016±0.0123	0.0603±0.0007	0.7952±0.0265
416	1.2877±0.0136	0.0514±0.0007	0.8688±0.0322
417	1.6119±0.0210	0.0506±0.0009	0.8399±0.0379
418	1.2314±0.0173	0.0482±0.0008	0.8208±0.0358
419	1.1597±0.0125	0.0613±0.0008	0.8301±0.0321
420	1.3581±0.0109	0.0565±0.0006	0.7466±0.0239
421	1.2558±0.0121	0.0582±0.0007	0.8157±0.0278
422	1.1137±0.0078	0.0573±0.0005	0.8900±0.0249
423	1.1023±0.0094	0.0630±0.0006	0.8490±0.0262
424	1.2999±0.0144	0.0504±0.0007	0.8505±0.0341
425	1.1364±0.0115	0.0549±0.0007	0.7822±0.0299
426	1.2188±0.0080	0.0609±0.0005	0.8458±0.0217
427	1.1434±0.0067	0.0608±0.0004	0.8502±0.0186
429	1.1551±0.0104	0.0642±0.0006	0.8436±0.0266
430	1.3918±0.0099	0.0575±0.0005	0.8154±0.0233
431	1.2382±0.0120	0.0644±0.0007	0.8672±0.0282
432	1.5977±0.0184	0.0510±0.0007	0.8284±0.0317
437	1.1261±0.0084	0.0597±0.0005	0.8290±0.0203
438	1.1707±0.0088	0.0687±0.0006	0.8098±0.0239
439	1.2840±0.0076	0.0683±0.0004	0.7913±0.0184
441	1.3881±0.0098	0.0609±0.0005	0.7681±0.0238
442	1.2824±0.0109	0.0661±0.0006	0.8306±0.0276
443	1.3567±0.0160	0.0523±0.0008	0.8894±0.0354
444	1.1392±0.0122	0.0594±0.0007	0.8913±0.0352
445	1.1530±0.0146	0.0518±0.0007	0.8193±0.0385
446	1.1406±0.0120	0.0525±0.0006	0.7770±0.0320
447	1.1071±0.0063	0.0725±0.0005	0.5937±0.0169
448	1.0864±0.0050	0.0702±0.0004	0.6411±0.0149
449	1.1095±0.0047	0.0763±0.0004	0.5874±0.0156
450	1.0135±0.0066	0.0602±0.0004	0.7009±0.0228
451	1.1371±0.0111	0.0541±0.0006	0.6736±0.0320
452	1.0722±0.0052	0.0862±0.0005	0.4928±0.0175

456	1.1352±0.0104	0.0573±0.0007	0.8682±0.0303
457	1.1380±0.0133	0.0601±0.0008	0.8887±0.0340
458	1.2274±0.0098	0.0637±0.0006	0.8116±0.0220
459	1.2158±0.0127	0.0596±0.0007	0.8185±0.0284
460	1.2340±0.0140	0.0627±0.0008	0.8518±0.0335
462	1.0981±0.0121	0.0669±0.0008	0.7958±0.0259
463	1.1196±0.0060	0.0681±0.0004	0.8384±0.0199
464	1.3184±0.0153	0.0486±0.0007	0.8050±0.0372
465	1.2520±0.0122	0.0541±0.0007	0.7971±0.0364
466	1.1489±0.0108	0.0561±0.0007	0.8144±0.0320
469	0.8490±0.0062	0.1285±0.0010	0.4030±0.0154
470	0.9143±0.0086	0.1570±0.0020	0.2950±0.0178
473	0.8379±0.0051	0.1502±0.0011	0.3614±0.0134
475	0.7912±0.0033	0.1215±0.0005	0.4174±0.0115
476	0.8567±0.0042	0.1252±0.0007	0.3718±0.0126
477	0.9231±0.0095	0.1177±0.0013	0.4670±0.0225
480	0.9915±0.0085	0.0818±0.0007	0.6130±0.0221
483	1.0157±0.0134	0.0536±0.0009	0.7423±0.0428
484	1.1365±0.0085	0.0600±0.0006	0.8355±0.0288
486	1.2098±0.0121	0.0620±0.0007	0.7956±0.0327
487	1.2197±0.0143	0.0629±0.0009	0.8574±0.0351
488	1.5333±0.0277	0.0671±0.0013	0.7901±0.0367
490	1.1862±0.0493	0.0685±0.0032	0.8027±0.0563
492	1.1623±0.0120	0.0614±0.0007	0.8353±0.0307
493	1.2702±0.0116	0.0636±0.0007	0.8467±0.0288
494	1.1435±0.0119	0.0631±0.0007	0.8268±0.0315
495	1.2241±0.0123	0.0608±0.0007	0.8796±0.0335
496	1.1606±0.0145	0.0566±0.0008	0.9142±0.0426
497	1.2174±0.0153	0.0565±0.0009	0.7828±0.0392
502	0.8446±0.0056	0.1233±0.0008	0.4996±0.0142
503	0.8467±0.0080	0.1622±0.0021	0.4312±0.0203
504	0.7636±0.0027	0.1775±0.0008	0.3406±0.0099
505	0.7883±0.0035	0.1772±0.0010	0.2347±0.0109
506	0.8227±0.0058	0.2681±0.0034	0.1202±0.0148
507	0.8463±0.0037	0.3215±0.0023	-0.0549±0.0089
508	0.8865±0.0027	0.4169±0.0025	-0.1680±0.0063

Supplementary Table 5

S^2 model-free order parameters of Ca^{2+}-bound state of CBD1

Residue number	S^2	τ_{int} (ps)	R_{ex} (1/s) †	Exclusion criteria*
373	0.917±0.007	24.028±8.060		
374	0.860±0.007	8.128±4.460		
376	0.942±0.006	0.000±7.021		
377	0.899±0.006	17.197±6.247		
378	0.927±0.003	19.246±5.054		
379	0.847±0.005	10.373±3.170		
381	0.853±0.004	7.704±3.083		
382	0.839±0.004	14.550±2.440		
383	0.940±0.004	14.603±5.900		1
384	0.865±0.005	3.221±3.007		
385	0.898±0.006	11.239±4.869		1, 2
387	0.945±0.004	8.328±6.234		
388	0.955±0.006	6.902±7.124		
389	0.852±0.004	6.168±1.985	0.858±0.112	2
391	0.898±0.004	5.516±3.892		
392	0.857±0.005	10.825±3.412		
393	0.830±0.004	8.081±2.476		
394	0.924±0.005	0.000±4.078		
395	0.931±0.006	6.604±6.632		
396	0.894±0.005	9.138±4.655		
397	0.940±0.005	23.929±9.725		
399	0.932±0.018	26.976±18.300	10.546±0.670	2, 3
402	0.973±0.006	1390.607±1166.636		3
403	0.950±0.008	59.249±30.291		3
404	0.915±0.006	24.773±5.400		
405	0.916±0.005	3.579±4.392		
406	0.908±0.006	15.472±5.462		1
407	0.935±0.006	12.721±7.899		
408	0.966±0.005	0.000±8.980		1
409	0.953±0.005	7.587±8.074		
411	0.948±0.006	38.942±11.870		
412	0.872±0.004	12.516±3.036		
413	0.920±0.005	0.000±3.406		
414	0.846±0.006	5.583±3.108		
415	0.872±0.006	3.185±3.551		
416	0.974±0.007	9.684±12.845		
417	0.854±0.007	3.213±2.749		
418	0.935±0.007	6.514±6.375		
419	0.879±0.005	0.148±2.641		
420	0.896±0.004	42.410±3.782		

421	0.902±0.007	6.300±4.816		
422	0.964±0.003	10.858±9.129		3
423	0.919±0.005	13.160±5.979		
424	0.917±0.005	7.297±5.210		
425	0.938±0.005	0.000±5.289		
426	0.884±0.004	9.175±3.812		
427	0.920±0.003	14.151±5.134		
429	0.904±0.005	11.431±5.059		
430	0.865±0.005	10.019±3.147		
431	0.871±0.005	11.860±3.667		
432	0.852±0.007	0.557±2.117		
435	0.925±0.005	19.106±6.050		
437	0.956±0.005	31.491±10.898		1
438	0.857±0.004	9.282±2.874		
439	0.826±0.003	11.093±2.015		
440	0.891±0.004	16.581±4.165		
441	0.836±0.003	6.040±2.366		
442	0.839±0.004	7.838±2.471		
443	0.917±0.007	6.436±5.518		
444	0.903±0.005	8.196±4.586		
445	0.933±0.007	18.545±8.307		
446	0.930±0.006	9.421±6.188		
447	0.765±0.003	16.273±1.210		
448	0.881±0.008	10.782±5.027		
449	0.905±0.006	7.232±3.172		2
450	0.955±0.011	0.000±6.840		2
451	0.935±0.008	2.752±6.818		
452	0.836±0.003	13.346±2.456		
453	0.861±0.003	14.944±2.245		
454	0.848±0.006	28.792±3.255		
455	0.878±0.006	1.229±2.932		
456	0.948±0.005	9.726±7.391		
457	0.933±0.006	18.276±8.093		
458	0.877±0.004	3.915±2.924		
459	0.904±0.006	3.949±4.635		
460	0.891±0.007	20.078±6.044		
462	0.881±0.006	14.930±4.749		
463	0.882±0.003	12.327±3.768		
464	0.911±0.012	3.052±6.253	3.472±0.472	2
465	0.907±0.009	31.606±7.967	1.675±0.301	2
466	0.969±0.007	272.966±90.771		1, 3
469	0.729±0.003	76.603±2.153		4

470	0.631±0.003	65.540±1.802	2, 4
472	0.701±0.002	77.234±1.723	2, 4
473	0.666±0.002	76.592±1.853	4
475	0.783±0.002	119.862±3.260	2, 3, 4
476	0.734±0.002	88.204±1.896	2, 4
477	0.751±0.004	73.521±2.990	4
480	0.862±0.006	74.233±6.257	4
483	0.873±0.020	1138.501±190.402	1, 2, 3
484	0.939±0.005	39.750±11.149	
486	0.917±0.008	7.420±7.446	1
487	0.894±0.009	9.238±7.080	
488	0.769±0.007	7.524±2.467	
490	0.880±0.015	11.402±7.876	
492	0.916±0.006	8.119±5.108	2
493	0.863±0.005	7.310±3.472	
494	0.924±0.005	21.559±7.000	
496	0.889±0.006	5.449±4.439	
497	0.942±0.006	14.605±8.599	
498	0.928±0.009	12.747±9.274	
500	0.900±0.005	3.882±3.974	
501	0.865±0.003	71.456±3.489	1, 2
502	0.745±0.005	54.064±3.295	1, 2
503	0.578±0.004	55.042±1.814	2, 4
504	0.623±0.001	48.871±0.484	2, 4
505	0.563±0.001	79.845±0.801	2, 4
506	0.462±0.002	77.478±1.044	2, 4
507	0.428±0.008	79.067±4.881	2, 4
508	0.373±0.001	77.748±0.410	2, 4

† Only non-zero values are listed.

* Criteria used to exclude residues from the characterization of the rotational diffusion tensor. 1) RDC not consistent with the Ca^{2+}-bound crystal structure. 2) Signs of conformational exchange. 3) High τ_{int} value in the original fit that includes a site-specific overall correlation time. 4) Not represented in the Ca^{2+}-bound crystal structure (see Materials and Methods).

Supplementary Table 6

S^2 model-free order parameters of apo state of CBD1

Residue number	S^2	τ_{int} (ps)	R_{ex} (1/s)†	Exclusion criteria*
374	0.806±0.007	0.000±3.088		
376	0.897±0.008	12.334±8.288		
377	0.864±0.008	22.705±7.038		
378	0.899±0.005	6.937±6.270		
379	0.820±0.009	4.779±4.823		
380	0.916±0.005	17.553±7.659		
383	0.961±0.008	12.490±22.746		1
384	0.883±0.008	18.407±8.527		
385	0.840±0.005	16.853±4.247		
387	0.950±0.006	4.031±11.129		
388	0.987±0.003	1248.741±473.763		3
389	0.856±0.004	3.926±3.815		
391	0.878±0.006	3.394±5.004		
392	0.823±0.007	11.302±5.078		
393	0.809±0.006	5.738±3.746		
394	0.889±0.007	0.000±6.055		
395	0.888±0.007	0.000±4.589		
396	0.845±0.007	8.534±5.608		
397	0.901±0.006	24.152±8.751		
399	0.871±0.021	14.693±9.569	10.193±0.746	2, 3
400	0.921±0.008	29.534±13.143		
403	0.917±0.011	32.083±16.029		
404	0.887±0.007	16.647±6.121		
405	0.869±0.007	17.569±6.279		
406	0.885±0.007	0.000±4.384		1
407	0.876±0.006	5.336±5.573		
408	0.932±0.007	17.060±12.183		1
409	0.920±0.006	4.180±7.286		
411	0.912±0.007	11.020±8.806		
412	0.841±0.006	12.081±4.369		
413	0.887±0.006	9.027±7.031		
414	0.819±0.008	8.597±5.078		
415	0.873±0.008	17.184±6.857		
416	0.924±0.008	2.227±7.690		
417	0.836±0.010	3.616±4.464		
418	0.913±0.015	16.155±11.864	2.497±0.417	2

419	0.886±0.008	9.950±7.824		
420	0.846±0.006	22.706±4.215		
421	0.884±0.008	13.345±7.452		1
422	0.937±0.006	0.000±7.476		
423	0.895±0.007	6.552±6.512		
424	0.927±0.009	2.144±8.997		
425	0.934±0.008	41.694±16.793		
426	0.868±0.005	3.108±3.711		
427	0.898±0.004	4.722±5.199		
429	0.867±0.007	5.801±5.746		
430	0.838±0.006	8.767±4.249		
431	0.853±0.007	0.000±3.371		1
432	0.835±0.008	5.467±4.035		
437	0.924±0.006	16.123±8.558		1
438	0.826±0.005	11.353±4.451		
439	0.794±0.004	10.991±2.769		
441	0.808±0.005	14.287±3.519		
442	0.812±0.005	5.878±4.134		
443	0.891±0.010	0.000±5.596		
444	0.911±0.008	0.000±8.120		
445	0.978±0.010	81.614±114.208		1
446	0.955±0.010	68.005±38.993		3
447	0.799±0.004	48.588±3.057		
448	0.826±0.003	47.352±3.316		
449	0.797±0.003	51.828±3.060		1
450	0.797±0.006	1048.263±66.216		3
451	0.923±0.018	444.444±109.028		1, 3
452	0.752±0.003	60.112±2.750		1
456	0.927±0.008	0.000±8.967		
457	0.906±0.009	0.000±6.907		
458	0.841±0.006	10.078±4.404		
459	0.889±0.008	13.454±7.785		1
460	0.851±0.008	1.634±5.228		
462	0.861±0.008	18.813±6.209		
463	0.849±0.004	7.628±3.921		
464	0.931±0.010	23.223±15.068		
465	0.879±0.011	17.766±8.705	1.117±0.333	2
466	0.931±0.008	24.445±15.758		
469	0.685±0.004	76.462±3.495		4
470	0.587±0.005	65.167±2.458		2, 4
473	0.635±0.003	71.823±2.385		4
475	0.730±0.003	99.203±3.154		4

476	0.686±0.003	83.006±2.707		4
477	0.693±0.006	59.771±3.873		4
480	0.818±0.006	59.467±5.878		4
483	0.928±0.016	664.624±246.570	0.831±0.426	2, 3
484	0.905±0.006	11.204±9.042		
486	0.871±0.007	17.595±7.519		1
487	0.856±0.009	1.643±4.963		
488	0.731±0.010	6.649±3.738		
490	0.822±0.028	12.112±10.076		
492	0.884±0.008	7.934±7.211		
493	0.831±0.006	2.002±3.561		
494	0.877±0.008	10.704±7.956		
495	0.872±0.007	0.000±4.606		
496	0.921±0.009	0.000±12.846		
497	0.899±0.010	26.679±11.183		
502	0.713±0.004	64.330±2.911		1
503	0.617±0.005	55.752±2.909		2, 4
504	0.612±0.002	77.995±1.771		4
505	0.590±0.003	89.396±1.963		4
506	0.465±0.004	73.725±1.866		2, 4
507	0.405±0.003	81.657±1.396		2, 4
508	0.344±0.001	78.274±0.705		2, 4

† Only non-zero values are listed.

* Criteria used to exclude residues from the characterization of the rotational diffusion tensor. 1) RDC not consistent with the Ca^{2+}-bound crystal structure. 2) Signs of conformational exchange. 3) High τ_{int} value in the original fit that includes a site-specific overall correlation time. 4) Not represented in the Ca^{2+}-bound crystal structure (see Materials and Methods).