

Supporting Information for “Characterization of protein-protein interfaces in large complexes by solid state NMR solvent paramagnetic relaxation enhancements”

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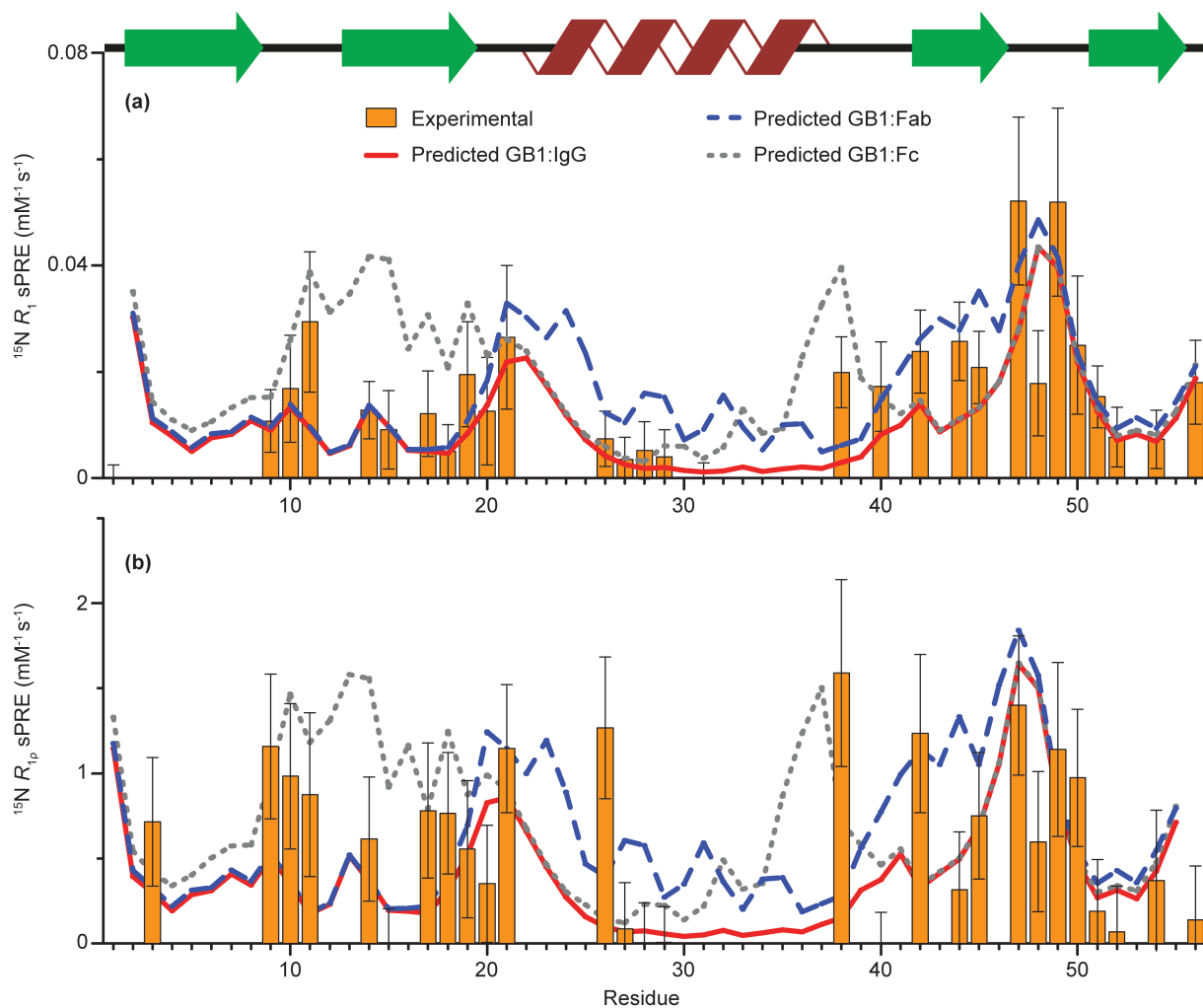
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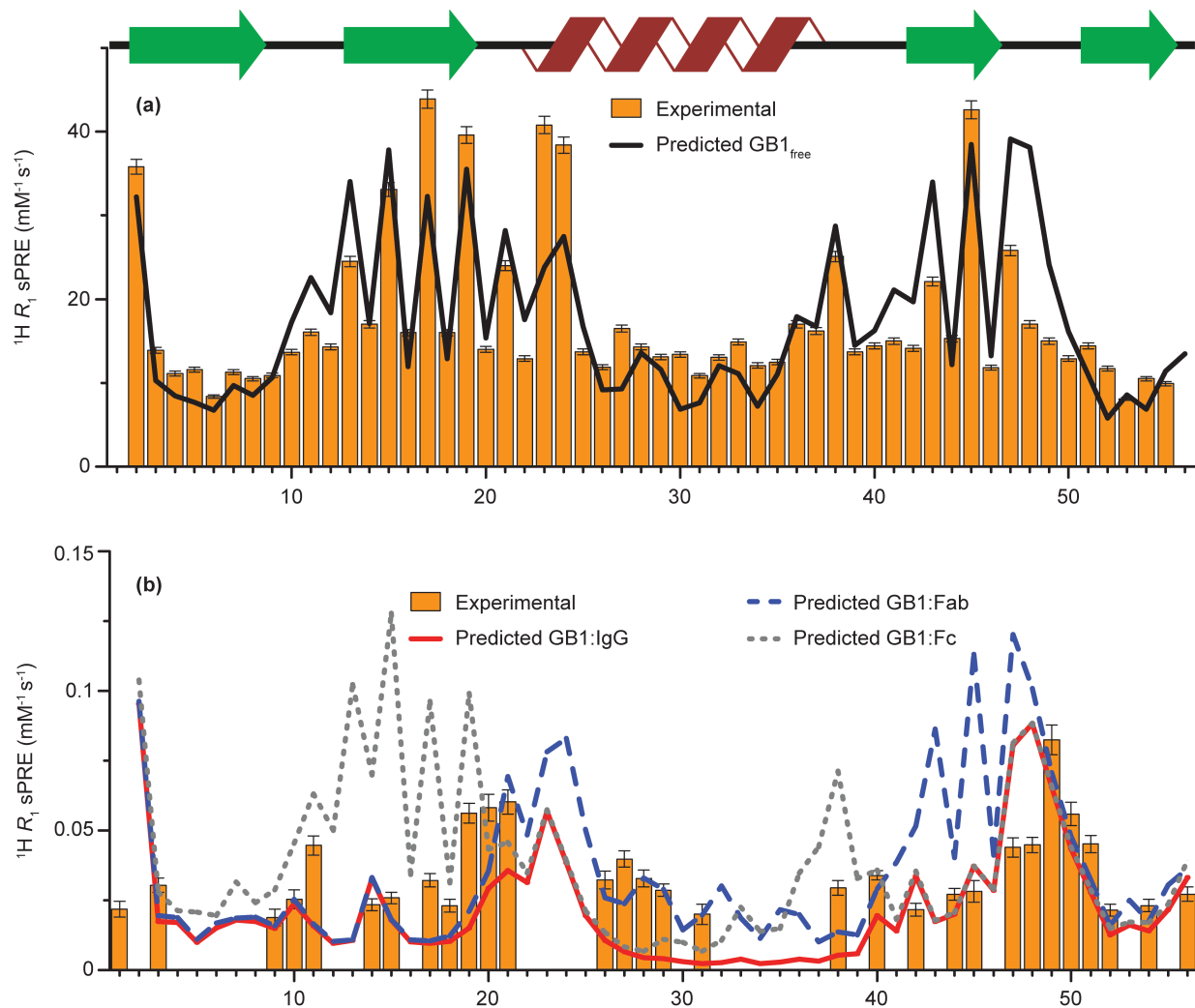
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Direct comparisons between experimental and predicted sPREs of GB1_{IgG} are presented in SI figure 1 for ¹⁵N data, SI figure 2 for ¹H data including a comparison of predicted ¹H sPREs for GB1_{free} with published experimental sPRE data¹.

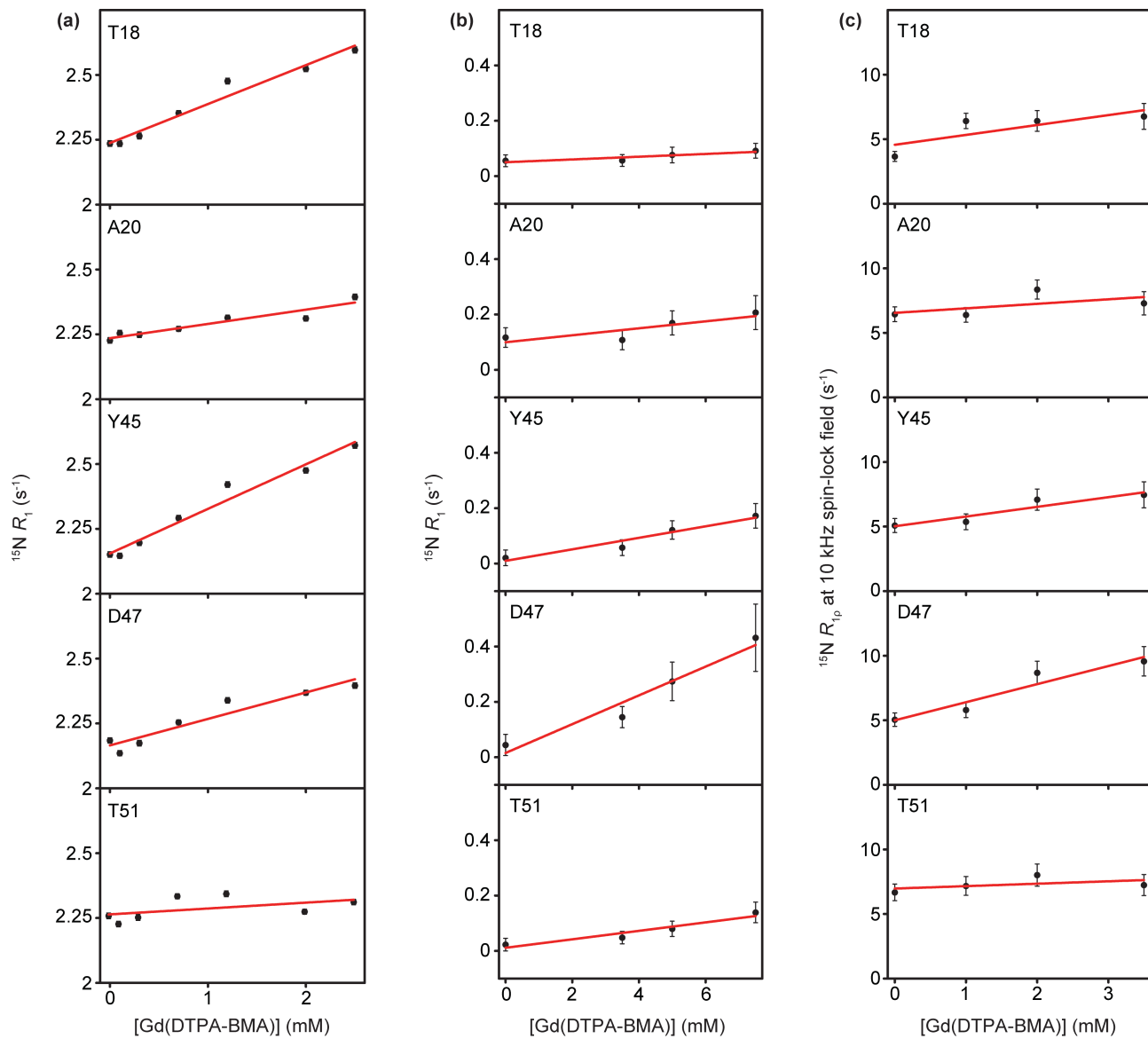
Examples of linear fits used to calculate sPREs from relaxation rates measured at different concentrations of Gd(DTPA-BMA) in GB1_{IgG} samples are compared to linear fits obtained for GB1_{free} in SI figure 3. The model of GB1 in complex with full length IgG that was used for the calculation of theoretical sPREs is presented in SI figure 4. C α secondary chemical shifts for GB1_{free} and GB1_{IgG}, based on data from ref² are shown in SI figure 5. All data used in SI figures 1-3 are detailed in SI tables 1-9. SI tables 10 and 11 contain relaxation delays and spin-lock lengths used for all relaxation measurements. SI table 12 contains results from a χ^2 -based best fitting comparison between experimental and predicted Δ sPRE data sets.



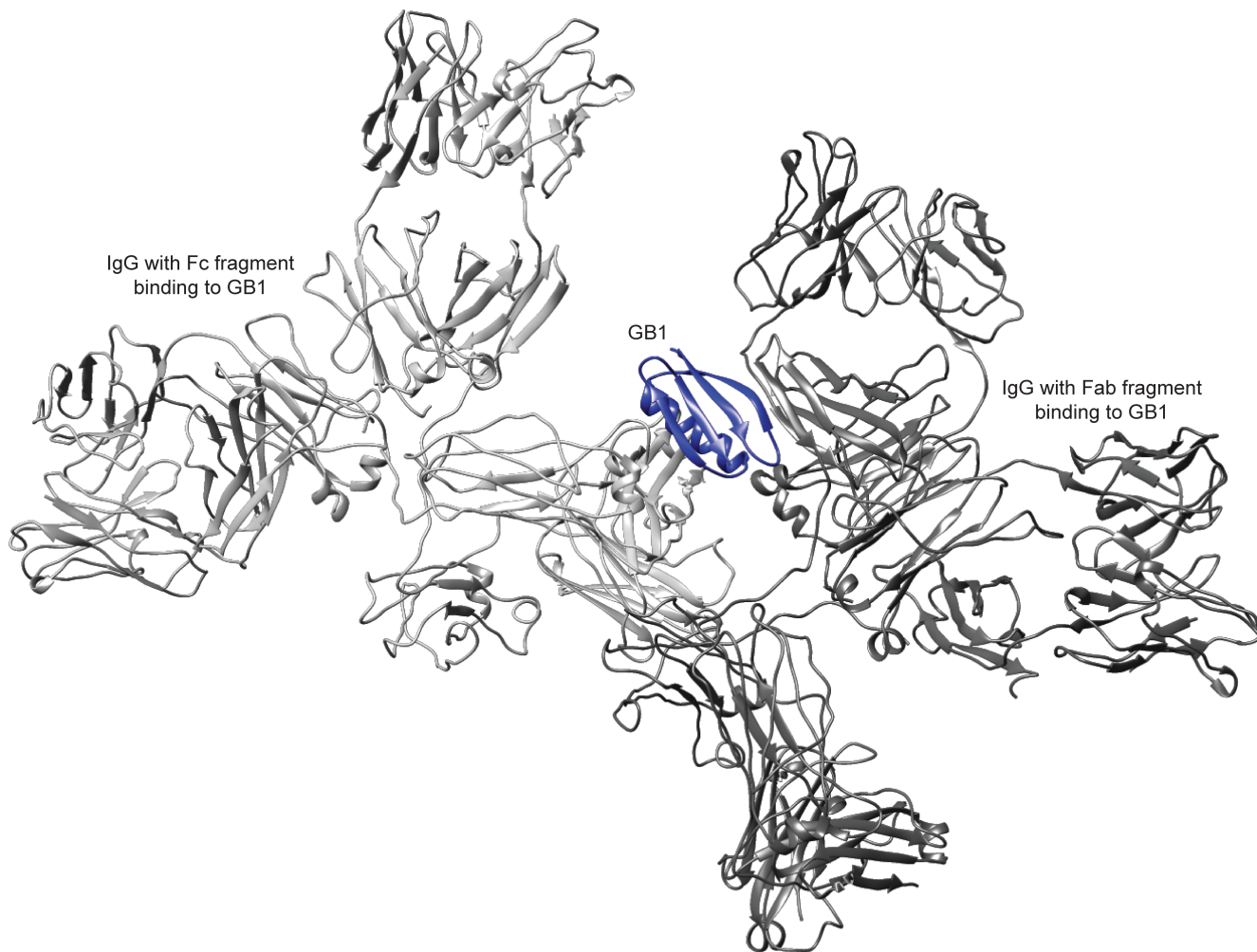
SI figure 1. Comparison between experimental and predicted ^{15}N sPREs for GB1 in complex with IgG. For visualization purposes the predicted sPREs were scaled so that the average values are the same in the data sets that are compared. (a) GB1_{IgG} based on $^{15}\text{N } R_1$, (b) GB1_{IgG} based on $^{15}\text{N } R_{1p}$. The lines represent predicted sPREs; red line for GB1 in complex with both fragments of IgG, dashed blue line for GB1 in complex with the Fab fragment of IgG and dotted grey line for GB1 in complex with the Fc fragment of IgG.



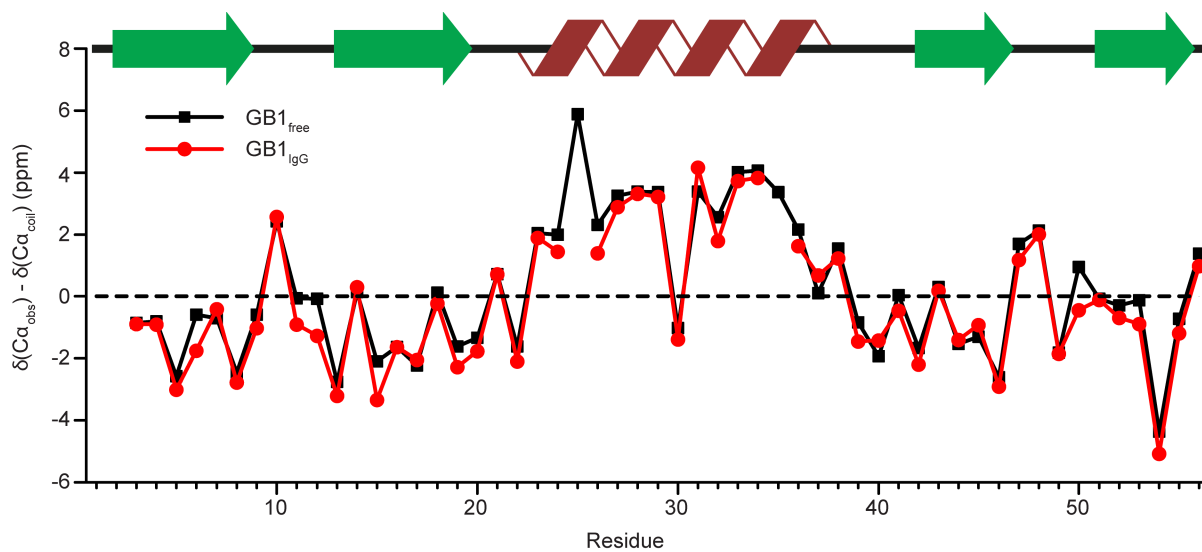
SI figure 2. Comparison between experimental and predicted ^1H sPREs for GB1 free in solution (a) (experimental data from ref¹) and GB1 in complex with IgG (b). For visualization purposes the predicted sPREs were scaled so that the average values are the same in the data sets that are compared. The lines represent predicted sPREs; black line for GB1 free in solution, red line for GB1 in complex with both fragments of IgG, dashed blue line for GB1 in complex with the Fab fragment of IgG and dotted grey line for GB1 in complex with the Fc fragment of IgG.



SI figure 3. Examples of linear fits used to extract ^{15}N sPREs for (a) GB1_{free}, (b) GB1_{IgG} based on R_1 and (c) GB1_{IgG} based on R_{1p} .



SI figure 4. Model of GB1 in complex with IgG used for calculations of theoretical sPREs. The model is based on crystal structures, solution NMR and solid state NMR: Crystal structures of the Fab fragment of IgG in complex with GB3³ and the Fc fragment of IgG in complex with GB2⁴; Solution NMR of GB2 in complex the Fab fragment⁵, GB2 in complex with the Fc fragment⁶ and GB1 in complex with the Fc fragment⁷; and solid state NMR of GB1 in complex with full length IgG².



SI figure 5. C^α secondary chemical shifts for GB1 free in solution (black squares) and GB1 in complex with IgG (red circles), based on published data².

SI table 1. ^{15}N R_1 rates (s^{-1}) for GB1_{free} with varying concentration of $\text{Gd}(\text{DTPA-BMA})$

Residue	0 mM		0.1 mM		0.3 mM		0.7 mM	
	R_1	Error	R_1	Error	R_1	Error	R_1	Error
2	2.2326	0.0109	2.2001	0.0110	2.2237	0.0113	2.3445	0.0104
3	2.2463	0.0111	2.2032	0.0110	2.2397	0.0111	2.3218	0.0103
4	2.2599	0.0115	2.3086	0.0117	2.3171	0.0119	2.3321	0.0103
5	2.3500	0.0118	2.3674	0.0124	2.3522	0.0121	2.3909	0.0103
6	2.2624	0.0110	2.2501	0.0116	2.2608	0.0116	2.3240	0.0099
7	2.2469	0.0111	2.2131	0.0112	2.2011	0.0110	2.2641	0.0098
8	2.1480	0.0108	2.1297	0.0110	2.1450	0.0108	2.1735	0.0095
9	2.2315	0.0111	2.2020	0.0109	2.2193	0.0111	2.2531	0.0097
10	2.1400	0.0106	2.1291	0.0107	2.1306	0.0110	2.1557	0.0091
11	2.0404	0.0096	2.0031	0.0101	2.0173	0.0102	2.0595	0.0088
12	1.8230	0.0087	1.8143	0.0089	1.8224	0.0090	1.9066	0.0083
13	2.0546	0.0103	2.0336	0.0101	2.0411	0.0103	2.1427	0.0093
14	2.0068	0.0098	2.0026	0.0099	2.0255	0.0099	2.0932	0.0090
15	2.0886	0.0103	2.0634	0.0104	2.1244	0.0107	2.1948	0.0096
16	2.2233	0.0111	2.2152	0.0113	2.2348	0.0113	2.2870	0.0101
17	2.1667	0.0104	2.1296	0.0103	2.1982	0.0109	2.3272	0.0100
18	2.2355	0.0112	2.2350	0.0112	2.2646	0.0113	2.3528	0.0101
19	2.0743	0.0101	2.0720	0.0102	2.1024	0.0107	2.1472	0.0088
20	2.2268	0.0109	2.2541	0.0114	2.2486	0.0113	2.2709	0.0099
21	2.2359	0.0112	2.2269	0.0112	2.2485	0.0115	2.3144	0.0100
23	2.2456	0.0112	2.2371	0.0113	2.2659	0.0113	2.3357	0.0103
24	2.1352	0.0105	2.1307	0.0108	2.1566	0.0108	2.2235	0.0096
25	2.2187	0.0107	2.1634	0.0105	2.1800	0.0109	2.2584	0.0098
26	2.3589	0.0117	2.3282	0.0117	2.3465	0.0122	2.4935	0.0107
27	2.2470	0.0110	2.2287	0.0111	2.2247	0.0112	2.2986	0.0101
28	2.2584	0.0112	2.2122	0.0111	2.2250	0.0113	2.3432	0.0101
29	2.2448	0.0112	2.2419	0.0116	2.2698	0.0112	2.3653	0.0102
30	2.2877	0.0114	2.2647	0.0116	2.2797	0.0116	2.3507	0.0103
31	2.2924	0.0114	2.3002	0.0117	2.2807	0.0115	2.3041	0.0098
32	2.2207	0.0112	2.2073	0.0114	2.2151	0.0116	2.2687	0.0098
33	2.2454	0.0114	2.2710	0.0115	2.2798	0.0115	2.2853	0.0099
34	2.3471	0.0118	2.3515	0.0117	2.3744	0.0126	2.4396	0.0104
35	2.1855	0.0111	2.1431	0.0105	2.1576	0.0109	2.2884	0.0100
36	2.2268	0.0116	2.2242	0.0113	2.2342	0.0116	2.2964	0.0102
39	2.1725	0.0109	2.1820	0.0114	2.1982	0.0110	2.2718	0.0096
40	1.9386	0.0097	1.9496	0.0099	1.9333	0.0098	1.9150	0.0084
42	2.1449	0.0106	2.1689	0.0112	2.1897	0.0110	2.2368	0.0098
43	2.1709	0.0109	2.1990	0.0113	2.2064	0.0108	2.2368	0.0098
44	2.2814	0.0110	2.2893	0.0117	2.3434	0.0120	2.4124	0.0105
45	2.1529	0.0108	2.1477	0.0103	2.1984	0.0109	2.2936	0.0101
46	2.2105	0.0107	2.2404	0.0113	2.2648	0.0110	2.2829	0.0096
47	2.1837	0.0105	2.1346	0.0102	2.1733	0.0109	2.2536	0.0097

48	2.0891	0.0103	2.0544	0.0104	2.0930	0.0105	2.1823	0.0095
49	2.1031	0.0101	2.0504	0.0099	2.0625	0.0103	2.1770	0.0095
50	2.3415	0.0115	2.2964	0.0113	2.3074	0.0119	2.3909	0.0105
51	2.2567	0.0109	2.2252	0.0108	2.2506	0.0113	2.3320	0.0100
52	2.2550	0.0110	2.2045	0.0110	2.2195	0.0110	2.2853	0.0103
53	2.2307	0.0106	2.1749	0.0105	2.1867	0.0106	2.2419	0.0097
54	2.4056	0.0122	2.3584	0.0117	2.3854	0.0120	2.4970	0.0111
55	2.2265	0.0108	2.2040	0.0112	2.2162	0.0112	2.2248	0.0095
56	2.2278	0.0112	2.2380	0.0112	2.2400	0.0113	2.2976	0.0098

SI table 2. ^{15}N R_1 rates (s^{-1}) for GB1_{free} with varying concentration of $\text{Gd}(\text{DTPA-BMA})$

Residue	1.2 mM		2 mM		2.5 mM	
	R_1	Error	R_1	Error	R_1	Error
2	2.3745	0.0110	2.3765	0.0102	2.4624	0.0114
3	2.3449	0.0110	2.2817	0.0097	2.2944	0.0102
4	2.3566	0.0109	2.3138	0.0098	2.3593	0.0104
5	2.4162	0.0112	2.3725	0.0099	2.3969	0.0114
6	2.3466	0.0104	2.2964	0.0099	2.3474	0.0106
7	2.3069	0.0107	2.2922	0.0100	2.3115	0.0104
8	2.1914	0.0101	2.1964	0.0095	2.1935	0.0099
9	2.2947	0.0104	2.2868	0.0099	2.2989	0.0106
10	2.2125	0.0101	2.2257	0.0096	2.2647	0.0101
11	2.1274	0.0095	2.1581	0.0093	2.2132	0.0099
12	1.9534	0.0087	1.9788	0.0085	1.9910	0.0092
13	2.2675	0.0105	2.3586	0.0100	2.3710	0.0106
14	2.1876	0.0099	2.2328	0.0097	2.3300	0.0104
15	2.3092	0.0105	2.4385	0.0104	2.4739	0.0111
16	2.4347	0.0111	2.5293	0.0109	2.5890	0.0118
17	2.4779	0.0117	2.5131	0.0106	2.5884	0.0117
18	2.4764	0.0113	2.5235	0.0109	2.5959	0.0117
19	2.2528	0.0100	2.2856	0.0100	2.3276	0.0107
20	2.3137	0.0103	2.3113	0.0101	2.3941	0.0110
21	2.3260	0.0106	2.3189	0.0097	2.3325	0.0107
23	2.4389	0.0112	2.3803	0.0104	2.4513	0.0109
24	2.2774	0.0104	2.2337	0.0095	2.2892	0.0102
25	2.2907	0.0105	2.2897	0.0101	2.3690	0.0106
26	2.4992	0.0112	2.3722	0.0105	2.3540	0.0108
27	2.3379	0.0104	2.3243	0.0101	2.3736	0.0107
28	2.3463	0.0108	2.2651	0.0095	2.2421	0.0097
29	2.3480	0.0108	2.3023	0.0099	2.3096	0.0105
30	2.3671	0.0110	2.3621	0.0097	2.4090	0.0109
31	2.3353	0.0108	2.3103	0.0101	2.3137	0.0105
32	2.3000	0.0104	2.2500	0.0096	2.2757	0.0103
33	2.3335	0.0110	2.3394	0.0099	2.3386	0.0105
34	2.4259	0.0112	2.3442	0.0101	2.4010	0.0110

35	2.3018	0.0108	2.2492	0.0097	2.2746	0.0104
36	2.3313	0.0108	2.2946	0.0096	2.3394	0.0107
39	2.2842	0.0106	2.2449	0.0096	2.2691	0.0101
40	1.9780	0.0089	2.0013	0.0087	2.0483	0.0095
42	2.2913	0.0103	2.3274	0.0102	2.3359	0.0105
43	2.3219	0.0105	2.3774	0.0101	2.4369	0.0107
44	2.4561	0.0111	2.4673	0.0110	2.5077	0.0112
45	2.4224	0.0111	2.4768	0.0105	2.5738	0.0113
46	2.3895	0.0110	2.4126	0.0102	2.4464	0.0110
47	2.3385	0.0107	2.3676	0.0100	2.3951	0.0107
48	2.2256	0.0099	2.2382	0.0094	2.3414	0.0107
49	2.2145	0.0100	2.2701	0.0096	2.2642	0.0100
50	2.4307	0.0111	2.4533	0.0105	2.4683	0.0112
51	2.3415	0.0110	2.2728	0.0097	2.3099	0.0104
52	2.3211	0.0105	2.3414	0.0099	2.3961	0.0107
53	2.2821	0.0104	2.2498	0.0099	2.2661	0.0102
54	2.4939	0.0115	2.4206	0.0104	2.4426	0.0112
55	2.3001	0.0103	2.3009	0.0098	2.3139	0.0105
56	2.3409	0.0107	2.3299	0.0100	2.3663	0.0106

SI table 3. ^{15}N R_1 rates (s^{-1}) for GB1_{cryst} with 0 and 2 mM Gd(DTPA-BMA)

Residue	0 mM		2 mM	
	R_1	Error	R_1	Error
2	0.0616	0.0060	0.0783	0.0080
3	0.0343	0.0041	0.0474	0.0065
6	0.0157	0.0025	0.0392	0.0056
8	0.0343	0.0043	0.0461	0.0065
9	0.0466	0.0052	0.0594	0.0070
10	0.0814	0.0090	0.0954	0.0098
11	0.0993	0.0104	0.1605	0.0171
12	0.0986	0.0102	0.1193	0.0115
14	0.0542	0.0062	0.0573	0.0067
15	0.0330	0.0047	0.0377	0.0060
16	0.0416	0.0046	0.0358	0.0056
17	0.1044	0.0118	0.1063	0.0110
18	0.0650	0.0069	0.0826	0.0088
19	0.1047	0.0106	0.1255	0.0133
24	0.0358	0.0047	0.0627	0.0075
26	0.0223	0.0033	0.0238	0.0045
28	0.0252	0.0041	0.0362	0.0058
29	0.0271	0.0041	0.0422	0.0058
32	0.0259	0.0042	0.0419	0.0064
33	0.0279	0.0043	0.0327	0.0058
35	0.0316	0.0044	0.0457	0.0066
36	0.0264	0.0043	0.0393	0.0059

39	0.0514	0.0056	0.0610	0.0069
40	0.1590	0.0185	0.1644	0.0175
44	0.0217	0.0034	0.0211	0.0047
45	0.0163	0.0034	0.0258	0.0050
46	0.0246	0.0037	0.0333	0.0056
49	0.0614	0.0068	0.0902	0.0096
51	0.0205	0.0035	0.0239	0.0054
52	0.0112	0.0030	0.0174	0.0047
53	0.0110	0.0029	0.0173	0.0047
54	0.0149	0.0034	0.0192	0.0051
55	0.0225	0.0040	0.0370	0.0058
56	0.0531	0.0056	0.0722	0.0078

SI table 4. ^{15}N R_1 rates (s^{-1}) for GB1_{IG} with varying concentrations of Gd(DTPA-BMA)

Residue	0 mM		3.5 mM		5 mM		7.5 mM	
	R_1	Error	R_1	Error	R_1	Error	R_1	Error
1	0.0334	-	0.0526	0.0269	0.0610	0.0248	-	-
9	0.0373	-	0.0819	0.0272	0.0877	0.0260	0.1194	0.0282
10	0.0547	-	0.1512	0.0445	0.1100	0.0367	0.1943	0.0502
11	-	-	0.1066	0.0296	0.0828	0.0300	0.2619	0.0594
14	0.0126	-	0.0858	0.0243	0.1057	0.0308	0.1039	0.0255
15	0.0620	-	0.0841	0.0324	0.0672	0.0257	0.1401	0.0377
17	0.0449	-	0.0595	0.0290	0.0623	0.0231	0.1436	0.0462
18	0.0556	-	0.0563	0.0214	0.0763	0.0284	0.0917	0.0266
19	0.0487	-	0.1452	0.0362	0.1540	0.0396	0.1971	0.0542
20	0.1158	-	0.1068	0.0352	0.1686	0.0436	0.2058	0.0614
21	0.0781	-	0.2517	0.0553	0.2270	0.0584	0.2838	0.0758
26	0.0309	-	0.0909	0.0237	0.0614	0.0224	0.0927	0.0267
27	0.0044	-	0.0270	0.0236	0.0555	0.0213	0.0225	0.0185
28	0.0296	-	0.0746	0.0236	0.0299	0.0244	0.0795	0.0278
29	0.0110	-	0.0432	0.0276	0.0540	0.0258	0.0370	0.0174
31	0.0305	-	0.0374	0.0249	0.0330	0.0212	0.0212	0.0201
38	0.0264	-	0.0557	0.0278	0.1207	0.0364	0.1716	0.0417
40	0.0644	-	0.0763	0.0311	0.0540	0.0245	0.2138	0.0484
42	0.0322	-	0.0854	0.0297	0.1276	0.0290	0.2133	0.0483
44	0.0005	-	0.0073	0.0174	0.0706	0.0260	0.2697	0.0644
45	0.0204	-	0.0573	0.0285	0.1210	0.0333	0.1722	0.0445
47	0.0422	-	0.1429	0.0384	0.2719	0.0697	0.4298	0.1216
48	0.0530	-	0.1578	0.0416	0.1331	0.0344	0.1951	0.0518
49	0.0277	-	0.3069	0.0774	0.1149	0.0329	0.4797	0.1182
50	0.0344	-	0.2602	0.0512	0.2072	0.0486	0.2279	0.0735
51	0.0227	-	0.0481	0.0227	0.0798	0.0277	0.1389	0.0374
52	0.0150	-	0.0668	0.0250	0.0999	0.0300	0.0630	0.0272
54	0.0256	-	0.0495	0.0266	0.0819	0.0278	0.0748	0.0249

56	0.0372	-	0.1102	0.0318	0.1166	0.0353	0.1765	0.0437
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SI table 5. ^{15}N $R_{1\rho}$ rates (s^{-1}) at 10 kHz nutation frequency for GB1_{IgG} with varying concentrations of Gd(DTPA-BMA)

Residue	0 mM		1 mM		2 mM		3.5 mM	
	$R_{1\rho}$	Error	$R_{1\rho}$	Error	$R_{1\rho}$	Error	$R_{1\rho}$	Error
3	6.04	0.57	5.39	0.49	7.72	0.92	8.04	1.04
9	5.78	0.61	6.57	0.68	10.03	1.13	9.32	1.15
10	6.74	0.58	5.94	0.65	10.63	1.03	9.20	1.21
11	6.85	0.73	7.18	0.60	9.38	0.88	9.58	1.34
14	5.78	0.50	6.75	0.68	11.10	1.04	7.23	0.99
15	6.09	0.60	7.80	0.67	7.70	0.86	6.11	0.90
17	3.27	0.36	7.18	0.61	6.17	0.85	6.78	1.18
18	3.66	0.39	6.41	0.59	6.41	0.80	6.76	1.00
19	4.89	0.54	7.62	0.75	6.49	0.86	7.45	1.09
20	6.44	0.57	6.39	0.57	8.36	0.74	7.29	0.90
21	5.76	0.57	7.59	0.68	8.74	1.05	9.86	1.04
26	4.89	0.63	5.80	0.60	7.17	0.89	9.26	1.20
27	8.47	0.71	6.27	0.65	7.55	0.72	8.23	0.93
28	9.14	0.81	7.21	0.69	5.93	0.73	7.25	1.06
29	6.73	0.70	7.48	0.70	6.25	0.66	7.09	0.85
38	5.76	0.57	9.97	0.92	8.75	1.00	12.23	1.59
40	7.84	0.67	5.48	0.56	7.55	0.60	6.37	0.79
42	6.97	0.66	6.19	0.61	9.99	1.02	10.50	1.28
44	6.58	0.74	5.28	0.55	6.24	0.64	7.34	0.85
45	5.08	0.54	5.37	0.61	7.09	0.82	7.46	1.01
47	5.05	0.52	5.80	0.59	8.68	0.90	9.57	1.14
48	6.19	0.57	6.69	0.68	8.03	0.91	8.12	1.13
49	7.27	0.69	8.56	0.79	9.99	1.10	11.23	1.42
50	4.85	0.49	6.14	0.68	8.02	0.93	8.12	1.13
51	6.62	0.64	7.12	0.73	7.96	0.86	7.19	0.82
52	6.94	0.64	4.88	0.56	7.16	0.81	6.46	0.97
54	6.21	0.72	7.65	0.73	7.47	0.84	7.76	1.10
56	5.50	0.56	5.25	0.58	6.53	0.79	5.70	1.06

SI table 6. ^1H R_1 rates (s^{-1}) for GB1_{IgG} with 0 and 100 mM Cu(EDTA)

Residue	0 mM		100 mM	
	R_1	Error	R_1	Error
1	1.925	0.166	4.102	0.171
3	1.151	0.109	4.188	0.179
9	1.913	0.210	3.794	0.155
10	1.952	0.229	4.492	0.183
11	1.223	0.145	5.680	0.255

14	1.046	0.098	3.387	0.165
15	0.948	0.099	3.531	0.144
17	1.124	0.118	4.336	0.174
18	1.172	0.119	3.487	0.161
19	0.958	0.104	6.577	0.289
20	1.945	0.219	7.762	0.350
21	1.556	0.166	7.580	0.338
26	1.645	0.189	4.868	0.206
27	1.457	0.146	5.439	0.208
28	1.683	0.200	4.964	0.176
29	0.977	0.116	3.841	0.155
31	1.845	0.270	3.847	0.151
38	1.071	0.166	4.008	0.173
40	0.636	0.073	4.024	0.129
42	1.433	0.159	3.603	0.136
44	0.975	0.108	3.686	0.149
45	2.227	0.256	5.043	0.225
47	1.344	0.143	5.731	0.251
48	1.000	0.102	5.482	0.218
49	1.470	0.176	9.712	0.427
50	1.275	0.151	6.866	0.328
51	1.279	0.135	5.802	0.228
52	1.250	0.116	3.394	0.142
54	1.098	0.113	3.412	0.151
56	1.194	0.114	3.911	0.185

SI table 7. Experimental ^{15}N sPRE values ($\text{mM}^{-1} \text{s}^{-1}$) for GB1_{free}, GB1_{cryst} and GB1_{IgG} and ^1H sPREs for GB1_{IgG}

Residue	^{15}N R_1 GB1 _{free}		^{15}N R_1 GB1 _{cryst}		^{15}N R_1 GB1 _{IgG}		^{15}N $R_{1\rho}$ GB1 _{IgG}		^1H R_1 GB1 _{IgG}	
	PRE	Error	PRE	Error	PRE	Error	PRE	Error	PRE	Error
1	-	-	-	-	0	0.0025	-	-	0.0218	0.0028
2	0.0944	0.0053	0.0084	0.0056	-	-	-	-	-	-
3	0.0271	0.005	0.0065	0.0045	-	-	0.7156	0.3773	0.0304	0.0025
4	0.0228	0.0052	-	-	-	-	-	-	-	-
5	0.0145	0.0055	-	-	-	-	-	-	-	-
6	0.0317	0.0051	0.0117	0.0035	-	-	-	-	-	-
7	0.0378	0.0052	-	-	-	-	-	-	-	-
8	0.0248	0.005	0.0059	0.0046	-	-	-	-	-	-
9	0.0357	0.0051	0.0064	0.0051	0.0107	0.0059	1.1588	0.4248	0.0188	0.003
10	0.0541	0.0048	0.0070	0.0073	0.0168	0.0101	0.9828	0.4281	0.0254	0.0034
11	0.0789	0.0047	0.0306	0.0115	0.0294	0.0132	0.8748	0.483	0.0446	0.0034
12	0.0762	0.0043	0.0103	0.0090	-	-	-	-	-	-
13	0.1495	0.005	-	-	-	-	-	-	-	-
14	0.1296	0.0048	0.0016	0.0035	0.0128	0.0054	0.6142	0.3647	0.0234	0.0022
15	0.1706	0.0053	0.0024	0.0034	0.0091	0.0074	0	0.2029	0.0258	0.002
16	0.1593	0.0055	0.0010	0.0024	-	-	-	-	-	-

17	0.1832	0.0054	0.0010	0.0053	0.0121	0.008	0.7815	0.3969	0.0321	0.0024
18	0.15	0.0054	0.0088	0.0066	0.005	0.005	0.7663	0.3577	0.0231	0.0023
19	0.1072	0.0049	0.0104	0.0096	0.0195	0.0099	0.5544	0.4032	0.0562	0.0036
20	0.055	0.0053	-	-	0.0126	0.0101	0.3511	0.3448	0.0582	0.0048
21	0.0408	0.0052	-	-	0.0265	0.0135	1.1452	0.3779	0.0602	0.0043
22	-	-	-	-	-	-	-	-	-	-
23	0.0822	0.0053	-	-	-	-	-	-	-	-
24	0.059	0.0049	0.0134	0.0051	-	-	-	-	-	-
25	0.0675	0.0052	-	-	-	-	-	-	-	-
26	0.0065	0.0053	0.0010	0.0019	0.0074	0.0052	1.2675	0.4171	0.0322	0.0032
27	0.0548	0.0052	-	-	0.0035	0.0042	0.0857	0.2732	0.0398	0.003
28	0.0074	0.005	0.0055	0.0041	0.0052	0.0054	0	0.2381	0.0328	0.0031
29	0.0238	0.0052	0.0076	0.0041	0.004	0.0051	0.0054	0.2093	0.0286	0.0022
30	0.0508	0.0054	-	-	-	-	-	-	-	-
31	0.0103	0.0053	-	-	0	0.0028	-	-	0.02	0.0036
32	0.0238	0.0053	0.0080	0.0043	-	-	-	-	-	-
33	0.0358	0.0052	0.0024	0.0033	-	-	-	-	-	-
34	0.0089	0.0055	-	-	-	-	-	-	-	-
35	0.0451	0.0051	0.0070	0.0045	-	-	-	-	-	-
36	0.043	0.0053	0.0065	0.0042	-	-	-	-	-	-
37	-	-	-	-	-	-	-	-	-	-
38	-	-	-	-	0.0199	0.0067	1.5898	0.5496	0.0294	0.0027
39	0.0344	0.0049	0.0048	0.0048	-	-	-	-	-	-
40	0.0426	0.0046	0.0027	0.0097	0.0172	0.0084	0	0.1836	0.0339	0.0017
41	-	-	-	-	-	-	-	-	-	-
42	0.077	0.0051	-	-	0.0238	0.0078	1.2338	0.465	0.0217	0.0023
43	0.1036	0.0052	-	-	-	-	-	-	-	-
44	0.0869	0.0054	0.0010	0.0019	0.0257	0.0074	0.3167	0.3382	0.0271	0.0021
45	0.1717	0.0053	0.0047	0.0034	0.0208	0.0068	0.7502	0.3728	0.0282	0.0039
46	0.0929	0.0053	0.0043	0.0038	-	-	-	-	-	-
47	0.102	0.0051	0.0053	0.0044	0.0521	0.0158	1.4001	0.4093	0.0439	0.0034
48	0.1009	0.005	-	-	0.0178	0.0099	0.5972	0.4123	0.0448	0.0028
49	0.0875	0.0048	0.0144	0.0068	0.0519	0.0177	1.1401	0.5106	0.0824	0.0053
50	0.0667	0.0054	-	-	0.025	0.013	0.974	0.4039	0.0559	0.0042
51	0.0226	0.0051	0.0017	0.0026	0.0153	0.0058	0.1878	0.3055	0.0452	0.0031
52	0.0668	0.0052	0.0031	0.0031	0.0077	0.0056	0.0688	0.2669	0.0214	0.0021
53	0.0283	0.0049	0.0031	0.0030	-	-	-	-	-	-
54	0.0215	0.0055	0.0022	0.0028	0.0073	0.0055	0.3692	0.4143	0.0231	0.0022
55	0.0447	0.0051	0.0073	0.0040	-	-	-	-	-	-
56	0.054	0.0051	0.0096	0.0056	0.018	0.0079	0.1379	0.3161	0.0272	0.0025

SI table 8. Predicted ^{15}N sPRE values ($\text{mM}^{-1} \text{s}^{-1}$) for GB1_{free}, GB1_{cryst}, GB1_{IgG} and GB1 in complex with IgG fragments

Residue	GB1 _{free}		GB1 _{cryst}		GB1 _{IgG}		GB1 _{IgG} (Fab)		GB1 _{IgG} (Fc)	
	PRE	Error	PRE	Error	PRE	Error	PRE	Error	PRE	Error
1	-	-	-	-	-	-	-	-	-	-
2	4.234	0.275	0.241	-	3.564	-	3.652	-	4.128	-
3	1.944	0.134	0.179	-	1.219	-	1.328	-	1.685	-
4	1.593	0.07	0.159	-	0.929	-	1.021	-	1.288	-
5	1.245	0.028	0.092	-	0.594	-	0.677	-	1.054	-
6	1.344	0.023	0.081	-	0.892	-	0.974	-	1.251	-
7	1.554	0.093	0.097	-	0.964	-	1.021	-	1.561	-
8	1.826	0.11	0.203	-	1.267	-	1.343	-	1.782	-
9	2.030	0.111	0.262	-	1.060	-	1.134	-	1.795	-
10	3.447	0.098	0.603	-	1.570	-	1.640	-	3.046	-
11	4.965	0.062	0.516	-	1.106	-	1.139	-	4.556	-
12	4.079	0.078	0.175	-	0.541	-	0.569	-	3.666	-
13	4.337	0.188	0.132	-	0.715	-	0.733	-	4.072	-
14	4.217	0.161	0.100	-	1.601	-	1.617	-	4.906	-
15	4.557	0.192	0.074	-	1.134	-	1.146	-	4.838	-
16	3.029	0.043	0.116	-	0.607	-	0.636	-	2.854	-
17	3.990	0.112	0.290	-	0.588	-	0.639	-	3.616	-
18	3.016	0.103	0.454	-	0.547	-	0.676	-	2.440	-
19	4.470	0.084	0.853	-	0.986	-	1.285	-	3.871	-
20	3.142	0.06	0.234	-	1.613	-	2.158	-	2.717	-
21	4.445	0.108	0.109	-	2.565	-	3.866	-	3.072	-
22	3.773	0.037	0.133	-	2.664	-	3.563	-	2.818	-
23	3.106	0.058	0.374	-	2.047	-	3.105	-	2.103	-
24	3.899	0.032	0.444	-	1.396	-	3.705	-	1.442	-
25	3.046	0.026	0.187	-	0.844	-	2.764	-	0.946	-
26	1.666	0.032	0.118	-	0.488	-	1.452	-	0.705	-
27	1.557	0.015	0.087	-	0.304	-	1.229	-	0.443	-
28	2.441	0.035	0.097	-	0.210	-	1.881	-	0.372	-
29	2.297	0.067	0.236	-	0.230	-	1.789	-	0.714	-
30	1.357	0.023	0.191	-	0.172	-	0.845	-	0.699	-
31	1.373	0.029	0.095	-	0.133	-	1.083	-	0.435	-
32	2.322	0.094	0.153	-	0.158	-	1.837	-	0.678	-
33	2.259	0.062	0.321	-	0.240	-	1.127	-	1.523	-
34	1.483	0.023	0.129	-	0.147	-	0.626	-	0.994	-
35	2.225	0.079	0.170	-	0.195	-	1.177	-	1.094	-
36	4.091	0.162	0.214	-	0.247	-	1.198	-	2.686	-
37	4.257	0.07	0.138	-	0.207	-	0.582	-	3.836	-
38	5.536	0.136	0.138	-	0.349	-	0.721	-	4.667	-
39	2.980	0.068	0.124	-	0.472	-	0.868	-	2.211	-
40	2.808	0.09	0.221	-	0.971	-	1.740	-	1.795	-
41	3.629	0.128	0.295	-	1.166	-	2.405	-	1.429	-
42	3.854	0.071	0.219	-	1.637	-	3.084	-	1.725	-
43	4.062	0.104	0.087	-	1.023	-	3.530	-	1.059	-

44	3.141	0.046	0.063	-	1.289	-	3.267	-	1.313	-
45	4.404	0.086	0.066	-	1.544	-	4.141	-	1.557	-
46	3.362	0.049	0.081	-	2.121	-	3.265	-	2.140	-
47	4.889	0.225	0.180	-	3.273	-	4.713	-	3.294	-
48	6.265	0.154	0.147	-	5.107	-	5.714	-	5.122	-
49	5.042	0.049	0.171	-	4.663	-	4.889	-	4.695	-
50	2.830	0.041	0.183	-	2.568	-	2.764	-	2.623	-
51	1.813	0.031	0.121	-	1.475	-	1.685	-	1.554	-
52	1.176	0.017	0.064	-	0.839	-	1.100	-	0.937	-
53	1.455	0.016	0.069	-	0.971	-	1.333	-	1.057	-
54	1.340	0.017	0.089	-	0.815	-	1.106	-	0.960	-
55	1.999	0.047	0.164	-	1.323	-	1.695	-	1.474	-
56	2.695	0.075	0.386	-	2.208	-	2.473	-	2.501	-

SI table 9. Predicted ^1H PRE values ($\text{mM}^{-1} \text{s}^{-1}$) for GB1_{free}, GB1_{IgG} and GB1 in complex with IgG fragments

Residue	^1H GB1 _{free}		^1H GB1 _{IgG}		^1H GB1 _{IgG} (Fab)		^1H GB1 _{IgG} (Fc)	
	PRE	Error	PRE	Error	PRE	Error	PRE	Error
1	-	-	-	-	-	-	-	-
2	6.05579	0.86467	5.713	-	5.771	-	6.225	-
3	1.92983	0.07241	1.043	-	1.166	-	1.674	-
4	1.58913	0.06759	1.020	-	1.125	-	1.278	-
5	1.44369	0.04194	0.592	-	0.658	-	1.247	-
6	1.26859	0.02899	0.907	-	1.015	-	1.165	-
7	1.8265	0.07138	1.075	-	1.117	-	1.890	-
8	1.59691	0.04574	1.038	-	1.142	-	1.442	-
9	2.00112	0.07334	0.889	-	0.951	-	1.727	-
10	3.23847	0.13902	1.424	-	1.518	-	2.725	-
11	4.24353	0.18799	0.946	-	0.992	-	3.780	-
12	3.45689	0.13274	0.577	-	0.617	-	2.996	-
13	6.39924	0.26087	0.641	-	0.653	-	6.128	-
14	3.20512	0.19916	1.964	-	1.986	-	4.184	-
15	7.10608	0.63004	1.078	-	1.087	-	7.666	-
16	2.24653	0.10432	0.608	-	0.645	-	2.049	-
17	6.05796	0.23198	0.576	-	0.622	-	5.773	-
18	2.42318	0.11199	0.614	-	0.731	-	1.866	-
19	6.66838	0.63787	0.908	-	1.262	-	5.941	-
20	2.88295	0.18841	1.753	-	2.123	-	2.589	-
21	5.294	0.25301	2.133	-	4.159	-	2.745	-
22	3.29529	0.11104	1.884	-	2.901	-	2.086	-
23	4.47693	0.33442	3.417	-	4.690	-	3.447	-
24	5.16172	0.15534	2.304	-	4.973	-	2.349	-
25	3.13895	0.14487	1.172	-	3.001	-	1.265	-
26	1.72057	0.05982	0.634	-	1.556	-	0.812	-
27	1.74493	0.07566	0.388	-	1.427	-	0.500	-
28	2.55056	0.27893	0.264	-	1.976	-	0.408	-

29	2.17533	0.13373	0.245	-	1.737	-	0.660	-
30	1.29119	0.04752	0.181	-	0.863	-	0.594	-
31	1.43688	0.09264	0.138	-	1.179	-	0.399	-
32	2.26622	0.18417	0.163	-	1.806	-	0.642	-
33	2.08873	0.10234	0.229	-	1.120	-	1.346	-
34	1.35966	0.0466	0.142	-	0.676	-	0.825	-
35	2.07551	0.14472	0.172	-	1.297	-	0.889	-
36	3.36134	0.17582	0.231	-	1.191	-	2.085	-
37	3.14332	0.10107	0.195	-	0.611	-	2.650	-
38	5.39785	0.25964	0.324	-	0.823	-	4.271	-
39	2.72259	0.1352	0.349	-	0.751	-	1.971	-
40	3.05651	0.28448	1.174	-	1.745	-	2.147	-
41	3.9637	0.91033	0.841	-	2.320	-	1.087	-
42	3.69336	0.14428	2.023	-	3.097	-	2.124	-
43	6.38352	0.62965	1.038	-	5.179	-	1.065	-
44	2.28854	0.06131	1.198	-	2.417	-	1.234	-
45	7.23329	0.11884	2.227	-	6.785	-	2.234	-
46	2.4899	0.04131	1.713	-	2.467	-	1.738	-
47	7.35167	0.0862	4.824	-	7.204	-	4.875	-
48	7.15681	0.10108	5.291	-	6.043	-	5.305	-
49	4.5353	0.0803	3.932	-	4.236	-	3.955	-
50	3.03221	0.09807	2.602	-	2.868	-	2.641	-
51	2.05768	0.0396	1.671	-	1.933	-	1.726	-
52	1.09254	0.01821	0.759	-	0.958	-	0.893	-
53	1.61171	0.0239	0.967	-	1.498	-	1.029	-
54	1.28433	0.02151	0.839	-	1.047	-	1.026	-
55	2.13988	0.08549	1.295	-	1.824	-	1.415	-
56	2.53396	0.17187	1.992	-	2.183	-	2.354	-

SI table 10. Relaxation delays (s) used and total experimental time for R_1 measurements of $GB1_{free}$ and $GB1_{cryst}$

	15N R_1 , GB1 free in solution, Gd(DTPA-BMA)							15N R_1 , GB1 crystals, Gd(DTPA-BMA)	
	0 mM	0.1 mM	0.3 mM	0.7 mM	1.2 mM	2 mM	2.5 mM	0 mM	2 mM
	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.001	0.001
	0.1	0.1	0.1	0.075	0.075	0.075	0.075	0.2	0.1
	0.2	0.2	0.2	0.1	0.1	0.1	0.1	0.5	0.4
	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.8	0.8
	0.5	0.5	0.5	0.3	0.3	0.3	0.3	1.2	1.5
	0.75	0.75	0.75	0.4	0.4	0.4	0.4	2.2	3
	1	1	1	0.5	0.5	0.5	0.5	4	5.5
	1.5	1.5	1.5	0.75	0.75	0.6	0.75	8	9
	2			1	1.1	0.75	1	15	15
				1.2		1		22	
Total	46 h	35 h	35 h	42.5 h	42 h	46.5 h	42.5 h	12 h	12 h

SI table 11. Relaxation delays (s) and spin-lock lengths (s) and total experimental time used for R_1 and $R_{1\rho}$ measurements of GB1_{IgG}

	$^{15}\text{N } R_1$, Gd(DTPA-BMA)				$^{15}\text{N } R_{1\rho}$, Gd(DTPA-BMA)				$^1\text{H } R_1$, CuEDTA	
	0 mM	3.5 mM	5 mM	7.5 mM	0 mM	1 mM	2 mM	3.5 mM	0 mM	100 mM
	0.01	0.001	0.001	0.001	0.002	0.002	0.002	0.002	0.25	0
	15	0.01	0.01	0.01	0.005	0.005	0.005	0.005	0.5	0.02
		0.05	0.04	0.04	0.01	0.01	0.01	0.01	0.75	0.04
		0.2	0.1	0.1	0.02	0.02	0.02	0.02	1	0.07
		0.5	0.5	0.5	0.04	0.04	0.04	0.04	1.25	0.1
		1.5	1.5	1.5	0.07	0.06	0.06	0.06	1.5	0.14
		3.2	3	3	0.1	0.09	0.09	0.09	1.75	0.2
		6	7.5	7.5	0.15	0.13	0.13	0.13	2.2	0.3
Total experimental time	87 h	89 h	65.5 h	65.5 h	120 h	24 h	18h	23.5 h	30 h	37 h

SI table 12. Result of fitting of experimental Δ sPREs against Δ sPREs back-calculated for several different models with global scaling as the only fit parameters and weighted by experimental errors.

Experimental data set	Predicted data set	Scaling factor	χ^2
$^{15}\text{N } R_1$	GB1:IgG (model B Fig. 5)	16.34	4.10
$^{15}\text{N } R_1$	GB1:IgG	13.33	4.34
$^{15}\text{N } R_1$	GB1:Fab	11.86	9.63
$^{15}\text{N } R_1$	GB1:Fc	11.26	14.09
$^{15}\text{N } R_{1\rho}$	GB1:IgG (model B Fig. 5)	16.27	3.29
$^{15}\text{N } R_{1\rho}$	GB1:IgG	13.60	4.30
$^{15}\text{N } R_{1\rho}$	GB1:Fab	12.40	8.64
$^{15}\text{N } R_{1\rho}$	GB1:Fc	11.10	12.58
$^1\text{H } R_1$	GB1:IgG (model B Fig. 5)	59.07	5.27
$^1\text{H } R_1$	GB1:IgG	51.27	6.77
$^1\text{H } R_1$	GB1:Fab	50.91	14.44
$^1\text{H } R_1$	GB1:Fc	36.18	19.23

SI table 13. Predicted ^1H sPREs for GB1_{IgG} based on modified models with an additional interaction site (model B) or anisotropic motion (1-5).

Residue	Model B	Motion 1	Motion 2	Motion 3	Motion 4	Motion 5
2	5.593	5.753	5.612	5.685	5.614	5.748
3	0.956	1.087	1.030	1.052	1.013	1.095
4	0.690	1.039	1.026	1.029	1.018	1.041
5	0.308	0.593	0.612	0.598	0.594	0.600
6	0.185	0.917	0.911	0.912	0.923	0.899
7	0.187	1.049	1.137	1.087	1.125	1.033
8	0.239	1.054	1.051	1.053	1.095	0.997
9	0.275	0.885	0.931	0.902	0.978	0.814

10	0.971	1.459	1.447	1.432	1.613	1.286
11	0.616	0.974	0.994	0.955	1.166	0.799
12	0.308	0.583	0.618	0.586	0.704	0.492
13	0.178	0.583	0.763	0.653	0.778	0.532
14	0.311	1.831	2.197	1.991	2.141	1.764
15	0.420	0.965	1.276	1.089	1.166	0.999
16	0.285	0.589	0.656	0.613	0.619	0.606
17	0.458	0.563	0.632	0.577	0.544	0.621
18	0.537	0.650	0.614	0.622	0.594	0.658
19	0.894	1.114	0.781	0.912	0.797	1.082
20	1.736	1.885	1.638	1.760	1.593	1.918
21	2.134	2.358	1.979	2.139	1.710	2.650
22	1.880	1.990	1.804	1.892	1.666	2.103
23	3.343	3.323	3.447	3.390	3.141	3.536
24	2.251	2.205	2.334	2.278	1.883	2.595
25	1.157	1.232	1.097	1.168	0.946	1.417
26	0.618	0.671	0.608	0.637	0.555	0.729
27	0.357	0.407	0.375	0.388	0.343	0.440
28	0.250	0.280	0.248	0.259	0.219	0.317
29	0.238	0.255	0.241	0.243	0.222	0.275
30	0.157	0.197	0.168	0.179	0.174	0.190
31	0.110	0.144	0.125	0.131	0.132	0.136
32	0.150	0.153	0.168	0.154	0.161	0.157
33	0.217	0.265	0.195	0.223	0.247	0.214
34	0.114	0.159	0.125	0.137	0.157	0.125
35	0.155	0.192	0.153	0.166	0.209	0.142
36	0.224	0.250	0.215	0.226	0.256	0.225
37	0.183	0.236	0.161	0.191	0.233	0.179
38	0.311	0.436	0.252	0.319	0.479	0.247
39	0.315	0.439	0.293	0.348	0.483	0.268
40	1.087	1.367	1.030	1.173	1.449	0.958
41	0.736	0.964	0.742	0.842	0.977	0.725
42	1.518	2.260	1.773	2.028	2.139	1.929
43	0.567	1.447	0.769	1.039	1.147	0.956
44	0.260	1.413	1.007	1.198	1.247	1.153
45	0.578	3.006	1.677	2.218	2.283	2.144
46	0.515	1.868	1.572	1.710	1.702	1.710
47	2.902	5.642	3.927	4.840	4.597	5.052
48	2.794	5.524	5.015	5.300	5.231	5.345
49	1.890	4.024	3.861	3.946	3.932	3.951
50	1.743	2.658	2.568	2.611	2.594	2.622
51	0.762	1.722	1.638	1.677	1.670	1.682
52	0.288	0.786	0.747	0.765	0.764	0.764
53	0.183	1.050	0.892	0.967	0.985	0.949
54	0.176	0.876	0.813	0.847	0.870	0.822
55	0.615	1.417	1.153	1.300	1.359	1.245

56	1.083	2.035	1.957	2.003	2.090	1.913
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SI table 14. Predicted ¹H sPREs for GB1_{IgG} based on modified models with an additional interaction site (model B) or anisotropic motion (1-5).

Residue	Model B	Motion 1	Motion 2	Motion 3	Motion 4	Motion 5
2	3.477	3.630	3.491	3.559	3.487	3.625
3	1.099	1.254	1.213	1.227	1.195	1.263
4	0.649	0.945	0.940	0.939	0.924	0.951
5	0.281	0.600	0.609	0.602	0.600	0.601
6	0.192	0.894	0.910	0.900	0.912	0.884
7	0.165	0.954	1.004	0.976	1.008	0.932
8	0.239	1.268	1.300	1.284	1.339	1.204
9	0.367	1.059	1.097	1.072	1.159	0.976
10	0.938	1.566	1.639	1.581	1.775	1.422
11	0.657	1.095	1.200	1.114	1.357	0.928
12	0.255	0.532	0.596	0.551	0.665	0.456
13	0.186	0.664	0.829	0.730	0.848	0.607
14	0.318	1.455	1.859	1.626	1.783	1.408
15	0.376	1.036	1.305	1.146	1.212	1.064
16	0.318	0.579	0.667	0.611	0.615	0.605
17	0.453	0.581	0.635	0.593	0.564	0.627
18	0.487	0.591	0.541	0.552	0.522	0.594
19	0.968	1.152	0.880	0.992	0.879	1.137
20	1.602	1.783	1.466	1.618	1.403	1.843
21	2.565	2.759	2.414	2.572	2.174	2.959
22	2.660	2.769	2.579	2.673	2.424	2.882
23	1.999	2.028	2.049	2.040	1.869	2.165
24	1.356	1.364	1.399	1.384	1.154	1.595
25	0.832	0.900	0.783	0.841	0.672	1.050
26	0.473	0.523	0.466	0.489	0.424	0.568
27	0.273	0.322	0.291	0.303	0.272	0.341
28	0.195	0.222	0.199	0.205	0.179	0.246
29	0.223	0.231	0.233	0.227	0.215	0.248
30	0.149	0.189	0.155	0.169	0.169	0.175
31	0.103	0.141	0.119	0.125	0.132	0.126
32	0.145	0.151	0.162	0.149	0.162	0.147
33	0.229	0.281	0.205	0.234	0.262	0.222
34	0.121	0.168	0.130	0.143	0.167	0.129
35	0.178	0.224	0.170	0.189	0.247	0.158
36	0.241	0.275	0.226	0.243	0.285	0.244
37	0.197	0.256	0.167	0.203	0.246	0.199
38	0.332	0.480	0.271	0.345	0.528	0.259
39	0.430	0.603	0.393	0.471	0.667	0.356

40	0.901	1.140	0.844	0.971	1.215	0.782
41	1.039	1.307	1.049	1.168	1.320	1.027
42	1.249	1.883	1.408	1.640	1.754	1.539
43	0.509	1.342	0.786	1.025	1.115	0.953
44	0.292	1.613	1.031	1.289	1.355	1.229
45	0.393	1.949	1.246	1.538	1.567	1.506
46	0.664	2.387	1.876	2.120	2.103	2.122
47	1.929	3.679	2.882	3.278	3.169	3.373
48	3.274	5.277	4.937	5.121	5.064	5.157
49	2.664	4.735	4.624	4.681	4.668	4.680
50	1.735	2.611	2.549	2.578	2.565	2.586
51	0.723	1.514	1.458	1.483	1.476	1.488
52	0.275	0.875	0.818	0.844	0.844	0.842
53	0.173	1.029	0.918	0.972	0.988	0.957
54	0.195	0.867	0.771	0.822	0.846	0.796
55	0.554	1.414	1.218	1.331	1.382	1.280
56	1.389	2.276	2.136	2.217	2.301	2.131

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